Supplementary File 2 [Ek Dosya 2]



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High pKa variability of cysteine residues in structural databases and the effect of H-bond contributions

[Yapısal veritabanlarındaki sistein kalıntılarında pKa değerinin yüksek oranda değişkenlik göstermesi ve H-bağı katkılarının etkisi]

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RESULTS of ppka3 on PDB-crystal dataset prot=protein name res_num=residue number H-bond=hydrogen bond contribution to pKa prediction (pKa) Coul=electrostatics (from Coulombic interactions) contribution to pKa prediction (pKa) Solv=Solvation effect contribution to pKa prediction (pKa)

prot,res num,pKa,H-bond,Coul,Solv

2P4D,ASP_147,2.36,-1.59,-0.73,0.88 4FD6,LYS_106,10.24,-0.23,0,-0.03 301C.HIS 155.2.75.-3.17.0.-0.57 1LZL,ARG_303,12.35,-0.31,0,0.17 3K8J,ASP 114,3.92,0,0,0.12 1K95,ARG_145,12.08,-0.45,0,0.03 1AK1,HIS 88,2.92,-2.57,0.04,-1.06 301C,ARG 156,13,13,-0,41,0,38,0.67 1XFK,ARG_313,12.56,-0.34,0,0.4 3AUF,ASP_20,3.26,-0.84,-0.51,0.82 1JKS,GLU 18,4.09,0.3,-0.42,-0.29 1NJ4,LYS_186,10.14,-0.35,0,-0.01 3PP8,GLU 183,3.56,0.42,-1.03,-0.33 106D.GLU 54,4,7,0,42,0,-0,22 3V55,ARG_374,10.7,-1.83,0,0.03 2EDM,TYR_69,11.12,0,-0.42,1.54 4H4J,LYS_222,10.81,-0.23,0.11,0.42 1UAJ,GLU 116,4.7,0.2,0,0 2QZQ,HIS_163,5.59,-0.99,0.29,-0.2 1T6L,ARG_218,12.28,-0.23,0,0.01 2IRM,GLU_80,5.74,0.88,0,0.36 3FWU,HIS_14,6.53,-0.25,0,0.3 3EVP,HIS_297,5.84,-0.98,0.37,-0.06 3SMD,LYS 142,10.02,-0.44,0,-0.04 3HVM.CYS 28,10.29,0.0.18,1.11 3IL3,TYR_203,10.48,0,0.17,0.31 3BCH.ARG 186.11.49.-1.01.0.0 3LJI,LYS_62,10.43,-0.1,0,0.03 1IAP,HIS 200,6.07,-0.52,0,0.09 1JT9,LYS 248,10,52,-0,13,0,0,15 1JKS,LYS_50,10.45,-0.05,0,0 1MUF,ARG_103,12.58,-0.22,0,0.32

109G,ARG_34,12.12,-0.59,0,0.22 200K,ASP_242,3.77,-0.11,-0.1,0.18 3U2A,ARG 88,13.48,-0.25,0.79,0.43 2YWX,LYS_126,10.54,-0.09,0,0.13 208P,GLU_10,4.37,0.33,-0.46,0.01 3M16,LYS_323,10.29,-0.25,0,0.04 2W0G,GLU 207,3.67,0.35,-0.67,-0.51 2GKG,GLU_114,4.67,0.21,0,-0.04 2XJ4,HIS 262,6.25,-0.18,0,-0.07 1SQW,HIS_77,6.33,-0.2,0,0.03 4EF5,ARG_310,12.07,-1.17,0.06,0.66 3BPP,ARG 121,12.67,-0.31,0,0.48 2OSA.ASP 335,3.65,-1.06,-0.06,0.98 3RFF,TYR_122,10.26,-0.09,-0.2,0.55 3PZ9,TYR_291,10.79,-0.28,0.07,0.99 3CRM,GLU_229,4.65,0.15,0,0 1FO9,TYR_185,9.97,-0.84,2.78E-17,0.82 3KT9,ARG_18,12.35,-0.27,0,0.12 2BLL,GLU_412,4.5,1.14,-0.69,-0.45 1ES9,HIS_106,5.3,-0.61,0,-0.59 3FNI,ARG_149,12.31,-0.3,0,0.11 3CRM,GLU_237,4.68,0.23,0,-0.05 3ETV,LYS_234,10.15,-0.35,0,0 3KT9,ASP 11,2.95,-1,-0.45,0.59 4DNU,LYS_115,10.41,-0.09,0,0.01 2AZL.LYS 217,10.48,-0.07,0.0.05 2IXM,GLU_115,3.98,0.31,-0.74,-0.09 3COU,HIS_99,5.4,-1.07,0,-0.02 2B6P,ARG_153,12.28,-0.53,0,0.32 4EKU,ARG 39,12.35,-0.46,0,0.33 2CI3,LYS_280,10.23,-0.43,0,0.16

3GE9,ASP 22,3.44,-0.54,0,0.18 20HT.GLU 203.4.4.0.16.0.-0.26 2D7J,LYS 174,10.52,-0.17,0,0.19 4E9E,ASP_568,3.98,0,-0.17,0.35 2V4U,GLU_356,4.69,0.28,0,-0.08 1MHN,ARG_133,12.36,-0.14,0,0 2YYO, ASP_14, 3.92, 0, 0, 0.12 2WB8,CYS_762,8.91,-0.1,-0.51,0.51 2GAU,HIS_74,4.95,-0.86,0,-0.69 2IQT,LYS_164,10.19,-0.32,0,0.02 1RZ2,LYS_55,10.25,-0.25,0,0 3FHF,ASP_20,3.46,-0.85,-0.43,0.95 2Z0M,ASP 78,2,93,-0,79,-0,48,0,4 2PP6,GLU_92,4.81,0.25,0,0.06 3M66,LYS_299,10.41,-0.14,0,0.05 2IF4,LYS_117,10.67,-0.46,0,0.62 1HF8,TYR_222,12.05,0,0.79,1.26 1WYC,HIS_191,6.43,-0.08,0,0.01 3JZN,ASP 438,4,11,-0.85,-0.44,1.61 3H8Y,ARG_70,12.66,-0.07,0,0.23 3EOD,ARG_115,12.78,-0.29,0.06,0.51 2FZ4,ARG_152,11.66,-0.85,0,0 2G5X,LYS_125,11.51,-0.31,0.83,0.49 2X4G.TYR 154.11.08.0.0.27.0.8 3DZ1,LYS_2,10.41,-0.21,0,0.13 10XZ,ASP_285,4.13,0,0,0.33 3SMD,TYR_92,10.07,-0.57,-0.01,0.65 3GV0,GLU_175,5.07,1.2,-0.82,0.21 2AHE,CYS 35,9.17,-2.17,-0.31,2.65 4H4J,CYS_58,10.14,-0.65,0.14,1.64 3MEW, ARG_202, 13.87, -0.4, 1.22, 0.54

3FK5,GLU_171,4.62,0.25,0,-0.12

3KEY,TYR_438,10.08,0,0,0.08 1LZL,ASP 34,4.62,0,-0.07,0.88 3M7G,GLU 262,4.94,0.26,0,0.18 2W1R,ASP_78,2.85,-1.86,-0.06,0.98 3ASA,GLU_349,3.77,0.31,-0.73,-0.31 2FM9,LYS_133,10.54,-0.31,0,0.35 2H14,CYS_334,9.83,0.13,0.29,0.42 2X5Y,CYS_798,11.86,-0.01,-0.02,2.89 3S0A, ASP_77, 2.41, -1.83, 0, 0.43 2B02,LYS_394,10.41,-0.29,0,0.2 2P5D,ARG_123,12.43,-0.07,0,0 2Q34,ARG_85,12.37,-0.3,0,0.16 3UAH,GLU 276,4.77,0.19,0,0.08 2RIS,TYR 87,11.39,-0.02,0.84,0.57 1RI6,ASP_70,3.05,-0.57,-0.34,0.17 1XKR,LYS_33,11.49,-0.49,0.82,0.66 1MUF,GLU_220,4.91,0.25,0,0.16 1Q42,ASP_89,3.52,-0.27,-0.38,0.36 1ILW.LYS 121.10.58.-0.17.0.0.25 2ZCO,TYR_24,10.83,0,-0.04,0.87 4DNU,HIS_258,3.67,-2.17,0.17,-0.82 2B0A,LYS_65,10.6,-0.2,0,0.3 3G9T,TYR_125,13.14,0,0,3.14 1ZP2,ASP 148,4.1,0,-0.15,0.45 2APL.GLU 17.3.88.0.36.-0.7.-0.28 2YLF,ASP_93,3.55,-0.65,0.01,0.4 2RIS,ARG 142,13.01,-0.49,0.53,0.48 1XEU,GLU_195,5.24,1.18,0,-0.44 3CE7,TYR_23,10.16,0,-0.03,0.19 2C2Y,HIS 160.5.87,-0.77,0.0.13 1QQE,GLU_282,4.56,0.2,0,-0.14

1YM5.GLU 245.4.56.0.08.0.-0.02 1XIP.GLU 303.5.56.0.91.0.0.16 3EJC,ARG_107,12.39,-0.11,0,0 3B21,ASP_198,3.71,-0.35,-0.04,0.31 2HXB.LYS 52,10.42,-0.08.0.0 1X7F.TYR 22.13.1.-0.85.0.35.3.6 3IO0,LYS_245,10.49,-0.15,0,0.14 4FZN,GLU_4,4.61,0.11,0,0 1P6F,TYR_173,11.15,-0.56,0.48,1.23 3IBT,ASP_67,3.07,-0.47,-0.63,0.37 3ILC,HIS 0,5.97,-0.3,0,-0.23 3TOW, ARG_153, 12.17, -0.63, 0, 0.29 4AF2,ASP_37,3.29,-0.54,-0.3,0.33 1BYI,GLU_12,4.46,0.13,-0.07,-0.11 1U3Y,ASP 297,3.98,0,-0.07,0.24 1NAF,ASP_247,3.89,0,-0.09,0.18 1FKM,ARG_460,12.72,-0.2,0.04,0.38 3CGW,GLU_170,4.29,0.36,-0.6,0.04 2DFL,ASP_16,3.9,0,-0.08,0.18 10GL,ARG 9,12,43,-0,14,0,0.07 2D7U,GLU_162,4.02,1.58,-1.51,-0.55 3BWT,GLU_861,4.68,0.24,0,-0.07 1YTD.TYR 361,12.03.0.-0.06,2.09 1BN6.HIS 199.5.5.-1.02.0.0.02 3AU3,GLU_582,3.05,0.67,-1.83,-0.29 2PGX,ARG_112,12.66,-0.34,0,0.49 1UXO,ARG_46,13.75,-0.22,0.94,0.52 3JSN,ARG 172,13.22,-0.67,0.77,0.62 2RFA,GLU_68,4.64,0.13,0,0.01 4AE7,TYR_149,10.16,0,0,0.16 1DTO,ARG 27,13.57,-0.18,0.77,0.48 1RKA,GLU_126,3.53,0.39,-0.99,-0.38 1YTD, ARG 378, 11.28, -1.88, 0, 0.65 1Y2O,ARG 108,12.86,-0.4,0.32,0.45 2ATR,TYR_45,10.88,-0.1,0.15,0.83 3BCY,HIS_85,5.64,-1.02,0,0.16 2EYI,GLU_143,4.56,0.06,0,0 1NAF,HIS_235,7.25,-0.24,0.77,0.21 2ZTY,GLU_96,4.05,0.32,-0.78,0 3FTT.GLU 123.4.56.0.3.0.-0.24 3TMO, ASP_236, 3.68, -0.53, 0.09, 0.33 2EEY,CYS 124,11.78,0,0,2.78 2VGM,LYS 2,10,74,-0,23,0,0,48 3N2T,HIS_149,5.98,-0.6,0.08,0 2VGM,GLU_304,4.58,0.78,-0.77,0.06 2V1L,HIS_108,6.31,-0.42,0,0.23 1R53,LYS_237,10.58,-0.19,0,0.27 3U0V,ARG_117,12.98,-0.63,0.72,0.4 1P4X,HIS_153,5.83,-0.42,0,-0.25 4FH3,ARG_293,11.21,-1.77,0,0.48 1L2F,GLU 128,3.28,0.24,-0.85,-0.61 1MHN,ASP 96,3.22,-0.83,-0.34,0.6 3ZSL,ASP_215,2.87,-0.85,-0.38,0.3 109G,TYR_4,10.64,0,-0.21,0.85 3MIX,GLU_507,4.64,0.28,0,-0.14 4AE7,LYS 191,10.02,-0.24,0,-0.24 3NZL,ASP_32,4.03,0,0.05,0.17 2CXY,LYS_89,10.11,-0.3,0,-0.08 1NAR,ASP_20,3.8,-0.72,-0.68,1.39 3KEY,LYS_363,10.55,-0.18,0,0.23 309P.HIS 90.6.4,-0.1.0.0 4FCU,ASP_43,2.94,-0.86,-0.42,0.41 4AF2,CYS_95,10.63,-0.03,-0.03,1.68 3GT0,GLU_158,4.67,0.17,0,0 105J,GLU_44,4.6,0.1,0,0 2AZL,GLU 141,4.63,0.2,0,-0.07 2NRR,HIS_488,6.44,-0.3,0,0.24 1JKS,GLU_187,4.42,3.51,-2.32,-1.28 3CQ1,ARG_46,13.63,-0.35,0.81,0.66

3GV0,GLU_78,4.81,1.3,-1.05,0.08 3H6O,LYS 97,11.34,-0.31,0.4,0.77 2F4Q,TYR_77,12.16,0,-0.16,2.33 2YX0.ARG 227.12.48.-0.33.0.0.29 2G2D,GLU_101,4.46,0.34,-0.36,-0.02 4DVD.LYS 59.10.6.-0.38.0.04.0.44 2X5Y,LYS 882,11.01,-0.72,0.78,0.45 3CS1,LYS_64,11.16,-0.38,0.53,0.51 3I4T,LYS_13,10.91,-0.14,0,0.55 3RE9,GLU_84,4.56,0.06,0,0 3IO0,ASP 98,3,18,-0,8,-0,08,0,26 2JKF,GLU_107,3.63,0.41,-0.81,-0.47 3CIV.CYS 147,11.14,-1.01,-0.8,3.95 2FPN,TYR_37,10.46,-0.05,-0.04,0.55 3R87.ARG 77.13.11.-0.61.0.8.0.43 20JO.LYS 583,10.38,-0.25,0.0.14 3V1Q,HIS_594,6.09,-0.32,0,-0.08 3BCY,ASP_117,3.94,0,-0.21,0.34 1JKS,ASP_268,3.12,-1.27,-0.02,0.62 3KV0,ARG 140,12.37,-0.15,0,0.02 1DUN,ASP_116,3.32,-0.79,0,0.31 2FL4,LYS 37,10.68,-0.09,0,0.27 3JSN,ARG_252,12.46,-0.28,0,0.24 2E3C,ASP 206,2.27,-2,-0.91,1.38 3LOE, ASP 231, 4.04, -0.18, -0.08, 0.5 3FXH,HIS_33,6.02,-0.89,0.34,0.06 1GXN,TYR_573,10.22,0,0,0.22 1ILW,ARG_64,13.24,-0.44,0.8,0.38 3MEW,ASP_172,3.93,0,0,0.13 2CE6,ASP_12,2.78,-2.08,-0.59,1.64 3F7M,ASP_288,3.64,-1.5,-0.03,1.38 1YM5,GLU_15,4.29,0.26,0,-0.48 3I47,ASP_186,2.15,-2.17,0,0.52 2E3S,ARG 406,12,34,-0,28,0,0,12 2YX0,TYR_274,10.59,0,0,0.59 1QQL,GLU_90,4.01,0.7,-0.8,-0.39 1YOY,TYR_141,10.01,0,-0.2,0.2 3DTE,ARG 241,13.16,-0.24,0.59,0.31 3H04,LYS_11,10.46,-0.04,0,0 1RI5,ARG_112,11.77,-0.76,0,0.03 3RFY,ASP_193,4.44,-0.05,0.33,0.36 30NH.ARG 466.11.78.-0.96.0.0.24 3CCYARG 75,13.83,-0.44,0.68,1.09 1SFE,ARG_172,11.61,-1.53,0,0.64 3BJV,GLU_42,4.58,0.3,0,-0.22 3JZ9,LYS_382,10.87,-0.28,0.27,0.38 1DZF,ARG 17,13.28,-0.63,0.77,0.64 1XTZ,TYR_99,10.3,0,-0.04,0.34 1AD6,ARG_544,12.44,-0.25,0,0.2 2RGY,HIS 164,5.46,-1.05,0,0.01 1ZCE,TYR 7,13,24,0,0,27,2,97 1WP5,HIS 321,7.6,-0.31,0.8,0.62 3ADO,LYS_307,11.15,-0.73,0.85,0.52 3GOZ,ASP_316,2.12,-1.72,-0.37,0.41 1QYI,HIS_357,6.12,-0.4,0,0.02 4F3J,ASP_120,4,0,0.01,0.19 1TD6.LYS 34.10.54.-0.08.0.0.12 3ETV,LYS_301,10.63,-0.19,0.05,0.27 1X8F,ARG_120,12.21,-0.29,0,0 2HP7.GLU 145.4.68.0.19.0.-0.01 106D.GLU 33.3.84.0.83.-0.68.-0.8 1R7J,ARG_39,12.4,-0.15,0,0.06 3I4T,CYS_98,10.61,0,-0.05,1.66 1YW5,GLU_165,3.91,0.69,-0.93,-0.34 3R2E,ARG_85,12.54,-0.17,0,0.21 1X1E,GLU_118,4.56,0.1,0,-0.04 1RHS,HIS_51,5.57,-1.58,0.63,0.02 1XTZ,GLU 257,3.49,0.57,-0.85,-0.75 4FD6,GLU_114,3.74,1.23,-1.53,-0.47

4F85,HIS 57,4,46,-2,24,0,36,-0,15 3IBT,CYS_52,12.37,-0.36,0.23,3.5 1A8Q,HIS_52,6.07,-2.74,0.87,1.44 4EKU,CYS 61,9.81,-0.76,-0.03,1.59 1KN3,GLU_33,4.84,0.28,0,0.05 2X4J,ASP_33,2.09,-1.64,-0.75,0.69 3IO0,ASP_295,3.89,0,-0.12,0.21 3P28,TYR_103,10.5,0,0.19,0.31 1WYC,TYR_13,10.9,0,0.11,0.78 1R3F,LYS_265,11.23,-0.53,0.85,0.41 1ZYL,GLU 262,6.37,2.68,-0.78,-0.04 10XZ.LYS 213.10.63.-0.31.0.32.0.12 4DND,LYS_16,10.41,-0.09,0,0 1T95,LYS_160,10.42,-0.08,0,0 1PZC.GLU 4.4.6.0.22.0.-0.11 30KO,TYR 558,11,74,0.85,0.46,0.43 1X04,GLU_56,4.72,0.25,0,-0.03 2V4U,ARG_477,12.23,-0.38,0,0.11 3IU5,ASP_59,2.43,-1.48,-0.39,0.5 3LPZ,ARG 98,12.15,-0.51,0,0.16 1GOE,TYR 244,12,22,-0.66,0.46,2.42 3BA1,ASP_123,2.49,-1.26,-0.45,0.41 4EVF,GLU_63,5.45,1.52,-0.68,0.11 1SIG.ARG 122.13.09.-0.43.0.6.0.42 4ETX.ARG 381.13.49.-0.38.0.82.0.56 1YB2,TYR_190,10.94,0,0.25,0.68 4DBX,ASP_286,4.02,0,0.07,0.14 1XTD,LYS_169,10.08,-0.42,0,0 3EX9, ASP 96, 3.42, -0.79, -0.22, 0.63 3BWT,ARG 788,13.21,-0.6,0.57,0.74 3HZQ,GLU_36,4.47,0.21,0,-0.24 4F8A,ASP_631,3.65,-0.3,-0.19,0.34 2G5X,ARG_195,13.89,-0.36,1.28,0.47 2FM9.GLU 153,4.71,0.25,0,-0.04 3ETV,GLU_158,3.79,0.52,-0.85,-0.37 2QK0,ASP_66,2.46,-1.45,-0.46,0.57 1XEU,GLU_269,4.97,0.3,0,0.18 1TD6,GLU_53,4.54,0.22,0,-0.18 1DTO.CYS 140.11.83.0.0.23.2.6 1L2F,TYR_35,10.74,0,0,0.74 3G9B,TYR_42,13.81,-0.7,0.9,3.61 2P5D,LYS 73,11.37,-0.27,0.68,0.47 3H13.LYS 245.10.59.-0.16.0.0.26 4FH3,GLU_124,4.18,0.41,-0.56,-0.17 3P28,LYS_65,10.28,-0.52,0,0.3 3F1X,LYS_31,10.77,-0.24,0,0.51 3G9G,TYR_8,11.72,0.49,0.3,0.94 3GS9,ASP_22,4.15,-0.2,0.2,0.35 3H8Y,ASP_73,3.87,0,-0.08,0.14 2ZO5.TYR 169.10.47.0.0.25.0.22 3H5T,GLU_348,4.66,0.12,0,0.04 1AK1,LYS 205,10.57,-0.29,0,0.36 3RRO.GLU 136.4.68.0.23.0.-0.05 20PJ,ARG_113,12.31,-1.41,0.74,0.48 1YLN,GLU_117,4.65,0.15,0,0 1YM5,GLU_161,5.11,1,-0.12,-0.27 3QKY,TYR_146,10.99,0,0.12,0.88 4EUG,GLU_211,4.82,0.32,0,0 2RH3.GLU 164.4.63.0.13.0.0 3GS9,GLU_111,4.5,0,0,0 3COU,ASP 66,2.07,-2.45,-0.43,1.16 205X.GLU 761.4.37.0.18.0.-0.31 3H13,ASP_343,3.16,-0.75,-0.34,0.44 4EVF,LYS_37,10.33,-0.18,0,0 3ONH,ASP_530,4.21,0,0.03,0.39 1WRU,GLU_278,5.27,1.71,-0.84,-0.1 3C38,LYS 225,10.29,-0.46,0,0.24 2CXY,LYS 43,10.13,-0.41,0.0.04 2X4G,GLU_63,4.84,0.19,0,0.15

1RL0,LYS_235,10.69,-0.1,0,0.29 1ES9,HIS 53,5.66,-0.8,0,-0.03 1RKA,GLU_172,4.41,0.18,0,-0.26 3CS1,LYS_92,10.31,-0.24,0,0.06 3PM2,GLU_26,4.81,0.29,0,0.02 3RFY,ASP_141,3.93,0,-0.17,0.3 200K,ARG_30,11.98,-0.63,0,0.11 3LH5,GLU_675,4.41,0.3,0,-0.39 1R3D,HIS_186,6.27,-0.23,0,0 2AZP,ASP_202,2.76,-1.67,-0.01,0.65 2D8N,TYR 158,10.04,0,-0.3,0.34 1RAJ,ASP_381,1.85,-3,-0.5,1.56 1FO9,TYR_390,13.35,0,0.24,3.11 1XAW,TYR 517,10.82,0.13,0.02,0.68 2CXY,GLU_13,2.5,0.61,-2.04,-0.57 3I0C, ASP 194, 2.85, -1.06, -0.44, 0.56 1HF8.ARG 125.12.11.-0.39.0.0 2FBQ,GLU_25,4.44,0.11,0,-0.18 2X4J,ARG_104,13.17,-0.28,0.67,0.28 1ZP2.LYS 112.10.48.-0.12.0.0.1 2BDV.ARG 4,10.58,-2.02,0,0.11 1X6J,ASP_37,3.7,0,-0.35,0.25 3RJX,LYS 214,10,42,-0,13,0,0,04 3PM2.HIS 167.5.25.-2.0.7.0.05 3CCY,GLU 42,4.43,0.1,0,-0.17 3MIX.TYR 643.11.02.0.0.48.0.54 1DTO,CYS_195,7.79,-1.65,-0.19,0.63 2VGY,ASP_87,3.98,0,0,0.18 1R3F,GLU_106,4.6,0.1,0,0 1WP5,GLU_104,4.5,0.18,0,-0.19 2P0L,CYS_227,9.32,0,-0.04,0.36 3JZN,ARG 313,13,-2,16,0,45,2,21 1MTZ,CYS_269,11.8,0,1.25,1.55 1LTU,LYS 86,11.24,-0.38,0.63.0.48 3PP8,ASP_214,4.07,0,-0.05,0.32 1X7F,HIS_147,2.79,-3.51,0,-0.2 1WRU,ARG_115,13.02,-0.55,0.58,0.49 2RGY,TYR_309,10.06,0,-0.02,0.08 2FZP,GLU 235,3.73,0.3,-0.68,-0.39 1ZP2,CYS_27,9.98,-0.42,-0.64,2.04 1IDK,CYS_161,12.43,-0.17,0.41,3.19 2B0J,LYS_116,10.57,-0.25,0,0.32 3IVF,LYS 306,10.52,-0.15,0,0.17 2ZO5.GLU 135,4.03,0.33,-0.78,-0.02 2IRM,GLU_111,5.61,4.04,-1.7,-1.24 1AKO,ARG_116,13.76,-0.47,1.1,0.63 2EHG,GLU_100,4.78,0.24,0,0.04 2CYG,ARG_84,12.27,-0.25,0,0.02 2B61,LYS_316,11.36,-0.41,0.85,0.42 1DOV,GLU_110,4.57,0.18,0,-0.11 1X9G,HIS_78,5.61,-0.76,0,-0.13 2ZTY,LYS 82,11.16,-0.3,0.68,0.28 3RFF,CYS 80,10.27,-0.02,-0.16,1.45 10I7,GLU_215,2.66,1.68,-2.9,-0.61 2PPN,GLU_102,4.63,0.59,0,-0.47 3EGN,TYR_443,13.5,0.52,0.16,2.82 2BV9,HIS_288,5.48,-0.45,0,-0.58 2OSA,HIS_380,6.22,-0.35,0,0.07 2P0Y,ARG_30,12.01,-0.6,0,0.11 3LJC,GLU_124,4.85,0.16,0,0.2 1QQH,LYS_88,10.22,-0.28,0,0 2G5X.LYS 227.10.55.-0.22.0.0.27 1EYH,ARG_141,12.47,-0.1,0,0.07 3AU3,ASP_491,3.19,-0.89,-0.11,0.38 106D,GLU_17,4.58,0.14,0,-0.06 1D2K,LYS_274,11.5,-0.32,0.85,0.47 3I0C.TYR 126,10,55,0,0,36,0,19 2B0J,HIS_123,5.63,-1.26,0,0.39 3GEC,ARG_533,12.3,-0.53,0,0.33

1NAR.HIS 19.6.33.-0.19.0.04.-0.02 2PP6,ARG 80,11.98,-0.3,0,-0.22 3FRR,ARG_61,12.44,-0.52,0.14,0.32 3JZN,LYS_375,10.56,-0.24,0,0.29 2Z84,ASP 87,4,24,0,-5,20E-18,0,45 2IRM,ARG 308,12,78,-0,15,0,0,44 3QAV,ARG_199,12.83,-1.47,0.84,0.95 1YB2,ASP_169,2.55,-1.35,-0.58,0.69 3EVN,GLU_115,4.54,0.16,0,-0.12 1MIX,LYS_324,10.45,-0.05,0,0 2D0A.HIS 180.4.76.-3.15.0.61.0.81 3MTT,LYS_529,10.56,-0.09,0,0.15 1FHL,TYR_258,10.15,0,0,0.15 4DNU,LYS_252,10.59,-0.18,0,0.26 1H4U,ARG 488,10.18,-3.33,0,1 1059,ARG_339,11.64,-1.98,0,1.11 3K9I,GLU_89,4.43,0.27,0,-0.34 3LOD,HIS_118,6.18,-0.24,0.01,-0.09 1AK1,LYS_307,10.28,-0.38,0,0.16 1BKR.GLU 83.4.87.0.13.0.0.25 3EVP,LYS_69,10.33,-0.19,0,0.02 2D7U,LYS_144,11.5,-0.35,0.85,0.5 3DHN,GLU_204,3.29,2.58,-2.81,-0.99 1MTZ.GLU 186,5.19,0.54,0,0.14 1RZ2,GLU_41,5,0.31,0,0.19 4EKU,GLU_314,4.67,0.17,0,0 2GS5,ARG_12,13.12,-0.47,0.68,0.42 3K9I,ARG 91,12.42,-0.09,0,0.01 1K95,HIS_141,5.64,-0.56,0,-0.31 3CNU,LYS_108,10.45,-0.05,0,0 3ETV,GLU_167,3.64,0.23,-0.83,-0.26 3H04,LYS_7,10.31,-0.19,0,0 3IBT,LYS 38,10.89,-0.54,0.33,0.6 2IRM,ASP_337,3.97,0,-0.2,0.38 3EUR,TYR_106,13.88,-0.08,0.45,3.51 3H9W,LYS_55,10.42,-0.12,0,0.04 1Z3X.LYS 192.10.48.-0.02.0.0 3N2T,ASP 47,2.85,-0.85,-0.47,0.37 1A8Q,LYS_40,11.5,-0.23,0.85,0.38 2FBO,TYR 44,10.08,0,0,0.08 2CBE,TYR_51,13.66,0,0,3.66 3FTT,GLU 3,2.86,0.56,-1.67,-0.53 2PPN.ASP 32,3.05,-0.93,-0.23,0.41 4FH3,HIS_41,5.19,-0.94,0,-0.36 2CWC,TYR_266,10.5,-0.31,0.08,0.73 3DSH,ARG_252,12.42,-0.22,0,0.14 2IRM, ARG_278, 12.42, -0.37, 0, 0.28 1JKS,ASP_14,3.72,0,-0.43,0.36 3KEY,GLU_461,4.04,0.27,-0.73,0 2IRM,TYR_44,10.04,0,0,0.04 3E0H,GLU 82,4.55,0.09,0,-0.04 10XZ.GLU 199.4.7.0.3.0.-0.1 3ETV,LYS_27,10.05,-0.34,0,-0.12 3Q1C,GLU_352,4.5,0.08,0,-0.08 2EYI,LYS_95,10.34,-0.61,0.14,0.3 1R6Y,GLU 34,6.78,2.22,0,0.06 1X8F,LYS_79,11.26,-0.2,0.34,0.61 3EVP,LYS_259,11.48,-0.21,0.57,0.62 3CGW,LYS_214,9.75,-0.98,0,0.23 2W2S, ASP 183, 4.8, -0.07, -0.45, 1.52 2GAU.GLU 166.4.37.0.17.0.-0.3 3RKV,GLU_200,4.62,0.19,0,-0.07 3BCY,TYR_129,9.65,-0.57,-0.34,0.56 1HF8,LYS_149,10.44,-0.06,0,0 3JV1,LYS_94,9.79,-0.69,0,-0.02 200K,CYS_179,12.49,0,0.04,3.44 2GEN,GLU_111,3.99,0.33,-0.46,-0.38 3RJZ,LYS_110,11.1,-0.19,0.55,0.24 2CXC,ARG_129,11.72,-0.78,0,0

2A6B,ARG_173,12.05,-0.55,0,0.1 2FC3.GLU 17.2.94.0.41.-1.59.-0.38 2DVK,ASP_154,4.07,0,0.15,0.12 3RE9,HIS 152,4,19,-2,6,0,78,-0,49 1UOH,ARG_184,12.45,-0.37,0,0.32 3P2F.TYR 47.12.46.0.59.0.59.1.27 3IPZ,GLU_165,4.78,0.17,0,0.11 2E3C,GLU_396,5.18,0.69,0,0 2IF4,LYS_57,10.42,-0.18,0,0.1 2QRX,GLU_110,4.08,0.66,-0.66,-0.42 3M70,GLU_51,4.54,0.15,0,-0.12 3LOD, ARG_110, 11.78, -1, 0.23, 0.04 4EVF,LYS 40,10.43,-0.09,0.0.02 2Q98,HIS_59,4.8,-2.27,0.14,0.43 2ZCX.ARG 197.13.32.-0.12.0.94.0 2PLO.LYS 321,10.07,-0.16,0,-0.27 3RJX,ARG_189,12.15,-2.26,1.2,0.7 2H30,CYS_68,8.29,-1.92,0.05,1.17 1ZCE,LYS_20,11.64,-0.5,0.87,0.76 3GOZ,CYS 184,9.93,0,-0.01,0.94 4EKU,LYS_98,10.6,-0.4,0.17,0.33 2V81,LYS_198,11.53,-0.2,0.85,0.38 4FH3,ARG_349,12.12,-0.51,0,0.12 1G8P,ARG_202,11.97,-1.11,0,0.57 1AKO,ARG 170,12.17,-0.31,0,-0.03 3HUE,ASP_178,3.97,-0.37,-0.05,0.59 100X,GLU_120,3.76,0.26,-0.62,-0.37 3OBS,ASP_123,3.96,-0.78,-0.03,0.98 1QQE,CYS 208,12.18,-0.03,-0.09,3.31 2IF4,ASP_169,3.84,-0.11,0,0.15 3EZ7,GLU_31,4.42,0.23,-0.31,0 2QVT,ARG_122,12.28,-0.22,0,0 2D7U,CYS 131,9.67,-1.92,-0.15,2.74 3GOZ,HIS 297,5.85,-0.3,0,-0.35 3C6B,GLU_251,4.98,1.09,-0.54,-0.06 3EVP,LYS_71,10.56,-0.31,0,0.37 2FL7,LYS_129,10.11,-0.41,0,0.02 2D59,TYR 109,9.42,-1.47,-0.04,0.92 3A4C,CYS_498,9.14,-0.7,0.08,0.76 3GA2,GLU_161,4.69,0.13,0,0.07 3CAX,ASP_472,3.8,0,0,0 2AHE,ASP 180,1.96,-2.98,-0.55,1.69 20DJ.CYS 278,10.81,-0.07,0.38,1.49 1R29,ARG_122,12.8,-0.19,0.09,0.4 2H01,HIS_132,4.39,-2.26,0.15,0 2Q34,GLU_22,3.92,0.27,-0.85,0 3HYQ,GLU_114,4.67,0.17,0,0.01 1NWA,LYS 104,10.9,-0.22,0,0.61 2Q12,GLU_255,4.59,0.09,0,0 1QQH,HIS_188,6.56,-0.79,0.85,0.01 1NJ4.HIS 146.5.88.-0.6.0.-0.03 4EF5,ARG 284,11.84,-0.88,0.0.22 3PP8,LYS_298,10.62,-0.14,0,0.26 3PU6,ASP_143,2.8,-0.79,-0.77,0.56 1SIG,GLU_152,4.6,0.42,0,-0.32 4ANN,GLU_149,4.25,0.67,-0.54,-0.38 3NR5.GLU 109.4.73.0.16.0.0.06 4AM1,TYR_168,10.16,-0.53,-0.28,0.98 3BB7,GLU_263,4.26,0.64,-0.39,-0.5 1R53.HIS 271.6.55.-0.54.0.57.0.01 2A4D,GLU 197,4.29,1.06,-0.83,-0.43 2AXO,LYS_171,10.46,-0.08,0,0.04 1PV5,ARG_247,12.76,-0.19,0.21,0.25 2OJQ,GLU_474,4.57,0.07,0,0 2ZTY,ASP_85,2.14,-1.82,-0.53,0.68 3M66, ARG_181, 12.44, -0.22, 0, 0.17 30IP,LYS_22,11,-0.15,0.2,0.44 1VJG,GLU 130,4.18,0.8,-0.72,-0.4 2B61,CYS_167,13.62,-0.05,1.03,3.65

2R51.LYS 230.10.9.-0.19.0.0.59 3FXH,GLU_34,4.45,0.21,-0.16,-0.09 1L2H,TYR_68,11.66,0,0.08,1.58 2HP7.TYR 89.12.51.-0.68.0.46.2.74 4EZB,GLU_228,4.34,0.34,0,-0.49 1FOLGLU 349.4 67.0 22.0 -0.05 3GEC,LYS_446,10.02,-0.36,0,-0.12 1DZF,GLU_102,4.39,0.14,0,-0.26 3EUR,GLU_74,3.36,0.43,-1.47,-0.1 2OGQ,TYR_462,10.96,0.27,0.29,0.41 20KT,GLU 303,4.32,0.2,0,-0.38 1XEU.LYS 185,10.16,-0.28,0,-0.06 2G2D,ARG_137,12.56,-0.19,0,0.25 3LD1,CYS_110,9.17,-0.17,0,0.34 3RJX.ARG 106.13.53.-1.73.1.29.1.47 3IBT,ARG 56,12,54,-0.91,0.36,0.59 3S0A, ASP_58, 2.61, -1.39, -0.38, 0.6 20KT.HIS 165.6.11.-0.25.0.-0.14 3BQE,LYS_363,11.27,-0.46,0.67,0.56 1UAJ,GLU 80,4.56,0.08,0,-0.02 2P52.HIS 230.5.69,-0.87.0.0.06 1G5Z,GLU_109,4.73,0.24,0,-0.01 3IBT,ARG_167,12.22,-0.28,0,0 3LJN.GLU 300.4.86.0.36.0.0 3RVC.ARG 200.12.46.-0.1.0.0.06 4EKU,ASP_37,4.07,0,-0.11,0.38 2XMZ,LYS_262,10.4,-0.11,0,0.01 1XEU,LYS_217,10.36,-0.12,0,-0.02 1ZCE,GLU_10,3.99,0.32,-0.47,-0.36 2Q13,ASP_49,3.84,0,-0.37,0.4 1X7F,LYS_288,10.63,-0.16,0,0.28 1W24,LYS_21,10.81,-0.35,0.12,0.55 3MIX,GLU_668,4.64,0.14,0,0 3BB7,HIS 179,6.15,-0.44,0,0.1 1XFK,HIS_15,6.45,-0.32,0.27,0 1RAJ,ARG_379,11.97,-0.69,0,0.16 1PVT,ARG_2,12.51,-0.1,0,0.1 1NJ4,ARG_304,13.69,-0.6,1.07,0.72 2G9D,ASP_298,3.82,0,-0.16,0.17 3Q6L,ASP_3,3.74,0,-0.23,0.17 3F7M,GLU_345,3.72,1.06,-1.4,-0.43 2H85,ASP 16,2.83,-0.81,-0.71,0.56 1SQH,ARG 72,12.08,-0.43,0,0.02 3E5T,GLU_145,1.78,3.52,-1.79,-4.46 3CE7,ASP_66,4.57,0,0,0.77 3Q9P,CYS_137,9.24,0,-0.18,0.43 1UXO,HIS 161,7.26,-0.24,0.73,0.27 3PAC, ASP_70, 4.13, -0.19, -0.01, 0.53 3CIV,ARG_33,12.12,-0.41,0,0.03 2HXB,ASP 25,3.84,0,-0,14,0,18 1AKO,GLU_95,4.85,0.35,0,0 1YR6,GLU_174,3.46,0.33,-1.02,-0.35 108B.CYS 48.11.13.-0.14.0.4.1.87 3PAC, ASP_143, 3.21, -0.93, -0.19, 0.53 1SJY,ARG_64,13.26,-0.53,0.16,1.12 3C2E,LYS_84,11.46,-0.19,0.66,0.49 1Q42,ASP_110,2.38,-2.11,-0.35,1.03 3MIX,GLU_321,4.45,0.15,0,-0.2 1SOH,ASP 15,2,45,-1,18,-0,96,0,78 2JHY,TYR_175,10.5,-0.08,-0.39,0.96 3M16,LYS_226,10.35,-0.25,0,0.1 1NKD,HIS 44,6,55,-0,48,0,21,0,33 3I47,TYR_8,11.42,0,0.17,1.26 3UAH,TYR_170,13.67,0.04,0.81,2.82 3QKY,GLU_93,4.35,1.71,-0.96,-0.9 2B61,ASP_334,3.03,-0.85,-0.33,0.41 1J7G,LYS_41,10.95,-0.34,0,0.79 3ANJ,LYS 88,10.62,-0.3,0.03,0.38 1S7K,ARG_147,12.34,-0.1,0,-0.06

2FG1,LYS_146,10.54,-0.58,0.41,0.21 3DTE, ARG 75, 12.47, -0.22, 0, 0.2 208P,GLU_184,4.65,0.2,0,-0.04 1WRU,GLU_133,3.9,0.29,-0.91,0.02 2EFK,ARG_226,12.41,-0.59,0,0.5 3FXH,HIS 11.6.16,-0.34,0.0 3GW3.GLU 63.3.05.0.4.-1.5.-0.35 2H30,LYS_80,10.55,-0.22,0,0.27 3K8U,LYS_7,9.99,-0.4,0,-0.1 2GAU,ASP_173,1.61,-2.56,-0.27,0.64 3H5T.CYS 274.13.12.0.0.29.3.83 1MUF,LYS 233,10.23,-0.33,0,0.06 1V43,GLU_62,4.28,0.88,-0.43,-0.67 2EHG,ASP 142,3.86,0,-0,15,0,21 3LMF,HIS_40,5.78,-0.51,0.02,-0.23 3GE9,GLU 152,4.6,0.1,0,0.01 1JB3,LYS 38,11.32,-0.68,0.74,0.77 3T57,GLU_296,4.55,0.5,-0.05,-0.4 2BLL,HIS_361,7.41,-0.34,0.85,0.4 4ECC,ASP 75,3.63,-0.02,-0.29,0.15 1SJY.GLU 65.6.14.1.34.0.0.31 1YM5,TYR_64,10.31,-0.12,0.03,0.4 1U53,LYS 68,10,39,-0,11,0,0 2AH5,TYR 71,13.06,0,-0.02,3.07 4FH3,TYR 52,9.69,-0.84,-0.81,1.34 3GS3,GLU_221,4.67,0.15,0,0.02 1Z3X,ARG_193,13.7,-0.35,1.17,0.38 1SIG,ARG_260,11.78,-0.85,0,0.13 4AM1,LYS_303,10.64,-0.13,0,0.28 2G9D,HIS_295,6.27,-0.24,0,1.04E-17 3AUF,ARG_189,13.27,-0.4,0.39,0.78 2H2W.GLU 83.3.96.0.21,-0.75.0 2Z0M, ARG_257, 12.33, -0.2, 0, 0.04 2H2Z,ARG_217,12.23,-0.35,0,0.08 20KT.ARG 321.12.31.-0.19.0.0 2Q99,GLU_11,5.57,3.95,-1.67,-1.22 109G,ASP_153,3.89,-0.71,0.13,0.67 3COU, ARG_67, 12.49, -0.05, 0, 0.04 3BCY,HIS 60,6.62,-0.28,0,0.4 3EOD,LYS_8,10.62,-0.27,0,0.39 3TOW, ARG 190, 12, 59, -0.32, 0, 0, 42 4FZN,ARG_163,12.78,-0.28,0.22,0.34 3L7N,LYS 62,10.9,-0.3,0.31,0.39 3HVM,LYS 74,10.25,-0.57,0,0.33 10I7,GLU_19,4.43,0.28,0,-0.34 1ILW,CYS_133,13.41,-0.02,1.19,3.24 3DTE,ARG_54,12.37,-0.22,0,0.09 1V43,GLU_66,4.4,0.24,0,-0.34 3ETV,LYS_182,10.44,-0.06,0,0.01 3CZC,HIS_62,6.65,-0.31,0.24,0.21 3TMO,LYS_253,10.64,-0.16,0,0.29 2RJD,GLU_214,4.86,0.32,0,0.04 30NH.GLU 534.4.65.0.12.0.0.03 2BQQ,TYR_70,12.33,0,0.6,1.74 2FG1,ASP_88,1.7,-2.14,-0.62,0.66 4ANN,ASP_60,2.94,-0.85,-0.66,0.65 2VGM,LYS_25,11.35,-0.42,0.45,0.83 4DNU.TYR 82.10.9.-0.66.0.1.56 3D9H,GLU_231,4.36,0.29,-0.31,-0.12 2W1R,GLU_100,4.4,0.15,-0.06,-0.2 2G9D,ARG_90,11.93,-1.99,0.62,0.8 4H4J.ARG 139.12.59.-0.18.0.11.0.17 2JKF,GLU_149,4.58,0.08,0,0 3BWT,HIS_783,6.24,-0.19,0,-0.07 2XJ4,ARG_44,13.79,-0.33,1.19,0.42 1NWA,GLU_101,3.77,0.3,-0.46,-0.56 2JEO,CYS 40,13.04,-0.09,0.79,3.33 3EVP,ARG_254,9.57,-3.11,0,0.17 1VJG,HIS_182,5.82,-1.78,0.85,0.24

1YTD.LYS 230.11.39.-0.39.0.85.0.44 2G9D,ARG 242,12.81,-1.52,0.76,1.07 3RNV,ASP_410,2.57,-1.29,-0.38,0.45 3DSH,ASP_239,4.55,0,0.03,0.72 3DSH,CYS 340,10.23,-0.01,-0.13,1.36 2DG7.TYR 47.10.68.0.0.0.68 3ERF,CYS_86,11.05,-0.18,-1.15,3.36 3G9B,ARG_46,12.6,-0.37,0,0.47 3AU3,LYS_523,10.38,-0.27,0,0.15 1R5Q,CYS 45,9.36,-0.01,0,0.37 3GS9.TYR 212.10.22.0.0.0.22 1P1L,GLU_102,5.06,0.41,0,0.16 3CX2,ASP_245,4.04,0,-0.05,0.29 3LD1,CYS_212,11.26,-0.03,-0.02,2.29 2HRZ.ARG 22.12.21.-0.41.0.0.12 3JZ9,GLU_344,4.79,0.21,0,0.08 3CAX,LYS_126,10.99,-0.41,0.52,0.38 2EDM,ARG_67,12.19,-0.69,0,0.38 3LJN,GLU_307,4.88,0.24,0,0.14 3K8J.GLU 67.4.49.0.06.0.-0.08 1G8P,ARG_262,12.5,-0.4,0.13,0.27 1DCF,LYS_95,10.43,-0.07,0,0 2FI9,GLU_85,4.63,0.11,0,0.03 2BAA, ARG 110, 12.4, -0.43, 0, 0.34 3VJ8,GLU_113,4.3,0.27,-0.11,-0.36 1VSM,GLU_187,4.47,0.1,0,-0.13 3RJX,LYS_274,10.43,-0.07,0,0 3JZ9,ASP 388,3.31,-0.85,-0.16,0.53 1PGV,HIS_266,5.94,-0.52,0,-0.03 1D2K,TYR_219,12.87,0.71,0.47,1.69 1RI6.LYS 297.10.54.-0.2.0.0.23 2X4L,LYS_56,10.31,-0.22,0,0.02 1DUN,LYS 42,10.48,-0.18,0,0.15 1SNT.TYR 59,11.2.0.0.06,1.14 2Z0M,HIS_199,4.98,-1.53,0,0.03 2ZCO,ARG_271,12.44,-0.16,0,0.09 3CNU,CYS_12,12.45,0.53,0.72,2.21 2AXO, ARG_143, 12.64, -0.09, 0, 0.23 2V5B,ARG_55,12.32,-0.3,0,0.12 2VAN,GLU_172,4.67,0.2,0,-0.03 3IVF,ASP_27,4.15,-0.12,-0.15,0.61 3M16,ARG 135,11.86,-0.71,0,0.05 1YTO.HIS 106.6.6.-0.44.0.71.-0.17 2ZQ5,LYS_22,10.4,-0.07,0,-0.03 1MUF,GLU_279,4.47,0.19,-0.2,-0.03 1EYH,TYR_101,10.18,0,0.05,0.14 1YG2,TYR_137,13.78,1.41,1.08,1.29 2P52,HIS_176,5.88,-0.74,0.43,-0.31 1XIP,TYR_243,13.25,-0.34,0.8,2.78 1AD6,LYS_548,10.09,-0.3,0,-0.11 1YTQ,TYR 163,11.34,-0.07,0.09,1.32 2D7U,LYS 65,11,36,-0.37,0.85,0.38 2OGQ,LYS_589,10.35,-0.23,0,0.08 3IRA,GLU_64,4.79,0.25,0,0.04 1PVT,TYR_71,10.89,0,0.53,0.36 4ECC,CYS 151,9.55,0,0.12,0.42 3PBH,LYS_166,10.42,-0.42,0,0.33 2WOZ,LYS_602,10.29,-0.25,0,0.05 3H04,CYS_77,11.03,-0.01,0.59,1.47 3EX9,GLU_36,4.67,0.22,0,-0.05 2ZCX.GLU 133.4.21.0.3.-0.59.0 3LD1,GLU_128,4.69,0.21,0,-0.03 1WP5,ARG_248,13.78,-0.9,1.55,0.63 2BLL,CYS_383,11.68,0,-0.24,2.91 10IS,LYS_236,11.45,-0.32,0.83,0.44 3TRE, ARG 54, 12.41, -0.36, 0, 0.28 2PLQ,ASP_303,3.85,0,-0.1,0.16 3IL3,ARG_17,11.78,-1.36,0.01,0.63 1IDK,TYR 254,10.39,0,0.18,0.21

10I7,GLU_278,4.31,0.36,-0.84,0.28 2IOT.GLU 190,5.94,3.97,-1.66,-0.87 1RWZ,LYS_233,10.45,-0.45,0,0.4 4FZR,LYS_79,10.57,-0.17,0,0.24 1NAR,HIS 133,6,36,-0,73,0,29,0,3 1XIP.TYR 108,10.51,0,0,0.51 2RJD.TYR 255,13,33,0.0.62,2.72 3ETV,LYS_145,10.27,-0.23,0,0 3HUE,ARG_250,12.5,-0.1,0,0.1 2WB8,ASP_703,2.95,-1.45,-0.01,0.6 1W7B,LYS_206,10.45,-0.05,0,0 4GA2,TYR_116,9.83,0,-0.43,0.26 1LTU,LYS_167,10.18,-0.29,0,-0.03 3ASA,ASP_378,4.44,-0.03,-0.01,0.69 3CIV.HIS 113.6.78.-0.34.0.0.61 3JZN,ASP_237,3.64,-0.67,-0.15,0.65 2WB8,ARG_590,13.96,-0.43,1.26,0.64 3ADO,TYR_255,10,-0.04,-0.2,0.23 20EW,GLU_144,4.84,0.24,0,0.1 1IAP,ARG 152,12.31,-0.22,0,0.03 3OA7,TYR_534,10.65,0,0.31,0.34 1NJ4.GLU 230.5.01.0.7.0.-0.19 3IVF,HIS_124,6.22,-0.45,0,0.17 2WZ9,GLU 75,4.34,0.24,-0.4,0 3K1H.GLU 130.4.79.0.25.0.0.04 1V6T,GLU_23,4.66,0.24,0,-0.08 1FKM,ARG_303,12.38,-0.12,0,0 1KCM,GLU_102,3.72,0.57,-0.85,-0.49 3RNV,GLU_375,3.67,0.41,-0.85,-0.38 1QQE,LYS_261,10.49,-0.09,0,0.09 3ELI,ARG_8,11.79,-0.68,0,-0.03 1V43,LYS_370,10.38,-0.13,0,0 2DG7,ASP_139,2.66,-1.6,0,0.45 1046.GLU 116.4.51.0.23.0.-0.22 3CRM,GLU_272,3.59,0.29,-0.9,-0.3 1EW4,HIS_58,6.14,-0.52,0.04,0.12 1AD6,ARG_418,11.76,-1.77,0.19,0.84 3H6Q,ASP_113,3.73,0,-0.24,0.18 1IAP,GLU_169,4.17,1.28,-1.11,-0.5 3GE9,HIS_69,6.17,-0.31,0,-0.02 1UOH,LYS_206,10.62,-0.25,0,0.37 1ZCU.CYS 88.13.14.-0.53.0.09.4.57 3GYW.TYR 127.10.49.0.-0.05.0.54 1QYI,TYR_27,10.66,-0.06,-0.21,0.93 1PGV,ARG_312,12.21,-0.31,0,0.03 1YB2,GLU_20,4.11,0.41,-0.56,-0.23 3RLE, ARG 101, 13.25, -0.54, 0.83, 0.46 2H01.GLU 19.4.85.0.41.0.-0.06 3N2T,LYS_228,10.46,-0.04,0,0 3F1X,LYS_122,10.24,-0.35,0,0.09 2AD1.LYS 202.11.15.-0.31.0.28.0.67 1PV5,ARG_28,12.35,-0.22,0,0.07 1L2F,ARG_119,12.41,-0.17,0,0.08 3QKY,ARG_52,12.75,-0.33,0.26,0.31 1TR9,HIS_108,5.6,-2.31,1.22,0.19 2P0Y,LYS_143,10.37,-0.17,0,0.04 3BA1.GLU 240.4.07.0.4.-0.49.-0.35 3JV1,GLU_114,5.16,0.3,0,0.37 1DOV,ASP_114,3.26,-0.85,0,0.31 3GS3,TYR_131,11.51,-1.29,-1.14,3.92 2Q34,CYS_103,10.76,-0.72,-0.5,2.99 3IRA,ARG_128,12.54,-0.29,0,0.33 2FZP,ARG_231,13.38,-0.11,0.68,0.3 2CW4,ARG_51,11.91,-1.03,0,0.45 3EGN,LYS_437,10.34,-0.27,0,0.12 2NRK,GLU_18,4.79,0.16,0,0.13 2BDD,LYS_144,10.19,-0.31,0,0 3RFF,ASP_112,3.16,-0.62,-0.38,0.36 3P2F,GLU_81,4.04,0.45,-0.85,-0.06

1SQW,LYS_100,10.29,-0.21,0,0 2ZCO,GLU 180,4.52,0.12,0,-0.09 3EVN,GLU_60,4.72,0.17,0,0.05 3OA7,TYR_501,10.08,0,-0.07,0.15 3MIX,TYR_501,10.33,0,0.1,0.22 2RIS.LYS 204,10.46,-0.04,0.0 1UOH, ASP 68, 4, 12, 0, -0, 15, 0, 46 2Q99,ARG_52,12.27,-0.29,0,0.06 2FG1,TYR_97,9.95,-0.74,-0.05,0.75 2VGM,GLU_132,4.17,1.09,-0.6,-0.82 2VGM,GLU_333,4.55,0.24,0,-0.19 2E3S.TYR 435,10.41,-0.01,-0.46,0.87 3U2A, ARG_79, 13.06, -0.54, 0.79, 0.31 2IDC, ASP_20, 3.09, -0.84, -0.47, 0.59 2007, ARG 436, 13, 2, -0, 64, 0, 12, 1, 23 3GFP.HIS 441.5.82,-1.04.0.0.36 2PIM,ASP_32,3.28,-0.8,-0.02,0.3 1Z9L,TYR_78,10.27,0,0.08,0.2 3P2F,ARG_44,12.6,-0.35,0,0.46 3P28,GLU 165,2.74,0.63,-1.57,-0.81 3L3P.ARG 445,13,29,-0.51,0.6,0,71 3HKX,HIS_37,5.92,-0.53,0,-0.05 2QVT,ARG_123,12.32,-0.25,0,0.07 3BWT,ASP 610,3,36,-1,47,-0,12,1,16 1W7BLYS 302.10.53.-0.39.0.0.42 3H6Q,TYR_103,10.71,0,0.1,0.61 1S7K,ASP_101,0.79,-3.4,-0.38,0.78 2W2S,ARG_73,12.64,-0.3,0.07,0.37 20KT,LYS 147,10.21,-0.4,0,0.11 1WXF,GLU_137,5.01,0.51,0,0.01 2WOZ,ASP_421,3.39,-0.64,-0.24,0.48 3CE7,GLU_88,3.62,0.72,-1.42,-0.18 1NIJ,GLU_42,4.41,0.08,0,-0.17 1ZBP,GLU 10,4.62,0.15,0,-0.03 2Q99,LYS_215,12.32,-0.9,1.7,1.02 1TLV,TYR_202,9.76,-0.73,-0.05,0.53 3M70,GLU_86,4.61,0.29,0,-0.19 2BQQ,TYR_103,9.92,0,-0.34,0.26 3JSN,TYR 52,10,42,-0,11,0,23,0,3 3CGW,GLU_142,4.87,0.22,0,0.15 3ONH,LYS_457,10.88,-0.19,0,0.57 30IP.TYR 95,11.52,0.75,0.38,0.39 1AM2,HIS 187,6.62,-0.46,0.37,0.21 1L2F,LYS_179,10.46,-0.68,0,0.65 2PP6,LYS_23,10.69,-0.19,0,0.38 1TP6,ARG_66,12.48,-0.98,0.66,0.3 3TOW, ASP 67, 4.02, 0, -0.15, 0.38 1ZCU,TYR_94,13.09,0.8,0.73,1.55 1ZP2,LYS_66,10.48,-0.15,0,0.13 2V4X.LYS 70.10.3.-0.51.0.0.31 2ATR,LYS_5,10.4,-0.11,0,0.01 2H01,TYR_160,9.81,-0.4,0,0.21 4FZN,TYR 13,13,58,0,0,09,3,5 1L2F,LYS_173,10.7,-0.09,0,0.28 1N81,ARG_92,13.3,-0.31,0.53,0.57 2FBI,GLU_122,4.29,0.18,-0.39,0 2WOZ,LYS 575,11.05,-0.23,0.1,0.68 2R57,GLU_321,5.52,3.9,-2.8,-0.08 2IF4,GLU 192,4,51,0.06,0,-0.05 3NR5,ASP_62,2.86,-1.4,0,0.46 3GG6,GLU 79,4.72,0.32,0,-0.1 2X4G,GLU_246,4.97,0.35,0,0.11 2R51,GLU_98,4.96,0.36,0.19,-0.08 4F85,GLU_94,4.62,0.64,-0.36,-0.15 3ASA,ARG_268,12.71,-0.32,0.16,0.38 3DTE,TYR_103,10.56,0,0.08,0.48 3U4K,TYR_113,12.73,0,-0.1,2.83 2EFK.LYS 66,10.24,-0.34,0.0.08 3I47,TYR_230,10.72,0,0.25,0.48

3BQW,LYS_184,9.81,-0.78,0,0.09 1Y2Q,LYS 18,10.38,-0.06,0,-0.07 3DB9,ASP_117,3.74,-0.36,-0.01,0.31 3L7N,ARG_231,13.22,-0.36,0.57,0.51 3M70,GLU_58,3.57,0.4,-0.85,-0.47 2GS5.TYR 78.10.75.-0.08.-0.8.1.63 4D8LARG 121.10.71.-1.55.0.-0.23 3UV9,ASP_447,3.12,-0.92,-0.32,0.56 1NIJ,ASP_189,3.82,0,-0.24,0.27 1X8F,LYS_130,10.42,-0.08,0,0 1T95,ASP 143,3.24,-0.77,-0.55,0.77 2FG1,GLU_141,3.12,0.38,-1.43,-0.33 2Q99,LYS_368,10.44,-0.06,0,0 2PLO.TYR 171.11.25.0.0.63.0.62 1MJS,GLU_346,6.04,1.65,-0.04,-0.06 3RHE,HIS 114,6.83,-0.25,0,0.58 3QAV,ASP_33,3.31,-0.55,-0.39,0.45 3Q1C,HIS_186,6.11,-0.77,0,0.37 2C2Y,GLU_106,4.24,0.65,-0.8,-0.11 2W2S,LYS 115,11,16,-0,31,0,44,0,53 2YT4.GLU 574.4.88.0.74.0.-0.36 3PP8,GLU_136,3.02,0.7,-1.72,-0.45 1RWZ.LYS 130,11.05,-0.28,0.45,0.38 1L2F,LYS 269,9,36,-0.55,0,-0.59 1U3Y,LYS 312,10.76,-0.15,0,0.42 1S7K.ASP 165.3.82.0.-0.18.0.2 2AHE,CYS_234,11.87,0,-0.01,2.88 1Q5Z,GLU_603,4.51,0.27,0,-0.26 200P.ARG 168.12.11.-1.12.0.03.0.7 1X91,ASP_106,4.19,0,0.09,0.29 3C38,ARG_72,12.12,-0.43,0,0.04 1AIL,GLU_26,4.57,0.07,0,0 1T6L,LYS_78,11.03,-1.24,0.77,0.99 3JZN, ASP 362, 3.35, -0.81, 0, 0.36 2IXM,HIS 318,6.98,-0.4,0.85,0.03 2QDJ,GLU_315,4.58,0.28,0,-0.2 2QEV,LYS_34,9.95,-0.58,0,0.02 2WB8,LYS_771,10.35,-0.29,0,0.13 4H4J,GLU 47,2.66,1.81,-2.19,-1.46 2Q12,ARG_72,12.42,-0.08,0,0 3HVM,GLU_161,4.41,1.07,-0.96,-0.2 1QZN,ASP_83,2,-1.79,-0.51,0.5 3RLE,LYS 50,10.41,-0.13,0,0.05 1X1E,CYS 173,10.62,-1.1,-0.14,2.85 1M5I,ARG_232,13.05,-0.36,0.66,0.25 2BAA,LYS_109,10.36,-0.27,0,0.13 1NKD,GLU_5,3.87,0.41,-0.87,-0.16 2EA9,CYS 100,9.27,0,-0.09,0.36 2YX0,TYR_158,10.36,0,0.02,0.34 3U0V,LYS_163,10.38,-0.12,0,0 4ANN,ARG_153,12.65,-0.93,0.54,0.53 2BT8,ARG_316,12.28,-0.26,0,0.04 4FCU.ASP 64.3.12.-0.85.-0.53.0.7 2DFL,ARG_180,12.52,-0.44,0,0.46 2HXB,ASP_7,2.46,-1.63,-0.12,0.41 4EVF,LYS_169,10.39,-0.15,0,0.03 1QQE,GLU_224,4.47,0.62,-0.1,-0.55 3O2C,GLU 92,4.55,0.39,-0.14,-0.2 3H8Y,CYS_68,10.36,-0.22,0.16,1.42 2Z84,CYS_186,9.23,0,-0.02,0.24 1X8F,ASP_243,3.98,-0.13,-0.11,0.43 2E3S.GLU 409.4.68.0.26.0.-0.09 4HDE,HIS_158,5.36,-1.82,0.68,0 3C5V,ARG_369,12.24,-0.26,0,0 1WXQ,LYS_241,10.44,-0.06,0,0 1NJ4,LYS_246,10.42,-0.17,0,0.1 2RJD.LYS 442.10.14.-0.36.0.0 2B78,ARG_248,12.19,-0.31,0,0 1BYI,GLU_44,4.6,0.27,-0.19,0.02

1R53.LYS 183.10.23.-0.23.0.-0.04 3048,ASP 12,2.85,-1.16,-0.21,0.41 1JKS,TYR_83,12.49,0.49,0.5,1.49 1YR6,TYR_238,10.77,0.27,0.38,0.11 3M7G,ASP 178,3.9,-0.03,0.0.14 1WPA.GLU 419.4.5.0.32.0.-0.32 2FI9,TYR_45,9.63,-0.85,-0.06,0.54 3G6S,LYS 35,10,48,-0,35,0,0,32 1CHD,HIS_270,5.75,-0.66,0,-0.1 1NRI,HIS_114,6.31,-0.26,0.13,-0.05 1P6F,LYS 186,10.36,-0.13,0.0 30DJ,LYS_88,10.44,-1.16,0.75,0.34 2GZR,GLU_165,5.92,2.5,-0.6,-0.48 1W7B,ARG_178,12.43,-0.19,0,0.12 3F7M.ARG 120.11.8.-0.81.0.0.11 3ULX,GLU_26,3.73,0.33,-0.91,-0.19 3RLE,CYS_192,11.55,0,0.05,2.5 1EV8,TYR_209,11.97,0.33,0.85,0.79 300P,ARG_106,12.78,-0.7,0.35,0.63 3I0C,TYR 71,10.83,0.02,0.46,0.35 3Q1C,HIS_40,6.58,-0.35,0.14,0.3 1TWU,GLU_121,4.6,0.76,-0.34,-0.32 1MD6,LYS_11,10.36,-0.36,0,0.22 2BDD,ASP 120,1.71,-2.38,-0.4,0.7 3BA1,GLU_44,3.77,0.29,-0.63,-0.38 3CGW,LYS_176,11.04,-0.28,0.43,0.39 2G9D,ASP_336,3.98,0,0,0.18 2H8O, ARG 44, 12.41, -0.25, 0, 0.17 1PBV,GLU_117,3.86,0.6,-0.63,-0.61 2D0A,LYS_132,11.33,-0.71,0.65,0.89 1O5T,TYR_248,10.22,0,0,0.22 2IQT,LYS_203,10.46,-0.23,0,0.19 2YX0,CYS_81,12.11,-1.24,0.86,3.48 1TXJ.TYR 134,12.06.0.0.69,1.36 3BA1,GLU_272,2.29,1.02,-2.26,-0.97 3GW3,GLU_270,4.88,0.15,0,0.23 2Z61,TYR_308,10.55,-1.5,-1.62,3.67 1ZBS,TYR_277,10.22,-0.27,-0.66,1.15 1DVO,LYS_138,10.51,-0.11,0,0.12 2BV9,HIS 137,7.12,-0.85,0.85,0.62 3CIV,TYR_247,10.43,-0.04,-0.26,0.72 3T57,ARG_259,12.66,-0.21,0,0.37 10IS.TYR 358,10,42,0,-0,11,0,53 1T95,LYS_139,10.4,-0.23,0,0.13 1PBV,ARG_152,12.51,-0.19,0,0.2 3GEC,ARG_460,12.77,-0.71,0.33,0.65 1X1E,ASP_51,2.94,-0.93,-0.52,0.59 1HUF,GLU_118,2.9,1.14,-1.7,-1.04 1XTZ,ASP_63,3.09,-0.79,-0.4,0.48 4EKU,GLU_301,4.46,0.6,-0.51,-0.14 2W0G,TYR 248,12.07,0,0.18,1.88 2GZO.ASP 87.3.89.0.-0.15.0.24 2R2Y,HIS_58,6.62,-0.57,0.12,0.56 1SQH,GLU_175,4.65,0.19,0,-0.04 4HDE,GLU_120,4.51,0.07,0,-0.06 2EA9,HIS 87,5.51,-0.61,0,-0.38 3QKY,LYS_85,11.16,-0.22,0.5,0.38 3UAH,TYR_396,9.5,-0.73,-0.71,0.94 2P0L,LYS_187,11.48,-0.37,0.85,0.5 1YOY,GLU 41,4.08,0.39,-0.82,0 1XWM,LYS 102,10,41,-0,23,0,0,15 2CI3,TYR_223,11.97,-0.03,0.02,1.98 2BQQ,ARG_56,12.2,-0.6,0,0.31 1059,LYS_140,10.52,-0.35,0,0.38 208P,HIS_62,6.91,-0.7,0.85,0.26 2XJ4,GLU_94,4.5,0.44,0,-0.44 2H30,LYS_157,10.35,-0.15,0,0 2RIK,LYS_193,10.73,-0.11,0,0.34 3VHJ,ASP_104,4.31,0,0.21,0.3

1LZL.ASP 233.4.19.0.0.21.0.18 2P52.HIS 211.4.81.-1.62.0.-0.08 1WXQ,LYS_295,10.41,-0.09,0,0.01 2P1W,GLU_199,4.41,0.15,0,-0.23 1Q42,ASP_66,2.83,-1.33,-0.5,0.86 1RSS.ARG 143.13.3.-0.29.0.67.0.42 2PGX,ASP_87,3.87,0,-0.04,0.11 2FD4,TYR_547,10.88,0,0.12,0.77 3IBT,ASP_161,2.73,-1.13,-0.41,0.47 4AE7,CYS_142,12.27,-0.81,0.08,4 2HP7,GLU_111,4.63,0.13,0,0 3IV4,LYS_4,10.73,-0.19,0,0.41 3T5B,GLU_389,4.44,0.26,0,-0.31 1ZBS,ARG_230,12.43,-0.07,0,0 2ATR.GLU 8.4.49.0.1.0.-0.11 1HUF,CYS 23,9.86,-0.04,0.04,0.86 1R29,HIS_116,6.54,-0.14,0,0.18 1WRU,ARG_244,11.99,-0.41,0,-0.11 2AZL,LYS_53,10.36,-0.53,0,0.39 2ZCO,CYS 11,12.49,-0.07,0.12,3.43 2E3S,ASP_385,3.07,-0.91,-0.14,0.33 1BN6,ASP_167,3.89,-0.04,-0.09,0.22 3P51,GLU_139,3.85,0.94,-1.13,-0.45 2RFA,GLU_164,3.21,2.12,-2.49,-0.92 2NMU/HIS 29.6.21,-0.82,0.0.53 3T57,GLU_248,4.66,0.2,0,-0.03 2XMZ,HIS_243,4.99,-3.3,0.85,0.95 1RWZ,TYR_197,12.02,0.85,0.45,0.72 3N0K,TYR 136,10.85,0,0.12,0.73 1SI7,ARG_56,11.77,-1.09,0,0.36 3CNU, ARG_102, 12.41, -0.12, 0, 0.03 1RI5,ARG_113,12.61,-0.14,0,0.25 4DIU,LYS 82,10.25,-0.29,0,0.04 1RWZ.TYR 236,13.63.0.0.17,3.45 3FS3,ARG_222,12.17,-0.49,0,0.16 1NKD,ARG_52,12.99,-0.19,0.4,0.28 1NRI,GLU_99,3.22,0.4,-1.06,-0.63 204D,GLU 77,4.53,0.13,0,-0.11 4DNU,GLU_138,3.48,0.25,-0.84,-0.43 3EJC,ARG_9,12.48,-0.02,0,0 2XHC,LYS_25,9.6,-0.9,0,0 1RHS.TYR 70.10.67.0.0.02.0.64 20JO.LYS 564,10.52,-0.07,0.0.1 2R57,CYS_193,11,-0.04,-0.13,2.17 3Q1C,ARG_106,12.4,-0.42,0,0.32 2EYI,HIS_88,6.83,-0.4,0.6,0.14 2GAU, ASP 221, 2.74, -1.26, -0.33, 0.53 1SNT,ARG_134,12.4,-0.33,0,0.23 2AHE,ARG_227,13.59,-0.88,1.31,0.65 3VJ8,CYS_303,11.89,0,-0.18,3.06 3DSH,ARG 249,12,25,-0,34,0,0.09 3M66,ASP 202,2.83,-0.87,-0.38,0.29 2D7J,LYS_28,10.45,-0.16,0,0.11 3ZXY,GLU_200,5.29,0.33,0,0.46 1Y0K,ARG_46,13.27,-0.13,0.81,0.09 1YW5,ARG_132,12.53,-0.26,0.04,0.24 1U7U.GLU 402.3.62.0.43.-0.89.-0.41 2ZCX,GLU_152,3.99,0.82,-0.71,-0.63 3IDW,LYS_59,10.43,-0.08,0,0.02 1U3Y,ASP_277,2.78,-1.65,-0.07,0.69 1W24,GLU_178,2.45,0.3,-1.67,-0.68 3G9B,TYR_27,13.58,0.74,0.63,2.21 3LPZ,GLU_23,4.11,0.3,-0.45,-0.24 3RKV,LYS_278,10.4,-0.2,0,0.1 1XTZ,TYR_170,10.16,0,0,0.16 3LJN,LYS_165,11.47,-0.47,0.85,0.59 1V6T,LYS_47,10.36,-0.55,0,0.41 20BI,GLU_50,4.03,0.38,-0.85,0 2FI9,ARG_61,12.62,-0.45,0,0.57

2XHC,GLU_15,3.36,1.44,-2.28,-0.29 1FQI,LYS 308,10.32,-0.35,0,0.16 100E,HIS 109.6.56,-0.17.0.04.0.2 3FNI,LYS_2,10.47,-0.03,0,0 105T,GLU_115,4.98,0.15,0,0.33 1EV8,ARG 49,12,45,-0,28,0,0,23 3L7N,HIS 4,4.61,-1.96,0.0.07 3KB5,ARG_356,13.45,-0.85,0.42,1.38 1LZL,TYR_134,11.44,0,0.21,1.23 2EFK,LYS_51,10.35,-0.12,0,-0.02 3LE4,GLU_323,4.46,0.09,0,-0.13 306L.GLU 130.3.45.0.32.-0.7.-0.67 2IXM,GLU_90,4.04,0.4,-0.5,-0.37 3K9I,LYS_62,10.38,-0.14,0,0.02 2HP7.LYS 46.10.32.-0.14.0.-0.04 1JKS.GLU 237.5.05.0.27.0.0.28 1UCH,ARG_5,11.34,-1.17,0,0.01 2OZO,HIS 169,5.88,-0.52,0,-0.09 1ZKZ,LYS_87,10.35,-0.15,0,0 3H13,ASP_441,3.97,0,-0.21,0.38 3V75.ARG 169.12.41.-0.19.0.0.1 2YLF,LYS 189,10.38,-0.13,0,0.01 1NAR,ARG_74,12.34,-0.26,0,0.1 3ILC.HIS 113.6.61,-0.28.0.47,-0.08 2V1LARG 100.12.66.-0.13.0.0.29 1XKR,ASP_134,4.04,0,0.05,0.19 3M70,GLU_269,4.58,0.08,0,0 3EAZ,GLU_143,4.84,0.12,0,0.22 2BLL,HIS 618,5.75,-0.67,0,-0.09 3M70.LYS 95.10.15.-0.37.0.0.02 1S7K,GLU_160,4.74,0.54,0,-0.3 3PM2,GLU_127,2.95,0.93,-2.05,-0.44 1Q2Y,LYS_115,10.27,-0.21,0,-0.02 2V4U,ARG 532,12.32,-0.26,0,0.08 3HYQ,GLU_135,3.69,1.03,-0.88,-0.96 1VJG,GLU_109,4.5,0,0,0 2CXA,GLU_118,4.51,0.26,0,-0.26 2ZTY,LYS 12,10.41,-0.07,0,-0.02 2RIS.ASP 180.4.31.0.-0.03.0.54 2B61,ARG_79,12.75,-0.34,0.02,0.56 4DBX,LYS_156,11.45,-0.52,0.43,1.04 2GKG.ARG 93.12.38.-0.4.0.0.29 2CXA,HIS 180,6.69,-0.36,0.41,0.14 4DVD,GLU_74,4.72,0.39,0,-0.17 2E3C,ARG_426,11.62,-1.18,0,0.31 2Q5X,ASP_813,1.78,-2.11,-0.32,0.42 2GEN,ARG_129,12.95,-0.44,0.57,0.32 3GS3,LYS_51,10.57,-0.28,0,0.35 3U2A,CYS_55,11.12,0,0.11,2 4FZR.HIS 0.6.09.-0.18.0.-0.23 1QQE,GLU_34,4.88,0.31,-0.02,0.1 4H4J,ASP 100,2.16,-1.48,-0.63,0.47 20G0.GLU 399.4.68.0.23.0.-0.06 4FCU,ARG_53,12.49,-0.28,0,0.27 3H6Q,HIS_114,6.87,-0.32,0.49,0.19 3GV0,ASP_300,3.53,-0.58,-0.44,0.75 3GE9,ASP_123,2.18,-1.47,-0.6,0.45 1G5Z,LYS_48,10.71,-0.19,0,0.4 3LJI,ARG 31,13,49,-0,36,0,58,0,77 3M3P,HIS_108,6,-0.35,0,-0.14 1U53,ARG 23,9.27,-3.36,0,0.14 3C2E,HIS 295.6.2,-0.08,0,-0.21 2Q13,TYR_190,10.04,0,-0.19,0.22 1BN6,ARG_157,12.38,-0.39,0,0.27 2VC8,CYS_47,9.16,-0.39,-0.05,0.6 1XTZ,ARG_158,13.19,-0.44,0.43,0.69 2YX0,ASP_326,3.17,-0.88,-0.3,0.55 3G6S,TYR_13,10.43,-0.17,0.15,0.45 2HRZ,LYS_30,10.47,-0.11,0,0.07

1NFN,ARG_134,13.11,-0.57,0.39,0.8 1ILW, ARG 173, 12.28, -0.28, 0, 0.07 3BWT,LYS_583,10.15,-0.4,0,0.04 3G9G,LYS_162,10.45,-0.05,0,0 2PWQ,LYS_92,10.59,-0.13,0,0.22 3IVF,ASP 261,3.63,-0.34,-0.13,0.31 1AK1.GLU 19.4.73.0.3.0.-0.08 2BV9,TYR_87,12.98,-0.85,0.43,3.39 4DNU,GLU_43,3.81,0.19,-0.67,-0.21 2CI3,HIS_46,4.46,-2.17,0.12,0 4EVF.GLU 49.4.91.0.23.0.0.17 2VGM,LYS 84,10,42,-0.33,0,0,25 2ZCO,ARG_181,12.76,-0.85,0.06,1.05 2JEO,ARG 172,12.8,-1.06,0.64,0.71 3FXH,LYS_48,10.61,-0.26,0,0.38 1PSW,LYS 79,11.11,-0.32,0.24,0.69 1BN6,ARG 133,13,14,-0,73,0,77,0,61 3A7L,GLU_61,4.78,0.27,0,0.01 1TR9,GLU_104,4.62,3.61,-3.14,-0.35 2Z84,ASP 25,3.97,0.0.0.17 3H9W.GLU 81.4.68.0.27.0.-0.09 2NRK,GLU_80,3.8,0.3,-0.82,-0.18 3M7G,ARG_231,13.31,-1.46,1.41,0.86 3GS9.GLU 292,4,44,0,49,-0.37,-0.18 3TRE, ASP 18, 3.87, 0, -0.06, 0.12 3HUE,GLU 308,3,78,0,23,-0,57,-0,38 3PZ9, ASP_362, 1.88, -2.28, -0.56, 0.93 3CZC,LYS_45,11.27,-0.36,0.85,0.27 3RFF,ARG_50,11.86,-1.09,0,0.45 1QYI,HIS_160,6.28,-0.2,0,-0.03 3M7D,GLU_13,4.66,0.16,0,0 1PSW,HIS_74,5.62,-0.42,0.17,-0.63 2J8A,HIS_340,6.37,-0.1,0,-0.04 1ZP2,LYS 198,10.31,-0.21,0,0.01 3P51.TYR 65.12.29.0.0.26.2.02 1MIX,LYS_334,10.54,-0.2,0,0.24 4F8A,ARG_583,12.29,-0.21,0,0 3DB9,ASP_72,4.03,0,0.04,0.18 3M66,GLU 256,4.63,0.12,0,0.01 3QAV,GLU_70,4.54,0.25,0,-0.22 2RJD,LYS 216,10.3,-0.23,0,0.03 2V4U,GLU_513,6.04,3.63,-2.01,-0.08 3H6Q,GLU_100,4.19,0.27,-0.4,-0.19 200P,ASP 186,2,79,-0.94,-0.59,0.51 2IRM,LYS_35,10.49,-0.22,0,0.21 3RLE,GLU_117,3.58,0.27,-0.85,-0.35 1J85,LYS_81,10.34,-0.16,0,0 3CAX,ARG 253,12.82,-0.69,0.58,0.43 2GZR,LYS_109,10.69,-0.29,0,0.48 2OBI,ASP_6,2.56,-1.11,-0.64,0.51 3EGN,ARG_392,12.45,-0.11,0,0.07 3CRM,LYS_317,10.4,-0.11,0,0.01 3TIR.GLU 176.4.91.0.56.0.-0.16 1TR9,GLU_88,4.59,0.09,0,0 3CX2,GLU_223,4.14,0.48,-0.27,-0.58 2ZQ5,ASP_147,4.37,0,-0.06,0.63 2AZL,ARG_150,12.71,-0.24,0,0.44 2G9D,ARG 261,12,74,-0,47,0,0,7 1KCM,TYR_141,10.43,-0.7,0.18,0.96 2CXA,HIS_130,2.94,-3.18,0,-0.38 2DG7,ASP_163,3.97,0,-0.17,0.34 2FPN.LYS 71.10.53.-0.06.0.0.09 1EQ6,TYR_199,13.02,-0.02,0.58,2.46 3CNU,GLU_40,5.17,0.84,0,-0.16 3GT0,LYS_142,11.69,-0.25,0.72,0.72 4ANN,ASP_75,4.13,-0.29,0.11,0.5 2O99,TYR 119,13,18,0.63,0.44,2,11 3RAZ,ASP_86,3.91,0,-0.04,0.15 1MTZ,ARG_206,12.28,-0.3,0,0.08

2E3C.ARG 314.12.46.-0.07.0.0.02 2EYI,LYS 157,9.91,-0.46,0,-0.13 1UAJ,HIS_46,6.49,-0.17,0,0.15 2FD5,ASP_74,3.26,-0.81,-0.04,0.31 1JYH.GLU 140.4.78.0.16.0.0.12 2B2H,TYR 92,13.63,-0.85,0,4.48 3I4T,CYS_119,10.46,-0.24,0,1.7 3FS3.ASP 34.3.92.0.0.0.12 2OB5,ASP_24,4.22,-0.19,-0.06,0.67 1CBY,GLU_106,4.15,0.29,-0.63,-0.01 2D59,ASP_76,2.91,-0.67,-0.57,0.34 3LPZ,ARG_107,13.67,-1.29,1.6,0.87 1J33,HIS_56,3.84,-3.11,0,0.45 2AHE,LYS 130,10,36,-0,14,0,0 2V81.HIS 90.6.19.-0.36.0.0.05 2CL3,TYR_191,11,-0.33,-0.36,1.69 3RFY,ASP_255,3.33,-0.44,-0.38,0.36 3L3P,HIS_461,4.7,-1.86,0.17,-0.11 2EJX,TYR 111,10.37,0,0,0.37 2FZ4,ARG 221,8.86,-2.75,0,-0.88 3H5T,ASP_130,3.6,-0.43,-0.03,0.27 1NIJ,ASP_85,2.54,-1.35,-0.4,0.49 4FH3,LYS_133,10.4,-0.09,0,-0.01 4F3J,TYR 160,9.9,0,-0.39,0.29 2RH3,GLU_176,4.61,0.31,0,-0.2 1V6T,CYS_35,12.13,-0.54,0,3.66 3AUF,GLU_164,3.88,0.36,-0.53,-0.45 1WXF,LYS 14,10.43,-0.3,0,0.24 3IVF,ASP_55,2.9,-0.8,-0.55,0.43 3CXS,LYS_73,10.41,-0.09,0,0 2CIU.ASP 121.3.25,-0.82.0.0.27 2GZQ,TYR_171,10.68,0,0.31,0.38 4EUG,ARG 116,12.46,-0.26,0,0.22 3RJZ,ARG 126,13,43,-0.64,0.31,1.27 3HZQ,LYS_62,10.27,-0.23,0,0 2BDD,GLU_92,5.2,0.78,0,-0.07 3V3T,ASP 39,3.34,-1.29,-0.12,0.95 1RKA.GLU 93.4.06.0.32.-0.66.-0.1 2P0Y,GLU_235,5.65,1.42,-0.3,0.03 1X04.GLU 159.4.13.0.31.-0.42.-0.27 30NH,CYS_442,9.64,0,-0.44,1.08 2W0G.ARG 270,13.27,-0.42,0.8,0.4 3KT9.GLU 101.4.7.0.25.0.-0.04 3PBH,LYS_86,9.53,-0.45,0,-0.52 2E0T,GLU_64,4.1,0.58,-0.85,-0.13 2FPN,CYS_130,9.24,0,-0.05,0.29 2X4J,ASP_52,3.58,-0.29,-0.16,0.23 1SIG,HIS 338,8.15,-0.39,1.48,0.56 3CCY,ARG_47,13.27,-0.25,0.34,0.67 1O3X,ARG_258,12.34,-0.23,0,0.07 1YTQ,TYR 136,12.62,0,0.36,2.26 1GXN.GLU 396.6.79.4.25.-1.96.-0.01 1V8E,TYR_69,12.03,0,0.4,1.63 1MML,ASP_28,3.81,0,-0.33,0.34 3JZ9,ARG_506,12.32,-0.2,0,0.02 2JKF,LYS_50,11.31,-0.94,0.85,0.9 4ETX,ASP_182,3.07,-0.85,-0.4,0.51 1J85,GLU_56,5.4,1.18,0,-0.27 1ZBM,TYR_60,11.27,-0.31,-0.16,1.74 3GA2,GLU 74,3.12,1.1,-2.48,0 3HVM,HIS 167.6.14,-0.36.0.0 1NFN,ARG_147,13.69,-0.45,0.85,0.78 1GVP,TYR_61,10.92,-0.08,0.1,0.91 106D,ASP_83,4.02,0,-0.04,0.26 3HVM,GLU_174,3.25,0.73,-1.57,-0.41 1PNE, ASP_8, 4.09, -0.02, 0, 0.31 10LR,ASP_172,3.25,-0.83,-0.24,0.52 3M66,GLU_396,4.16,0.34,-0.82,0.14 2R51,GLU_175,5.32,0.6,0,0.22

2QV2,ASP_324,3.83,-0.32,-0.07,0.42 3N2T,ASP_93,3.4,-0.96,0,0.56 3EAZ,ARG_94,12.41,-0.09,0,0 4DBX,ARG_2,12.84,-0.16,0.17,0.32 4D8L,LYS_196,10.48,-0.2,0,0.18 1ILW.ARG 116.12.16.-0.34.0.0 1EDG,ASP_290,3.44,-0.62,-0.75,1.01 2YX0,ARG_119,11.61,-0.9,0,0 3VJ8,LYS_117,10.46,-0.14,0,0.1 1V8E,ARG_215,12.79,-0.25,0.23,0.31 2D59,TYR_50,12.52,0,0.11,2.41 2RFA,ASP_90,3.74,-0.82,0.02,0.74 1NWA,LYS 81,10.46,-0.08,0.0.03 2VAN,TYR_271,10.44,0,0.12,0.32 2NRK.TYR 149.12.33.0.0.34.1.99 1YM5.GLU 35.5.05.0.25.0.0.3 3LJN,ASP_237,3.46,-1.18,-0.38,1.23 1HUF,ARG_28,12.45,-0.05,0,0 2G7O,ARG_110,13.95,-0.29,1.18,0.56 2AZL,GLU 94,4.17,0.38,-0.45,-0.25 2X4J,LYS_64,10.37,-0.13,0,0 1L2F,LYS 81,10,41,-0,27,0,0,18 2RGY,TYR_301,13.46,-0.01,-0.52,4 1JKS,ASP 88,3.31,-1.44,-0.56,1.51 1ZCU,HIS 87.6.35,-2.2.1.35.0.7 1M5I,ASP_156,4,0,-0.07,0.28 3IVF,LYS_263,10.54,-0.13,0,0.16 1ES9,ARG_206,12.42,-0.22,0,0.14 3I82.ARG 8,12.02,-0.51,0,0.02 1AM2,HIS_143,6.54,-0.41,0.22,0.23 2FG1,LYS_42,10.43,-0.58,0.12,0.39 3T57,GLU_91,4.67,0.18,0,-0.01 4ECC,LYS 91,10.53,-0.15,0,0.19 3LPZ.LYS 112.10.53.-0.22.0.0.25 3U4K,LYS_137,9.93,-0.63,0,0.06 1SIG,LYS_324,10.35,-0.15,0,0 2EFK,GLU_189,4.89,0.2,0.03,0.15 3VJ8,ASP 194,2.95,-0.84,-0.38,0.37 2QK1,LYS_361,10.3,-0.29,0,0.09 4D8L,ASP_207,2.42,-2.08,-0.61,1.3 2V4U,GLU_347,3.46,0.35,-0.85,-0.54 3M3P.HIS 176.11.22,-2.85,2.45,5.12 20JO.LYS 621.10.51.-0.13.0.0.14 2I6I,ASP_69,3.99,-0.08,-0.23,0.5 2|88,HIS 427,5,49,-1,21,0,43,-0,23 3JRT,LYS_100,9.9,-0.2,0,-0.4 1DTO,GLU 149,4.78,0.31,0,-0.04 20YZ.GLU 5.4.59.0.11.0.-0.02 3EGN,GLU_417,4.61,0.11,0,0 2YLF,ARG_188,12.38,-0.12,0,0 2IDC.LYS 71,10.37,-0.36,0.0.23 105J.GLU 16.3.27.0.33.-0.68.-0.89 2E0T,ASP_184,2.76,-0.85,-0.62,0.42 1GVP,ASP_50,2.8,-0.99,-0.55,0.54 1MIX,LYS_272,10.42,-0.08,0,0 2EDM,ARG_57,12.34,-0.16,0,0 1V43,ASP 117,3.89,-0.13,0.05,0.17 20KT,TYR_108,11.18,0,-0.04,1.22 2ZCX,ASP_144,3.91,0,-0.18,0.29 2B3M.ARG 117.12.03.-0.55.0.0.08 3M70.CYS 232.9.18.-0.84.0.1.02 1TJE,ASP_161,2.44,-1.42,-0.46,0.53 1UAJ,GLU_120,4.79,0.23,0,0.06 2R57,CYS_333,12.43,-0.06,0.6,2.89 3GW3,TYR_133,12.47,0,0.11,2.36 1UOH,HIS_52,5.91,-0.79,0.27,-0.08 2B61,TYR_313,11.72,0.85,0.4,0.47 3IU5,TYR 84,12.17,0,0.49,1.68 3F6F,GLU_136,4.87,0.38,0,-0.01

3V3T.ASP 221.3.14.-1.03.0.0.38 1DTO,TYR 115,11.23,0,0.09,1.14 3Q6L,ASP_99,3.84,-0.01,-0.18,0.24 100X,LYS_19,10.94,-0.4,0.38,0.46 109G,LYS_218,9.68,-0.34,0,-0.48 375L LYS 139.10.66 -0.2.0.0.36 1FHL,ASP_318,3.12,-1.36,0,0.68 3ANJ,LYS_8,10.55,-0.13,0,0.18 2CW4,ARG_111,12.27,-0.25,0,0.02 1X04,GLU_219,4.55,0.23,0,-0.18 1MIX,CYS 236,11.12,0,-0.17,2.29 1DCF.HIS 51.4.8.-1.59.0.3.-0.41 2B78,GLU_346,3.19,0.95,-1.7,-0.57 2PGX,ASP_221,4.03,0,-0.2,0.42 3GOZ.ASP 120.4.43.0.0.0.63 1T6L.HIS 248.6.74,-0.09.0.28.0.05 2D59,GLU_92,5.23,0.71,0,0.01 1SUU,LYS 519,9.87,-0.71,0.0.09 1YTD,ARG_335,13.2,-0.38,0.66,0.43 2IXM,TYR 68,11.47,0,0,1.47 3TOW.GLU 157.4.11.0.18.-0.34.-0.23 4ACJ,LYS_695,10.43,-0.27,0,0.2 2A1V,HIS_140,6.56,-0.16,0,0.22 2P65.GLU 135.4.61.0.11.0.0 3ERF.ARG 156.12.99.-0.37.0.32.0.54 3K1H,ARG_80,12.67,-0.23,0,0.4 1TR9,ASP_284,4.03,0,-0.1,0.33 2EJX,ASP_68,3.96,0,-0.18,0.34 2RJD,ARG_374,12.25,-1.76,0,1.51 2XHC.ARG 229,12,41,-0,23,0,0,14 1RAJ,GLU_76,4.96,0.46,0,-0.01 3T5B,GLU_23,5.7,2.56,-1.55,0.19 3ON1,HIS_79,6.37,-0.1,0,-0.02 1U3YLYS 275.10.99.-0.19.0.31.0.37 2FG1,GLU_71,3.9,0.37,-0.77,-0.2 2BLL,GLU_374,4.68,0.09,0,0.09 1HF8,GLU_249,4.44,0.24,0,-0.3 2RFA,TYR_154,11.12,0,0.46,0.66 3B79,ARG 56,12,45,-0,15,0,0,11 2DVK,ARG_111,12.27,-0.33,0,0.1 1BYI,HIS_184,7.59,-0.56,0.85,0.81 3S0A.GLU 48,4.22,1.24,-0.61,-0.92 3UX2,GLU 137,3.85,0.2,-0.85,0 2P52,TYR_199,10.27,0,0.12,0.15 2YWK,GLU_7,3.34,0.28,-0.82,-0.62 3FFM,GLU_66,4.57,0.07,0,0 3BQE,TYR_296,10.39,0,-0.22,0.62 1N81,GLU_134,6.06,1.74,0,-0.18 3UC9,HIS_157,6.79,-0.23,0.48,0.03 20DJ.TYR 155,12.06,-0.85,0.22,2.69 1Q46,GLU_78,4.57,0.11,0,-0.04 3V55,ASP 662,4,-0.05,-0.03,0.28 2PLQ,ARG_24,12.32,-0.34,0,0.16 2OB5,ASP_100,3.09,-1.27,0,0.55 2B02,TYR_386,10.33,-0.1,-0.42,0.85 4E9E,GLU_552,3.23,0.8,-1.68,-0.4 3UV9,ARG_484,13.24,-1.83,1.51,1.06 1I60,TYR_54,12.25,0,0.54,1.7 2Y2T.ASP 74.3.99.0.0.08.0.11 1AKO,ARG_224,13.02,-0.36,0.5,0.38 3RFY,TYR 229,10.66,0,0.13,0.53 2RIS.CYS 165.10.36.-2.48.0.75.3.07 3BB7,ASP_58,4.08,0,0,0.28 10I7,GLU_159,4.82,0.3,0,0.01 208I,ASP_90,3.28,-0.58,-0.19,0.25 3K9I,GLU_137,3.93,0.54,-0.55,-0.55 4H4J,LYS_35,11.33,-0.48,0.83,0.48 3EJC,ASP_20,4.09,0,-0.02,0.31 2APL,HIS_11,6.02,-0.62,0,0.14

1WLY,HIS_141,5.97,-1.74,0.85,0.38 3V75,ARG 268,12.26,-0.49,0,0.25 1SQW,LYS_115,10.04,-0.44,0,-0.02 3CIV,ASP_211,3.98,-0.01,-0.06,0.25 1IDK,TYR_215,11.75,0.24,0.23,1.28 1NIJ.GLU 230.3.88.1.57.-1.45.-0.73 1NKD.ASP 31.3.72.-0.2.0.0.13 2B0A,GLU_104,4.67,0.23,0,-0.06 1RI6,TYR_65,11.98,0,-0.02,2 2P0L,TYR_136,10.23,0,0.05,0.19 2FBI,GLU_50,3.64,0.94,-1.58,-0.22 3RLE,GLU_81,3.86,0.28,-0.54,-0.38 3ADO,TYR_152,12.53,0,0.96,1.56 1MTZ,LYS_30,11.09,-1.12,0.85,0.85 1X7F,GLU_234,4.09,2.2,-2.3,-0.31 3QAV,TYR 10,11.44,0.06,0.45,0.93 3CS1,LYS_197,10.27,-0.98,0,0.74 1UW7,ASP_25,3.55,-0.38,-0.06,0.19 4EVF,LYS_3,10.42,-0.08,0,0 2CBE.TYR 114.11.12.0.0.02.1.1 1BKB,ARG_136,12.58,-0.15,0,0.23 1AT0,ARG_304,12.18,-0.32,0,0 3DZ1,ASP 244,4.02,0,-0,17,0,4 3G9G,TYR 213,10.27,-1.03,-0.02,1.32 1ZBM,ASP_235,3.98,0,0,0.18 2VGM,TYR_196,12.28,0.13,0.55,1.61 3BJV,TYR_57,11.44,-0.56,0.01,1.99 3LJN,ASP_201,3.13,-0.65,-0.43,0.4 2Z0M,ASP_118,3.26,-0.34,-0.75,0.55 2Q98,TYR_168,12.47,0,0.33,2.14 2YWK,ARG_20,13.31,-0.33,0.6,0.53 3BOE, ASP 257, 3.59, -0.79, 0.01, 0.58 1ES5,TYR_206,11.19,-0.4,-0.44,2.04 1R53,HIS 338,6.45,-0.36,0.02,0.29 3ETU,LYS 89,10.36,-0.09,0,-0.05 105T,CYS_274,7.99,-1.41,-0.13,0.53 3RLN,LYS_597,11,-0.25,0,0.74 4E8B,ARG_33,12.21,-0.24,0,-0.04 3GFP,ASP 458,4.01,0,-0.1,0.3 3ETU,CYS_245,9,-0.28,0,0.28 200K.GLU 326.4.77.0.19.0.0.08 2D8N,ARG_71,10.69,-2.1,0,0.29 1V43,ASP 174,3.27,-0.95,0,0.42 20KT,HIS 58,6.8,-0.37,0,0.67 10LR,ARG_159,12.98,-0.77,0.27,0.97 3O48,TYR_14,11.82,0,0.64,1.18 2QRX,GLU_40,4.61,0.22,-0.02,-0.09 2A4D,ASP 175,3.06,-0.9,-0.38,0.54 3G9B,LYS_99,10.41,-0.11,0,0.01 2Z0M,ARG_66,12.36,-0.2,0,0.06 4AM1,LYS_43,10.49,-0.25,0,0.23 3RAZ,LYS_65,10.59,-0.09,0,0.18 3EZ7.TYR 367.10.34.-0.64.0.0.99 3HKX,HIS_219,6.51,-3.49,1.68,1.82 3B21,TYR_76,11.49,0.35,0.47,0.66 4F8A,ARG_573,12.19,-0.33,0,0.02 11LW,LYS_171,10.31,-0.14,0,-0.04 2A4D.GLU 112.4.15.0.43.-0.27.-0.53 1ZYL,TYR_42,10.59,-0.03,-0.52,1.15 1RHS,ARG_20,12.39,-0.28,0,0.17 1T3J,LYS_731,10.43,-0.07,0,0 2BOO.GLU 137.4.54.0.09.0.-0.06 3E7P,TYR_241,12.7,0,0.47,2.24 2EEY,LYS_108,10.17,-0.35,0,0.03 3EOD,ARG_74,11.5,-1.19,0,0.19 2R51,TYR_270,12.23,-1.65,0.24,3.63 1X7F.TYR 129.13.94.0.85.0.66.2.43 3DZ1,ASP_26,4.52,0,-0.15,0.88 3E0H,ARG_86,12.08,-0.48,0,0.06

3P28,TYR 97,13.59,0,0.32,3.28 3PZ9,ARG 63,12,4,-0,19,0,0.08 3EOD,GLU_118,4.4,0.23,-0.06,-0.26 1YM5,ARG_213,12.79,-2.28,1.14,1.44 3FHF.ARG 98,11.99,-0.51,0.0 3UAH,LYS 260,11,46,-0.27,0.85,0.38 1C3K,LYS_51,10.44,-0.06,0,0 1YR6.LYS 87.11.48.-0.57.0.85.0.69 30NH,GLU_526,4.4,0.53,-0.3,-0.35 3M7D,GLU_194,3.83,0.26,-0.56,-0.37 3PP8,GLU_131,4.84,0.29,0,0.06 2F4Q,ARG_15,11.68,-0.83,0,0.01 1ZBS,CYS_106,11.49,0,0.3,2.2 1RL0,GLU_125,4.36,1.66,-1.42,-0.37 3S0A.GLU 39.4.73.0.29.0.-0.06 3BPP,GLU_54,5.49,1.87,-0.79,-0.08 4FH3,CYS_48,12.45,-0.04,0.01,3.49 1T3J,LYS_713,10.3,-0.2,0,0 2EJB,HIS 157,6.39,-0.26,0,0.15 4E9E,LYS 562,9.88,-0.52,0,-0,1 3U0V,LYS_222,9.92,-0.63,0,0.05 3GW3,ARG_37,12.21,-1.23,0,0.95 2H30,TYR_118,10.4,0,0.09,0.31 1A8Q,GLU 10,4.71,0.21,0,0 3ODJ,TYR_40,11.64,0,0.35,1.3 2R51,HIS_111,6.37,-0.13,0,0.01 2D7J,GLU_113,4.27,1.02,-0.9,-0.36 3TIR,ARG 125,11.63,-1.28,0,0.41 3UX2,ASP_135,3.09,-1.12,0,0.42 1R29,ASP_29,2.46,-1.38,-0.43,0.48 2BT8, ARG_321, 12.49, -0.16, 0, 0.14 1T6L,CYS_117,9.48,0,-0.05,0.53 4FZR,ARG 198,12.42,-0.15,0,0.07 4DVD,ARG 82,12,76,-0,27,0,21,0.32 3FWU,CYS_88,10.88,0,0.03,1.85 1T3J,ASP_685,3.67,-0.38,0,0.25 3QKY,ARG_160,11.65,-0.94,0,0.08 2ZCO.HIS 148.6.53.-0.18.0.0.21 3MIX,ARG_367,12.33,-0.65,0,0.48 1P2F,LYS 193,9.81,-0.26,0,-0.42 3EYE,ASP_44,4.08,-0.02,0.11,0.18 3CZC, ARG 27, 12.88, -0.37, 0.41, 0.35 3HUE,TYR 112,10,51,0,-0,08,0.59 1FKM,ASP_403,3.95,0,-0.16,0.31 2E3H,CYS_265,10.71,0,0.2,1.51 1XEU,LYS_100,10.52,-0.21,0,0.23 1SUU,GLU_628,5.06,0.27,0,0.29 3FWU,ASP_36,3.21,-0.51,-0.28,0.2 3EVN,LYS_5,10.46,-0.07,0,0.04 3BPV,ARG_70,12.1,-0.35,0,-0.04 3VHJ,GLU_152,3.9,0.39,-0.8,-0.19 1PSW,ARG_70,12.3,-0.2,0,0 1V6T,TYR_86,10.55,0,0.27,0.28 1JB3,ASP_75,3.75,-0.24,-0.55,0.73 1MUF,GLU_142,4.19,0.3,-0.2,-0.41 2OBI,HIS 25,7.21,-0.32,0.79,0.25 2Z84,ARG_93,12.28,-0.3,0,0.08 3KB5,CYS_313,10.69,-0.47,0.28,1.87 3GOZ,HIS_226,6.39,-0.87,0.76,0 3NBI,GLU_28,4.73,0.24,0,-0.01 2D0A,LYS 307,10,46,-0,23,0,0,18 2G2D,GLU_83,4.6,0.1,0,0 1AD6,CYS_407,10.64,-0.24,0,1.88 1J8B,CYS_52,9.6,-0.01,-0.02,0.63 1EV8,TYR_4,13.36,-0.01,0.16,3.21 1XIP,GLU 7,5.15,0.33,0,0.32 1DUN,TYR_75,10.44,0,0.04,0.4 1NKD,ASP_38,4.14,0,0.11,0.23 1MTZ,ASP_277,3.92,-0.5,0,0.62

1P1L.LYS 45,11.1,-0.45,0.67,0.38 1MML,ARG 80,12.05,-0.54,0.0.08 1TUL,HIS_43,5.57,-0.98,0.44,-0.39 3JSN.GLU 21.4.9.0.36.0.0.03 2D0A.ARG 141.12.29.-0.28.0.0.06 1P4X,LYS 24,10.24,-0.17,0,-0.09 1UAJ,GLU_142,4.31,2.6,-2.21,-0.59 20GQ,ASP_438,1.77,-2.59,-0.54,1.11 1CHD,ASP_249,2.63,-0.85,-0.62,0.31 3JZN,ARG_264,11.96,-1.32,0.07,0.7 3US6,ASP_51,3.96,0,-0.13,0.3 2BCF,ARG_250,12.35,-0.81,0.19,0.47 1X1E,HIS 115,5.86,-0.68,0,0.04 3GT0,LYS_112,10.47,-0.05,0,0.02 1YLN.HIS 154.5.98.-0.36.0.-0.16 2Z0W.TYR 39,10,14,0,0,0,14 2CIU,LYS_139,10.55,-0.17,0,0.22 3FK5,GLU_141,3.74,0.37,-0.79,-0.35 4GA2,GLU_88,4.14,0.41,-0.29,-0.49 1LTU,ARG 58,12.37,-0.48,0,0.35 1PVT,HIS_104,4.84,-3.1,0.7,0.74 2D0A,ASP_136,2.94,-0.75,-0.8,0.69 2XJ4,ARG_167,11.44,-1.2,0,0.14 1X9G,GLU 46,3.36,0.93,-1.3,-0.77 1PSW,ARG 22,11.92,-0.79,0,0.2 3A4C,LYS_537,10.15,-0.33,0,-0.01 3TMO,HIS_315,6.26,-0.27,0,0.03 3ZTA,LYS_67,10.44,-0.24,0,0.18 1RKA,GLU_236,4.61,0.11,0,0 3M7G,GLU_259,4.89,0.2,0,0.19 3I4T,ASP_210,3.88,-0.51,0.22,0.37 3U2R,ARG_141,13.88,-0.26,1.25,0.39 3V1Q,LYS 614,10.41,-0.12,0,0.03 1RZ2,ASP 156,3.31,-0.83,-0.01,0.34 3EX9,CYS_145,9.36,0,-0.09,0.45 3ETV,CYS_257,6.5,-2.93,0.03,0.39 1YTD,ARG_262,12.9,-0.81,0.64,0.56 2JEO,LYS 69,10.37,-0.44,0,0.31 2D59,TYR_68,10.35,0,-0.24,0.58 3H8Y,GLU 22,4.87,0.28,0.0.09 3BPP,LYS_200,10.12,-0.35,0,-0.03 2RFA.GLU 177.4.49.0.29.-0.05.-0.26 3V3T,LYS 260,10.37,-0.53,0.0.4 3ULX,ARG_19,12.05,-0.21,0,-0.24 1MML,ARG_187,11.27,-1.29,0,0.06 1YTD,LYS_218,12.14,-0.45,1.31,0.77 3UAH, ASP_275, 3.93, 0, 0, 0.13 2CN1.GLU 276.4.74.0.23.-0.36.0.37 1DOV,ASP_96,3.78,-0.05,-0.29,0.32 3CAX,ARG_156,12.46,-0.24,0,0.19 3EVN.CYS 117.9.45.-0.12.0.0.57 4E8B,ASP 120,3.36,-0.64,-0.1,0.3 3ELI,HIS_98,5.01,-1.14,0,-0.34 1KN3,ASP_144,3.67,-0.2,-0.15,0.22 3VJ8,CYS_172,12.34,-0.02,-0.42,3.77 2FPN,LYS_59,10.36,-0.14,0,0 1EYH.GLU 90.4.36.0.18.0.-0.32 2XJ4,ARG_202,11.95,-0.68,0,0.12 3C5V,GLU_353,6.95,4.17,-2.1,0.39 3ZRI,LYS 58,10,43,-0,1,0,0.02 105T.GLU 121.4.69.0.3.0.-0.11 3M7D,ASP_124,2.58,-1.25,-0.5,0.54 3F1X,HIS_167,4.96,-1.41,0,-0.13 2IDC,ARG_49,12.62,-0.27,0,0.38 4ETX,ARG_205,13.21,-0.73,0.82,0.63 1BYI,ASP_110,3.04,-1.02,-0.28,0.54 2QVT,HIS_85,5.56,-0.75,0,-0.18 1D2K,LYS_60,10.39,-0.3,0,0.19 1Q42,ARG_116,11.56,-2.78,0.74,1.1

2G3A.HIS 55.5.51,-0.72.0,-0.26 3LPZ.ARG 292.12.41.-0.09.0.0 1NJ4,TYR_312,11.63,0.74,0.35,0.54 3P2F,HIS_14,6.23,-0.3,0,0.03 3EX9,ASP_57,3.71,-0.35,0,0.26 3CGW,LYS 183,10.38,-0.32,0.0.2 2NYC, ARG 294, 10.92, -1.61, 0, 0.04 3LH5,LYS_564,10.36,-0.14,0,0 1AD6,LYS_462,10.15,-0.7,0,0.34 2GS5,GLU_41,4.72,0.25,0,-0.03 1TLV,ARG 203,12.39,-0.13,0,0.02 3CJW.GLU 214,4.67,0.19,0,-0.02 3BWT,HIS_639,6.47,-0.39,0.17,0.2 2GAU,GLU_159,3.86,1.3,-1.31,-0.62 3JRT.TYR 55,11,58,0,0,09,1,49 3CJW,ARG 385,12.59,-0.14,0,0.23 3BB7,TYR_120,11.64,0.22,0.22,1.2 2EEY,LYS 106,10.25,-0.3,0.0.05 3FHF,ARG_84,12.28,-0.22,0,0 2A0J,ASP 90,3.39,-0.31,-0.38,0.28 3I82, ASP 118, 3.06, -0.85, -0.14, 0.25 3JZN, ASP_140, 3.22, -1.16, -0.9, 1.47 3CGW,ARG_60,13.26,-0.83,0.84,0.75 2E3S.TYR 404,10,59,0,-0,1,0,68 1RAJ.GLU 396.3.99.0.41.-0.44.-0.47 4EZB,ASP_220,4.05,-0.75,-0.1,1.1 307K,LYS_122,10.5,-0.61,0,0.6 2DFL,HIS_186,6.29,-0.28,0,0.07 1J7G,GLU_34,4.07,1.04,-0.85,-0.61 3GEC,ASP_238,3.7,0,-0.34,0.24 3G9T,LYS_225,10.48,-0.07,0,0.05 3GFP,LYS_382,10.41,-0.15,0,0.06 3ETV.GLU 202.4.22.0.3.-0.36.-0.21 1CHD,CYS_207,10.53,0,-0.08,1.61 3LD1,ARG_6,12.3,-0.24,0,0.05 2Q98,ASP_17,4.07,0,0,0.27 3ASA,LYS_96,10.58,-0.09,0,0.17 1WPA,GLU 449,4.77,0.43,0,-0.16 2099,ASP 361,4.37,0,-0.37,0.94 1IDK,HIS_232,6.06,-1.56,0.47,0.64 3IO0,LYS_179,10.44,-0.12,0,0.06 2IDC,GLU_25,4.37,0.33,0,-0.47 2X4L.GLU 340,4.67,0.19,0,-0.02 2E3I,TYR_108,9.93,-0.86,0,0.79 3Q2C,TYR_38,10.5,-0.61,0.54,0.57 1NAR,LYS_106,10.31,-0.36,0,0.17 2ZCX,GLU 65,4.58,0.63,-0.6,0.04 3TOW,HIS_106,6.36,-0.25,0,0.11 2D59,ARG_5,12.46,-0.04,0,0 3RE9.GLU 118.4.59.0.09.0.0 3B21,GLU_80,5.14,0.61,-0.02,0.07 1BGF,LYS 88,10.32,-0.09,0,-0.09 2RJD,HIS_291,4.48,-2.88,0.85,0.01 3OKQ,ASP_579,4.15,0,0.1,0.24 3JZN,TYR_308,10.67,0,0.33,0.35 2E3C,CYS_296,11.1,0,-0.07,2.17 1XAW.ASP 426.2.95.-0.78.-0.34.0.26 2NRR,ARG_484,12.36,-0.63,0,0.49 2E3C.GLU 261,4.72,0.44,0,-0.23 2X4L,LYS 198,10,59,-0,51,0,0,59 1Q42,ARG 48,13.12,-0.57,0.5,0.69 1R3F,HIS 43,5,49,-0,96,0,-0,05 4E9E,TYR_509,10.23,0,0.01,0.22 1AT0,GLU_337,3.18,0.48,-1.79,0 3DHN,ARG_36,12.42,-0.15,0,0.07 3FS3,ARG_83,12.76,-0.3,0,0.55 2CXY,GLU_71,4.56,0.24,0,-0.18 4H4J.TYR 41.11.98.0.04.0.98.0.96 3V4G,GLU_142,3.82,0.3,-0.49,-0.48

10I7,HIS_62,6.96,-0.29,0.7,0.06 2XMZ,CYS 235,10.56,0,-0.15,1.7 2DG7.CYS 173.9.69,-0.18,-0.05,0.93 3R2E,HIS_63,6.56,-0.96,0.84,0.18 1M5I,GLU_136,4.85,0.22,0,0.13 2R57.CYS 376.9.2.0.0.0.2 4F85.ARG 268.13.13.-1.75.0.67.1.71 3GS3,GLU_169,4.55,0.08,0,-0.03 2PGE,ARG_72,12.33,-0.35,0,0.18 2RJD,ASP_420,3.95,0,0,0.15 1XTZ.TYR 60.11.89.0.66.0.22.1.01 3CIV,LYS_111,10.51,-0.12,0,0.13 2V4U,LYS_353,10.97,-0.16,0,0.63 1Y2O.GLU 107.3.94.0.32.-0.83.-0.05 3U0V,HIS_53,6.15,-0.35,0,0 30DJ,LYS 131,10.39,-0.11,0,0 1JB3,HIS_32,7.27,-0.34,0.85,0.25 208P,TYR_222,11.21,0,0.15,1.07 2BCF,TYR_233,10.27,0,-0.03,0.3 2AZP.HIS 208,5.9,-3.34,0.85,1.89 4EUG,CYS_200,11.38,-0.87,0.46,2.79 1WNH,LYS_114,10.47,-0.03,0,0 2H85,TYR_88,10.98,-0.36,-0.46,1.8 2B0J.HIS 120.7.13.-3.38.2.23.1.78 4FLE,ASP 138,3.98,0,0,0.18 3PP8,GLU_79,3.89,0.37,-0.66,-0.32 2IQT,ARG_95,11.81,-0.81,0,0.12 3AU3,LYS_586,10.53,-0.46,0.21,0.29 1SI7.ARG 188.12.29.-0.2.0.-0.02 1G5Z,ASP_105,4.4,0,-0.1,0.7 4ANN,GLU_164,4.44,0.16,0,-0.21 1AKO,ARG 78,12,19,-0,59,0,0,3 1ZBS,ARG_226,13.16,-0.23,0.31,0.59 10GL,GLU 265,4.58,0.08,0,0 3MIX.GLU 318.4.34.0.06.0.-0.22 1IAP,ARG_137,13.01,-0.17,0.19,0.49 2IDC,LYS_129,10.46,-0.09,0,0.04 1DZF,ARG_55,13.27,-1.72,1.41,1.09 1WNH,CYS 144,12.77,0,0,3.77 3GT0,GLU_106,4.6,0.47,-0.78,0.41 2CXY,LYS 55,10.65,-0.25,0,0,4 1JB3,GLU_126,4.49,0.15,0,-0.17 3LJC,GLU 191,4.79,0.18,0,0.11 2ZO5,ARG 72,12,51,-3,23,1,43,1,81 4EVF,GLU_76,4.68,0.59,-0.47,0.06 1R3F,ARG_81,12.56,-0.43,0.26,0.22 2X4G,ASP_66,3.66,-0.3,-0.17,0.33 1TD6,GLU_226,5.13,0.85,-0.19,-0.03 1BKB,GLU_19,4.73,0.17,0,0.06 4DIU,LYS_86,10.69,-0.24,0,0.42 3B4D,ASP_180,1.73,-2.3,-0.53,0.76 3KB5,TYR_427,10.47,-0.74,0,1.21 208P.LYS 119.10.49.-0.07.0.0.06 3GT0,GLU_145,3.85,0.29,-0.72,-0.22 200K,ASP_201,4.22,-0.09,-0.25,0.76 2YWX,LYS_151,10.42,-0.08,0,0 2B78,TYR_143,12.93,0,0.11,2.82 2EEY,TYR 129,10,41,0,0,0,41 1WP5,ARG_114,12.44,-0.67,0.09,0.52 1JT9,GLU_122,3.25,2.32,-2.85,-0.73 2YX0,GLU_230,3.55,0.38,-0.85,-0.48 1T95.GLU 62.4.76.0.28.0.-0.04 2YLF,TYR_217,13.86,0,1.17,2.71 3V3T,LYS_304,10.45,-0.05,0,0 3CJW,HIS_291,6.45,-0.73,0.53,0.14 2WB8,GLU_461,4.68,0.25,0,-0.07 2012.TYR 147.10.15.0.0.0.15 3M66,HIS_309,6.26,-0.74,0.18,0.31 3CN5,LYS_64,10.48,-0.17,0,0.15

1X1E.ARG 198.12.34.-0.48.0.0.33 20DJ.LYS 192,10.64,-0.36,0.0.5 1FO9,GLU_215,4.14,1.15,-0.73,-0.78 2FI9,GLU_79,4.64,0.14,0,0 1T07,ASP 18,3,5,0,-0,53,0,23 2|88,LYS 470,10.33,-0.22,0.0.04 2Q07,ASP_396,3.49,-0.47,-0.61,0.77 3RRQ,CYS_93,7.88,-1.35,-0.1,0.32 3P2F,ASP_182,2.93,-1.55,-0.38,1.06 1XEU,ASP_256,3.99,0,0,0.19 2FBI,CYS_59,9.2,0,-0.32,0.53 2B6P,ARG_85,12.73,-1.1,0.68,0.65 3DHN,GLU_129,4.63,0.13,0,0 2EJB,GLU_46,3.61,0.51,-1.36,-0.04 1TWU,ASP 78,3.88,0,-0.29,0.37 1AKO,HIS_118,6.51,-0.47,0.33,0.16 1A8Q,ASP_44,2.9,-0.85,-0.38,0.33 1YTD,LYS_313,10.42,-0.12,0,0.04 3JRT,LYS_115,10.44,-0.28,0.04,0.18 1ILW.GLU 42,4,47,0,21,0,-0,24 3OA7,ARG_556,13.11,-0.17,0.79,0 1R7J,LYS_4,10.41,-0.26,0,0.17 1GVP.ASP 79,1.77,-1.56,-0.86,0.4 4FCU,ASP 164,3.25,-0.66,-0.28,0.4 2BDD,ARG_100,12.24,-0.26,0,0 1BN6,GLU_268,4.6,0.1,0,0 1YB2,GLU_45,3.82,0.81,-0.85,-0.63 3V1Q,HIS 503,6.42,-0.24,0.16,0 2WB8,LYS 663,8.91,-1.86,0.0.26 3BWT,ARG_696,12.51,-0.43,0,0.45 2YX0,ASP 329,3.32,-0.84,0,0.36 2AXO,LYS_230,10.2,-0.43,0,0.13 2EDM.TYR 46,10.54,-0.38,0.03,0.89 1WXF.HIS 260.5.53.-0.52.0.15.-0.59 1J7G,ASP_135,3.78,0,-0.27,0.25 3MTT,GLU_543,4.31,0.39,-0.08,-0.51 3IL3, ASP_238, 3.97, -0.82, -0.11, 1.1 2ZCX.ARG 218,12.7,-0.23,0.0.43 1G5Z,GLU_51,4.03,0.21,-0.31,-0.37 1T95.TYR 189.11.85.0.85.0.47.0.53 1GVP,LYS_46,11.19,-0.48,0.85,0.32 1ES9,HIS 144,6.18,-0.3,0,-0.01 100L.GLU 91,4.59,0.06,0.0.03 2HXB,TYR_90,9.3,-0.7,-0.41,0.41 3GV0,TYR_99,10.83,0,0.26,0.57 2QRX,TYR_141,11.81,0,0.09,1.73 2HNG,ASP_38,3.35,-0.51,-0.28,0.35 2D2S,LYS_613,11.46,-0.67,0.83,0.81 3CRM,ARG_54,12.67,-0.09,0,0.26 1TD6,ARG_144,12.26,-0.33,0,0.09 1PDB,ASP_186,2.69,-1.2,-0.63,0.73 4DNU,HIS_268,5.92,-0.8,0,0.22 1SNT,TYR_359,10.49,-0.65,-0.29,1.43 1WLY,GLU_107,4.58,0.28,0,-0.19 4DIU,HIS_46,4.25,-2.64,0.42,-0.03 3PZ9,ASP 158,2.74,-1.48,-0.4,0.82 3V3T,LYS_271,10.85,-0.73,0.65,0.44 3IVF,LYS_57,10.45,-0.19,0,0.15 2EFK,LYS_30,11.22,-0.25,0.45,0.52 3H5T,ARG 41,12.22,-0.33,0,0.05 2FC3.GLU 120.3.72.0.33.-0.72.-0.39 1T07,GLU_52,4.6,0.1,0,0 2G5X,GLU_91,4.41,1.62,-1.42,-0.29 10TM,GLU_129,4.61,0.41,0,-0.3 2BT8, ARG_225, 13.75, -0.75, 1.07, 0.93 2V5B,GLU 134,4.62,0.98,-0.99,0.13 3GS9,TYR_179,12.53,-0.01,0.7,1.84 3RKV,LYS_328,10.43,-0.18,0,0.11 2D8N,LYS_119,10.81,-1.06,0.67,0.7

1R50,ASP 6,3.75,-0.4,0,0.36 1HF8,TYR 118,9.61,-0.65,0.01,0.25 2EFK,GLU_15,4.08,0.44,-0.38,-0.47 2C2Y,ASP 247,3,73,0,-0.36,0.29 3I0C.GLU 242,4.3,0.44,-0.1,-0.54 2IOT.LYS 194.10.74.-1.02.0.82.0.44 1F2V,LYS 155,10,25,-0,25,0,0 100X,CYS_155,10.14,-0.3,-0.21,1.65 1MN3,ARG_438,12.52,-0.06,0,0.08 2WB8,CYS_792,9.87,0,-0.02,0.89 3M66,ARG_257,12.2,-0.31,0,0 2AD1,HIS_142,5.58,-0.66,0.07,-0.33 1U53.CYS 152.10.8.0.0.04.1.75 1K95,TYR_86,11.29,0.11,0.35,0.83 2AD1.GLU 161.3.48.0.74.-1.32.-0.43 1R29,ARG 44,13.08,-0.4,0.53,0.44 2E3C,ARG_252,12.73,-0.24,0.11,0.37 1F2V,LYS_69,10.29,-0.16,0,-0.06 1LZL,HIS_283,6.86,-0.92,0.85,0.43 3V1Q,HIS 634,5.83,-1.13,0.71,-0.25 2EJX,ARG_118,11.84,-0.68,0,0.01 3N2T,ASP_36,3.18,-0.58,-0.34,0.3 3E5T,ARG_230,12.56,-0.13,0,0.18 3RHE,HIS 61,6.33,-0.1,0,-0.07 3PP8.GLU 211.4.59.0.13.0.-0.04 2FGG,ASP_49,3.89,-0.06,0,0.14 10I7,GLU_216,4.03,0.39,-0.74,-0.12 4EZB,GLU_208,4.76,0.14,0,0.12 2PPN.GLU 5,4.39,0.19,-0.05,-0.26 3OA7,GLU_565,4.8,0.14,0,0.17 1EV8,ARG_107,12.78,-0.21,0.5,0 2YT4,LYS_659,10.68,-0.2,0,0.38 4F85,ASP 65,3.43,-0.69,-0.03,0.34 3G6S,ASP 71,2.82,-1.42,-0.13,0.57 2BT8,GLU_194,4.58,0.08,0,0 3JZN,GLU_347,4.42,0.44,-0.61,0.09 1ZCU,TYR_194,10.38,0,0,0.38 3OA7,GLU 518,4.5,0.38,0,-0.38 3RJX,TYR_181,12.74,0,0.06,2.68 3CNU,LYS_5,11.25,-0.77,0.85,0.67 1RSS,CYS_47,11.32,-0.5,0.05,2.78 2G2D,ASP 61,4.03,0,-0.08,0.31 3RJX.GLU 239.4.39.0.24,-0.08,-0.28 2VAN,TYR_142,12.7,0.51,0.59,1.61 3M66,LYS_329,10.29,-0.17,0,-0.05 1SUU,ASP_578,3,-0.8,0,0 3CE7,LYS 30,10.35,-0.13,0,-0.02 1SOW,LYS 148,10.6,-0.22,0.0.33 1Z9L,GLU_103,4.56,0.09,0,-0.03 1HF8,LYS_24,10.41,-0.09,0,0 1PGV.GLU 268.4.32.0.31.-0.01.-0.48 3K8J,ARG_221,13.18,-0.31,0.67,0.32 20BI,ARG_69,12.1,-0.8,0,0.4 2GZQ,ASP_22,3.32,-0.83,-0.03,0.37 4GCO,HIS_165,6.77,-0.71,0.85,0.12 2ZQ5,GLU_84,4.13,0.46,-0.8,-0.03 1H09.LYS 330.10.45.-0.08.0.0.03 3GV0,LYS_205,11.21,-0.25,0.67,0.29 1DUN,CYS_83,11.76,0,0,2.76 1KN3,HIS 86,2.99,-3.47,0.88,-0.93 1SIG.LYS 121.10.69,-0.2.0.0.4 3G9G,ARG_128,12.72,-0.26,0,0.48 2QEV,LYS_140,10.67,-0.15,0,0.32 1TLV,ARG_238,12.41,-0.21,0,0.11 2X5Y,LYS_761,11.15,-0.68,0.85,0.48 1J33,ARG_269,12.01,-0.58,0,0.09 1WP5,ARG_234,12.12,-0.38,0,0 3GV0,GLU 178,4.92,0.46,0,-0.04 1YW5,GLU_119,4.65,0.23,0,-0.09

2013.GLU 120.4.56.0.25.0.-0.18 3VJ8,GLU 222,4.97,0.39,0,0.09 2VAN,LYS_168,10.62,-0.21,0,0.34 3GA2,CYS 60,13,33,0,0,83,3,49 2CI3,ARG_11,12.21,-0.32,0,0.03 3IO0.TYR 259,10.08,0.0.0.08 2OSA,LYS 453,10.53,-0.61,0.14,0.52 2EA9,HIS_79,6.28,-0.22,0,0 2D2S,LYS_534,10.51,-0.1,0,0.12 1WYC,GLU_28,4.71,0.21,0,1.39E-17 1TWU,TYR 66,10.6,0,0.39,0.2 3GW3.LYS 178.9.91.-0.59.0.0 3IVF,ARG_194,11.5,-1.1,0,0.1 3LD1,HIS_329,5.09,-1.82,0.61,-0.2 4EKU,HIS 122,5,91,-0,54,0,-0,04 2FD5,ARG 121,12,54,-0.2,0,0,24 2C2Y,TYR_94,13.57,0,0.54,3.04 1W24,HIS_88,5.19,-1.28,0,-0.02 2XWS,TYR_71,11.41,0.03,0.38,1 3JZ9,LYS 396,11.39,-0.42,0.77,0.54 3TMO.GLU 241.4.03.0.16.-0.01.-0.62 1XEU,GLU_187,4.42,0.28,-0.36,0 3N0K,GLU_9,3.72,0.5,-0.85,-0.43 1TJE,ASP 8,2,4,-1,76,-0.03,0,39 1NU.HIS 294.6.03.-0.84.0.35.0.02 2Q34,ASP_34,2.13,-2.43,-0.06,0.81 3PU6,HIS_119,6.31,-0.21,0,0.02 2FI9,ARG_118,12.62,-0.18,0,0.3 2IDC,TYR_117,10.45,-0.58,0.05,0.98 2AZP,CYS_49,12.21,0,-0.39,3.59 4DIU,GLU_128,5,0.27,0,0.23 10IS,ASP_195,3.59,0,-0.39,0.18 2AZL.GLU 61.4.67.0.11.0.0.05 3CAX.LYS 403.10.25.-0.25.0.0 3H13,ASP_452,2.75,-1.03,-0.38,0.36 2B02, ASP_410, 3.22, -0.84, -0.07, 0.33 3K9I,ASP_141,2.42,-1.79,0,0.42 1L2H,LYS 94,10.3,-0.2,0,0 4D8LASP 134.3.94.0.0.01.0.12 4EF5,CYS_309,11.74,0,-0.12,2.85 2GAU,ARG_128,12.41,-0.1,0,0.01 2VAN, ASP_145, 2.91, -1.37, -0.59, 1.06 1AM2.LYS 98,10.59,-0.42,0.28,0.24 1RI5,HIS_163,5.16,-1.99,0.79,-0.14 1XWM,ARG 21,13.35,-0.31,0.77,0.38 2O0K,LYS_31,10.34,-0.53,0,0.38 2P5D,LYS 95,11.34,-0.5,0.85,0.49 4EF5,CYS_292,11.36,-0.16,0.16,2.36 3HUE,CYS_222,11.24,-0.02,0.16,2.11 3H9W,LYS 78,11.54,-0.2,0.77,0.47 1X04, ARG_45, 13.02, -0.27, 0.42, 0.37 3ANJ,TYR 260,10.89,0,0.08,0.81 3FHF.GLU 130.4.43.2.09.-1.39.-0.76 1X7F,GLU_255,4.35,0.32,-0.58,0.11 3MTT,LYS_477,10.05,-0.55,0,0.1 3ZXY,HIS_179,6.45,-0.26,0.11,0.1 3EJC,GLU_112,2.89,0.41,-1.61,-0.4 2X4G,ARG_223,12.32,-0.74,0.17,0.39 2F9F,GLU 119,3.93,0.69,-0.68,-0.59 3M16,GLU_176,4.73,1.88,-1.66,0.02 1XIP,ASP_254,3.84,0,-0.05,0.09 2EHG,LYS 108,10,44,-0,14,0,0.09 2QRX,ARG_154,12.85,-0.29,0.28,0.36 1C44,GLU_21,4.42,0.22,0,-0.31 3CJW,LYS_389,10.44,-0.06,0,0 1C44,GLU_25,4.27,0.15,0,-0.38 3BA1,LYS_137,10.93,-0.57,0.85,0.15 3N0K.GLU 140.6.08,2.48,-0.82,-0.08 2FXT,GLU_390,4.58,0.08,0,0

2NRK,LYS_162,10.41,-0.09,0,0 2V81,ARG 95,12.76,-0.31,0.33,0.24 3M7G,GLU_41,4.25,0.27,0,-0.52 2Q5X,ASP_747,3,-1.16,-0.04,0.4 1NIJ,ASP_285,3.59,-0.77,-0.08,0.62 4AM1.GLU 18,4.5,0.35,-0.06,-0.29 4DBX.CYS 192.12.39.0.0.58.2.82 1SQH,TYR_82,13.09,-0.85,0,3.94 2H8O,ARG_144,12.69,-0.22,0,0.41 3ZSL,GLU_184,3.77,0.54,-0.69,-0.59 2DFL,GLU_307,5.85,1.74,-0.04,-0.36 2WB8,GLU_735,2.75,0.52,-1.54,-0.73 2PP6,GLU_91,4.75,0.31,0,-0.06 1NIJ.ARG 175.12.03.-0.93.0.0.47 2E3I,ASP_57,3.85,0,-0.07,0.12 2P65,CYS 155,12.45,0,0,3.45 2YT4.GLU 626.3.65.0.45.-0.85.-0.45 1QQE,LYS_69,10.6,-0.23,0,0.34 4DVD,ARG_23,12.45,-0.9,0.4,0.46 2A6B,LYS 35,10.24,-0.26,0,0 2BAA, TYR 96, 11, 75, 0, 85, 0, 37, 0, 52 307K,ARG_120,13.34,-0.4,0.75,0.49 3RJX,LYS_94,10.56,-0.09,0,0.15 1R3D,TYR_156,11.52,-0.55,-1.24,3.31 3TOW,GLU 132,4.73,0.23,0,0 2IRM.LYS 100.10.49.-0.3.0.0.28 200K,HIS_176,3.87,-2.84,0.13,0.09 3CIV,ARG_140,12.37,-0.34,0,0.2 10TM,LYS 109,11.52,-0.24,0.85,0.41 3CSR,LYS_95,10.36,-0.27,0,0.13 3G9G,GLU_172,4.43,0.34,0,-0.41 3V46,TYR_392,11.44,0,-0.45,1.89 2A6B,ARG_204,11.21,-1.34,0,0.05 3CS1,ASP 26,3.11,-0.64,-0.48,0.44 1T6L,LYS 224,10,23,-0,24,0,-0.03 4AM1,LYS_351,10.64,-0.25,0,0.38 2P65,GLU_61,4.65,1.04,-0.65,-0.24 2E3C,HIS_392,6.08,-0.73,0.19,0.12 3EVN,ASP_265,3.22,-0.85,-0.02,0.3 4ECC,LYS_27,10.15,-0.37,0,0.02 2AHE,GLU_16,3.14,0.49,-1.32,-0.53 4DND,GLU_65,3.24,0.79,-1.62,-0.42 2E0T.ARG 80,11.83,-0.34,0,-0.33 1RHS.GLU 136.4.17.0.87.-0.85.-0.35 4FD6,LYS_118,10.59,-0.18,0,0.27 3T5B,TYR_290,12.67,-0.14,-0.55,3.36 2P4D,GLU_154,3.07,1.35,-2.01,-0.77 3UAH,LYS_366,10.58,-0.34,0,0.42 3GFP,TYR_405,12.68,0,0.61,2.07 2A1V,ASP_11,2.87,-1.08,-0.1,0.25 1O0X,LYS_126,12.18,-0.35,1.23,0.79 3S0A,LYS_64,10.51,-0.25,0,0.25 1AK1.GLU 90.2.77.0.77.-2.15.-0.35 3I47,TYR_196,10.82,0,0,0.82 2I88,GLU_468,4.68,0.43,0,-0.24 1YR6,LYS_166,10.36,-0.52,0,0.39 3I82,HIS_127,4.66,-1.73,0,-0.12 1SNT.GLU 319,3.98,0.32,-0.73,-0.1 1YIB, TYR_217, 10.43, 0, 0.26, 0.17 3K8J,ARG_112,12.46,-0.33,0,0.3 2RGY,ARG_191,12.99,-0.37,0.43,0.43 1ES5.GLU 249.4.69.0.92.-0.61.-0.12 1R53,GLU_239,4.74,1.2,-0.78,-0.17 3UV9,GLU_317,4.55,0.05,0,0 3CS1,TYR_67,11.93,0,0.35,1.57 1XTD,TYR_41,10.28,0,-0.38,0.66 2Z61,ASP 90,3.65,0,-0.48,0.32 1J33,TYR_66,10.14,0,0,0.14 2CVB,ARG_127,11.26,-1.49,0,0.25

3IPZ.ASP 152.3.98.0.-0.02.0.2 3GMS,ARG 92,11,41,-1,71,0,0.63 1YR6, ARG_146, 10.97, -1.77, 0, 0.24 2RJD,ARG_521,12.32,-0.18,0,0 2DVK.GLU 169.4.65.0.24.0.-0.08 1SJ8.CYS 750.10.68.0.0.1.68 1RI5,TYR_124,12.59,-1.7,0.61,3.68 3LJI,GLU_187,4.25,1.63,-1.57,-0.31 2B78,LYS_12,9.93,-0.21,0,-0.36 2C2Y,ARG_166,12.1,-0.35,0,-0.05 2D7U,HIS 110,5.89,-0.8,0,15,0.04 2IXM,CYS_167,11.85,0,0.12,2.73 2BDV,HIS_82,5.63,-0.38,0,-0.49 2JHY,LYS 200,10.66,-0.09,0.0.25 10LR.ARG 186.12.28.-0.37.0.0.15 4DVD,TYR_142,10.45,0,-0.06,0.51 2BT8,ARG_201,12.55,-0.17,0,0.22 1JKS,ASP_169,3.85,0,-0.28,0.33 3LJC,CYS 39,10.29,0,0.03,1.26 2H2Z,TYR 101,11.1,-0.04,0.3,0.85 3T5B,ARG_379,13.51,-0.5,0.83,0.68 3FWU,ARG_24,13.28,-0.39,0.51,0.66 2Y2T,LYS_66,10.37,-0.13,0,0 1R3D,HIS 259,6.2,-0.36,0,0.06 2FXT,GLU_407,4.89,0.11,0,0.28 3RJX,ARG_262,13,-0.47,0.34,0.63 1PSW,ARG_244,11.94,-0.73,0,0.17 2AD1,ASP_67,3.04,-0.85,-0.62,0.71 1UOH, ARG 222, 12, 37, -0, 13, 0, 0 1FO9,ARG_419,12.72,-0.81,0,1.03 3D9H.HIS 162.6.08,-0.96.0.32.0.21 2H14,HIS_300,5.03,-2.6,0.81,0.31 1NRI.GLU 15,4.78,0.41,0,-0.13 3KV0.ARG 165.12.41.-0.68.0.0.6 4EZB,ASP_58,3.11,-0.89,-0.16,0.35 1J33,ARG_149,12.96,-0.41,0.44,0.42 3COU, ARG_114, 12.63, -0.17, 0, 0.3 3B79,ARG_14,11.92,-0.59,0,0.01 3ETV,ARG_205,12.67,-0.45,0.36,0.26 2RIK.GLU 124.4.43.0.19.0.-0.26 2YT4,LYS 582,10.34,-0.16,0,0 2YX0.GLU 270,3.1,3.73,-2.01,-3.11 1ZYL.ARG 190.12.33.-0.64.0.0.47 3T5B,GLU_361,5.14,0.85,0,-0.21 2BT8, ASP_325, 3.64, -0.5, -0.19, 0.53 2P0Y,ASP_184,3.78,-0.52,0,0.5 2O8P,LYS_35,11.36,-0.62,0.85,0.65 2GZR,LYS_171,10.29,-0.21,0,0 2Q12,TYR_41,10.43,-0.03,0.1,0.36 3U2A, ASP_12, 2.74, -1.37, 0, 0.31 3QAV,ASP 127,3.53,-0.63,-0.04,0.4 2RJD,ARG 267,10.9,-2,78,0,1.18 1059,HIS_214,6.88,-0.41,0.58,0.22 3B7X,ARG_36,12.38,-0.3,0,0.18 3HVM,HIS_323,1.5,-3.76,0.85,-2.09 3FHF,HIS_83,4.84,-1.81,0.72,-0.56 2EYI,ASP_98,4.14,0,0,0.34 1EV8,LYS_96,10.19,-0.83,0.08,0.44 2JHY,ASP_185,4.51,0,0.5,0.2 2FB6,ARG 33,12.28,-0.22,0,0 3EX9,HIS 32,6.03,-0.42,0,-0.04 3L3P,ASP_339,4.49,-0.04,-0.05,0.78 3CIV,GLU_31,3.86,0.3,-0.73,-0.2 2B6P,TYR_149,13.28,0,0.4,2.87 3AU3,GLU_428,4.55,0.09,0,-0.04 2X4G,HIS 207,6.44,-0.35,0.29,0 1SNT,HIS_64,6.15,-0.37,0,0.02 3DSH,HIS 453,6.35,-0.15,0,0 3F1X,ARG_127,11.78,-0.69,0,-0.03

3B21,HIS 199,6,14,-0,29,0,-0.07 1H09,CYS_239,10.78,-0.15,0.08,1.85 2V1L,HIS_58,6.91,-1.2,0.85,0.75 10IS,ASP_339,2.62,-1.52,-0.2,0.54 1NJ4.ASP 127.3.99.0.0.0.19 3N2TLYS 192.10.57.-0.14.0.0.22 2R0S,HIS 230,5.8,-1.13,0.35,0.07 2GYZ,ARG_15,12.05,-0.19,0,-0.25 1P4X,HIS_219,6.79,-0.89,0.85,0.33 3BCY,ASP_27,3.3,-0.79,-0.05,0.35 1X9G,HIS_45,5.04,-1.78,0.25,0.07 10TM,LYS_120,10.47,-0.1,0,0.07 1H09,TYR 137,10,13,-0,89,0,27,0,76 2QK1,LYS_460,11.31,-0.52,0.51,0.81 4DBX.LYS 209.10.66.-0.11.0.0.26 3ZXY,HIS 61,4,51,-2,63,0,71,-0.07 1SIG,ARG_339,12.33,-0.19,0,0.02 3I0C,LYS_125,10.45,-0.05,0,0 1R9W,ARG_320,12.44,-0.06,0,0 2YYO,GLU 44,4.51,1.45,-1.18,-0.26 1KW4,ASP_21,2.9,-1.28,0,0.38 3FXH,GLU_37,4.69,0.17,0,0.03 3P2F,GLU_63,4.87,0.16,0,0.22 3CAX,LYS 215,10.3,-0.13,0,-0.07 3V46,ASP 365,3,3,-0,47,-0,52,0,5 2OJQ,TYR_660,9.97,-0.85,0.01,0.81 1RL0,GLU_70,4.09,0.61,-0.52,-0.51 2D8N,ASP_165,3.2,-0.67,-0.34,0.4 3MIX,GLU 588,4.76,1.36,-1.11,0 2CXC,ARG_80,12.89,-0.26,0.1,0.54 2PWQ,GLU_124,4.88,0.28,-0.08,0.19 3OBS,ARG_23,13.19,-0.3,0.54,0.44 1CHD,LYS 246,10.45,-0.68,0.04,0.58 20DJ.LYS 122.11.23.-0.72.0.85.0.59 20EW,TYR_223,10.59,-0.85,0.08,1.35 3GMS,CYS_134,12.8,0,0,3.8 1NIJ,GLU_307,4.6,0.09,0,0.02 2EEY,TYR 145,10.52,0,-0.17,0.68 100X,LYS_63,10.37,-0.43,0,0.3 208P,GLU_47,2.71,1.14,-2.45,-0.48 1ZCE,ARG_33,13.28,-0.52,0.76,0.53 3ULX.LYS 35,10.82,-0.87,0.85,0.34 2B0A,HIS 50,4,43,-1,35,0,-0,71 1RL0,ASP_152,3.22,-0.36,-0.5,0.29 3MIX,ASP_517,3.39,-0.97,-0.17,0.74 1AT0,LYS_379,11.34,-0.46,0.85,0.45 4FCU,ASP 135,3.8,0,-0.17,0.18 20GO,HIS 382,6.27,-0.19,0,-0.03 3I47,LYS_254,10.45,-0.05,0,0 2QHT,CYS_138,12.54,-0.37,-0.17,4.08 1MML,ASP 108,3,15,-0,76,-0.09,0,2 2CWY,LYS 64,9.85,-0.26,0,-0.4 3MEW,GLU_198,4.63,0.07,0,0.06 2CI3,CYS_177,12.3,0,-0.24,3.54 2WB3,HIS_369,6.2,-0.3,0,0 4FCU,ASP_71,3.24,-0.46,-0.32,0.22 1J33.TYR 97.12.17.0.73.0.22.1.23 100X,GLU_137,4.59,0.22,0,-0.13 2ZTY,GLU_81,4.29,0.22,-0.05,-0.37 2V4U,LYS 490,11,49,-0,24,0,85,0,38 30NH,ARG 443,12,86,-0,3,0,3,0,37 3JZN,ASP_279,3.91,0,-0.13,0.24 3TMO,ASP_221,3.8,0,-0.16,0.16 1W24,ARG_60,12.63,-0.31,0.07,0.36 1YB2,TYR_139,9.79,-0.85,0,0.64 100X,ARG_133,11.81,-0.87,0,0.18 3JZN,ARG_439,12.15,-0.6,0,0.26 2WB8,GLU 548,4.73,0.23,0,0 2A1V,ASP_18,4.05,0,-0.09,0.34

1EYH, HIS 146, 7, 21, -0, 2, 0, 8, 0, 12 3CO1,HIS 29,6.34,-0.15,0,-0.02 1MJS,ARG_242,12.07,-0.77,0,0.35 3EVZ.HIS 59.6.28.-0.72.0.26.0.24 1X7F,ARG_271,11.34,-1.17,0,0.02 3H13,TYR 276,13,26,-0.85,0.38,3,73 1SNT,ARG 41,12,29,-0,26,0,0.06 1YW5,ASP_131,3.61,-0.17,-0.34,0.32 3LPZ,LYS_119,10.18,-0.25,0,-0.06 2E0T,HIS_129,6.36,-0.97,0.76,0.07 1JSX,GLU 179,4.09,0.32,-0.77,0.04 105T.LYS 458.10.25.-0.29.0.0.05 2RIS,TYR_53,10.01,0,-0.35,0.37 1H4U,ASP_606,3.46,-0.66,-0.19,0.51 2IDC,ASP 118,2,81,-1,11,-0,48,0,6 1ZYL.ARG 50,12,41,-0,18,0,0.09 2P65,LYS_43,9.62,-0.83,0,-0.05 2X4L.LYS 67.10.8.-0.54.0.46.0.38 3GS9,ASP_285,3.76,-0.79,0,0.75 2BDV,GLU 12,4.19,0.32,-0.61,-0.02 4F85,ASP_287,3.39,-1.57,-0.02,1.18 1A8Q,ASP_84,2.85,-0.74,-0.44,0.23 2OJQ,GLU_460,4.45,0.27,0,-0.31 3EX9.CYS 104.12.18.0.0.29.2.89 3CXS.ASP 10.3.01.-1.06.-0.1.0.36 3CGW,ARG_161,12.38,-0.2,0,0.08 2EYI,LYS_147,10.55,-0.73,0.2,0.59 2D2S,LYS_751,10.21,-0.37,0,0.09 3JZ9,TYR 403,11.41,0,0.03,1.38 4EZB,ARG_201,12.52,-0.06,0,0.09 1TD6,LYS_23,10.3,-0.15,0,-0.05 1Y2Q,ASP_17,3.86,0,-0.1,0.16 10TM,GLU_55,3.72,0.45,-0.85,-0.38 1DVO,CYS 135,9.14,-0.1,-0.24,0.48 1ES5,ASP_65,3.72,-0.11,-0.37,0.41 3ULX,TYR_120,9.89,-0.02,-0.58,0.5 3M70,GLU_79,4.23,0.61,-0.52,-0.37 3BQW,LYS_97,10.6,-0.12,0,0.22 20RX/HIS 49.6.18,-1.37,0.71,0.34 2R51,ARG_240,12.39,-0.11,0,0 1ZBS,ASP_83,4.11,0,0.01,0.3 1V6T,HIS_107,3.75,-3.25,0.83,-0.33 1V43,GLU 39,5.25,2.62,-1.27,-0.6 1U53,ASP_168,4.16,0,-0.11,0.48 2X4L.LYS 307.10.3.-0.24.0.0.04 3CAX,LYS_462,10.54,-0.17,0,0.21 3O16,ARG_175,11.46,-1.76,0.08,0.64 2YLF,ARG_76,12.42,-0.07,0,-0.02 2G9D,ASP_78,4.94,0,0.13,1.02 3US6.CYS 104.12.25.0.26.0.88.2.13 1l60,CYS_149,11.19,-1.28,0.1,3.37 2DVK,ARG 179,12.67,-0.33,0.01.0.49 3CSR.LYS 32,11.63,-0.52,0.85,0.81 1VJG,LYS_74,10.44,-0.06,0,0 2FZ4,GLU_103,4.83,0.25,0,0.08 2PWQ,GLU_131,4.51,0.26,0,-0.25 2B0J.GLU 306.3.93.0.31.-0.74.-0.15 3BCY,TYR_53,13.05,0,0.09,2.96 1R7J.CYS 17.11.43.0.-0.01.2.43 1NAR,GLU_107,4.47,0.17,0,-0.2 208P,LYS 166,10.52,-0.23,0,0.25 3D9H,ASP 161,4.38,-0.82,0.25,1.14 3MTT,GLU_466,4.57,0.29,0,-0.23 1W7B,GLU_253,4.99,0.58,0,-0.07 1YLN,CYS_168,13.25,0,0.43,3.82 1X8F,GLU_75,4.7,0.22,0,-0.01 2EFK,LYS_187,10.63,-0.24,0,0.37 3BB7.GLU 216.3.68.0.48.-1.05.-0.24 3DSH,ASP_227,3.96,0,0,0.16

3RJZ,CYS_213,8.68,-0.55,0,0.23 2R2Y,TYR 48,12.58,0.62,1,0.95 1MD6,GLU_93,4.53,0.28,0,-0.26 1VJG,ARG_139,13.61,-0.96,1.54,0.52 1RWZ,GLU_92,3.89,0.29,-0.49,-0.41 3EJG.CYS 123.11.2.0.0.25.1.96 2YWK.HIS 59.6.28.-0.27.0.0.04 2CN1,ASP_140,3.35,-0.73,-0.25,0.53 3ONT,HIS_126,6.32,-0.17,0,-0.01 2H8O,ARG_136,13.76,-1.43,1.44,1.25 200K,ASP_54,3.43,-0.53,-0.31,0.46 3T5B,ARG 41,12.2,-0.36,0.0.06 2JKF,LYS_133,10.81,-0.8,0.56,0.56 1JYH,GLU_23,4.18,0.23,-0.55,0 3ILC, ARG_100, 13.44, -0.31, 0.81, 0.44 2Q13,GLU 239,4.74,0.24,0,0 2R0S.TYR 226.10.72.0.0.06.0.67 4ECC,ASP_90,3.93,0,-0.22,0.34 2P0L,ASP_109,4.28,0,-0.17,0.64 2GAU,ARG_144,10.62,-1.91,0,0.03 2ZCO.GLU 220.4.75.1.2.-0.68.-0.27 3EZ7,ARG_104,13.28,-0.45,0.48,0.75 2D7U.GLU 169.5.12.0.28.0.0.34 2ZCO.TYR 105,13,46,0.83,0.5,2,13 3G9G,GLU 222,4.67,0.2,0,-0.03 1J7G.CYS 113.12.12.-0.3.-0.01.3.42 2CBE,ASP_71,2,-1.85,-0.39,0.44 3ERF,GLU_109,3.38,0.41,-1.31,-0.21 2A1V,HIS_84,6.14,-0.29,0,-0.07 1KCM,HIS_85,6.67,-0.84,0.85,0.15 3RE9,GLU_129,2.99,0.49,-1.54,-0.46 3IBT,ASP_82,4,0,0,0.2 3FXH,ASP_22,3.91,0,-0.02,0.13 3O48, ASP_101, 3.39, -0.72, -0.63, 0.93 3CN5.TYR 53.10.36.0.0.0.36 3G9G,HIS_147,4.24,-1.65,0,-0.62 1WRU,ARG_160,11.11,-1.47,0,0.09 1YW5,GLU_114,3.55,0.31,-1,-0.26 2CBE,ARG 227,12.59,-1.18,0.84,0.44 3A4C,ASP_520,3.94,0,-0.03,0.17 3C38, ARG_146, 12.07, -0.57, 0, 0.13 1LZL,ARG_211,11.9,-0.6,0,0 2BLL,GLU 377,3.65,0.42,-0.93,-0.35 1SOH.GLU 173.3.7.0.37.-0.91.-0.26 2A4D,CYS_145,12.89,0,0.36,3.53 4ESS,LYS_134,10.09,-0.49,0,0.07 2PLQ,ARG_267,10.4,-2.47,0,0.37 2JKF,GLU 165,5.31,1.56,-0.37,-0.37 2BLL,GLU_586,3.83,0.63,-0.88,-0.41 2H2Z,LYS_97,10.41,-0.12,0,0.03 3CBN,ARG_25,13.13,-0.35,0.59,0.39 3BZT,ASP_342,3.01,-1.04,0,0.26 3MIX,ARG 372,11.64,-0.86,0,-0.01 2CVB,GLU_155,3.72,0.37,-0.85,-0.31 1Y0K,TYR_45,11.92,0.83,0.07,1.02 1DTO, ARG_47, 12.23, -0.27, 0, 0 3FWU,HIS_13,6.31,-0.17,0,-0.03 3BWT,LYS 786,10,73,-0,39,0,26,0,36 3LQE,GLU_342,4.15,0.54,-0.58,-0.3 2FZ4,ARG_62,12.53,-0.94,0.39,0.59 1A8Q,LYS_177,11.29,-0.46,0.82,0.43 2013.TYR 168.9.7.-0.24.-0.24.0.19 1GXN,TYR_635,12.68,0,-0.32,3 3B21,LYS_34,11.34,-0.31,0.77,0.38 1YB2,HIS_210,5.07,-1.34,0,-0.1 3RKV,GLU_297,3.25,0.42,-0.94,-0.72 3F6M,LYS 31,10.2,-0.48,0,0.18 3CO1,LYS_83,10.44,-0.06,0,0 2NSN,LYS_70,10.69,-0.22,0,0.41

3UPD.ARG 96.13.14.-0.36.0.7.0.29 2XMZ.LYS 36,10.72,-0.36,0.0.57 4D8L,LYS_48,10.26,-0.12,0,-0.12 3H9W,ASP_85,3.07,-0.82,-0.49,0.58 1ZBP,GLU_247,4.58,0.08,0,0 2NRK.TYR 168.10.37.0.0.01.0.36 1Y0K,GLU_191,4.48,0.12,0,-0.14 3LJC,GLU_151,4.59,0.09,0,0 4E8B,ARG_151,13.58,-0.91,1.27,0.71 2W2S,GLU_58,4.38,0.75,-0.12,-0.74 3RRO,ARG 115,12.84,-0.26,0.04,0.56 3CCY,GLU_31,4.63,0.12,0,0.01 2FM9,HIS_209,6.28,-0.19,0,-0.03 2X4G.GLU 204.4.65.0.15.0.0 3H5T.GLU 49.4.97.0.14.0.0.33 1ZCE,CYS_85,12.19,0.2,1.07,1.92 2A0J,LYS_23,10.6,-0.16,0,0.26 3U0V,TYR_58,13.52,0,0.21,3.31 2G9D,ASP_342,4.14,0,0.2,0.15 3LJN.GLU 236,4,53,0,29,0,-0,26 2NRK,GLU_170,3.53,0.25,-0.83,-0.39 1DUP,GLU_115,4.76,1.26,-0.8,-0.2 3GFP,ASP_395,4.4,-0.23,-0.13,0.96 1XDZ.TYR 64,11.29,0,0,1.29 3B21,TYR_115,12.01,0,0.46,1.56 2H14,TYR_35,12.99,-0.39,1.13,2.25 3E0H,GLU_157,4.42,0.17,0,-0.25 20EW,LYS 151,10.22,-0.33,0,0.05 2XWS,ARG_3,12.43,-0.37,0,0.3 1AD6,TYR_454,12.45,0,-0.02,2.47 1ES9,ARG_83,12.92,-3.89,0.59,3.72 3K8J,GLU_175,5.73,1.03,0,0.2 2E0T,ASP 73,2.28,-1.73,-0.7,0.91 30NH,ASP 544,3.01,-0.65,-0.38,0.24 2ZQ5,HIS_164,5.45,-1.11,0,0.06 1W7B,TYR_316,10.78,0,0.27,0.5 2B61,ASP_325,3.07,-0.81,-0.56,0.64 1AKO.TYR 52,12.09.0.0.13,1.96 2CXA,ASP_32,1.38,-2.72,-0.5,0.8 2A6B,ARG 80,10,99,-1,52,0,0.01 20KT,TYR_194,13.52,-0.09,0.61,3.01 2D7J,ARG 95,12.51,-0.06,0,0.08 2AD1.LYS 223,10.82,-0.16,0.0.48 3DB9,ARG_87,13.22,-0.67,0.73,0.65 1059,HIS_194,6.32,-0.16,0,-0.02 3EIZ,HIS_137,6.29,-0.31,0,0.09 3H13,ASP_306,2.81,-1.74,-0.57,1.31 1FKM,ASP_330,4.09,-0.43,-0.04,0.76 1EYH,GLU_143,3.29,0.48,-0.94,-0.74 3ASA,LYS_83,9.7,-1.03,0,0.23 2CWY,GLU 22,5.04,0.2,0,0.35 2EJB.GLU 127,3.63,0.33,-0.76,-0.44 1SJY,GLU_151,3.65,0.36,-0.78,-0.43 4ETX,GLU_356,3.92,0.26,-0.33,-0.51 2WB8,CYS_564,11.85,0,0.06,2.79 1SNT,GLU 72,4.56,0.32,-0.05,-0.22 3EYE,ARG_62,12.05,-0.45,0,0 3K1H,GLU_129,4.7,0.2,0,0 2F4Q,LYS_172,10.3,-0.13,0,-0.07 3CJW,GLU 339,4.64,0.17,0,-0.03 2EHG.GLU 87.4.57.0.28.0.-0.21 3F5D,LYS_4,11.06,-0.54,0.85,0.25 3EZ7,LYS_331,10.45,-0.25,0,0.2 1MD6,ARG_47,12.47,-0.38,0,0.35 3IPZ,GLU_168,4.7,0.2,0,0 3GE9,LYS 6,10.93,-0.27,0.21,0.49 3CBN,ASP_140,3.64,-0.98,0.15,0.67 2JEO,GLU_196,3.62,0.36,-0.82,-0.42 1UAJ,GLU_243,3.86,0.41,-0.85,-0.19

2CE6.ASP 26.2.51.-1.2.-0.54.0.46 2D7U.GLU 307.4.52.0.29.0.-0.27 3JZ9,ASP_445,5.16,-0.03,0.12,1.28 2YX0,GLU_54,4.11,0.32,-0.07,-0.65 3RJX.LYS 147.11.09.-0.28.0.48.0.38 2IXM.GLU 262,4.84,0.51,0,-0.17 1R53,HIS_174,6.23,-0.23,0,-0.05 3GV0,GLU_299,3.63,2.82,-0.73,-2.96 1RKA,GLU_188,5.26,1.19,-0.19,-0.24 1PVT,GLU_209,3.85,1.06,-1.16,-0.55 2V4X,GLU_21,4.7,0.22,0,-0.02 3ON1,GLU_3,4.54,0.04,0,0 3A0X,LYS 682,11.06,-0.33,0.65,0.25 1J33,LYS_115,11.34,-0.44,0.85,0.43 1P1L.TYR 76.12.95.0.85.0.62.1.48 3EVN,TYR 8,13.07,-0.85,0.22,3.69 3GA2,GLU_212,4.42,0.17,0,-0.25 3VJ8,HIS_268,6.03,-1.19,0.81,-0.08 2FG1,LYS_73,10.34,-0.16,0,0 3FWU,ARG 94,12.14,-0.63,0,0.27 1JKS,LYS_108,11.29,-0.47,0.85,0.4 2FXT,GLU_267,4.64,0.16,0,-0.03 1YB2,ASP_140,3.41,-0.59,0,0.21 1UAJ,CYS 112,13.75,0,1.06,3.7 2OK0.GLU 35.3.38.0.61,-1.23,-0.5 1M5I,ASP_170,4.11,0,-0.05,0.35 1WYC,CYS_216,12.57,-0.85,0.51,3.92 2YWX,GLU_136,4.29,0.33,0,-0.54 4ETX,HIS 338,5.59,-1.31,0,0.4 1GVP,LYS_69,11.08,-0.54,0.85,0.27 3DHN,LYS_42,10.28,-0.22,0,0 1K95,GLU_116,3.84,0.47,-0.59,-0.54 200K,LYS 112,10.56,-0.32,0,0.37 1KCM.GLU 41.3.63.0.3.-0.85.-0.32 3KB5,ARG_408,12.8,-0.16,0,0.45 1U3Y,ASP_276,3.42,-0.31,-0.4,0.33 2H85,GLU_220,4.41,0.29,-0.22,-0.17 1RHS,ASP_200,4.99,0.26,0.35,0.58 3PU6,ARG_99,12.89,-0.62,0.35,0.65 1RI5,TYR_254,11.65,0,0.17,1.48 2CVB,TYR_47,9.95,0,-0.36,0.31 2AZP,ARG 313,12,29,-0,23,0,0.02 1J85,GLU 117,3.96,0.2,-0.72,-0.02 3LJN,CYS_50,10.96,-0.01,-0.12,2.08 3ETU,ARG_316,12.42,-0.13,0,0.05 2BT8,HIS_158,6.38,-0.12,0,0 3EGN,CYS 420,9.58,-0.19,0.13,0.64 1L3K.GLU 132,4.61,0.31,0,-0.19 3Q2C,LYS_42,11.04,-0.2,0.59,0.16 3FK5,GLU_173,4.65,0.57,-0.27,-0.16 3BWT.TYR 615.9.9.0.-0.48.0.38 2A6B.GLU 102.4.53.0.19.0.-0.16 2E3C,ARG_330,11.7,-1.43,0,0.63 1HF8,ARG_126,11.86,-0.81,0,0.17 1QYI,GLU_16,4.61,1.15,-0.51,-0.52 2G9D, ASP_16, 3.13, -0.67, -0.37, 0.37 1042.GLU 36.4.62.0.12.0.0 2Q12,GLU_28,4.71,0.16,0,0.05 1RKA,ASP_306,4.07,0,0.01,0.26 3ETV.GLU 88.4.75.0.25.0.0 3ELI,ARG 111,13,1,-0,29,0,0,89 2X5Y,LYS_748,10.08,-0.52,0,0.11 1DZF,LYS_152,10.3,-0.35,0,0.15 1DVO,ARG_111,13.04,-0.43,0.65,0.32 1YR6,GLU_94,4.5,0.32,0,-0.33 1LTU,GLU_39,4.92,0.3,0,0.12 3CO1,CYS_45,12.57,-0.03,0.1,3.51 3GS3,GLU 143,4.57,0.07,0,-0.01 1HF8,LYS_239,11.3,-0.29,0.77,0.32

1FHL.LYS 166.10.22.-0.8.0.0.52 1GPP,TYR_146,11.62,-0.34,-0.3,2.26 2AHE,LYS_177,10.27,-0.19,0,-0.04 3EUR.LYS 132,10.4,-0.25,0.0.15 2AZL,LYS_265,9.65,-0.82,0,-0.02 3GS3,ARG 113,12,12,-0,38,0,0 2IRM.CYS 189,12.0,-0.04,3.04 3RFY,LYS_411,10.74,-0.59,0.16,0.67 1TR9,ARG_276,13.43,-1.24,1.11,1.05 1GPP,LYS_128,11.44,-0.31,0.85,0.39 2EHG,ASP_28,3.68,-0.19,-0.07,0.13 1UXO,ASP 136,1,56,-2,48,-0,28,0,53 2H01,ASP_109,3.98,0,-0.06,0.24 2C2Y,ARG_267,12.38,-1.51,0.78,0.59 20K1.GLU 476.4.44.1.91.-1.51.-0.45 3M3P.HIS 152,5.95,-1.49,1,-0.06 1DTO,TYR_154,11.96,-0.47,0.51,1.91 2J8A,CYS_248,8.88,-0.37,-0.47,0.71 4GA2,GLU_73,4.42,0.68,-0.41,-0.35 3OKQ,GLU_585,3.1,0.36,-1.07,-0.69 3RVC.TYR 89.10.21.0.0.0.21 3M3P,ASP_219,3.86,0,-0.17,0.23 2EJB,LYS_158,10.47,-0.03,0,0 2A6B,TYR_127,10.53,-0.44,0.41,0.56 3CIV.GLU 5.4.55.0.31.0.-0.26 1R53,GLU_15,4.59,0.2,-0.07,-0.03 2QDJ,GLU_112,4.65,0.19,0,-0.04 3EZ7,ASP_72,4.03,0,0,0.23 1LTU,ASP_257,3.21,-0.82,-0.17,0.4 1DZF,ARG_14,12.12,-0.32,0,-0.06 1Q42,CYS_67,9.94,-0.05,0.1,0.89 3ASA,ARG_362,12.49,-0.07,0,0.06 20PJ.ARG 169.13.79.-0.66.1.21.0.74 1WXF,LYS 257,10.37,-0.13,0,0 1TD6,ARG_288,12.43,-0.35,0,0.29 20KT,ARG_160,11.47,-1.16,0,0.13 4ACJ,HIS_653,5.47,-0.82,0.22,-0.42 2Q34,LYS 33,10.6,-0.17,0,0.27 1BKB,LYS 10,10.33,-0.17,0.0 3ETU,LYS_289,11.29,-0.56,0.85,0.5 1WNH,GLU_43,4.13,0.46,-0.21,-0.6 2WB8,ARG 616,12,27,-0.36,0,0.13 1T95.LYS 153.9.87.-0.38.0.-0.25 1X04,GLU_188,4.7,0.15,0,0.06 1TWU,GLU_67,4.74,0.2,0,0.04 2QHT,CYS_170,9.64,0,0.25,0.39 3GEC,ARG 316,12.79,-0.79,0.23,0.87 1WYC,CYS_118,12.47,-0.66,0.33,3.8 1GPP,GLU_141,4.64,0.29,0,-0.15 3GS9,LYS 71,11,51,-0,58,0,85,0,74 1A8Q,GLU_262,3.53,0.47,-1.21,-0.24 2P5D,ASP 74,2.53,-1.29,-0.43,0.45 1V6T.ARG 168.11.84.-1.03.0.0.35 2OB5,CYS_126,11.82,0,0.05,2.76 2G2D,ARG_185,12.42,-0.08,0,0 3T5B,ASP_130,4.01,-0.15,-0.2,0.57 3FK5,LYS_39,10.64,-0.14,0,0.28 3C0C,GLU_324,4.26,0.58,-0.82,0 3FRR.ARG 10.12.25,-0.26.0.0.01 1DTO,HIS_53,5.76,-0.38,0,-0.36 2D7U,ARG 138,11.83,-0.87,0,0.21 4FCU,LYS 114,11,44,-0,23,0,79,0,38 3LQE,ARG_238,12.56,-0.31,0,0.38 1SQW,LYS_94,11.06,-0.2,0.38,0.39 1L2F,GLU_122,4.48,0.27,0,-0.29 4EZB,GLU_245,3.47,0.42,-1.07,-0.38 3JRT,LYS_152,11.25,-0.6,0.85,0.51 20K1.TYR 376.12.96.-0.72.0.3.68 4ANN,ARG_134,11.07,-2.46,0.19,0.84 3JSN,GLU_187,3.91,0.27,-0.56,-0.3 2NRR,LYS 389,10.5,-0.3,0,0.3 2R0S.CYS 130.10.21.-0.98.0.05.2.14 3I47,ARG_239,12.33,-0.17,0,0 3H5T,ARG_23,12.41,-0.09,0,0 4AE7,ARG 92,13,41,-0,15,0,45,0,61 3ETU.ASP 349.3.96.0.-0.04.0.2 3LMF,ARG_23,12.37,-0.13,0,0.01 1EQ6,ASP_73,3.88,-0.1,0,0.18 4FH3,HIS_336,5.21,-1.35,0,0.05 2ZQ5,ASP_323,3.64,-0.47,-0.06,0.37 4DEZ,TYR_83,12.63,0.17,0.73,1.74 20EW,ARG_56,12.27,-0.21,0,-0.02 3GS3,ASP_167,3.93,0,-0.04,0.18 1QQE,ASP_151,3.98,0,-0.28,0.46 1L2F,ASP 278,3.92,-0.15,-0.12,0.39 3V55,ARG 467,12,72,-0.3,0.46,0.06 3V75,ASP_267,3.97,-0.15,-0.31,0.64 1RZ2,TYR_168,13.54,-0.07,0.43,3.18 1XEU,ASP_268,3.9,-0.13,0,0.24 1NJ4.GLU 278.4.13.0.5.-0.74.-0.12 1JB3,ASP_58,3.88,0,-0.18,0.26 3VJ8.GLU 344.4.39.0.78.-0.71.-0.17 1BYI.TYR 74,10.77,-0.8,0.11,1.47 1R6Y,GLU 67,3.3,0.3,-0.85,-0.65 2Q99,ASP_40,4.12,0,-0.06,0.38 3LPZ,LYS_4,10.61,-0.16,0,0.28 2X4L,CYS_331,12.99,0,0.21,3.77 2XJ4,ARG_198,12.18,-0.19,0,-0.13 3TIR,ARG_21,12.61,-0.13,0,0.24 1X9G,ARG_84,12.55,-0.19,0,0.24 2Z0M.GLU 329.4.73.0.2.0.0.03 1X8F,GLU_83,3.71,0.39,-0.85,-0.33 4FCU,ASP 242,3.46,-0.74,0.01,0.39 3B21.GLU 174.4.48.0.1.0.-0.12 3B21,TYR_200,13.16,0,0.25,2.9 3RVC,ARG_140,12.65,-0.28,0.04,0.38 1DUP,ARG_34,11.74,-0.6,0,-0.18 1G8P,TYR 147,12.55,0,-0.33,2.88 2CI3,ARG_144,13.15,-1.56,0.53,1.67 1T3Y,LYS 72,10.58,-0.2,0.28,0 3V75,ARG_74,12.4,-0.21,0,0.11 1ZBP,GLU 214,4.38,0.18,0,-0.31 2XWS.GLU 36,5.03,0.85,-0.06,-0.26 3EIZ,LYS_132,10.22,-0.61,0,0.35 2QOP,GLU_176,4.6,0.36,-0.09,-0.17 3H8Y,LYS_94,10.42,-0.15,0,0.07 3OBS,TYR 15,12.18,-0.82,0.05,2.95 4E9E,LYS_472,10.43,-0.07,0,0 3LPZ,ASP_76,4.01,-0.32,-0.28,0.81 1WP5,ARG_215,12.38,-0.62,0.2,0.29 4DIU,GLU_15,4.74,0.32,0,-0.08 3KT9.GLU 99.3.82.0.59.-0.76.-0.51 3COU, ARG_5, 12.48, -0.26, 0, 0.24 3P2F,ASP_170,3.81,0,-0.12,0.13 2EFK,ASP_82,3.42,-0.41,-0.4,0.43 1SJY,ASP_126,3.77,-0.3,0.02,0.25 3BOW.ARG 101,12,36,-0.24,0,0,1 2A1V,HIS_139,6.42,-0.08,0,0 1G8P,LYS_133,10.32,-0.24,0,0.06 1Y2Q,TYR_13,12.04,0,0.17,1.86 3A2Z,ASP 49,4.01,0.0.06,0.16 3GV0,ASP_248,2.99,-1.97,-0.46,1.63 1KCM,GLU_250,4.51,0.24,0,-0.22 1ES9,GLU_126,4.74,0.24,0,0 3C5V,ARG_325,12.65,-0.08,0,0.23 3CRM,ASP 244,1.86,-2.05,-0.38,0.49 3Q2C,GLU_68,3.06,0.33,-0.97,-0.81 3M7G,GLU_266,4.75,0.2,0,0.05

4F8A.CYS 568.9.2.-0.04.-0.22.0.47 3F5D,ASP 168,3.89,0,-0.09,0.18 1SUU.LYS 648.10.5.0.0.0 3IV4,HIS_26,4.87,-1.77,0.04,0.1 1KW4,ARG 27,12,39,-0,18,0,0,06 1UOH, ASP 181, 3.07, -0.85, -0.42, 0.54 2J8A,HIS_294,5.6,-1.46,0.45,0.1 3CO1,TYR_119,10.73,0,0.12,0.61 2AZL,GLU_268,4.74,0.29,0,-0.05 3FRR,TYR_165,12.72,0.54,0.78,1.42 3ETV,LYS_111,10.38,-0.12,0,0 2X4J,LYS_30,10.44,-0.06,0,0 3NR5,LYS_2,10.42,-0.11,0,0.02 3C5V,ARG_106,11.92,-0.86,0,0.29 1P6F.LYS 136.9.76.-0.74.0.0 1RHS,ASP_195,3.8,0,-0.46,0.46 1S7K.TYR 95.11.38.0.62.0.26.0.51 2RJD,ARG_467,12.39,-1.41,0.82,0.46 20KT,ARG_76,12.89,-0.35,0.41,0.33 2ILR,ARG 365,11.8,-0.85,0.0.14 2BV9,TYR_54,10.42,0,0,0.42 3G9G,GLU_23,3.73,0.51,-0.84,-0.43 205X.LYS 865,10.64,-0.31,0.22,0.24 2XHC.ARG 272.12.45.-0.08.0.0.03 1H09,LYS_236,10.4,-0.09,0,0 3H13,HIS_417,6.48,-0.23,0.29,-0.08 4DBX,HIS_131,5.67,-3.26,0.85,1.58 3RJZ,LYS 90,10.46,-0.05,0,0 1XTZ,LYS 65,10.69,-0.19,0,0.38 3GYW,HIS_120,7.02,-0.6,0.76,0.36 1T95,LYS 228,10.52,-0.09,0,0.11 1SQH,GLU_20,3.98,0.42,-0.69,-0.25 3L7N,LYS 111,10.33,-0.62,0,0.45 10TM,GLU_194,5.27,0.62,0,0.15 1LFP,LYS_119,10.14,-0.36,0,0 1P4X,LYS_54,9.75,-0.78,0,0.03 3I82,TYR_70,9.68,-0.43,-0.05,0.16 2C2Y,ARG_150,12.7,-0.65,0.55,0.3 4ECC,HIS_160,6.47,-0.18,0,0.15 1R5O.GLU 59.3.69.0.43.-0.94.-0.3 2E0T,ASP_75,4.13,0,0.13,0.19 3PP8,HIS 109,5.78,-0.96,0,0.24 1J7G,TYR 52,10,12,0,-0,14,0,27 30NH,ARG_522,12.01,-0.66,0,0.17 2JEO,TYR_187,10.32,-0.23,-0.52,1.08 3K8J,TYR_49,12.37,0,0.68,1.69 3P28,ASP_228,4.22,0,-0.17,0.6 1PZC,ASP_37,3.25,-0.82,-0.17,0.43 2F4Q,GLU_228,4.13,1.64,-1.46,-0.55 2D7J,LYS_138,10.56,-0.08,0,0.14 1ZP2,GLU_70,3.99,0.13,-0.29,-0.35 1UCH,HIS 179,6.68,-0.41,0.26,0.33 1W7B,LYS_81,10.3,-0.11,0,-0.08 2ZCO,LYS_9,10.38,-0.12,0,0 2HRZ,HIS_86,2.79,-2.87,0,-0.84 1J85,LYS_42,10.5,-0.07,0,0.07 10IS,LYS_271,10.47,-0.25,0,0.22 1TXJ,GLU_66,4.96,0.42,-0.07,0.11 3EZ7,GLU_301,3.49,0.39,-0.85,-0.56 2Q98,GLU_39,3.15,0.33,-0.85,-0.83 4DIU.ARG 62,12.22,-0.28,0,0 3EX9,ARG_117,12.36,-0.23,0,0.1 1L3K,ASP_80,2.72,-1.7,-0.09,0.71 3EJC,GLU_87,3.55,0.43,-0.75,-0.64 3QAV,LYS_119,10.83,-1,0.85,0.48 1XAW,TYR_443,10.08,0,-0.32,0.4 1YTQ,GLU_122,3.52,0.38,-0.63,-0.73 1IAP,ARG_136,12.44,-0.23,0,0.17 3G6S,ARG_26,10.26,-2.71,0,0.48

3CAX,LYS_137,10.96,-0.27,0.31,0.41 3V3T,ASP 133,3.44,-0.16,-0.44,0.24 2GZR,ARG_167,12.09,-0.45,0,0.04 2JKF,TYR_35,11.03,-0.32,0.05,1.3 1G8P.HIS 159,7.95,-0.37,1.23,0.6 1BN6.CYS 139.13.06.0.0.65.3.41 3ADO,GLU_52,5.71,1.33,0,-0.12 3D9H,HIS_103,5.65,-1.18,0,0.32 1FQI,LYS_319,10.43,-0.21,0,0.14 2BLL,ARG_317,13.4,-0.28,0.34,0.84 1DZF,GLU_6,4.33,0.1,0,-0.28 1P1L,HIS_2,5.77,-0.84,0,0.1 2B78,TYR_222,12.46,-0.59,-0.06,3.12 3K9I,ARG_111,12.68,-0.7,0.55,0.32 3RLN.GLU 592.3.36.0.67.-1.47.-0.32 1SOH,TYR 288,13.03,-0.85,0,3.88 2X5Y,ASP_803,2.2,-1.59,-0.64,0.64 2Q34,LYS_205,10.47,-0.14,0,0.11 2AZL,ARG_46,12.25,-0.28,0,0.03 1059,HIS 76,6.22,-0.23,0,-0.04 2CVB,GLU_17,3.71,0.45,-0.61,-0.62 1YR6,GLU_41,4.39,0.14,0,-0.26 3NR5,ASP_39,3.68,0,-0.26,0.13 2ATR,CYS 128,9.29,0,0,0.29 3JV1.CYS 147.10.05.-0.07.-0.33.1.45 1ZBP,HIS_205,5.72,-1.53,0.59,0.16 2CWC,ARG_107,12.42,-0.2,0,0.13 3KEY,ASP_375,4.63,0,-0.19,1.02 1MHN,TYR 127,12.7,0.29,0.67,1.74 1OXZ,GLU_257,4.03,0.76,-0.65,-0.57 3COU,GLU_8,4.71,0.1,0,0.12 2YWX,LYS_17,10.03,-0.42,0,-0.05 3ADO,HIS 145,5.95,-2.09,0.85,0.7 4FZR.GLU 77.4.6.0.1.0.0 3ASA,GLU_296,4.58,0.11,0,-0.03 1R3F,ASP_90,3.79,-0.87,-0.46,1.32 1NAF,LYS_226,10.48,-0.12,0,0.1 2YX0,GLU 297,4.94,0.22,0,0.21 3M7G,GLU_123,4.76,0.08,0,0.18 2RIS,LYS_191,10.59,-0.26,0,0.35 1WJG,ARG_61,12.47,-0.26,0,0.23 100X.ASP 151.2.75,-1.43,-0.14,0.52 3RJZ,ARG 60,12,11,-0,55,0,0,15 1NKD,ASP_45,3.99,0,-0.11,0.3 2ZCX.TYR 63.10.05.0.-0.42.0.47 1NJ4,LYS_309,10.46,-0.16,0,0.11 3T8R,GLU 43,4.6,0.5,-0.15,-0.25 1P2F,LYS 16,10.67,-0.1,0,0.27 2V4U,ASP_341,5.28,0,0.17,1.32 3K8J,LYS_237,10.37,-0.19,0,0.06 4EKU,LYS 249,10.32,-0.21,0.0.02 1XIP.TYR 248,13.07.0.42,0.64,2.01 2OJQ,ASP_452,4.11,0,-0.31,0.63 1R3F,TYR 208,13.92,-0.85,0.92,3.85 3GW3,GLU_315,4.67,0.12,0,0.05 3GYW,ARG_68,12.5,-0.23,0,0.22 1TD6.TYR 128,12,88,0.85,0.54,1.49 4HDE,ARG_188,13.56,-0.39,0.57,0.87 3CO1,GLU_36,4.68,0.31,0,-0.13 2E3C,LYS 415,11,48,-0.36,0.67,0.67 1KCM.GLU 113.3.89.1.89.-1.-1.48 1GPP,LYS_148,10.27,-0.2,0,-0.02 3V3T,ASP_41,3.65,-0.05,-0.46,0.37 2D7J,LYS_140,10.85,-0.34,0,0.68 1UJ8,HIS_44,7.36,-0.68,1.53,0.02 2RFA,ARG_134,12.5,-0.31,0.05,0.26 208P,ARG_136,12.3,-0.89,0,0.68 3F1X,ARG_158,12.36,-0.6,0,0.46 2ATR,ASP_62,1.66,-2.69,0,0.55

1V6T.HIS 38.0.97.-3.26.0.-2.27 4ETX,TYR 427,11.33,0,0.15,1.18 1AKO,ASP_143,3.89,0,-0.11,0.2 3OBS,CYS_87,12.91,0,0.09,3.82 3C0C,TYR_315,10.24,0,0.03,0.2 1FO9,ARG_121,12.73,-0.25,0.02,0.47 1PDB,ARG_70,10.54,-1.96,0,0 4ETX,ASP_318,3.08,-0.84,-0.23,0.35 1Z9L,LYS_31,10.4,-0.25,0,0.15 2FG1,LYS_44,10.58,-0.38,0.2,0.27 2J8A,LYS 366,10.45,-0.22,0.16,0 3CIV.HIS 136.6.09,-0.32,0,-0.09 2GZQ,LYS_11,11.4,-0.36,0.85,0.41 1RI6,TYR_53,12.74,0,0.31,2.43 2FXT,LYS 330,10,38,-0,12,0,0 3M7D,ARG 93,12,54,-0,18,0,0,22 2QZQ,LYS_151,10.49,-0.05,0,0.05 4E8B.CYS 115.8.55.-1.83.-0.05.1.42 2BDD,TYR_128,10.39,0,0.08,0.3 3G9G,ARG_175,12.67,-0.23,0,0.4 2D0A, ASP_40, 4.02, 0, 0, 0.22 2P4D,ASP_100,2.15,-2.87,-0.19,1.4 1RI5,GLU_257,5.2,0.96,0,-0.27 2EJB,HIS 81.6.18,-0.24,0,-0.08 2YT4.HIS 632.6.41.-0.09.0.0 4H89,ARG_45,12.45,-0.29,0,0.25 2X4L,GLU_154,3.63,0.31,-0.85,-0.33 3K8J,HIS_141,6.26,-0.22,0,-0.02 1TWU,ARG_27,13.42,-0.39,0.55,0.76 1ZCE,CYS_134,11.53,-0.26,0.06,2.73 3C38,GLU_176,4.74,0.24,0,0 2EFK,ASP_281,3.87,0,0,0.07 3EVN,TYR 81,10.88,0.32,0.01,0.55 1AD6,GLU_464,3.32,0.62,-1.42,-0.38 1FHL,TYR_113,13.24,0,0.16,3.08 2FZP,GLU_201,4.71,0.15,0,0.07 2FD5,GLU_72,4.73,0.2,0,0.04 4AM1,HIS_212,5.41,-1.65,0.83,-0.28 1VSM.GLU 172.4.43.0.36.0.-0.43 3HUE,LYS_71,10.45,-0.21,0,0.16 1AK1,LYS_135,10.73,-0.18,0,0.41 2X4G,GLU_312,4.63,0.17,0,-0.05 1ZP2,ARG 61,10.45,-3.11,0.1,0.95 1DVO,ARG_49,12.29,-0.21,0,0 4F3J,ASP_137,3.05,-1.15,-0.02,0.41 1ZP2,HIS_178,6.48,-0.81,0.51,0.28 3DZ1,ASP 226,4.2,0,-0.11,0.5 30DJ,GLU_45,4.83,0.27,0,0.07 3HUE,LYS_84,10.77,-0.17,0.11,0.32 3RRO,ASP 77,4.01,0,-0.05,0.26 2ZCO,GLU_178,3.87,0.34,-0.85,-0.12 3K9I,GLU 129,4.48,0.48,-0.36,-0.13 2D59,LYS 66,10,7,-0,21,0,0,41 1L3K,GLU_135,4.6,0.3,0,-0.2 1QYI,GLU_183,3.67,2.64,-2.69,-0.77 1P2F,ARG_27,12.45,-0.07,0,0.02 3QKY,GLU_268,3.16,0.55,-1.29,-0.6 1XEU,HIS_192,6.02,-0.7,0.01,0.2 4E8B,ASP 72.2.87,-1.04,-0.44,0.55 2P65,ASP_171,2.76,-1.59,-0.51,1.08 1QZN,TYR 101,11.92,-0.84,0.64,2.12 2FM9,LYS 164,10,27,-0,3,0,0,06 2B78,TYR_356,13.67,0.85,0.52,2.31 2QEV,LYS_117,10.21,-0.47,0,0.18 3G6S,LYS_73,10.56,-0.07,0,0.13 2IQT,GLU_44,4.35,0.17,-0.28,-0.04 1NAR,LYS 69,11.23,-0.35,0.47,0.61 3A4C,ARG 526,12,4,-0,1,0,0 2GZR,TYR_219,9.62,-1.53,0.01,1.13

1PNE,ARG_88,12.05,-0.49,0,0.04 3E7P,TYR 244,12.04,0.85,0.44,0.75 2CYG,LYS_302,10.24,-0.18,0,-0.08 2CN1,TYR_170,12.48,0.85,0.37,1.26 2ZQ5,HIS_255,6.66,-1.74,0.96,0.94 1KN3.LYS 156.10.38.-0.19.0.0.07 3IL3.GLU 64.4.59.0.23.0.-0.15 1ZCE,TYR_53,11.66,0,0.11,1.55 2QK1,TYR_369,12.31,0,0.25,2.05 1NAR,ARG_73,12.93,-0.26,0,0.69 2P4D.LYS 87.10.78.-0.17.0.0.45 3V75,ASP_33,3.49,-0.31,-0.33,0.34 2RJD,GLU_352,4.43,2.87,-2.71,-0.24 2B78.LYS 66.10.39.-0.11.0.0 3FTT,GLU_34,4.06,0.32,-0.39,-0.37 2IRM,GLU 193,4.57,0.07,0,0 1WRU,ASP_258,2.95,-1.76,-0.03,0.94 1Z3X,GLU_123,4.2,0.88,-0.8,-0.38 1Y0K,ARG_36,12.95,-1.56,0.74,1.27 2W1R.TYR 62,10.82,0,0,0.82 3DSH.ASP 323.3.63.-0.84.-0.45.1.11 3AUF,ARG_94,12.19,-0.38,0,0.07 1RI5.GLU 97.4.59.0.12.0.-0.04 1J85,LYS 92,9,78,-0,31,0,-0,42 3BCH,ASP_200,4.08,-0.07,-0.06,0.41 1V6T,ASP 173,2.53,-1.81,0,0.54 2BAA,TYR_123,10.58,0,0,0.58 4DNU,TYR_241,10.22,0,-0.19,0.42 1XFK,ARG_173,13,-0.36,0.74,0.13 2Q13,LYS_361,10.73,-0.79,0.66,0.36 3HKX,GLU_172,4.18,0.51,-0.77,-0.06 1UAJ,ASP_177,3.72,-0.05,-0.25,0.22 2Q34,CYS_52,10.71,0,-0.02,1.73 2WB8,ASP 519,3.99,-0.15,-0.08,0.42 2RJD,TYR 490,9.2,-0.85,-0.28,0.33 1TD6,LYS_78,10.31,-0.2,0,0 1X7F,HIS_213,3.81,-2.72,0,0.03 1GQE,LYS_292,11.82,-0.68,0.95,1.04 3RFY,ARG 280,12.65,-0.14,0,0.3 3MEW,TYR_245,11.34,0.22,0.53,0.59 3JZN,LYS 332,10.07,-0.77,0.0.33 3L3P,GLU_383,5.39,0.83,0,0.06 3BQW,ARG 119,12.71,-0.67,0.25,0.62 1X04,HIS 135,6.74,-0.71,0.74,0.21 2ZQ5,ASP_33,3.25,-0.85,0.04,0.26 3K1H,CYS_54,12.16,0,0.19,2.97 3G9G,HIS_169,7.04,-0.24,0.65,0.14 3ON1,LYS 49,10.14,-0.42,0,0.05 2J8A,GLU_249,4.19,0.83,-0.71,-0.45 1UXO,HIS_62,6.8,-0.64,1.05,-0.11 1EYH,GLU_21,3.85,0.51,-0.98,-0.18 3LMF,GLU_106,4.06,0.21,-0.1,-0.55 2PGX.ASP 136.3.1.-1.12.-0.07.0.49 2R57,CYS_372,13.93,0.57,1.01,3.35 3PP8,LYS_150,10.48,-0.17,0,0.15 3CAX,TYR_433,10.06,0,-0.24,0.3 4ESS,ASP_17,2.35,-1.95,-0.37,0.86 2CIU.GLU 188.4.18.1.16.-0.98.-0.51 3ADO,TYR_251,10.47,0,0.11,0.36 2P0Y,GLU_164,4.1,0.26,-0.45,-0.21 1TXJ,CYS_14,11.35,-1.18,0.11,3.42 1MUF.CYS 119.10.4,-0.69,-0.16.2.26 4H4J,ARG_259,13.73,-1.03,1.61,0.65 1P1L,GLU_16,4.61,0.3,0,-0.18 1U7U,ARG_342,11.52,-1.22,0,0.25 1NAF,LYS_174,11.01,-0.22,0.12,0.62 3CIV.GLU 257,3.63,0.94,-1.43,-0.38 3H04, ASP_12, 1.03, -2.87, -0.42, 0.52 2RIK,ASP_68,2.91,-2.2,-0.14,1.44

2H85.ASP 183.3.61.-0.14.-0.32.0.26 2FGG.GLU 22,4.5,0.33,-0.02,-0.32 2CL3,GLU_70,4.23,0.95,-0.57,-0.65 2VGM,ASP_241,3.94,0,-0.42,0.55 3BOW,LYS 222,11,24,-0.35,0.23,0.85 3LMF,HIS 107.6.4,-0.65.0.47.0.07 1MUF,CYS_303,11.69,0,0.01,2.68 3H5T,GLU_330,4.65,0.58,-0.11,-0.33 2IN0,ARG_96,11.63,-0.93,0,0.06 1BN6,ASP_93,4.38,0,0.06,0.52 2XMZ,ARG 73,12,47,-0.22,0,0,18 106D,GLU_147,3.11,0.51,-1.25,-0.65 1QZN,LYS_117,10.23,-0.37,0,0.11 3I82,GLU_27,4.61,0.11,0,0 102Y.TYR 17.10.21.0.0.01.0.2 2YYO,ARG_34,12.41,-0.18,0,0.09 1WXQ,TYR_323,13.54,0,0.53,3 2GZR,ARG_161,12.1,-2.59,0.79,1.4 1TXJ,GLU_86,4.7,0.2,0,0 1X7F.GLU 208.4.53.1.55.-0.75.-0.77 3GW3,HIS_189,5.37,-1.01,0,-0.13 1WRU,LYS_304,10.39,-0.11,0,0 3A0X.LYS 723.10.43.-0.18.0.0.12 2EFK,ARG 222,13.98,-0.33,0.87,0.94 3ADO,LYS_264,10.45,-0.05,0,0 200K,LYS_192,10.34,-0.2,0,0.03 2CL3,LYS_182,10.5,-0.14,0,0.13 1NIJ,ARG_257,11.02,-3.37,1.04,0.85 2OJQ,GLU_442,4.7,0.2,0,0 3OKQ,LYS_632,10.51,-0.17,0,0.18 3LJI.TYR 290,10,53,0,0,1,0,43 3F6F,LYS_188,11.02,-1.14,0.85,0.81 100X,ASP 122,1.12,-2.72,-0.51,0.55 1RL0.GLU 199.4.23.0.66.-0.73.-0.2 2H85,LYS_264,10.75,-0.18,0.08,0.35 2GZQ,LYS_106,10.17,-0.12,0,-0.21 3M70,ASP_251,2.68,-1.12,-0.62,0.62 3BWT,LYS_751,10.4,-0.11,0,0.01 3Q2C,TYR_35,10.33,-0.64,-0.02,1 4DVD,GLU_56,4.53,0.42,0,-0.39 1YLN,GLU_142,4.62,0.18,0,-0.05 1V43.ASP 357,4.19,-0.66,-0.02,1.07 3AU3,ARG 499,12.31,-0.66,0,0.47 3PZ9,LYS_167,10.53,-0.32,0,0.34 2P65,ASP_112,4.08,0,0,0.28 2JEO,ARG_22,12.69,-0.26,0.12,0.34 2QOP,GLU_111,5.19,1.72,-0.2,-0.83 1QQH,ASP_205,2.71,-1.37,-0.09,0.37 2XWS,ASP_81,2.42,-1.49,-0.41,0.52 2HP7,ASP_108,2.99,-1.21,0,0.41 1ZCE,ASP_60,4.65,-0.05,-0.24,1.13 4EVF.GLU 277.4.54.0.23.0.-0.18 1PVT,LYS_167,10.62,-0.15,0,0.27 4ECC,GLU_104,3.53,0.27,-0.71,-0.53 1SJY,HIS_3,6.41,-0.09,0,0 3L7N,TYR_105,9.43,-1.7,0.5,0.63 1AK1,HIS_28,5.17,-0.84,0.01,-0.51 2CWC,ARG_295,12.17,-0.44,0,0.11 1SFE,ARG_72,12.14,-0.37,0,0.01 3CN5,ASP_241,2.64,-1.7,-0.86,1.38 3U0V.CYS 87.9.6.-0.31.-0.17.1.08 2VAN,CYS_239,12.6,0,-0.18,3.78 3CNU,LYS_54,11.78,-0.33,0.85,0.75 3AUF,ARG_30,12.17,-0.26,0,-0.07 3EAZ,LYS_137,10.52,-0.19,0,0.21 3QAV,GLU_27,4.63,2.58,-1.69,-0.77 1S7K,HIS_62,5.2,-1.98,0.94,-0.26 1SJ8,ASP_515,3.13,-0.73,-0.31,0.37 1QQH,LYS_66,10.46,-0.05,0,0

30NH,TYR_471,13.45,0,0.29,3.16 3BCY,HIS 83,5.83,-0.42,0,-0.25 2PGE,ARG_74,12.42,-0.12,0,0.04 4F3J,TYR 136,12.27,-0.73,0.14,2.85 3ULX,LYS 123,10.34,-0.16,0.0 3RKV.ARG 220.12.85.-0.29.0.38.0.25 1JT9,ARG 253,12.5,-0.12,0.0.12 1NRI,CYS_110,9.13,-0.09,0.04,0.18 1YM5,ASP_169,2.76,-1.34,-0.15,0.44 2CBE,HIS_3,6.11,-0.11,0,-0.27 3Q9P,ASP_93,4.07,0,0,0.27 3ULX,ASP_141,2.95,-0.73,-0.44,0.33 3M3PLYS 238,10.22,-0.19,0,-0.09 1GVP,TYR_56,10.45,-1.02,0.11,1.36 3BA1.ARG 118.13.3.-1.26.1.41.0.64 2ZCO.TYR 75,10.31.0.0.0.31 2QEV,GLU_25,3.73,0.52,-0.85,-0.43 1Y2Q,LYS_128,12.4,-0.59,1.7,0.79 3BQW,GLU_24,4.08,0.72,-0.75,-0.38 2D59,LYS 77,10.38,-0.16,0,0.04 1CBY,HIS_30,6.32,-0.18,0,0 3GMS,GLU_272,4.72,0.33,0,-0.1 1YW5,ARG_94,12.44,-1.04,0.36,0.63 2QEV,GLU 130,4.7,0.2,0,0 2P5D,TYR 31,10,-0.03,-0.38,0.41 2A6B,LYS_101,10.5,0,0,0 208I,GLU_23,4.01,0.34,-0.61,-0.22 2WOZ,CYS_451,12.69,0,0.02,3.67 3H8Y,GLU_89,3.94,0.41,-0.39,-0.58 300P,GLU_101,5.04,0.72,0,-0.19 3IDW,GLU_7,4.55,0.24,-0.37,0.17 2P52,GLU_204,4.51,0.3,0,-0.29 3ANJ,TYR 383,12.94,-0.42,0.05,3.31 1G8P.GLU 125.4.83.0.3.-0.27.0.3 1WP5,TYR_131,11.97,0.85,0.58,0.54 1XIP,GLU_83,4.33,0.37,-0.16,-0.37 1MJS,LYS_340,11.34,-0.44,0.85,0.43 1PDB,ASP 141,4.09,-0.04,0,0.33 3U2R,LYS_94,10.66,-0.17,0,0.33 3E5T,ASP_196,3.41,-0.75,-0.45,0.82 2Z61,HIS_33,8.19,-1.12,1.61,1.2 3BJV,HIS_11,6.21,-0.22,0,-0.06 3H13.GLU 414.4.66.0.23.0.-0.07 2CXA,CYS_228,9.29,-0.35,-0.14,0.77 1RZ2,TYR_40,9.94,0,-0.14,0.08 2H14,TYR_228,9.71,-0.35,-0.28,0.34 2A6B,GLU_36,3.24,0.82,-1.65,-0.42 200K,GLU_16,4.94,0.44,0,0 20YZ,GLU_43,5.71,1.49,-0.3,0.03 2X4G,ARG_233,13.53,-0.36,0.26,1.13 2VAN,GLU_144,2.42,0.67,-2.22,-0.52 2BLL,GLU_407,4.74,0.31,0,-0.07 1MUF,ASP_88,3.91,0,0,0.11 4H89,ARG 168,12,1,-0.63,0,0.23 2V4U,ARG_411,11.88,-1.14,0.04,0.48 1G8P,GLU_346,3.79,0.35,-0.85,-0.21 1L2F.GLU 264.4.47.2.19.-1.13.-1.1 2ATR,HIS_40,6.28,-0.22,0,0 1UCH,GLU_40,4.59,0.09,0,0 3ANJ.TYR 391.10.7.0.11.0.07.0.53 3IU5,ASP 62,1.97,-2.04,-0.54,0.75 1UCH,ASP_79,3.87,0,-0.09,0.15 105J,LYS_13,11.2,-0.35,0.68,0.37 4EVF,ARG_187,11.79,-0.67,0,-0.04 2NYC,TYR_316,10.39,0,0,0.39 1TJE,HIS_89,6.33,-0.28,0,0.11 1RI5,CYS_223,11.02,0.26,0.64,1.11 4EVF,ARG_278,13.69,-0.3,0.55,0.94 2B2H,HIS_305,3.4,-3.1,0,0

3E0H,LYS 51,10.32,-0.31,0,0.13 1WP5,GLU 295,4.77,0.31,-0.18,0.14 1UJ8,ASP_49,4.03,0,-0.02,0.24 2EJB.GLU 26.4.7.0.25.0.-0.05 1059,GLU_78,4.54,0.06,0,-0.02 3HKX,ARG 112,11,11,-1.6,0,0,21 3ELI,ASP_121,3.57,-0.62,0.03,0.36 3JZ9,LYS_464,11.46,-0.57,0.85,0.68 1WOU,CYS_110,11.58,-0.05,0.16,2.46 2XWS,ARG_123,12.43,-0.07,0,0 2D59,ASP_37,4.14,0,-0.09,0.45 3A2Z,LYS 127,10.6,-0.12,0,0.22 1W7B,TYR_24,9.83,0,-0.28,0.12 3GOZ,TYR_259,11.14,0,0.44,0.7 20GO.CYS 544,9.65,-0.93,-0.01,1.59 2IXM,HIS 308,4,95,-0.94,0,-0.61 3FHF,GLU_91,4.35,0.29,0,-0.43 2NMU.CYS 45.11.66.0.0.04.2.62 1YLN,ARG_194,12.57,-0.15,0,0.22 3LOD,GLU_13,3.74,0.41,-1.05,-0.11 1JT9.ARG 18.12.15.-0.83.0.0.48 1RL0,LYS_254,10.26,-0.3,0,0.07 3GS3,LYS_29,10.39,-0.11,0,0.01 1J33.HIS 271.5.5.-1.73.0.66.0.09 3GW3.ARG 247.12.11.-0.61.0.0.22 1SQW,LYS_53,10.61,-0.17,0,0.28 1XAW,TYR_432,10.87,-0.53,0.09,1.3 1U3Y,ASP_271,3.88,0,-0.26,0.34 2P52,GLU_283,3.06,0.84,-1.65,-0.62 1SJ8,ARG 589,12.31,-0.39,0.0.2 2YLF,CYS_221,11.97,-0.05,-0.02,3.04 3LH5,GLU_530,3.68,0.47,-1.06,-0.24 3AU3,LYS_670,10.33,-0.17,0,0 1VJG,HIS 173,6.4,-0.19,0,0.09 1R3D,HIS_78,5.52,-1,0.02,0 2QEV,ASP_67,1.64,-2.02,-0.7,0.56 2IRM,TYR_34,11.48,-0.52,-0.71,2.72 2P65,ARG 32,12.38,-0.12,0,0 1SUU,ARG 735,12,31,-0,4,0,0,21 2CI3,LYS_252,10.25,-0.25,0,-1.39E-17 3F1X,LYS_40,10.45,-0.05,0,0 1KCM,ASP 238,3,99,0,-0,14,0,33 2P0L,ASP 257,3.46,-0.41,-0.12,0.2 2B78,TYR_286,10.45,-1.7,0.01,2.14 3ZTA,GLU_23,4.12,0.32,-0.32,-0.38 4FZR,GLU_251,4.89,0.83,-0.02,-0.42 2D0A,TYR 46,11.88,-0.01,0.21,1.68 2B61,TYR_252,10,0,-0.15,0.15 1G8P,ARG_230,12.92,-0.68,0.8,0.3 2HXB,ASP_135,3.98,-0.01,0.01,0.18 2VAN,TYR_322,11.1,0,0.29,0.79 2PWQ,ASP 28,3.86,0,-0.13,0.19 1XAW,LYS 444,10,46,-0,18,0,0,15 1R3F,LYS_176,10.62,-0.17,0,0.28 1TUL,CYS_90,9.39,0,0,0.39 1RHS,ARG_146,12.4,-0.16,0,0.06 3ASA,ASP_42,3.86,-0.78,-0.29,1.13 10I7,LYS_25,10.32,-0.18,0,0 3BB7.TYR 212.10.4.0.-0.09.0.49 3F5D,CYS_100,11.83,-0.09,1.15,1.78 1ZBP,HIS 73,6,-0.38,0.06,-0.18 3CXS.TYR 170,12.24,-0.85,0.1,2.99 2AD1,CYS_26,10.17,-0.41,0.17,1.41 3HKX,ASP_255,3.56,-0.84,-0.4,1.01 1XDZ,LYS_13,10.22,-0.48,0,0.2 4GA2,GLU_136,4.78,0.21,0,0.07 4EKU,ASP_100,3.42,-0.3,-0.51,0.42 3ZSL,HIS_217,5.85,-0.51,0,-0.14 3COU,GLU_119,4.12,0.51,-0.75,-0.14

3IRA,TYR_91,11.8,0,0,1.8 3U0V,GLU 189,3.81,0.66,-0.97,-0.38 1XTZ.HIS 262.6.8.-0.21.0.71.-0.19 1FOILLYS 283.10.49.-0.01.0.0 4DEZ,ASP_72,3.95,0,0,0.15 10I7,GLU_208,5.71,1.5,0,-0.27 3CAN.GLU 53.3.9.0.35.-0.5.-0.45 2F4Q,ASP_276,4.26,0,0.02,0.45 3IVF,LYS_106,10.74,-0.29,0,0.54 3G9T,LYS_16,10.42,-0.12,0,0.05 1L2F,GLU_158,4.33,0.36,-0.16,-0.37 3E7P.CYS 18.10.94.-0.09.0.26.1.77 2GZQ,ASP_48,3.56,0,-0.47,0.23 3DZ1.GLU 175.3.3.0.29.-1.11.-0.38 1WLY,ARG_269,12.02,-0.58,0,0.11 3GG6,ARG 37,12.47,-0.03,0,0 4EZB.GLU 163.4.6.0.1.0.0 1LFP,LYS_202,11.17,-0.85,0.85,0.67 1XTZ,GLU_254,3.9,0.42,-0.6,-0.42 2CBE,TYR 40,10,24,0,-0,1,0,34 2FPN,LYS 44,10,18,-0,32,0,0 1RI6,ASP_161,2.56,-1.28,-0.38,0.41 3PBH,ARG_40,11.6,-1.07,0,0.17 2DFL.ASP 70.3.82.0.-0.26.0.27 3CAN.GLU 22.4.77.0.16.0.0.11 2ILR,CYS_421,9.96,-0.85,-0.27,2.08 3LD1,CYS_20,11.11,-0.53,-0.05,2.69 1RAJ,LYS_250,10.59,-0.16,0,0.24 2VAN,GLU_335,4.8,0.13,0,0.17 3RJX,HIS_264,4.37,-2.13,0,0 2IQT,GLU_281,4.72,0.32,0,-0.1 2R51,ARG 60,12,96,-0.2,0.06,0.6 1PVT,ARG_226,12.42,-0.08,0,0 4HDE,LYS 88,10.64,-0.16,0,0.3 20VT.ASP 60.2.68,-2.32,-0.12,1.31 2R57,CYS_277,9.19,-0.25,0.02,0.43 2E0T,TYR_166,11.97,0,0.07,1.91 2H2W,GLU_208,3.68,0.42,-0.6,-0.64 2DFL,LYS 137,10.33,-0.21,0,0.04 1WNH,ARG_214,12.45,-0.35,0,0.3 2Y2T,ARG 32,12,27,-0,4,0,0,16 1DUN,ASP_26,3.09,-0.83,-0.22,0.34 3M66,ARG 302,12.28,-0.24,0,0.02 300P,LYS 75,10,78,-0,78,0,69,0,38 3LJC,GLU_62,4.11,0.27,-0.23,-0.42 2JHY,HIS_157,5.41,-0.51,0,-0.58 2EDM,ASP_158,2.82,-0.85,-0.46,0.33 3EYE,CYS 86,12.69,0,0.12,3.58 1ZBM,ARG_102,12.64,-0.19,0,0.34 1L3K,ARG_146,12.31,-0.31,0,0.12 3ASA,TYR_327,10.79,-0.85,-1.25,2.89 2NRK,LYS_167,11.54,-0.27,0.83,0.47 105Z,ARG 571,12.4,-1.55,0.74,0.72 1TR9,LYS_236,10.31,-0.1,0,-0.09 3IDW,CYS_19,10.49,-0.03,0.21,1.32 2EEY,GLU_116,6.33,2.31,-0.58,0.1 3L7N,TYR_34,11.15,0,0.15,1.01 4H4J.ASP 136.2.99.-0.85.-0.41.0.46 4E8B,HIS_15,7.12,-0.29,0.74,0.17 3CXS,CYS_45,9.72,-1.64,0.41,1.96 2YWJ,LYS_118,11.61,-0.34,0.85,0.6 3FWU,ARG 61,12.63,-0.31,0.0.44 2G9D,LYS_304,10.64,-0.54,0.33,0.36 3EZ7,ARG 217,13,21,-0,23,0,39,0,54 2V5B,GLU_186,4.8,0.43,0,-0.14 2NRR,GLU_464,4.93,0.43,0,0 1X8F.ASP 32.3.45.-0.32.-0.28.0.26 3L3P,ARG_378,13.09,-1.33,1.26,0.66 1SI7,GLU_97,4.56,0.06,0,0

3K8J.ASP 166.2.81.-1.29.-0.59.0.89 3BOW,ASP 321,3,93,0,0,0,13 3RLN.TYR 591,10,99,0,-0,1,1,09 1Z9L,GLU_124,4.51,0.23,0,-0.21 3GYW, ARG 222, 12, 28, -0, 37, 0, 0, 14 2B61,HIS 130,6.11,-0.39,0,0 1NJ4,LYS_253,11.3,-0.45,0.85,0.39 2Q13,ARG_171,12.21,-0.34,0,0.05 2FL4,GLU_44,4.85,0.49,-0.1,-0.04 2HRZ,ASP_124,2.47,-1.32,-0.52,0.51 2EEY,GLU 95,4.55,0.07,0,-0.02 1PNE,TYR_6,10.52,0,0.17,0.34 2YLF,ARG_70,12.06,-0.44,0,0 1L3K.CYS 43.11.44.0.0.18.2.25 1YR6.ARG 227.13.45.-0.45.0.78.0.64 10I7,LYS_226,11.39,-0.29,0.8,0.38 1MML.TYR 222,10,14,-0,26,0,11,0,29 3E7P,ARG_225,13.23,-0.1,0.46,0.37 1M5I,ASP_149,2.97,-0.77,-0.38,0.32 2B3M,LYS 16,10,51,-0,26,0,0,27 1NRI,GLU_31,3.9,0.33,-0.63,-0.3 1YR6,GLU_62,3.05,0.51,-1.58,-0.38 1WXF,GLU_239,4.56,1.4,-0.8,-0.54 3RKV.GLU 192,3.67,0.25,-0.75,-0.33 1BKB,LYS_60,10.37,-0.16,0,0.02 3T57,LYS_159,10.61,-0.49,0,0.61 3ELI,HIS_147,6.83,-0.23,0.26,0.3 4FZR,GLU 83,4.5,0.35,0,-0.36 2Q5X,GLU_796,4.8,0.3,0,0 1DOV,LYS_186,11.3,-0.29,0.71,0.38 4DND,GLU_101,4.47,0.21,0,-0.24 3K8J,GLU_224,3.85,0.38,-0.67,-0.35 1N81,LYS 68,10.36,-0.28,0,0.14 1BN6,ARG 32,12,65,-0,43,0,04,0.55 1PGV,GLU_290,4.4,0.37,-0.42,-0.05 1ZYL,GLU_155,4.91,0.82,0,-0.41 4ANN,LYS_41,10.45,-0.12,0,0.08 3BA1.GLU 69.2.89.0.98.-1.8.-0.79 1MHN,GLU_134,2.78,0.8,-2.55,0.03 2XJ4.LYS 35,11.09,-0.4,0.23,0.76 3TOW,HIS_195,4.86,-1.11,0,-0.52 3GFP,ARG 432,12.04,-0.39,0,-0.07 1UCH.TYR 137.11.16.0.0.27.0.89 3EUR,ASP_85,4.07,0,-0.44,0.7 1RAJ,ASP_412,3.66,0,-0.43,0.29 1SJ8,LYS_592,11.01,-0.46,0.52,0.46 2QV2,GLU_26,5.26,0.91,0,-0.16 3ELI,HIS_37,6.17,-0.33,0,0 1MN3,GLU_451,4.63,0.13,0,0 2VGM,LYS_124,9.96,-0.54,0,0 3CSR,ASP 149,3.07,-0.72,-0.3,0.3 3LOD,LYS 149,10.63,-1.06,0.79,0.41 3MEW,TYR_273,10.62,0,0.27,0.35 1A8Q,LYS_130,10.6,-0.14,0,0.24 1LN4,ASP_55,2.8,-1.29,-0.03,0.32 4H86,ASP_84,3.59,-0.76,-0.27,0.82 2YLF,ASP_138,4.14,0,-0.08,0.42 2B61,LYS_349,11.41,-0.29,0.85,0.35 3UX2,GLU_51,3.47,0.41,-1.11,-0.32 2P0L,ASP_214,3.37,-0.78,-0.09,0.44 3I82,LYS 29,10,44,-0.06,0,0 1SBX,CYS_153,7.7,-3.6,0.26,2.03 2CVB,TYR_79,9.72,-0.04,-0.64,0.39 3CX2,ASP_152,3.88,0,-0.06,0.14 2RGY,LYS_169,10.61,-0.27,0,0.38 1J7G,LYS 95,10.57,-0.38,0,0.45 3H13,CYS_310,12.42,0,0,3.42 1X6J,GLU_48,4.53,0.22,0,-0.18 3E5T,HIS_197,6.61,-2.73,1.7,1.13

1X7F,ASP 293,3.29,-0.71,-0.11,0.31 2ATR.GLU 35.4.82.0.19.0.0.12 1YB2,HIS_211,5.52,-1.59,0.09,0.53 1WP5,LYS_124,10.83,-0.2,0,0.52 3ONT,LYS_10,10.43,-0.07,0,0 1XIP.GLU 11.4.84.0.44.-0.05.-0.04 3O48,GLU_107,4.9,0.64,-0.03,-0.22 2CN1,ASP_128,3.82,0,-0.2,0.22 2BV9,ARG_143,12.11,-0.82,0,0.43 1RWZ,ASP_62,2.76,-0.85,-0.45,0.26 3C2E.GLU 61.4.32.1.38.-1.14.-0.41 1K95,ARG_186,13.01,-0.85,0.59,0.77 1C44,LYS 14,10.3,-0.31,0.0.11 4DEZ,GLU_123,5.03,0.2,0,0.34 1C3K.HIS 91.6.4.-0.1.0.0 1T07.GLU 41.3.53.0.44.-0.85.-0.55 1AKO,ASP_40,3.26,-0.45,-0.32,0.23 2Q13,LYS_193,10.31,-0.19,0,0.01 3IBT,GLU_141,4.47,0.14,0,-0.17 3MTT,GLU 537,4.76,0.27,0,-0.01 2QDJ,LYS_294,10.33,-0.17,0,0 2EHG,LYS_40,10.38,-0.13,0,0.02 1YTQ,GLU_166,4.75,0.25,0,0 4F8A,LYS 679,10.47,-0.15.0.0.11 3M66,ARG 365,11.9,-2.07,0.82,0.64 3U2A,GLU_105,4.71,0.21,0,0 3OKQ,CYS_643,9.39,0,0.1,0.29 2QVO,LYS_53,10.47,-0.25,0,0.22 1FO9,GLU_298,3.95,0.36,-0.74,-0.17 2A6B,TYR 55,12.35,0.59,0.59,1.17 4EVF,ASP_275,3.22,-1.31,-0.19,0.91 4FH3,ARG_78,13.92,-0.38,0.75,1.05 3UC9,GLU 171,4.13,0.55,-0.41,-0.52 1TWU,LYS 36,10.3,-0.21,0.0.01 2W0G,LYS_202,10.82,-0.18,0.2,0.3 2X4G,GLU_71,4.81,0.36,0,-0.04 2NMU,ARG_12,13.54,-0.37,0.81,0.6 4F8A,CYS 658,9.5,-0.12,-0.26,0.88 1X6J,ASP_38,3.82,0,-0.23,0.25 1Q42,TYR_88,11.39,0.63,0.3,0.46 2P0L,ASP_223,4.25,0,0.03,0.42 3EVZ,LYS 226,10,19,-0,21,0,-0,1 2DG7.ARG 117.12.22.-0.98.0.1.0.59 3ELI,ASP_44,4.05,-0.05,-0.42,0.72 1JYH,GLU_8,4.41,1.03,-0.62,-0.5 2VGM,LYS_45,9.5,-0.93,0,-0.07 3I47,LYS 13,10.12,-0.25,0,-0.13 1ZBPLYS 59,10.47,-0.09,0.0.05 1EQ6,HIS_210,6.1,-0.32,0,-0.08 3LH5,TYR_669,12.3,0,0.23,2.07 3GEC.TYR 414,12.06.0,-0.07,2.13 3HOX,LYS 93,10,13,-0,48,0,0,1 1AD6,GLU_413,4.57,0.11,0,-0.03 2P5D,LYS_142,10.65,-0.15,0,0.31 1X9G,LYS_26,10.52,-0.07,0,0.09 3TMO,LYS_211,11.21,-0.55,0.85,0.41 2R51,LYS 180,11.3,-0.91,0.85,0.86 3M7D,ARG_37,12.55,-1.67,0.54,1.17 3CS1,ASP_177,2.84,-1.62,0,0.66 1XTZ.HIS 263.8.15,-0.43,1.7.0.38 3I82,ARG 35,12.02,-0.43,0,-0.05 1R9W,ARG_349,13.52,-0.14,0.85,0.31 3V46,ARG_369,13.4,-1.11,1.26,0.75 2GZQ,GLU_13,4.11,0.56,-0.45,-0.5 3LJI,GLU_74,5.83,3.27,-0.53,-1.41 3N2T,LYS_245,10.32,-0.23,0,0.05 1FKM,ARG_310,12.25,-0.28,0,0.03 2V81,LYS_142,9.93,-0.73,0,0.16 2FBI,CYS_101,9.81,0,-0.09,0.9

3H6Q,TYR_93,11.74,0,0.63,1.09 2HRZ,ARG 309,11.64,-0.9,0,0.04 1QQE,GLU_73,4.41,0.31,-0.04,-0.37 3EOD,ARG 20,12,25,-0,45,0,0,2 2W0G,LYS_242,11.31,-0.42,0.85,0.38 2R4O,ASP 233,3,31,-0.81,-0.17,0.48 4ANN,LYS 180,10,44,-0,06,0,0 1NIJ,LYS_254,10.26,-0.36,0,0.12 1CBY,GLU_112,4.77,0.2,0,0.06 3V4G,ARG_22,13.28,-0.38,0.72,0.44 2A0J,GLU 18,4.36,0.14,-0.01,-0.27 3M70,ARG 199,12.24,-0.48,0,0.22 2PGE,TYR_351,12.77,0,0.48,2.3 2FL7,LYS_202,10.44,-0.06,0,0 1R3F.GLU 235.4.77.0.27.0.0 1ZHV.CYS 65,12,51,-0.03,0,3,54 3K8U,CYS_17,12.66,-0.83,0.45,4.04 2OJQ,LYS_638,10.53,-0.15,0,0.18 10IS,TYR_270,11.02,0,0.17,0.85 3LD1,LYS 335,10.14,-0.2,0,-0.15 2AXO,ARG 106,13.53,-0.35,0.95,0.43 1J74,ASP_99,3.56,-0.46,-0.38,0.6 2QEV,GLU_20,3.98,0.47,-0.66,-0.33 3TMO.CYS 247,10.67,0.0.28,1.39 3FHELYS 6.10.58.-0.23.0.0.31 200K,HIS_264,6.4,-0.22,0,0.12 2FGG,ASP_46,4.11,-0.05,-0.08,0.44 1ANU,ASP_133,3.88,-0.8,-0.03,0.92 2Q12,LYS 63,10.54,-0.11,0,0.15 3H5T,HIS_143,4.55,-1.95,0.09,-0.1 3TIR,ARG_100,12.02,-0.3,0,-0.18 1UJ8,TYR_30,10.52,0,0.08,0.44 2P5D,TYR_72,10.02,-0.85,-0.45,1.32 4ACJ,ASP 698,3.99,0,-0.08,0.27 1BGF,LYS_73,10.46,-0.04,0,0 1X04,HIS_125,6.85,-0.35,0.68,0.02 1J74,LYS_66,10.25,-0.26,0,0.01 3GMS,ARG 287,12.29,-0.36,0,0.16 2FZP.GLU 245,4,5,0.85,-0.57,-0.28 1ZCU,ASP_129,3.98,0,-0.07,0.25 1XKR,GLU_104,4.59,0.06,0,0.03 3CAN, ARG_127, 13.83, -0.47, 1.14, 0.67 10QE,GLU 237,3.9,0.61,-0.85,-0.35 1DUP,ASP_6,3.82,0,-0.17,0.19 2IF4,GLU 102,4.86,1.95,-0.82,-0.77 10TM,LYS_102,10.56,-0.41,0.16,0.3 2RIS,LYS 186,10.34,-0.18,0,0.02 3BB7,ASP_248,4.87,0,0.16,0.9 1YLN,HIS_64,6.23,-0.24,0.1,-0.13 3EVN,ARG_25,12.19,-0.57,0,0.27 2IIA,TYR_51,11.41,0,0.02,1.38 3N2T,GLU 254,5.23,0.46,0,0.27 1UOH,GLU 186,4,47,0,27,0,-0,3 2YLF,GLU_127,4.22,0.41,-0.74,0.06 2NRK,CYS_31,10.54,-0.15,-0.21,1.89 10I7,TYR_53,10.75,0,0.03,0.73 4E9E,TYR 566,13,15,0,0,35,2,81 1EW4,GLU_85,4.85,0.28,0,0.07 2Z0M,ARG 255,11.87,-0.65,0.0.02 3BB7.LYS 146.10.46.-0.04.0.0 2B78,HIS 283,6.36,-0.14,0,0 3CAX,LYS 223,10.7,-0.23,0.11,0.32 3CIV,GLU_81,4.6,0.18,0,-0.08 3EVZ,GLU_82,3.02,1.45,-2.51,-0.42 1JYH,LYS_6,10.77,-0.18,0,0.46 2PLQ,HIS_281,6.15,-0.58,0.36,-0.13 3LJI,GLU 261,4.65,0.15,0,0 4EUG,HIS 67.6.44,-0.52,0.33,0.12 3CJW,GLU_225,4.46,1.08,-0.81,-0.3

1X9G,LYS_147,10.4,-0.1,0,0 4E9E,GLU 533,3.39,0.5,-1.53,-0.08 3L7N,ASP_196,3.76,-0.26,0,0.22 2RIS,ARG_177,12.7,-0.29,0,0.48 2DFL,LYS_289,10.02,-0.28,0,-0.2 3CXS,ASP 83,4,22,-0.05,-0.52,0.99 1RI5.ARG 162.11.76.-0.83.0.0.1 1TR9,GLU_232,4.27,0.41,-0.57,-0.08 1PSW,ASP_150,3.6,-0.39,-0.38,0.57 1NKD,LYS_3,10.41,-0.09,0,0 2WB8,LYS 727,10,42,-0,1,0,0,01 2X4G,ARG_44,12.11,-0.39,0,0.01 3EUR,CYS_40,8.13,-1.52,0,0.65 3HQX,TYR_18,10.32,0,0.07,0.24 3NBI,GLU_200,4.7,0.27,0,-0.07 2BCF,GLU 82,3.86,0.52,-0.85,-0.31 3CSR.TYR 153,10,21,0,-0,18,0,39 2D2S,LYS_721,10.44,-0.06,0,0 2FZ4,TYR_87,10.56,0,0.41,0.15 20GO,ARG 584,12,42,-0,34,0.02,0.24 1VSM,ASP 165,2.87,-0.64,-0.69,0.4 1XEU,LYS_162,10.06,-0.38,0,-0.06 4E8B,GLU_203,3.76,1.37,-2,-0.12 1PVT.LYS 176.11.75.-0.48.0.68.1.06 2FC3,ASP 56,3.33,-1.1,-0.49,1.11 3ONT,LYS_64,10.47,-0.42,0,0.38 2CW4,GLU_116,5.6,1.1,0,0 2YX0, ARG_70, 11.97, -0.87, 0, 0.34 2NMU,CYS_128,7.67,-2.01,0.17,0.5 10I7,GLU_196,3.5,0.28,-0.8,-0.47 3G9G,ASP_197,3.93,0,-0.15,0.28 2EFK.ASP 26,2.98,-1.6,-0.47,1.25 2CXY,LYS_67,10.37,-0.13,0,0 2A4D,TYR 189,10.19,0,-0.16,0.35 1AK1.TYR 253.13.93.-0.85.1.2.3.59 1T95,ARG_238,13.08,-0.37,0.52,0.44 2YWJ,ARG_31,12.42,-0.47,0,0.39 1AK1,ASP_228,3.95,0,-0.13,0.28 3G6S,LYS 235,11.13,-0.82,0.62,0.84 1X9G,HIS_7,6.58,-0.79,0.63,0.24 2Q07,TYR_272,10.79,-0.63,0.01,1.4 2FL7,ARG_195,12.69,-0.37,0,0.56 10IS,GLU 335,3.12,0.54,-1.5,-0.42 3CGW.GLU 185.4.49.0.59.-0.35.-0.24 3M9A,LYS_97,10.58,-0.12,0,0.21 3MTT,ARG_587,12.36,-0.14,0,0 3ETU,TYR_82,9.96,-0.85,0.27,0.54 1XAW,ASP_479,2.85,-0.92,-0.38,0.35 3K1H,ASP_66,3.97,0,-0.01,0.19 3QAV,ARG_55,12.54,-0.1,0,0.14 3P2F,ASP_50,2.52,-1.32,-0.35,0.39 2P0Y,ARG_214,12.41,-0.21,0,0.12 2AD1.ASP 278.3.41,-0.85,-0.76,1.22 4H4J,CYS_63,11.45,-0.58,0.75,2.27 1H09,TYR_287,11.11,0,0.37,0.74 3GV0,GLU_319,4.77,0.29,0,-0.02 2ZQ5,GLU_375,3.81,0.29,-0.79,-0.2 3GG6.GLU 110.4.65.0.2.0.-0.05 2R57,CYS_288,9.17,-0.08,0,0.26 3T57,GLU_147,4.76,0.49,-0.03,-0.19 1JSX,HIS_110,6.45,-0.15,0,0.11 1V43.GLU 297.3.69.0.42.-0.76.-0.47 2QHT,GLU_26,3.76,0.34,-0.72,-0.35 3L3P,ASP_388,3.41,-0.56,-0.22,0.4 3FK5,CYS_123,12.07,-0.2,0.15,3.13 1J85,ARG_43,13.16,-0.24,0.53,0.37 2RJD.LYS 408.10.35.-0.26.0.0.11 1MTZ,ASP_73,2.59,-1.34,-0.13,0.26 1MHN,LYS_93,10.86,-0.15,0.17,0.34

1ZCU.ARG 116.12.03.-0.52.0.0.04 10LR/CYS 216,13.03,-0.37,0.37,4.03 3GEC,LYS_512,10.24,-0.49,0,0.23 3JRT,ASP_20,4.14,0,-0.11,0.45 2007.LYS 432.10.38.-0.13.0.0.01 1AK1.ARG 128.12.4.-1.23.0.4.0.72 2F8H,ASP_205,4.05,0,0,0.25 2012.LYS 172.10.4,-0.1.0.0 3G6S,ARG_214,12.94,-0.37,0.3,0.52 1RKA,LYS_215,11.39,-0.39,0.85,0.43 2F4O,ARG 74,12,46,-0,16,0,0,12 2R51,LYS_23,10.11,-0.29,0,-0.11 4AM1,GLU_87,4.85,0.37,0,-0.02 2FXT,ARG 272,12.23,-0.27,0.0 2F8H.ARG 174.12.96.-0.34.0.59.0.21 3VHJ,TYR_16,10.85,0,0,0.85 1EDG,ASP_92,3.36,-0.59,-0.19,0.34 3ADO,TYR_200,10.4,0,0.13,0.27 3TRE,HIS_83,6.13,-0.6,0,0.23 20ZO.LYS 78,10,18,-0,54,0,0,22 2YLF,GLU_122,4.96,1.31,-0.61,-0.24 2YT4,TYR_530,12.23,0,0.07,2.15 2WOZ,HIS 493,5.68,-1.57,0.85,-0.1 1059.GLU 255.4.7.0.29.0.-0.09 1TJE,ASP_54,3.36,-0.67,-0.19,0.41 3N2T,ASP_310,3.69,-0.66,-0.51,1.06 1BN6,ASP_277,3.53,-0.73,0,0.47 3T8R,LYS 20,10.29,-0.26,0,0.05 2Q5X,ARG_840,12.59,-0.16,0,0.25 1VSM,LYS_191,10.47,-0.33,0,0.3 3FS3,LYS_51,10.88,-0.17,0.17,0.38 4DIU,TYR_137,11.11,0,0.2,0.91 2F9F,ARG 162,13.23,-0.28,0.53.0.48 3HYO,LYS 149,10,15,-0,16,0,-0,19 3LJC,LYS_218,10.21,-0.22,0,-0.07 4AF2,ASP_57,3.4,-0.47,-0.38,0.45 2F8H,ASP_149,3.98,0,-0.13,0.32 3B21,CYS_70,12.69,0,0,3.69 3V55,LYS_557,10.6,-0.3,0,0.41 2BAA, TYR 125, 12.79, -0.82, -0.55, 4.17 2EFK,ASP_218,3.53,-0.3,-0.26,0.28 1DUP,ASP 32,3.94,-0.05,-0.66,0.86 2VAN, ASP 321, 4, 27, 0, 0, 16, 0, 32 3RE9,GLU_242,4.54,0.04,0,0 3ZXY,ASP_92,2.65,-1.23,-0.32,0.41 1L2F,LYS_274,10.74,-0.42,0.26,0.4 1XIP,TYR_277,13.95,0,1.33,2.62 1DVO,ARG_122,12.16,-0.36,0,0.02 1JYH,ASP_53,2.28,-1.8,-0.42,0.71 2A6B,HIS_137,6.11,-1.04,0.61,0.04 3PBH,TYR 151,12.24,-0.18,-0.44,2.85 2P0Y,ASP 127,3.92,0,-0.07,0.2 4ESS,LYS_40,11.58,-0.61,1.06,0.63 1ZBP,TYR_116,10.37,0,0,0.37 4DND,ARG_55,12.22,-0.27,0,-0.01 1KCM,TYR_190,10.34,0,0.06,0.28 1SNT,ARG_172,12.17,-0.64,0,0.31 1LZL,GLU_176,4.64,0.23,0,-0.09 3Q1C,CYS_279,10.25,0,-0.07,1.33 2E3S,LYS 402,10.96,-0.22,0,0.68 2|6|,LYS 155,10,42,-0,08,0,0 4ETX,ARG_207,12.54,-0.34,0,0.37 4DIU,GLU_149,3.31,0.37,-1.1,-0.47 1PVT,GLU_216,4.73,0.33,0,-0.1 3DSH,LYS_299,10.78,-0.16,0.05,0.38 3PU6,ARG 13,12.31,-0.27,0,0.09 3MIX,LYS_520,10.42,-0.23,0,0.15 2Q12,ASP_29,3.17,-0.81,-0.24,0.41 3IV4,ASP_48,3.95,0,-0.03,0.18

1XKR,GLU_89,4.12,0.27,-0.44,-0.2 3LMF.GLU 54.4.67.0.17.0.0 2V81,CYS_170,11.66,-0.02,-0.11,2.8 1V43,ARG_138,12.26,-0.27,0,0.04 4ETX,ARG 423,12.07,-0.29,0,-0.14 2AHE.ASP 152.4.16.-1.24.0.03.1.57 20V2.TYR 189.10.23.0.-0.02.0.25 3M7D,GLU_89,4.55,0.23,0,-0.17 1M5I,ARG_141,13.27,-0.3,0.74,0.33 3B21,CYS_212,8.62,-0.81,-0.13,0.57 3Q1C,GLU_47,4.86,0.24,-0.01,0.14 2Y2T,CYS_29,9.59,-0.19,0.17,0.61 1RAJ,HIS 413,6.61,-0.6,0.78,-0.07 2H14,LYS_207,9.93,-0.65,0,0.08 4DEZ,ARG_20,11.75,-0.8,0,0.05 1MUF.GLU 151.4.84.0.3.0.0.05 1FO9,TYR_228,11.43,0,0.15,1.28 1P1L,CYS_30,9.37,-0.21,-0.36,0.94 3CS1,LYS_79,10.31,-0.24,0,0.05 2FL4,GLU 138,5.62,1.29,-0.55,0.38 1X9G,HIS_110,6.21,-0.98,0,0.69 2R57,ARG_234,10.2,-2.94,0,0.64 3ILC,LYS_87,10.62,-0.43,0.03,0.51 2FZ4.ARG 55,13.11,-0.78,0.68,0.71 4AF2,ARG 93,13.08,-0.36,0.47,0.47 1TXJ,LYS_116,10.5,-0.28,0,0.27 2CL3,ARG_68,12.26,-0.32,0,0.08 3AU3,GLU_484,3.97,0.9,-1.43,0 3R2E,LYS 40,11.31,-0.34,0.62,0.52 3AU3,LYS_534,10.5,-0.15,0,0.15 1X7F,ARG_168,13.46,-0.52,0.82,0.67 4F3J,ASP_224,3.94,0,-0.44,0.58 1FHL,TYR_214,13.75,0,0.35,3.4 3H8Y.GLU 87.4.6.0.1.0.0 1QQE,LYS_186,10.43,-0.07,0,0 1WLY,LYS_114,10.51,-0.08,0,0.09 2RH3,ARG_117,12.29,-0.19,0,-0.02 1PV5,GLU 167,5.04,0.24,0,0.29 1WRU,CYS_64,13.75,0.34,0.85,3.56 3B79,GLU_97,3.51,0.26,-1.25,0 2B78,GLU_178,4.88,4.55,-1.68,-2.49 4E6S.CYS 34,9.88,0,-0.08,0.96 3JRT,LYS 45,10.34,-0.22,0.0.07 3ADO,LYS_54,10.41,-0.3,0,0.21 1YG2,ARG_93,12.4,-0.1,0,0 1Y0K,ARG_170,13.94,-1.14,1.59,0.98 4HDE,CYS_73,13.16,0.58,1.18,2.42 1WXO,LYS 347,9.64,-0.75,0,-0.11 3B21,ASP_40,4.06,0,0.03,0.23 1JYH,GLU 132,6.37,3.66,-1.8,0 2099,ARG 366,13,17,-0,49,0,81,0,36 2D7J,LYS 98,10.52,-0.25,0,0.27 2QOP,CYS_117,10.81,-0.48,0.12,2.18 105T.TYR 329,10.3,-0.95,-0.52,1.77 1UCH,LYS_74,11.26,-0.45,0.8,0.4 2B6P,TYR_89,11.79,-0.81,0.15,2.46 3ELI,ASP 89,4,2,0,0,25,0,15 1NFN,ARG_92,12.84,-0.2,0.23,0.32 1TP6,TYR_118,10.69,0.22,0.12,0.35 1XFK,HIS 184,4.87,-1.33,0,-0.3 3ANJ,TYR 222,10.25,0,0.01,0.24 3GYW,LYS_45,10.37,-0.13,0,0 2DG7,GLU_53,4,1.23,-0.9,-0.83 3BQE,CYS_349,9.89,-0.71,0.04,1.55 3CIV,CYS_98,11.06,0,0.21,1.86 3F7M,ASP_202,1.74,-2.02,-0.82,0.78 1T95,GLU_169,3.74,0.41,-0.92,-0.25 2IF4,LYS 165,10.45,-0.05,0,0 1AD6,LYS_475,10.49,-0.06,0,0.05

3RVC,ASP_139,3.91,-0.07,0,0.19 3EVZ,LYS_185,10.68,-0.57,0.27,0.48 2EEY,LYS_82,10.33,-0.19,0,0.02 4F85,ARG 147,12,79,-0.3,0,13,0,46 3V3T,TYR_238,12.98,0,0.29,2.69 1UOH,TYR_199,11.68,0.79,0.38,0.51 4DBX,TYR 186,11.06,-0.07,0.24,0.9 2D0A, ARG_182, 13.62, -0.85, 1.4, 0.57 1GXN,ARG_413,13.57,-0.42,0.6,0.88 3NBI,LYS_183,10.29,-0.63,0,0.42 2E3I,LYS 115,11.45,-0.34,0.78,0.51 1059,LYS 305,10,25,-0,25,0,0 2NYC,ARG_219,12.26,-0.24,0,0 2B0J,ASP_164,2.94,-0.7,-0.43,0.28 4H4J.LYS 251.10.4.-0.13.0.0.04 1KCM,ASP 107.3.75.0.-0.4.0.35 3LPZ,ASP_213,3.51,-0.36,-0.3,0.37 3T57,CYS_138,10.84,-0.28,-0.12,2.24 1EDG,TYR_325,11.58,-0.06,-0.09,1.72 3I47,TYR 175,10.2,0,0.06,0.15 3AU3.CYS 447.10.84.0.0.14.1.69 1MML.LYS 258,10,79,-0,22,0,0,51 2HP7,GLU_147,3.26,0.82,-1.69,-0.38 3BB7.LYS 205.10.6.-0.24.0.0.33 3EVP.LYS 284.10.48.-0.26.0.0.24 2BCF,ARG_114,12.45,-0.44,0,0.39 2AZL,LYS_34,10.8,-0.43,0.3,0.43 2IN0,GLU_434,5.5,2.28,-0.76,-0.51 3IL3,GLU 74,4.86,0.69,-0.04,-0.28 2YWX,ARG 32,12,4,-0,43,0,0,33 1X1E,ASP_233,3.31,-1.75,0,1.26 1ZBS,HIS_239,5.17,-1.33,0,0 3G9T,ASP_242,3.65,-0.95,-0.21,1.01 3D9H,ASP_133,3.41,-0.57,-0.3,0.48 3JZN,ARG_287,12.49,-0.37,0,0.36 1RWZ,ARG_222,13.43,-1.17,1.41,0.69 2H8O,HIS_143,5.95,-1.08,0.01,0.51 4DEZ,ASP_84,3.91,-0.21,0,0.32 4AM1.LYS 42.11.3.-0.41.0.85.0.36 2IN0,GLU_86,4.37,0.24,-0.07,-0.29 1SIG,LYS_220,10.51,-0.56,0,0.57 4F3J.TYR 218.10.31.-0.11.0.0.41 1TR9,HIS 161,4.72,-2.6,0.85,-0.02 3M3P,ASP_202,3.25,-0.82,-0.03,0.31 2F8H,HIS_51,5.41,-1.34,0,0.25 1IAP,LYS_90,10.43,-0.08,0,0.01 3I0C,GLU_215,5.09,0.85,0,-0.25 2AZP,ASP_126,1.51,-2.04,-0.82,0.57 4EKU,GLU_342,5.55,2.01,0,-0.97 3GW3.CYS 308.9.85,-0.25.0.46.0.64 3LPZ,ASP_299,3.95,-0.15,0,0.3 1DVO,LYS 118,10.16,-0.1,0,-0.25 1XTZ,ASP 176,3.22,-0.78,-0.38,0.57 3LH5,LYS_553,10.35,-0.15,0,0 3G9G,ASP_66,3.18,-0.68,-0.37,0.43 4F85,ARG_149,12.22,-0.28,0,0 2O4D,ARG_135,12.12,-0.38,0,0 1RL0,ARG_60,12.33,-0.29,0,0.12 2012.ASP 49.3.33.-0.51.-0.38.0.42 3MIX,ASP_416,3.49,-0.39,-0.13,0.22 2P5D,GLU 98,4.53,0.38,0,-0.35 2YT4.CYS 535.8.79.-0.78.0.12.0.44 3E5T,HIS_216,5.88,-0.57,0,-0.07 1EV8,ARG_53,12.18,-0.33,0,0.01 1VJG,LYS_6,10.59,-0.22,0,0.32 4E8B,LYS_118,10.51,-0.13,0,0.14 3E5T,ASP_223,3.78,0,-0.21,0.19 20BI.CYS 75,10.99,-1.13,0.27,2.83 1G8P,GLU_157,3.6,0.26,-0.85,-0.3

1T95,ARG_63,13.17,-0.15,0.48,0.34 2H8O, ARG 187, 12.32, -0.18, 0, 0 3PZ9,ARG 160,13,2,-0,36,0,65,0,41 3KEY,GLU_394,3.9,0.45,-0.71,-0.34 1Z3X,ASP_180,3.94,0,-0.09,0.23 3ETV.TYR 93,11.5,-0.68,0.22,1.95 2P4D.ASP 61.3.46.-0.4.-0.14.0.19 4FD6,LYS_38,11.53,-0.53,0.85,0.72 1TLV,ASP_113,3.75,0,-0.22,0.17 2FG1,LYS_55,10.46,-0.11,0,0.07 1Q46,LYS_66,9.82,-0.33,0,-0.35 3BPP.TYR 25,10.87,0.28,-0.22,0.81 3EJC,CYS_142,12.07,0,0.19,2.88 2O34,LYS 63,10,-0,48,0,-0.01 1V43,ASP_83,3.79,0,-0.37,0.34 2YWX,LYS 142,10.72,-0.18,0.24,0.15 1AD6.GLU 466.4.7.0.11.0.0.09 3BA1,ARG_117,12.35,-0.2,0,0.05 3CXS,ASP_91,4.18,0,-0.15,0.53 3U4K,ASP_43,3.8,-0.08,-0.06,0.13 2QV2,ARG_11,12.53,-0.08,0,0.1 4FH3,ARG_351,11.69,-0.72,0,-0.08 3AU3.HIS 492.6.37.-0.18.0.06.-0.01 3OKO,LYS 602,10,31,-0.22,0,0.03 3JV1,ASP 82,3.1,-0.48,-0.54,0.33 3ERF.GLU 150.4.55.0.11.0.-0.06 2ZCO,HIS_92,5.25,-0.86,0,-0.4 1EYH,LYS_117,10.62,-0.19,0,0.32 3CIV,CYS_254,8.73,-1.01,0.15,0.6 10TM,LYS_143,10.16,-0.29,0,-0.05 3LJC,LYS_223,10.42,-0.08,0,0 3RNV,LYS 393,11.38,-0.43,0.85,0.46 1WXQ,LYS_346,9.72,-0.7,0,-0.08 4FCU,HIS 3,6.83,-2.15,1.7,0.78 4F3J.TYR 152.10.27.0.0.0.27 2R4Q,LYS_234,10.23,-0.37,0,0.1 1XKR,GLU_158,5.63,0.32,0.25,0.58 1DZF,GLU_85,4.76,0.22,0,0.04 2AZL,ARG 88,12.85,-0.39,0.45,0.29 1VJG,HIS_73,6.2,-0.34,0,0.04 2E3C,LYS 293,10,47,-0,03,0,0 3PM2,GLU_115,3.66,0.41,-0.51,-0.74 2H14,LYS 227,11.16,-0.19,0.35,0.5 3ZTA, ASP 47, 3, 97, -1, 39, -0, 25, 1, 82 4H89,ARG_79,12.3,-0.2,0,0 1AD6,GLU_428,4.69,0.27,0,-0.08 1X9G,LYS_125,9.78,-0.89,0,0.18 2Z0M,LYS 32,10.43,-0.29,0,0.22 3I47,ASP_224,3.28,-0.93,0,0.41 3KT2,HIS_69,5.6,-0.94,0,0.04 1BGF,LYS_93,10.46,-0.37,0,0.33 1KCM,LYS_50,10.19,-0.42,0,0.11 3FFM,ASP 89,3.93,0,-0.07,0.2 3GV0,LYS_310,11.25,-0.31,0.72,0.33 2R0S,TYR_94,10.02,0,-0.04,0.06 1R7J,ASP_46,3.74,0,-0.38,0.32 2EFK,ARG_199,12.36,-0.13,0,-0.02 1V43.GLU 133.4.2.0.39.-0.65.-0.04 2BLL,HIS_379,4.71,-1.6,0,-0.19 2ZQ5,GLU_259,4.31,0.63,-0.74,-0.08 2JHY,TYR_128,12.51,-1.76,0.06,4.21 3TRE,LYS 108,10,35,-0,37,0,0,22 1U7U,GLU_258,5.13,0.69,0,-0.06 3LH5,TYR_588,10.12,0,0,0.12 3K8J,TYR_128,10.71,-0.85,0.23,1.32 1T07,ARG_53,12.31,-0.33,0,0.13 1R7J,ARG 51,13,17,-0.33,0.61,0.39 1X9G,GLU_97,4.66,0.18,0,-0.02 2A6B,HIS_31,6.11,-1.68,0.85,0.45

3M7GLYS 116.10.23.-0.78.0.1.0.4 4FCU,HIS 132.6.31,-0.26.0.0.06 2E0T,LYS_183,10.36,-0.13,0,-0.01 3EJC,LYS_48,10.31,-0.19,0,0 1H4U,HIS 536,7.26,-0.39,0.85,0.3 2D59.LYS 119.11.3.-0.38.0.72.0.47 2QVO,LYS_69,10.32,-1.11,0.19,0.73 3EYE, ASP_104, 3.55, -0.8, -0.19, 0.74 2WOZ,GLU_395,5.89,1.96,-0.86,0.3 3M7D.HIS 260.7.18.-0.84.0.85.0.68 20JO,ASP 467,3.86,-0.1,-0.25,0.41 1XDZ,LYS_202,11.49,-0.36,0.85,0.5 3EVZ,TYR_178,9.35,-0.37,-0.54,0.26 3DTE,ASP_106,3.44,-0.47,0,0.11 3K9I.LYS 157.11.09.-0.27.0.45.0.41 1Q8B,LYS_76,10.58,-0.12,0,0.2 3OKQ,LYS_641,11.34,-0.27,0.73,0.38 3BCY,HIS_46,6.37,-0.34,0,0.22 3B4D,LYS 213,10.61,-0.12,0,0.23 1EDG.LYS 373,10.63,-0.26,0.0.38 2CW4,TYR_16,10.08,-0.51,-0.01,0.6 1XTD,LYS_150,10.38,-0.12,0,0 1ZBM,HIS_-1,6.68,-0.25,0.32,0.12 3GYW,GLU 61,4.72,0.27,0,-0.05 3EVN,ARG_7,12.5,-0.51,0,0.51 1YR6,GLU_92,5.01,1.84,-0.83,-0.49 3HUE, ASP_213, 3.91, 0, -0.04, 0.15 3H04,LYS 137,11.43,-0.3,0.47,0.76 3Q2C,HIS_36,5.68,-0.83,0,0.01 1R5Q,TYR_96,9.92,-0.58,0.04,0.46 4DND,ASP_84,4.06,0,-0.05,0.31 3ANJ,ARG_22,12.94,-0.31,0.62,0.12 1UXO,LYS 127,10.64,-0.19,0,0.34 2YWJ.ASP 39.3.1.-0.84.-0.24.0.38 2Q13,LYS_70,10.23,-0.26,0,-0.02 1TR9,TYR_213,9.84,-1.15,0.07,0.92 2HXB,HIS_128,6.39,-1.28,0.64,0.52 1RHS,GLU_165,3.31,0.44,-1.25,-0.38 3ETU,ASP_174,3.53,-0.47,-0.25,0.45 1P6F.GLU 83,4,46,0,12,0,-0,16 3BA1,ARG_127,13.98,-0.16,1.26,0.38 3T5B,ASP 135,3.93,0,-0.03,0.15 105J,LYS 61,10.37,-0.62,0.0.49 1X04,GLU_104,4.66,0.3,0,-0.15 3C6B,TYR_119,11.22,0,0.12,1.09 2F8H,ARG_95,12.23,-0.47,0,0.19 2YYO, ARG_91, 12.37, -0.13, 0, 0 1WXF,ARG_263,13.12,-0.41,0.39,0.65 3UAH,HIS_228,5.33,-1.18,0,0.01 3E5T,HIS_118,5.86,-0.75,0,0.12 1EV8,LYS_235,10.62,-0.29,0,0.42 3U0V.HIS 138,4.77,-1.58,0,-0.15 1TD6,ARG_66,13.01,-0.33,0.38,0.46 3M66,GLU_292,4.48,0.14,0,-0.16 1PNE, ASP_54, 1.66, -2.43, -0.13, 0.41 3U2A,GLU 33,4.62,0.12,0,0 1UAJ,ARG_220,12.49,-0.17,0,0.16 3MIX,ASP_609,3.85,0,-0.08,0.13 2G2D,ASP_40,4.08,0,0.03,0.25 1XIP,LYS 81,10.47,-0.15,0,0.12 3RJZ,ARG 84,12.66,-0.22,0,0.38 1TD6,GLU_221,4.79,0.4,0,-0.11 3LD1,LYS_78,11.44,-0.29,0.85,0.38 4H4J,ARG_122,13.04,-0.66,0.63,0.57 2CL3,HIS_87,6.49,-1.03,0.85,0.15 2ZCX,ARG_208,12.24,-0.26,0,0 3AU3,TYR_486,11.32,0,0.5,0.83 1FQI,GLU_302,4.62,0.33,0,-0.21 3E5T,LYS_25,10.72,-0.23,0,0.45

3H5T,ARG_32,12.24,-0.26,0,0 1FKM,ARG 329,12,43,-0.07,0.0 2OGQ,ARG_396,12.71,-0.3,0,0.51 4F85,CYS_129,11.1,-0.29,0.13,2.26 1WYC,ARG_99,12.96,-0.58,0.51,0.53 1P4X.GLU 16.5.21.2.36.-0.69.-0.97 2Z61.TYR 185.10.47.0.-0.01.0.49 3F6F,GLU_185,3.62,0.64,-0.85,-0.67 1TLV,ARG_252,12.42,-0.15,0,0.07 1MTZ,TYR_170,10.99,-1.64,0.27,2.36 3T5B,ARG_221,12.09,-0.5,0,0.1 3EZ7,LYS_240,9.43,-1.21,0,0.14 20KT.HIS 339.6.53,-0.22.0.26.0 1X7F,GLU_342,4.65,0.11,0,0.04 3D9H,ARG 180,13.3.-0.32,0.73,0.39 2CXA.GLU 176.3.71.0.86.-0.89.-0.76 3FTT,TYR_71,12.44,-0.15,0.37,2.22 2NRK,ARG_122,10.97,-1.15,0,-0.37 3T8R,GLU_91,4.54,0.04,0,0 4H4J,GLU 160,4.36,0.14,0,-0.27 1SNT,ARG_314,12.26,-0.27,0,0.03 3P51,ASP_103,3.23,-1.07,0.03,0.47 3M66,HIS_172,6.15,-0.47,0.18,-0.05 1LN4.HIS 10,6.08,-0.47,0.05,0 3LJN,LYS 19,10,44,-0.23,0,0,17 1IAP,ARG_183,12.35,-0.42,0,0.27 1A8Q,GLU_150,3.48,0.48,-1.44,-0.06 3CCY,TYR_49,10.29,0,-0.1,0.39 1ZCE,ARG_119,12.4,-0.1,0,0 1HF8,ARG_261,12.41,-0.33,0,0.25 1T07,LYS_37,10.53,-0.27,0,0.3 4DEZ,ARG_69,12.2,-0.23,0,-0.07 1ZYL,ARG 40,12.54,-0.64,0.03,0.65 1TD6.GLU 68.5.88.1.5.0.-0.11 1RKA,LYS_154,11.25,-0.27,0.65,0.38 3GS9,TYR_160,13.73,0.06,1.02,2.64 3CO1,LYS_98,10.6,-0.18,0,0.28 1QYI,LYS 64,10.26,-0.23,0,-0.01 2GZQ,TYR_69,10.11,0,-0.17,0.28 1NRI,TYR_226,10.81,0.31,0.33,0.17 1DUP,HIS_76,6.26,-0.15,0,-0.09 2GOV.TYR 69.11.1.0.0.02.1.09 3T5B,ARG 244,12.81,-0.21,0,0.51 3GE9,ARG_190,12.8,-0.29,0.3,0.29 1ILW,GLU_63,4.93,0.4,0,0.03 2IF4,CYS_253,11.29,-0.02,-0.55,2.85 1GXN,LYS_485,10.4,-0.12,0,0.02 3P28,ARG 74,13,71,-0.5,1.02,0.69 2G2D,TYR_107,11.36,0,0.18,1.19 3V55,LYS_466,10.01,-0.69,0,0.2 2H2Z.CYS 16.11.83.0.0.02.2.81 1TWU.TYR 103,10.89,-0.55,-0.05,1.48 3P28,LYS_78,10.52,-0.18,0,0.2 4F8A,GLU_596,4.85,0.44,0,-0.09 1TJE,LYS_137,11.35,-0.27,0.74,0.38 3ASA,ARG_244,12.38,-0.15,0,0.03 2CBE.ASP 165.3.69.0.-0.32.0.21 2WB8,ASP_709,4.1,0,0.13,0.17 106D,CYS_30,11.53,0,-0.09,2.63 1X1E,ARG_212,13.82,-0.28,1.03,0.56 1SFE.GLU 73.4.7.0.34.0.-0.14 4FLE,TYR_124,10.21,0,0.11,0.1 3B4D,ASP_233,3.36,-0.82,-0.07,0.45 3RRQ,GLU_141,3.64,0.41,-0.89,-0.38 20PJ,GLU_151,4.73,0.17,0,0.06 109G,ARG_215,12.85,-0.59,0.36,0.58 1WP5,GLU_225,4.67,0.32,0,-0.15 2H2W,TYR 240,9.95,-0.01,-0.37,0.32 4DIU,ASP_198,2.53,-1.69,-0.05,0.47

2X5Y.GLU 795.4.52.0.14.0.-0.12 2NRR,ARG_410,13,-0.29,0.31,0.49 4DNU,GLU_375,4.85,0.15,0,0.21 3RFY,LYS 158,10,43,-0.07,0,0 2CL3,ARG_221,12.05,-0.65,0,0.19 3LMO,GLU 58,4,56,0.09,0,-0.03 2W2S,LYS_176,10.07,-0.43,0,0 4FLE,ASP_102,4.03,0,0.01,0.22 1R3F,GLU_171,3.95,0.91,-0.94,-0.51 1PSW,ASP_293,3.71,-0.26,-0.11,0.28 2Z84,TYR 41,11.58,-0.74,0.86,1.47 2FBI,GLU_134,4.69,0.19,0,0 3BPV,ARG_95,12.85,-0.15,0.02,0.48 1V8E,GLU_176,4.6,0.1,0,0 4GCO,TYR 166,12.02,-0.51,0.25,2.29 3CBN.ARG 91,12.9,-0.42,0.38,0.43 1R29,GLU_99,3.85,0.24,-0.76,-0.13 3DSH,ASP_430,3.93,0,0,0.13 3RFY,ARG_393,12.23,-0.27,0,0 2F4Q,ASP 296,4.53,0,0.02,0.7 3EAZ,GLU_90,3.82,0.24,-0.71,-0.21 1TR9.GLU 180.3.82.0.5.-0.85.-0.32 1SNT,HIS_132,5.88,-0.43,0,-0.19 1UOH,LYS 189,10.54,-0.19,0.0.23 2DFLLYS 163.10.45.-0.11.0.0.06 3A0X,CYS_721,11.65,-0.29,0,2.95 2F4Q,TYR_51,10.44,0,-0.01,0.45 2A0J,ARG_84,13.3,-0.29,0.32,0.78 3UAH,ASP_200,3.04,-0.98,-0.16,0.39 3CN5,CYS_132,9.56,-0.08,0,0.63 3JV1,ARG_149,12.03,-1.04,0.07,0.5 1U3Y,LYS_249,10.41,-0.3,0,0.2 3RKV,GLU_209,4.51,0.35,-0.64,0.31 3BOW.LYS 90,10.21,-0.38,0,0.09 4DIU,LYS_230,10.91,-0.39,0.42,0.38 3CXS,HIS_34,6.33,-0.21,0,0.04 1NWA,ARG_-1,12.45,-0.05,0,0 1RI6,GLU_176,4.73,0.09,0,0.14 3ADO,LYS 104,10.38,-0.12,0,0 3C5V,GLU_239,4.56,0.07,0,-0.02 3CAN,LYS_86,10.33,-0.22,0,0.05 2ZCX,HIS 200.6.31,-0.1,0,-0.09 1R9W,ASP_228,3.9,0,-0.26,0.36 3K8J,LYS_91,10.39,-0.11,0,0 4E9E,LYS 480,10.87,-0.15,0.18,0.34 3GEC,ARG_394,12.01,-0.57,0,0.07 1NJ4,ASP 337,3.44,-0.41,-0.48,0.53 3AU3,HIS_464,6.39,-0.29,0.01,0.17 2OBI,LYS_151,11.48,-0.46,0.85,0.59 4E8B,ARG_190,12.88,-1.84,1.5,0.73 2F8H,ASP_229,3.71,-0.14,-0.19,0.23 1TWU,ASP_23,4.01,0,0,0.21 2A1V,LYS 126,10,45,-0.05,0,0 2PWQ,GLU_21,3.78,0.49,-0.8,-0.41 2ZQ5,TYR_317,9.95,-0.06,-0.38,0.39 2F4Q,ASP_82,3.77,-0.01,-0.63,0.6 3M66,LYS_168,11.48,-0.25,0.85,0.38 3O16, ARG_225, 11.85, -0.68, 0, 0.02 1NAF.ARG 299.12.43.-0.07.0.0 1N81,ARG_100,12.71,-3.33,1.62,1.93 4DNU,ASP 380,2.86,-1.1,-0.25,0.42 2AZL.TYR 39,11,76,0,0,35,1,4 2V4U,ARG_425,13.28,-0.36,0.47,0.66 2YWJ,GLU_112,4.01,0.31,-0.85,0.05 2FG1,HIS_114,6.54,-0.45,0.49,0 2BQQ,LYS_140,10.36,-0.1,0,-0.04 2GAU,LYS_39,10.37,-0.13,0,0 1WRU,GLU_171,4.42,0.61,-0.31,-0.38 100X,LYS_220,10.53,-0.6,0,0.64

2CI3,CYS_221,11.24,-1.41,0,3.65 3EGN,LYS 425,10.06,-0.6,0,0.16 2ILR,ARG_290,12.54,-0.15,0,0.19 1X04,ARG_38,13.27,-0.25,0.6,0.42 3RJX,HIS_226,1.43,-3.8,0,-1.27 3OA7, HIS 563, 6, 25, -0, 32, 0, 0, 07 1059.LYS 237.11.49.-0.31.0.85.0.44 300P,LYS_100,10.55,-0.16,0,0.22 3GOZ,CYS_273,10.43,-0.09,0.11,1.41 3AU3,GLU_460,4.54,0.12,0,-0.09 1T3Y,CYS 10,11.37,-0.04,0.13,2.28 2FI9,ASP_19,4.17,0,0.03,0.34 3M70,TYR_249,12.5,-0.81,0.06,3.25 1X04,ASP 147,2,43,-1,48,-0,55,0,67 3RFF.GLU 49.4.92.0.64,-0.36.0.14 2WB8,ASP_592,3.52,-0.55,-0.17,0.44 1J74,GLU_17,4.79,0.36,0,-0.08 2FM9,LYS_146,11.6,-0.22,0.85,0.47 3H13,GLU_241,3.8,0.32,-0.6,-0.42 3I4T,GLU_70,3.63,0.37,-0.85,-0.38 4E8B,ASP 51,4,12,-0,26,0,1,0,49 3RFF,HIS_17,3.83,-2.58,0,-0.09 1ZBM,ASP 133,3.91,0,-0,13,0.24 2NMU/HIS 86,5,96,-0,5,0,-0,04 3T8R,TYR 9,10.13,0,-0.1,0.23 2V4X,LYS 23,10,45,-0,14,0,0,09 3A2Z,HIS_152,5.53,-1.45,0,0.48 1TR9,HIS_142,5.83,-1.37,0.8,-0.1 3F5D,LYS 87,10.25,-0.25,0.0 1PSW,TYR_200,10.57,0,0.02,0.55 3NZL,TYR_73,10.55,-0.05,-0.21,0.82 2HXB,ASP 10.4.14.0.0.05.0.28 4F8A,ARG_702,13.15,-0.51,0.34,0.81 3P51,HIS 25,5.74,-1.02,0.55,-0.29 1IAP.CYS 77,13,4,0,0.68,3,72 1F2V,ASP_26,3.38,-0.5,-0.14,0.23 1ZBM,TYR_232,13.37,-0.34,0.55,3.15 3TMO,GLU_323,3.51,0.28,-0.83,-0.44 2XWS,LYS 99,9.86,-0.79,0,0.16 2FBI,LYS_97,10.48,-0.25,0,0.23 1DTO.GLU 39,4.89,1.5,-0.79,-0.32 1G8P,GLU_176,4.43,0.23,-0.12,-0.18 3GW3,ASP_239,3.56,-0.78,-0.58,1.12 2XJ4,LYS 168,10.66,-0.13,0.0.29 2FG1,GLU_58,4.73,0.15,0,0.08 2B2H,LYS_83,10.45,-0.05,0,0 2PLQ,ASP_40,3.93,0,-0.15,0.28 1R3D,GLU 66,4.66,0.16,0,0 1P6F,ASP_93,2.95,-1.43,-0.36,0.94 4AM1,GLU_254,4.68,0.73,0,-0.55 2H01,HIS_157,6.32,-0.3,0,0.12 3ZXY,ASP_27,3.32,-1.23,-0.19,0.93 2AHE,ARG 250,12,43,-0,29,0,0,21 3LPZ,ASP_321,3.95,0,0,0.15 3GEC,GLU_431,4.08,0.21,0,-0.64 2X4L,LYS_281,12.27,-0.42,1.33,0.85 2YX0,ARG_38,12.79,-0.67,0.43,0.53 4HDE,LYS 85,10,48,-0,13,0,0,1 1R5Q,TYR_81,10.81,0,0.03,0.78 3JRT,ARG_62,11.44,-1.05,0,-0.01 2IF4,TYR_246,10.71,0.18,0,0.52 2D59,ARG 21,12.6,-0.33,0.03,0.4 1PBV,HIS_127,6.48,-0.4,0,0.38 1SIG.LYS 393,10.07,-0.29,0,-0.13 3ADO,GLU_212,4.84,0.18,0,0.17 3DZ1,ASP_115,4.12,0,0,0.32 200K.ARG 202.11.88.-0.76.0.0.15 2CIU,TYR_213,11.41,0.57,0.38,0.46 2F8H,CYS_137,13.28,-1.21,1.86,3.64

1N81.GLU 148.3.34.0.44.-1.23.-0.37 1T3Y,ASP 6.3.32,-0.86,-0.01,0.4 3K8J,GLU_181,4.44,1.58,-1.64,0 3GS9,GLU_142,4.95,0.33,0,0.11 1W7B.LYS 119.10.23.-0.14.0.-0.14 2X5Y.GLU 781.2.92.0.31.-1.49.-0.39 3LMO,LYS_49,10.39,-0.14,0,0.04 1X1E.GLU 193.4.75.0.25.0.0 30NH,ASP_451,2.16,-2,-0.3,0.67 2QOP,ARG_106,12.35,-2.06,0.65,1.26 2GYZ,TYR_75,10.02,0,-0.35,0.37 1PBV,ARG_239,12.45,-0.16,0,0.12 3FFM,ARG_146,13.22,-0.72,0.42,1.02 2AHE,LYS 257,10.47,-0.03,0,0 20SA.ASP 440.3.41.-1.28.-0.16.1.04 2NRR,HIS_474,6.1,-0.5,0,0.11 2PPN,ARG_40,11.74,-1.06,0.11,0.19 4F8A,ARG_674,12.56,-0.35,0,0.41 2Q5X,TYR_849,12.47,0,0.07,2.4 1PGV.LYS 247,10.2,-0.27,0,-0.03 1059,GLU_72,5.58,1.65,-0.51,-0.06 3GT0,ARG_197,13.89,-0.32,0.82,0.88 1PSW,ARG 69,12.65,-0.44,0.25,0.34 1MJS.HIS 398,6.63,-1.01,0.78,0.36 3L3P,ASP_363,2.61,-1.44,-0.38,0.63 1JKS,GLU_113,3.31,1.12,-2.3,-0.01 3FXH,LYS_92,11.27,-0.27,0.85,0.19 2P65,HIS 125,5.83,-1.45,0.08,0.7 1PDB,GLU_183,4.62,0.56,0,-0.44 3I47, ASP_46, 3.27, -0.82, -0.17, 0.47 4H4J,TYR_179,11.1,0,0.45,0.66 3CJW,HIS_175,6.53,-0.22,0,0.25 1NIJ,ASP 236,3.46,-0.86,0,0.52 2CXY,LYS 3,10.51,-0.07,0,0.08 1WP5,HIS_322,7.01,-0.53,0.85,0.2 3E5T,HIS_72,4.95,-2.84,0.79,0.5 1G8P,GLU_347,4.77,0.27,0,0 3LH5,LYS_629,10.54,-0.07,0,0.12 2F9F,CYS_88,11.32,-0.23,-1.2,3.76 10YI.ARG 58,13,14,-0.63,0.42,0.85 2A6B,ASP_134,2.59,-1.56,-0.63,0.99 3E5T,ASP 31,3.45,-0.67,-0.31,0.62 3IRA.GLU 65.4.81.0.27.0.0.04 1G5Z,ASP_188,4.14,0,-0.09,0.43 1J33,ARG_39,12.4,-0.29,0,0.19 2l6l,LYS_151,10.21,-0.12,0,-0.17 3GS9,ASP_121,3.22,-0.72,-0.22,0.36 4H86,LYS_47,10.4,-0.24,0,0.14 2Z84,GLU_109,4.65,0.16,0,0 1PVT,TYR_39,12.63,0.85,0.64,1.14 2R57,GLU 300,4.13,0.28,-0.64,0 1YDL.LYS 32,10.4,-0.41,0.0.31 3F6M,GLU_14,4.56,0.09,0,-0.03 3C6B,ASP_92,4,0,0.1,0.1 2BT8,TYR_295,13.25,-0.13,-0.01,3.38 3G9G,ARG 58,12.61,-0.36,0.22,0.25 3LJN,ASP_221,2.95,-0.86,-0.37,0.38 1NRI,GLU_48,4.63,0.13,0,0 3F6M,ARG_115,12.33,-0.28,0,0.11 3HUE,HIS 241,6.46,-0.48,0.41,0.03 3EX9,LYS 136,11,45,-0,5,0,85,0,59 3V3T,HIS_120,4.35,-1.83,0,-0.32 2D59,ARG_16,12.48,-0.38,0,0.35 3RNV,LYS_433,10.32,-0.18,0,0 3QKY,TYR_217,10.5,-0.13,-0.21,0.83 2Q99,LYS 32,11.35,-0.38,0.85,0.38 3ETV,TYR_136,9.74,-0.62,-0.13,0.49 1NJ4,LYS_143,10.41,-0.11,0,0.02 2F4Q,ASP_163,4.09,0,0,0.29

1XIP,GLU_117,4.61,0.19,0,-0.08 2CL3.LYS 167.10.38.-0.12.0.0 1T95,LYS_166,10.63,-0.28,0,0.4 1C3K,ASP 78,4,2,0,-0,68,1,1 3H5T,LYS 175,10.5,-0.13,0,0.14 2013.GLU 336.3.51.0.49.-1.04.-0.43 1DZF,LYS_122,10.41,-0.09,0,0 1ZP2,ASP_201,4.05,0,-0.01,0.26 3BQW,ARG_127,11.93,-0.47,0,-0.11 1JT9,CYS_228,9.7,-0.54,0,1.24 2Z0M,LYS 23,11.38,-0.97,0.85,1 1SQH,ARG_56,13.59,-0.38,0.86,0.61 1TUL.LYS 97,10.64,-0.27,0.0.41 1W24,ASP_95,4.04,-0.01,0,0.25 3M16.ARG 235.13.14.-1.2.0.99.0.86 2G9D,TYR 341,9,79,-0.02,-0.54,0.35 3UPD,TYR_-5,10.02,0,0,0.02 3ZRI,GLU_22,4.58,0.26,0,-0.19 1LZL,ASP_62,3.51,-0.36,-0.42,0.49 1AM2,GLU 14,4.67,0.14,0,0.03 3L3P,GLU_321,4.59,0.09,0,0 2CWY.GLU 7.4.92.0.16.0.0.26 2CL3,HIS_93,6.02,-1.26,0.69,0.09 3GW3,GLU 45,2.62,1.14,-2.48,-0.55 4GA2,ASP 145,3.85,0.0.0.05 3RVC,HIS_169,5.45,-1.2,0,0.15 2B0J,LYS_107,10.53,-0.39,0,0.42 2GYZ,ARG_37,12.43,-0.07,0,0 3H04,GLU_134,4,0.32,-0.44,-0.38 3C2E,LYS_75,10.41,-0.09,0,0 2EDM,ARG_56,11.45,-1.21,0,0.16 2CXA,CYS_102,11.21,-0.61,0.12,2.7 1VJG,ARG 97,11.97,-0.8,0,0.26 3JRT.GLU 12.4.87.0.21.0.0.17 3DZ1,ARG_236,13.8,-0.24,1.06,0.48 1H09,GLU_24,4.7,0.15,0,0.05 2B0J,ASP_194,1.43,-2.87,-0.44,0.94 1M5I,ARG 216,12.04,-0.34,0,-0.13 1D2K,LYS_187,11.76,-0.28,0.85,0.69 2CWC,ARG 49,12,45,-0.05,0,0 3L3P,ASP_434,3.1,-0.89,-0.21,0.4 3GYW.TYR 272,10.17.0,-0.07.0.24 2G9D,LYS 329,10,18,-0,32,0,0 1NIJ,LYS_32,10.46,-0.25,0,0.23 1SNT,ASP_306,3.26,-0.76,-0.34,0.56 4D8L,LYS_18,10.2,-0.31,0,0.01 3Q1C,LYS 56,10.05,-0.45,0,0 1IDK.TYR 286,11,43,-0,55,0,58,1,41 2X4G,ARG_119,11.69,-0.97,0,0.16 3N2T,ARG_143,12.47,-0.19,0,0.16 3ILC,ARG 102,12,43,-0.07,0.0 4EKU.GLU 357.4.56.0.1.0.-0.04 1R3F,GLU_221,4.64,0.24,0,-0.11 3LOD,HIS_107,6.86,-0.46,0.72,0.1 4DEZ,CYS_47,10.07,-1.14,-0.34,2.55 3M66,HIS_346,6.12,-0.34,0,-0.04 2WOZ,LYS 459,10.56,-0.11,0.0.17 3EVP,ARG_267,13.02,-0.32,0.36,0.48 3KV0,ARG_136,12.86,-0.31,0.34,0.33 1DZF,TYR_46,11.53,0,0.28,1.25 1TD6.GLU 273.4.77.0.94.0.-0.68 1YLN,ARG_217,12.05,-0.34,0,-0.11 3BQW,GLU_172,4.85,0.24,0,0.11 3IRA,ASP_86,1.66,-2.32,-0.38,0.56 1ZBS,ASP_90,3.7,0,-0.32,0.22 3IO0,ASP_236,3.2,-0.67,-0.38,0.45 1HF8,ASP_111,2.24,-2.4,-0.02,0.85 1SJY,GLU_69,7.47,3.11,-0.55,0.41 2FXT,ASP_412,4.2,0,0.21,0.19

1D2K.TYR 322.13.11.0.09.1.04.1.98 2JHY,ASP 143,2.57,-1.02,-0.84,0.63 3JZ9,LYS 533,10,5,0,0,0 3CAX,ASP_154,3.4,-0.72,-0.05,0.37 3Q1C,LYS_53,10.31,-0.59,0,0.39 3RLN,ASP_731,2.41,-1.64,-0.41,0.66 3GMS,HIS 56,6,38,-0,12,0,0 1PSW,HIS_300,6.31,-0.17,0,-0.02 2RGY,ASP_108,3.49,-0.32,-0.42,0.43 2CXA,ARG_8,12.38,-0.13,0,0 3V55.GLU 607,4.56,3.58,-2.3,-1.22 3LH5.LYS 673,10.44,-0.12,0.0.06 2HRZ,GLU_210,4.45,1.74,-1.2,-0.59 1J74,TYR_63,11.89,-0.17,-0.28,2.33 3ANJ.ARG 104.10.97.-2.49.0.0.96 1RSS,LYS 35,10,38,-0,12,0,0 3GA2,TYR_165,10.13,-0.01,-0.14,0.27 3EUR/HIS 41.6.45,-0.09.0.0.05 3GE9,ARG_95,12.98,-0.26,0.35,0.38 3A7L,ARG_17,12.71,-0.78,0.55,0.44 1X91,ASP_122,2.78,-1.72,-0.25,0.95 3EAZ,CYS_119,11.67,0,-0.31,2.99 3R87,ARG_118,13.36,-0.27,0.75,0.38 1ZP2.GLU 76.4.42.0.82.-0.89.0 1YTD.LYS 195.10.67.-0.23.0.0.4 3BPP,LYS_167,11.53,-0.25,0.85,0.43 1XIP,CYS_300,10.76,-1.33,-0.49,3.58 3EVP,GLU_163,4.45,0.62,-0.28,-0.39 1G8P,GLU 258,4.39,0.3,-0.13,-0.27 1BYILLYS 182,10.39,-0.13,0,0.02 1PV5,HIS_3,6.15,-0.32,0,-0.02 1DCF,LYS_52,10.27,-0.29,0,0.06 1WP5,LYS_191,10.32,-0.12,0,-0.06 2PLQ,HIS 10,6.28,-0.11,0,-0.11 2WB8,LYS_462,10.52,-0.21,0,0.22 3LJC,LYS_49,10.28,-0.45,0,0.23 2A4D,GLU_206,4.77,0.27,0,0 2Q07,HIS_404,4.34,-2.43,0.65,-0.37 10YLCYS 125,9.27,0,-0.03,0.3 1PSW,GLU_126,4.74,0.07,0,0.16 1PGV,LYS_327,10.7,-0.83,0.34,0.68 3RFF,ARG 153,12,95,-0.33,0.33,0.45 1MD6.TYR 115.10.96.0.0.24.0.72 3GV0,HIS_108,6.19,-0.26,0,-0.04 2WOZ,GLU_584,4.6,0.16,0,-0.06 2Q5X,GLU_836,4.67,0.42,0,-0.25 2XMZ,ASP_249,4.05,-0.54,0.12,0.67 2H2W,ASP_266,4.1,0,0.01,0.29 1J85,GLU_102,3.93,2.25,-3.03,0.21 1WXF,LYS 275,10.37,-0.13,0.0 3EVP,GLU_126,0.83,0.59,-3.29,-0.97 2Q13,TYR 302,11.96,0,0.26,1.7 1DTO,ASP 173,4,17,0,0.06,0.31 3ADO, ARG_116, 12.54, -0.23, 0, 0.28 1KW4,GLU_28,4.54,0.2,0,-0.15 2CW4,ASP_44,2.92,-1.04,-0.27,0.43 20EW,LYS 313,10.55,-0.12,0,0.17 2CE6,TYR_81,9.98,-0.77,-0.24,0.98 2FBI,LYS 111,10,47,-0,16,0,0,13 2VAN,LYS_280,10.46,-0.11,0,0.07 3VJ8,ARG 348,11.7,-1.11,0,0.31 2BOO,LYS 66,10.33,-0.16,0,-0.01 1WYC,LYS_246,9.96,-0.73,0,0.2 3EVN,HIS_197,6.14,-0.36,0,0 3RNV,TYR_422,10.03,0,0,0.03 3IVF,GLU_269,4.01,1.55,-1.35,-0.69 1X04,LYS_28,10.44,-0.06,0,0 1JSX,ASP_171,3.97,0,0.03,0.14 2A0J,GLU_46,4.74,0.31,0,-0.06

1X1E,ARG_63,12,-0.59,0,0.08 3H9W,CYS 76,11.72,-0.05,0.5,2.27 3LMF,LYS 39,10,35,-0,19,0,0,04 2OSA,GLU_381,3.94,0.32,-0.21,-0.67 3PU6,LYS_104,11.34,-0.51,0.85,0.5 2GEN/HIS 160,4,73,-1,7,0,-0.08 2Q98,ASP 20,3.57,-0.14,-0.55,0.46 2RFA,ASP_188,3.57,-0.76,-0.18,0.72 2JKF.TYR 10.11.34.0.31.0.27.0.75 2G3A,ARG_58,12.13,-0.42,0,0.05 3CE7,ARG 97,12.91,-0.29,0.14,0.56 2EYI,ASP 200,3.45,-0.85,0.06,0.44 3HQX,ARG_66,13.01,-0.28,0.41,0.39 3K9I.TYR 119.10.12.0.0.0.12 2AXO,ASP 246,3.01,-0.95,-0.38,0.55 3DB9,HIS 199,6.35,-0.84,0.76,-0.07 2DG7,ARG 104,10.32,-2.39,0,0.21 3GEC,TYR_468,11.28,0,-0.06,1.35 3ADO,ASP_253,4.02,0,-0.03,0.25 3US6.GLU 44.4.79.0.29.0.0 1TJE,LYS 91,10.51,-0.34,0,0.35 2F4Q,ARG_330,12,-0.65,0,0.14 1P4X/HIS 246,7.02,-0.45,0.1,0.89 2YWJ.TYR 24.11.78.0.0.3.1.48 1V6T.LYS 238.10.35.-0.29.0.0.15 1Y2O,LYS 51,10,49,-0,31,0,0,29 2B0A,LYS_25,10.4,-0.1,0,0 3ZXY,ARG_103,13.05,-0.44,0.7,0.29 1ES5,LYS_3,10.1,-0.4,0,0 3QKY,GLU_150,4.69,0.11,0,0.07 1ZBP,GLU_22,4.69,0.29,-0.04,-0.06 3E5T,GLU_47,4.6,0.25,0,-0.14 1JT9,LYS_183,10.44,-0.06,0,0 1MML,HIS 161,6.07,-0.43,0,0 2FG1.CYS 125,9.37,-0.11,-0.2,0.69 2BV9,HIS_285,5.96,-0.24,0,-0.31 1QZN,GLU_85,4.62,0.12,0,0 1X6J,ASP_53,4.28,0,0.16,0.32 1RAJ,TYR 450,11.81,-0.05,0.54,1.33 106D,GLU_89,4.92,0.86,0,-0.43 2VGM,LYS 46,10,41,-0,16,0,0,07 1Q5Z,LYS_518,10.47,-0.12,0,0.09 2WB3,LYS 338,10.52,-0.26,0,0.29 3LJN,ARG 283,12,19,-0.35,0,0.03 2QV2,LYS_132,10.02,-0.34,0,-0.14 3GT0,LYS_213,10.94,-0.26,0.13,0.56 1N81,LYS_149,9.84,-0.87,0,0.21 1MTZ,ARG 278,13.11,-0.77,0.66,0.72 2QHT,ARG_22,12.5,-0.13,0,0.13 3RFY,LYS 236,10.21,-0.29,0.0 2XHC,TYR_143,10.32,0,-0.1,0.41 1ZBM,ARG_181,12.74,-0.55,0.21,0.58 3D9H,ASP 101,3.8.0,-0.22,0.23 3GW3,ARG_142,11.05,-1.45,0,0 2IRM,GLU_293,6.35,3.46,-0.63,-0.98 4EKU,ARG_306,12.59,-0.35,0.08,0.36 1EV8,LYS_10,11.36,-0.38,0.83,0.41 3M7D.GLU 129.5.77.4.55.-0.85.-2.42 3ADO, ARG_19, 11.45, -1.06, 0, 0.01 3RAZ,GLU_59,5.93,1.74,-0.36,0.05 2B3M,HIS_67,4.72,-1.57,0,-0.22 3HYO.GLU 91.3.69.0.4,-0.82,-0.38 1X1E,GLU_20,4.8,0.35,0,-0.05 3I47,GLU_243,3.09,1.37,-2.21,-0.57 3K8U,LYS_118,10.33,-0.17,0,0 1MD6,LYS_34,10.33,-0.41,0,0.24 1YTD.GLU 252,4.05,0.41,-0.8,-0.05 3V1Q,LYS_571,10.21,-0.2,0,-0.08 3H6Q,LYS_148,10.4,-0.54,0,0.45

3MEW.LYS 189.10.36.-0.17.0.0.02 2H01,ARG 106,13,4,-0,34,0,79,0,44 2IF4,HIS_83,6.16,-0.37,0.06,-0.04 3FNI,TYR_15,11.77,-0.58,0.8,1.55 1W7B.ARG 63.13.19.-1.66.1.49.0.85 109G.ARG 113,13.08,-0.38,0.61,0.34 2P0L,ARG_255,12.41,-0.13,0,0.04 1RSS,LYS_53,10.18,-0.37,0,0.05 3M7D,ARG_131,10.32,-2.31,0.1,0.02 2B0A,GLU_54,4.6,0.1,0,0 2JKF.GLU 62.4.93.0.43.0.0 3K8U,LYS_124,10.28,-0.46,0,0.24 4FCU,ARG_181,12.46,-1.24,0.47,0.73 1FO9,ARG_303,12.87,-1.52,1.37,0.53 2YLF.ARG 74.12.42.-0.08.0.0 2CWY,ARG_68,12.08,-0.4,0,-0.02 2H01,ARG_119,12.55,-0.74,0.21,0.58 3PU6,GLU_51,4.59,0.1,0,-0.01 1ZCE, ARG_42, 13.75, -0.47, 1.33, 0.39 3IL3,ARG 40,12,58,-0.22,0,0,31 3LQE,ARG_390,13.11,-0.33,0.42,0.53 100X,ARG_169,12.22,-0.58,0,0.3 3SMD,LYS_97,10.69,-0.51,0.41,0.29 1D2K,TYR 106,12.49,0.7,0.63,1.15 1SBX,ASP_95,3.9,0,0,0.1 1K95,GLU_126,4.7,0.27,0,-0.07 3M66,HIS_152,5.82,-0.78,0.05,0.05 1C3K,GLU 55,4.32,0.31,0,-0.49 3CBN,TYR_26,11.89,0.81,0.45,0.63 3IV4,HIS_74,4.82,-1.04,0,-0.64 3UV9,LYS_400,10.45,-0.39,0,0.34 1YLN,LYS_243,10.15,-0.35,0,-0.01 2PGE,GLU 176,4.53,0.45,0,-0.42 1G5Z.LYS 161.10.54.-0.1.0.0.15 1L2H,LYS_97,10.26,-0.27,0,0.03 1059,GLU_260,3.75,0.4,-0.57,-0.58 2B3M.LYS 22,10.41,-0.09.0.0 3F6M,CYS_150,12.41,-0.01,0.36,3.06 4FZR,ASP_58,4.07,0,0,0.27 3H04,LYS 264,10.89,-0.25,0.14,0.5 3FNI,LYS_134,10.48,-0.13,0,0.1 2QV2,GLU 95,4.7,0.22,0,-0.02 1X04,ASP 119,3,16,-0,76,-0,38,0,51 2EYI,ARG_82,12.32,-0.22,0,0.04 2HRZ,GLU_72,4.63,0.54,0,-0.41 2OJQ,HIS_633,5.14,-1.15,0,-0.21 20EW,ASP_206,4.03,0,-0.15,0.39 1GPP,HIS_170,7.16,-0.26,0.85,0.08 3BZT,LYS_261,10.57,-0.48,0.23,0.33 3F1X,ARG_269,12.41,-0.16,0,0.06 1FKM,ASP_317,2.75,-0.83,-0.63,0.42 2C2Y,ARG 112,13,11,-0.38,0.57,0.42 1WYC, ASP_132, 3.33, -0.87, 0, 0.4 2RJD,HIS_398,4.54,-2.12,0,0.17 1Z3X,GLU_100,4.69,0.3,0,-0.11 3RFY.ARG 361,12.47,-0.03,0,0 1UW7,TYR_89,12.48,-0.43,0.25,2.66 3V55,TYR_490,12.41,0.23,0.12,2.07 2IF4,ASP_159,3.46,-0.28,-0.39,0.33 1P4X,LYS_25,10.3,-0.29,0,0.09 4ACJ.ARG 681.12.32.-0.18.0.0 1DZF,ARG_11,11.87,-0.29,0,-0.34 1WXF,CYS_60,12.55,0,0,3.55 1Z3X,GLU_139,3.11,0.84,-1.85,-0.38 1GPP,LYS_97,10.42,-0.08,0,0 2QZQ,GLU 90,3.75,1.44,-1.78,-0.42 1DCF,ASP_94,3.42,-0.75,-0.07,0.44 1QYI,LYS_68,10.32,-0.28,0,0.1 3TOW,GLU_138,4.58,0.17,0,-0.09

3KEY,ASP 366,3.3,-0.37,-0.47,0.34 3D9H,ARG 23,12,15,-0,35,0,0 1HF8,HIS_281,6.42,-0.08,0,0 1P6F,HIS_108,6.24,-0.27,0,0.02 2ATR,ASP_49,3.1,-0.85,-0.15,0.3 3LH5.ASP 667.3.68.0.-0.27.0.16 3VJ8,LYS_160,12.51,-0.66,1.64,1.02 1SJY,ASP_4,3.97,0,0,0.17 3FRR,LYS_23,10.77,-0.15,0,0.43 3KEY,HIS_486,6.44,-0.47,0,0.41 2Q98,GLU_101,5.03,0.7,0,-0.16 2XWS,ARG_44,12.33,-0.28,0,0.1 4AM1.ARG 329.12.45.-0.94.0.34.0.56 3U0V,LYS_70,10.46,-0.04,0,0 3GS9,GLU_128,3.71,0.33,-0.85,-0.27 3H13,ARG 243,12.54,-0.36,0.02,0.36 2EFK,LYS_52,10.37,-0.13,0,0 2YWJ,LYS_155,10.45,-0.81,0,0.76 1FHL,TYR_20,10.64,0,0.34,0.31 2C2Y,CYS 140,12.91,-0.3,0.93,3.28 3UPD,ARG_100,12.41,-0.08,0,-0.01 1JKS,ARG_47,12.22,-0.38,0,0.11 1SJ8,GLU_601,3.9,0.51,-0.37,-0.75 1TD6,GLU 70,6.16,1.52,0,0.13 2P1W.GLU 233,4.27,1.5,-1.06,-0.67 2IRM,GLU_84,5.24,1.45,-0.71,0 2GAU,GLU_32,4.62,0.3,0,-0.19 2P65,GLU_184,4.7,0.16,0,0.03 3N2T,GLU 244,4.12,0.45,-0.72,-0.11 3ONT,GLU_137,4.15,0.33,-0.68,0 3DB9,ARG_17,12.72,-0.23,0,0.45 2RGY,CYS_186,12.22,0,0.52,2.69 1GQE,LYS_177,11.41,-0.33,0.85,0.38 1P2F.ARG 110.11.63.-1.56.0.0.7 2GKG,GLU_124,4.73,0.07,0,0.16 3A2Z,TYR_197,10.16,0,0.15,0.01 4AM1,ARG_245,11.58,-1.82,0.42,0.48 2CIU,LYS 179,10.7,-0.19,0,0.39 1WRU,TYR_121,11.22,0,0.43,0.78 4FD6,GLU_153,4.5,0.4,0,-0.4 2BV9,TYR_176,10.27,0,-0.06,0.33 4ACJ,LYS 677,10,28,-0,1,0,-0,13 100H,LYS 178,10.96,-0.25,0.01,0.69 3CQ1,ARG_98,12.48,-0.15,0,0.13 1MML.TYR 133.10.98.0.26.0.37.0.35 2HP7,ARG_75,12.22,-0.23,0,-0.05 2EDM,LYS 192,10.9,-0.93,0.85,0.48 3NBI.GLU 128,4,72,0,22,0,0 2NRK,LYS_148,10.4,-0.1,0,0 2XHC,TYR_84,10.42,0,0.01,0.41 2XHC.TYR 6.11.2.0.0.1.2 3B79.GLU 23.4.35.0.18.-0.32.-0.01 2V4U,LYS_297,10.13,-0.37,0,0 3P2F,ARG_49,13.91,-0.99,1.68,0.73 3FFM,HIS_118,7.43,-0.93,0.9,0.96 3G9T,LYS_257,10.4,-0.1,0,0 2F4O,ARG 158,13,-0.36,0.5,0.36 200K,ARG_349,12.4,-0.35,0,0.26 3BWT,GLU_664,4.61,0.28,0,-0.18 2FD4,ARG 449,11.5,-1.12.0.0.12 1H4U,ASP 473,3.45,-0.61,-0.18,0.44 2QDJ,LYS_341,10.47,-0.11,0,0.07 1M5I,GLU_138,3.4,0.44,-0.79,-0.75 3V1Q,HIS_638,6.48,-0.22,0.16,0.04 1X7F,LYS_16,11.49,-0.25,0.37,0.86 3ULX,ASP_58,4.31,0,0.12,0.39 3H5T,LYS_334,10.81,-0.26,0.11,0.48 1W7B,LYS_227,10.22,-0.41,0,0.13 3U0V,LYS_114,10.11,-0.27,0,-0.13

1RL0,ARG 166,12.06,-0.57,0.0.13 1G5Z,LYS 127,10.31,-0.39,0.07,0.13 3M7G,LYS_28,11.05,-0.59,0.7,0.44 1T6L/HIS 212.6.39,-0.38,0.0.26 1XTZ,LYS_148,10.16,-0.6,0,0.25 3CCY,ASP 180,3.54,-0.29,-0.38,0.41 2OSA,LYS 368,10,71,-0,3,0,0,51 1WOU,HIS_59,6.52,-0.31,0,0.34 2P0L,ASP_263,4.15,0,-0.04,0.39 2F9F,LYS_51,10.41,-0.09,0,0 3EX9,TYR 120,13.25,0,0.47,2.78 2APL.ASP 116.4.09.0.0.07.0.22 2R0S,TYR_73,11.27,0,0.23,1.04 3UX2,ASP_128,3.79,-0.26,0,0.25 100X,ASP 170,4,25,-0.07,-0.04,0.55 1SOH, LYS 242, 10, 49, -0, 28, 0, 0, 27 2EHG,GLU_39,4.26,0.8,-0.69,-0.36 2FB6,CYS_78,11.01,-0.07,0.37,1.71 1TP6,ASP_112,1.73,-2.27,-0.55,0.76 3OA7,TYR_43,10.09,0,0,0.09 4F85.HIS 99.6.03.-1.3.0.77.0.06 208I,ARG_124,12.51,-0.36,0,0.36 1Q5Z,GLU_607,3.57,0.29,-0.85,-0.37 3K8J.HIS 66.6.29,-0.29.0.0.08 4E6S,TYR 17,10.56,0,0.15,0.42 3UV9,ASP_318,3.36,-0.8,0,0.35 2GKG,ARG_25,12.14,-0.41,0,0.05 2RJD,HIS_512,4.67,-2.12,0.83,-0.54 3C5V,GLU 129,4.16,0.66,-0.81,-0.2 2ATR,GLU_32,4.97,0.35,0,0.11 1T07,ASP_29,2.35,-1.64,-0.55,0.74 2JEO,LYS_81,10.35,-0.13,0,-0.02 1T95,GLU_23,3.42,0.29,-0.8,-0.56 100L.ARG 119,12.47,-0.31,0,0.27 3CBN,GLU_152,3.81,0.18,-0.75,-0.12 1Q46,ARG_175,12.85,-0.08,0,0.42 3JZN,LYS_293,10.12,-0.32,0,-0.06 106D,GLU_47,4.27,0.23,-0.14,-0.33 2B0J.GLU 86,4,76,0,3,0,-0,04 2AZL,ARG_249,12.1,-0.49,0,0.09 3IV4,GLU_28,4.26,0.32,-0.39,-0.17 1LPL/ARG 163/12/21/-0.51/0/0/21 3PBH.CYS 240,11.92,0,0.27,2.65 1U7U,GLU_330,4.72,0.47,-0.2,-0.05 1BN6,ARG_144,11.82,-1.86,0.62,0.57 2FD5,ARG_67,11.69,-0.76,0,-0.06 2QHT,ARG_208,12.59,-0.22,0.07,0.24 2WB8,ARG_695,13.19,-0.87,0.7,0.87 2H85,ARG_126,12.81,-1.9,1.13,1.07 3GW3,LYS 289,10.69,-0.15,0,0.34 3CX2,GLU_258,4.57,0.1,0,-0.03 2P5D,ARG 134,11.88,-0.72,0,0.1 2013.LYS 91.10.37.-0.22.0.0.09 1RHS,ASP_65,3.45,-0.68,-0.11,0.45 3KB5,ARG_386,13.4,-0.35,0.72,0.53 2GZQ,HIS_93,3.99,-2.91,0.65,-0.24 2VGM.TYR 311.10.01.0.-0.17.0.17 4FZN,ASP_184,3.04,-0.82,-0.46,0.52 3GEC,LYS 457,10.64,-0.17,0,0.31 3HOX.CYS 23.10.09.-0.85.0.1.94 1L2F,ARG 199,12.31,-0.36,0,0.18 3ETU,LYS 270,10,4,-0,31,0,0,21 2B78,LYS_65,10.42,-0.08,0,0 3UAH,ASP_421,3.87,-0.01,-0.19,0.27 1DUN,GLU_11,3.96,0.33,-0.85,-0.02 2NRK,ARG_118,12.2,-1.56,0.71,0.55 3LPZ,HIS_133,5.32,-1.35,0,0.16 3GV0,ASP_275,3.13,-0.8,-0.35,0.48 2ZCX,ARG_154,12.38,-0.43,0,0.3

2Q07,TYR_245,10.9,0,0.1,0.8 3RLE,CYS 103,9.25,-0.85,-0.41,1.5 1LTU.TYR 232.11.4.0.0.12.1.28 1RHS,ARG_186,12.33,-1.83,1.33,0.33 3LJI,ASP_278,3.28,-0.74,-0.07,0.29 2AZL/ARG 55/12.92/-0.52/0.47/0.48 3N2TARG 109.13.05.-0.35.0.55.0.36 2QEV,HIS_35,4.23,-2.31,0.14,-0.1 2HXB,ARG_58,12.73,-0.28,0.25,0.26 1J33,GLU_28,4.71,0.5,0,-0.3 2YX0,GLU_316,4.42,0.21,0,-0.29 2RJD,HIS_233,6.25,-0.2,0,-0.04 2CXA,HIS_121,6.45,-0.55,0.23,0.27 3L7N,ASP 42,3.98,0,-0.05,0.23 1DTO,TYR_44,10.15,0,-0.14,0.29 3TMO,ASP_231,3.09,-0.84,-0.39,0.52 3U2R,GLU_40,4.47,0.11,0,-0.14 1MN3,ASP_430,4.26,0,0.19,0.27 2P0L,ARG_129,11.83,-0.82,0,0.16 1PGV.GLU 379.3.83.0.41.-0.69.-0.39 3UPD.LYS 55,9.91,-0.76,0.0.18 10LR,HIS_112,6.74,-0.87,0.85,0.26 1160.HIS 46.7.45.-0.55.1.3.0.21 1XIP.GLU 14.4.49.0.15.-0.22.0.07 10LR,ARG 146,12.06,-0.45,0,0.01 1NWA,TYR_65,13.16,0,0.13,3.03 2F4Q,ARG_69,12.28,-0.49,0,0.26 4FCU,ASP_140,3.74,-0.06,-0.18,0.19 3RJX,TYR_287,10.52,0,-0.14,0.65 2QK1,LYS_489,10.66,-0.11,0,0.27 4DIU,GLU_123,4.64,0.46,0,-0.32 3MIX.LYS 565,10.63,-0.14,0.0.26 3H13,CYS_426,11.28,0,-0.23,2.51 3B7X,LYS 85,10.49,-0.01,0,0 1JT9.HIS 81.6.21.-0.44.0.0.14 2V5B,ARG_227,12.49,-0.24,0,0.24 3CRM,ARG_258,13.09,-0.32,0.49,0.43 2AHE,TYR_205,11.09,0,-0.01,1.1 3CBN,ASP_57,3.51,-0.39,-0.31,0.41 1RAJ,GLU_426,4.83,0.28,0,0.05 1RI5,LYS_132,11.01,-0.7,0.85,0.37 2P52,TYR 160,11.94,-0.07,5.55E-17.2.01 4EUG,ARG_105,13.56,-0.47,1.07,0.46 3A4C,GLU_488,4.69,0.12,0,0.07 1GXN,TYR_569,10.5,0,0.03,0.46 1RWZ,LYS_158,10.57,-0.06,0,0.13 2VAN,ARG_137,12.44,-0.33,0,0.27 1WNH,ASP_155,4.18,0,0.04,0.34 2FL7,LYS_209,11.57,-0.31,0.85,0.53 4E8B,HIS_17,6.49,-0.47,0.39,0.07 2OB5,ASP_51,3.93,-0.13,-0.41,0.67 3LE4,TYR 319,10.23,-0.16,-0.21,0.6 3BB7,ARG_353,13.07,-0.94,0.42,1.09 3ZXY,ARG_82,12.34,-0.44,0,0.27 2JHY,CYS_79,8.76,-1.36,0.02,1.1 2ATR,TYR_78,11.67,0.85,0.38,0.44 3I47, ARG_173, 12.29, -0.31, 0, 0.1 1YM5,LYS_202,10.38,-0.44,0,0.32 3VJ8.HIS 269.2.63.-2.36.0.-1.52 3BQE,ARG_217,13.01,-0.33,0.48,0.37 3UC9,GLU 77,4.44,0.2,0,-0.26 3LJN.CYS 57.12.66,-0.08,0.08,3.67 1YG2,TYR_136,10.11,0,0,0.11 3F1X,GLU_135,4.7,0.4,0,-0.2 4ESS,ASP_138,2.75,-0.81,-0.44,0.2 4HDE,LYS 53,10.61,-0.1,0.0.22 1V8E,LYS_89,9.85,-0.72,0,0.07 2PLQ,ASP_95,3.08,-0.81,-0.48,0.56 2Q98,LYS_187,10.58,-0.43,0.03,0.49

1DCF.ASP 117.3.82.0.-0.17.0.18 3RFY,LYS_246,10.03,-0.33,0,-0.14 1L2H,LYS_92,11.85,-0.49,1.09,0.74 3FFM,LYS_131,10.47,-0.04,0,0.01 1PSW.CYS 262.12.28.0.0.07.3.22 1D2K.LYS 271.10.13.-0.49.0.0.12 1ZBP,LYS_5,10.34,-0.16,0,0 2CBE,LYS_76,10.95,-0.33,0.42,0.35 2RIK,LYS_236,10.4,-0.15,0,0.05 3UX2.HIS 89.6.39.-0.1.0.-0.01 1FHL,GLU_323,4.87,0.31,0,0.07 3Q2C,TYR_73,11.28,-0.92,-0.34,2.55 2B2H,ASP_66,2.48,-1.5,-0.49,0.67 1NJ4.GLU 65.4.49.1.08.-0.7.-0.4 3A7L.GLU 122.4.92.0.29.0.0.13 1BN6,TYR_35,11.07,0,0.09,0.98 1V43,LYS_112,9.77,-0.61,0,-0.11 1GQE,ARG_262,12.22,-0.82,0,0.54 2DG7.GLU 60.5.12.1.87.-0.53.-0.73 1WRU,GLU_27,4.58,1.05,-0.23,-0.74 2HRZ,GLU_290,4.55,0.05,0,0 1RL0,ARG_182,12.25,-0.65,0,0.4 3ETU,GLU_202,4.85,0.63,0,-0.28 1RSS,ARG 41,12.33,-0.22,0.0.05 3MEW, ARG_157, 12.63, -0.09, 0, 0.23 2IQT,GLU_110,4.63,0.36,0,-0.22 1JB3,LYS_48,10.25,-0.17,0,-0.07 2P5D,TYR 141,11.79,0,0.24,1.55 2DG7,ARG_42,12.45,-0.05,0,0 3F7M,ASP_221,3.06,-1.54,-0.47,1.26 1NAF,GLU_220,3.89,0.24,-0.6,-0.25 1WYC.ASP 105.2.28.-1.39.-0.69.0.56 4EKU.CYS 310.11.52.0.0.37.2.15 2Q99,ASP_100,2.92,-0.81,-0.42,0.34 2AHE,ARG_61,12.64,-0.08,0,0.23 1G8P,GLU_291,4.97,0.52,-0.09,0.03 3I47, TYR 217, 10.51, 0, 0.15, 0.37 105J.GLU 64,4.53,0.31,0,-0.28 1V6T,HIS_162,5.17,-1.68,0,0.34 1SIG,GLU_136,5.29,1.53,-0.29,-0.45 2B0J.LYS 160,10.5,-0.1,0,0.1 3GYW, ARG 132, 13.87, -1.41, 1.34, 1.44 3EVP,HIS_82,4.09,-2.74,0,0.32 2D2S.LYS 747.10.56.-0.16.0.0.22 300P,HIS_20,6.3,-0.19,0,-0.01 3KT9,GLU_78,4.15,0.65,0,-1 2R0S,ASP 269,2,55,-1,57,-0.08,0,4 2NRR,GLU_444,2.97,0.36,-1.16,-0.73 1LZL,ASP_60,4.12,0,0.14,0.18 2FL4.ASP 40.3.96.0.0.16 1SBX.TYR 191,10.49,0.0.33,0.16 1AK1,HIS_183,4.9,-2.43,0.81,0.02 1MD6,GLU_39,4.88,1.12,-0.82,0.07 1NAF,GLU_188,4.83,0.12,0,0.21 3BPP,TYR 179,10.41,0,0.17,0.23 2Q07,TYR_453,10.11,0,-0.19,0.3 1R29,HIS_14,6.37,-0.22,0,0.09 2FPN,ARG 13,12.47,-0.19,0,0.15 3RKV,ARG_316,12.78,-0.34,0.28,0.34 3O48,GLU_127,3.91,0.26,-0.85,0 2HRZ,ARG_104,12.95,-0.35,0.34,0.47 1LFP,ARG_50,12.24,-0.42,0,0.17 4E8B,ARG_188,12.7,-0.63,0.19,0.64 2QDJ,TYR_292,11.33,0,0.56,0.77 1S7K,CYS_74,9.72,0,0.09,0.62 3IL3,GLU_301,7.87,3.59,-0.22,0 10LR,ARG_127,11.67,-1.06,0,0.23 2A0J,HIS_67,5.29,-1.56,0.84,-0.49 3V4G,LYS_19,10.11,-0.23,0,-0.16

3H5T.ARG 148.13.07.-0.49.0.45.0.61 1YB2,LYS_248,10.23,-0.62,0,0.35 2D0A, ARG_309, 12.22, -0.33, 0, 0.04 3EZ7,TYR_105,10.06,0,-0.13,0.19 3NBI.GLU 54,4.67,0.27,0,-0.1 2NRK.TYR 103,12,99,0.6,-0.12,2.51 3ULX,ARG_155,12.36,-0.14,0,0 2G5X.ARG 26.12.6.-0.3.0.01.0.39 3U0V,LYS_228,10.73,-0.95,0.68,0.51 1O6D,LYS_38,10.39,-0.16,0,0.04 20GO,ARG 581,12,28,-0.33,0,0,11 3V4G,LYS_117,10.41,-0.09,0,0 2YWX,LYS_143,11.05,-0.42,0.59,0.38 1NAR.GLU 29.4.47.0.07.0.-0.11 1G5Z,GLU_44,4.73,0.23,0,0 3HVM,TYR_27,10.19,0,0.1,0.09 3EAZ,TYR 112,10.09,0.0.0.09 3GMS,LYS_322,10.5,0,0,0 1TUL,GLU_30,4.36,0.3,-0.57,0.14 1RI6.GLU 225.4.52.0.1.0.-0.08 2RJD,HIS_477,5.52,-0.99,0,0.03 1NFN,GLU_109,4.67,0.26,0,-0.09 1J33.GLU 137.4.9.0.25.0.0.14 1XFK.LYS 225.10.82.-0.23.0.27.0.27 1EQ6,LYS_34,10.39,-0.11,0,0 1WXQ,LYS_51,10.71,-0.15,0,0.35 2B0A,LYS_60,10.41,-0.13,0.13,-0.08 2P0Y,ARG_289,12.79,-0.11,0,0.39 2H01.LYS 93.10.39.-0.19.0.0.08 1RI5,ARG_59,12.53,-0.27,0,0.3 1BN6,ARG_129,13.07,-1.36,1.31,0.62 3E7P,GLU_91,4.6,0.25,0,-0.16 3G9G.CYS 221.9.7.0.0.42.0.29 3FHF,HIS_149,5.53,-0.7,0,-0.28 3EYE,ASP_126,4.02,-0.68,0.26,0.62 2FPN,HIS_203,6.26,-0.24,0,0 3EIZ,TYR_142,12.87,-0.04,0.15,2.75 1YTQ,GLU_22,3.77,0.29,-0.84,-0.17 3FRR,ASP_122,3.54,-0.68,-0.57,0.99 3LH5,ARG_742,13.83,-0.55,1.45,0.42 3EZ7,ASP_322,3.98,0,-0.03,0.21 2RIK,ARG 230,12.66,-0.22,0,0.38 3IPZ.GLU 156.4.5.0.2.0.-0.2 2EJX,ARG_78,12.32,-0.4,0,0.22 1MTZ,ASP_224,3.15,-1.63,-0.03,1 3LMF,HIS_20,6.26,-0.35,0,0.12 2H2W,LYS 255,10.38,-0.12,0,0 3UV9,TYR_389,10.29,0,-0.06,0.35 1RAJ,TYR_350,13.56,0.85,0.78,1.93 3EVP,TYR_301,12.35,-0.15,0.14,2.36 3I0C,GLU 276,4.39,0.77,-0.45,-0.43 2RGY,HIS 115.6.28,-0.16.0,-0.06 20BI,ASP_23,3.2,-0.85,-0.16,0.41 1T3Y,LYS_98,10.6,-0.8,0.85,0.05 2YT4,GLU_604,5.1,0.77,0,-0.17 1AM2,ARG_68,12.35,-0.21,0,0.06 1H09,LYS_128,10.19,-0.4,0,0.09 1MTZ,LYS_158,10.55,-0.18,0,0.23 3EJC,GLU_16,4.82,0.18,0,0.15 4D8L,ARG 288,11.72,-0.99,0,0.2 3PZ9.GLU 252.4.58.0.24.0.-0.16 3RLN,HIS_719,5.84,-0.6,0,-0.06 1FHL,GLU_326,4.68,0.18,0,0 2AZL,GLU_14,4.57,0.32,0,-0.25 2CBE,GLU_238,3.76,0.29,-0.83,-0.21 3CXS,ARG_180,12.36,-0.14,0,0 1JT9,ASP_141,2.18,-1.88,-0.61,0.86 1SIG,TYR_228,10.46,0,-0.2,0.66 3P28,HIS_189,6.81,-0.21,0.64,-0.12

3M9A.GLU 13.4.41.0.16.0.-0.24 2R0S,LYS 239,10.57,-0.24,0,0.3 3RVC,ARG_193,12.42,-0.09,0,0.01 100X,LYS_138,10.72,-0.45,0,0.67 10IS.GLU 280.4.77.0.3.0.-0.03 3A7L,ASP_127,3.93,0,0,0.13 3FK5,ARG_231,12.47,-0.23,0,0.2 1YM5,GLU_168,4.68,0.25,0,-0.07 3RFY,TYR_223,10.52,0,0.28,0.25 2RJD,LYS 302,10.85,-0.19,0.14,0.4 3CGW,LYS 123,10.91,-0.22,0.0.63 4EKU,GLU_205,5.12,1.19,-0.64,0.07 3V75,ASP_258,2.93,-1.08,-0.13,0.35 2XHC.ARG 279,13,24,-0,76,0,68,0,81 2D7U.TYR 186,10.42,0,0.2,0.22 30IP,ASP_178,3.58,-0.8,0,0.58 1DOV.TYR 245.10.8.0.0.05.0.74 3M7G,TYR_226,10.84,-0.83,-1.45,3.1 2H2W,LYS 295,10,49,-0.01,0,0 2EYI,LYS 106,10.38,-0.12,0.0 1RKA, ASP_66, 3.43, -0.88, 0.13, 0.39 3F1X.HIS 66.6.58.-0.14.0.22.0 3BJV,TYR_44,10.4,0,-0.08,0.47 4FLE,ARG 121,12.92,-0.34,0.16,0.6 2B0J.HIS 201,5.25,-3,1,0.85,1 2Z14,ARG_100,12.45,-0.15,0,0.09 4EZB,ARG_45,12.32,-0.33,0,0.15 2H14,HIS_128,4.87,-2.9,0.85,0.41 200K,ARG 278,12.4,-0.1,0,0 2VGM,GLU_189,3.26,0.69,-1.38,-0.55 3FHF,GLU_153,3.66,1.59,-1.69,-0.74 2OJQ,LYS_471,10.61,-0.17,0,0.28 1YR6,GLU 183,4.64,0.65,-0.13,-0.37 2V1L.ARG 120,12,34,-0.22,0,0,06 2AXO,ARG_65,12.42,-0.29,0,0.21 3UV9,TYR_466,10.62,-0.48,0.06,1.04 3IO0,ARG_282,12.68,-1.21,0.45,0.94 1MUF,TYR 217,11.81,0.85,0.39,0.57 1YDL,LYS_6,10.43,-0.07,0,0 3HQX,ASP_71,3.86,0,-0.08,0.15 2CXC,ARG_53,12.46,-0.04,0,0 3US6,CYS 112,10.55,-0.28,0,1.83 2NMU,HIS 6,6,46,-0.04,0,0 1ZBM,HIS_22,6.21,-0.58,0.3,-0.02 3I47,LYS_221,10.06,-0.45,0,0.01 3PP8,GLU_182,4.19,0.32,-0.72,0.09 3LJI,ASP_115,4,0,-0.34,0.54 1DVO.ARG 143.13.96.-1.08.1.1.54 2ILR,GLU_318,4.7,0.22,0,-0.02 2FD5,ARG_170,12.42,-0.08,0,0 3ANJ,TYR_204,12.6,0.8,0.42,1.37 1TWU.GLU 31.4.6.0.28.0.-0.18 3BJV,GLU_155,4.65,0.14,0,0.02 3JSN.TYR 35,11,72,0,-0,11,1.83 1TJE,LYS_130,11.49,-0.38,0.85,0.52 3LD1,LYS_13,10.42,-0.4,0,0.32 3E5T.GLU 200.4.49.0.36.0.-0.36 3A4C,ARG_528,12.46,-0.04,0,0 2Q12,LYS_152,10.36,-0.14,0,0 3AUF,ARG_167,12.96,-0.44,0.53,0.37 2CWC/HIS 48.6.54,-0.27.0.0.31 3IO0,ASP_243,3.87,0,-0.07,0.14 3L7N,HIS 141,2.56,-3.33,0.4,-1.02 1TXJ,ASP_111,3.92,0,-0.05,0.18 1FKM,ARG_482,13.15,-0.99,1.07,0.57 3COU,ASP 52,2.54,-1.35,-0.67,0.74 2D59,LYS_23,9.43,-1.08,0,0.01 3P28,GLU_197,3.94,1.45,-0.85,-1.17 2DG7,ASP_141,4.1,0,0.16,0.13

1160.TYR 42.11.81.0.0.28.1.53 2Z0M.ARG 312.12.41.-0.09.0.0 3PM2, ASP_98, 4, 0, -0.14, 0.34 4DVD,ARG_68,11.75,-0.56,0,-0.19 3E7P,GLU_229,4.03,0.31,-0.46,-0.32 2QRX,LYS_75,10.14,-0.18,0,-0.18 2Q5X,ASP_763,4.09,0,0.05,0.24 3V55,TYR_620,10.47,0,0.17,0.3 2EEY,ASP_136,3.66,-0.5,0.02,0.34 2D2S,GLU_681,4.51,0.09,0,-0.08 2P65,LYS 77,10.41,-0.34,0,0.24 1RHS,ARG 110,13,33,-3,52,0.8,3.54 3AU3,GLU_601,3.37,0.34,-1.21,-0.26 2X4L,ASP_158,3.13,-0.7,-0.28,0.32 3A0X.GLU 645.5.08.0.37.0.0.22 1U53,LYS 41,10.69,-0.22,0.03,0.38 3T5B,ARG_199,11.69,-1.52,0.36,0.34 1P6F,ARG_70,12.3,-0.22,0,0.02 1NRI,ARG_26,12.39,-0.22,0.03,0.08 2R51,LYS 28,10.43,-0.29,0,0.23 2OSA,CYS_391,10.53,0,0.11,1.42 2FL4,TYR_51,10.24,0,0,0.24 1PSW,GLU_249,4.43,0.21,0,-0.28 1059.GLU 311.4.92.0.5.0.-0.08 1C3K,ASP 136,4.02,0.0.0.22 4FH3,ARG_66,12.32,-0.27,0,0.09 1XKR,ASP_127,4.02,0,-0.04,0.26 2VGM,LYS_103,10.31,-0.2,0,0.01 3LJC,ARG_97,12.21,-2.47,0.97,1.21 3I47.GLU 78.4.58.0.08.0.0 2QV2,GLU_126,3.55,0.5,-0.9,-0.55 4FZR,ASP_167,4.05,0,0.05,0.2 2CWC.TYR 112.12.43.0.85.0.58.0.99 2GZO.LYS 124.10.-0.24.0.-0.26 3O16,GLU_69,4.64,0.12,0,0.02 1ZP2,ARG_115,12.38,-0.27,0,0.15 2WB8,TYR_667,11.27,-0.57,0.23,1.61 2E3S,LYS_488,10.58,-0.35,0.11,0.31 20YZ,LYS 84,10.3,-0.29,0.0.1 2FG1,ARG_122,12.88,-0.61,0.11,0.87 2H30,ASP_45,1.66,-2.43,-0.38,0.67 2BAA,ARG_55,12.46,-0.88,0,0.84 1MTZ,TYR 152,9.72,-0.57,-0.1,0.4 4H89,ARG_116,12.37,-0.36,0,0.22 1W7B,ARG_37,12.66,-0.14,0,0.29 3ANJ,GLU_10,2.81,1.3,-2.38,-0.6 3GG6,TYR_169,10.41,0,0.11,0.3 30IP.GLU 172.3.73.0.23.-1.01.0 2G9D,LYS_249,10.48,-0.12,0,0.1 105T,HIS_375,5.44,-0.7,0,-0.36 2OJQ,GLU_617,4.62,0.17,0,-0.05 2QZQ,ASP 146,2.06,-2.08,-0.26,0.6 1FO9,GLU_258,3.32,0.79,-1.56,-0.41 10GL,ASP_187,3.9,0,-0.09,0.19 2GEN,ARG_74,12.45,-0.05,0,0 1Y2Q,ARG_2,12.27,-0.34,0,0.11 4GA2,LYS_115,10.95,-0.18,0.18,0.44 208P,ASP_9,2,-1.65,-0.47,0.33 2EDM.LYS 59.10.35.-0.24.0.0.09 1LN4,GLU_38,4.06,0.7,-0.75,-0.4 30DJ,TYR 53,10.69,0,0.26,0.43 2JEO.GLU 111.4.42.0.21.-0.29.0 3CXS,ASP_126,3.89,0,-0.15,0.24 3GS9,ASP_201,4.08,-0.64,0.22,0.71 2D7U,GLU_14,4.6,4.69,-2.48,-2.12 2FL7,TYR_101,12.05,0,0.53,1.52 3M66,ASP_165,1.71,-2.09,-0.42,0.42 1RI5,ARG_126,12.51,-0.1,0,0.11 2BDV,LYS_63,11.38,-0.32,0.71,0.49

2B02.LYS 432.11.58.-0.31.0.85.0.53 3E7P,LYS_100,10.31,-0.19,0,0 2188,LYS 469,10.31,-0.4,0,0.2 3DTE,ASP_98,4.44,0,0.35,0.29 1WOULYS 89.10.43.-0.07.0.0 2GKG,ARG 115,13,43,-0.32,0.77,0.48 200K,TYR_77,11.53,0.18,0.6,0.75 1YG2,HIS_5,5.16,-0.97,0,-0.37 1RI6,ARG_141,13.51,-0.27,0.84,0.43 3BCH.ASP 44.3.33.-0.8.-0.09.0.41 3CN5,CYS_127,11.38,0,0,2.38 3B21,HIS 145.6.02,-2.29,0.85,0.96 2ZCO,GLU_250,3.28,1.04,-1.32,-0.94 1WXO.ASP 47,3.81,0,-0.36,0.37 3AU3,ASP 432,3.66,-0.29,0.0.14 1RKA, ARG_129, 13.5, -0.37, 0.99, 0.38 1WNH,ARG_171,13.26,-0.45,0.51,0.7 1J8B,ARG_54,12.79,-0.3,0.32,0.27 3CN5.TYR 90.10.15.0.0.08.0.08 3DSH,ARG_328,11.66,-1.35,0.21,0.31 2P0L, ASP_134, 3.85, 0, -0.17, 0.22 3OA7,ARG_528,12.27,-0.16,0,-0.07 1YLN,ARG 140,12.52,-0.24,0,0.26 1NAR.HIS 234.6.22,-0.28.0.0 2H2Z,ASP_245,3.88,0,-0.09,0.17 1ES9,ARG_154,12.91,-0.3,0.4,0.3 1R29,HIS_46,6.01,-1.05,0.43,0.13 1L2F,GLU 15,4.48,0.14,0,-0.16 3ZRI,TYR_84,10.34,0,0.07,0.26 3R87,ASP_42,4.17,0,0.21,0.15 2X4L,LYS_264,10.91,-1.12,0.85,0.67 1D2K.TYR 418.11.34.0.0.29.1.05 2RIK,LYS 82,10.42,-0.1,0,0.02 2GAU,TYR_140,9.97,0,-0.44,0.39 3PP8,GLU_300,4.51,0.27,0,-0.26 1ZHV,ASP_41,3.84,-0.18,0,0.23 4AE7,LYS 231,10.22,-0.16,0,-0.12 3VJ8,LYS 241,10.41,-0.08,0.0 1MTZ,LYS_23,10.52,-0.21,0,0.23 2QK1,LYS_469,10.43,-0.07,0,0 2ZTY,CYS 147,11.08,-1.25,0,3.33 2AD1.LYS 86.10.85.-0.25.0.19.0.41 3GE9,HIS_91,6.05,-0.25,0,-0.21 3RKV,ASP_331,3.96,0,-0.1,0.26 3IU5,GLU_133,4.74,0.77,-0.54,0 1D2K,TYR 350,11.47,-0.75,0,2.22 2AZL.GLU 18,3.66,0.32,-0.78,-0.38 1RI6,HIS_237,6.33,-3.16,0.95,2.03 1C3K,LYS_67,10.6,-0.39,0.08,0.4 2H01.LYS 126.11.47.-0.53.0.7.0.81 2IXM,LYS 62,9.68,-0.83,0,0 2W0G,ASP_170,3.95,0,-0.21,0.37 3PP8,LYS_170,10.18,-0.39,0,0.07 1XEU,HIS_103,7.37,-0.91,0.85,0.93 2AXO,ARG_137,12.6,-0.62,0.37,0.35 1U7U,ASP_375,3.83,-0.27,0.06,0.25 2CBE, ASP_190, 2.9, -1.05, -0.42, 0.57 2I6I,TYR_50,10.28,0,0.05,0.23 1GQE,ARG_150,13.13,-0.35,0.63,0.35 3BPV.LYS 61,10.39,-0.16,0,0.04 2A4D,ASP_116,1.68,-2.49,-0.37,0.73 3C2E, ARG_150, 12.24, -0.55, 0, 0.29 2PPN,LYS_105,10.79,-0.4,0.42,0.26 3EX9,GLU 146,4.45,0.35,-0.02,-0.39 2ZCX.GLU 81.3.79.0.96.-1.36.-0.32 1Y2Q,GLU_55,3.08,0.61,-1.65,-0.38 4H4J,ASP_91,3.98,0,-0.12,0.3 2P0Y,ASP_316,3.65,-0.23,-0.21,0.3 3NBI,ASP_195,3.99,0,0,0.19

3BB7.GLU 44.4.8.0.3.0.0 2FZ4,ARG_110,10.59,-1.86,0,-0.04 1XIP,GLU_288,4.79,0.22,0,0.07 2E0T,ARG_203,12.41,-0.09,0,0 30KY,ARG 175,13,23,-0.59,0,4,0,92 1RHS,ARG 121,12,25,-0,51,0,0.27 2CN1,GLU_136,4.24,0.45,-0.78,0.08 1J33,GLU_280,5.75,2.53,-0.41,-0.87 200K,ASP_131,3.96,0,0,0.16 2Q99,ASP_159,3.79,0,-0.44,0.42 2IN0.ARG 54,12.83,-0.35,0.04,0.64 3FK5,HIS_113,7.22,-0.13,0.85,0 2GAU,ARG_15,13.3,-0.18,0.46,0.51 1L2H,LYS 16,10,58,-1,49,0,85,0,72 3V46.TYR 341.13.32.-0.85.0.81.3.35 1RKA,LYS_160,10.43,-0.07,0,0 3JZN,LYS_106,10.03,-0.53,0,0.06 1VJG,ARG_63,13.02,-1.93,1.3,1.14 2FD4,GLU 537,4.64,0.18,0,-0.04 3BQW,GLU_273,4.44,0.16,0,-0.21 2R0S,LYS_188,10.48,-0.15,0,0.13 1XDZ,ASP_30,4.44,0,0.04,0.61 3S0A,LYS_18,10.3,-0.25,0,0.06 1JSX,GLU 130,4.6,0.1,0,0 4FLE,HIS_33,6.32,-0.13,0,-0.05 1X6J,ARG_74,13.04,-0.16,0.46,0.24 2PGX,ARG_74,12.28,-0.29,0,0.07 2RIK,LYS_126,10.61,-0.12,0,0.23 1SIG.ARG 232,12,57,-0.31,0,0.38 1UXO,ASP_110,3.49,-0.83,0,0.52 2YLF,HIS_80,6.07,-0.62,0.22,-0.04 2QEV,TYR_127,11.49,0,0.49,1.01 2Z61,ASP 111,3.61,-0.26,-0.17,0.23 2DG7,ASP_74,3.22,-0.79,0,0.22 3RFY,GLU_302,4.59,0.09,0,-0.01 2PLQ,HIS_107,6.14,-0.7,0,0.33 1PVT,HIS 81,5.89,-1.39,0.37,0.41 1WYC,GLU_199,4.14,0.61,-0.82,-0.15 2Q12,HIS_100,5.59,-0.91,0,0 2AZL.GLU 213,4.62,0.12,0,0 3DZ1,LYS_268,10.29,-0.26,0,0.05 2WB8,LYS 773,10.11,-0.36,0,-0.02 2G9D,GLU_29,4.52,0.08,0,-0.07 3HVM,CYS_312,12.46,-0.48,0.31,3.62 1EW4,ASP_29,4.03,0,0.01,0.21 3EVP,LYS_79,10.56,-0.19,0,0.26 1DVO,TYR_144,10.69,0.21,0.2,0.28 2BCF,HIS_178,7.11,-1.14,0.85,0.91 1U3Y,ASP_302,3.14,-1.02,-0.03,0.4 1MUF,LYS_168,10.46,-0.18,0,0.14 3ADO, ASP 221, 3.82, -0.46, -0.42, 0.91 2B61,LYS 308,11,41,-0,34,0,77,0,48 3FHF,HIS_0,7.06,-0.53,0.7,0.39 2D7J,CYS_186,11.84,-0.07,-0.12,3.03 2CN1,LYS_117,10.26,-0.42,0,0.18 3F5D,TYR_131,11.86,0,0,1.86 2B78,HIS 354,7.46,-1.16,1.66,0.47 3EGN.GLU 433.4.78.0.25.0.0.03 3I4T,LYS_234,11.46,-0.25,0.41,0.8 3EOD,CYS 123,11.76,0.46,0.56,1.74 1PDB,ARG 32,12,37,-0.27,0,0,15 3GFP,ASP_363,3.13,-0.38,-0.54,0.24 3PM2,ASP_73,3.3,-0.92,0,0.41 2F9F,HIS_54,6.3,-0.16,0,-0.04 1FO9,ARG_363,13.37,-0.52,0.81,0.58 2FZP,HIS_312,5.74,-0.37,0,-0.38 2PGX,ASP_48,2.79,-0.98,-0.47,0.45 3CJW,LYS_362,10.24,-0.2,0,-0.06 1GVP,LYS_87,10.43,-0.07,0,0

3M7D,GLU_372,3.84,0.34,-0.61,-0.41 2PIM.CYS 114,9.87,-0.24,0.08,1.04 3EUR,GLU_75,5.02,0.2,0,0.32 3UPD,HIS_149,4.67,-2.05,0.72,-0.5 3OBS, ASP_104, 2.21, -2.11, -0.19, 0.7 1RZ2,TYR 53,12.85,0,0.43,2.41 2X4G,LYS 151,10.61,-0.35,0.12,0.34 3E7P,HIS_68,6.91,-0.41,0.82,0 2PPN,LYS_35,11.27,-0.39,0.8,0.37 2YWJ,LYS 135,10.85,-0.4,0.37,0.38 1EV8.HIS 57.5.03.-1.26.0.-0.21 20PJ,ARG_128,13.59,-3.53,0.8,3.81 1MTZ.TYR 9,10.61,0.0.2,0.41 2ZQ5,ARG_66,11.82,-0.66,0,-0.02 3GS9,ASP 102,3.98,0,-0.02,0.21 3SMD.GLU 12,4,76,0,26,0,0 1WLY,ARG_279,12.2,-1.68,0.58,0.81 3U2R,GLU_135,4.96,0.38,0,0.08 3U2R.HIS 56.6.15.-0.46.0.0.11 3RJX.CYS 319,11.9.0.-0.05,2.93 2HP7,GLU_154,3.55,1.55,-2.01,-0.5 1YTD.GLU 23.4.63.0.23.0.-0.1 1J7G,GLU_104,4.49,0.3,0,-0.31 1MTZ.HIS 181,4.27,-2.62,0.69,-0.31 1T6L.LYS 35,9.94,-0.33,0,-0.22 3V75,ARG_173,13.11,-0.33,0.55,0.39 3PBH,TYR_214,11.3,0,0.24,1.08 3T5B,GLU_345,4.42,0.17,0,-0.25 2FB6,GLU 109,3.6,1.32,-1.7,-0.52 4F8A,ASP_587,3.82,0,-0.15,0.17 2PWO.GLU 3,3,77,0,48,-0,98,-0,24 3I0C,TYR_246,12.83,0,-0.05,2.89 1KN3,ASP 134,2.48,-1.21,-0.38,0.26 3IV4.ASP 50.4.28.0.0.03.0.45 2FD5,ARG_66,11.94,-2.04,0,1.48 3EVZ,ASP_55,3.49,-0.1,-0.64,0.42 1IAP,ARG_232,12.66,-0.14,0,0.29 2E0T,ARG 112,12.27,-0.16,0,-0.06 3LPZ,ARG_14,12.48,-0.19,0,0.17 3EJG,ASP_139,4.14,0,-0.15,0.49 2H85,GLU_266,4.43,0.36,-0.08,-0.35 2ZCO, ARG 34, 12.92, -0.67, 0.43, 0.65 3ETV,ARG 104,12.65,-0.26,0.05,0.35 3V3T,GLU_61,4.54,0.21,0,-0.18 2H8O,LYS_206,9.57,-0.56,0,-0.37 2B0A,GLU_19,3.99,0.16,-0.65,-0.02 3M7G,ARG 108,12.44,-0.2,0,0.14 2B78,ARG 200,13,28,-2,19,1,24,1,72 3RLE,GLU_154,4.72,0.15,0,0.07 1MML,ASP_235,4.12,0,0.06,0.26 1NIJ,GLU_171,4.13,0.26,-0.03,-0.61 2X4L.LYS 250,11.08,-0.82,0.85,0.55 3BCY,HIS_156,6.92,-0.41,0.78,0.05 2AZP.ARG 272,12,75,-0,48,0,33,0,39 3E7P,ASP_19,4.96,-0.01,-0.33,1.5 3CO1,LYS_76,10.33,-0.17,0,0.01 4ACJ.TYR 728,10.26,0.0.01,0.25 1PV5,GLU_208,4.74,0.36,0,-0.12 3Q9P,ARG_140,12.72,-0.26,0.1,0.38 10GL,LYS_251,10.22,-0.4,0,0.12 1SFE,ASP 42,3.01,-0.69,-0.42,0.32 3PZ9,LYS_205,10.08,-0.77,0,0.35 3BA1,ARG 146,13.88,-0.51,1.35,0.54 1Z9L,ARG_51,13.03,-0.81,0.78,0.57 2WB8,ASP_578,3.08,-0.89,-0.39,0.56 3M70,ASP 114,3.62,-0.21,-0.3,0.33 2VGM,HIS_290,7.35,-0.92,1.53,0.25 20KT,LYS_40,10.88,-0.31,0.21,0.48 2IQT,TYR_240,11.22,0,0.19,1.03

3GV0,GLU_274,4.7,0.13,0,0.07 2H2W,ARG 56,13.82,-1.64,1.78,1.18 1YM5,CYS_88,12.12,-0.2,-0.02,3.35 2EEY,ARG 158,12.69,-0.18,0,0.37 1JYH,GLU_124,4.85,0.29,-0.04,0.09 1U7U,CYS 274,13.81,0,0.57,4.24 1A80,CYS 195,11.85,0,-0.72,3.57 2YX0,LYS_133,10.44,-0.2,0,0.15 1UCH,ARG_215,11.29,-2.07,0,0.87 10I7,LYS_222,10.64,-0.13,0,0.27 1Q46,GLU_124,4.7,0.28,0,-0.08 1059.HIS 228.6.66.-0.16.0.0.32 2EA9,HIS_61,6.12,-0.5,0.12,0 3CCY,CYS_41,10.08,-0.1,-0.09,1.27 3RAZ.GLU 142.4.34.0.23.-0.24.-0.14 3H13,TYR 463,11.96,-0.38,0.39,1.95 3LMO,ARG_20,12.44,-0.45,0.14,0.25 1PVT,HIS_125,4.65,-1.55,0.47,-0.77 3TRE,TYR_76,10.52,0,0.16,0.37 1WJG,ARG_108,12.25,-0.25,0,0 3ZTA.LYS 22,10.36,-0.17,0.0.03 1RKA,ARG_276,12.28,-0.39,0,0.17 2QOP,ARG_45,12.5,-0.11,0,0.11 3LJN.GLU 311,3.97,0.24,-0.38,-0.39 3PP8.CYS 164.10.64.-0.28.-0.09.2.01 2H14,LYS_296,10.37,-0.22,0,0.09 1UXO.HIS 83.6.4.-0.26.0.0.16 2JKF,TYR_101,12.59,0,0.25,2.33 1R6Y,GLU_35,4.49,0.15,0,-0.16 1SI7.LYS 293.10.46.-0.06.0.0.02 2Z0W,GLU_15,3.78,0.23,-0.95,0 3RAZ,ARG_103,12.02,-0.5,0,0.02 3OAV.ASP 124.3.66.-0.35.0.0.22 3GFP,GLU 356,4.56,0.19,0,-0.12 4DIU,GLU_206,4.92,0.61,0,-0.19 2V4U,HIS_480,2.88,-2.83,0.08,-0.88 4ECC,HIS_31,6.06,-0.54,0,0.11 2Z61,ASP_86,3.42,-0.54,-0.05,0.21 3G6S,GLU_145,4.06,0.39,-0.82,-1.39E-17 3GA2,GLU_159,4.26,0.17,-0.34,-0.07 2AD1,ASP_30,3.97,0,-0.06,0.23 3FHF,LYS 30,11.36,-0.42,0.85,0.43 1PSW,LYS 92,10.36,-0.18,0.0.03 4H4J,LYS_233,10.4,-0.13,0,0.03 3PP8,ARG_55,11.52,-1.01,0,0.03 4EKU,LYS_198,10.49,-0.01,0,0 2VGY,TYR_47,11.24,0,0.46,0.78 3VJ8,GLU_229,5.25,0.89,0,-0.14 1L2F,LYS_134,11.4,-0.35,0.85,0.4 1N81,TYR_49,12.66,0,0.52,2.14 1X7F,GLU_343,4.47,0.48,-0.39,-0.12 3EYE.GLU 55.4.61.0.11.0.0 105T,LYS_96,10.46,-0.04,0,0 3BQW,TYR_159,13.77,-0.31,0.75,3.33 2RJD,TYR_275,10.57,0,0,0.57 2CN1,GLU_185,4.28,0.22,-0.79,0.35 2IF4,ASP_285,3.31,-0.26,-0.47,0.24 3CX2,HIS_206,6.25,-0.49,0.02,0.23 1JSX,CYS_151,12.08,0,0.04,3.05 1P6F,GLU_137,4.72,0.89,-0.21,-0.47 1YTD, ARG 127, 11, 95, -2, 2, 0, 71, 0, 94 1PZC,LYS_24,10.44,-0.4,0,0.35 2CXY,LYS 65,10.39,-0.11,0,0 2IF4,CYS_239,11.1,-0.35,-0.02,2.47

1PDB,HIS_130,6.31,-0.61,0.36,0.07

1JT9,GLU_73,5.36,3.29,-2.17,-0.26

4FZR,GLU_159,4.68,0.25,0,-0.08

3M16,LYS 322,10,41,-0.09,0,0

1X04.ARG 142.12.28.-0.41.0.0.19 3BPP,ARG 66,12,7,-0,18,0,0.38 1PZC,LYS_117,10.92,-0.17,0.22,0.37 20KT,LYS_88,10.56,-0.19,0,0.24 3EJC.GLU 28,3.64,0.39,-0.83,-0.42 2PP6.ARG 19.12.26.-0.24.0.0 1LTU,ASP_105,3.91,-0.28,0,0.39 1LTU,ARG_226,13.05,-1.88,1.51,0.92 3L7N,CYS_162,10.9,-1.61,0.49,3.04 1TP6,CYS 127,9.78,0,0.21,0.57 3JZN,HIS_185,5.79,-0.4,0,-0.31 2B6P,HIS_122,6.19,-0.31,0,0 3S0A,GLU_73,4.78,0.29,0,0 3GS3,ARG_27,12.61,-0.24,0,0.34 105T.LYS 432.10.48.-0.15.0.0.12 1P4X,LYS_8,9.87,-0.93,0,0.29 4AM1,ASP_41,2.62,-0.85,-0.68,0.35 3ADO,CYS_141,12.75,0,0.21,3.54 2B02,ARG_379,13.92,-0.56,1.35,0.63 3A7L,ASP 86,3,95,0,0,0,15 2FBI,LYS_139,10.46,-0.11,0,0.07 3B7X,HIS_67,6.17,-0.35,0,0.02 3EVZ,ASP_192,3.45,0,-0.57,0.21 1WNH, ASP 186, 3.32, -1.85, -0.2, 1.56 2YT4, ARG_570, 13.39, -0.49, 0.66, 0.72 3SMD, ASP_96, 2.07, -1.64, -0.71, 0.62 10LR,HIS_138,5.82,-0.6,0,-0.08 3CX2,CYS 249,9.75,0,0.1,0.64 1RWZ,LYS_199,11.54,-0.28,0.85,0.47 1KN3,ASP_96,3.98,0,-0.16,0.34 3DB9,LYS_100,10.46,-0.2,0,0.16 1TD6,LYS_185,10.43,-0.07,0,0 1G8P,ARG 229,12.57,-0.12,0,0.18 20K0,ARG 80,13,39,-0,4,0,84,0,44 1ZBM,LYS_24,10.55,-0.21,0,0.26 2R57,CYS_359,11.29,-0.23,-0.28,2.8 1ZBS,GLU_80,3.91,0.26,-0.46,-0.38 4H86.GLU 45.4.58.0.26.0.-0.18 1ZCE,LYS_13,11.14,-0.21,0.47,0.38 3ASA,GLU_377,4.7,0.1,0,0.1 3ZTA,HIS_29,6.43,-0.16,0,0.1 2YWJ.TYR 104,13.47,0.85,0.57,2.05 3PZ9,LYS 265,10.62,-0.22,0.0.34 3FFM,GLU_143,4.84,0.23,0,0.11 1XWM,GLU_91,5.29,1.31,-0.68,0.16 4DBX,ARG_178,13.62,-0.27,0.64,0.75 3BZT,TYR_272,10.31,0,0,0.31 2ZQ5,GLU_172,7.03,3.2,-1.43,0.76 3O16,GLU_172,4.65,0.28,0,-0.13 3UC9,ASP_55,2.57,-1.64,-0.66,1.08 204D,GLU 22,4.2,1.6,-1.49,-0.41 1RZ2,GLU 59,3.95,0.56,-0.8,-0.3 4EVF,HIS_146,4.32,-1.93,0,-0.24 1TR9,GLU_307,3.68,0.26,-0.95,-0.14 3B4D,LYS_223,10.35,-0.1,0,-0.05 1T6L,HIS_145,5.88,-1.15,0.85,-0.31 3LJI,HIS_180,6.59,-0.61,0.79,-0.1 3SMD,LYS_73,10.39,-0.11,0,0 3K8J,ARG_61,12.51,-0.36,0,0.36 1ZBS,TYR 248,12.11,-0.97,0.03,3.06 3F1X,ARG 164,13,25,-2,83,1,36,2,22 1XIP,ASP_74,2.9,-0.69,-0.44,0.23 4DBX,ASP_237,3.98,0,0,0.18 3I4T,ASP_225,2.98,-0.96,-0.35,0.49 3LJC,LYS_239,10.42,-0.08,0,0 30IP,LYS 147,11.46,-0.28,0.85,0.38 2CI3,GLU_77,5.47,4.2,-1.64,-1.59 10I7,ARG_117,11.81,-0.88,0,0.19 3RFY,ARG 196,11.96,-0.44,0,-0.1

3M70,TYR_103,12.37,0.85,0.36,1.16 1TD6.HIS 140.5.85.-0.39.0.-0.26 1S7K,CYS_134,10.91,0,-0.03,1.93 3EJC,LYS 6,10,44,-0.06,0,0 3RJX,TYR 267,10.39,-0.24,-0.29,0.92 4H89.TYR 33.11.95.-0.42.0.62.1.74 2CWY,ARG 13,12,58,-0.33,0.06,0.35 1UAJ,ARG_183,12.46,-0.04,0,0 2FM9,ASP_223,3.03,-1.38,-0.13,0.73 3EVZ,LYS_244,9.96,-0.71,0,0.17 2WB8,GLU_530,3.92,0.31,-0.85,-0.04 2R51,TYR_194,10.68,0,0.32,0.36 2FL4,LYS_14,10.33,-0.31,0,0.12 3FTT,LYS_127,10.2,-0.36,0,0.06 2EYI,HIS_170,5.35,-0.95,0.04,-0.24 2PGX.ASP 58.3.47,-1.08,-0.3,1.05 3CN5,HIS_260,5.14,-1.11,0,-0.25 1SQH,ARG_207,12.13,-0.41,0,0.05 1YTD,ASP_49,3.79,-0.18,-0.06,0.23 1V8E,ARG 54,12.61,-1.29,0.54,0.85 3N0K,ARG_33,12.22,-0.28,0,0 2EEY,HIS 97,5.92,-0.62,0.0.04 1MUF,ARG_323,12.38,-0.34,0,0.21 2DFL.ARG 242,12.91,-0.23,0.3,0.34 1CHD.GLU 156.5.04.1.0.-0.45 3CN5,TYR_122,12.45,-0.7,0.08,3.07 3SMD,TYR_7,11.71,0,0.39,1.31 3M3P,ARG_82,12.41,-0.27,0,0.18 2EFK,ARG 35,13.11,-0.57,0.73,0.45 1HF8,ASP_263,4.3,0,0.22,0.28 2AD1,ASP_280,3.88,-0.85,-0.65,1.59 2CN1,TYR_103,13.62,0,0.69,2.92 3EVZ,ARG 40,12.15,-0.35,0,0 2W1R.GLU 159.4.53.0.43.0.-0.4 2AHE,GLU_241,4.84,0.6,0,-0.25 1JB3,ARG_84,11.7,-1.02,0,0.24 1J85,GLU_53,2.59,0.69,-2.2,-0.41 3G9G,LYS 152,9.76,-0.61,0,-0.13 2CVB,LYS_49,10.66,-0.29,0,0.44 1P1L,ARG_88,12.43,-0.07,0,0 3M3P,GLU_135,4.94,1.68,-0.76,-0.46 3MEW.ARG 208,12.31,-0.13,0,-0.06 2B78,ARG 281,12,23,-0,31,0,0,04 2WZ9,ARG_114,12.39,-0.24,0,0.13 4FCU,ARG_165,12.44,-0.07,0,0.01 4AE7,GLU_179,4.75,0.25,0,0 4EF5,HIS 332,5.42,-1.29,0.66,-0.45 4F3J,HIS 237,6,44,-0,38,0,04,0,27 3CS1,LYS_165,11.17,-0.31,0.37,0.61 2QV2,TYR_51,10.97,0,0.43,0.55 3LJN.GLU 119.3.57.0.27.-0.76.-0.44 2l6l,ARG 127,12.31,-0.62,0.11,0.32 2ATR,LYS_110,9.95,-0.29,0,-0.26 2H85.TYR 278.12.34.0.0.63.1.71 3M7G,GLU_186,4.67,0.39,-0.11,-0.1 3LJC,HIS_24,5.91,-0.75,0,0.15 1NAF.ASP 171.2.88,-0.39,-0.63,0.1 4ETX,ARG_376,12.08,-0.26,0,-0.17 4HDE,TYR_183,10.94,-0.06,0.04,0.96 1F2V,ARG 87,12.1,-0.5,0,0.1 2ATR/LYS 89/10.36/-0.14/0/0.01 3OIP,TYR_70,13.8,0,0.7,3.1 1EQ6,ASP_126,3.72,-0.85,0,0.77 2BCF,LYS_106,10.7,-0.2,0.08,0.34 1RI6,TYR_51,9.68,-0.58,-0.38,0.64 2GZQ,ARG_190,12.45,-0.22,0,0.16 4D8L,TYR_49,10.01,0,-0.07,0.08 3NR5,GLU_70,3.97,0.94,-1.65,0.18 1ILW,ARG_135,13.53,-0.64,1.2,0.47

2CWC,ARG 234,12.2,-0.36,0,0.06 2IRM,ARG_173,12.38,-0.17,0,0.05 3LQE,ARG_322,12.33,-0.74,0,0.57 2BQQ,ASP_81,4.05,0,0,0.25 3H5T,ARG_222,12.67,-0.99,0.6,0.56 1KN3,ASP 174,2.87,-2.25,-0.05,1.37 3EIZ.TYR 130.10.23.0.0.0.23 3DSH,ARG_396,12.5,-0.04,0,0.04 4E9E,ASP_495,3.05,-0.91,-0.28,0.43 2H2Z,ASP_216,4.06,-0.54,-0.17,0.98 2H14,GLU 322,4.11,0.34,-0.77,0.04 2AH5,TYR_103,11.69,0,0.46,1.22 2PGE,ARG_80,12.25,-0.39,0,0.14 1XTD,GLU_109,4.55,0.07,0,-0.02 1WLY,CYS 89,13,24,0,0,31,3,92 1DTO.HIS 56.6.28,-0.22.0.0 3GV0,GLU_121,4.45,0.13,0,-0.19 3CAX,ARG_394,12.51,-0.28,0.04,0.25 3JSN,ASP_135,2.34,-1.74,-0.13,0.41 3LQE,GLU 292,4.88,0.38,0,-0.01 3F6F.GLU 196.4.45.1.06.-0.48.-0.63 1WXQ,ASP_98,4.44,-0.18,0.25,0.57 3DHN,HIS_47,6.72,-0.34,0,0.55 208I,ASP_136,3.91,0,-0.12,0.23 2WZ9.LYS 111.11.26.-0.49.0.85.0.41 2OSA,GLU_334,4.7,0.19,0,0.01 1AT0,GLU_307,3.56,0.29,-0.85,-0.38 1MTZ,TYR_159,11.51,0.68,0.38,0.45 3IVF,GLU 252,3.41,0.18,-0.76,-0.51 3ADO,HIS 294,7,4,-0,34,0,85,0,38 2X4L,ASP_262,3.17,-0.85,-0.02,0.24 1IDK,ARG_236,11.39,-2.19,0.1,0.98 1LZL,GLU_307,3.48,1.25,-1.7,-0.57 3T57,HIS 119,6.06,-0.38,0,-0.07 2H85,TYR_324,12.11,-0.85,0.04,2.91 3PM2,ARG_74,13.16,-0.51,0.81,0.36 2O0K,LYS_99,10.3,-0.19,0,-0.01 4EVF,ASP 16,3.82,0,-0.37,0.39 2IXM,ASP_113,3.98,0,-0.33,0.5 2DG7,ASP_5,2.16,-1.64,-0.52,0.53 1NIJ,GLU_115,4.55,0.09,0,-0.04 1SFE,GLU_111,4.69,0.19,0,0 105T,HIS 387,6.01,-0.97,0.5,-0.03 3T8R,GLU_33,4.74,0.25,0,0 20KT,ARG_100,13.48,-1.89,1.58,1.3 1RI5,ASP_203,3.89,0,0,0.09 3FS3,LYS 170,10.5,-0.06,0,0.06 1DCF,HIS_81,5.83,-0.28,0,-0.39 2PLQ,TYR_227,11.52,0,0.15,1.37 1RI5.GLU 202.4.6.0.1.0.0 2H85,GLU_41,4.98,0.38,-0.14,0.24 1Y2Q,LYS 59,12.23,-0.58,1.46,0.84 3HUE, ARG 316, 12, 78, -0.21, 0, 11, 0, 38 2F9F,GLU_79,3.75,0.18,-1.04,0.1 2FZP,CYS_291,10.53,-0.18,0.23,1.49 2ZCO,HIS_78,6.62,-0.83,0.8,0.14 1X04,GLU_68,4.19,1.02,-0.85,-0.48 1ZHV,LYS_114,11.07,-0.22,0.47,0.33 2B3M,ARG_111,12.81,-0.21,0.27,0.25 2R0S,HIS_177,6.17,-0.3,0,-0.03 2C2Y,ARG_12,12.65,-0.8,0.35,0.6 1ZHV.HIS 124,5.87,-1.36,0.81,-0.08 1YLN,ARG_94,12.02,-0.42,0,-0.06 1WYC,HIS_38,6.79,-0.68,0.82,0.14 1X7F,CYS_165,10.98,-0.63,0.09,2.52 3VHJ,LYS_121,11.29,-0.17,0.55,0.41 3GA2,ARG_180,11.93,-0.74,0,0.16 2E3S,ARG 582,12.31,-0.29,0,0.09 10LR,ARG_84,12.57,-0.18,0,0.25

30IP,CYS_124,12.47,0,-0.05,3.52 3CQ1,GLU 22,4.92,0.24,0,0.18 3CJW,ASP_235,3.89,0,-0.07,0.16 3CBN,ARG_118,12.9,-1.22,0.82,0.79 2E0T,HIS_119,6.24,-0.21,0,-0.05 2W0G.GLU 201.4.63.0.09.0.0.04 1XTZ.LYS 185.10.72.-0.13.0.0.35 2V1L,GLU_40,4.72,0.12,0,0.09 3P28,GLU_94,3.62,0.33,-1.22,0 1WXF,CYS_94,9.63,-0.27,-0.07,0.97 20YZ,TYR_93,11.74,0.08,1.11,0.56 3KT9.TYR 94,11.9.0.85,0.41,0.64 2AXO,GLU_47,4.24,3.93,-2.16,-2.03 4GCO,ASP 241,2.59,-1.6,-0.04,0.44 1N81,LYS_156,10.27,-0.15,0,-0.08 2JEO,ASP_159,3.62,-0.36,-0.52,0.69 2012.TYR 48.10.52.0.0.18.0.34 2D0A,HIS_226,5.39,-1,0,-0.1 3GE9,ARG_97,12.41,-0.09,0,0 3AU3,ASP_397,3.63,-0.24,0,0.06 3SMD,LYS 9,10,39,-0,11,0,0 3JSN,ARG_202,13.43,-0.57,1.06,0.44 1J33.ASP 14.4.08.0.-0.18.0.46 1ZBS.ARG 103.12.87.-1.51.0.33.1.55 2AHE, HIS 196, 4.07, -2.22, 0, -0.21 3CRM,ASP_302,3.54,-0.84,-0.01,0.59 3U2A, ARG_109, 12.37, -0.33, 0, 0.21 3IL3,GLU_57,4.14,0.91,-0.85,-0.42 1Z3X.ARG 189.12.19.-0.48.0.0.17 1JKS,TYR_129,10.15,-0.72,0.06,0.82 4DVD,GLU_103,3.87,0.42,-0.72,-0.33 2QVO,GLU_56,4.56,0.13,0,-0.07 3EX9,CYS_80,10.16,0,0,1.17 2AZL,ASP_35,2.79,-1.15,-0.54,0.68 2007.LYS 470,10.43,-0.07.0.0 1059,GLU_129,3.01,0.99,-1.7,-0.78 1HF8,LYS_221,10.11,-0.53,0,0.14 2NMU,ARG_125,13.24,-1.3,1.25,0.79 4AM1,ARG 256,12.17,-0.35,0,0.02 1XIP,ARG_181,11.79,-1.38,0.22,0.45 3M66.LYS 275.10.28.-0.16.0.-0.06 2PWQ,GLU_42,4.88,0.29,0,0.08 2GZQ,ARG_84,12.32,-0.08,0,-0.1 2H8O,ARG 42,13.84,-0.68,1.13,0.9 2CXC,GLU_33,3.9,0.35,-0.61,-0.35 3PZ9,TYR_114,12.68,0.85,0.64,1.19 1WRU,LYS_257,10.44,-0.09,0,0.03 4FZR,ASP 200,4.01,-0.23,0,0.44 30NH,ASP_479,2.71,-2.09,-0.35,1.36 3V46,GLU_374,4.2,0.25,-0.29,-0.26 2WB8,GLU_516,4.35,1.75,-1.26,-0.64 2PP6,CYS_31,10.66,0,0.05,1.61 3K8U,LYS 43,10.63,-0.23,0,0.36 2YWJ,CYS_75,12.04,-0.1,0.02,3.12 3FTT,HIS_114,6.29,-0.6,0,0.39 3JZ9,ASP_512,2.88,-0.85,-0.4,0.34 4DBX,LYS_155,10.55,-0.11,0,0.16 2CIU.LYS 118.10.5.0.0.0 10GL,LYS_60,10.46,-0.26,0,0.21 2CIU,HIS_221,6.82,-0.29,0.63,-0.03 3DHN,TYR_92,11.57,0,0,1.57 2C2Y,ASP 105,3.61,-0.5,0.0.32 2G3A,LYS_80,10.4,-0.1,0,0 1X9G,LYS_185,10.2,-0.26,0,-0.05 3F7M,HIS_173,10.74,-2.17,2.45,3.96 3V75,GLU_272,4.76,0.49,0,-0.23 1R5O,LYS 35,10,25,-0,34,0,0.08 3G9T,HIS_74,3.67,-3.19,0.84,-0.49 3IV4,LYS_19,10.86,-0.26,0.27,0.34

2VAN.ASP 130.3.39.-0.51.-0.28.0.38 4FCU.LYS 169.10.47.-0.03.0.0 3V75,GLU_191,4.69,0.18,0,0.02 3CIV,ASP_30,4.03,0,0.09,0.14 2CWC,ARG 176,12.29,-0.82,0.49,0.13 4D8L.GLU 7.4.08.0.24,-0.46,-0.19 3C5V,GLU_225,4.33,0.7,-0.85,-0.03 1AK1,GLU_23,3.53,0.31,-0.85,-0.43 2C2Y,ARG_195,12.5,-0.06,0,0.07 1J33,ARG_12,13.56,-0.78,1.46,0.38 3P28,TYR_58,13.39,-0.85,0.09,4.15 2H8O,ARG_137,12.04,-0.35,0,-0.11 1DTO,GLU_74,4.91,0.41,0,0 3IL3,LYS 234,10.35,-0.33,0,0.18 2B3M.GLU 151.4.09.0.32.-0.27.-0.47 3V75,ARG_12,13.92,-0.36,1.3,0.48 2E0T,GLU_117,4.36,0.31,-0.02,-0.43 3ELI,ARG_93,12.12,-1.08,0.41,0.29 3ETU,ARG_269,11.41,-1.21,0,0.13 2PIM.GLU 39,3.85,0.53,-0.51,-0.66 3DHN,ASP_181,4.12,0,0.04,0.28 3C6B,TYR_123,13.18,-0.01,0.06,3.14 1X91.GLU 74.5.45.0.66.0.0.3 2CWY.ARG 60.12.41.-0.09.0.0 1EV8,ASP_89,3.65,-0.82,0.34,0.33 1YDL,TYR_22,10.11,0,0,0.11 1ZP2,TYR_84,10.17,-0.57,-0.07,0.82 2A0J,ARG 35,12.55,-0.08,0,0.13 3DB9,ASP_98,3.79,0,-0.22,0.21 3ERF,GLU_204,5.21,0.19,0.18,0.35 2QOP,HIS_51,5.54,-0.71,0,-0.25 1BKR,LYS_2,10.38,-0.12,0,0 1YB2,ASP 195,4,0,0,0.2 3GS3.ASP 194.4.23.0.0.24.0.19 1UXO,LYS_24,10.45,-0.24,0,0.19 1SJY,GLU_68,4.66,0.36,0,-0.2 1G5Z.LYS 92,10.26,-0.28,0.0.04 3H04,LYS 29,9,94,-0.61,0,0.05 1JSX,ARG_106,12.19,-0.28,0,-0.04 1JKS.GLU 17.3.71.0.24,-0.65,-0.38 4ETX,ARG_239,12.5,-0.25,0,0.25 1S7K,GLU 153,2.99,0.6,-1.69,-0.41 3IL3,LYS 132,10,45,-0,34,0,0,29 3LH5,ASP_547,3.45,-0.72,0,0.37 2E3C,LYS_435,9.93,-0.59,0,0.02 3RLN,LYS_627,10.29,-0.21,0,0 1ES5,LYS_61,10.8,-0.19,0.11,0.37 3LMO,ASP_42,4.17,0,0.06,0.31 1MUF,ARG_312,11.93,-2.4,0,1.82 1XEU,LYS_175,10.72,-0.31,0,0.54 3E7P,HIS_205,6.57,-0.73,0.26,0.54 2FBO.GLU 20.3.88.0.43.-0.78.-0.28 1ZCU,CYS_97,12.08,-0.79,0.05,3.82 2CWY,ASP_4,3.2,-0.93,-0.01,0.35 3M7G,TYR_238,11.93,0,0.59,1.35 2PP6,ASP_3,4.02,0,0,0.22 2XWS,ARG_47,13.15,-0.25,0.49,0.41 3EZ7,LYS_316,10.41,-0.09,0,0 1YR6,ARG_155,12.21,-0.37,0,0.09 2P5D,GLU 66,3.95,0.68,-0.53,-0.7 2Z0M,ARG 230,12.39,-0.34,0,0.22 1W7B,LYS_204,11.1,-0.25,0.47,0.38 3ETU,GLU_155,3.59,0.25,-0.85,-0.31 2VAN, ASP_332, 2.78, -0.85, -0.56, 0.39 1KCM,GLU_249,4.56,0.29,0,-0.23 1YG2,CYS 55,9.43,0,0,0.43 1YOY,ARG_166,12.33,-0.17,0,0 1NIJ,LYS_220,10.51,-0.17,0,0.17 20PJ,ARG_170,12.29,-0.31,0,0.11

3K8J,TYR_127,10.72,-0.18,0.02,0.89 4D8L,ASP_241,2.86,-0.75,-0.59,0.41 1H4U,LYS_407,11.12,-0.37,0.61,0.38 1ZYL,TYR_128,9.79,-0.31,-0.42,0.52 1YB2,LYS 115,10,43,-0.07,0,0 2Z61.LYS 280.10.38.-0.15.0.0.02 3P51,TYR_46,9.78,-0.31,-0.29,0.38 1SJY,GLU_40,4.72,0.25,-0.02,0 4AM1,ARG_129,11.67,-3.4,0,2.57 1ZHV,ARG_18,12.54,-0.24,0,0.28 1V43,LYS_187,10.49,-0.14,0,0.13 1TR9,LYS_47,10.47,-0.11,0,0.08 2PLO.LYS 278,10,34,-0,33,0,0,16 1SQH,ARG_47,12.56,-0.11,0,0.17 1R3F.CYS 193.10.21.-0.6.-0.08.1.88 20EW.GLU 174.4.6.0.1.0.0 2F8H,ARG_360,12.16,-0.8,0,0.46 2IF4,GLU_43,3.98,0.12,-0.64,0 1JB3,HIS_122,6.65,-0.17,0.12,0.2 1GXN,LYS 592,10.56,-0.34,0,0.4 1ZCE,LYS_82,11.52,-0.23,0.75,0.5 2|6|,ARG 130,12.38,-0.35,0.0.22 3ONT,ASP_39,4.33,0,0.3,0.23 3DHN,TYR 219,11.33,-0.66,0.59,1.41 4GCO,LYS 189,10.61,-0.33,0.03,0.4 3C2E,CYS_255,9.96,0,0.16,0.81 2GAU,GLU_142,4.72,0.23,0,-0.01 1JSX,GLU_196,3.37,0.37,-1.1,-0.39 3ASA,GLU_283,4.05,0.9,-0.9,-0.46 2HRZ,GLU_216,4.36,0.26,-0.16,-0.23 1ZHV,ARG_4,12.37,-0.13,0,0 2FD5,GLU_118,4.53,0.27,0,-0.24 1AIL,LYS 62,10.23,-0.43,0,0.15 2H85,LYS 289,10.6,-0.38,0.0.49 2H8O,LYS_178,10.04,-0.73,0,0.27 1RI5,GLU_133,4.52,0.35,0,-0.33 1JKS,GLU_100,6.31,1.15,0,0.66 1CHD,TYR 243,10.82,-0.19,-0.11,1.11 1XFK,CYS_246,11.39,-0.06,-0.29,2.73 2BLL,ARG_426,10.75,-2.57,0,0.83 2H01,GLU_60,4.74,0.25,0,-8.67E-18 3RLE,ASP 106,4,0,0,0,2 2AHE, TYR 128, 13, 36, 0, 59, 0, 43, 2, 33 3EAZ,ASP_141,2.54,-2.08,-0.05,0.87 3DSH,LYS_401,10.19,-0.11,0,-0.21 3PP8,GLU_233,5.12,1.49,-0.9,0.02 3KV0,TYR 186,13.53,0,0.07,3.46 3IO0.GLU 80.4.12.0.32.-0.66.-0.03 3EVP,LYS_237,10.91,-0.29,0.22,0.47 3O48,GLU_73,4.54,0.14,0,-0.1 2F8H.ARG 298.12.98.-0.24.0.25.0.47 1ZCE,ASP 147,3.97,0.0.02,0.15 1ZBM,LYS_66,10.63,-0.16,0,0.29 3A4C,GLU_516,4.86,0.48,0,-0.11 3FK5,TYR_33,11.78,-0.68,0.31,2.16 3CO1,HIS_57,5.76,-0.23,0,-0.52 2F8H,LYS 202,10,28,-0,36,0,0,14 3P51,GLU_109,3.99,0.78,-0.8,-0.49 4EF5,CYS_257,13.17,0,0.23,3.94 2HRZ,ARG 176,12.33,-0.15,0,-0.02 1R9W,ASP 342,3,98,0,-0.06,0.24 1IAP,CYS_78,11.57,-0.06,0.03,2.6 2VGM,ARG_332,12.63,-1.76,0.85,1.04 3CAX,ASP_365,4.22,-0.81,-0.46,1.69 1WP5,ARG_23,12.34,-0.15,0,-0.01 1YG2,ARG_42,12.16,-0.35,0,0.01 4DIU,LYS_80,10.72,-0.2,0,0.42 2H8O,ARG_299,12.78,-0.38,0.29,0.37 3IRA,GLU_37,4.05,0.31,0,-0.76

3M7G,ARG 193,13.27,-0.52,0.47,0.82 3BB7.HIS 305.3.07.-3.43.0.0 3GW3,LYS_242,10.42,-0.1,0,0.01 2H14.LYS 165.9.94.-0.65.0.0.09 2IXM,HIS_31,6.44,-0.35,0.25,0.04 2QV2,GLU_148,3.99,0.26,-0.76,0 2YX0,HIS_69,4.88,-1.87,0.85,-0.61 3FFM,ASP_150,4.12,0,-0.28,0.6 3CQ1,ASP_35,3.56,-0.38,-0.26,0.4 2PGX,LYS_2,10.59,-0.11,0,0.2 1Z3X,GLU 200,2.68,0.56,-1.92,-0.46 2WB3,LYS 304,10.38,-0.12,0.0 1EW4,CYS_80,8.04,-2.36,0.28,1.12 2JKF,TYR_89,10.51,0,0.3,0.21 1TJE.ARG 72.11.72.-0.9.0.0.12 3ANJ,ASP 241,3,43,-0,39,-0,29,0,31 2A1V,LYS_122,10.4,-0.09,0,-0.01 1YM5.GLU 118.4.6.0.1.0.-0.01 2XMZ,GLU_144,4.49,0.16,0,-0.17 1ANU,LYS_7,10.6,-0.22,0,0.32 2PLO,ARG 264,13.8,-0.73,1.41,0.61 3LJN.LYS 133.10.48.-0.02.0.0 1EYH,ARG_25,12.48,-0.53,0.09,0.42 2GYZ,ARG 71,12.61,-0.17,0.0.28 1YW5,ARG 175,12.4,-2.68,1.2,1.39 10TM,LYS_187,10.41,-0.12,0,0.03 3ZSL,GLU_185,4.39,1.08,-0.79,-0.4 3LJN,GLU_31,3.64,0.37,-0.82,-0.41 2D7J,ASP_130,4.51,0,-0.09,0.79 3VJ8,TYR_174,11.32,0.53,-0.03,0.81 3HVM,TYR_137,10.55,0,0.19,0.36 3G9G,GLU_45,4.67,0.2,0,-0.03 2EHG.GLU 120.4.87.0.38.0.-0.01 2D7U,ASP 297,4.26,-0.07,0.11,0.41 1WOU,CYS_69,12.55,0,0.07,3.48 1PNE,LYS_69,9.69,-0.56,0,-0.25 2EYI,ASP_138,3.5,-0.44,-0.45,0.58 3M70,LYS_164,11.05,-0.38,0.52,0.4 4F85,ARG 204,12.56,-1.01,0.58,0.48 4AE7,LYS_53,10.51,-0.27,0,0.28 1M5I,ARG_168,12.41,-0.3,0,0.21 3V46,ASP_348,2.99,-0.74,-0.48,0.4 3EYE.TYR 57,10.26,0,0,0.26 3IVF,LYS_322,10.42,-0.08,0,0 2EA9,ASP_56,4.13,0,0,0.33 2W0G,HIS_148,6.11,-0.14,0,-0.25 1FQI,LYS 368,10.53,-0.05,0,0.08 30NH,TYR 489,10.85,0,0.64,0.2 1FHL,ASP_60,4.03,0,0,0.23 100E,ASP 171,3.85,-0.23,-0.02,0.3 1QQH,TYR_159,11.22,-0.37,0.82,0.77 2PGX,GLU 49,3.18,0.59,-1.38,-0.53 1KCM,LYS 117,9.85,-0.69,0,0.04 4FZR,ASP_375,2.18,-1.66,-0.4,0.44 2D8N,ASP_110,4.34,-1.18,-0.01,1.74 2D2S,GLU_593,4.79,0.29,0,0.01 1ZP2,CYS_190,9.43,-0.12,0.07,0.49 1QQE,ASP_58,4.66,0,-0.25,1.12 2EJX.GLU 5.4.38.0.37.0.-0.49 2G9D,CYS_91,12.75,0,0.32,3.44 1EDG,ASP 268,4.02,0,-0.01,0.23 2X4L.GLU 128,4.56,0.09,0,-0.03 2H85,GLU_215,4.85,0.28,0,0.07 2P0Y,LYS_305,10.55,-0.11,0,0.16 1NIJ,HIS_114,6.25,-0.59,0,0.33 3Q9P,ASP_149,2.7,-1.53,0,0.43 2QDJ,ARG_355,12.23,-0.46,0,0.19 3CRM,ARG_311,12.22,-0.25,0,-0.02 1VJG,LYS_116,10.25,-0.25,0,0

4DND.CYS 29.9.25.-0.37.0.07.0.56 2QHT,GLU 134,4.94,0.26,-0.02,0.2 2BV9,ASP_201,3.6,-0.85,0,0.65 1AK1,ARG_3,12.31,-0.41,0,0.22 1EV8,ASP_13,3.95,-0.23,0.06,0.31 3H5T,LYS 139,10,78,-0.84,0.85,0.26 2EHG.GLU 119.3.91.0.26.-0.75.-0.09 3HYQ,GLU_173,5.07,0.21,0.25,0.12 1PBV,ARG_205,12.46,-0.04,0,0 2PP6,ARG_70,12.7,-0.17,0.05,0.31 2W0G,GLU_185,3.15,0.43,-1.27,-0.52 3EUR,LYS_7,10.16,-0.35,0,0.01 2Q13,CYS_335,9.72,0,-0.04,0.75 3LH5,TYR_550,10.11,0,0,0.11 2NYC,ARG_291,12.53,-0.09,0,0.12 2QEV,TYR 94,13.05,0,0.06,2.99 2D7U,ARG_257,12.52,-0.48,0,0.51 3FHF,GLU_14,4.62,0.08,0,0.04 4DNU,GLU_140,4.12,0.28,-0.5,-0.16 1RI5,LYS 185,10.85,-0.22,0.11,0.46 2BAA.TYR 31.10.95.0.-0.06.1.01 2D7J,GLU_111,3.9,0.28,-0.65,-0.22 2CXC,GLU 46,4,24,0,45,-0,38,-0,33 3A2Z,ARG 65,13.06,-2.72,1.44,1.83 20DJ.LYS 130.11.61.-0.42.0.85.0.69 2E3S,HIS_378,5.05,-2.1,0.65,0 3PBH,HIS_7,6.68,-0.49,0.63,0.04 1TJE,ARG_183,12.46,-0.58,0,0.54 4HDE,LYS_56,10.27,-0.16,0,-0.06 2FXT,GLU_269,4.59,0.09,0,0 3H5T,ARG_312,12.05,-0.53,0,0.07 2H85,GLU_44,4.54,0.24,0,-0.2 3CXS,LYS_80,10.46,-0.04,0,0 1NJ4,ARG 243,13.83,-0.35,1.07,0.62 2F8H,ASP 121,3.87,-0.17,-0.1,0.35 1X1E,LYS_54,11.15,-0.16,0.33,0.48 2Q98,GLU_162,4.98,0.38,0,0.1 2W0G,GLU_198,4.58,0.74,-0.47,-0.19 1FO9,ARG 358,13.71,-0.27,1.05,0.42 105T,LYS_249,10.36,-0.13,0,-0.01 3T8R,ASP_78,2.45,-1.88,-0.27,0.8 2YWK,TYR_76,10.23,0,-0.07,0.3 1DVO,GLU 52,4.54,0.16,0,-0.11 3EVN,GLU_292,4.74,0.3,0,-0.06 3F6F,LYS_79,10.4,-0.1,0,0 2YT4,TYR_621,10.51,0,-0.02,0.53 1AT0,LYS_273,11.06,-0.36,0.42,0.5 3EVN,GLU_238,4.94,0.54,0,-0.1 3PZ9,HIS_152,6.72,-2.21,1.59,0.84 3LJN,ARG_175,12.3,-2.59,0.63,1.77 1P2F,LYS_189,10.33,-0.14,0,-0.03 3CIV,ASP 308,4.19,0,-0.02,0.41 105Z.GLU 628.3.59.0.34.-0.85.-0.4 1XDZ,LYS_53,10.66,-0.41,0,0.57 1RHS,GLU_218,4.74,0.09,0,0.15 2HNG,GLU_49,4.82,0.09,0,0.23 3C2E,LYS_191,10.35,-0.17,0,0.02 1RAJ.ARG 408.12.48.-0.06.0.0.05 2OB5,LYS_143,9.75,-0.65,0,-0.09 1WLY,HIS_193,5.67,-0.83,0,0 1R6Y,HIS_71,6.79,-0.42,0.31,0.41 1RZ2,LYS 111,11,29,-0.46,0.6,0.65 1XIP,ARG_321,12.86,-0.48,0,0.84 3PP8,ASP_82,2.3,-1.64,-0.14,0.29 1DUN,GLU_95,4.82,0.18,0,0.14 2Q13,TYR_147,10.1,0,-0.07,0.17 3BPV.HIS 18.7.95.-1.37.1.7.1.12 1SQW,CYS_69,9.95,-0.74,-0.43,2.12 1WJG,ARG_96,12.22,-0.46,0,0.17

1GVP,TYR 41,10.14,0,0.08,0.05 2IOT.HIS 182.6.51.-0.12.0.0.13 2AXO,TYR_135,12.46,0.85,0.48,1.13 3GEC,ASP_260,4.16,0,0.12,0.24 3I0C,ARG 198,13.67,-0.31,1.06,0.41 4DBX.GLU 14.4.66.0.17.0.-0.02 3MTT,ASP_552,4.06,-0.03,-0.04,0.32 3M9A,GLU 72,3.43,0.53,-1.03,-0.57 2B0J,GLU_94,4.32,0.66,-0.35,-0.49 1YR6.LYS 205.10.29.-0.22.0.0.01 3LH5,ARG_561,13.09,-1.19,0.88,0.92 2D7U,ARG_269,12.67,-0.3,0.17,0.31 3EIZ,ASP_11,4.04,0,0.03,0.22 1PSW,GLU_65,3.87,0.16,-0.25,-0.54 1X1E.TYR 192.10.12.-0.52.0.19.0.45 3COU, ARG_6, 13.37, -0.48, 0.81, 0.53 3CBN,GLU_141,4.41,0.25,-0.08,-0.26 2VAN,ARG_253,11.52,-1.64,0,0.66 1X6J,ASP_33,2.83,-0.79,-0.58,0.4 3TMO,HIS 246.6.27,-0.28,0.0.05 3RVC,ASP_173,2.82,-1.34,-0.14,0.5 2IQT,HIS_227,7.11,-0.52,0.85,0.28 4HDE.ASP 185.3.86.0.-0.28.0.34 2VGM.LYS 44.10.22.-0.37.0.0.08 4D8L,ARG_130,12.28,-0.25,0,0.04 1T07,LYS_44,11.58,-0.27,0.85,0.5 1SI7,ARG_247,13.01,-0.4,0.64,0.27 2CN1,GLU_85,5.95,2.08,0,-0.63 1NJ4,ARG_40,11.6,-1.14,0,0.24 1X7F,GLU_361,4.79,0.32,0,-0.02 2B0J,ASP_157,3.63,0,-0.39,0.22 3DB9,LYS_18,10.41,-0.09,0,0 1S7K,ARG 123,12.36,-0.14,0,0 2G5X.ARG 93.12.48.-0.08.0.0.06 1MML,HIS_143,6.47,-0.87,0.75,0.08 3HVM,GLU_236,4.18,0.42,-0.26,-0.48 3PU6,LYS_3,11.77,-0.57,1.07,0.76 1LZL,GLU_258,3.52,0.71,-1.57,-0.11 1T6L,CYS_175,9.05,-0.04,-0.03,0.12 1ZCU.TYR 196.10.16.0.0.0.16 1A8Q,GLU_190,4.48,0.8,-0.51,-0.31 2OJQ,LYS 627,10.59,-0.17,0,0.26 3F7M,ARG 251,13.3,-0.39,0.76,0.43 2A1V,HIS_22,6.48,-0.6,0.56,0.02 3JZN, ASP_339, 3.44, -0.37, -0.25, 0.27 3ASA,GLU_142,4.56,0.23,0,-0.17 3V4G,ASP_128,3.84,-0.43,0.18,0.29 2FB6,ASP_17,3.92,0,-0.03,0.15 2XJ4,LYS_197,11.52,-0.22,0.84,0.4 1ES9,ARG_141,11.32,-1.31,0,0.13 2DFL,ARG_291,12.35,-0.15,0,0 4FCU.GLU 200.3.76.0.15.-0.74.-0.15 2NYC,ASP_227,3.09,-1.38,-0.01,0.68 2FL4,ARG_80,13.86,-0.29,1.27,0.38 1G8P,GLU_76,4.71,0.22,0,-0.01 1XDZ,TYR 51,13.41,0,0.78,2.64 3EVN,ARG_247,12.5,-0.28,0,0.28 2BLL,ARG_334,13.69,-1.13,0.94,1.38 3JSN,ASP_257,3.17,-0.59,-0.29,0.26 1Z9L,ASP_24,3.39,-0.68,0,0.27 3CIV.ARG 217,13,15,-0.37,0.45,0.57 1P6F,GLU_13,3.91,0.32,-0.65,-0.26 3FS3,LYS_47,10.45,-0.14,0,0.08 3CX2, ASP_198, 2.76, -1.32, -0.17, 0.45 4ECC,ASP_148,3.85,0,-0.37,0.42 3U2A,GLU 73,3.74,0.9,-1.19,-0.45 3DTE,ASP_131,3.95,-0.04,-0.4,0.59 3KB5,GLU_396,3.48,0.6,-1.63,0 3LPZ,ASP_254,3.84,0,-0.15,0.19

1ILW.GLU 147.3.63.0.48,-0.85,-0.51 2V4U.GLU 528.6.64.3.69.-1.55.0 1R7J,TYR_57,10.38,-0.29,-0.08,0.75 1BKR,ASP_88,3.68,0,-0.26,0.14 2CXC,ARG 62,12,22,-0,29,0,0.01 3LJI.ASP 93.3.64.0.-0.43.0.28 1WRU,ASP_239,3.96,-0.24,0,0.4 1GVP,GLU_51,4.58,0.07,0,0.01 3VJ8,ASP_62,3.29,-0.82,-0.08,0.4 4F85,GLU_231,4.58,0.08,0,0 3FRR,ARG_21,12.27,-0.47,0,0.24 3PP8,ARG_308,11.69,-0.92,0,0.11 1Q46,GLU_28,4.51,0.07,0,-0.06 2ZQ5,HIS_154,6.25,-0.25,0,0 2FI9.GLU 128.4.86.0.14.0.0.22 3EGN,ARG 505,12,46,-0.04,0.0 3OA7,ARG_531,12.42,-0.31,0,0.23 2PWQ,LYS_2,10.93,-0.19,0,0.63 3OA7,CYS_567,9.27,0,-0.1,0.37 3MTT,GLU 526,4.58,0.19,0,-0.12 3I4T,TYR_86,10.49,0,0.06,0.43 3EUR,TYR 94,10.36,0,-0.32,0.69 3L3P,GLU_517,4.11,0.31,-0.63,-0.07 1GXN,LYS 645,11.16,-0.43,0.71,0.38 1TLV.HIS 200.6.17.-0.21.0.-0.11 2P52,GLU_177,3.9,0.42,-0.8,-0.21 1PV5,GLU_145,4.64,0.24,0,-0.1 3C6B,LYS_77,11.21,-0.3,0.48,0.54 3IRA,TYR_18,10.4,0,0.09,0.31 3CXS,GLU_90,4.59,0.95,-0.53,-0.34 1XKR,GLU_179,4.56,0.15,0,-0.09 1L3K,GLU_67,3.61,0.94,-1.81,-0.04 1TD6,TYR 32,10.71,0,0.09,0.62 3BPP,ASP 39,4.35,0,0.05,0.5 1PV5,GLU_16,4.32,0.29,-0.42,-0.05 2B3M,GLU_125,3.77,0.52,-0.82,-0.43 2AZL,ASP_188,3.94,0,-0.04,0.17 1WRU,LYS 89,9.97,-0.77,0,0.23 3I0C, ASP_154, 2.99, -1.22, -0.27, 0.69 4F85,HIS_124,6.49,-0.86,0.74,0.11 3016,ASP_40,2.83,-1.38,-0.07,0.47 3HVM,HIS 93,6.02,-0.15,0,-0.34 3CBN,ARG 148,12.09,-0.38,0,-0.03 1YB2,ASP_161,3.63,-0.85,-0.2,0.87 1X7F,GLU_120,5.73,3.91,-0.19,-2.49 2AXO,GLU_96,4.26,0.3,-0.56,0.02 3G6S,ARG 201,12.42,-0.1,0,0.02 2PIM,GLU_107,4.17,0.22,-0.33,-0.23 1WXQ,GLU_238,5.54,0.68,0,0.37 2XWS,GLU_95,4.59,0.18,0,-0.09 3K1H,LYS 67,10.29,-0.31,0.0.1 2VGM,LYS_77,10.66,-0.09,0,0.26 4FCU,ARG_14,12.75,-0.16,0.14,0.27 3N2T,ARG 222,12.68,-0.11,0.29,0.01 3N2T,ASP_229,3.94,0,0.02,0.12 2Q13,HIS_140,5.7,-0.85,0,0.06 3PZ9,LYS 264,10.29,-0.49,0.0.29 3VHJ,LYS_68,10.39,-0.12,0,0.01 1BN6,HIS_24,6.06,-0.68,0,0.23 1T3Y,ASP 32,3,95,0,0,0,15 1M5I,TYR 158,10.63,-0.21,0.24,0.59 1Y2Q,TYR_10,10.19,0,-0.06,0.25 1T3J,GLU_693,4.62,0.2,0,-0.08 2YWK,ARG_45,12.46,-0.04,0,0 1MUF,ASP_270,3,-1.01,-0.23,0.44 2FGG,ASP_14,3.78,-0.01,-0.26,0.24 2R51,HIS_83,6.43,-0.34,0,0.27 3RJZ,HIS 225,8.41,-0.41,1.7,0.62 3K8J,HIS_196,6.84,-0.28,0.56,0.06

1GPP,ARG_147,12.28,-0.26,0,0.04 1YG2,ARG 151,11.99,-0.49,0,-0.02 3FHF,GLU_73,4.69,0.23,0,-0.04 1QQH,GLU_175,4.48,1.12,-0.73,-0.4 1CBY,TYR_242,10.39,0,0.23,0.16 1MIX TYR 199 10 89 0 0 18 0 7 4EVF.GLU 36.5.28.0.92.-0.02.-0.11 2DFL,ARG_107,12.78,-0.41,0.17,0.52 1HF8,ASP_276,4.91,-0.07,0,1.17 1JKS,ASP_220,3.93,0,0,0.13 2D8N,LYS 97,10.16,-0.19,0,-0.15 2AD1.LYS 184,10.33,-0.43,0.0.26 3RVC,ARG_148,12.54,-1.32,0.79,0.56 2AD1,GLU_158,3.94,0.23,-0.79,0 1FOI,LYS 342,11,4,-0,25,0,7,0,44 3MIX.ARG 400.12.63.-1.29.0.38.1.04 2D0A,LYS_174,9.85,-0.73,0,0.08 3ASA,GLU_160,4.57,0.07,0,0 1WJG,ARG_58,12.18,-0.48,0,0.17 2GZQ,ARG 12,13.23,-0.25,0.45,0.55 2HRZ,ARG 192,11.54,-1.01,0.0.05 2B0J,LYS_339,10.45,-0.07,0,0.03 1PSW,CYS_171,10.27,0,-0.02,1.29 3MIX.GLU 576.4.33.0.26.0.-0.43 3HNX.ASP 61.3.26.-0.45.-0.41.0.31 1NAF,ARG_260,12.13,-0.45,0,0.09 4AM1,HIS_99,3.61,-2.61,0,-0.27 1XWM,CYS_104,10.68,-0.06,0,1.74 2YX0,GLU_164,4.98,0.82,0,-0.34 2IF4,ARG 121,13.31,-0.69,0.71,0.78 1Q42,ARG_169,12.73,-0.29,0.1,0.43 4GA2,GLU_74,4.09,0.2,-0.28,-0.33 3VJ8,ASP 200,2.24,-1.8,-0.67,0.92 1IAP,GLU 195,4.17,0.7,-0.63,-0.38 2FB6,TYR_96,10.87,-0.06,0.62,0.32 1Y2Q,LYS_66,10.65,-0.15,0,0.3 3LJI,ASP_92,4.77,0.32,0.22,0.42 1XDZ,GLU_180,5.01,0.31,0,0.2 3O2C,HIS 69,5,22,-1,23,0,-0.05 2FD5,TYR_45,10.29,0,0,0.29 1L2F,ARG_36,12.26,-0.24,0,0 2YWK,GLU_28,4.79,0.22,0,0.08 3EVN,TYR 186,13.3,-0.15,0,3.45 4F85,GLU_170,4.59,0.1,0,-0.02 1IAP,ARG_196,13.05,-0.29,0.56,0.29 2O8P,TYR_16,10.21,0,-0.01,0.22 1YB2, ASP 124, 3.11, -0.94, -0.13, 0.37 3L3P,ARG_374,12.53,-0.84,0.68,0.19 1ZYL,LYS_138,11.08,-0.44,0.72,0.3 3BB7,GLU_232,4.18,1.02,-0.85,-0.48 1L2F,LYS_164,10.1,-0.15,0,-0.25 1X7F,LYS_53,10.24,-0.42,0,0.16 2FI9.ASP 117.3.94.0.-0.03.0.17 20PJ,CYS_253,11.83,-0.08,-0.38,3.29 1UAJ,ARG_215,12.31,-0.35,0,0.16 2D59,ASP_51,3.1,-0.65,-0.47,0.42 2IOT.GLU 206.4.79.0.29.0.0 2DFL,TYR_178,12.66,0.85,0.31,1.5 2G70.ASP 126.3.88.0.0.0.08 3LMF,HIS_32,6.44,-0.29,0,0.23 1PSW.TYR 287,13.05,0,0.79,2.28 2EJX,ASP_75,3.16,-0.81,-0.41,0.58 3OBS,ASP_34,3.99,0,-0.08,0.26 20GQ,ARG_392,12.14,-0.5,0,0.15 3N2T,ARG_188,13.54,-1.48,1.41,1.11 1G5Z,LYS_167,10.98,-0.47,0.5,0.44 2V4U,ASP_312,3.76,-0.12,-0.06,0.14 4EVF.TYR 215.10.61.0.0.25.0.36 3H6Q,TYR_140,10.23,0,0.11,0.11

3V1Q,ARG_534,12.17,-0.33,0,0 1N81,ASP_164,3.32,-0.57,-0.49,0.56 1W24,CYS_41,12.1,-0.05,0.81,2.33 105J,GLU_62,4.14,0.55,-0.85,-0.06 3RVC,ASP_189,4.23,0,0.21,0.21 3V75,HIS 255,5,35,-0.61,0,-0.55 2GS5.TYR 188.10.2.0.0.0.2 1FQI,LYS_375,10.44,-0.1,0,0.04 3LJC,GLU_93,4.6,0.33,0,-0.23 3F6F,TYR_207,9.89,-0.43,-0.46,0.8 3RE9,TYR_223,10.13,0,-0.18,0.31 1DUP,ASP_11,2.23,-1.74,-0.38,0.56 1RWZ,ASP_76,3.79,0,-0.23,0.23 3QKY,GLU_172,4.53,0.63,-0.22,-0.38 3FFM,ARG_35,12.23,-0.29,0,0.02 1U3Y,GLU 350,4.91,0.17,0,0.24 2ZCO,TYR_260,12.15,0.78,0.31,1.07 2YWJ,LYS_21,10.57,-0.25,0,0.33 1160,GLU_24,3.35,1.02,-1.62,-0.56 4ANN,ASP 141,4.04,0,-0.07,0.31 1SJY,HIS 46,5,49,-1,87,0,84,-1,73E-17 1P1L,ARG_67,13.95,-0.34,1.34,0.45 1AK1,LYS_162,10.47,-0.25,0,0.22 3ADO,HIS 173,5,46,-0.62,0,-0.43 2QDJ,HIS 69,6.29,-0.27,0,0.06 4H89.HIS 164.5.82.-0.86.0.0.18 4F85,ASP_187,3.08,-0.97,-0.27,0.52 2DG7,ASP_32,2.63,-1.41,-0.19,0.44 2PGE,ARG 244,12,41,-0.09,0,0 3BPV,ARG_132,12.49,-0.13,0,0.11 2GS5,GLU_28,4.57,0.07,0,0 3ASA/GLU 196,4,7,0,17,0,0.03 103X,ARG_207,13.17,-0.26,0.47,0.46 3EJG,TYR 52,10.17,-0.4,0.08,0.48 1U7U,ASP_250,3.78,-0.34,-0.41,0.73 2AXO,ASP_213,2.39,-1.64,-0.04,0.27 3BQE,GLU_250,7.93,3.88,-0.65,0.2 2CBE,GLU_214,3.71,0.62,-1.24,-0.17 1QQE,ASP 38,4.39,0,0.13,0.45 3JV1,ARG_193,13.66,-0.98,1.27,0.88 3V4G,GLU_153,2.69,0.47,-1.55,-0.74 1MTZ,HIS_179,5.55,-0.97,0,0.01 2E3C,GLU 425,7.02,4.79,-2.26,-0.01 4FLE,ASP 58,3.97,0,-0.09,0.25 2P5D,LYS_32,11.85,-0.27,0.85,0.76 2B02,GLU_403,3.96,0.18,-0.34,-0.37 2O4D,ARG_97,13.27,-0.51,0.85,0.43 2PPN,GLU_54,2.96,0.5,-1.65,-0.38 2PPN,ARG_13,12.52,-0.05,0,0.07 1T6L,ASP_120,3.91,0,0,0.11 3QAV,ARG_95,12.55,-0.47,0.03,0.49 1YTQ,LYS_47,11.17,-0.3,0.57,0.39 1NJ4,TYR 52,12,46,0,23,0,5,1,73 4ANN,ASP_169,4.09,0,0.02,0.27 1PDB,TYR_121,13.52,0,0.51,3.01 1PV5,HIS_214,5.45,-1.9,0.72,0.13 3GT0,LYS_88,11.67,-0.42,0.85,0.74 1XAW,ASP 516,2,57,-1.02,-0.65,0.45 3V75,GLU_80,5.05,0.58,0,-0.03 2QK1,ASP_490,4.07,0,0.08,0.19 3K8J,ARG_260,13.19,-0.67,0.66,0.7 2B0J,ASP_280,4.01,0,0,0.21 3HVM,GLU_9,3.61,1.83,-2.18,-0.53 3GMS,HIS_265,4.9,-0.91,0,-0.7 3E5T,LYS_188,10.36,-0.14,0,0 1O5T,LYS_153,10.39,-0.1,0,-0.01 1V43,LYS 314,10.51,-0.11,0.0.12 4ACJ,CYS_776,9.82,-1.63,0.02,2.44 3GA2,LYS_104,10.74,-0.24,0.12,0.36

1X6J.ARG 45.13.82.-0.46.1.03.0.74 3CAX.GLU 382.4.56.0.11.0.-0.05 1DTO,GLU_162,4.72,0.21,0,0.01 2HRZ,HIS_-5,6.65,-0.12,0.27,0 20EW,ASP 222,3.59,-0.56,-0.68,1.03 2B61,HIS 327,6.74,-0.71,0.81,0.14 208P,ASP_49,2.24,-1.92,-0.68,1.02 3ELI,ARG_5,13.15,-0.38,0.35,0.68 2HRZ,GLU_150,4.13,0.27,-0.63,-0.01 2B2H,ARG_33,12.47,-0.23,0,0.19 3MTT,ARG_527,12.25,-0.25,0,0 4EF5,TYR_186,10.43,-0.92,-0.28,1.63 1YB2,ARG_220,12.38,-0.16,0,0.04 1BN6.GLU 234.4.89.0.41.0.-0.01 20ZO.LYS 158.10.31.-0.19.0.0 3CIV,HIS_249,6.93,-0.46,0.74,0.16 2FBI,ARG_44,12.07,-0.43,0,0 3H13,ARG_303,13.2,-0.15,0.37,0.47 2Q13,LYS_191,11.07,-0.61,0.77,0.42 2W0G,LYS 160,10.25,-0.31,0,0.07 2XJ4,ARG_242,12.32,-0.18,0,0 3HYQ,GLU_116,5.37,1.29,0,-0.43 20KT,TYR 291,9,98,-0,47,-0,48,0,94 3B79,LYS 74,10.63,-0.28,0.19,0.22 4DNU,GLU_364,4.58,0.08,0,0 3HUE, ASP_97, 4, 0, -0.12, 0.32 4F8A,GLU_578,4.48,0.25,0,-0.27 2GEN,CYS_17,9.68,-0.31,-0.2,1.18 1MUF,HIS_181,6.4,-0.22,0,0.11 3T8R,LYS_29,10.63,-0.09,0,0.23 2H14,GLU_292,3.92,0.23,-0.79,-0.02 3H13,HIS_443,4.13,-2.46,0.12,-0.04 3GEC,ASP 381,3.95,-0.02,-0.23,0.41 3FS3.LYS 93.10.5.-0.08.0.0.08 2QOP,ASP_84,3.15,-1.13,-0.12,0.59 2PP6,ASP_30,3.07,-0.68,-0.35,0.3 3PZ9,ASP_56,3.92,-0.85,-0.31,1.28 2QOP,ASP_157,3.42,-0.52,-0.32,0.46 1TD6,LYS_158,10.58,-0.69,0.37,0.4 1GOE,ASP 330,2.81,-0.65,-0.64,0.31 3BPP,ARG_43,12.86,-0.79,0.21,0.94 3M66.ASP 278,3.17,-0.73,-0.58,0.68 1EO6.ASP 53.3.23.-1.53.0.0.95 2WOZ,GLU_564,4.03,1.13,-1.59,0 3RFF,ARG_90,11.66,-0.86,0,0.02 3H9W,ASP_89,2.81,-1.44,-0.49,0.94 2YX0, ARG_325, 13.08, -1.3, 0.84, 1.04 1SJ8,TYR_570,10.89,-0.08,0.01,0.95 2XJ4,ARG_196,12.41,-0.33,0,0.24 1YLN,ARG_161,13.26,-0.3,0.7,0.37 3C6B,LYS 25,10.34,-0.18,0,0.02 2V4X,ARG 9,13.31,-0.62,0.82,0.61 3GOZ,LYS_189,10.57,-0.13,0,0.19 4FD6,CYS_189,9.71,-0.17,-0.18,1.05 1J74,LYS_85,10.2,-0.34,0,0.04 1SNT,ARG 55,11.64,-1.06,0,0.2 2EJB,LYS_140,10.34,-0.16,0,0 3GA2,LYS_13,10.37,-0.26,0.14,0 2CXA,ARG_44,12.02,-0.51,0,0.03 1MIX,ARG 220,13.58,-0.92,0.89,1.12 1X8F,LYS 284,10.36,-0.17,0.03,0 1LZL,GLU_108,4.62,0.25,0,-0.13 1R5Q,ARG_97,13.64,-0.17,1.27,0.04 2FXT,ASP_345,3.9,0,-0.18,0.27 1Q5Z,TYR_640,11.87,0,0.48,1.39 1KCM,GLU_38,4.71,0.17,0,0.04 4H86,GLU_147,4.6,0.62,-0.44,-0.08 1RI6,ASP_241,2.68,-1.66,-0.64,1.16 3MTT,GLU_486,4.66,0.2,0,-0.04

3ES3.ASP 192.3.88-0.09-0.02.0.18 1FKM,ARG 343,13.33,-0.25,0.75,0.34 2B0J,LYS_113,10.32,-0.1,0,-0.08 1J85,TYR_51,10.16,-0.05,-0.16,0.37 3NBI.GLU 65.4.63.0.13.0.0 3PBH.ARG 1.12.54.-0.22.0.04.0.23 1DCF,GLU_41,4.64,0.06,0,0.07 2E3C,GLU_222,3.95,0.25,-0.35,-0.45 3BQW,TYR_275,10.12,0,-0.13,0.26 3LQE,TYR_435,10.41,-0.04,-0.18,0.62 2QK1,ARG_454,12.49,-0.18,0,0.18 3H8Y,GLU_69,5.09,0.2,0.3,0.09 3M7G,ARG_267,13.9,-0.34,0.85,0.88 20KT,GLU_319,4.66,0.38,0,-0.22 1HUEASP 7.2.93.-0.73.-0.45.0.31 1NIJ.ARG 270.12.62,-1.17.0.69.0.59 3BQW,GLU_56,4.96,0.55,0,-0.1 2P1W,GLU_232,4.57,0.21,0,-0.13 3JZ9,LYS_380,10.39,-0.14,0,0.03 2CL3,HIS_171,5.59,-1.5,0.58,2.08E-17 3RFY,GLU_175,4.3,0.26,0,-0.46 1YM5,ARG 257,11.87,-0.41,0,-0.22 1EV8,TYR_94,13.02,-0.04,0.24,2.82 3M7D.HIS 281,6.87,-0.63,0.61,0.39 2D59.LYS 33.10.52.-0.18.0.0.19 2XJ4,LYS_155,10.4,-0.22,0,0.12 3CNU,ASP_70,4.05,0,0.05,0.2 3B4D,ASP_206,3.82,0,-0.23,0.25 1J85.GLU 64,5,0.32,0,0.17 2GAU,ARG_230,12.4,-0.11,0,0.01 2AHE,TYR_225,13.47,0,0.63,2.83 3H13,LYS_247,10.26,-0.3,0,0.06 1SQH,HIS 61,7,-1.07,1.65,-0.08 1RSS,ARG 155,12.33,-0.17,0.0 3CAN, ASP_139, 3.9, 0, -0.04, 0.14 3I0C,TYR_150,12.3,0,0.16,2.14 2QHT,LYS_21,9.44,-0.81,0,-0.25 3M7D,ARG 351,12.36,-0.49,0,0.35 2V81,CYS_105,12.22,0,-0.16,3.37 2QOP,ARG_90,12.05,-0.62,0,0.17 3Q6L,LYS_80,10.69,-0.3,0.18,0.31 3LOD, ASP 11, 3, 31, -0.76, -0.14, 0.41 20DJ.ARG 150.11.81.-0.8.0.0.11 3AUF,CYS_135,12.38,-0.1,0.7,2.77 1U7U,GLU_336,4.9,0.35,-0.03,0.08 2EFK,LYS_247,12.41,-0.51,1.33,1.09 1U53,TYR 144,10.29,-0.78,-0.24,1.3 1LPL/ARG 162,11.96,-1.22,0.02,0.66 3T57,GLU_255,4.18,0.21,0,-0.54 2IF4,GLU_105,4.74,0.75,-0.36,-0.16 4FH3,ASP_371,4.11,0,0,0.31 1HF8,ARG_150,11.79,-0.63,0,-0.08 4FH3,TYR_49,10.97,0,0.12,0.85 3A0X,LYS_732,10.43,-0.11,0,0.03 2DG7,ASP_175,4.32,0,0.24,0.27 1SI7,ARG_291,12.32,-0.79,0.36,0.23 3BWT,HIS 569,5,98,-0,58,0,0.05 2QV2,ASP_72,3.85,-0.02,-0.25,0.33 3I47,ARG_37,12.02,-0.5,0,0.02 10YLASP 124.3.84.0.-0.14.0.17 2D59.GLU 35.3.95.0.48.-0.75.-0.28 3QKY,GLU_55,4.3,0.25,-0.17,-0.27 3EVZ,GLU_86,7.58,3.35,-0.14,-0.14 1V8E,ARG_139,13.2,-1.08,1.25,0.54 3MIX,ASP_676,2.78,-0.97,-0.38,0.33 3V46,ARG_235,12.4,-0.05,0,-0.05 1F2V,ASP_174,3.41,-0.4,-0.47,0.48 4EVF,LYS_119,10.38,-0.12,0,-0.01 3F1X,GLU_125,4.09,0.32,-0.34,-0.4

1P6F.TYR 63,10.47,0.0.01,0.46 1XEU,TYR 254,10.68,-0.7,0.22,1.15 3F6F,LYS_46,10.43,-0.08,0,0.01 3P2F,ASP 89,4.01,0.0.0.21 1L2F,ASP_50,2.29,-1.7,-0.26,0.45 1J8B,ASP_64,3.97,0,0,0.17 2P65.LYS 80.10.26.-0.56.0.0.32 1NAR,CYS_246,12.84,0,0,3.84 4ACJ,ASP_789,3.87,0,-0.24,0.32 2CBE,LYS 213,11.19,-0.8,0.85,0.65 3H04,TYR 194,10.16,-0.03,-0.19,0.38 2EJX.TYR 84,10.6.0.0.06.0.55 3E5T,GLU_111,4.84,0.2,0,0.14 1TLV,TYR_201,11.35,-0.01,-0.6,1.96 2WB3,LYS 384,10,44,-0.06,0,0 2BLL/HIS 593,5,73,-0,4,0,-0.37 3EYE, ARG_10, 11.26, -2.77, 0.44, 1.09 1FKM,LYS_265,10.34,-0.34,0,0.18 2X4G,GLU_163,4.08,0.87,-0.41,-0.89 1X7F,GLU 284,3.51,0.3,-0.85,-0.44 2WB3.GLU 382.4.36.0.21.0.-0.35 2IOT.GLU 43,4.61,0.18,0,-0.06 1WP5,LYS_127,10.5,-0.21,0,0.21 1MML.GLU 201,3.21,1.04,-2.05,-0.27 3LOE.ASP 255.3.14.-1.37.-0.27.0.97 2Z61,ARG_287,12.63,-0.29,0.16,0.26 2B78,TYR 129,10.39,-0.03,-0.05,0.47 3M70,GLU_163,4.61,0.12,0,-0.01 3EVP,LYS_127,10.43,-0.08,0,0.01 20YZ.ARG 56,13.86,-0.72,1.19,0.89 3KV0,ASP_133,3.5,-0.34,-0.27,0.3 3CO1,LYS_60,10.29,-0.19,0,-0.02 2X4L,LYS_347,10.34,-0.19,0,0.03 1RAJ,ARG_415,12.64,-0.24,0,0.38 3CXS,GLU_5,3.93,0.41,-0.66,-0.33 2F9F,GLU_129,4.43,0.18,0,-0.25 1Z3X,LYS_120,10.86,-1.16,0.8,0.71 2CN1,GLU_20,4.68,0.19,0,-0.01 1DZF.GLU 40.4.63.0.09.0.0.04 1Q46,ARG_112,12.44,-0.26,0,0.2 2RIK,GLU_54,4.56,0.08,0,-0.01 2Z84,LYS 88,11,12,-0,58,0,65,0,56 2FPN,GLU 123,4,0.31,-0.81,0 3ETV,GLU_309,4.69,0.19,0,0 1YR6,GLU_228,5.26,0.69,0,0.07 1FHL,ASP_91,4.02,-0.37,0.17,0.42 2W0G,GLU 261,4.16,0.22,-0.32,-0.24 3GMS.ARG 283,13.21,-0.49,0.71,0.49 3RFY,TYR_109,13.26,0.85,0.77,1.65 3CBN,LYS 119,10.52,-0.25,0,0.28 2HNG,GLU_116,4.09,0.31,-0.7,-0.02 1SIG,HIS 242,6.38,-0.12,0,0 1D2K.HIS 66.0.92.-3.2.0.-2.38 4DIU,HIS_176,7.25,-0.42,0.52,0.64 2RJD,GLU_472,4.78,0.7,0,-0.42 1TUL,LYS_105,10.03,-0.78,0,0.31 3IVF.ARG 30,12.63,-0.17,0.0.31 3LJI,TYR_250,12.83,0,0.74,2.1 2|88,GLU 518,4.63,0.21,0,-0.07 2B78,ARG_132,13.64,-0.95,0.88,1.21 3IOC, LYS 131, 11.47, -0.26, 0.85, 0.38 10IS,GLU_255,4.69,0.19,0,0 3GOZ,GLU_15,3.95,0.27,-0.82,0 2EFK,LYS_138,10.67,-0.22,0,0.4 3RFY,ASP_409,4.34,0,0,0.53 1AKO, ARG_184, 12.01, -1.75, 0.51, 0.75 1NWA,TYR_98,10.27,0,-0.22,0.49 20GQ,ARG_563,13.71,-0.36,0.79,0.78 3M66,ASP_388,3.18,-1.33,-0.07,0.77

3M70,GLU_211,4.35,0.38,0,-0.53 1NIJ,GLU 306,4,0.87,-0.76,-0.62 2GAU,LYS_121,11.07,-0.27,0.43,0.41 2Q5X,LYS_801,10.39,-0.22,0,0.1 3DHN,CYS_62,9.45,0,-0.11,0.57 1RW7 LYS 32 10 92 -0 45 0 39 0 47 1S7K.LYS 92.10.43.-0.22.0.0.15 3CSR,LYS_116,10.2,-0.3,0,0 3VJ8,HIS_98,5.95,-0.55,0,0 1R3F,ASP_230,3.9,0,0,0.1 3GS9.ASP 216.2.83.-1.49.0.0.53 3M3P.CYS 159,12,74,-0.89,1.77,2.85 2RH3,ARG_133,12.26,-0.28,0,0.04 2D7U,GLU_240,4.37,0.33,-0.48,0.02 2ZQ5,ASP_341,4.02,0,0.08,0.14 2ZTY,LYS 60,10.47,-0.13,0,0.11 3CQ1,ARG_91,12.5,-0.37,0.02,0.35 1P4X,LYS_76,10.39,-0.11,0,0 2IF4,LYS_39,10.07,-0.39,0,-0.03 4AM1.LYS 15.10.54.-0.25.0.06.0.24 1H4U.GLU 558,4,71,0,19,0,0.02 3FS3,LYS_45,10.39,-0.14,0.03,0 20GQ,ASP_402,2.8,-1.15,-0.38,0.53 1TR9.GLU 295.4.62.0.22.0.-0.11 1LFP,ARG 68,12.45,-0.19,0,0.13 3OBS.HIS 102.6.31.-0.68.0.67.-0.18 109G,CYS_60,13.83,-0.17,1.9,3.1 3IO0,LYS_183,10.41,-1.34,0.75,0.5 3KB5,ARG 447,12.51,-0.19,0,0.2 2CIU,TYR_171,11.26,0.13,0.5,0.63 3PM2,TYR_166,11.05,-0.13,0.02,1.16 10YI.GLU 273.4.21.0.52.-0.81.0 3EZ7,ARG_378,12.34,-0.39,0,0.22 2JHY,HIS 155,5.7,-0.65,0,-0.16 1NRI.LYS 241.10.34.-0.16.0.0 3M70,GLU_71,4.66,0.47,-0.3,-0.02 3B4D,GLU_224,4.78,0.11,0,0.17 4AM1,LYS_340,11.41,-0.38,0.85,0.44 3LMF,GLU 35,4.65,0.21,0,-0.06 200K,GLU_122,4.06,0.71,-0.76,-0.39 3FS3,LYS_198,10.27,-0.23,0,0 1L2F,GLU_14,5.05,0.25,0,0.31 4ECC,CYS 98,8.36,-1.09,0.06,0.4 3L3P.GLU 400.5.75.0.31.0.04.0.9 3QKY,GLU_238,4.79,0.22,0,0.07 1AK1,ASP_76,3.78,0,-0.21,0.19 2R57,ASP_215,3.71,-1.44,-0.15,1.51 3EX9,GLU_28,4.19,0.64,-0.57,-0.38 3DHN,ASP_203,3.71,-0.71,-0.49,1.11 2Q98,LYS_69,10.44,-0.3,0,0.25 1MUF,GLU_166,4.6,0.23,0,-0.13 1WXF,TYR_231,11.09,0,0.06,1.04 3SMD.GLU 17.3.81.0.17.-0.41.-0.45 3GG6,ARG_65,12.43,-0.07,0,0 1TD6,GLU_266,4.28,0.15,-0.37,0 2EA9,ARG_40,12.08,-0.38,0,-0.04 1KN3,ASP_56,3.8,0,-0.16,0.16 3P28,ARG 186,13.63,-0.27,1,0.41 1ZCU,HIS_70,6.99,-0.49,0.79,0.19 3HYQ,CYS_37,10.64,-1.88,0.03,3.5 4DVD,ARG_121,13.25,-0.35,0.72,0.38 2XJ4.GLU 87.4.78.0.15.0.0.13 2B0J,LYS_232,11.71,-0.33,0.84,0.7 2QEV,ARG_23,13.58,-0.38,0.85,0.61 1AD6,LYS_417,11.49,-0.22,0.82,0.39 1MIX,LYS_316,10.27,-0.26,0,0.04 3SMD.TYR 6,10.32,0.0.05,0.27 1MIX,CYS_286,10.88,0,-0.03,1.9 1AT0,GLU_351,4.64,0.25,0,-0.1

1SJ8.GLU 780.6.85.2.22.0.0.13 3D9H,HIS 166,6,29,-0,13,0,-0,08 1P4X,ARG_101,11.78,-0.81,0,0.09 2QV2,ARG_325,11.94,-0.59,0,0.03 3ZXY.GLU 122.3.6.0.47.-0.96.-0.41 1ZBM.GLU 256.4.95.0.28.0.0.16 1RI6,LYS_289,11.27,-0.28,0.15,0.91 3MTT,ARG_510,12.34,-0.22,0,0.05 2CWY, ARG_37, 12.2, -0.45, 0, 0.14 3GS9,GLU_184,4.56,0.06,0,0 3NZL,LYS 27,10.08,-0.19,0,-0.23 3CNU,LYS_9,10.36,-0.37,0,0.22 2GAU,LYS_136,10.54,-0.15,0,0.2 3FS3,LYS 44,10.21,-0.29,0,0 3DSHLYS 449.11.23.-0.2.0.54.0.39 3HVW,TYR_324,10.45,0,-0.02,0.48 1SQW,GLU_7,3.23,0.36,-1.24,-0.39 3C6B,ASP_153,3.54,-0.44,-0.1,0.28 1SQH,HIS_35,3.44,-3.06,0,0 4EKU.CYS 267.11.48.0.0.28.2.2 1BN6,ASP_175,4.04,0,-0.07,0.32 1ILW,ASP_153,3.69,-1.31,-0.07,1.27 2AD1,LYS_186,10.52,-0.06,0,0.08 4ECC.ASP 114.4.14.0.-0.09.0.43 1PVT,GLU_151,4.68,0.39,0,-0.21 1GPP,GLU_69,4.54,0.11,0,-0.07 1NIJ,GLU_97,4.2,1.79,-1.79,-0.3 1BN6,ASP_150,3.29,-0.63,-0.12,0.24 3JZN,ASP_142,3.38,-0.79,-0.11,0.5 1R53,GLU_36,3.78,0.77,-1.51,0.02 2OJQ,GLU_596,3.1,0.95,-1.94,-0.4 208P,CYS_161,10.97,0,0.04,1.93 2VAN,GLU 147,3.4,0.62,-1.35,-0.37 2NRR.GLU 384,4.67,0.35,0,-0.19 4E8B,HIS_27,6.1,-0.58,0,0.18 4ACJ,LYS_787,10.53,-0.08,0,0.11 4FH3,LYS_63,10.41,-0.13,0,0.03 1R3D,HIS_99,5.65,-0.79,0,-0.05 2IRM,TYR_247,10.32,0,-0.26,0.58 2B78.TYR 150.12.03.0.02.0.59.1.41 2EJB,TYR_156,9.99,0,-0.13,0.12 3GG6,GLU 62,4.51,2.28,-1.02,-1.24 2AZL.GLU 187.4.78.0.21.0.0.08 2VAN,CYS_267,11.89,0,-0.02,2.92 3VHJ,ASP_62,3.48,-0.73,-0.23,0.65 1ZKZ,LYS_71,10.35,-0.16,0,0.01 3I4T,TYR_268,11.01,0,0.68,0.32 2R57,ASP_247,2.47,-2.21,-0.75,1.61 3BCH,ARG_184,11.7,-1.17,0.22,0.17 2XMZ,LYS_236,10.01,-0.7,0,0.21 2OBI,CYS 66,9.58,0,0.13,0.45 3D9H,HIS 81,5.97,-0.88,0.49,-0.14 2V4U,LYS_560,10.5,0,0,0 2GAU,ASP_213,3.08,-0.56,-0.38,0.21 2GKG,LYS_3,10.34,-0.34,0,0.18 4E8B,ARG 174,12.45,-0.06,0,0.01 1CHD,GLU_326,4.52,0.96,-0.72,-0.22 1X91,ASP_39,3.42,-0.85,-0.47,0.95 1AK1,ASP_171,3.67,-0.44,-0.02,0.34 20YZ,ARG 44,13.54,-0.27,0.45,0.86 3P51.GLU 115.4.5.0.21.0.-0.21 2AH5,TYR_197,10.85,0,0.27,0.58 2ZCO,TYR_41,13.67,-0.24,0.46,3.44 10LR,TYR_11,11.85,0.28,0.57,1 2CL3,LYS_23,10.44,-0.06,0,0 2NRR,LYS 390,10.25,-0.41,0,0.17 2IRM,GLU_264,4.57,0.28,0,-0.2 10GL,LYS_92,9.85,-0.73,0,0.08 3EVN,TYR_157,12.26,0,0.1,2.16

1BKB,GLU_72,5.02,0.52,0,0 20KT.TYR 44,11.01.0.0.23.0.77 1TWU,TYR_59,9.7,-0.31,-0.3,0.32 3IO0,LYS_283,10.42,-0.08,0,0 1PV5.GLU 49.4.63.0.4.0.-0.27 4F3JLYS 109.10.09.-0.38.0.-0.02 1A80,ARG 20,11,33,-1,6,0,01,0,41 2JKF,ARG_14,13.02,-0.27,0.06,0.73 4FZR,ARG_362,12.25,-0.39,0,0.14 3ZTA,GLU_14,4.71,0.19,0,0.01 2RFA,ARG_139,13.03,-0.44,0.6,0.37 2H30,ASP_56,3.79,0,-0.2,0.2 2JEO,LYS_78,10.49,-0.14,0,0.13 3O16, ARG_176, 12.41, -0.21, 0, 0.13 307K,ARG 41,12.53,-0.44,0,0.47 2E3C,GLU 247,4.29,1.35,-0.73,-0.83 1QQL,HIS_93,6.24,-0.27,0,0.01 1LTU,ARG_123,13.46,-2.95,1.58,2.32 1WRU,TYR_67,9.93,-0.1,-0.4,0.42 1X8F,ASP 107,3.58,-0.53,0,0.32 1XDZ,LYS_224,10.96,-0.25,0.41,0.3 3RNV.LYS 414,10.22,-0.18,0,-0.09 1W7B,HIS_224,6.16,-1.52,0.85,0.33 4DNU.ASP 96,4.16,-0.07,-0.03,0.46 3BPP.GLU 162.4.61.0.36.0.-0.25 3PAC,LYS_135,11.18,-0.35,0.64,0.38 3NBI,GLU_75,4.79,0.12,0,0.17 2Z0M,ASP_220,2.73,-0.85,-0.68,0.46 3GV0,ARG 185,13.4,-0.91,0.8,1 1SJ8,ASP_600,4.27,0,0.15,0.32 1H4U,LYS_500,11.36,-0.3,0.84,0.32 1YTQ,TYR_61,9.88,-0.63,-0.14,0.65 3I47,LYS 59,10.41,-0.09,0,0 20ZO,TYR 141,12,13,0.85,0.51,0.77 3VJ8,GLU_234,4.87,0.33,0,0.04 1ES9,HIS_166,5.86,-0.57,0,-0.07 2PGE,ARG_212,11.5,-2.75,0,1.75 1J7G,GLU 18,4.6,0.09,0,0.01 2GQV,GLU_75,3.58,0.37,-0.83,-0.46 1WRU,ARG_108,12.33,-0.44,0,0.27 1A8Q,LYS_274,11.28,-0.32,0.57,0.54 3E5T.CYS 222,8.72,-0.77,0.06,0.43 3LPZ.LYS 92.10.2.-0.61.0.0.32 1Q46,ASP_83,3.72,-0.61,-0.26,0.79 2AZL,LYS_17,10.36,-0.37,0,0.23 1QZN,TYR_58,12.16,0,0,2.16 2RGY,GLU 230,4.84,0.78,-0.22,-0.22 3E7P.GLU 173.5.51.1.42.-0.34.-0.06 1Q46,CYS_5,11.1,-0.11,0.11,2.1 3ELI,GLU 9,4.15,0.21,-0.45,-0.12 1MML,ASP_174,4.02,-0.45,-0.62,1.29 3NZL,ASP 28,3,63,0,-0,4,0,24 2B61,ARG_291,12.65,-0.62,0.03,0.73 208I,ASP_132,4.06,0,0.06,0.21 3C0C,TYR_344,10.99,0,0.17,0.83 2X4L,ASP_336,3.79,-0.53,-0.28,0.8 1V43.ARG 74.12.22.-0.48.0.0.21 3M7G,GLU_129,6.03,3,-0.92,-0.55 2Z0M,ARG_309,12.53,-0.4,0.12,0.31 1WP5.GLU 308,3.65,0.35,-0.85,-0.34 1046.GLU 9.4.47.0.44.0.-0.46 1R6Y,GLU_7,4.54,0.33,-0.38,0.08 3M16,LYS_277,10.3,-0.2,0,0 4FZN,ARG_228,12.4,-0.31,0.03,0.18 1VJG,LYS_95,10.5,0,0,0 2R2Y,ARG_27,12.63,-0.21,0,0.34 1A8Q,ARG_48,13.97,-0.79,1.65,0.62 3GV0,ASP_245,3.05,-0.72,-0.38,0.35 3RNV,CYS_344,10.19,-0.32,0.59,0.93

3KEY,LYS_340,10.46,-0.04,0,0 2P0Y,HIS 328,6.92,-0.19,0.63,-0.02 1LFP,LYS_23,10.37,-0.36,0,0.22 208P,ARG_99,13,-0.48,0.51,0.46 3P51,GLU_57,4.87,0.37,0,0 1KN3,LYS_47,10.12,-0.27,0,-0.1 4FZR,TYR 117,13.5,-0.12,0.17,3.46 105T,ARG_162,10.78,-2.12,0,0.4 2A1V,ASP_132,3.25,-0.25,-0.51,0.2 3ASA,ASP_161,3.99,0,-0.01,0.19 2FXT,ARG 347,12.61,-0.09,0,0.21 1T6L.GLU 36,4.52,0.08,0,-0.07 3GYW,ASP_73,3.85,0,-0.18,0.23 3IVF,LYS_284,11.42,-0.22,0.76,0.38 3K8U,LYS 27,10.27,-0.23,0.0 109G,TYR 178,9,92,-0,55,-0,49,0,97 2CXY,GLU_15,4.62,0.41,-0.39,0.09 3FNI.ASP 150.3.75.-0.14.-0.67.0.75 3EOD,GLU_45,4.74,0.11,0,0.13 3FS3,LYS 81,10.34,-0.16,0,0 1XEU.ARG 39.12.42.-0.08.0.0 3B7X,ASP_141,3.48,-0.58,-0.14,0.39 2ATR,GLU_90,4.72,0.22,0,-0.01 1W7B,TYR 317,10.11,0,-0.14,0.25 1Z3X.ARG 91.12.21.-0.29.0.0 3F6F,GLU_38,4.02,0.38,-0.83,-0.03 2CYG,TYR 141,10,29,0,-0,12,0,4 3H6Q,ARG_81,9.83,-2.69,0,0.02 2CYG,LYS 51,10.16,-0.34,0,0 3RE9.TYR 87.10.08.-0.03.-0.13.0.23 2HRZ,TYR_145,9.42,-0.91,-0.32,0.65 3L3P,GLU_507,4.72,0.21,0,0 3KB5,GLU_443,4.57,0.7,-0.77,0.14 3BWT.GLU 606.4.64.0.19.0.-0.05 3EJC,ARG_80,13.31,-0.32,0.75,0.38 1PV5,ARG_9,12.41,-0.33,0,0.24 2RGY,HIS_117,6.23,-0.23,0,-0.04 2X4G,ARG_308,12.78,-0.11,0,0.4 2BAA.ARG 221.11.57.-1.55.0.0.62 3NBI,HIS_19,5.69,-0.72,0,-0.09 3UC9,LYS_149,10.56,-0.32,0,0.39 2FC3.GLU 72.4.84.0.27.0.0.07 3V55.LYS 538.10.77.-0.25.0.14.0.37 1Z9L,ARG_55,12.55,-0.09,0,0.15 3HVM,TYR_191,10,0,-0.16,0.16 4EZB,ASP_277,3.57,-0.65,0,0.42 2Q34,GLU_236,4.94,2.69,-2.22,-0.03 3IVF,LYS_318,10.31,-0.16,0,-0.03 1KN3,LYS_93,10.47,-0.2,0,0.16 3JRT.GLU 125.4.29.0.86.-0.35.-0.71 3HUE,ASP_221,3.99,-0.15,0.12,0.22 1GXN,GLU 384,4.56,0.14,0,-0.08 3CN5.CYS 69.9.24.0.0.0.24 1XFK,HIS_127,7.5,-3.53,0.91,3.61 3RLN,LYS_683,10.3,-0.2,0,0 1R6Y,LYS_89,11.07,-0.28,0.85,0 3I47, ASP_187, 4.12, 0, 0.18, 0.14 2A6B,ASP_221,3.8,0,0,0 1VJG,ASP_179,1.45,-2.76,-0.68,1.09 4FH3,GLU_50,4.74,0.29,0,-0.05 1J8B,GLU 86,4.58,0.23,0,-0.16 3ASA,GLU_384,4.65,0.16,0,-0.01 3CAX,ASP_208,3.56,-0.41,-0.47,0.65 1PGV,GLU_308,4.28,0.48,-0.79,0.1 2EFK,HIS_266,6.54,-0.17,0,0.22 3LJN,CYS_61,10.09,-0.02,-0.02,1.14 1059,ARG_238,12.49,-0.11,0,0.1 2IF4,ARG 284,12.39,-0.11,0,0 20EW,LYS_285,10.46,-0.11,0,0.07

1MUF,HIS_252,7.11,-0.46,0.69,0.38 2PLQ,LYS_106,9.84,-0.53,0,-0.13 4AM1,HIS_284,5.9,-0.95,0.28,0.07 1PBV,ARG_98,13,-0.23,0.27,0.45 1WYC,ARG_130,12.79,-0.32,0.16,0.45 205X.ASP 731.4.07.0.0.12.0.15 3RJX.LYS 254.10.86.-0.18.0.0.54 4E9E,LYS_565,10.27,-0.23,0,0 3ON1,TYR_59,10.22,0,-0.12,0.33 3NR5,GLU_5,4.56,0.08,0,-0.02 1J33,TYR 25,10,47,-0,27,-0,24,0,97 3GE9,CYS_215,12.6,0,0.11,3.49 2Q98,HIS_46,6.12,-0.32,0,-0.06 1PV5,ARG_101,11.6,-1.28,0,0.39 3F7M,TYR_163,11.03,0,0.07,0.97 1JSX,ARG 87,12.78,-1.05,0.84,0.49 3M7D,LYS_335,10.67,-0.45,0.14,0.49 2JKF,ASP_92,3.45,-0.55,-0.39,0.6 1WJG,ARG_17,13.28,-0.3,0.64,0.44 10TM,LYS 64,10.53,-0.04,0.0.07 2D2S,TYR 739,9.56,-0.85,-0.11,0.53 2H2Z,CYS_156,9.4,0,-0.31,0.71 2JEO.ARG 66,11.37,-1.28,0.0.14 2ATR.GLU 109.4.56.0.06.0.0 1GPP,ASP 429,3.59,-0.47,-0.01,0.28 1M5I,CYS_207,9.39,0,0.14,0.24 2NRR,LYS_447,10.1,-0.4,0,0 2XJ4,ARG_213,13.69,-0.9,1.54,0.55 2GZR,ASP_99,3.6,-0.85,-0.32,0.97 30KQ,GLU_622,4.69,0.22,0,-0.02 3GE9,ARG_199,12.19,-0.94,0.32,0.3 3RFF.ARG 23,13.07,-0.34,0.46,0.44 2C2Y,ASP_237,3.89,0,0,0.09 30NH,ARG 497,12.64,-0.31,0,0.45 3LH5,ASP_701,3.88,0,-0.12,0.21 2BLL,ASP_445,2.75,-1.49,-0.74,1.17 3ETV,LYS_282,10.38,-0.28,0,0.16 3FRR,LYS_7,10.29,-0.11,0,-0.1 1ZBS,CYS 15,9.78,-0.85,-0.09,1.72 3T57,LYS_126,10.48,-0.18,0,0.15 3BJV.GLU 147.3.4.0.43.-1.14.-0.38 1T3Y,ASP_19,3.34,-0.8,0.03,0.31 1EW4,ASP 22,3.99,0,0,0.19 2Z14.LYS 121.10.45.-0.05.0.0 1F2V,GLU_171,3.89,0.38,-0.97,-0.02 4ECC,GLU_30,5.96,2.55,0,-1.09 1BGF,ARG_114,13.88,-0.33,1.34,0.38 2QV2,GLU 155,4.05,0.4,-0.85,0 2CI3,GLU_243,3.79,0.26,-0.58,-0.38 1RKA, ARG_239, 12.31, -0.3, 0, 0.1 2OJQ,GLU_439,4.86,0.26,0,0.1 1Z3X,ARG_133,12.4,-0.12,0,0.03 1DOV.GLU 158,4.36,0.7,-0.83,-0.01 4D8L,ASP_88,3.6,-0.56,-0.33,0.69 2FPN,ASP_104,3.8,0,-0.16,0.15 3Q1C,GLU_52,4.47,0.59,-0.7,0.08 3ZXY,TYR_190,12.69,-0.84,0,3.53 3EVP,LYS 289,10.63,-0.28,0.0.42 3B7X,ARG_24,12.33,-0.24,0,0.07 1N81,ARG_75,12.52,-0.29,0,0.32 4H86,ASP_163,4.09,-0.31,0.18,0.42 1PVT,GLU_164,1.9,0.39,-2.24,-0.76 105T,LYS_418,10.57,-0.1,0,0.17 1C3K,LYS_105,10.3,-0.28,0,0.08 106D,GLU_46,4.33,0.15,-0.33,0.01 2B0A,LYS_170,10.56,-0.15,0,0.21 3U0V.TYR 158,12.62,-0.55,0.5,2.68 4EUG,LYS_15,9.6,-0.94,0,0.03 4EKU,ARG_79,12.14,-0.36,0,0

2WB8.GLU 451.4.6.0.1.0.0 2G9D.TYR 211.11.41.0.-0.16.1.58 3EAZ,GLU_142,4.49,0.21,0,-0.22 2CI3,GLU_239,4.53,0.25,-0.21,-0.01 2B0A,ARG 21,12.34,-0.18,0.0.02 2B0J.ARG 12,12.86,-1.18,0.75,0.79 3BPV,ARG_19,12.44,-0.22,0,0.17 3I82,HIS 106,5.97,-0.86,0,0.33 2J8A,TYR_296,12.68,0,0.37,2.31 1NRI,ARG_34,13.28,-0.26,0.63,0.41 1ZYL,ARG 242,12.63,-0.1,0,0.23 3IVF,ASP_201,2.14,-2.14,-0.2,0.69 3RLN,CYS_679,9.79,-0.18,0.04,0.93 4FCU,TYR_155,12.13,0.71,0.53,0.89 20RX.ARG 24.12.89.-0.54.0.46.0.47 3EJG,LYS_104,10.93,-0.25,0.42,0.26 1QYI,LYS_33,10.2,-0.33,0,0.03 1XDZ,TYR_141,12.53,-0.82,1.32,2.04 3RFF,ASP_139,2.34,-1.65,-0.1,0.29 2XMZ.GLU 165,4.04,0.38,-0.84,-0.01 2R2Y,CYS_127,10.55,-0.01,0.13,1.43 3I47,CYS_183,10.06,0,0.12,0.94 4ETX,GLU_254,4.72,0.3,0,-0.08 4DIU.GLU 132,4.75,0.19,0,0.06 208P,ASP_50,3.63,-0.44,-0.2,0.46 3ILC,ASP_176,3.75,0,-0.41,0.36 2VGM,ASP_340,4.18,0,0,0.38 2FZP,ARG 213,12.25,-0.25,0,0 3I0C,CYS_209,11.45,-0.85,-0.33,3.63 3NJM,LYS_12,10.3,-0.2,0,0 1NIJ,ASP_161,3.94,-0.07,-0.07,0.28 3M66,LYS_237,10.52,-0.1,0,0.12 1RWZ,LYS_84,10.46,-0.04,0,0 2GAU.GLU 114.4.11.0.31.-0.74.0.05 1AD6,LYS_537,10.39,-0.5,0,0.4 3PP8,ARG_227,12.4,-0.95,0.36,0.5 3GOZ.ARG 175,12.03,-0.68,0,0.21 3HNX,ARG 20,13.09,-0.28,0.54,0.33 1P6F,LYS_118,10.42,-0.08,0,0 3KEY,GLU 330,3.76,0.31,-0.7,-0.36 2ZQ5,ARG_101,12.05,-0.67,0,0.22 1KCM,ASP_154,3.25,-0.75,-0.71,0.9 3BWT,ASP 846,3.61,-0.34,-0.54,0.7 2FZ4,GLU_69,4.88,0.29,0,0.09 1UW7,CYS_14,11.94,0,0.24,2.7 2P1W,ASP_84,1.84,-1.96,-1.42,1.42 3ADO, ARG_261, 12.33, -0.17, 0, 0 3ELI,ARG_49,12.26,-0.97,0.05,0.68 1IAP,ARG_126,12.36,-0.14,0,0 3GS3,GLU_91,3.85,1.68,-1.44,-0.89 3EYE, ASP 147, 2.93, -0.85, -0.88, 0.85 3JZN.ARG 173.13.94.-1.13.0.94.1.63 2X4J,LYS_88,10.71,-0.25,0.17,0.29 2YYO,LYS_100,10.44,-0.13,0,0.06 2Z84,CYS_162,11.72,0.16,0.42,2.14 3M66,GLU_270,4.29,0.24,-0.08,-0.36 1JT9,GLU_148,1.77,0.75,-2.62,-0.86 4FH3,ASP_109,3.62,-0.67,-0.02,0.51 2RGY,ASP_182,3.97,-0.02,-0.27,0.45 4EZB,TYR 222,10.48,0,-0.02,0.5 3BWT.ASP 711.3.84.0.-0.21.0.25 3DSH,TYR_325,10.16,0,-0.25,0.41 3BWT,ASP_853,3.65,-0.21,-0.15,0.21 1RL0,ASP_49,3.86,0,-0.53,0.59 2BLL,GLU_333,4.39,0.98,-0.36,-0.74 1F2V,CYS_98,11.24,-0.79,0.59,2.45 2A6B,TYR_220,13.18,0.85,0.3,2.03 2GAU,HIS_12,6.08,-0.32,0,-0.11 2CBE,LYS_18,10.23,-0.38,0,0.1

2PGE,ARG 64,12.37,-0.19,0.0.07 3LJN,ASP 232,3,49,-0,81,0,0,5 3QAV,LYS_183,10.52,-0.23,0,0.26 3FK5.GLU 177.7.1.2.31.0.25.0.05 1U7U,HIS_188,6.02,-0.21,0,-0.27 3LOE.GLU 516.4.1.0.57.-0.49.-0.48 3PZ9,ASP 84,3.02,-0.67,-0.48,0.36 1NFN,GLU_79,3.72,0.46,-0.85,-0.38 1KN3,HIS_48,5.85,-0.42,0,-0.22 3H13,ARG_337,11.36,-1.17,0,0.03 2RIS,ARG_29,13.02,-0.32,0.42,0.42 1RKA,ASP_175,2.89,-0.85,-0.38,0.32 1YOY,ARG_34,12.44,-0.06,0,0 2HRZ,HIS_-4,6.43,-0.07,0,0 4AF2.ASP 34.2.4.-1.73.-0.05.0.39 2P0L.GLU 66.4.51.0.19.0.-0.18 3CGW,HIS_278,6.32,-0.18,0,1.91E-17 3FFM,ARG_100,12.69,-0.47,0,0.66 3GT0,GLU_47,4.28,0.26,-0.48,0 3EZ7.LYS 320.10.41.-0.09.0.0 1ES5,TYR_108,11.19,-0.3,0,1.49 1ES5,ARG_86,13.51,-0.41,0.82,0.61 3VJ8,GLU_131,3.6,1.25,-2.13,-0.02 2XHC,GLU 273,4.24,0.85,-0.82,-0.29 1DOV.ARG 241,12.18,-0.99,0.25,0.42 2C2Y,LYS_59,10.81,-0.28,0.31,0.27 3UX2,ARG_149,12.28,-0.22,0,0 3IL3,CYS_92,8.93,-0.77,0.13,0.58 3NZL,GLU 15,3.97,0.38,-0.78,-0.12 3RNV,HIS_411,6.68,-0.64,0.8,0.02 1V43,LYS_306,10.59,-0.07,0,0.16 3DHN,GLU_221,3.7,0.23,-0.69,-0.34 2Z0W,LYS 47,10.47,-0.1,0,0.07 3O9P.TYR 133,10.02,0.0,0.02 3ERF,GLU_57,3.69,0.59,-1.22,-0.19 1W24,HIS_33,6.77,-0.85,0.85,0.28 1PVT,ASP_73,2.64,-1.43,-0.24,0.51 2CI3,LYS 158,10.54,-0.06,0,0.1 3UPD,GLU_20,3.39,1.16,-1.73,-0.55 3M16,GLU_267,4.33,0.21,0,-0.38 2A6B,TYR_110,12.6,0,0.49,2.11 2OK1,LYS 558,10,7,-0,12,0,0,31 4F3J,TYR 214,10.38,0.0.19,0.19 3LJI,ARG_289,13.52,-0.59,0.83,0.78 3IL3,ARG_36,12.24,-0.26,0,0 3EGN,LYS_484,10.41,-0.11,0,0.03 3EGN,LYS 461,10.37,-0.13,0,0 2Q12,ASP_241,3.95,-0.05,0,0.2 2QVT,HIS_81,7.13,-0.41,0.7,0.34 2BDV,LYS_116,10.41,-0.72,0,0.63 4ETX,ASP_351,1.88,-2.09,-0.43,0.59 3DHN,ASP 97,4.03,-0.54,-0.27,1.05 3EJG,GLU_37,4.44,0.28,0,-0.34 3EX9,ARG_149,12.73,-0.29,0.02,0.5 3ASA,CYS_168,12.25,0,0.13,3.12 3E5T,ASP_112,3.91,0,0,0.11 1NAF,LYS 206,10,43,-0,1,0,0,03 3R87,HIS_7,4.9,-1.14,0,-0.46 3JZ9,LYS_401,10.3,-0.4,0,0.21 3M66.GLU 221.3.8.0.35.-0.85.-0.21 2VGY.ARG 105.12.4.-0.82.0.04.0.68 3LQE,TYR_501,10.67,0,0.08,0.59 4E8B,ARG_209,12.62,-0.28,0,0.4 2YT4,ASP_549,3.59,0,-0.6,0.38 208P,LYS_15,12.61,-0.75,1.7,1.16 4GA2,LYS_5,10.93,-0.18,0.12,0.5 1JYH,LYS_40,10.09,-0.48,0,0.07 3LJC,LYS_113,10.46,-0.26,0,0.22 3F6F,TYR_77,11.97,0.93,0.43,0.63

2HXB,TYR_103,11.74,0.85,0.38,0.51 2OSA,GLU 291,4.31,0.97,-0.79,-0.37 4DIU,GLU_58,3.67,1.16,-1.5,-0.49 1ZBM.TYR 18.11.8.0.85.0.4.0.56 3IPZ,TYR_132,11.08,0,0.35,0.74 2P5D,LYS 116,10.63,-0.26,0.0.39 1C44,LYS 122,10.09,-0.31,0,-0.1 3GOZ,ASP_98,3.81,-0.17,-0.01,0.18 3CCY,LYS_45,10.39,-0.16,0,0.05 1FHL,TYR_296,12.9,-1.56,0.18,4.29 2E3C,GLU_324,5.14,3.68,-2.09,-0.96 3GE9.GLU 10.4.06.0.21.-0.3.-0.35 2QV2,ARG_319,12.44,-0.09,0,0.03 2RH3,HIS_169,5.23,-0.74,0,-0.53 10GL/ARG 37,13.21,-0.3,0.56,0.45 3V75.GLU 190.4.62.0.3.0.-0.18 4DVD,ARG_166,13.35,-0.23,0.82,0.27 2Z14,ASP 81,3.61,-0.47,0.0.28 1FO9,LYS_335,10.24,-0.91,0.27,0.38 1SJ8,LYS_745,10.4,-0.14,0,0.06 2BV9,ARG 90,13,15,-0,26,0,28,0.62 1PZC,ASP_100,3.98,0,0,0.18 1PNE,GLU_129,4.64,0.29,0,-0.15 1RWZ.LYS 203,11.11,-0.3,0.74,0.17 2EYI.GLU 254.4.64.0.14.0.0 1DZF,HIS_147,6.11,-0.38,0,0 4AM1,GLU_11,3.75,0.49,-0.85,-0.38 1N81,TYR_76,10.87,0,0.06,0.82 3M7D,LYS 116,11.21,-0.26,0.55,0.42 3V46,HIS 344,6.26,-1.17,0.57,0.38 1FQI,HIS_381,6.52,-0.51,0.5,0.03 1DUP,TYR_93,10.46,0,0,0.46 1YTD,ASP_274,3,-1.34,-0.3,0.85 1LZL,ASP 150,1.89,-2.22,-0.32,0.63 2RIK,ASP_205,3.19,-0.79,-0.29,0.46 2CXA,ASP_192,3.91,0,0,0.11 1DTO,TYR_43,11.49,-0.44,0.52,1.41 3B21,GLU 100,4.63,0.08,0,0.05 1SUU.TYR 569,12,75,0.84,0.59,1.32 4ETX,HIS_440,6.57,-0.26,0.17,0.15 3KEY,GLU_432,4.47,0.14,0,-0.16 2CVB,HIS 132,6.83,-2.43,1.17,1.59 4GA2,LYS 40,10.67,-0.14,0,0.31 1V8E,HIS_170,5.4,-0.78,0,-0.32 3GEC,GLU_528,4.7,0.33,0,-0.12 2RIK,ASP_83,2.74,-1.45,-0.24,0.63 3LQE,GLU 296,5,0.29,0,0.2 4DEZ,ASP_209,2.92,-1.16,0,0.28 2H85,ARG_257,12.82,-0.86,0.56,0.62 3IBT.GLU 186.4.01.1.-1.08.-0.42 2P4D,TYR_9,11.78,0.62,0.22,0.95 3P28,ASP_132,4.06,-0.21,-0.33,0.81 2FZ4,ASP 180,4,0,-0.01,0.21 3FWU,GLU_74,4.51,0.18,0,-0.17 4AM1,TYR_145,11.99,-0.03,-1.38,3.39 1JT9,ARG_156,13.8,-0.88,1.17,1.01 1X7F,LYS_290,10.44,-0.13,0,0.07 2H2W,LYS_87,10.29,-0.21,0,0 2CWC.ARG 156.11.98.-0.71.0.0.19 2ZQ5,ARG_131,10.61,-3.08,0.51,0.68 20V2,ASP 76,2.52,-1.48,-0.83,1.03 1HF8,HIS 32,5.99,-0.34,0,-0.18 2FD4,ARG_550,12.03,-0.48,0,0.01 1L3K,CYS_175,10.73,-0.2,0.04,1.9 1VSM,GLU_68,4.95,1.8,-0.82,-0.52 1R5Q,ASP_62,4,0,-0.1,0.3 2EEY,ASP_23,3.33,-0.58,-0.15,0.26 1Y2Q,ASP_9,1.97,-1.74,-0.54,0.45 3E7P,LYS_243,10.53,-0.21,0,0.24

2Q07,ARG_244,12.42,-0.08,0,0 3IO0,HIS 224,7.89,-2.95,0.83,3.51 2CW4,LYS_107,10.47,-0.03,0,0 1SUU,GLU_784,4.57,0.41,0,-0.34 3H9W,ASP_68,1.8,-2.76,-0.64,1.39 2P1W/HIS 41.6.15,-0.35,0.0 3EIZ.HIS -13.6.37.-0.13.0.0 3V75,ASP_38,3.27,-0.68,-0.32,0.46 2F4Q,ARG_186,12.45,-0.07,0,0.01 3B7X,ASP_35,1.61,-2.8,0,0.6 3CS1.GLU 149.4.42.0.21.0.-0.29 2ZO5,LYS 91,10,49,-0,15,0,0,14 3V55,GLU_521,4.68,0.4,0,-0.21 1X04,HIS 204,6.02,-0.42,0,-0.06 1XAW,TYR_481,10.71,0.22,0.06,0.42 2BAA,ASP_20,3.22,-0.83,-0.35,0.6 1TJE,ASP_167,3.52,-0.38,-0.1,0.2 1XEU,ARG_153,12.49,-0.23,0,0.22 1PSW,ARG_306,12.03,-0.61,0,0.14 10XZ.GLU 203,3,98,0,33,-0,42,-0,43 2XMZ,ARG 28,13.87,-1.07,1.5,0.95 1Q46,ARG_52,12.43,-0.07,0,0 1JB3,GLU_118,4.71,0.2,0,0 2D7U,LYS 89,11,44,-0.33,0.58,0.68 1L2ELYS 339.11.14.-0.39.0.7.0.32 1BKB,ASP_68,3.62,-0.38,-0.05,0.25 3EVZ,HIS_238,6.68,-1.35,1.13,0.4 20YZ,CYS_91,11.8,0.22,0.81,1.77 2V5B,LYS_218,10.76,-0.19,0,0.46 4EF5,ARG_197,12.61,-1.06,0,1.17 2CN1,CYS_70,10.21,0,-0.02,1.23 3RKV.ARG 305,12.34,-0.16,0,0 3RFY,ARG_290,12.26,-0.73,0.06,0.42 4GA2,CYS 82,11.58,-0.02,0.2,2.4 2P4D.GLU 104,3.72,0.53,-0.65,-0.67 3FNI,TYR_11,11.4,0,0.46,0.94 1160,LYS_87,10.39,-0.2,0,0.09 3IVF,LYS_364,10.44,-0.06,0,0 2CXY,LYS 42,10.47,-0.03,0,0 1QYI,LYS_197,11.14,-0.85,0.85,0.64 2H85,TYR 225,11,76,0.85,0.22,0.69 3ETU,ARG_92,12.48,-0.36,0,0.34 4HDE,LYS 91,10.46,-0.04,0,0 2VGM,LYS 307,11.68,-0.34,0.85,0.67 2RFA,TYR_222,10.57,0,0.01,0.56 2QEV,HIS_70,5.71,-1.42,0.41,0.21 1JB3,GLU_6,4.35,0.08,0,-0.23 3JZN, ASP 341, 3.82, -0.07, -0.41, 0.52 3KEY,TYR_459,10.15,0,-0.01,0.16 3C6B,HIS_122,5.57,-1.15,0,0.22 3IVF,ASP_69,4.08,-0.1,0,0.38 3FWU,HIS_43,6.15,-0.52,0.15,0.01 20ZO,LYS 132,10.23,-0.33,0.0.06 2CBE,HIS_119,4.73,-3.58,0.85,0.96 3TMO, ARG_227, 12.64, -0.58, 0.22, 0.49 1Q42,LYS_106,10.08,-0.33,0,-0.08 2X4J,GLU_116,3.83,0.28,-0.67,-0.28 3U0V.ARG 19.12.43.-0.07.0.0 3HUE,GLU_220,3.05,0.42,-1.48,-0.38 3ILC, ARG_132, 12.64, -0.16, 0, 0.3 2CXC,ASP_32,2.4,-1.9,-0.96,1.47 1AD6.GLU 492.5.98.3.72.-1.51.-0.74 1BN6,GLU_171,4.94,0.21,0,0.23 1YOY,GLU_37,5.53,2.86,-1.46,-0.35 3EZ7,GLU_218,3.89,0.34,-0.57,-0.38 1MUF,GLU_183,4.53,0.13,0,-0.1 3RJX.GLU 308.4.25.0.59.-0.34.-0.5 2EFK,LYS_166,10.45,-0.05,0,0 2IXM,ASP_35,1.31,-2.47,-0.58,0.57

1UXO.HIS 119.5.92.-0.72.0.0.14 20JO,ASP 459,3.74,-0.51,-0.41,0.87 1H4U,TYR_388,10.3,0,0,0.3 2XHC,TYR_247,9.97,-0.16,-0.23,0.37 2BDV.LYS 113,10,46,-0,04,0,0 1SOW, ARG 174, 12, 53, -0, 22, 0, 0, 25 3U0V,LYS_82,10.52,-0.15,0,0.17 1TR9,LYS 141,10.34,-0.21,0.0.05 4FLE,LYS_115,10.41,-0.09,0,0 3ONT,ARG_106,12.45,-0.05,0,0 3FHF,LYS_5,10.59,-0.09,0,0.18 3CIV,ARG_290,13.81,-0.46,0.8,0.97 2E3C,GLU_199,4.71,0.32,0,-0.11 2PWO,LYS 9,11.32,-0.22,0.68,0.36 1XFK,ARG 203,13.48,-0.44,0.76,0.66 3K8J,HIS_123,6.29,-0.21,0,0 3PBH,TYR_146,10.22,0,-0.36,0.59 1P4X,LYS_206,9.27,-0.96,0,-0.27 3RLN,LYS_743,10.55,-0.42,0.03,0.45 1MTZ.GLU 242,3.64,0.47,-1.11,-0.22 4ANN,HIS_46,6.19,-0.36,0.08,-0.02 1EYH,ASP_108,3.89,0,-0.15,0.25 3A7L,CYS_57,11.75,0,0.52,2.25 2XWS,TYR 63,10.29,0,-0.06,0.35 1MUF,TYR_335,10.41,0,0.14,0.26 3KT9,ASP_69,3.45,-0.76,-0.08,0.49 1NJ4,LYS_92,10.25,-0.24,0,-0.01 1PZC,GLU_113,4.56,0.3,0,-0.24 1L2F.GLU 79.4.65.0.17.0.-0.01 3RRQ,GLU_146,4.01,0.28,-0.61,-0.15 1EDG,ASP_52,2,-2.28,0,0.47 2B0J,CYS_10,9.32,-2.41,-0.15,2.87 2Q07,ARG 497,12.92,-0.19,0.12,0.49 2R51.TYR 222.10.7.0.0.21.0.49 3ADO,LYS_33,10.01,-1.02,0,0.53 1TUL,TYR_61,11.88,0,0.61,1.27 3EX9,ARG_105,12.94,-0.31,0,0.74 1NJ4,ASP_120,4.53,0,0.01,0.71 1GPP,ASP_163,3.08,-1.64,-0.57,1.49 10YI.LYS 301.10.35.-0.43.0.0.27 2X4G,ASP_335,4.18,0,0.1,0.29 1ANU,ASP 34,3.7,-0.82,0,0.73 4E8B.GLU 22.3.59.0.38.-0.95.-0.33 3BCY,LYS_118,10.47,-0.2,0,0.18 2B3M,LYS_147,10.31,-0.26,0,0.07 1LZL,GLU_281,5.44,0.81,0,0.13 1AKO,ARG_251,11.02,-2.04,0,0.56 4FCU,ARG_59,12.51,-0.36,0,0.37 3L7N,GLU_9,4.63,1.02,-0.88,0 3T8R,ARG_112,12.46,-0.25,0.03,0.19 1N81, ARG 78, 11.99, -0.3, 0, -0.21 3GW3,ASP 17,3.89,-0.26,-0.28,0.62 100X,HIS_181,4.4,-1.72,0,-0.37 2P5D,LYS_109,11.1,-0.63,0.85,0.38 10TM,GLU_236,4.9,0.4,0,0 1TR9,GLU 182,4.42,0.09,0,-0.18 3E7P,LYS_135,10.44,-0.12,0,0.06 1RWZ,ARG_117,12.24,-0.32,0,0.06 1PZC,HIS_40,5.8,-1.48,0.64,0.15 3L3P,ARG 490,12.45,-0.37,0,0.32 2F4O,TYR 298,11.68,0,0,38,1,31 2CWC,TYR_119,9.81,-0.84,-0.64,1.28 3M66,LYS_381,11.34,-0.39,0.85,0.38 2GYZ,ASP_44,2.92,-1.11,-0.3,0.53 2EA9,ASP_95,3.91,-1.35,-0.06,1.53 3C6B,HIS 140,5.5,-0.8,0,-0.19 1LZL,TYR_139,10.92,0,0.14,0.78 2B0A,LYS_160,10.25,-0.29,0,0.04 3U4K,ARG 69,12.74,-0.24,0.48,0

3HVW,ASP_316,4.06,0,0.11,0.16 3IVF.HIS 176.5.82,-1.36.0.74,-0.06 3LJI,ASP_127,3.5,-0.79,0,0.48 3LJI,ASP_106,2.5,-1.37,-0.38,0.46 1NAR,GLU_61,4.66,0.12,0,0.05 2O34.TYR 144.11.81.0.0.22.1.59 4FCU,GLU_52,4.62,0.28,0,-0.16 1V43,GLU_229,3.76,0.26,-0.79,-0.21 2JHY,LYS_127,10.61,-0.29,0.17,0.22 4F8A,ARG_564,12.64,-0.12,0,0.26 3H13,LYS_430,11.35,-0.63,0.54,0.95 3CXS,LYS_146,10.34,-0.25,0,0.09 2CXY,GLU_112,4.5,0,0,0 3T8R,CYS_25,9.56,0,-0.09,0.65 1FOLLYS 346.11.14.-0.63.0.85.0.42 3JZ9,ASP 457,3.42,-0.81,-0.04,0.47 1V6T,LYS_251,10.54,-0.32,0,0.36 1N81,ASP_176,3.71,0,-0.26,0.16 3P2F,ARG_69,13.55,-2.86,1.66,2.25 30DJ,TYR 106,10.05,0,0,0.05 2Z61,ASP_172,3.36,-0.83,-0.06,0.46 1NAF,ARG_191,12.41,-0.09,0,0 2FBI,GLU_123,4.68,0.18,0,0 2NMU,TYR 14,9.72,-0.81,-0.23,0.76 3V10.GLU 666.4.57.0.08.0.-0.01 1BYI,LYS_217,10.56,-0.21,0,0.27 1SFE,ARG_165,12.86,-0.97,0.69,0.64 2V4U,GLU_476,6.93,3.74,-1.38,0.07 3OKQ,LYS 665,10.38,-0.12,0,0 3GW3,GLU_316,3.44,0.27,-1.3,-0.02 4GA2,LYS_106,10.95,-0.26,0.28,0.42 20GQ,LYS_475,11.96,-1.33,1.7,1.09 1N81,GLU 42,3.92,4.85,-2.1,-3.32 2FL4,ARG 92,12.27,-0.26,0.0.03 1NRI,LYS_208,10.47,-0.26,0,0.24 3FHF,GLU_184,5.22,0.27,0.16,0.29 2B61,ASP_190,3.05,-1.76,0,1.01 3PBH,GLU 171,9.61,5.35,-0.79,0.55 3GG6,GLU_138,5.02,0.6,0,-0.09 4GCO,LYS_229,10.55,-0.14,0,0.19 1ILW,ARG_51,11.05,-1.45,0,0 3BQW,GLU_78,4.53,0.93,-0.82,-0.07 1RWZ.GLU 24,5.01.0.35.0.0.16 2R51,GLU_20,4.21,0.19,-0.72,0.24 3PP8,LYS_58,11.07,-0.31,0.21,0.68 1MIX,LYS_343,10.58,-0.13,0,0.21 2RGY,ARG_112,13.01,-0.19,0.32,0.38 2YWX,GLU_28,4.58,0.16,0,-0.08 1YB2,ARG_89,12.4,-0.12,0,0.02 1T95,ASP_11,2.83,-0.67,-0.38,0.09 208I, ASP_65, 3.61, -0.81, -0.02, 0.64 3H5T,ARG_190,12.19,-0.34,0,0.03 2FG1,ASP_9,2.56,-1.71,-0.27,0.75 1BN6,GLU_31,5.26,0.46,0,0.29 2H14,LYS_87,10.47,-0.12,0,0.09 4FCU,ASP_236,2.84,-1.03,-0.57,0.64 2IXM,LYS 103,10,13,-0,18,0,-0,19 1XFK,LYS_233,10.42,-0.19,0,0.11 3HUE,GLU_193,5.02,0.37,0,0.14 3RJX.GLU 259.4.65.0.4.0.-0.26 2O34,LYS 80,10,28,-0,54,0,0,32 1RAJ,CYS_212,11.29,-0.09,-0.05,2.43 1YB2,LYS_30,10.45,-0.07,0,0.02 1MIX,LYS_234,11.01,-0.47,0.41,0.57 2B2H,GLU_387,4.58,0.26,0,-0.18 208PLYS 227.10.5.0.0.0 3M66,GLU_311,4.1,0.94,-0.83,-0.5 3C38,HIS_120,6.34,-0.18,0,0.03 1RZ2,TYR_202,12.5,0,-0.04,2.55

1YR6.GLU 134.4.58.0.18.0.-0.1 1WNH,LYS_64,10.41,-0.12,0,0.03 3T57,LYS_268,10.35,-0.08,0,-0.08 2OB5.HIS 15.6.36.-0.19.0.0.05 4EKU,ASP_116,3.86,-0.23,-0.06,0.35 4DVD CYS 123.9 35 -0.03.0 01.0 37 1PV5.CYS 102.11.78.0.0.35.2.42 3V3T,CYS_87,10.66,-0.21,-0.04,1.92 2R0S,LYS_206,10.54,-0.04,0,0.09 3PM2,HIS_34,7.11,-0.67,0.85,0.43 3R2E,GLU 81,4.61,0.29,0,-0.19 200K,LYS 182,10,48,-0.08,0,0.07 2AZP,ARG_34,12.17,-1.05,0.08,0.64 3GEC,TYR_459,12.49,-1.21,0,3.7 2XJ4,GLU 88,3.77,0.5,-0.85,-0.38 2RFA,LYS 54,10.7,-0.24,0.0.43 2YWX,LYS_13,10.63,-0.16,0,0.29 3KEY,ASP 471,4.36,-0.14,0.02,0.67 4EVF,LYS_133,10.42,-0.08,0,0 2FPN,GLU 35,3.74,0.35,-1.07,-0.05 2ZCX.GLU 34.4.83.0.25.0.0.08 3EZ7,LYS_43,11.3,-0.46,0.38,0.89 1NAR,TYR_45,10.51,0,0.23,0.27 3M7G,GLU 169,4,41,0.27,0,-0.36 1TD6.LYS 122.9.89.-0.69.0.0.09 3ETV,GLU_235,4.1,0.3,-0.7,0 3CIV,GLU_156,6,3.81,-1.61,-0.69 3RE9,ARG_96,12.02,-0.49,0,0.02 1V8E,GLU_22,4.18,1.06,-0.6,-0.77 1YTD.GLU 96.4.24.1.77.-1.06.-0.98 3EJC,GLU_23,4.38,0.22,-0.5,0.16 4F85,GLU_278,3.1,1.52,-2.41,-0.52 2CVB,ASP_124,3.17,-1.42,-0.64,1.43 3IVELYS 83.10.34.-0.4.0.0.24 2B3M,LYS_133,10.27,-0.08,0,-0.16 3CAX,ASP_370,2.15,-2.14,-0.45,0.93 200K,LYS_136,9.88,-0.56,0,-0.06 1T3Y,GLU 44,4.4,0.15,0,-0.25 1GOE,LYS 30,9.62,-0.89,0.0 2D59,GLU_60,4.53,0.09,0,-0.07 2BCF,HIS_159,6.14,-0.36,0,0 1AD6.GLU 458,4,58,1,26,-0,72,-0,46 2P4D.CYS 99.11.06.-0.05.-0.03.2.14 20KT,HIS_66,6.21,-0.28,0,-0.02 1NAR,LYS 181,10.07,-0.53,0,0.1 2V4U,CYS_362,10.15,0,-0.04,1.18 2GKG,LYS 36,10.47,-0.07,0,0.05 3UV9,GLU_410,3.72,0.29,-0.67,-0.4 3PAC,TYR_137,10.28,-0.61,-0.26,1.14 2RIS,ASP 26,2,52,-1,65,-0,03,0,4 2AZP,ARG_289,12.94,-0.48,0.4,0.52 4E8B,ARG 114,12.51,-0.26,0,0.27 1NJ4,ASP_67,2.47,-1.44,-0.38,0.5 1X7F,GLU_200,2.55,1.56,-3,-0.51 3EZ7,ASP_337,3.17,-0.76,-0.23,0.36 4FD6,TYR_18,10.19,-0.04,-0.05,0.29 3M66,ARG_285,11.66,-0.84,0,0 1YOY,GLU_101,4.62,0.08,0,0.05 4AF2.LYS 167.10.39.-0.16.0.0.05 3COU,TYR_95,10.76,-0.85,-0.09,1.7 2WOZ,TYR 291,10.05,0,0,0.05 1JKS.GLU 173.4.89.0.66.0.-0.28 2YX0,LYS_134,11.1,-0.57,0.65,0.53 2NMU,GLU_60,4.47,0.1,0,-0.13 1WJG,LYS_77,10.38,-0.09,0,-0.03 1EV8,GLU_250,4.51,0.24,0,-0.23 3IVF,GLU_186,4.47,0.19,0,-0.22 1MIX.LYS 320.10.45.-0.05.0.0 1NAF,LYS_198,10.42,-0.08,0,0

3V46,GLU_306,4.18,0.22,-0.13,-0.41 3RE9,LYS 163,10.31,-0.24,0,0.05 2GEN,ARG_101,12.44,-0.67,0.32,0.28 2B2H,TYR_76,10.49,-0.01,0.21,0.29 1X9G,LYS_139,10.67,-0.11,0,0.28 4F85,ASP_98,3.28,-0.81,-0.58,0.87 3LJN.ARG 225.12.98.-0.18.0.27.0.4 2RIK,LYS_108,10.47,-0.48,0,0.45 2CI3,LYS_266,11.23,-0.79,0.85,0.68 3RE9,ASP_169,2.55,-1.06,-0.75,0.56 1SBX,GLU_99,3.98,0.31,-0.84,0.01 1ZKZ,ASP_89,3.91,0,0,0.11 1T07,LYS_72,11.52,-0.35,0.85,0.52 30N1,LYS 64,11.2,-0.5,0.82,0.38 2AHE,ASP_209,3.06,-0.76,-0.39,0.41 3GA2,LYS 138,11.28,-0.68,0.85,0.61 3HZQ,ASP_72,4.37,-0.08,0,0.65 2H30, ASP_175, 2.52, -1.52, -0.06, 0.31 2E0T,HIS_61,6.92,-0.44,0.68,0.18 3A4C,ARG 474,11.98,-0.4,0,-0.12 3O2C,LYS 5,11.52,-0.31,0.85,0.48 3FK5,ARG_52,11.58,-2.9,0.59,1.39 3CJW,CYS_260,9.89,-0.32,-0.36,1.57 1N81,TYR_118,12.22,0,0.71,1.51 2IDC,GLU 166,4.35,0.23,-0.19,-0.19 1JT9,LYS_250,10.44,-0.11,0,0.05 2CL3,TYR_158,10.49,0,0.22,0.27 3M3P,HIS_245,6.31,-0.14,0,-0.05 1WXO.GLU 63.4.48.0.86.-0.46.-0.41 20V2.GLU 241.5.02.1.19.-0.77.0.1 3V3T,HIS_45,6.14,-0.41,0,0.05 1PBV,GLU_87,4.44,0.11,0,-0.17 2EEY,LYS_51,10.3,-0.21,0,0.01 3KB5,GLU 342,4.4,0.29,-0.09,-0.3 1ZBM,TYR 238,10.14,0,-0.13,0.27 2JHY,ARG_111,12.15,-0.38,0,0.03 3V55,GLU_624,4.02,0.36,-0.79,-0.05 3BZT,TYR_301,10.22,0,-0.15,0.37 1ANU,ARG 38,12.48,-0.22,0,0.2 2OSA, ASP_456, 3.72, -0.34, -0.12, 0.37 1XTD.LYS 37.10.37.-0.13.0.0 3JSN,GLU_110,6.42,3.51,0,-1.59 2JEO,ARG 57,11.89,-0.7,0,0.08 4FD6.LYS 150.10.25.-0.3.0.0.06 3C0C,GLU_320,4.89,0.17,0,0.22 3US6,ARG_92,13.61,-0.7,1.26,0.54 1LZL,GLU_265,10.04,4.86,-1.47,2.16 2EDM,ASP_199,3.91,0,0,0.11 3HVM,LYS_232,11.16,-0.8,0.24,1.22 20EW,LYS_96,9.97,-0.24,0,-0.29 2PIM,TYR_6,10.48,0,0.01,0.48 1EYH,GLU 26,4.81,0.27,0,0.04 3EZ7,HIS 327,6.78,-0.28,0.59,-0.02 1Q5Z,HIS_535,7.26,-0.36,0.85,0.27 1AIL,ASP_24,3.04,-0.74,-0.41,0.39 2B78,GLU_205,5.06,0.43,0,0.13 3NR5,ARG 93,12.42,-0.12,0,0.03 3RLN,TYR_705,12.59,0,0.62,1.98 1QYI,GLU_153,4.64,0.21,-0.06,0 1R7J,LYS_61,10.81,-0.15,0,0.45 10GL,HIS_228,6.08,-0.44,0,0.03 3M9A,ASP_22,3.96,0,0,0.16 4GCO,ARG_248,12.31,-0.28,0,0.09 1WPA,ARG_519,13.32,-0.23,0.74,0.3 3M70,GLU_64,4.24,0.28,-0.54,0 2W1R,ASP_127,3.36,-0.69,0,0.25 2IXM,ARG 236,12.62,-0.26,0,0.37 3BB7,ARG_254,12.09,-0.48,0,0.07 2IDC,ARG_145,12.37,-0.31,0,0.18

1MMLLYS 193,10.67,-0.64,0.32,0.49 3CJW.CYS 326.9.15.0.0.01.0.14 2AZP.CYS 246.12.63.0.1.0.31.3.21 1PGV,LYS_239,10.68,-0.26,0.01,0.43 2WB3,LYS 278,10.38,-0.12,0.0 3O2C,LYS 41,10.46,-0.09,0.0.05 4D8L,HIS_180,3.12,-3.18,0,-0.2 1UOH,ARG_35,12.52,-0.27,0,0.28 2A6B,ASP_5,3.91,-0.02,-0.07,0.2 3U2A,ARG_36,12.73,-0.19,0,0.41 1AT0.HIS 316.5.59.-0.64.0.-0.28 2OSA,GLU_455,5.52,0.89,0,0.12 3LMO,HIS_28,6.44,-0.4,0,0.33 2PWO,LYS 127,10.66,-0.11,0.0.27 3CCY.CYS 112.10.51.-0.15.0.11.1.56 1ES9,LYS_22,10.61,-0.22,0,0.32 2E3S,CYS_433,9.8,-3.6,0.56,3.84 2QV2,TYR_293,10.69,0.15,0.36,0.18 1W7B,ARG_77,12.36,-0.15,0,0.02 4DEZ,LYS 189,10,46,-0,04,0,0 10I7,LYS_261,11.32,-1.94,1.68,1.09 3A4C,GLU_464,4.8,0.27,0,0.03 3CSR,ASP 57,3.61,-0.47,0.0.28 1GXN,TYR 443,11.19,-0.03,0.3,0.93 2WB3,LYS_334,10.37,-0.13,0,0 1XDZ,ARG_105,13.11,-1.33,1.28,0.66 2QDJ,ASP_111,2.87,-0.85,-0.38,0.31 3I4T,ARG 97,12.23,-0.33,0,0.07 2C2Y,GLU_14,3.6,0.41,-0.83,-0.48 2VAN,GLU_309,4.61,0.15,0,-0.05 3G9G,GLU_135,3.56,0.37,-1.14,-0.18 1WNH,LYS_208,10.42,-0.22,0,0.14 1ZBM.TYR 236,11.82,0.69,0.56,0.57 3P28,LYS 233,10,58,-0,23,0,0,31 2E0T,ARG_158,12.6,-0.91,0.39,0.63 1MUF,TYR_191,11.49,0,0.04,1.45 1YM5,LYS 8,11,91,-1,25,1,7,0,96 1X9G,LYS_10,10.21,-0.27,0,-0.02 1K95,HIS_142,6.57,-0.19,0,0.27 1W24,LYS 180,11,38,-0,3,0,85,0,32 1R5Q,LYS_66,10.56,-0.15,0,0.21 3V75,ARG 115,13.49,-0.28,0.6,0.67 3GFP.LYS 433,10.62,-0.11,0.0.24 1Y0K,ARG_108,11.98,-0.86,0,0.33 3IDW,ASP_34,3.22,-0.86,0,0.29 3BA1.GLU 216.4.71.0.2.0.0.01 4F8A,CYS_589,11.29,-0.01,0,2.3 3VHJ,GLU_56,4.68,0.24,0,-0.06 2FBO.ARG 113.11.93.-0.62.0.0.04 2HRZ,LYS_75,10.29,-0.26,0,0.04 1NWA, ARG 83, 12.17, -0.19, 0, -0.14 2D2S.GLU 557.4.79.0.23.0.0.06 1O3X,HIS_235,6.65,-0.48,0.63,0 3R2E,ARG_39,12.8,-0.09,0,0.38 1ES9,TYR_193,10.38,0,0.02,0.36 1VSM,HIS_104,2.96,-3.15,0,-0.39 1LTU,ASP_34,3.45,-0.49,-0.18,0.32 300P,LYS_59,10.41,-0.09,0,0 3GV0,ARG_246,12.3,-0.36,0,0.16 1WYC,LYS 315,10.44,-0.06,0,0 2007,ARG 282,13.02,-2.38,1.37,1.53 3A4C,GLU_506,3.54,0.3,-1.02,-0.25 2BDD,LYS_132,10.36,-0.11,0,-0.03 3CIV,HIS_84,6.71,-1.26,0.85,0.61 3BA1,TYR_29,10.86,0,-0.03,0.9 3B4D,GLU 219,3.63,0.43,-0.68,-0.62 1L3K,ASP_48,2.2,-1.96,-0.09,0.44 3CXS,GLU_127,4.83,0.2,0,0.13 1I60,LYS 274,10.49,-0.14,0,0.12

3ZXY,HIS_114,4.33,-1.71,0,-0.46 4FCU,ARG 139,12.52,-0.31,0,0.32 2H8O,LYS_49,10.34,-0.27,0,0.11 2XMZ,ASP_39,3.95,-0.09,-0.03,0.27 3HVM,GLU_297,3.59,0.32,-0.85,-0.38 1RZ2,GLU 207,4.83,0.34,-0.01,0 3EVN,LYS_54,10.4,-0.12,0,0.02 2PGE,LYS_173,10.2,-0.72,0,0.42 3LE4,ARG_341,12.47,-0.03,0,0 2F9F,ASP_53,3.74,-0.35,0.02,0.27 1NRI,GLU_89,5,0.65,0,-0.16 2D0A,TYR_20,12.65,0.12,0.4,2.13 4DIU.LYS 164,10,78,-0,13,0,0,41 3Q1C,TYR_394,13.04,0.42,0.12,2.51 1GXN.ARG 557,13.59,-0.46,0.85,0.71 2OK0.ASP 30.3.3.-0.61.-0.12.0.22 2QHT,GLU_107,5.95,1.5,0,-0.05 4FCU,HIS_24,6.6,-0.54,0.68,-0.03 200K,LYS_19,10.4,-0.1,0,0 2Q98,GLU 107,4.66,0.16,0,0 1SUU,ARG_626,11.83,-1.19,0.17,0.34 2I88.TYR 507.13.59.0.0.22.3.36 3EZ7,CYS_326,9.57,-0.05,0.29,0.33 4H89,GLU 25,4.45,0.43,-0.32,-0.15 20K1.CYS 443,12.5,-0.01,0.27,3.25 3KV0,ASP_53,3.69,-0.44,0,0.34 2WB8,GLU_497,5.97,4.14,-2.29,-0.4 3EYE,LYS_137,10.27,-0.34,0,0.11 1JKS,LYS 154,10.45,-0.12,0,0.07 2D7U,GLU_79,3.41,0.24,-0.85,-0.48 3F7M,ARG_229,12.3,-0.2,0,0 1J7G,ASP_14,2.57,-1.42,-0.38,0.57 2R57,ASP_337,3.75,-0.3,-0.22,0.47 1AKO.GLU 114.3.29.0.31.-0.88.-0.65 4FH3,LYS_282,10.44,-0.13,0,0.07 2XJ4,HIS_24,3.59,-3.2,0,0.28 3H04,ARG_130,12.87,-1.41,1,0.78 2ZQ5,ARG_304,13.4,-1.34,1.61,0.64 4ACJ,ASP_767,4.23,0,0.2,0.23 1DVO,ARG_170,13.12,-0.33,0.39,0.56 3BA1,GLU_261,4.04,2.21,-1.61,-1.07 2O4D.TYR 15.10.26.0.0.01.0.26 4ESS.GLU 131.4.06.0.35.-0.26.-0.53 3RJX,LYS_74,10.29,-0.57,0,0.36 3G6S,CYS_220,10.69,0,0.42,1.28 2FBQ,HIS_125,6.41,-1.26,1.39,-0.22 3IVF,GLU 342,4.9,0.6,0,-0.19 1J85,ARG 28,12.87,-0.85,0.22,1.01 3EGN,ARG_398,12.11,-0.68,0,0.28 2A0J,LYS_74,10.31,-0.24,0,0.04 1WLY,LYS 182,10.09,-0.41,0.0 1KN3,HIS 85,4.11,-2.71,0.82,-0.5 2FPN,GLU_111,4.7,0.27,0,-0.06 4FH3,TYR_205,9.74,0,-0.41,0.16 3OBS,HIS_119,5.92,-0.63,0,0.04 2W0G,LYS_149,10.26,-0.25,0,0.01 1A80.LYS 261.11.34.-0.76.0.85.0.76 3ETU,LYS_350,10.64,-0.15,0,0.28 1059,TYR_314,11.7,-0.18,0,1.88 3OKQ,LYS_576,11.11,-0.28,0.49,0.39 1XKR.GLU 176.3.39.0.19.-0.85.-0.45 2YT4,LYS_500,10.46,-0.04,0,0 3ODJ,ARG_187,12.19,-0.2,0,-0.1 4DEZ,ARG_26,12.2,-0.33,0,0.03 1RHS,TYR_6,10.34,-0.72,-0.59,1.65 1C3K,ASP_5,2.53,-1.28,-0.55,0.56 1AKO,LYS_60,10.29,-0.12,0,-0.09 3T57,GLU 137,4.76,0.23,0,0.02 1ZCU,LYS_180,10.54,-0.48,0,0.52

301C,LYS 374,10,47,-0,47,0,07,0.36 3IV4,TYR 37,11.94,0.11,0.55,1.29 2AD1,GLU_195,6.35,3.57,-1.78,0.06 1RI5.GLU 279.4.17.0.7.-0.46.-0.57 1059,GLU_11,4.43,0.28,-0.6,0.24 3DB9.GLU 14.4.53.0.2.0.-0.17 3BB7.LYS 140,10.57,-0.54,0.18,0.43 2G9D,ASP_50,2.59,-1.38,-0.4,0.56 3U0V,LYS_202,10.47,-0.23,0,0.19 2CXA,HIS_124,5.66,-1.55,0.72,-0.01 3CBN,GLU_156,3.31,0.56,-0.97,-0.78 2FXT,LYS 239,10.38,-0.12,0.0 1IDK,ASP_159,4.54,0,-0.03,0.77 3RE9,HIS_158,6.79,-0.95,0.85,0.39 3L7N,TYR 67,11,59,-0,29,0,48,1,4 1FHL.TYR 191,9.88,-0.37,0.02,0.23 2YX0,LYS_135,9.94,-0.64,0,0.09 2RH3,ARG 196,12.81,-0.26,0.16,0.41 1MTZ,GLU_256,4.34,0.39,0,-0.55 3M7D,GLU 175,2.94,0.43,-1.55,-0.44 4F8A,GLU 651,4,14,0,33,-0,34,-0,35 2IOT.GLU 75.2.84.0.85.-1.52.-0.98 3CXS,CYS_179,8.99,-0.28,0,0.28 3MM4.ASP 979.3.33.-0.42.-0.41.0.36 4EKU.GLU 243.3.84.1.71.-0.77.-1.61 3MIX,LYS_573,10.76,-0.12,0,0.38 2AZP,TYR_84,13.52,0.61,0.22,2.7 1ILW,LYS_32,11.45,-0.39,0.63,0.7 2W2S,ARG 117,12.23,-0.2,0,-0.06 2W2S,LYS 160,10.69,-0.12,0.0.31 3EUR,ASP_16,2.64,-0.85,-0.76,0.45 3I47,LYS_209,10.76,-0.55,0.34,0.46 3GOZ,TYR 94,10.37,0.0.19,0.18 2BAA,CYS 223,11.65,-0.45,-0.07,3.18 30NH,LYS_551,10.42,-0.12,0,0.03 1DZF,LYS_71,10.66,-0.63,0.17,0.61 1QQE,ASP_214,3.33,-0.81,-0.11,0.44 4FCU,GLU_129,4.67,1.19,-0.47,-0.54 3BQW,ASP_94,2.42,-1.61,-0.2,0.43 2EFK,GLU_135,4.38,0.4,0,-0.52 1QQE,LYS_279,10.32,-0.31,0,0.13 3RFF,ASP_29,2.26,-1.44,-0.35,0.26 2GKG,ASP_30,3.6,-0.55,-0.25,0.61 2Y2T,HIS_90,6.24,-0.25,0.04,-0.05 3VHJ,TYR_129,10.39,0,0.03,0.37 2P0Y,HIS_251,5.18,-1.8,0.92,-0.44 2ILR,ARG 371,11.56,-1.34,0.01,0.4 1T95,GLU_198,4.67,0.21,0,-0.04 1PV5,ARG_108,11.49,-1.06,0,0.05 1R7J.GLU 8.3.57.0.29.-0.83.-0.4 1JB3,ARG_128,13.33,-0.25,0.69,0.38 3SMD,GLU 99,3.87,0.49,-0.63,-0.49 2IRM,ARG_304,12.18,-0.37,0,0.05 3RVC,GLU_97,3.57,0.78,-1.26,-0.45 2IRM,CYS_288,11.4,-0.04,-1.05,3.5 1WRU,ARG_231,12.26,-0.24,0,0 3H13,TYR_347,9.66,-0.37,-0.21,0.24 2XWS,ASP_60,3.29,-0.65,-0.17,0.3 2DFL/HIS 238.6.03,-0.47,0,-0.01 3CCY,HIS_50,6.05,-0.22,0,-0.23 3I82,TYR 65,9.88,-0.18,-0.24,0.31 1GPP.CYS 75.12.77,-0.11.0.25.3.64 3LJC,ARG_216,12.12,-0.24,0,-0.14 1Z3X,ASP_93,4.29,0,0.16,0.33 3F6F,ARG_97,10.86,-1.66,0,0.03 1IDK, ARG_308, 13.3, -1.63, 1.41, 1.02 2E0T,ASP_125,2.63,-1.48,-0.01,0.32 3E5T.CYS 26.12.11.0.0.3.11 3EAZ,GLU_147,3.63,0.15,-0.8,-0.21

2OSA,TYR_396,10.6,-0.23,0.07,0.75 1ZKZ,HIS 54,6.42,-0.22,0,0.14 1RSS,TYR_44,12.05,0.21,0.56,1.27 1J7G,GLU_107,5.11,0.61,0,0 3ZTA,TYR_74,10.55,0,0.22,0.33 2V5B.GLU 130.4.42.3.32.-2.94.-0.48 2099.LYS 358.10.35.-0.13.0.-0.02 2XHC,TYR_14,10.22,0,0.02,0.2 1JKS,ARG_150,12.77,-0.39,0.17,0.5 1H09,LYS_225,10.3,-0.19,0,-0.01 2Q98,GLU_145,4.63,0.13,0,0.01 1PBV,GLU_229,4.6,0.22,0,-0.13 2R4Q,ARG_256,12.28,-0.22,0,0 3RHE,ARG 84,13.31,-0.15,0.48,0.49 1F2V,ASP_59,4.03,0,0,0.23 1Y0K,GLU 138,4.72,0.22,0,-1.39E-17 1RAJ,LYS 348,10.33,-0.2,0,0.03 3NR5,ARG_150,12.31,-0.58,0,0.39 1NRI,LYS_175,10.51,-0.05,0,0.07 105T,GLU_199,5.01,1.95,-0.71,-0.73 4F85.GLU 181.7.88.4.92.-1.6.0.06 2FD4,LYS_529,11.06,-0.28,0.69,0.15 3FK5.TYR 95.9.71.-0.7.0.2.0.21 3IL3,GLU_23,4.37,0.36,-0.62,0.14 2FPN,LYS_20,10.46,-0.17,0,0.13 1LTU.GLU 62.4.92.1.13.-1.02.0.31 1J33,GLU_220,5.13,0.43,0,0.19 1T07,ASP_71,4.18,0,-0.22,0.6 20K1,LYS 382,10.35,-0.15,0.0 3BCY,LYS_106,10.47,-0.29,0,0.27 2F9F,TYR_133,11.09,0,0.12,0.97 2GOV.TYR 55.11.18.-0.22.0.43.0.97 1LFP,HIS_120,5.55,-0.82,0,-0.13 2FBQ,TYR 141,13.25,0,0,3.25 1MTZ,LYS 117,12,29,-0,4,1,32,0.86 1N81,CYS_46,11.85,-0.13,-0.57,3.55 3NBI,ASP_71,3.93,0,0,0.13 2PIM,GLU_14,4.62,0.12,0,0 3PM2,CYS 54,10.2,-1.56,0.2,2.55 2VGY,TYR_86,10.5,0,0.14,0.36 1NRI.GLU 39,3.72,1.06,-1.33,-0.52 4E8B,CYS_160,11.89,-0.04,-0.02,2.94 1SUU,LYS 745,10.44,-0.15,0,0.09 3LJI.GLU 175,4.96,0.63,0,-0.18 2RIS,LYS_140,10.22,-0.28,0,0.01 1RI6,LYS_149,10.25,-0.4,0,0.14 3UAH,ASP_235,4.07,0,0,0.27 3M7G,GLU 237,4.65,0.1,0,0.05 3JRT,GLU_11,4.14,0.34,-0.61,-0.1 1X7F,HIS_29,6.95,-0.7,0.85,0.29 2B78, ASP_83, 3.76, 0, -0.33, 0.29 3M3P,ASP_217,3.8,0,-0.22,0.22 1YM5.TYR 210.12.38.0.0.5.1.88 2ZCO,GLU_149,4.4,0.76,-0.67,-0.18 1ZBS,HIS_88,6.32,-0.16,0,-0.02 3F1X,GLU_47,4.33,1.3,-0.7,-0.76 3VJ8,HIS_161,6.35,-0.31,0,0.16 3EZ7,TYR_82,10.08,-0.38,0.09,0.37 3FRR,TYR_75,12.25,0.14,0.49,1.61 3M66,LYS_189,11.43,-0.23,0.77,0.38 3GW3,TYR_182,10.34,0,0,0.34 3ADO,ARG 103,12,32,-0,24,0,0.06 1VJG,ASP_59,3.02,-0.99,-0.54,0.75 2D2S,ASP_537,3.08,-0.85,-0.51,0.65 1Q8B,GLU_67,6.45,2.62,-0.63,-0.04 3B79,GLU_108,4.73,0.14,0,0.09 2012.LYS 124.10.41.-0.12.0.0.04 1RI6,GLU_305,4.27,0.41,0,-0.65 2V5B,HIS_48,6.18,-0.36,0,0.04

1L2H.GLU 25.4.64.0.32.-0.07.-0.11 3ADO,HIS 137,6.98,-0.77,0.76,0.49 2CWY,HIS_50,5.85,-0.56,0,-0.08 3GYW,TYR_151,10.69,-0.24,0.18,0.75 1EDG.ARG 155.12.09.-0.64.0.0.24 3KEY,TYR 421,9.97,-0.62,0.28,0.32 2Z14,ARG_69,12.45,-0.17,0,0.11 3RFY,ASP_402,4.18,0,-0.06,0.43 1MJS,ARG_278,12.55,-1.08,0.53,0.58 2FC3,ARG 8,12.95,-0.37,0.08,0.73 3RLE.LYS 60.10.42.-0.08.0.0 1Z9L,GLU_82,2.76,0.35,-1.63,-0.47 1ZKZ,ASP_47,3.8,-0.12,0,0.13 20EW.GLU 137.4.24.0.4.-0.3.-0.35 3PZ9.ARG 157.12.96.-0.71.0.04.1.14 2HRZ,GLU_267,4.09,0.58,-0.76,-0.23 1SNT,HIS_185,6.04,-0.24,0,-0.21 2YLF,LYS_187,10.36,-0.13,0,-0.01 1JKS,LYS_28,10.88,-0.35,0.42,0.31 3C2E,ARG 131,12.25,-0.33,0.0.07 3D9H,HIS_124,6.03,-0.45,0,-0.02 1JT9,GLU_102,4.62,0.15,0,-0.03 3BCY,HIS_63,6.41,-0.15,0,0.06 1KN3,ARG 141,12.41,-0.24,0,0.15 1UXO,GLU_82,3.78,1.4,-1.45,-0.65 2CE6,ARG_29,12.06,-1.23,0.39,0.41 2GKG,ASP_11,3.1,-0.93,-0.16,0.4 1R9W,LYS_292,10.12,-0.5,0,0.13 105T,ARG_127,13.13,-0.36,0.53,0.46 3F6M,LYS_61,10.4,-0.17,0,0.06 2CN1,GLU_122,3.47,0.33,-0.68,-0.68 3ASA,CYS_383,10.9,0,0.02,1.87 2B0J,ASP 134,3.4,-0.71,-0.1,0.4 2F4O,ARG 336,12.7,-0.42,0.0.62 1TD6,LYS_134,10.11,-0.24,0,-0.15 3I0C,GLU_135,3.61,0.42,-0.85,-0.46 2IXM,LYS_28,9.69,-0.71,0,-0.1 3F1X.TYR 226.11.54.0.0.79.0.75 2XJ4,ARG_194,13.44,-0.26,0.82,0.38 1DVO.CYS 98,9,79,0.08,0.15,0.57 1CBY.CYS 19.8.3.-0.73.0.0.03 1AD6,GLU 539,4.62,2.2,-1.45.-0.63 1EYH,ASP 31,3.17,-0.82,-0.29,0.48 3B4D,ARG_227,12.42,-0.08,0,0 1ZCU,TYR_145,12.19,-0.85,0.48,2.56 3N2T,CYS_212,12.09,0.02,-0.06,3.13 1DTO,GLU_90,3.29,1.26,-1.66,-0.8 3PBH,TYR_148,10.22,0,0.08,0.14 1QQL,TYR_125,10.68,0.23,0.17,0.28 1NFN,GLU_59,3.46,0.54,-1.58,0 10LR,CYS 175,13.19,0,0.36,3.83 3M7G.TYR 38,10.06.0.-0.14.0.2 1SJ8,GLU_657,4.97,0.78,0,-0.3 2OGQ,ARG_560,13.82,-0.65,0.7,1.28 1L3K,TYR_124,10.31,-0.77,0.06,1.02 3HZQ,LYS 45,10.43,-0.07,0,0 2X4J,TYR_111,10.15,0,0.06,0.1 1YM5,LYS_291,10.27,-0.29,0,0.06 3KB5,LYS_330,10.46,-0.13,0,0.1 2CN1,GLU 19,4.53,0.21,0,-0.18 2H01,ARG 149,12,72,-0,32,0,0.54 3HVM,LYS_258,10.62,-0.11,0,0.24 1SUU,ASP_762,4.03,0,0.05,0.18 3ANJ,TYR_239,10.21,0,0.04,0.17 2B78, ASP_309, 3.78, 0, -0.42, 0.41 1J33,TYR 241,10.75,0,0.25,0.51 1IDK,HIS_210,4.33,-3.19,1.05,-0.02 3GEC,CYS_467,8.7,-1.42,-0.13,1.25 1MTZ,GLU_279,4.13,0.25,-0.72,0.1

1LFP.HIS 115.6.68.-0.26.0.75.-0.3 4ANN.GLU 65,3.6,0.33,-0.85,-0.38 3PP8,LYS_73,10.28,-0.28,0,0.07 1Z9L.LYS 83.10.45.-0.05.0.0 1T3J,ARG 679,12.38,-0.12,0,0 2007.LYS 431,10.47,-0.03,0,0 3DHN,LYS_209,10.44,-0.11,0,0.05 3L7N,GLU_73,5.53,3.8,-0.85,-1.93 3ERF,GLU_205,3.84,0.3,-0.73,-0.23 3HYQ,LYS_55,10.91,-0.73,0.85,0.27 1UW7,GLU_-7,4.99,0.5,0,-0.01 2RIS,ASP_170,2.14,-1.6,-0.45,0.4 2X4G,TYR_54,10.6,-0.58,-0.53,1.71 2B78,ASP_117,4.19,0,-0.01,0.41 2R2YLYS 42.10.46.-0.06.0.0.01 2BAA.HIS 121.5.57.-0.99.0.0.06 10I7,ARG_263,12.95,-0.22,0.08,0.59 3EJG,LYS_147,11.25,-1.21,0.85,1.11 1H4U,GLU_616,4.65,0.15,0,0 2IQT,TYR 33,10.21,-0.77,-0.41,1.39 3HKX,GLU_209,5.24,1.4,0,-0.66 3CCY,ARG 87,12.06,-0.45,0,0.01 3K8J,TYR_227,11.46,0,0,1.46 1RZ2,TYR 191,10.14,0,-0.07.0.2 2XJ4.GLU 53.4.75.0.71.0.-0.45 4AF2,CYS_82,12.37,-0.59,0.42,3.54 2F9F,LYS_6,11.54,-0.33,0.85,0.51 1XKR,LYS_86,11.49,-0.83,1,0.81 2B61,GLU 38,4.05,0.32,-0.77,0 2Q99,HIS_286,6.12,-0.38,0,0 1BN6,ARG_164,10.84,-1.86,0,0.2 1L2F,GLU_96,4.66,0.33,0,-0.17 2F9F,ASP 138,3.15,-1,-0.05,0.41 2EYI,ARG 185,12,52,-0,23,0,0,25 2H85,ARG_206,11.27,-1.22,0,-0.01 3TIR,LYS_29,10.36,-0.14,0,0 4DIU,TYR_127,11.07,0,0,1.07 3BQW,HIS_332,4.46,-2.2,0.08,0.09 2H85,ASP_239,2.15,-1.67,-0.43,0.45 1KN3,LYS_77,10.44,-0.06,0,0 1JKS,TYR_128,10.16,-0.03,0,0.19 3CGW.ARG 266,12,41,-0,13,0,0,04 20VT.HIS 117.5.6.-0.36.0.-0.54 3GEC,HIS_492,6.21,-0.62,0.05,0.28 3GFP.TYR 325,12.66,-0.85,0,3.51 4GCO,ARG_232,12.45,-0.22,0,0.17 3P28, ASP 81, 4.03, 0, -0.01, 0.24 2CVB,ARG 159,13.08,-0.29,0.36,0.51 3NR5,LYS_149,10.36,-0.17,0,0.03 3H9W,GLU_67,4.33,0.16,0,-0.33 20EV.ASP 59.4.03.0.-0.04.0.27 1A80.LYS 245,11.87,-0.53,0.97,0.93 2QV2,LYS_53,10.6,-0.68,0,0.78 3E7P,TYR 140,10.81,0.0.21,0.6 2QK1,LYS_342,10.59,-0.08,0,0.17 4F85,GLU_260,4.81,0.31,0,0 4F8A, ASP 562, 3, 72, -0.25, 0, 0, 17 3I47,GLU_136,5.53,1.82,-0.79,-0.01 1FO9,LYS_301,11.14,-0.34,0.81,0.17 1NJ4,ASP 37,2.44,-1.58,-0.43,0.65 2EFK.CYS 99.10.11.-0.19.-0.43.1.74 1UAJ,ASP_51,3.49,-0.54,-0.08,0.32 3HVM,GLU_97,3.1,0.81,-1.53,-0.69 2D7J,LYS_184,10.11,-0.22,0,-0.17 3LJN,ARG_120,12.03,-0.64,0,0.17 3ETV,ARG_13,11.95,-0.56,0,0.02 2CXC,ARG_56,12.32,-0.18,0,0 3CXS,ARG 118,13.01,-0.53,0.17,0.87 1RAJ,LYS_359,10.43,-0.08,0,-1.39E-17 4H86.GLU 157.3.79.2.72.-3.24.-0.18 2WZ9,LYS 92,10.01,-0.45,0,-0.04 3EOD, ASP_42, 4.4, 0, 0.32, 0.28 3L3P.GLU 411.4.51.0.08.0.-0.07 3LH5,LYS_763,10.42,-0.08,0,0 2P0L/ASP 119/2.7,-1.38,-0.06/0.34 3V55,HIS 356,5.04,-1.29,0,-0.17 2C2Y,HIS_191,5.67,-0.42,0,-0.4 3CGW,ARG_91,12.51,-0.17,0,0.18 3ILC,ARG_103,12.32,-0.37,0,0.19 1R53,LYS 84,10.55,-0.11,0,0.16 1YDL,ASP 40,4,25,-0.03,0,13,0,36 1C44, ASP_77, 3.88, -1.49, -0.16, 1.73 3EVN,ASP_192,3.19,-0.75,-0.46,0.6 2B61,ASP 161,3,26,-0.85,-0.63,0.94 3PBH,ASP 34,3,36,-0.32,-0.61,0.48 2PLQ,LYS_160,10.34,-0.25,0,0.09 1FKM,ARG_274,12.02,-0.64,0,0.17 1LN4,GLU_42,4.07,0.34,-0.56,-0.22 2Z0M,ARG 37,11.51,-1.48,0.03,0.46 2F9F.GLU 166.3.71.0.4.-0.75.-0.43 1PBV,HIS 200,6.39,-0.7,0.82,-0.23 3P51,ASP_11,2.68,-1.25,-0.33,0.47 2GKG,ASP 72,2.14,-1.74,-0.49,0.57 2YLE.CYS 120.9.76.-0.04.-0.3.1.1 2AZL,TYR_190,10.8,-0.12,-0.49,1.41 1SQW,ASP_32,2.57,-1.4,-0.34,0.51 2Z61,LYS_269,10.64,-0.11,0,0.25 2QEV,HIS 55,6.47,-0.28,0,0.25 2D59,LYS 144,10,48,-0.02,0,0 2Q99,ARG_369,12.21,-0.28,0,-0.01 3Q2C,GLU_40,4.13,0.41,-0.23,-0.55 1K95,ASP_196,2.92,-1.57,-0.07,0.77 3EVN,LYS 137,10.43,-1.28,0.75,0.46 4H4J,GLU_53,4.68,0.16,0,0.02 2F8H,ASP_19,1.71,-2.05,-0.97,0.93 3IBT,ASP_151,4.05,-0.06,0,0.31 1SNT,LYS 183,10.11,-0.41,0,0.02 1TD6,ARG 159,12.05,-2.48,0.16,1.88 3GE9,HIS_63,6.46,-0.23,0,0.2 2Q13,ARG_287,13.13,-0.26,0.26,0.62 2NRK.LYS 159,10.6,-0.14,0.0.24 2X4G,ARG_279,12.45,-0.07,0,0.02 3CJW,ASP_398,3.88,0,-0.16,0.24 2AHE,LYS_203,11.24,-0.41,0.76,0.38 2G5X,LYS_82,10.54,-0.15,0,0.19 3BPP,TYR 126,10.22,0,0,0.22 3C38,CYS_264,10.9,-0.67,-0.03,2.61 1P1L,GLU_43,4.69,0.19,0,0 2CWC.HIS 144.6.55,-0.48.0.27.0.25 1LTU,CYS_60,12.23,-0.86,0.81,3.28 2XHC,ARG 228,12.59,-0.25,0,0.35 2I88.TYR 363.11.51.-0.25.0.1.76 2H2Z,LYS_90,10.57,-0.16,0,0.23 3E5T,TYR_22,10.41,0,0,0.41 3ILC,GLU_98,4.4,2.23,-1.6,-0.73 3K8J.GLU 129.4.91.0.24.0.0.17 1EDG,ASP_97,3.75,0,-0.28,0.23 2DVK,LYS 63,10.09,-0.18,0,-0.23 3GFP,ASP_416,2.66,-1.78,-0.31,0.95 3M7G,GLU 175,4.74,0.29,0,-0.06 1J85,LYS 119,10.02,-0.54,0,0.06 1PV5,CYS_134,9.87,-0.05,0.55,0.36 1ES9,HIS_66,6.49,-0.26,0,0.25 3RLN,LYS_578,11.18,-0.56,0.25,0.98 1X1E,HIS_72,5.15,-1.32,0,-0.04 3M70,TYR_92,10.65,-0.02,-0.04,0.71 1EDG,LYS_331,9.75,-0.66,0,-0.09 3CBN,GLU_160,4.59,0.25,0,-0.16

20PJ,ARG_145,12.25,-0.39,0,0.14 2R0S,LYS 208,11.34,-0.27,0.73,0.37 3HVW,ARG_277,13.43,-0.36,0.83,0.45 2FC3,GLU_61,4.65,0.2,0,-0.06 3RLN,GLU_706,3.85,0.7,-0.59,-0.75 3JZ9,LYS 484,10.39,-0.15,0.0.04 1U7U.TYR 280.10.19.0.-0.02.0.21 4FZR,LYS_108,10.31,-0.11,0,-0.07 1LZL,ASP_8,3.62,-0.64,-0.05,0.5 4ANN,ARG_125,12.44,-0.13,0,0.07 2W2S,CYS_170,9.93,-1.09,0.02,2 10I7.GLU 201,3.97.0.34,-0.48,-0.39 3I4T,GLU_169,4.51,0.01,0,0 1XAW,ARG_434,12.38,-0.14,0,0.02 3H13,GLU_301,4.08,0.4,-0.77,-0.05 3LJI,ARG 37,12.3,-0.37,0,0.17 2B0J,LYS_237,10.13,-0.25,0,-0.12 1FHL,GLU_147,4.93,0.43,0,0 1NAF,LYS_210,10.67,-0.38,0,0.56 1MD6,HIS_21,6.23,-0.29,0,0.02 2Z84,ARG 117,12.32,-0.1,0,-0.08 1EDG,LYS_213,10.48,-0.17,0,0.14 2AXO,TYR_104,14,0.06,0,3.94 2APL.GLU 87.4.69.0.17.0.0.02 2NMU, ASP 134, 4.11, 0, 0.04, 0.26 1JKS.GLU 235.4.67.0.19.0.-0.01 2FBQ,GLU_15,5.15,2.35,-0.97,-0.74 2P5D,ASP_14,3.12,-0.52,-0.43,0.26 1JKS,ARG_31,12.39,-0.23,0,0.12 1J7G,GLU_72,4.37,0.74,-0.84,-0.03 2V5B,ARG_135,13.03,-1.27,0.6,1.2 1RI6.GLU 25.4.05.0.2.0.-0.64 1YG2,LYS_124,10.56,-0.18,0,0.24 3F7M,HIS 333,3,-3.36,0,-0.14 1TLV.TYR 236.10.15.0.0.09.0.06 3B21,GLU_124,4.85,0.26,0,0.09 1ES9,ASP_182,2.2,-1.73,-0.26,0.4 1ZBS,GLU_19,4.22,0.17,0,-0.45 3ZSL,ARG 129,13.65,-0.2,0.93,0.42 3IRA,GLU_72,4.59,0.23,0,-0.14 2Q98,GLU_121,4.24,0.31,-0.13,-0.43 1BN6,LYS_135,10.56,-0.45,0,0.51 3JRT,GLU 154,4.93,0.18,0,0.25 2IRM,ASP 37,3.66,-0.43,-0.03,0.32 4FLE,GLU_53,4.68,0.31,0,-0.13 3K8J,ARG_154,12.4,-0.19,0,0.09 1XEU,LYS_224,10.7,-0.09,0,0.29 3RJX,LYS 289,10.75,-0.32,0.08,0.5 3KT9,LYS_38,10.05,-0.1,0,-0.35 1R3D,LYS_207,10.46,-0.04,0,0 3GT0,CYS_134,10.1,-0.13,0.16,1.06 3EX9,TYR_115,10.31,0,0.06,0.25 1ZYL.GLU 254,4.59,0.5,0,-0,4 1Y2Q,ASP_29,3.96,0,0.02,0.14 208I,CYS_45,11.68,-0.02,0.32,2.38 2NMU,HIS_100,4.84,-0.73,0,-0.93 2V5B,GLU_245,4.77,0.3,0,-0.03 2CN1.LYS 175.10.08.-0.5.0.0.08 3EZ7,LYS_296,10.69,-0.12,0,0.31 3KV0,HIS_146,5.64,-0.45,0,-0.41 1SJ8,ASP_569,3.25,-0.87,0,0.32 20DJ.LYS 240.10.42.-0.29.0.0.21 1LPL,LYS_144,10.54,-0.12,0,0.16 1DCF,ARG_120,12.19,-0.44,0,0.13 1JB3,HIS_99,7.97,-1.05,1.7,0.82 2CIU,TYR_196,10.11,0,0,0.11 1ZYL, ARG 112, 12, 37, -0, 3, 0, 0, 17 2EYI,ARG_34,13.29,-0.51,0.73,0.58 3OIP,LYS_30,10.36,-0.14,0,0

1WPA,LYS 455,10,44,-0,16,0,0,09 1JYH.TYR 3.12.01.0.85.0.38.0.78 3T8R,TYR_41,10.76,0,0.1,0.65 1JT9,LYS_130,10.44,-0.28,0,0.22 1RHS.ASP 102.3.79.0.-0.34.0.35 2W2S.GLU 141.4.73.0.77.-0.54.0 2YLF,GLU_43,4.78,0.26,0,0.02 1YR6,GLU_212,4.49,0.2,-0.22,0 3BQW,ASP_21,2.66,-1.12,-0.4,0.37 4AF2,LYS_128,10.34,-0.23,0,0.07 2W0G,ASP_229,3.21,-0.78,-0.18,0.38 2AD1,LYS_17,10.31,-0.25,0,0.06 1ZP2,CYS_189,10.69,-0.78,0.3,2.17 1LZL,LYS 66,10.69,-0.36,0.0.55 2BT8.TYR 191.10.33.0.0.0.33 1U53,LYS_44,10.38,-0.27,0,0.14 3IPZ,LYS_108,10.32,-0.33,0,0.15 1NAR,HIS_219,6.41,-0.28,0,0.19 3CCY,TYR 29,11.9,0,0.31,1.59 2D7J.GLU 26.4.28.0.23.-0.01.-0.44 4D8L,LYS_96,9.98,-0.23,0,-0.29 2GYZ,ARG_28,12.03,-0.32,0,-0.15 2RGY,HIS_153,6.45,-1.91,0.36,1.5 1UOH,GLU 20,4.47,0.23,0,-0.26 2EA9,TYR_102,9.79,-0.03,-0.43,0.25 3UAH,ASP_189,3.13,-1.38,-0.25,0.96 1L2F,ARG_257,13.79,-0.5,0.96,0.84 3BA1,GLU 60,3.83,0.24,-0.72,-0.19 3B7X,ASP_89,3.95,-0.22,0,0.37 4E6S,GLU_6,3.91,0.32,-0.72,-0.19 1V6T,ASP_136,3.6,-0.79,-0.12,0.71 2D2S,LYS_621,10.74,-0.28,0,0.51 2B0J,GLU 31,4.81,0.53,0,-0.22 3EVP.GLU 135.6.63.3.02.-0.85.-0.05 3GG6,ARG_123,12.53,-0.22,0,0.24 3LMF,ARG_68,12.31,-0.19,0,0 2CVB.LYS 144,10.61,-0.09,0.0.2 2Q98,ASP_79,3.55,-0.46,-0.14,0.35 2OSA,GLU_293,4,1.38,-0.85,-1.03 3ASA,HIS 260,7.61,-0.23,0.85,0.49 3E7P.ARG 219,12,42,-0.08,0.0 3PP8.ARG 281,12.5,-0.27,0,0.26 1WXO,HIS 187.6.28,-0.25,0.0.03 2QDJ,ARG_272,12.13,-0.4,0,0.03 1L3K,LYS_8,10.29,-0.1,0,-0.11 1HF8,CYS_27,9.3,-0.04,-0.28,0.63 2FL4,TYR_122,12.47,0,0.65,1.82 1H09,HIS 60,2.76,-3.6,0.02,-0.16 1TLV,HIS_256,7.05,-0.83,0.85,0.54 1R53,ARG_345,11.99,-0.56,0,0.06 2AH5,GLU_94,5.01,0.29,0,0.22 1P4X,ASP 221,3.34,-0.94,-0.04,0.53 2JEO,ASP_179,3.64,-0.47,0,0.31 3T8R,ASP_116,3.2,-0.74,-0.38,0.53 3FHF,ASP_17,4.02,0,0.01,0.21 3PP8,GLU 20,4.8,0.31,0,-0.01 3RLE,GLU 145,4.66,0.13,0,0.02 1BN6,ARG_210,11.52,-1.11,0,0.12 2X4J,LYS_126,9.54,-1.09,0,0.14 3UV9,LYS 371,10.52,-0.08,0,0.11 3BB7,ASP 206,3.92,-0.68,-0.18,0.98 3ETV,GLU_334,4.55,0.28,0,-0.23 3COU,GLU_80,7.12,3.81,-1.55,0.36 3ANJ,TYR_321,11.73,0.15,0.4,1.17 1X1E,LYS_84,11.4,-0.27,0.71,0.45 1HF8,GLU_279,5.17,0.56,0,0.11 3HYQ,TYR_178,12.78,0.14,0.34,2.31 4DEZ,ARG_68,12.38,-0.12,0,0 1ZCE,GLU_129,4.52,1.09,-1.06,-0.01

1YM5,HIS_283,6.01,-0.87,0.09,0.3 3N2TARG 107.11.84.-1.81.0.1.15 2CVB,HIS_94,5.86,-0.96,0,0.31 103X.LYS 250.10.6.-0.12.0.0.22 1RAJ.HIS 389.5.59.-2.56.0.85.0.8 4D8L, ARG 166, 12, 14, -0, 57, 0, 0, 21 1AK1.TYR 285,11.91,0.65,0.44,0.82 3CO1,TYR_6,11.63,0.81,0.38,0.44 10TM,ASP_50,2.78,-2.39,-0.15,1.52 2Q98,TYR_44,10.83,-0.06,-0.04,0.93 200K.LYS 223,10.44,-0.06,0.0 208P,GLU_52,4.14,2.26,-2.28,-0.35 3LJI.ARG 48.10.76.-2.43.0.0.69 2CI3,GLU_43,5.27,0.6,0,0.17 3LJN.CYS 117.11.44.-0.08.0.63.1.89 1NJ4,ASP 175,2.94,-1.65,-0.69,1.48 2FI9,HIS_33,5.18,-0.87,0.13,-0.59 1L2F,ARG_306,12.75,-0.3,0,0.55 1J85,LYS_58,10.62,-0.33,0,0.45 2B0J,ASP 143,3.7,-0.32,-0.64,0.85 1T3Y,LYS_102,11.2,-0.59,0.85,0.44 2H2W,LYS 96,10,49,-0.01,0,0 2ZCX,GLU_26,4.9,0.18,0,0.21 3MIX.TYR 603,10.36,0,0.19,0.16 4EKU,TYR 162,11.84,0,-0.76,2.61 1ZBM,ASP_162,4.27,0,0,0.47 1P2F,LYS_12,10.46,-0.06,0,0.03 3R2E,GLU_7,4.93,0.2,0,0.23 1XEU,GLU_73,2.24,0.62,-2.5,-0.38 1Q46,ASP_39,4.39,0,-0.53,1.11 2XWS,LYS_38,10.52,-1.67,0.85,0.84 1XTD,HIS_64,6.31,-0.19,0,0 3NBI,TYR 100,10.22,-0.07,-0.06.0.36 3IV4.GLU 12.3.19.0.61,-1.51,-0.41 3LOD, ASP_81, 2.66, -1.43, -0.31, 0.61 3P28,HIS_190,5.98,-0.36,0,-0.14 2GZQ,ARG_191,12.31,-0.29,0,0.1 3ASA,TYR 191,10.93,0,0.04,0.89 1NIJ,LYS_292,10.52,-0.09,0,0.11 1W24,HIS_10,3.67,-2.22,0,-0.62 2G2D,LYS_160,10,-0.38,0,-0.12 1IDK.TYR 96.10.68.0.0.01.0.67 4H89,HIS_85,6.04,-0.32,0,-0.14 1QYI,ARG_215,12.55,-0.47,0.07,0.45 1FKM,ASP_272,3.98,0,-0.18,0.36 1YM5,LYS_259,10.42,-0.08,0,0 4ETX,GLU 248,3.77,0.4,-0.7,-0.44 3ETV.ARG 56.12.35,-0.26.0.0.11 3UC9,HIS_18,6.01,-1.2,0,0.71 3RE9,GLU_93,4.45,0.21,0,-0.27 3M3P.HIS 120.6.13,-0.35,0,-0.02 2CYG,LYS 332,11,36,-0.37,0.85,0.38 3MTT,ARG_511,12.54,-0.3,0.11,0.22 2A4D,LYS_100,10.43,-0.07,0,0 1ZBP,ARG_190,11.52,-1.05,0,0.06 1DZF,GLU_194,4.27,2.37,-1.48,-1.13 1T3J.GLU 725.4.07.0.27.-0.71.0 3MIX,GLU_483,3.88,1.09,-0.85,-0.86 100X,ARG_124,12.35,-0.48,0,0.34 3UV9.GLU 292.4.55.0.05.0.0 3LJC.HIS 46.6.65.-0.19.0.42.-0.08 2BDV,ARG_192,13.04,-0.5,0.6,0.44 1JSX,ARG_197,12.52,-0.63,0.18,0.47 3ILC,TYR_120,12.47,0,0.75,1.72 3GMS,HIS_236,5.87,-1.19,0.74,-0.18 3V4G,GLU_84,4.11,0.63,-0.93,-0.09 2JKF,LYS_56,10.28,-0.38,0,0.16 1059,ARG 317,13.32,-0.28,0.48,0.61 3PAC, ARG_125, 12.43, -1.5, 0.61, 0.81

1HF8,TYR 138,12,28,0.85,0.55,0.89 3CRM,ASP 27,3.27,-0.85,-0.16,0.49 2QZQ,GLU_130,5.65,0.77,0,0.37 2BV9,CYS 158,13,26,-0.07,1.26,3.08 1PDB,ASP_110,2.4,-1.87,-0.21,0.69 1BN6,LYS_128,9.99,-0.42,0,-0.09 3EVZ,ARG 121,13.83,-0.31,1.12,0.52 2F9F,ASP_99,4.1,0,0.06,0.25 3BQW,ARG_73,13.51,-0.66,0.79,0.88 3UV9,ARG_298,12.38,-0.12,0,0 1PDB,GLU_161,4.73,0.23,0,0 3I4T.TYR 265.10.17.0.0.06.0.11 1FO9,GLU_135,4.6,0.1,0,0 2FZ4,ARG_50,12.42,-0.27,0,0.18 2CI3.TYR 241.12.34,-0.03.0.56,1.81 20EW,HIS 259,5,17,-2,17,0,68,0,16 10XZ,ASP_171,2.92,-0.76,-0.49,0.37 2B61,ASP_222,3.58,-0.5,0.01,0.26 1YM5,GLU_39,4.31,0.22,-0.4,0 1PDB,GLU 78,4.16,0.23,-0.24,-0.33 3RLE,LYS_56,11.78,-0.32,0.85,0.74 2Q98,LYS_78,10.58,-0.39,0.04,0.43 2XMZ,LYS_77,10.6,-0.23,0,0.33 1SUU,LYS 633,10,55,-0,15,0,0,2 2GAU.CYS 127.9.52.-0.08.-0.03.0.62 2QVT,LYS_58,10.13,-0.37,0,0 1JYH,LYS_45,10.41,-0.27,0,0.19 2OJQ,TYR_485,12.35,-0.28,0.42,2.2 3JRT,CYS 106,10.26,0,-0.03,1.29 4EKU.HIS 365.6.07.-0.49.0.0.06 2NYC,TYR_236,11.61,0,0.15,1.45 300P,LYS_17,10.35,-0.15,0,0 3CX2,LYS_195,10.32,-0.14,0,-0.04 10GL.CYS 115,9.66,-0.25,-0.52,1.42 1ZBP,LYS_179,10.91,-0.33,0,0.74 1NIJ,TYR_31,10.01,0,-0.17,0.18 2RFA,CYS_70,9.85,-0.13,0.06,0.92 4DNU,HIS 102,4.66,-1.83,0.04,-0.05 4F85,CYS 114,12,83,-0.77,1.28,3.33 3ILC,GLU_124,3.92,0.41,-0.85,-0.14 3CS1,LYS_19,10.4,-0.11,0,0.02 3BPP.ARG 187,12,79,-0.2,0.01,0.48 1GQE,ASP_238,3.99,0,-0.17,0.37 3RKV,GLU_237,4.57,0.33,0,-0.26 3ZRI,LYS_18,10.47,-0.22,0,0.19 4FZN,ARG_97,13.57,-0.61,0.83,0.85 3BQW,ASP 106,3.12,-0.97,-0.05,0.34 1WYC.GLU 237.4.85.0.41.0.-0.07 4EKU,GLU_138,4.91,0.3,0,0.1 3LQE,GLU_427,4.07,2.66,-2.5,-0.59 2V4X,GLU_4,3.71,0.23,-0.75,-0.27 1SI7,CYS 152,10.01,-0.1,-0.02,1.13 3T57,ARG 291,12.03,-0.52,0.0.04 3EVN,ASP_65,2.41,-1.74,-0.36,0.7 2FB6,LYS_49,10.42,-0.19,0,0.1 3QAV,LYS_29,10.24,-0.2,0,-0.05 2R51,GLU 85,4.03,0.43,-0.55,-0.35 20KT,TYR_300,10.13,-0.85,-0.05,1.03 3FFM.GLU 67.4.66.0.09.0.0.07 2A1V.GLU 135.4.56.0.08.0.-0.02 3E7P,ARG_85,11.97,-0.56,0,0.03 3BOW,TYR 115,10.63,-0.13,0.25,0.52 2P65,ARG_154,10.64,-1.52,0,-0.34 3ZXY,ARG_273,12.12,-0.38,0,0 2VAN,LYS_167,10.36,-0.15,0,0 2A1V,ARG_109,12.72,-0.81,0.66,0.37 1EYH,ASP_115,4.25,0,0.26,0.18 3JZ9,LYS 447,9.83,-0.7,0,0.03 2GQV,HIS_62,6.31,-0.19,0,0

2EJB,ASP_163,4.02,0,-0.08,0.3 3M7D,ARG 249,13.8,-0.54,1.4,0.43 1PV5,GLU_170,4.62,0.12,0,0 1XTD,HIS_88,6.28,-0.32,0,0.11 2HRZ,ARG_285,13.5,-0.31,0.68,0.63 3H9W.GLU 117.5.02.0.27.0.0.25 1W7B.LYS 176.10.73.-0.88.0.85.0.26 1UAJ,GLU_203,4.47,0.2,0,-0.24 2RJD,TYR_416,11.89,0.74,0.5,0.66 2B6P,HIS_201,4.83,-1.83,0.17,-0.01 1BN6,ASP_22,3.83,0,-0.14,0.17 1RI5,ARG_119,12.44,-0.35,0,0.29 1R3F,GLU_287,4.55,0.05,0,0 1X1E,ARG_164,12.45,-0.05,0,0 3Q9P,LYS_114,10.23,-0.08,0,-0.18 3ELI,ASP 23,4.49,0,-0.03,0.72 1ES9,LYS_35,10.59,-0.09,0,0.18 1PDB,TYR_33,12.87,0,0.12,2.75 3P51,ASP_104,4.2,0,0.03,0.36 3ILC,ASP_189,4.05,0,0,0.25 1PGV.GLU 341.3.98.1.15.-1.64.-0.03 2B02,ARG_366,12.3,-0.57,0.01,0.36 1SOH.GLU 221.4.53.0.4.0.-0.37 1IAP.HIS 58,3.58,-2.37,0,-0.56 3DZ1,ARG 90,12,-0.27,0,-0.24 4FZR,HIS_295,2.63,-2.77,0,-1.1 1JKS,GLU_107,4.29,0.28,-0.17,-0.31 3E5T,GLU_7,4.71,0.25,0,-0.04 3LD1,ASP_120,3.59,-0.75,-0.53,1.06 1HF8,LYS_227,10.35,-0.15,0,0 2F4Q,TYR_79,11.27,0,-0.7,1.98 307K,GLU_147,2.78,1.19,-1.61,-1.3 1NAR,ARG_239,13.47,-0.58,1.13,0.42 2Q12,LYS_119,10.57,-0.39,0,0.45 1EYH.TYR 83,10.7,-0.63,-0.17,1.5 3JRT,ARG_38,12.78,-0.26,0.36,0.18 2FL7,ARG_43,13.87,-0.47,1.46,0.38 1NAF,GLU_209,3.97,0.2,-0.7,-0.03 1X6J,GLU 31,3.57,0.61,-0.9,-0.65 109G,ASP_12,2.95,-1.11,0.02,0.24 3LOE, ARG 373, 12, 24, -0, 29, 0, 0, 03 1LTU,ARG_69,12.48,-0.2,0,0.18 307K,GLU 144,4.23,2.8,-2.06,-0.99 3EIZ,HIS 163,5,54,-1,03,0,0,07 3COU,GLU_160,4.53,0.17,0,-0.14 1SFE,ASP_59,2.97,-1.06,0,0.23 2BT8,ASP_228,2.78,-1.14,-0.82,0.95 1NFN,HIS_140,5.67,-0.45,0,-0.38 1NRI,ARG_81,11.99,-0.51,0,0 1LFP,LYS_155,11.29,-0.5,0.69,0.6 2G5X,ASP_9,3.09,-0.88,-0.22,0.4 1LTU,ASP_267,3.96,0,0,0.16 4HDE,LYS 173,10,16,-0,52,0,0,19 3ELI,ARG_137,13.17,-0.29,0.62,0.34 2D59,ASP_12,2.25,-1.27,-0.68,0.4 1MML,ARG_253,11.52,-1.17,0,0.19 2B61,TYR_296,12.09,-1.55,0,3.64 3E7P,ARG 218,12.5,-0.32,0.0.32 106D,ASP_12,3.88,0,-0.17,0.25 3NJM,ARG_122,12.33,-0.2,0,0.03 3U0V,GLU_217,7.27,3.4,-0.7,0.06 2E3S,ARG 487,12.16,-0.6,0,0.25 1J85,GLU_70,2.96,1.14,-1.43,-1.25 2R0S.TYR 165,10.85,0,-0.04,0.9 3BQW,TYR_295,12.65,0,0,2.65 2DVK,ARG_112,13.05,-0.36,0.37,0.54 1SUU.ARG 685,12.35,-0.18,0,0.03 2Q07,ARG_486,12.59,-0.2,0,0.28 2Q34,GLU_182,4.36,0.21,-0.05,-0.3

1EDG.CYS 257.11.71.0.0.15.2.56 1F2V.ASP 5.3.95.0.0.0.15 1D2K,LYS_362,11.27,-0.33,0.69,0.41 3C0C,ASP_331,3.29,-0.84,-0.2,0.52 2H2W.ARG 192,10,47,-2,95,0,0,92 2FD4.CYS 477.9.22.-1.78.0.05.1.94 2IRM,ASP_116,3.83,0,-0.29,0.32 3I82,LYS 198,10.36,-0.46,0.0.32 10TM,LYS_45,10.37,-0.13,0,0 3ETV,ARG_100,11.17,-2.83,0.57,0.93 1TD6.LYS 58.10.44.-0.2.0.0.15 1SFE,GLU_50,5.33,1.35,-0.14,-0.38 3GEC,ARG_484,12.69,-0.21,0,0.4 2EYI,LYS 198,10.57,-0.15,0.0.22 1VSM.ARG 179.12.14.-0.36.0.0 2D59,LYS_86,9.91,-0.38,0,-0.21 3EGN,ARG_464,12.45,-0.08,0,0.03 4FH3,ASP_246,4.18,0,-0.17,0.54 208I,GLU_142,4.42,2.11,-1.51,-0.68 4H89,ARG 24,13.2,-0.46,0.85,0.31 4ECC,LYS_194,10.35,-0.23,0,0.08 3N2T,LYS_78,10.42,-0.08,0,0 105T,ARG_133,12.09,-1.08,0.57,0.09 3ILC.ASP 95,1.96,-2.5,-0.74,1.4 1RZ2,LYS_216,10.44,-0.06,0,0 1R53,HIS_17,6.36,-0.14,0,0 1UW7,LYS_86,10.57,-0.82,0.85,0.05 2IIA,HIS 103,7.47,-0.69,0.85,0.81 3PP8,HIS_275,7.09,-1.21,0.85,0.94 2Z61,ASP_295,2.94,-0.52,-0.66,0.33 3EJG,LYS 62,10,45,-0.08,0,0.03 1AKO,GLU_85,4.37,0.21,0,-0.35 1YR6,GLU 79,4.67,0.29,0,-0.13 1J33.HIS 323.6.12,-0.84,0.84,-0.38 10XZ,GLU_251,4.62,0.22,0,-0.09 3FTT,ASP_51,2.22,-2.46,-0.4,1.27 2OSA,GLU_431,4.94,0.25,0,0.2 1LTU,ASP_26,2.44,-1.68,-0.45,0.76 1SIG,LYS_377,10.63,-0.14,0,0.27 2F8H,GLU 275,4.13,1.69,-1.66,-0.39 2QDJ,GLU_97,3.7,1,-1.36,-0.44 106D,LYS 112,11.2,-0.45,0.75,0.4 4D8L.ARG 8,12,94,-1,04,0,98,0,49 20EW, ARG_276, 13.31, -1.7, 1.34, 1.18 2RJD,HIS_331,6.23,-0.27,0,0 2G5X,ARG_1,12.35,-0.92,0.46,0.31 3IO0,GLU_132,3.51,1.3,-1.58,-0.71 3L3P,ASP_291,4.43,0,-0.01,0.64 1IAP.HIS 206.6.23,-0.27.0.0 1YTD, ARG_373, 12.35, -0.29, 0, 0.13 1YR6,HIS 178,4.81,-1.61,0,-0.09 3PZ9,ARG 38,12.2,-0.78,0.0.48 1NIJ,CYS_64,10.78,-0.75,-0.05,2.58 3OA7,LYS_433,10.43,-0.07,0,0 1BN6,GLU_158,4.62,0.11,0,0.01 1SI7,ARG_47,13.95,-0.65,1.32,0.78 1WP5,ARG_90,12.52,-0.05,0,0.08 2QVT,CYS_83,8.91,-0.9,-0.27,1.08 3M70,CYS_7,9.38,-0.71,-0.14,1.23 2P0L,LYS 160,10.39,-0.2,0,0.09 4H89.GLU 12.4.66.0.24.0.-0.09 2HRZ,HIS_326,4.73,-1.93,0,0.16 1Q5Z,ASP_556,2.55,-1.46,-0.2,0.4 1MML,CYS_90,10.68,0,0,1.68 2H2W,TYR_71,11.25,-0.65,0.14,1.78 1GXN,TYR 456,12.33,0,0.21,2.12 1JSX,LYS_4,10.18,-0.32,0,0 3EUR,HIS_82,6.78,-0.55,0.52,0.31 4GA2,GLU_9,4.65,0.25,0,-0.11

2FB6.LYS 106.10.42.-0.08.0.0 3I4T,ASP 240,3.28,-0.64,-0.09,0.21 2HRZ,ASP_108,4.51,0,-0.09,0.79 1NKD,LYS_25,10.62,-0.12,0,0.23 2H30,TYR_113,12.43,0,0.24,2.18 2GYZ.CYS 69.9.29.0.-0.01.0.3 3ETU,ARG 88,11,77,-2,74,0.83,1.18 1WPA,GLU_442,4.43,0.44,0,-0.51 1LZL,GLU_117,5.47,1.74,-0.79,0.02 3CN5,TYR_177,10.28,-0.02,0,0.3 109G,TYR_124,10.11,0,-0.28,0.38 3TOW,GLU_181,4.04,0.48,-0.57,-0.37 4GCO,GLU_235,4.05,0.41,-0.81,-0.05 1R3D,ARG_169,11.8,-0.72,0,0.03 4ECC.GLU 22.4.2.1.91.-1.55.-0.66 4EKU,ARG 228,12,36,-0,32,0,0,18 1FKM,ARG_316,12.93,-0.89,0.57,0.75 1SI7,ARG_177,12.27,-0.23,0,0 3JSN,LYS_241,10.42,-0.1,0,0.01 1R3D,TYR 232,10.79,0,0.41,0.38 4ANN,GLU_147,4.6,0.12,0,-0.02 3H9W,GLU_44,4,0.3,-0.8,0 3LPZ,ASP_69,4.69,0,-0.06,0.95 1ES5,LYS 82,9.74,-0.69,0,-0.08 2X5Y,TYR 728,11,27,0,0,59,0,68 1TLV,LYS_191,10.44,-0.21,0,0.15 3TOW,HIS_197,6.08,-0.2,0,-0.23 1QYI,ARG_299,13.1,-0.18,0.24,0.53 1NAR,ASP 137,3.02,-0.85,-0.45,0.53 1QQE,ARG_115,11.53,-1.04,0,0.08 1TWU,LYS_139,10.49,-0.01,0,0 1DZF,TYR_168,9.91,-0.05,-0.38,0.34 3BPP,TYR 89,11.08,0,0.59,0.49 2R0S.TYR 275.11.04.0.0.05.0.99 1EYH,GLU_142,4.64,0.15,0,-0.01 2ZCX,ASP_48,3.52,-0.6,-0.16,0.48 3OA7,LYS_542,10.39,-0.21,0,0.1 3L3P,GLU 264,4.53,0.13,-0.06,-0.04 3A7L,ASP_55,3.35,-0.84,0,0.38 20JQ,GLU_461,3.78,1.5,-1.67,-0.55 3FWU,ASP_12,2.04,-1.55,-0.69,0.49 3A2Z.HIS 55.6.48,-1.54,1.15.0.38 1YTD.LYS 299,10.47,-0.09,0.0.06 1YM5,GLU_33,3.61,1.47,-1.37,-0.98 1R3F,ARG_202,11.35,-2.87,0.21,1.51 4FLE,GLU_106,4.58,0.08,0,0 1WXF,HIS_204,7.49,-0.34,0.85,0.47 4FH3.GLU 84.4.61.0.27.0.-0.17 2H30,TYR_140,12.33,-0.19,0.37,2.15 1WXQ,HIS_171,5.7,-0.82,0,0.02 1SOW, ASP 152, 3, 9, 0, -0, 18, 0, 27 1Y0K.GLU 131.4.64.0.14.0.0 3ILC,GLU_153,6.07,1.66,0,-0.08 4ETX.TYR 345.12.44.0.0.54.1.9 3F1X,HIS_251,5.61,-0.93,0.17,-0.12 1NAR,GLU_55,4.75,0.17,0,0.09 2FPN,LYS 86,10,17,-0,33,0,0 3EVP,CYS_206,9,-1.93,0.23,1.69 1ES5,ARG_191,13.93,-0.45,1.46,0.41 102Y,LYS 92,10,54,-0,1,0,0,14 1L2F,LYS_156,11.2,-0.42,0.7,0.42 2XJ4,ARG_84,13.48,-0.25,0.85,0.38 3A2Z,GLU_39,4.82,0.62,0,-0.3 3ZXY,HIS_160,4.99,-1.75,0.2,0.04 1SNT,LYS_263,10.37,-0.21,0,0.07 2IN0,LYS_36,10.47,-0.08,0,0.05 2CVB,TYR_131,13.38,0,0.37,3 1Q8B,GLU 57,4.64,0.14,0,0 2D7J,ARG_21,12.28,-0.26,0,0.04

3BZT.HIS 320.6.27.-0.23.0.0 3P51,ARG 71,12.11,-0.66,0,0.27 1UCH,HIS_169,6,-2.96,0.85,1.59 3LH5.LYS 529,10.49,-0.23,0.0.22 3HNX,HIS_47,5.8,-0.32,0,-0.38 208I,ASP_27,2.45,-1.37,-0.38,0.41 2X4L,ASP_207,3.64,-0.65,-0.46,0.95 4FCU,GLU_172,4.58,0.08,0,0 2YT4,LYS_614,10.55,-0.07,0,0.12 3FS3,ASP_223,3.8,0,-0.17,0.18 3ADO,GLU 70,4.75,0.25,0,0 2X4G,HIS 12.6.3,-0.18,0,-0.01 2A1V,GLU_127,3.95,0.27,-0.85,0.02 3CXS,GLU_16,4.07,0.29,-0.58,-0.15 3JSN.GLU 144,5.17,1.31,-0.72,0.08 2F8H,TYR 67,10.65,0,-0.08,0.73 1RSS,GLU_142,4.25,1.04,-0.78,-0.5 1059, ARG_177, 11.85, -1.98, 1, 0.32 1N81,GLU_145,4.66,0.16,0,0 3PZ9,ARG 185,12.44,-0.44,0.02,0.36 3IO0.GLU 209,4.33,0.61,-0.75,-0.03 1X7F,LYS 326,10.91,-0.23,0.0.64 1SQH,GLU_182,4.61,0.25,0,-0.14 1WYC.HIS 9.4.13.-2.35.0.-0.02 1NU.GLU 291.2.71.0.5.-1.43.-0.86 3G6S,CYS_237,11.45,-0.33,0.04,2.74 1MUF,GLU_228,3.54,0.54,-0.78,-0.72 3G9B,TYR_130,12.54,-0.12,0.06,2.61 2OJQ,GLU_426,4.62,0.14,0,-0.02 3FFM,ASP_55,4.13,0,0.14,0.19 2EEY,LYS_160,10.44,-0.26,0,0.19 3BJV,LYS_40,10.58,-0.14,0,0.22 3RRO,ARG 104,12.56,-0.21,0,0.27 3JZ9.GLU 513.4.58.0.08.0.0 2R0S,LYS_82,10.42,-0.08,0,0 3ON1,ARG_69,13.04,-0.34,0.42,0.46 2ZCO,TYR_77,9.22,-0.78,-0.38,0.38 2CBE,HIS_10,6.22,-0.18,0,-0.11 3H6O.GLU 87.4.59.0.2.0.-0.1 3E7P,LYS_186,10.55,-0.1,0,0.15 4EKU,TYR_155,13.71,0.06,-0.35,4 2PIM,ASP_78,2.29,-1.05,-0.77,0.32 2DG7,GLU_35,4.88,0.26,0,0.13 1WP5,LYS_36,11.41,-0.26,0.58,0.58 2E3S,ARG_471,12.4,-0.1,0,0 2Z14,TYR_87,10.31,0,0.04,0.27 1DUP,LYS 16,10.45,-0.05,0,0 2JHY,LYS_99,10.44,-0.06,0,0 103X,GLU_251,4.46,0.22,0,-0.25 3EVZ.GLU 180,3.54,0.67,-1.5,-0.12 1L3K,GLU_11,4.36,0.21,0,-0.34 1Q42,LYS 74,10.26,-0.26,0,0.01 2099, HIS 115.6.12,-0.19,0,-0.19 1XDZ,GLU_238,4.92,0.35,0,0.07 4DBX,ARG_125,13.05,-0.31,0.43,0.44 4F8A,ASP_668,3,-0.85,-0.51,0.57 3KEY,CYS 420,9.25,-0.46,-0.01,0.72 1Q2Y,TYR_48,12.24,0.85,0.47,0.93 20YZ.TYR 35.10.59.0.0.0.59 1R3F,ARG_302,12.39,-0.36,0,0.25 2D2S.ARG 549,12.62,-0.3,0.07,0.36 1ILW,LYS 100,10.13,-0.66,0.0.29 1TWU,TYR_47,10.22,0,0,0.22 3S0A,LYS_69,10.26,-0.26,0,0.02 1W7B,TYR_188,10.12,0,-0.09,0.21 4D8L,HIS_31,0.74,-3.19,0.32,-2.9 3VJ8,ARG_149,11.86,-0.71,0,0.09 3F6F,TYR 147,10.57,0.0.21,0.36 1SJY,HIS_8,6.27,-0.21,0,-0.02

3T5B,GLU_263,4.84,0.68,-0.38,0.04 1Y0K,ARG 194,12.33,-0.31,0,0.14 2R51.LYS 67.10.65.-0.34.0.0.5 3U2A,GLU_31,3.52,0.41,-0.83,-0.54 2VAN,ASP_276,3.65,-0.19,-0.15,0.2 1ZBP.GLU 48.4.72.0.1.0.0.11 3GFPARG 380,12,94,-0,14,0,34,0,24 208P,LYS_216,9.99,-0.48,0,-0.03 3JSN,ASP_286,3.65,-0.91,-0.03,0.8 3UPD,GLU_54,4.72,1.84,-1.68,0.06 3TIR.HIS 51.5.65,-1.06.0.0.22 2W0G,ARG 235,12,13,-0.39,0.0.02 3CCY,TYR_134,10.03,-0.68,0.06,0.66 1XDZ,GLU_157,3.88,2.38,-2.43,-0.57 2VAN,LYS_113,10.57,-0.11,0,0.18 3PBH,HIS 199,7.64,-3.34,2.5,1.97 1WYC, ASP_390, 2.28, -1.58, -0.47, 0.53 2HRZ,ASP_66,2.79,-1.83,-0.37,1.18 1IAP,LYS_53,11.9,-0.94,1.7,0.64 2IOT.GLU 165.4.9.0.47.0.-0.06 3RJX.GLU 129.4.25.0.29.0.-0.55 1L3K,GLU_176,4.52,0.37,-0.09,-0.27 2XMZ.LYS 119,10.35,-0.22,0,0.08 1YM5,TYR 237,13,5,0,0,59,2,91 3L3P.TYR 480.10.12.0.0.05.0.07 2H8O,HIS_79,5.79,-1.3,0.82,-0.23 1T3Y,ASP_55,3.38,-0.84,0.14,0.28 2D7U,LYS_306,10.43,-0.42,0,0.34 4ECC.GLU 129,4,49,0.35,0,-0.35 106D,GLU_75,3.23,0.34,-0.85,-0.76 2B78,LYS_53,10.63,-0.13,0,0.26 3GV0.LYS 110.10.94,-0.26.0.32.0.38 109G,ARG_241,12.14,-0.49,0,0.13 1NAR,GLU 213,4.51,1.49,-0.84,-0.65 2W0G.CYS 183,10.08,-1.18,0.1,2.15 2XHC,TYR_109,9.95,0,-0.19,0.14 3G9T,LYS_185,10.48,-0.11,0,0.09 2QRX,GLU_22,4.75,0.19,0,0.06 2G5X,ASP 43,2.29,-1.33,-0.6,0.42 3PBH,ASP_124,3.56,-0.26,-0.13,0.15 3FS3.TYR 272.10.09.0.-0.14.0.22 3PBH,TYR_165,10.25,0,0,0.25 1ZBS,HIS 206,6.08,-0.7,0,0.28 1ZKZ.HIS 62.5.78.-0.51.0.-0.21 2GAU,HIS_152,6.35,-0.14,0,-0.01 2F9F,GLU_80,3.56,0.36,-1.32,0.02 2V4X,GLU_41,2.73,0.49,-1.44,-0.82 1HUF,ARG 49,13.05,-0.24,0.3,0.49 2B78,LYS_342,10.3,-0.31,0,0.11 3AU3,LYS_516,9.37,-1.15,0,0.02 1X04,GLU_49,4.11,0.16,-0.52,-0.04 1TD6,HIS_127,5.08,-2.23,0.72,0.09 2D8N,LYS 161,10,98,-0,47,0,33,0.63 1OTM,LYS_145,10.8,-0.24,0.2,0.35 1WXQ,GLU_328,4.22,0.33,-0.6,0 1TD6,GLU_196,5.07,2.23,-0.31,-1.35 2F4Q,LYS 90,10.41,-0.1,0,0.01 3BOW.GLU 212.2.93.0.66,-1.87,-0.36 3OKQ,LYS_589,10.99,-0.16,0.36,0.29 3L7N,ASP_69,2.98,-0.95,-0.51,0.64 2OJQ,ARG_380,12.4,-0.1,0,0.01 2ZCO,LYS 20.9.68,-0.47,0,-0.35 10LR,ARG_73,12.38,-0.34,0,0.22 2B2H,GLU_376,3.85,1.88,-1.52,-1.02 1O59,LYS_159,10.41,-0.11,0,0.03 3E7P,TYR_126,11.15,-0.11,0.17,1.1 2B61.LYS 39.10.34.-0.2.0.0.04 3BQW,ARG_117,13.09,-0.96,1.01,0.54 1RSS,HIS_122,6.5,-0.72,0.82,-0.1

3RFF,ASP_154,4.01,0,-0.08,0.3 3UC9.CYS 76.9.58.0.0.02.0.56 2O4D,TYR_80,10.31,-0.01,0,0.32 3AUF,ARG_75,12.48,-0.39,0,0.37 2B0J.GLU 299.4.63.0.21.0.-0.08 2NSN.CYS 59,9.04.0.-0.16.0.2 2OSA,HIS_407,6.57,-0.44,0.58,-0.07 3I4T,HIS_109,6.35,-0.38,0,0.23 3GOZ,GLU_186,4.05,0.41,-0.49,-0.37 2Z0M,LYS_39,10.3,-0.2,0,0 1PBV,GLU_85,4.52,0.28,-0.17,-0.09 1JKS,LYS_276,10.27,-0.23,0,0 3DHN,GLU_39,3.33,0.38,-1.09,-0.46 2H2Z,ASP_34,3.43,-0.45,-0.26,0.35 2H01.TYR 108.12.97.0.0.06.2.91 1FO9,LYS_397,11.19,-0.5,0.42,0.76 2IRM, ASP_195, 3.83, -0.18, -0.08, 0.28 2PGE,ASP_362,3.25,-0.5,-0.38,0.32 4ACJ,GLU_708,4.69,0.87,-0.28,-0.4 3BJV.GLU 96.4.7.0.2.0.0 2BLL,CYS_629,10.95,-0.09,0.19,1.86 2F8H,ASP_302,4.18,0,-0.05,0.42 4GCO.GLU 175.4.68.0.26.0.-0.08 3NBI/LYS 109,10.21,-0.29,0,0 2FPN,ARG_42,12.09,-0.44,0,0.03 2A4D,ASP_104,2.27,-1.7,-0.23,0.39 2X4J,LYS_53,10.3,-0.97,0.18,0.59 1KCM,TYR 7,12.89,0,0.28,2.61 1RZ2,LYS_252,10.91,-0.47,0.46,0.41 3A4C,LYS_534,10.35,-0.16,0,0.01 3GV0,GLU_322,3.96,0.3,-0.73,-0.1 10IS,LYS_198,10.67,-0.12,0,0.3 4GA2,LYS 99,11.37,-0.71,0.84,0.75 4GCO.GLU 192,4,37,0,25,-0,13,-0,26 2H2W,GLU_37,5.2,1.38,-0.43,-0.25 3AU3,LYS_570,10.32,-0.69,0,0.52 3EVN,HIS_162,6.19,-0.23,0,-0.08 1T3Y,LYS 30,11.01,-0.84,0.79,0.57 2Q12,ARG_149,12.19,-0.2,0,-0.11 3BWT,LYS 573,10,41,-0.22,0,0,12 1UAJ,ASP_150,4.39,0,-0.07,0.65 2BLL,TYR 341,13.78,0.89,0.94,1.95 2DG7,ARG 68,12,28,-0,22,0,0 1SJ8,CYS_732,10.31,-1.95,0.4,2.85 3CZC, ASP_33, 3.47, -0.14, -0.44, 0.25 1YG2,ARG_112,12.16,-0.34,0,0 20EW,LYS_60,10.87,-0.23,0.3,0.31 3DTE,ASP_216,3.2,-0.65,-0.32,0.37 105J,GLU_23,4.41,0.34,0,-0.43 1X9G,GLU_93,4.87,0.31,0,0.05 1ZCE, ARG 135, 13.02, -0.39, 0.38, 0.54 2P0L.LYS 56.10.58.-0.2.0.0.27 1Y0K, ASP_135, 3.47, -0.53, -0.11, 0.31 3PAC,HIS_78,5.82,-0.7,0,0.02 3VHJ,LYS_45,10.13,-0.23,0,-0.13 2Q99,ASP_227,3.05,-1.49,-0.07,0.81 1WXF,LYS_274,10.29,-0.21,0,0 3RFY,ARG_259,13.47,-0.38,0.84,0.52 3UX2,CYS_66,8.39,-1.23,-0.19,0.8 2NRR,HIS 370,6.84,-0.26,0.23,0.38 4ACJ.LYS 777,10.69,-0.15,0.0.34 3GT0,CYS_34,12.27,0.59,0.68,1.99 103X,ARG_265,12.37,-0.13,0,0 2X5Y,LYS_760,10,-0.55,0,0.04 3OBS,HIS_115,6.42,-0.13,0,0.06 1JT9,LYS 28,10.35,-0.14,0,-0.01 4DIU,GLU_77,4.61,0.34,0,-0.23 2FM9,GLU_111,3.84,0.29,-0.67,-0.28 3V55,GLU_572,4.55,0.12,0,-0.07

3ASA,ASP 265,3,73,-0,16,-0,35,0,43 2R51.GLU 279.4.62.0.26.0.-0.14 1OXZ,ASP_272,2.63,-0.99,-0.48,0.31 3EVP,TYR_93,9.38,-0.57,-0.5,0.46 109G.GLU 126.4.6.0.19.0.-0.09 1RSS.LYS 63.10.8.-0.37.0.28.0.39 1T3Y,LYS 126,10.59,-0.37,0.0.46 3RFY,ARG_317,12.35,-0.15,0,0 1PZC,HIS_81,5.3,-0.87,0,-0.34 1WYC,GLU_96,4.48,1.15,-0.85,-0.33 3CIV,ASP_207,3.43,-0.39,-0.36,0.37 1AK1,LYS_190,10.43,-0.33,0,0.26 2CE6.GLU 99.4.5.0.0.0 3TMO, ARG_294, 11.91, -0.81, 0, 0.21 1H09.LYS 3.11.35.-0.55.0.28.1.11 2H14,ARG 196,12.37,-0.8,0.02,0.65 2H14,TYR_131,10.3,0,0.11,0.19 3ETU,LYS_304,9.46,-1.06,0,0.02 3LH5,TYR_527,12.18,0.62,0.25,1.31 3HNX,ARG 17,12.53,-0.22,0,0.25 3PAC,HIS_174,6.41,-0.2,0,0.11 2IN0,ARG 405,13,22,-0,35,0,75,0,33 2Q07,TYR_408,12.19,0,0.4,1.79 10IS,LYS 215,10.18,-0.4,0,0.08 1LN4,ARG 91,13.39,-0.31,0.63,0.58 1PDB,GLU_30,7.46,3.55,-0.7,0.11 3CN5,LYS_142,10.41,-0.09,0,0 2Q12,TYR_168,10.29,0,0.1,0.2 1S7K,GLU 88,3.33,0.38,-1.45,-0.09 3GEC,CYS_242,12.42,-0.45,0.09,3.77 2RH3,LYS_184,10.53,-0.29,0,0.32 3DSH,LYS_356,10.44,-0.34,0,0.28 3RFY,LYS 133,10.5,-0.08,0,0.08 3BOW,LYS 177,10,55,-0,23,0,0,28 3C6B,ASP_275,3.68,-0.38,-0.08,0.35 4E8B,GLU_93,4.17,1.42,-1.4,-0.34 1WNH,HIS_185,6.89,-0.51,0.84,0.06 2P52,GLU 284,4.57,0.2,0,-0.13 3I0C, ASP_103, 3.99, 0, -0.06, 0.25 3ON1,LYS_50,10.83,-0.3,0.42,0.21 1TP6,ARG_116,13.96,-0.31,1.11,0.65 1FO9,GLU_280,2.2,1.01,-2.18,-1.13 1KN3.TYR 64.10.87.-0.71.0.24.1.34 2FD4,HIS_476,6.37,-0.32,0,0.19 1WP5.ARG 181.12.39.-0.11.0.0 1ES9,GLU_40,4.44,0.38,0,-0.44 3FXH,GLU 74,6.38,3.31,-1.48,0.05 1SOW,LYS 155,9,91,-0,19,0,-0,4 1LZL,ASP_205,3.52,0,-0.6,0.32 2YWK,LYS_48,11.31,-0.41,1.22,0 2XMZ.ASP 149.3.97.0.-0.1.0.26 1EV8.ASP 124.3.96.0.-0.03.0.2 4F85,CYS_211,12.52,0,-0.09,3.61 4FZR,GLU_134,4.12,2.03,-1.65,-0.75 1AD6,LYS_412,10.3,-0.2,0,0 4DBX,LYS_188,10.47,-0.08,0,0.05 10IS.ASP 239.4.16.0.0.02.0.34 2OJQ,TYR_370,11.33,0,0.09,1.24 3T8R,LYS_101,10.26,-0.42,0,0.18 3C38,HIS 166,4.87,-1.54,0,-0.09 1XEU.GLU 35.4.51.0.16.0.-0.16 3MEW, ARG_255, 12.97, -0.25, 0.27, 0.45 3EGN,ARG_411,12.38,-0.16,0,0.04 2E3S,ASP_508,3.72,0,-0.29,0.21 2CWC,ASP_122,2.83,-0.79,-0.7,0.51 3ASA, ARG_302, 12.66, -1, 0.31, 0.85 3M9A,TYR_65,10.51,0,0.32,0.2 2A4D,ARG_177,13.05,-0.14,0.31,0.38 3FK5,TYR_157,12.59,-0.59,-1.07,4.26

2R51,LYS 265,10.02,-0.49,0.0.01 3MEW,TYR_283,10.01,0,-0.91,0.91 1UW7,TYR_32,9.48,-0.52,-0.61,0.6 3V75,ARG_137,12.63,-0.12,0,0.26 1MML,GLU_69,3.58,0.29,-1.21,-0.01 300P.TYR 5,10.32,0.0.04,0.27 10XZ.GLU 301.4.84.0.29.0.0.04 1LFP,LYS_57,9.88,-0.62,0,0 3A2Z,TYR_174,10.27,0,0.02,0.25 1ZBM,ASP_207,2.93,-0.79,-0.39,0.3 2V5B,ARG_192,11.18,-2.23,0.66,0.24 2FM9,CYS_190,11.11,-0.41,0.11,2.41 1RL0,LYS_113,10.39,-0.28,0.01,0.16 2F9F,ARG_163,12.77,-0.8,0.75,0.32 1PV5.HIS 70.6.01.-0.73.0.0.24 20EW.GLU 44.4.83.0.25.0.0.08 2P65,ARG_165,12.53,-0.19,0,0.22 3RLN,GLU_701,4.62,0.12,0,0 3GW3,GLU_125,4.92,0.14,0,0.28 2P0L,LYS 75,10.42,-0.15,0,0.06 3NZL,LYS 78,10.38,-0.12,0,0 20JQ,GLU_650,6.09,2.22,-0.5,-0.13 3BWT,LYS_768,11.66,-0.7,0.95,0.89 4FH3.GLU 242.4.76.0.18.0.0.08 1AK1.TYR 248.11.09.0.0.37.0.72 2HXB,LYS_78,10.69,-0.32,0,0.52 3O48,LYS_70,10.34,-0.15,0,-0.01 2R51,TYR_178,12.04,0,0,2.04 3HYQ,GLU_78,3.81,0.3,-1.11,0.13 2EA9,ARG_17,12.35,-1.07,0.14,0.78 1JSX,LYS_203,9.18,-1.06,0,-0.25 3CO1,ARG_59,12.43,-0.07,0,0 1ANU,LYS 104,11,22,-0,34,0,68,0,38 3GYW,HIS 72,6.09,-0.73,0,0.31 1P1L,GLU_13,4.34,0.16,-0.06,-0.26 2XWS,ASP_35,3,-0.8,-0.4,0.4 1BN6,GLU_181,3.43,0.84,-1.47,-0.43 4F85,GLU_194,2.93,2.1,-3,-0.68 4DIU.GLU 229.4.12.0.78.-1.37.0.21 1KCM,ARG_74,12.35,-0.15,0,0 2QK1,LYS_340,10.9,-0.2,0.15,0.45 20JO,ARG 702,12,48,-0.06,0,0.04 4AM1,GLU 142,3.61,0.24,-0.75,-0.38 3F5D,TYR_187,10.1,0,0,0.1 1ILW,LYS_176,10.36,-0.34,0,0.2 2YWJ,TYR_124,11.8,0.85,0.5,0.45 1WOU,LYS 74,10,-0.17,0,-0.33 2HXB,TYR_156,10.27,0,0,0.27 3GOZ,LYS_285,10.32,-0.3,0,0.12 3P51.GLU 67.3.89.0.44.-0.76.-0.29 4ETX,ARG_168,12.55,-1.44,0.68,0.81 3KV0,TYR 139,11.33,0,0.02,1.32 4EVF.ARG 148.10.05.-2.46.0.0.01 2JEO,LYS_102,11.06,-0.2,0.45,0.31 1L3K,ARG_47,12.34,-0.39,0,0.23 2ILR,TYR_394,11.02,-0.79,0.02,1.8 1W24,TYR 46,10,26,0,-0,25,0,51 1Q46,TYR_12,10.26,0,-0.08,0.33 4EUG,HIS 8,5.97,-0.26,0,-0.27 1NFN,GLU_80,4.69,0.12,0,0.08 1V8E,HIS 168,3.3,-3.2,0,0 2V4X.TYR 11.12.81.0.85.0.7.1.27 3V75,ASP_39,2.53,-1.67,-0.06,0.45 3PZ9,TYR_81,10.56,-0.22,0.11,0.66 3IVF,ARG_118,12.21,-0.29,0,0 1R29,GLU_81,4.66,0.25,0,-0.09 4HDE,ASP 189,3.19,-1.42,-0.83,1.65 2IOT,LYS 3,10.3,-0.2,0,0 2HXB,LYS_60,11.31,-0.24,0.43,0.61

1RAJ,ASP_238,3.63,-0.59,0,0.41 3HKX,GLU 110,4.61,0.13,0,-0.02 3M70,LYS_2,10.47,-0.03,0,0 1SIG,ASP_403,4.14,0,0,0.34 2QK0,GLU_52,4.62,0.12,0,0 1XFK.HIS 241.6.4.-0.31.0.0.21 3I0C.HIS 285.5.63.-1.21.0.0.34 2H01,ASP_162,3.21,-0.65,-0.1,0.16 2X4L,ARG_59,12.5,-1.25,0.65,0.59 2AH5,GLU_32,4.66,0.32,0,-0.16 3V46,ARG 390,12.32,-1.17,0,0.99 20JQ,ARG_386,12.74,-0.41,0,0.65 2YLF,ARG_194,12.51,-0.08,0,0.09 1IDK,ASP 79,4.01,0.0.01,0.19 4ACJ,GLU_645,4.36,0.15,0,-0.28 3GA2,TYR 123,10.34,0,0,0.34 1XTD,LYS_27,10.35,-0.15,0,0 3HVM,TYR_61,10.03,0,-0.22,0.25 105T,GLU_436,4.58,0.27,0,-0.19 20HT.ARG 75,10.69,-2.58,0.0.77 2AZL,GLU_146,6.07,3.32,-0.73,-1.02 3L7N,ASP_217,2.43,-1.69,0,0.33 1LTU,LYS 94,10.18,-0.21,0,-0.11 3CS1,LYS_42,11.57,-0.26,0.85,0.48 3KB5,GLU 348,4.27,1.87,-1.55,-0.55 3UX2.TYR 41.11.89.0.66.0.51.0.72 4DBX,TYR_17,9.31,-1.45,-0.08,0.84 2WZ9,GLU_81,4.37,0.12,0,-0.25 3RJX,LYS_108,10.24,-0.47,0,0.22 1K95,ARG_193,12.53,-0.27,0,0.31 3ELI,HIS_43,5.78,-0.92,0.06,0.14 3G6S.GLU 261.4.99.0.26.0.0.23 2CIU,HIS_186,4.68,-1.54,0,-0.27 1AD6,HIS 549,6.56,-1.65,0.85,0.86 208P.GLU 118.4.03.0.93.-0.79.-0.6 3MTT,GLU_515,4.7,0.21,0,0 3HVM,LYS_45,10.32,-0.22,0,0.04 1YTQ,LYS_17,10.57,-0.21,0,0.28 300P,ASP 6,4.1,0,0,0.3 2C2Y,ARG_151,13.62,-0.26,0.83,0.55 3BWT,TYR_564,10.4,0,-0.1,0.49 1I60,LYS_189,11.5,-0.29,0.7,0.59 2IF4,CYS 70,11.69,0,0.02,2.67 2D0A, ARG 222, 12.08, -0.32, 0, -0.09 3FNI,GLU_86,4.56,0.13,0,-0.07 1YTD,LYS_13,10.6,-0.19,0,0.29 1LN4,LYS_50,10.08,-0.24,0,-0.18 3LMF,HIS_45,6.03,-0.86,0,0.38 1U7U,LYS 306,10.75,-0.11,0,0.36 1DCF,CYS_101,10.6,-0.21,-0.02,1.83 3ANJ,LYS_5,9.91,-0.8,0,0.2 3UV9,GLU_392,5.96,2.86,-1.8,0.4 20PJ.GLU 23,4.27,0.65,-0.84,-0.04 2FBI,ARG_119,12.4,-0.1,0,0 3EIZ,ARG_44,13.35,-0.24,0.65,0.45 1TP6,ARG_120,12.51,-0.33,0,0.34 1DVO,ARG_94,12.55,-0.38,0,0.44 1G8P.GLU 243,4.54,0.18,0,-0.14 3N2T,ASP_134,3.92,0,-0.09,0.21 3QKY,ARG_179,12.23,-0.29,0,0.01 1RHS,TYR_187,12.53,0,0.28,2.26 3ULX.LYS 167.10.41.-0.12.0.0.03 3G9B,ARG_73,12.87,-0.55,0.5,0.42 1R53,GLU_70,4.71,0.21,0,0 1SQW,ASP_157,3.44,-0.8,0,0.44 2OSA,LYS_264,10.08,-0.4,0,-0.03 2G7O.LYS 99,10.44,-0.1,0,0.05 3VHJ,TYR_47,9.29,-0.85,-0.28,0.42 3FTT,HIS_142,6.28,-0.22,0,0

4FLE.TYR 44.10.58.0.0.13.0.44 2CWY,ARG 82,12,35,-0,36,0,0,21 2VGM,LYS_201,11.33,-0.32,0.76,0.38 2B78,ASP_274,4.3,0,0.19,0.3 2CN1.LYS 260.10.43.-0.21.0.0.13 2H8O,GLU 95,4.56,2.3,-1.62,-0.63 3U2R,ARG_126,12.52,-0.38,0,0.4 1V8E,ARG 202,13,71,-0.64,1.43,0.43 3AUF,CYS_22,11.33,-0.02,-0.04,2.38 1YM5.LYS 148.11.32.-0.32.0.76.0.38 1NFN.GLU 50.5.33.0.56.0.0.27 3T5B,ARG_142,12.41,-0.18,0,0.08 1R7J,GLU_48,4.47,0.12,0,-0.14 2ZCO.GLU 236.3.46.0.51,-1.54,-0.01 2X4G.HIS 27.4.59.-2.49.0.83.-0.26 1ZBS,ARG_194,11.66,-0.84,0,0 2EYI,LYS_89,10.12,-0.29,0,-0.1 3CN5,LYS_186,10.5,-0.06,0,0.06 1TXJ,GLU_104,4.59,0.13,0,-0.04 10ZN.GLU 20.2.38.0.38.-2.12.-0.38 1P1L,GLU_69,4.56,0.35,0,-0.3 2OGQ,CYS_572,11.68,-0.03,0.31,2.4 1NAR,LYS 275,10,31,-0.23,0,0.04 3M7D.ARG 332.13.7.-0.43.0.66.0.98 3FRR,ARG_137,12.9,-0.58,0.4,0.58 2CXA,GLU_175,4.78,0.34,0,-0.07 3IVF,ARG_328,13.37,-0.86,0.76,0.97 2OSA, ASP_320, 3.47, -1.3, -0.62, 1.59 1RWZ,HIS_35,5.98,-1.46,0.85,0.1 3V75,ARG_87,13.38,-1.51,1.36,1.03 4GA2,LYS_34,10.1,-0.41,0,0.02 20YZ,ASP_24,3.8,-0.25,-0.08,0.33 3EZ7,LYS 48,10.44,-0.06,0,0 1Y2O,ARG 100,12,73,-0.37,0.08,0.53 3BWT,ASP_739,4.77,-0.06,0.35,0.67 2CBE,TYR_88,12.3,-0.22,0.6,1.92 3A2Z,TYR 30,10.6.0.0.06.0.54 2X4G.TYR 338.10.88.0.0.05.0.83 3ULX,ASP_50,3.61,-0.36,-0.42,0.59 4ETX.GLU 428.4.93.0.34.0.0.09 3KT9,HIS_88,5.84,-0.9,0,0.25 3ANJ,LYS 232,10.13,-0.37,0,0 1MJS.CYS 337,9.41,0.0.01,0.4 3Q2C,LYS_57,10.19,-0.28,0,-0.03 2CBE,LYS_159,10.26,-0.29,0,0.05 2Z0M,LYS_4,10.4,-0.15,0,0.05 3E5T,TYR_117,13.08,-0.85,0.13,3.8 2F4Q,LYS_91,9.98,-0.64,0,0.11 3BPPLYS 148,10.6,-0.17,0.0.27 3AUF,ARG_168,12.58,-0.14,0,0.22 2E3C,GLU 410,4.14,0.29,-0.41,-0.24 1R9W,LYS 289,10,27,-0,29,0,0.06 1M5I,ASP_183,3.49,-0.09,-0.49,0.27 2H85,LYS_319,10.98,-0.21,0.31,0.38 3EX9,ARG_20,12.32,-0.45,0,0.27 3IVF,LYS 89,10.22,-0.31,0,0.03 20EW,ASP_100,3.97,-0.33,0.12,0.37 3RRQ,LYS_78,10.66,-0.22,0,0.37 1XIP,TYR_279,11.69,-0.75,-1.59,4.03 10IS,LYS 332,10.52,-0.22,0,0.24 4EUG.GLU 215.4.71.0.77.0.-0.55 4DNU,ASP_260,3.21,-0.68,-0.36,0.44 2X4J,GLU_40,4.06,0.33,-0.39,-0.38 2BV9,ARG_136,12.38,-0.46,0,0.34 1PNE,LYS_125,10.27,-0.24,0,0 3DSH,GLU_384,5.47,1.25,0,-0.28 1YM5,ARG_74,12.27,-0.23,0,0 3R87, ASP_17, 2.46, -1.6, -0.23, 0.5 3PM2,LYS_164,10.36,-0.14,0,0

2A6B,HIS 165,5,13,-1,37,0,0 2D8N,TYR 53,12,57,-0,12,0,11,2,58 3ELI,ASP_3,4.23,0,-0.04,0.47 3GW3,LYS_359,10.34,-0.17,0,0.02 20EW,LYS 164,10,53,-0,32,0,0,34 2BV9,LYS_25,11.51,-0.29,0.85,0.45 1SUU,LYS_770,10.64,-0.43,0,0.57 3JV1,GLU_137,4.62,0.33,-0.29,0.09 2H14,ASP_98,2.26,-2.11,0.01,0.58 1P1L,LYS_62,10.61,-0.33,0,0.44 3BCH,ARG_85,11.84,-0.37,0,-0.29 1UXO,ARG_129,11.89,-1.07,0.09,0.36 3GOZ,ARG_309,12.79,-0.33,0,0.62 1RHS,GLU_42,4.54,0.17,0,-0.13 1Q42,ARG_15,12.24,-0.75,0.09,0.4 2XMZ,LYS 224,10,46,-0,2,0,0,16 4FZR,TYR_192,12.02,-0.28,0.01,2.29 3K9I,LYS_133,11.16,-0.37,0.36,0.66 1AM2,HIS_56,6.79,-0.37,0.63,0.03 2GKG,LYS 68,9.83,-0.5,0,-0.17 2X4L,ASP_66,3.91,0,0,0.11 4GA2,TYR_70,10.86,0,0.28,0.58 2CVB,GLU_85,4.49,0.1,0,-0.11 3BB7,HIS 287,6.18,-1.48,0.85,0.29 10YI,LYS 196,10.59,-0.26,0.02,0.33 10TM,ASP_178,2.52,-1.66,0,0.38 3JV1,HIS_89,6.85,-0.67,0.62,0.4 1ZCU,ARG_76,12.26,-0.4,0,0.16 3BJV,GLU_139,4.37,0.27,-0.39,-0.02 1ZCU,HIS_181,5.49,-1.11,0,0.1 3UV9,CYS_493,9.77,-0.14,0.12,0.78 2ZCO,GLU_121,3.75,0.35,-0.73,-0.38 4GCO,CYS_200,12.63,-0.07,0.69,2.99 2A1V.ARG 14.13.47.-0.43.0.76.0.63 1P1L,ARG_21,12.44,-0.26,0,0.21 10TM,LYS_230,10.44,-0.06,0,0 2WB8,ASP_789,3.59,-0.89,-0.01,0.69 1PGV,ARG 367,12.38,-0.15,0,0.03 2F4Q,GLU_308,3.62,0.42,-0.96,-0.34 4FZR,ASP_258,3.66,-0.33,0,0.19 2EFK,GLU_250,4.72,0.22,0,0 1TLV.TYR 126,13.1,-0.85,0.39,3.56 1WLY.CYS 91.12.77.0.0.41.3.36 3NJM,GLU_21,4.63,0.2,0,-0.06 4FZN,HIS_140,4.62,-2.66,0.78,0 3ONT, ARG_25, 13.3, -0.2, 0.33, 0.67 1AK1,GLU_172,3.87,0.59,-1.4,0.18 1LTU,ARG 219,11.85,-1.33,0.0.67 1XWM,GLU_157,4.17,0.31,-0.23,-0.41 2YX0,GLU_223,4.16,0.39,-0.76,0.04 2013.GLU 80.4.61.0.06.0.0.04 1SIG,LYS 414,10.02,-0.55,0,0.08 2X5Y,ASP_834,2.91,-0.84,-0.36,0.3 1UXO,LYS_25,10.22,-0.24,0,-0.04 1W24,ASP_171,3.49,-0.12,-0.37,0.18 2ZTY,ASP_58,3.53,-0.4,-0.21,0.33 301C.GLU 135,4.07,0.29,-0.32,-0.39 2R51,LYS_163,10.98,-0.17,0,0.65 1RWZ,ASP_168,3.89,0,0,0.09 3T5B.CYS 42.12.78.0.0.19.3.59 1DUN,LYS_92,10.56,-0.16,0,0.22 3DHN,ARG_167,12.72,-0.14,0,0.37 4AE7,CYS_113,8.69,-0.47,-0.18,0.34 3HYQ,HIS_69,6.75,-0.88,0.75,0.37 3MEW,GLU_191,3.97,0.51,-0.85,-0.19 1V6T,ASP_67,1.72,-2.31,-0.38,0.62 1D2K,LYS_346,10.41,-0.11,0,0.02 3GMS,ARG_295,12.27,-0.27,0,0.04 2BDD,LYS_39,10.58,-0.17,0,0.26

1XIP,GLU_371,5.38,1.05,-0.41,0.24 2H85,LYS_155,10.3,-0.2,0,0 1VSM,ARG_114,12.25,-0.25,0,0 1P6F,ARG_80,13.11,-0.45,0.58,0.49 3UV9,HIS_423,6.39,-0.1,0,-0.01 2F3LARG 120.12-0.5.0.0 3DSH.GLU 368.4.69.0.37.0.-0.18 2B0A,GLU_148,7.45,4.18,-1.14,-0.09 2Q13,GLU_224,4.63,0.13,0,0 1P6F,ASP_101,3.05,-1.14,0,0.38 1NIJ,ASP_253,2.93,-0.75,-0.38,0.27 4ECC,ARG 195,12,4,-0.81,0.09,0.63 3VHJ,ASP_118,4.17,0,0.07,0.29 1TXJ,TYR_101,9.5,-0.81,-0.64,0.95 2DVK.HIS 117.5.94.-0.34.0.-0.21 2F4O,ARG 14,13,73,-0.24,0.55,0.91 3FK5,GLU_81,3.91,0.28,-0.69,-0.18 2R0S,LYS_312,10.31,-0.23,0,0.05 3A4C,HIS_551,5.85,-0.42,0,-0.23 109G,ARG 181,12.51,-1.31,0.42,0.91 2EA9,ARG 22,11.69,-0.83,0.0.02 3BZT,ASP_302,4.02,0,0.04,0.18 3FWU,GLU_63,4.96,0.53,0,-0.07 3CX2,ASP 151,3.87,-0.03,0.0.1 1FKM,ASP_325,3.77,0,-0.33,0.3 1DUN,LYS_12,10.38,-0.51,0,0.39 109G,GLU_247,4.65,0.11,0,0.04 2Q99,TYR_51,13.96,0,0.3,3.68 2V4U,ARG_454,12.27,-0.46,0,0.23 2OSA, HIS 390, 5, 43, -2, 16, 0, 86, 0, 23 1R3D,LYS_129,10.01,-0.55,0,0.06 1YLN,LYS_238,10.36,-0.16,0,0.02 3O48,ASP 54,3.25,-0.9,0,0.34 4F85,HIS_235,5.61,-2.27,0.81,0.56 2WB3,ASP_356,3.86,0,0,0.06 2BDV,TYR_62,10.75,0,-0.03,0.78 3RNV,TYR_343,9.99,0,-0.35,0.33 1Y2Q,GLU_63,4.62,0.5,0,-0.39 3ULX.GLU 61.4.89.0.28.0.0.1 1ZBS,TYR_187,10.14,0,-0.06,0.21 1J74,LYS_116,11.23,-0.62,0.84,0.5 3RLE,GLU_157,3.07,0.54,-1.89,-0.09 2F9F,ASP 68,3.9,0,-0.02,0.12 2APL,LYS_7,10.84,-0.23,0.11,0.46 1WP5,ARG_240,12.44,-0.22,0,0.17 3I47,GLU_191,4.05,0.32,-0.74,-0.02 4FH3,LYS 180,10.37,-0.19,0,0.06 2X5Y,GLU_732,3.54,0.34,-0.59,-0.7 3GA2,GLU_101,4.2,0.27,-0.12,-0.45 1V43,HIS_362,4,-1.98,0,-0.51 1ZYL,TYR_276,10.74,-0.17,-1.2,2.1 2GZR,LYS 273,9.95,-0.59,0,0.04 2ZCX,ARG 24,12,46,-0,28,0,0,24 3JZN,GLU_233,4.31,0.26,0,-0.45 2FC3,GLU_10,4.55,0.1,0,-0.05 1X7F,ASP_331,2.04,-2.1,-0.71,1.05 2O0K,TYR_142,12.39,0,-0.41,2.81 3B7X,ASP_49,3.74,0,-0.19,0.13 3D9H.GLU 212.4.77.0.25.0.0.02 2FD4,ASP_472,3.86,0,-0.01,0.07 1M5I,ASP_227,3.42,-0.57,-0.32,0.5 2Z61,TYR 202,9.84,-0.5,-0.11,0.45 3PZ9,LYS_166,11.13,-0.82,0.85,0.61 3RHE,ARG_47,11.87,-0.63,0,0 4H89,GLU_42,4.13,0.23,-0.69,0.08 1CHD,GLU_235,3.8,1.3,-0.86,-1.13 2FBQ,LYS_176,10.26,-0.16,0,-0.07 1R6Y,HIS_15,6.65,-0.43,0.62,-0.04 1GQE,ARG_10,13.91,-0.58,1.36,0.62

1D2K,ARG_75,12.69,-0.35,0.01,0.53 2WB3,LYS 373,10.5,0,0,0 3ZTA,LYS_136,10.41,-0.17,0,0.08 2FBI,ASP_86,3.32,-0.61,-0.22,0.35 3BB7,LYS_119,12.18,-0.43,1.1,1 3IOC,LYS 139,10,43,-0,15,0,0.09 3LOE,ASP 388,3,99,-0,68,0,0,86 100X,HIS_154,6.67,-0.43,0.37,0.23 2YWJ,CYS_183,11.35,0,-0.5,2.83 2Q07,ARG_480,12.64,-0.09,0,0.23 2P1W.CYS 197.10.78.-0.15.0.37.1.55 1I60.TYR 135.11.59.0.85.0.39.0.35 2BLL,ASP_637,3.83,-0.27,0.02,0.28 1SNT,LYS_329,10.56,-0.13,0,0.19 2EFK,GLU_101,4.54,0.27,0,-0.23 1FHL,HIS 159,6.94,-0.93,0.85,0.52 1RHS,CYS_263,10.58,0,-0.22,1.8 1QQL,ASP_26,3.1,-0.49,-0.69,0.48 2BLL,HIS_627,5.91,-0.76,0,0.16 2P52.ASP 205.2.28.-1.8.-0.17.0.46 2E3S,TYR_586,11.8,0,0.52,1.28 1SJ8,GLU_538,4.49,0.28,0,-0.29 2GQV,ARG_31,13.4,-0.24,0.83,0.31 3R2E.GLU 113.3.39.0.39.-1.15.-0.36 100X,ARG 130,13.09,-0.35,0.37,0.58 1HF8,ASP_153,3.9,0,0,0.1 4F85,HIS_195,3.29,-3.55,0.16,0.19 105T,TYR_100,11.99,-1.44,0.06,3.37 20BI,GLU_88,3.77,0.21,-0.9,-0.04 4EZB,GLU_54,4.78,0.32,0,-0.04 4ETX,ASP_227,3.78,-1,0,0.98 2W1R/CYS 77,12,43,-0.33,0.24,3,51 1YTD,ASP_11,2.05,-1.7,-0.55,0.5 2NMU,TYR 93,10.17,0,0.08,0.09 3HVM,GLU 237,5.3,2.16,-1.35,-0.01 1FKM,ASP_609,3.88,0,-0.11,0.19 3MTT,ARG_478,12.23,-0.29,0,0.02 3LQE,ASP_385,3.68,-0.1,-0.25,0.24 3LH5,LYS 753,10.42,-0.12,0,0.03 3GS9,HIS_75,6.19,-0.37,0,0.06 1X7F.ARG 28.12.55.-0.25.0.0.3 2PLQ,LYS_125,10.53,-0.14,0,0.17 3ILC,ASP 193,4.2,0,0.14,0.26 2VGM,ASP 327,3.8,0,-0.43,0.41 208I,GLU_164,4.78,0.21,0,0.08 1JB3,ARG_100,12.26,-0.24,0,0 1UAJ,ARG_121,13.58,-0.23,0.81,0.49 2G70,ASP_108,3.94,0,-0.07,0.2 4DNU,ASP_156,3.74,-0.61,0.02,0.53 3PZ9,ARG_53,13.12,-0.41,0.71,0.31 2EYI,LYS_31,10.56,-0.15,0,0.21 2CIU,CYS_128,10.51,-0.11,0.2,1.43 2F4O,ASP 53,3,37,-0.55,-0.38,0.51 1RI6,CYS_154,11.07,-0.07,-0.43,2.57 3LQE,LYS_349,10.45,-0.05,0,0 4EUG,ARG_80,12.93,-0.87,0.77,0.52 1YG2,ASP_15,3.31,-0.85,-0.02,0.38 4AM1,ARG 330,10.05,-2.55,0.0.1 3JV1,GLU_113,4.57,0.07,0,0 1ZBP,GLU_132,4.9,0.18,0,0.22 3VJ8,ARG_317,12.27,-0.23,0,0 1IDK.HIS 168.6.67,-1.95,1.03,1.09 1ZBS,GLU_184,3.76,0.22,-0.46,-0.49 3CAX,ARG_383,11.1,-1.55,0,0.16 2EYI,LYS_162,10.46,-0.04,0,0 3EX9,LYS_25,10.28,-0.26,0,0.04 10LR,TYR_154,9.74,-0.22,-0.38,0.35 200K,ASP_183,3.91,0,-0.16,0.26 3M7G,ARG_241,12.53,-0.05,0,0.08

2P0Y.ARG 292.12.33.-0.24.0.0.07 2V4U.GLU 475,4.53,0.26,0,-0.23 1T95,LYS_12,10.48,-0.05,0,0.02 1L2H,LYS_27,10.04,-0.53,0,0.07 2G9D,ASP 232,3.95,-0.1,-0.11,0.35 4EZB.GLU 194,4.06.0.51,-0.85,-0.1 1ZHV,ASP_42,3.95,0,-0.08,0.23 1NAR,ASP_215,4.72,0,-0.01,0.92 3HVM,HIS_20,4.01,-2.24,0.14,-0.4 3FTT,ASP_18,3.61,-0.78,0.02,0.57 1G8P,ARG_260,11.55,-1.31,0,0.36 1Q2Y,LYS_7,10.54,-0.22,0,0.25 2B78,HIS_282,5.91,-0.4,0,-0.19 3GS9,TYR_228,10.69,0,0.28,0.41 2FZ4.GLU 26.4.22.0.37.-0.48.-0.17 1RI5,LYS_266,10.44,-0.06,0,0 2GYZ,ARG_57,12.43,-0.07,0,0 2IIA,ASP_40,3.58,-0.4,0,0.18 3M70,ASP_83,3.83,0,-0.14,0.17 1L3K.GLU 9.3.81.0.38.-0.81.-0.26 1D2K,ASP_62,3.84,-0.36,-0.08,0.48 1WXF,GLU_21,4.44,0.24,0,-0.3 2V5B,GLU_136,4.05,0.24,-0.48,-0.2 3LD1.GLU 320,4.09,0.23,-0.31,-0.32 2EFK,LYS_44,10.42,-0.08,0,0 1MTZ,GLU_54,4.63,0.29,0,-0.16 1WXQ,HIS_326,6.16,-0.23,0,-0.11 4FH3,ARG 359,12.45,-0.29,0,0.24 2FL4,ARG_13,12.25,-0.39,0,0.14 3H13,LYS_436,10.52,-0.07,0,0.08 2VGM,GLU_360,5.19,0.3,0.14,0.25 2XWS,HIS_16,6.6,-0.24,0.17,0.17 2CYG,GLU 275,4.05,0.33,-0.77,0 4ACJ,LYS 711,10,79,-0,36,0,28,0,37 3V55,GLU_397,5.76,1.44,0,-0.2 3LH5,ASP_699,3.96,0,-0.17,0.33 1KCM,GLU_86,5.23,1.39,-0.23,-0.43 1UCH,ASP_142,3.34,-0.53,-0.17,0.24 2A0J,GLU_6,4.71,0.21,0,0 20KT,HIS 309.6.07,-0.22,0,-0.22 1I60,LYS_44,10.51,-0.14,0,0.15 2XJ4.ARG 219,12.2,-0.41,0,0.1 1UXO,CYS 74,13.2,-0.07,0,4.28 2VAN,HIS_134,6.25,-0.39,0.37,-0.23 2NRK,TYR_8,10.91,0,-0.07,0.97 4ESS,GLU_153,4.3,0.34,-0.4,-0.14 1V6T,TYR_75,11.49,0.53,0.47,0.49 1DTO,ARG_37,12.29,-0.29,0,0.08 1AT0,ASP_303,3.98,0,-0.1,0.28 3C38,ARG_67,11.44,-1.36,0,0.3 1SQW,GLU 176,5.02,0.08,0.44,0 3EZ7.TYR 325,10.5.0.0.21,0.29 2D7J,HIS_67,6.81,-0.43,0.19,0.54 1RWZ,HIS_214,4.53,-1.42,0,-0.56 1RZ2,GLU_211,4.48,0.19,0,-0.2 2NRK,LYS 158,11.38,-0.28,0.64,0.52 1K95,LYS_184,10.12,-0.46,0,0.07 2HRZ,GLU_287,3.98,0.33,-0.52,-0.34 1K95,ARG_154,12.31,-0.19,0,0 2CIU,GLU 191,4.47,0.14,0,-0.18 3NBLTYR 170.10.42.0.0.05.0.37 3UPD,ARG_59,12.1,-0.46,0,0.07 2XMZ,ASP_72,2.56,-2.5,-0.43,1.69 3CIV,ASP_193,1.96,-1.92,-0.59,0.68 2R0S,HIS_89,6.04,-0.46,0,0 2V4X,GLU 75,4.91,0.19,0,0.22 1AIL,GLU_66,4.59,0.23,0,-0.14 4EVF,CYS_137,10.76,-0.76,0.43,2.09 2YT4,LYS 673,10.18,-0.37,0,0.05

1CHD,HIS 256.6.08,-1.13.0.38.0.32 2EYI.GLU 70.4.39.0.94.-0.78.-0.27 3ZSL,HIS_223,5.07,-1.64,0.34,-0.13 2CL3,ASP 57,3,32,-0,79,-0,79,1.09 105J.GLU 60.2.8.0.49,-1.7,-0.49 4ESS.LYS 28.11.4.-0.44.0.85.0.49 1LFP,ARG_106,12.35,-0.44,0,0.28 3GMS,ASP_223,4.28,-0.09,-0.11,0.68 2FG1,TYR_50,13.19,-0.29,0.79,2.7 3GYW,ARG_83,12.58,-0.36,0.05,0.4 4D8L,ASP_82,3.4,-0.76,-0.16,0.51 3M7G,LYS_47,10.47,-0.05,0,0.02 2APL,TYR_67,11.13,0,0.06,1.07 106D,ASP_94,3.12,-0.84,-0.4,0.55 2B0J.TYR 267.10.97.0.0.0.97 2E0T,ARG 204,12.27,-0.23,0,0 3GW3,LYS_231,10.09,-0.41,0,0 1X7F,GLU_201,6.05,1.51,0,0.04 3GYW,HIS_115,6.32,-0.24,0,0.05 3L3P,GLU_278,4.01,0.56,-0.57,-0.48 2ILR,CYS_422,9.73,0,-0.05,0.78 2AXO,HIS 201,4.14,-2.73,0.77,-0.4 1T3J,CYS_681,9.36,0,0,0.36 1GPP.TYR 431,10.96,0,0.56,0.4 3RJX.GLU 252.4.14.0.32.0.-0.67 1S7K,GLU_102,4.34,0.23,-0.25,-0.14 2X4J,GLU_117,5.88,1.34,0,0.04 3G9G,LYS_227,10.58,-0.3,0,0.38 1UAJ,HIS_201,6.45,-0.16,0.08,0.02 1OXZ,GLU_279,4.7,0.38,-0.01,-0.18 2RIK,ARG_40,12.33,-0.08,0,-0.1 1X04,ASP_126,1.92,-1.74,-0.62,0.49 2PP6,GLU_18,4.61,0.11,0,0 1YW5,ARG 15,13,16,-1,4,0,91,1,15 3EVN,ASP_105,4.02,0,-0.02,0.23 1JT9,GLU_241,4.78,0.23,0,0.06 4EVF,HIS_264,5.89,-0.26,0,-0.35 3AU3,HIS 408,6.83,-0.28,0.43,0.18 1PV5,CYS_260,9.97,-0.32,0.61,0.69 1JKS,GLU_62,3.1,0.47,-1.27,-0.6 3N2T,ASP_295,4.01,0,-0.35,0.56 3GEC,ARG 494,12.27,-0.53,0.0.3 2BDV.GLU 189.4.05.0.22,-0.44,-0.22 3LPZ,HIS_177,6.61,-0.3,0,0.41 1R3F,ARG_220,12.44,-0.35,0.02,0.26 20BI,ASP_111,3.75,0,-0.16,0.11 4EF5,GLU 336,4.29,2.23,-1.94,-0.51 1WYC.GLU 128,4.89,0.63,0,-0.24 1DTO,ASP_174,3.72,-0.85,-0.1,0.88 1PBV,LYS_244,10.11,-0.4,0,0.02 4FH3.LYS 144.11.05.-0.52.0.44.0.63 2FM9.GLU 122.4.31.0.82.-0.72.-0.3 1NFN,ARG_32,13.87,-0.45,1.4,0.42 3BOW.GLU 238,3,42,0.91,-1,78,-0,21 1JKS,GLU_81,3.09,1.27,-2.03,-0.64 3LJN,TYR_273,11.3,-0.04,-0.21,1.55 1X9G,TYR 60,10,1,0,0,0,1 1UOH,TYR_15,10.12,0,-0.1,0.23 2G9D,ARG_264,13.26,-0.93,1.12,0.58 1NRI,ASP_23,4.13,0,0.03,0.3 3G9T.GLU 57.4.21.1.65.-1.39.-0.55 1SI7,ASP_215,3.99,0,-0.03,0.22 3VJ8,ARG_360,12.93,-0.38,0.25,0.56 4AE7,TYR_129,11.56,-1.98,0.14,3.41 3A7L,HIS_31,6.44,-0.79,0.38,0.36 1LTU,GLU_65,4.69,0.31,0,-0.12 3HKX,CYS_220,11.08,-0.16,0.17,2.06 10I7,LYS_143,10.71,-0.22,0.04,0.38 2P0Y,HIS_313,5.07,-2.27,0.83,0.01

2EEY,LYS 21,9.6,-0.58.0,-0.33 2YWJ,ASP_96,2.22,-1.69,-0.39,0.5 2P52,LYS_98,10.42,-0.08,0,0 4ETX,ARG_172,11.17,-0.72,0,-0.6 2OPJ,ARG_118,11.59,-1.06,0,0.15 3BWT,ASP_776,4.39,0,-0.03,0.62 3ZRI,HIS -2,7.07,-0.2,0.76,0 3HVM,GLU_31,3.93,0.63,-0.85,-0.36 1AT0,LYS_352,10.44,-0.07,0,0.01 3GG6,ARG_111,12.63,-0.52,0.36,0.29 2EEY,ASP_53,3.4,-0.79,0,0.39 1PVT.GLU 166.4.66.0.21.0.-0.07 1Q42,LYS_73,11.46,-0.27,0.85,0.38 2QVT,ARG_116,12.06,-0.3,0,-0.13 3L3P.GLU 481.5.08.0.32.0.0.27 2WOZ.GLU 527.4.68.0.18.0.0 2BV9,GLU_284,3.27,0.2,-0.78,-0.65 4ECC,LYS_204,10.48,-0.11,0,0.09 3O16,ASP_216,3.4,-0.68,-0.07,0.35 3TOW, ARG 61, 12.48, -0.11, 0, 0.09 2P0L/ARG 264,12,44,-0.23,0.0.17 1LZL,ASP_22,3.48,-0.67,-0.11,0.46 2X4L,ASP_109,2.78,-0.85,-0.62,0.45 1RKA, HIS 35.6.14, -0.26.0, -0.1 1JT9.ARG 119.12.7.-0.24.0.0.45 3MTT,GLU_473,4.21,0.32,-0.3,-0.31 200K,CYS_125,13.06,0,0.41,3.65 1YG2,TYR_111,11.8,0,0.29,1.5 3EVN,LYS 15,10.2,-0.25,0,-0.05 2NRK,GLU_76,3.15,0.36,-1.19,-0.52 2VGM,GLU_91,4.7,0.14,0,0.05 2IRM,HIS_131,6.39,-0.11,0,0 1Z3X,LYS_109,10.39,-0.15,0,0.04 3M66,GLU_218,4.61,1.12,-0.66,-0.34 3B7X,LYS_60,10.57,-0.13,0,0.2 3RFF,GLU_146,3.49,0.31,-0.93,-0.39 1H4U,TYR_531,10.57,0,0.14,0.43 2FZ4,ASP 48,2.03,-1.75,-0.71,0.69 3F6M,ARG 76,13,93,-0,78,1,26,0,95 3AU3,CYS_661,11.5,0,0,2.5 3IU5,LYS_77,10.28,-0.14,0,-0.07 2FG1.TYR 75.10.35.0.0.35 3UV9.ARG 320.13.69.-0.26.1.45.0 1V43,GLU_347,4.56,0.09,0,-0.04 1MML,GLU_233,4.73,0.26,0,-0.03 1RZ2,ASP_188,3.6,-0.45,-0.21,0.46 2Q13,HIS_100,5.67,-1.04,0.21,0 2XJ4,GLU_83,3.41,0.48,-1.19,-0.38 3K9I,GLU_142,4.56,0.06,0,0 1O5T,LYS_253,11.06,-0.66,0.7,0.52 3MIX,ASP_544,4.02,0,0,0.22 2ZCX,ARG 211,12.03,-0.31,0,-0.17 3ULX,ARG 138,12,76,-1,38,0,76,0,89 3T57,GLU_282,3.91,0.27,-0.87,0.01 1SNT,TYR_377,11.39,-0.16,0.31,1.24 2IRM,LYS_19,10.37,-0.17,0,0.04 3Q6L,LYS_10,10.69,-0.35,0.16,0.38 2YLF,GLU_227,4.84,0.52,-0.27,0.09 20EW/TYR 39/12/16/0.54/0.81/0.81 2D7U,GLU_30,3.91,0.28,-0.85,-0.02 1PVT,ASP_52,3.94,0,0,0.15 1PZC.GLU 62.3.91.0.57.-0.82.-0.34 1L2H,ASP_86,3.31,-0.84,-0.01,0.36 3EZ7,GLU_23,4.67,0.17,0,0 3M16,LYS_8,12.07,-0.74,1.47,0.84 3ZTA,GLU_61,4.65,0.9,-0.57,-0.17 3CNU,ASP_81,2.04,-2.28,0,0.52 1SIG,ARG_281,12.78,-0.37,0.23,0.42 4FZR,GLU_37,4.77,0.27,0,0

105J,CYS_29,9.19,-0.24,-0.39,0.82 1VJG,ARG 193,12.49,-0.12,0,0.11 2AZL,LYS 103,10,45,-0.05,0,0 3VJ8,TYR_220,13.06,-0.08,0.31,2.85 1R7J,TYR_28,10.16,0,0,0.16 3EVP.GLU 164.4.64.0.14.0.0 3CIV.ARG 170.13.28.-1.32.1.38.0.72 4FCU,ASP_240,1.8,-2.18,-0.46,0.64 3IVF,ASP_341,2.32,-1.69,-0.43,0.63 1LN4,LYS_80,11.39,-0.34,0.85,0.38 1XKR,ARG_94,12.58,-0.19,0,0.26 1RSS,ASP_126,2.13,-1.7,-0.87,0.9 3BA1,LYS_267,10.36,-0.14,0,0 2E3C,ASP_196,2.97,-0.85,-0.38,0.4 2FPN,GLU_114,4.82,0.41,0,-0.1 2H14,ASP_302,3.31,-1.47,0.05,0.94 3IU5,ASP_130,3.75,0,-0.19,0.14 3TOW,LYS_120,10.6,-0.08,0,0.18 200K,ARG_84,12.43,-0.1,0,0.04 1UAJ,LYS 238,10.37,-0.09,0,-0.04 30NH.TYR 469.12.3.0.0.15.2.13 1P2F,ASP_185,3.39,-0.77,-0.44,0.81 1QQH,GLU_177,4.57,0.23,0,-0.16 3BJV.LYS 109.10.41.-0.09.0.0 3V55,TYR 434,12.77,0,0.4,2.37 3PM2,ASP_83,3.74,0,-0.36,0.3 2IRM,ARG_216,12.84,-1.84,1.48,0.7 3HQX,ARG_79,13.41,-0.27,0.8,0.38 208P.GLU 77.4.7.0.2.0.0 1DCF,CYS_32,11.31,0,0.02,2.29 30N1,GLU_24,4.07,0.24,-0.37,-0.31 2EYI, HIS 247, 5, 56, -1, 76, 0, 79, 0, 04 2BLL,GLU_552,3.41,0.83,-1.67,-0.25 3PBH.HIS 110,3.8,-2.6,0.03,-0.13 3A2Z,HIS 131,4,58,-3,56,0,85,0,79 2Q12,ASP_157,3.76,0,-0.21,0.17 3FTT,HIS_120,6.46,-0.24,0,0.2 1J8B,GLU_90,4.57,0.34,0,-0.26 1WRU,GLU 197,4.98,0.21,0,0.27 2VAN, ASP_318, 3.44, -0.82, 0, 0.46 3BWT,LYS_796,10.73,-0.12,0,0.35 1P4X,GLU_182,4.66,0.13,0,0.03 1YW5,HIS_156,2.99,-2.97,0,-0.54 3LOD.GLU 98.4.25.1.93.-1.39.-0.79 2P0L,GLU_216,3.66,0.3,-0.85,-0.28 1GVP,ARG_21,12.44,-0.06,0,0 20YZ,GLU_80,5.14,0.39,0.09,0.17 100X,GLU 134,4.08,0.53,-0.37,-0.58 3B7X,ASP_73,3.6,-0.87,0,0.68 1NWA,CYS_13,11.77,-1.21,1.13,2.84 2BAA,LYS_54,10.33,-0.34,0,0.16 2X4G,GLU_96,4.63,0.13,0,0 2D7U,HIS 83.6.2,-0.35.0.0.05 1PNE,ARG_135,12.07,-0.96,0,0.53 3LJI,HIS_178,5.18,-1.61,0,0.3 3BWT,GLU_599,4.17,0.97,-1.27,-0.03 1RHS,GLU_46,3.55,1.1,-1.41,-0.63 20HT.ARG 186.12.33.-0.25.0.0.09 3B21,GLU_86,4.31,0.74,-0.78,-0.15 3H04,TYR_6,10.01,-0.32,-0.03,0.35 3NBI,TYR_85,11.14,0,0,1.14 3IL3.GLU 199.4.58.0.08.0.0 3IRA,GLU_8,5.49,0.83,0,0.17 3F5D,HIS_115,5.98,-1.1,0.57,0.01 2HRZ,LYS_41,10.13,-0.54,0,0.17 1RSS,LYS_131,11.56,-0.33,0.85,0.53 4E8B.GLU 90.4.68.0.1.0.0.08 1Q2Y,LYS_13,11.49,-0.24,0.85,0.38 1N81,LYS_121,9.56,-0.56,0,-0.38

3BZTLYS 255.10.33.-0.39.0.0.22 4DNU,ARG 217,12.68,-0.26,0,0.44 2WB8,HIS_525,6.33,-0.2,0,0.03 1R3D,LYS_252,10.41,-0.09,0,0 1AD6.CYS 438,10.05,-0.02,0.45,0.63 3CAX,LYS 153,10.29,-0.15,0,-0.05 2Q07,ARG_399,12.67,-0.29,0,0.46 1WXF,GLU_119,3.96,0.58,-0.66,-0.46 3US6,GLU_36,4.58,0.08,0,0 3GE9,GLU_210,5.76,1.12,0,0.14 1Z9L.GLU 113,3,38,0,44,-1,22,-0,34 2GKG,LYS_94,10.28,-0.2,0,-0.02 3I82,HIS_75,7.07,-0.22,0.79,0.01 10YI.TYR 242,10,42,0,0,02,0,39 2YWJ.GLU 114,4.71,0.26,0,-0.07 3OA7,TYR_572,10.13,0,0.09,0.04 1Z3X,GLU_13,4.06,0.33,-0.81,0.04 3HKX,ARG_17,12.47,-0.03,0,0 1H09,ARG_110,13.17,-0.37,0.59,0.45 3CRM,ARG 59,12.83,-0.29,0.08,0.54 2XMZ,HIS_103,7.53,-0.31,0.85,0.49 2E3S,LYS_470,10.3,-0.35,0,0.15 3HVW.ASP 294.4.37.0.0.16.0.41 1SJ8.ARG 692,13.35,-0.23,0.67,0.41 2F9F,ARG_21,12.22,-0.42,0,0.13 3M66,ASP_197,3.88,0,-0.13,0.2 2YX0,ARG_90,11.41,-1.34,0,0.24 2A6B,ASP_186,4.07,-0.83,0.07,1.02 3DTE,ARG_253,12.75,-0.2,0,0.45 1WXF,ARG_134,13.76,-0.38,0.79,0.85 1KCM,TYR_155,10.14,-0.26,-0.36,0.77 1SIG,ASP_360,3.47,-0.33,-0.44,0.44 3CXS,LYS 166,10.3,-0.22,0,0.02 1EO6.LYS 144,10.4,-0.1,0.0 3DZ1,ARG_154,12.2,-0.45,0,0.16 3M16,ARG_124,12.64,-0.3,0.05,0.38 3M7D,ARG_76,13.86,-1.3,0.88,1.77 1EDG,ARG_358,12.64,-0.25,0.01,0.38 1SQH,GLU_105,5.09,1.55,-0.8,-0.16 4AM1.TYR 134.11.61.0.44.0.19.0.99 2FPN,GLU_178,4.76,0.12,0,0.14 3N0K,ARG 27,12.46,-0.04,0,0 1P2F,LYS 4,10.37,-0.19,0,0.06 2CXC,GLU_79,3.97,0.24,-0.57,-0.2 1YTD, ARG_24, 12.41, -0.19, 0, 0.1 1O3X,LYS_226,10.65,-0.11,0,0.26 3GOZ, ASP_69, 3.36, -0.34, -0.32, 0.22 2QEV,TYR_47,10.56,0.14,0.13,0.28 3EJC,ARG 116,12,76,-0,19,0.02,0.42 4GCO,ARG_225,12.39,-0.13,0,0.02 1A8Q,ASP_137,3.22,-0.91,-0.05,0.38 1ZCU.HIS 241,5.92,-0.49,0,-0.09 3DTE,ASP_101,3.95,0,-0.05,0.2 1AK1,ASP_95,3.97,-0.68,0.17,0.69 3PBH,HIS_239,4.81,-1.71,0,0.01 2RJD,TYR 319,13.76,0.85,1.03,1.88 3ETU,LYS_214,10.27,-0.41,0,0.18 1YTD,ARG_98,13.41,-0.3,0.66,0.55 1V43,ASP_359,3.34,-0.37,-0.54,0.45 1XTZ,ARG 219,12.85,-0.26,0,0.61 3016.GLU 24.4.8.0.24.0.0.06 1W7B,LYS_49,10.48,-0.02,0,0 1T6L,LYS_237,10.28,-0.21,0,-0.02 3HVW,LYS_282,9.99,-0.56,0,0.06 3EX9,ARG_67,12.66,-0.47,0.32,0.3 2EJX,ARG 128,12.35,-0.2,0,0.05 1PGV,TYR_378,9.88,-0.17,-0.1,0.15 3FK5,ASP_200,3.81,0,-0.24,0.24 106D,LYS_71,10.12,-0.47,0,0.08

208P,GLU_147,4.5,0,0,0 2FXT,LYS 278,10.22,-0.3,0.0.02 2G70,HIS_93,6.42,-0.23,0,0.14 3SMD,TYR_100,12.63,0.57,0.75,1.32 4FCU,GLU_40,4.63,0.13,0,0 2YT4.GLU 512.4.74.1.39.-0.66.-0.49 2ZCX,GLU_85,3.44,0.33,-0.76,-0.63 1NIJ,GLU_167,4.55,0.13,0,-0.08 1DVO,GLU_158,2.7,0.46,-1.84,-0.42 2P5D,GLU_29,3.08,0.38,-1.18,-0.62 1RWZ,LYS_147,10.32,-0.18,0,0 1WXQ,LYS_197,10.28,-0.15,0,-0.08 3K9LARG 85,12,16,-0,46,0,0,12 3N2T,LYS_240,10.5,-0.05,0,0.05 3L7N.LYS 63.10.46.-0.04.0.0 1AM2,CYS_79,12.01,0,-0.02,3.02 2IDC,GLU_88,3.81,1.01,-1.07,-0.64 1LTU,ASP_275,3.2,-0.81,-0.17,0.37 3P2F,CYS_67,12.07,0,-0.56,3.61 20BI,GLU 65,4.54,0.08,0,-0.04 4DVD,ASP_83,3.7,-0.21,-0.37,0.46 3M16,ARG 120,13.25,-0.37,0.75,0.38 1XIP,LYS_332,11.11,-0.4,0.5,0.51 2CBE,LYS 112,9.97,-0.49,0,-0.03 2ATR.GLU 106.4.62.0.12.0.0 3BA1,GLU_266,4.64,0.14,0,0 2O4D,ASP_116,3.72,-0.91,0.38,0.46 2AXO,TYR_178,12.67,-0.03,0.63,2.07 1ES9,GLU 56,4.85,1.7,-0.8,-0.56 1D2K,LYS_117,9.84,-0.64,0,-0.02 3ANJ,LYS_62,10.31,-0.19,0,0 3RAZ,GLU_145,3.81,0.31,-0.82,-0.18 3IU5,GLU 63,4.46,0.09,0,-0.14 3EVP,ASP 110,3.68,0,-0.37,0.25 3AUF,CYS_85,12.77,-0.27,0.19,3.85 2EHG,TYR_35,10.8,0,0.01,0.79 1DOV,GLU_170,4.77,0.34,-0.05,-0.02 2NRK,GLU_7,3.7,0.33,-0.74,-0.38 3H13,LYS_474,11.27,-0.32,0.6,0.5 2Q07,ARG_276,12.43,-0.07,0,0 1QQE,LYS_136,11.35,-0.66,0.59,0.92 1YR6.TYR 204.10.12.0.-0.06.0.18 1046.GLU 151.4.5.0.25.0.-0.25 3ULX,TYR_31,11.35,0,0.01,1.34 2NRR,ARG_362,13.67,-1.02,1.29,0.9 30DJ,HIS_60,3.54,-2.45,0.07,-0.57 1G8P,LYS 265,10.35,-0.18,0,0.02 2FGG,GLU 50,4.86,0.21,0.06,0.1 1QQE,ARG_268,12.59,-0.1,0,0.19 2VGY,GLU_159,4.58,0.08,0,0 1YLN,TYR_179,11.91,0,0.41,1.51 2B6P.TYR 177.10.38.0.0.0.38 2Q13,HIS_59,6.73,-0.25,0.32,0.16 3EX9,LYS 40,10,41,-0.09,0,0 3G9T,ASP_211,3.14,-0.8,-0.19,0.34 3H9W,ASP_111,2.08,-2.28,-0.01,0.56 3V10,ARG 647,12.51,-0.27,0,0.29 3CAN,LYS_29,10.65,-0.23,0,0.37 2PWQ,GLU_47,3.93,0.3,-0.71,-0.16 2JEO.ARG 149.12.1.-0.84.0.01.0.42 2NYC.GLU 237.5.43.0.76.0.0.16 3JV1,LYS_153,10.56,-0.06,0,0.12 1L2F,ASP_337,3.12,-0.7,-0.58,0.6 2V4U,LYS_319,10.42,-0.11,0,0.04 3PZ9,CYS_201,12.14,-0.28,0.52,2.88 2BCF,ARG_238,12.56,-0.41,0.03,0.44 3RNV,HIS_454,7.12,-0.32,0.74,0.2 1K95,ARG_172,12.51,-0.44,0,0.45 3TRE,TYR_74,10.71,-0.81,0.32,1.21

1MIX.HIS 255.5.31.-0.95.0.-0.24 3HVW,ASP 191,3.16,-0.58,-0.53,0.47 1YM5,GLU_211,5.52,2.55,-1.03,-0.5 3T5B.GLU 92,4.66,0.37,-0.16,-0.05 3CAN,TYR_98,12.58,0,-0.06,2.64 3U2R,ARG 93,12.01,-0.24,0,-0.25 200K.LYS 51,10.66,-0.13,0.0.29 3F5D,GLU_158,3.65,1.16,-1.61,-0.39 4DBX,TYR_177,13.12,-0.85,0.69,3.28 2BDD,LYS_121,10.66,-0.17,0.33,0 1LTU,TYR 210,10.46,-0.14,0.02,0.58 4ANN, HIS 54, 7.2, -0.42, 0.85, 0.27 30IP,LYS_198,10.49,-0.12,0,0.12 1V6T,ARG_126,12.94,-0.36,0.38,0.41 2PIM.ASP 46.3.97.0.0.0.17 2IRM.ARG 219.12.22.-0.28.0.0 1T95,LYS_71,10.56,-0.13,0,0.19 3ANJ,TYR_82,10.34,0,-0.16,0.49 1X9G,CYS_87,10.94,-1.74,0.09,3.59 3BWT,ASP 683,4.27,-0.58,-0.16,1.2 3M16.GLU 154,4.53,3.74,-3.25,-0.46 3GS3,ASP_201,3.89,-0.79,-0.65,1.54 3U0V,GLU_108,3.65,1.76,-1.61,-1.01 2P0L.LYS 268,10.35,-0.14,0,-0.02 2P0Y.ARG 333.12.38-0.12.0.0 2FD5,GLU_122,4.78,0.22,0,0.05 3LD1,ARG_300,12.89,-0.28,0.31,0.36 3ZRI,HIS_-5,6.62,-0.2,0.32,0 3JZN,GLU_394,3.97,0.15,-0.85,0.17 10LR.ASP 27.3.3.-0.63.-0.24.0.36 3P51,GLU_123,4.57,0.1,0,-0.03 2FM9,LYS_77,10.68,-0.15,0,0.33 2Z0W,GLU 44,3.85,0.38,-0.73,-0.31 2RIK,ASP_266,2.78,-0.74,-0.53,0.25 2IQT,GLU_176,3.83,3.79,-0.6,-3.84 3R87,TYR_58,9.82,0,-0.34,0.15 2CXC,LYS_114,10.8,-0.23,0.17,0.36 1SJY,ASP_54,3.85,0,-0.08,0.13 2EJB.CYS 90.12.92.0.0.17.3.75 1WYC,HIS_373,5.98,-0.38,0,-0.14 2NSN,GLU_106,4.71,0.21,0,0 1ILW.TYR 103.11.33.-0.82.0.86.1.29 3TOW,LYS 115,10.36,-0.37,0,0.22 3ASA,LYS_2,10.47,-0.03,0,0 1J7G,LYS_44,10.53,-0.18,0,0.21 3KT9,ASP_76,3.82,0,-0.27,0.29 2FXT,TYR 274,11.12,0,0,1.12 1NAF,GLU_279,4.79,0.29,0,-0.01 2R51,LYS_182,10.28,-0.48,0,0.26 2HRZ,LYS 37,10.52,-0.29,0,0.31 1NIJ,ARG_278,13.39,-0.27,0.75,0.41 3JRT,GLU 39,4.04,0.27,-0.57,-0.16 1WXQ,LYS_259,10.31,-0.19,0,0 3RHE,TYR_104,11.73,0.77,0.41,0.54 2CN1,GLU_133,4.5,0.15,0,-0.15 1P2F,LYS_169,10.38,-0.21,0,0.09 1QQH,LYS_162,10.57,-0.44,0,0.51 3ASA,ARG_22,11.97,-0.95,0.1,0.33 20GQ,TYR_421,10.03,0,-0.18,0.21 3GS3,ARG_83,12.95,-0.8,0.67,0.58 2ZQ5,ASP_9,3.65,0,-0.45,0.3 2V5B,LYS 85,10,14,-0,31,0,-0,05 2HP7,GLU_177,4.7,1.05,-0.85,0 3CX2,HIS_225,6.38,-0.6,0.27,0.21 1DVO,GLU_45,4.69,0.19,0,0 3DTE,ASP_42,3.91,0,0,0.11 2YWX,CYS_3,11.09,-0.13,-0.07,2.29 2FZ4,GLU 229,4,92,0,15,0,1,0,18 1U53,LYS_92,10.32,-0.57,0,0.39

2Z14,GLU_80,4.79,0.28,0,0.02 1EDG,LYS 94,10.56,-0.23,0,0.29 2CE6.LYS 17,10.1,-0.36,0,-0.04 1RKA,ARG_74,11.98,-0.68,0,0.16 2V4U,LYS_391,10.39,-0.14,0,0.04 2GZO.GLU 141.3.28.0.43.-1.06.-0.59 2F8H.GLU 13.4.83.0.28.0.0.05 3COU,ASP_63,3.53,-0.74,-0.02,0.48 3G9G,LYS_131,11.37,-0.26,0.5,0.63 1XTZ,HIS_261,6.17,-0.26,0.02,-0.08 1GPP,ASP_116,1.95,-1.76,-0.63,0.55 2EFK.GLU 108,4.6.0.25.0,-0.16 3CGW,GLU_79,4.38,0.19,-0.31,0 2P0L,LYS_243,10.27,-0.23,0,0 4ECC,LYS_9,10.87,-0.28,0.21,0.44 3V46,LYS 385,10.26,-0.26,0,0.01 3BB7,LYS 46,11,55,-0,25,0,85,0,45 1YTD, TYR_72, 10.59, -0.3, -0.15, 1.04 2E3S,LYS_581,10.54,-0.17,0,0.22 3ILC,GLU_184,4.6,0.1,0,0 2RIS.GLU 45,3.77.0.28,-0.95,-0.07 1JT9,GLU_259,3.32,1.48,-2.1,-0.56 3V3T,ARG_268,11.98,-0.31,0,-0.21 208I.LYS 120.10.36.-0.14.0.0 1AK1,LYS 5,10.14,-0.37,0,0.01 1PGV,GLU_287,4.88,0.25,0,0.13 3CBN,CYS_117,12.06,0,-0.05,3.12 1X7F,TYR_161,11.43,-0.23,0.79,0.86 1U3Y,GLU_338,4.62,0.22,-0.04,-0.06 2Q98,ARG_125,12.44,-0.19,0,0.12 4E9E,ARG_546,13.29,-0.69,0.83,0.65 2B61.CYS 46.12.68.0.0.3.68 3G9G,CYS_202,10.78,-0.05,-0.12,1.95 1RL0,TYR 229,11.79,0.8,0.41,0.58 4EVF.ARG 83,13,47,-0,45,0,74,0.68 3N2T,GLU_304,4.56,0.12,0,-0.06 3I4T,TYR_146,11.97,0.09,0.45,1.43 1QYI,LYS_170,10.25,-0.21,0,-0.04 1Z9L, ASP 101, 3.38, -0.75, 0, 0.33 1X1E,GLU_178,3.87,0.39,-0.57,-0.46 3RFY,TYR_283,13.28,-0.13,0.26,3.14 1W24,TYR_165,10.98,0,0.09,0.89 3ASA,HIS_190,6.48,-0.2,0,0.17 2F4O.TYR 150.9.27.-0.5.-0.64.0.41 2FL4,TYR_102,9.88,-0.58,-0.31,0.77 2Q5X,ARG_779,11.99,-0.74,0,0.24 2ZCO,LYS_113,10.29,-0.37,0,0.16 3FHF,ARG_87,12.55,-0.19,0,0.24 3UPD,LYS_253,10.24,-0.26,0,0 3GT0,TYR_178,10.09,0,0,0.09 1MTZ,LYS_53,10.55,-0.13,0,0.17 3BCY,LYS_78,10.63,-0.15,0,0.27 106D,ARG 72,13.89,-0.53,1.35,0.57 1P2F,ARG_113,13.12,-1.46,0.83,1.26 2VGM,LYS_193,11.06,-0.29,0.27,0.59 3ON1,ASP_43,2.42,-1.59,-0.36,0.57 2I88,ASP_459,3.58,-0.51,-0.13,0.42 105T,ARG 298,12,51,-0,11,0,0,12 4DBX,LYS_280,10.37,-0.2,0,0.06 4ETX,ARG_161,11.73,-1.09,0,0.32 1S7K,ASP_137,2.89,-0.7,-0.65,0.44 2AZP.HIS 101.6.4,-0.37.0.0.26 10GL,HIS_83,3.74,-2.3,0.2,-0.66 4F3J,HIS_135,5.44,-1.06,0,0 3F6F,LYS_28,10.62,-0.14,0,0.26 1LN4,LYS_89,10.47,-0.03,0,0 3K8J.GLU 131.4.37.0.12.0.-0.25 4E8B,CYS_21,9.58,-1.04,0.32,1.3 4EVF,GLU_109,4.33,0.24,0,-0.4

4F85.ASP 166.4.08.0.0.1.0.18 1U3Y,TYR_348,10.68,-0.01,0.3,0.4 3K9LASP 140.3.9.0.0.0.1 3A7L,GLU_89,4.19,0.39,-0.81,0.11 3M70,HIS 109,4.93,-1.43,0.2,-0.35 10TM,ASP 112,3,57,-0,76,-0.01,0.55 2HRZ,LYS_279,10.43,-0.13,0,0.07 3CX2,LYS_218,10.5,-0.11,0,0.11 4FD6,TYR_113,9.95,-0.36,-0.19,0.5 1BGF,HIS 100,6.26,-0.42,0.11,0.07 2098.GLU 120.5.57.1.22.0.-0.16 1WPA,HIS_499,6.33,-0.42,0,0.25 1X7F,GLU_320,3.43,2.39,-2.3,-1.16 1UOH,CYS_11,11.52,-0.46,0.43,2.55 2PGX.GLU 117.6.18.2.78.-1.18.0.1 2P5D,GLU_70,3.91,0.21,-0.79,-0.01 3Q6L,ARG_107,11.43,-2.46,0,1.39 2R51,HIS_173,7.39,-0.4,0.85,0.44 4D8L,LYS_129,11.28,-0.25,0.5,0.53 1XTZ,LYS 137,10.52,-0.36,0.11,0.27 1HUF,LYS_114,11.17,-0.67,0.85,0.48 1SI7,LYS_81,10.5,0,0,0 3I4T,ASP 41,3.91,0,-0.08,0.19 1XTZ,ARG 172,13.41,-0.27,0.78,0.4 2WB8,ASP_720,3.53,-0.46,-0.27,0.46 2RGY,GLU_110,4.2,1.57,-1.37,-0.5 4D8L,HIS_65,6.52,-0.62,0.75,-0.1 1JYH,GLU 31,4.49,0.29,0,-0.3 3H9W,GLU_115,4.78,0.11,0,0.17 2JKF,ASP_109,3.71,-0.55,0.19,0.27 1XAW,LYS_494,10.02,-0.31,0,-0.18 3UAH,TYR_299,10.97,-0.77,0.01,1.72 1J74,CYS 69,12.9,-0.02,0.41,3.51 1KCM,TYR 94,13.1,-0.05,0.83,2.33 3GS9,ARG_99,12.84,-0.39,0.42,0.31 3U2R,ASP_107,3.82,0,-0.13,0.15 1FO9,TYR_130,10.35,0,-0.12,0.48 2ZCO,GLU_242,3.97,1.43,-1.45,-0.51 3O16,HIS_107,3.86,-2.75,0,0.11 2IIA.CYS 34,9.12,-0.55,0.1,0.57 3UAH,TYR_397,10.44,0,-0.29,0.73 1RI5,GLU 207,4.2,0.32,-0.21,-0.41 3V3T.GLU 220.4.91.0.32.0.0.09 2FPN,ARG_56,13.44,-0.32,0.43,0.82 3JZ9,GLU_452,4.63,0.16,0,-0.03 2FM9,GLU_170,3.95,0.3,-0.85,0 1MIX,LYS_318,10.38,-0.12,0,0 1QQH,ASP_122,2.91,-1.51,0,0.62 1XFK,HIS_83,5.62,-1.3,0.37,0.05 1BKB,GLU_122,4.92,0.23,0,0.19 2B02, ARG 430, 12.5, -0.5, 0.1, 0.4 2P5D.ASP 55.3.81.0.-0.12.0.13 1ZBM,LYS_87,11.35,-0.41,0.79,0.47 3PM2, ASP_159, 3.77, 0, -0.36, 0.32 3VHJ,TYR_131,10.27,-0.83,0.49,0.61 4ACJ,ASP 739,3.06,-0.79,-0.32,0.37 200K,TYR_132,10.04,0,-0.09,0.13 1XDZ,GLU_129,4.37,1.63,-1.46,-0.31 1G5Z,LYS_191,10.28,-0.22,0,0 1GXN,GLU_551,4.77,0.32,0,-0.05 1ZHV.HIS 132.6.34.-0.2.0.04.0 10IS,ASP_171,3.07,-0.67,-0.6,0.53 1DVO,LYS_39,10.42,-0.08,0,0 1YM5,GLU_171,4.81,0.13,0,0.18 2V81,ASP_54,4.05,0,0.01,0.24 20BI,LYS 118,10.4,-0.43,0,0.33 3CCY,TYR_79,10.39,0,0.19,0.2 2G3A,ARG_112,12.11,-0.28,0,-0.11 3U2A,ASP_24,4.07,0,-0.23,0.49

10GL,GLU_250,4.07,0.68,-0.53,-0.59 2XHC,ARG 107,12.51,-0.2,0.0.2 3BWT,TYR_676,10.24,0,0,0.24 1SUU,ARG 776,12.7,-1.01,0.61,0.59 2BLL,GLU_575,3.88,0.36,-0.6,-0.38 2AXO.TYR 199.12.44.0.0.81.1.63 1MTZ,HIS 35,3.89,-3.59,0.33,0.64 3U2R,LYS_114,10.4,-0.12,0,0.02 1ZBM,ARG_224,13.42,-0.28,0.55,0.64 2161,CYS_96,8.94,-2.76,-0.29,2.98 1XTZ,ARG_189,13.48,-1.76,1.66,1.08 1YTD,ARG_254,12.03,-0.52,0,0.04 4F3J,ASP_203,2.63,-1.64,-0.37,0.85 2D0A,HIS_152,5.74,-1.28,0.52,0 1R3F.GLU 296.3.82.0.38.-0.74.-0.32 3FTT.CYS 178.10.25.-0.56.-0.02.1.82 1JKS,GLU_70,4.23,0.92,-0.85,-0.33 2B0J,GLU_222,4.86,0.18,0,0.19 1QZN,GLU_131,4.89,0.56,0,-0.17 2EHG,ARG 129,12.75,-0.36,0.01,0.6 2AXO,ASP_186,2.87,-0.75,-0.38,0.2 3P28.LYS 218.10.6.-0.09.0.0.18 2GS5,HIS_42,5.98,-0.6,0,0.08 1TR9,ASP 171,2.46,-1.68,-0.16,0.5 108B,ARG 61,12,21,-0,42,0,0,13 1TD6,TYR_258,10.72,-0.27,0.08,0.92 3G9T,ASP_130,4.01,0,-0.09,0.3 1DUP,LYS_77,10.31,-0.16,0,-0.03 3DTE,TYR_58,10.81,0,0.07,0.74 1EV8,ASP_40,4.15,0,0.02,0.33 1R9W,LYS_259,10.65,-0.17,0,0.32 1AK1,LYS_274,10.88,-0.34,0.32,0.4 3E5T,LYS 182,10.13,-0.68,0,0.32 2FD5.HIS 127.3.68.-2.32.0.-0.49 2R51,LYS_55,10.45,-0.05,0,0 10IS,HIS_331,7.42,-0.45,0.85,0.51 2P1W,LYS_31,10.44,-0.06,0,0 2PGX,LYS 80,10.32,-0.18,0,0 4FLE,TYR_153,9.72,-0.38,-0.1,0.21 2E3S,HIS_453,6.05,-0.53,0.09,-0.01 4H4J,LYS_153,10.96,-0.29,0.41,0.34 1XDZ.GLU 49.4.42.0.34.0.-0.42 2WB3.ASP 374.4.28.0.0.31.0.17 2CXC,LYS_126,11.77,-0.71,1.28,0.69 1Y0K,GLU_55,4.54,0.11,0,-0.07 3PZ9, ASP_378, 1.96, -2.43, -0.69, 1.27 4GCO,GLU 245,4.25,0.12,-0.38,0.01 3HUE,GLU 69,5.03,0.81,0,-0.28 1NRI,GLU_187,4.91,0.88,-0.42,-0.05 1CBY,GLU_120,4.44,0.16,0,-0.22 1ZBM.ARG 126.13.22.-0.26.0.5.0.48 4FZN,CYS_59,12.34,0,0.21,3.12 2V4U,ARG_376,13.71,-0.87,1.29,0.77 1V43,ASP_324,3.89,0,-0.35,0.45 1GPP,LYS_173,10.37,-0.08,0,-0.04 1Q8B,GLU_41,3.43,0.35,-0.85,-0.57 1DOV.LYS 178,10,44,-0,11,0,0,05 2OB5,ASP_69,3.3,-0.84,-0.38,0.73 1WYC,GLU_310,3.87,0.23,-0.67,-0.19 2QRX,TYR_16,9.43,-0.68,-0.17,0.27 3I4T.GLU 138.4.58.0.08.0.0 3E7P,GLU_131,4.43,0.44,-0.31,-0.2 1MJS,HIS_248,6.1,-0.4,0,0 1G8P,ARG_299,11.75,-0.83,0,0.08 3LJN,TYR_202,9.97,-0.04,-0.35,0.36 3B21,GLU_89,2.99,0.49,-1.58,-0.42 1BN6,ARG_215,11.84,-1.22,0,0.55 4FCU,GLU_208,3.08,1.14,-2.39,-0.16 1KN3,LYS_62,10.57,-0.24,0,0.3

1JYH,LYS_108,10.61,-0.16,0,0.27 105T,LYS 366,10.44,-0.06,0,0 3JSN,ARG_212,11.39,-1.23,0,0.12 2FPN,GLU_57,4.48,0.16,0,-0.18 3ONT, ASP_71, 2.26, -1.62, -0.45, 0.53 1PBV,GLU_95,4.74,0.31,0,-0.06 1YR6.LYS 93.10.65.-1.19.0.83.0.5 3CGW,HIS_96,3.02,-2.67,0,-0.81 1T3Y,GLU 8,4.67,0.08,0.0.09 1SJY,GLU_23,4.47,0.17,0,-0.2 1W7B,ARG_68,10.06,-3.04,0,0.6 2X4G.CYS 59.10.16.0.0.04.1.12 3DHN,HIS_223,6.26,-0.26,0,0.02 1QYI,LYS_95,10.35,-0.47,0,0.32 1NAR,LYS 153,10.64,-0.27,0.0.42 3ULX,ARG 62,12,3,-0.35,0,0.15 2Q99,ARG_372,12.3,-0.39,0,0.2 3C2E,CYS 54,12,81,-1.63,1.31,4.13 3JZN,TYR_148,11.39,-0.09,0.27,1.21 1A8Q,ARG 111,13.16,-0.57,0.74,0.49 2IIA.TYR 15.11.84.0.85.0.51.0.48 3HKX,ASP_194,3.99,0,0,0.19 3R2E,LYS_98,10.42,-0.74,0.2,0.47 20RX,ARG 63,13,19,-0,49,0.66,0.53 2HNG.GLU 27.3.33.0.78.-1.56.-0.39 2JHY,LYS_141,11.23,-0.58,0.85,0.45 2WZ9,ARG_27,13.57,-0.23,0.92,0.38 4H86,ASP_13,3.87,0,-0.06,0.14 1SJY,LYS 152,10.53,-0.37,0,0.4 3L3P,LYS_465,10.14,-0.43,0,0.07 3OBS,LYS_36,10.44,-0.1,0,0.05 2DG7,ARG_127,13.01,-0.23,0.35,0.4 2XJ4,ARG_187,11.39,-0.79,0,-0.33 2I88,TYR 478,12.52,0,0.11,2.42 3U0V,GLU_89,3.96,2.79,-2.01,-1.32 20KT,CYS_31,13.69,-0.06,0.68,4.07 3CIV,TYR_134,12.49,-1.06,0.64,2.91 2F8H,TYR_326,11.29,-0.05,0.09,1.24 4E8B.GLU 68.3.69.0.16.-0.74.-0.23 2VGM,ASP_294,4.02,0,0.07,0.15 3EYE, ARG_87, 13.96, -0.74, 1.65, 0.54 2WOZ,ARG_388,10.3,-2.64,0,0.44 4DNU,ASP 51,1.85,-1.9,-0.59,0.55 2FZ4,GLU_74,4.63,0.13,0,0 1DTO,HIS_136,5.62,-0.69,0.02,-0.21 2OKT,HIS_28,6.19,-0.53,0,0.21 3UV9,LYS 485,10.49,-0.11,0,0.11 2RGY,TYR_337,13.33,0.84,0.66,1.84 2XHC,ASP_303,3.36,-0.74,-0.18,0.49 3F1X,LYS 274,10.67,-0.08,0,0.25 2GZQ,GLU_40,4.23,0.36,-0.58,-0.05 10I7,ARG 146,13.12,-0.25,0.48,0.39 3RVC.GLU 142.4.51.0.44,-0.04,-0.39 1XDZ,LYS_104,10.39,-0.11,0,0 2ZQ5,GLU_225,3.17,0.4,-1.54,-0.19 2YLF,GLU_55,3.77,0.85,-1.35,-0.22 1WYC,HIS 375,6.01,-1.8,0.61,0.7 2HP7,GLU_91,3.54,0.34,-1.3,0 3H6O,ASP 56,3.99,-0.13,-0.25,0.56 2X4L,GLU_155,3.89,0.32,-0.81,-0.12 1XEU,CYS 258,9.59,0,0.15,0.44 3LJN,TYR 148,10.6.0.0.15.0.45 2NRR,GLU_345,4.34,0.43,-0.69,0.1 3DB9,ASP_12,3.51,-0.34,-0.22,0.27 2FL4,LYS_88,10.15,-0.25,0,-0.1 2CXY,LYS_17,11.27,-0.43,0.82,0.38 4DND,GLU_87,4.83,0.2,0,0.14 3E5T.GLU 203,4,72,0,26,0,-0.04 3EZ7,ARG_351,13.44,-0.37,0.39,0.92

1FO9,LYS_401,10.51,-0.07,0,0.08 4E8B,GLU 187,4.7,0.2,0,0 4F3J,CYS_145,10.42,-0.88,0.15,2.13 2APL,GLU_89,4.27,0.46,-0.71,0.02 1Q42,HIS_91,6.4,-0.19,0,0.09 1Y2O,LYS 72,10,33,-0,23,0,0.06 2H2W,LYS 26,10.49,-0.01,0,0 3LJN,HIS_210,4.46,-2.07,0,0.03 3US6,LYS_120,10.25,-0.18,0,-0.06 1YR6,ASP_75,3.39,-0.85,-0.37,0.81 2B0A,ARG_56,12.21,-0.31,0,0.02 1SIG.ASP 189.3.7.-0.3.-0.13.0.32 1RZ2,GLU_158,4.78,0.24,0,0.04 3U4K,TYR_64,10.94,0,0.11,0.83 2QK1,GLU_554,4.14,0.38,-0.25,-0.49 3G9G,GLU 186,5.49,0.92,-0.11,0.19 2NRK,HIS_98,4.74,-1.86,0,0.11 1GVP,ASP_36,3.22,-0.72,-0.17,0.31 2PLQ,ARG_295,12.51,-0.09,0,0.1 3V55,ASP 697,3.8,-0.18,0,0.18 3JZN.GLU 392,4,71,0,24,0,-0.02 3MIX,GLU_322,4.79,0.3,0,-0.01 1L2F,GLU_268,4.88,3.52,-2.2,-0.95 3BQW,ASP_74,3.91,0,-0.02,0.12 2DFL,TYR 177,11.12,0.47,0.11,0.54 3K8J,LYS_120,10.66,-0.11,0,0.27 3GFP,ASP_468,4.25,-0.18,0.28,0.34 1QYI,GLU_378,3.84,0.42,-0.94,-0.13 1LN4,GLU_69,4.7,0.19,0,0.02 2VGM,CYS_155,11.37,-0.09,-0.01,2.47 3Q1C,GLU_118,4.41,0.66,0,-0.76 1SNT.HIS 200.6.47.-0.6.0.0.57 1RL0,ARG_252,12.97,-0.31,0.34,0.44 1J8B,ASP 65,3.27,-0.76,0,0.23 3F5D.LYS 177.10.34.-0.25.0.0.08 2B0J,LYS_226,10.19,-0.75,0,0.45 1W7B,LYS_286,11.17,-0.63,0.85,0.46 1U53,TYR_170,13.31,0,0.12,3.2 2W0G,LYS 173,11.36,-0.18,0.65,0.39 3UV9,ASP_440,4.13,0,0.04,0.29 3M7G,GLU_18,4.08,0.84,-0.54,-0.72 1YLN,HIS_215,5.72,-0.32,0,-0.46 3A7L,GLU 126,4.65,0.17,0,-0.02 3NR5,LYS 97,10.44,-0.06,0.0 2Z0M,LYS_86,9.97,-0.5,0,-0.03 2AZL,ARG_286,11.99,-0.51,0,0 1WXF,GLU_22,3.85,1.39,-0.8,-1.24 3ADO,GLU 293,4.58,0.08,0,0 3M7D,ARG_42,12.98,-0.62,0.6,0.51 2IDC,ARG_137,11.64,-2.51,0.16,1.5 2BAA,LYS_26,10.38,-0.12,0,0 2E3H,GLU 240,4.9,0.28,0,0.12 3PBH,ARG 116,13.09,-0.33,0.37,0.55 2VGM,GLU_137,4.66,0.41,0,-0.25 2VAN,GLU_165,3.97,0.65,-0.82,-0.37 2Z84,TYR_178,10.5,0,0.05,0.44 3S0A,LYS_52,10.94,-0.64,0.48,0.6 1WXF.ARG 82,13.6,-0.54,0.95,0.69 2JEO,GLU_51,4.65,0.12,0,0.04 2E3S,LYS_590,10.67,-0.29,0,0.47 1WLY,LYS_316,11.32,-0.45,0.85,0.42 2CYG,ARG 252,12,13,-0,38,0,0 2BLL,HIS_363,5.57,-1.14,0.22,-0.01 4FD6,ARG_134,13.44,-2.01,0.83,2.12 2HNG,GLU_95,3.12,0.48,-1.48,-0.38 1BN6,CYS_273,10.96,0,-0.22,2.18 3PZ9.GLU 388.3.3.0.5.-1.32.-0.39 2Q13,ARG_72,12.47,-0.03,0,0 2FZP,ARG_190,12.96,-0.55,0.22,0.79

2HXB.GLU 93.3.52.0.64.-1.63.0 2IF4.GLU 261.3.69.0.26.-0.7.-0.37 2RIK,GLU_138,3.19,0.49,-1.52,-0.27 1GXN,ARG_625,14,-0.91,1.51,0.89 4ETX.CYS 236,12.07.0.-0.04,3.11 3AU3.CYS 575.11.27.0.0.15.2.12 2YYO,TYR_30,10.99,0,0.06,0.93 2ZCX,ARG_155,13.12,-0.47,0.71,0.39 3T5B,HIS_176,4,-3.28,0.79,0 1U53,LYS 14,10.48,-0.35,0,0.33 2Z84, ARG_128, 11.7, -1.08, 0, 0.29 2WOZ,ARG_485,10.94,-2.83,0.54,0.72 3CIV,GLU_231,3.1,3.85,-2.44,-2.81 2PGX,ASP_199,2.82,-1.09,-0.41,0.52 30AV.HIS 144.6.49.-0.43.0.0.42 3JZ9,HIS_376,5.27,-0.88,0,-0.35 2CL3,GLU_119,4.1,0.29,-0.49,-0.19 3IRA,GLU_32,4.69,0.17,0,0.01 20EW,LYS_234,10.63,-0.19,0.05,0.28 3M70,ASP 144,4.09,0.0.02,0.28 2ATR,TYR_126,10.48,0,0.19,0.28 3JRT,TYR_89,11.99,0,0.29,1.69 2X4G,ASP_323,3.69,-0.09,-0.4,0.39 3CO1,TYR 71,11.2,0.05,0.52,0.63 1KCM,GLU_28,4.9,0.85,0,-0.44 3HQX,LYS_68,10.42,-0.33,0,0.25 3C5V,LYS_217,11.2,-0.36,0.85,0.21 1P2F,LYS 163,10.39,-0.12,0,0.01 2NSN,ASP_42,3.49,-0.7,0,0.39 3CCY,TYR_194,10,0,-0.08,0.07 1J33.ARG 189.12.2.-0.29.0.-0.02 1MD6,ASP_127,3.38,-0.85,-0.08,0.51 4FZR,CYS 9,10.72,-0.13,0.37,1.48 1R6Y,GLU 86,3.93,0.28,-0.85,0 3GW3,GLU_314,4.92,0.32,0,0.09 2Z84,GLU_130,4.28,0.66,-0.54,-0.34 3UC9,ASP_177,3.83,0,-0.16,0.19 3T8R, ARG_50, 13.35, -0.37, 0.58, 0.64 109G,GLU_117,4.63,0.15,0,-0.02 3ZSL,ARG 169,12,47,-0.66,0.37,0.26 1SUU,GLU_709,4.54,0.07,0,-0.04 3TRE,CYS 113,10.44,0,0.07,1.37 10YI,HIS 88,4.02,-2.66,0,0,18 3R87,CYS_74,11.52,-0.08,0.22,2.38 3CBN,ARG_29,12.24,-0.32,0,0.06 3UAH,HIS_382,7.05,-1.83,1.26,1.12 1MUF,GLU_138,4.8,0.34,-0.58,0.55 2Q13,ARG_314,13.44,-0.16,0.74,0.36 3CS1,GLU_115,3.96,0.37,-0.53,-0.37 1JSX,GLU_89,3.18,0.68,-1.59,-0.41 1WLY,LYS 294,11.27,-0.46,0.7,0.53 3COU,ARG 50,12,26,-1,12,0,39,0,5 1ZP2,TYR_34,10.54,0,0.24,0.3 3ETV,LYS_161,10.45,-0.05,0,0 2X4L,TYR_130,12.5,0,0,2.5 3IRA,LYS 36,10.62,-0.11,0,0.23 2ZQ5,ARG_144,12.51,-0.17,0,0.17 2R0S, ASP_71, 3.1, -0.52, -0.41, 0.22 2CVB,GLU_104,4.45,0.69,-0.61,-0.14 3H9W,GLU 129,3.2,0.39,-1.36,-0.34 3LH5.TYR 633.13.9.0.0.01.3.88 3FTT,LYS_4,11.36,-0.47,0.78,0.55 1EQ6,ASP_149,4.12,0,0.04,0.28 208I,GLU_75,4.69,0.19,0,0 2NRR,LYS_357,10.57,-0.04,0,0.11 2A6B,ASP 156,3.82,0,-0.11,0.13 3GOZ,LYS_130,10.08,-0.47,0,0.05 3BB7,ARG_171,12.31,-0.22,0,0.04 4H4J,ASP_28,3.18,-0.73,-0.32,0.43

3M7D,ARG_206,13.45,-0.4,0.78,0.57 4FD6.ARG 10.12.62.-0.28.0.04.0.36 3UX2,GLU_68,4.2,0.29,-0.55,-0.03 3PZ9,ARG_364,13.78,-0.36,0.75,0.9 2A0J,ARG_24,12.61,-0.23,0,0.34 1RHS.TYR 107.13.28.0.-0.09.3.38 4EVF,TYR_114,11.72,-0.09,0.12,1.7 2RIK,GLU_135,4.77,0.27,0,0 1UCH,TYR_35,10.82,0.24,0.34,0.24 1X8F,GLU_245,4.76,0.14,0,0.11 20PJ.CYS 93.10.35.-0.26.-0.32.1.94 2YWJ,TYR_58,9.54,0,-0.72,0.27 3LPZ.ARG 197,12.15,-0.38,0.0.04 3CGW,GLU_25,4.99,0.36,0,0.13 100E.LYS 281.10.37.-0.28.0.0.14 3RJX.LYS 137.11.44.-0.24.0.72.0.45 2IN0,LYS_89,10.48,-0.13,0,0.1 2Q5X,ARG_850,13.29,-0.58,0.67,0.7 3GA2,ARG_177,12.82,-1.55,0.56,1.33 1X6J,ARG 81,12.36,-0.25,0,0.11 2W2S,LYS_77,10.4,-0.11,0,0.01 1A8O,ASP 65,3,58,-0.33,-0.19,0.29 1H09,LYS_288,10.24,-0.42,0,0.16 3LJN,ARG 25,12.23,-0.29,0,0.02 20HT,ARG 101,13.09,-0.17,0.44,0.32 2FBQ,LYS_50,10.31,-0.18,0,-0.01 3JZ9,GLU_524,2.66,0.75,-2.32,-0.27 2FI9,GLU_70,4.54,0.15,0,-0.11 4EF5,GLU_249,3.84,0.39,-0.67,-0.38 3BPV,ARG_96,12.28,-0.3,0,0.08 1BYI,CYS_151,9.99,-0.86,-0.01,1.86 3K1H,LYS_76,10.08,-0.45,0,0.03 2D7U,LYS 142,10.53,-0.11,0,0.14 1XKR.ASP 97.3.58.0.-0.37.0.16 1LTU,GLU_71,3.67,0.18,-0.63,-0.38 2P1W,TYR_61,12.19,0,0.16,2.02 1YG2,HIS_89,6.39,-0.1,0,-0.01 2B0A,LYS 95,10.49,-0.18,0,0.16 3BWT,ARG_674,12.67,-0.32,0.18,0.31 2WOZ,GLU_321,5.01,0.16,0,0.35 4DNU,TYR_194,11.08,0,0.2,0.88 3FFM.GLU 28.4.7.0.41.0.-0.2 105T,LYS 256,10,42,-0.08,0,0 2PGX,ARG_208,12.21,-0.52,0,0.22 2B61,ASP_10,3.07,-1.06,0,0.33 3FNI,GLU_137,3.13,0.49,-1.4,-0.45 2CWC,ASP_146,3.54,-0.27,-0.27,0.28 2WOZ.LYS 570.10.85.-0.8.0.61.0.54 4DNU,LYS_16,10.35,-0.15,0,0 1NJ4,HIS_151,4.94,-1.45,0,-0.1 3T5B,GLU_266,4.46,0.08,0,-0.12 3GS9.GLU 242.4.63.0.13.0.0 3AU3,ARG_549,11.8,-0.7,0,0 3V46,ASP_372,3.85,-1.44,-0.41,1.9 3B4D,HIS_211,6.35,-0.09,0,-0.06 4AM1,ASP_238,3.79,-0.84,-0.15,0.99 1RAJ.ASP 339.4.39.0.0.19.0.41 3RE9,ARG_91,12.75,-0.47,0.03,0.68 1YB2,TYR_253,10.44,-0.08,-0.04,0.56 2A6B,ASP 197,1.49,-2.3,-0.72,0.69 3ANJ,LYS 89,10,47,-0,44,0,0,4 2E3C,GLU_271,4.52,0.35,-0.31,-0.02 3MIX,GLU_345,4.61,1.76,-0.85,-0.82 1FQI,HIS_315,5.93,-0.42,0,-0.15 3JSN,ARG_301,11.95,-0.55,0,0 3JV1,ASP_214,3.71,-0.95,-0.34,1.2 2H01,LYS_29,10,-0.7,0,0.2 3NBI,LYS 105,10.33,-0.17,0,0 100X,ARG_199,12.27,-0.23,0,0

3DZ1,GLU_6,4.57,0.37,-0.33,0.03 1XEU,ARG 128,12.39,-0.16,0,0.04 2HP7,ASP_79,4.04,-0.1,0,0.34 2FBQ,ASP_88,3.26,-1,-0.11,0.57 2XHC,LYS_219,10.3,-0.52,0,0.32 2YLF,ASP 198,3.14,-1.06,-0.2,0.6 1Y0K.CYS 34,13.24,-0.09,0.25,4.08 1MJS,GLU_360,4.66,0.22,-0.05,-0.01 3JSN,ASP_223,2.85,-1.61,0,0.66 3AU3,ASP_605,4.32,0,-0.3,0.82 3EGN,TYR 413,11.92,0,0,1.92 3T5B,ARG_365,13.01,-0.85,0.62,0.74 1VJG,CYS_12,11.94,0,-0.16,3.11 2GYZ,ARG_74,12.31,-0.22,0,0.03 2B78.HIS 164.6.66.-0.87.0.62.0.41 3V55.GLU 549.4.23.0.54.-0.38.-0.42 2ZTY,TYR_178,11.68,-0.6,-0.33,2.62 3TIR,ARG_225,12.61,-0.48,0.08,0.51 2RGY,ARG_223,13.83,-3.45,0.06,4.73 3H9W,HIS_94,5.8,-0.65,0,-0.05 1XTD,LYS 143,10.85,-0.23,0.16,0.42 2QV2,HIS_192,6.14,-0.39,0,0.03 3ERF,TYR_131,10.38,0,-0.21,0.59 2NRK.GLU 58,4.69,0.22,0,-0.02 3CS1.TYR 127.11.27.-0.37.0.26.1.4 2B0J,ARG_268,13.2,-0.28,0.56,0.41 1PBV,ASP_131,3.74,-0.2,-0.75,0.89 3G9G,LYS_16,11.36,-0.38,0.85,0.38 3RJZ,LYS 200,10.62,-0.23,0,0.34 2EYI,ASP 199,3.11,-0.6,-0.43,0.34 1MTZ,GLU_4,8.33,3.33,0,0.49 1DZF,GLU_34,4.61,0.48,0,-0.36 2034,ARG 252,12,45,-0,2,0,0,15 1WPA.GLU 452.5.2.0.33.0.0.36 2CWY,TYR_17,10.5,0,-0.46,0.96 2OB5,TYR_118,10.66,-0.2,-0.12,0.96 3F7M,GLU_154,3.88,0.6,-0.45,-0.78 3GA2,GLU_55,4.71,0.37,-0.05,-0.1 3M70,HIS 27,5,79,-1,56,0.83,0.02 2FI9,HIS_11,5.74,-0.39,0,-0.37 1QQL,ARG_11,12.64,-0.21,0,0.35 2DVK.LYS 116.10.34,-0.16.0.0 2C2Y.ARG 223.12.59.-0.46.0.23.0.32 2H2W,ASP_175,3.87,0,-0.09,0.17 3MTT,ASP_455,4.04,-0.06,-0.19,0.48 3ZXY,GLU_71,4.52,0.1,0,-0.08 2BAA,TYR_222,12.62,-0.85,-0.48,3.95 1XAW,ASP_518,2.25,-1.57,-0.53,0.55 3BB7,TYR_270,10.32,-0.03,-0.2,0.56 3M70,ARG 284,12.81,-0.34,0.08,0.56 3G6S,LYS_122,10,-0.29,0,-0.21 1JSX,HIS 198,6.23,-0.6,0.28,0.05 1JT9.HIS 90.5.26.-1.42.0.0.18 3V46,GLU_261,4.49,0.27,0,-0.28 3LD1,LYS_43,10.36,-0.12,0,-0.02 2RGY,GLU_262,4.65,0.24,0,-0.1 1X9G,LYS_62,10.43,-0.07,0,0 3US6,TYR_13,10.38,-0.27,-0.34,0.99 2BV9,ARG_124,12.26,-0.26,0,0.02 1YM5,ASP 289,2.86,-0.85,-0.48,0.38 3B21,GLU 105,4.65,0.15,0,0 2D8N,LYS_170,10.81,-0.15,0,0.45 1FQI,ARG_403,13.57,-0.2,0.9,0.38 3C5V,LYS_358,10.54,-0.17,0,0.2 2V5B,HIS_123,4.61,-1.46,0,-0.42 3N2T,ASP_230,1.92,-2.17,-0.4,0.68 3LJC,LYS_219,10.07,-0.44,0,0.02 4EKU.CYS 89.12.8.0.0.7.3.1 2XMZ,HIS_180,5.78,-0.63,0,-0.1

2V81,GLU_71,4.12,0.33,-0.53,-0.19 1U53,LYS 32,10.2,-0.42,0,0.11 3C6B,LYS 5,10.21,-0.22,0,-0.06 4HDE,ASP_46,2.8,-0.85,-0.53,0.39 2Q07,ASP_259,2.55,-1.34,-0.43,0.53 2XMZ,HIS 168,6.25,-0.24,0,-0.01 1U7U.ASP 319.3.83.0.-0.14.0.17 2PGE,ARG_201,10.84,-1.69,0,0.03 2O8P,TYR_186,10.59,-0.85,-0.15,1.59 2D59,ASP_121,4.04,0,-0.01,0.25 1ZBM,GLU_242,3.92,0.13,-0.71,0 1P4X,ARG_21,12.97,-1.17,1,0.64 3LH5,GLU_526,4.53,0.33,0,-0.3 2XJ4,GLU_12,4.56,0.96,-0.52,-0.38 2RGY,ASP_188,3.58,-0.89,-0.17,0.84 3A7L,GLU 12,4.72,0.37,0,-0.16 1TLV,HIS_100,4.17,-2.34,0,0.01 3HZQ,LYS_92,10.45,-0.05,0,0 2YWJ,GLU_116,3.61,0.34,-0.85,-0.38 2HNG,ASP_120,3.91,0,0,0.11 1PDB.LYS 98,10.62,-0.21,0.0.33 1UAJ,GLU_126,5.13,1.32,0,-0.69 2W1R,ASP_143,2.87,-0.84,-0.43,0.35 3CS1,GLU_151,3.98,0.81,-1.55,0.23 3RLE,ARG 130,12.05,-0.37,0,-0.09 1YB2,TYR_160,9.96,-1.26,0.07,1.15 3M66,TYR_377,13.31,0,0,3.31 1TLV,TYR_94,9.42,-0.85,-0.26,0.54 2E3C,TYR_272,9.95,-0.17,-0.39,0.53 3F1X,ASP_34,3.77,-0.22,-0.29,0.49 1CHD,GLU_169,4.61,0.16,0,-0.04 1P4X.GLU 135.5.3.1.08.-0.47.0.17 3S0A,ASP_117,3.91,0,-0.55,0.66 1JT9,GLU 246,4.78,0.26,0,0.02 1MUF.TYR 98.10.41.0.0.0.41 1Y2Q,GLU_14,3.83,0.37,-0.49,-0.55 4ETX,ARG_199,12.49,-0.16,0,0.15 1YTD,GLU_315,4.67,0.2,0,-0.03 1K95,ASP 134,3.96,0,0,0.16 2B0J,GLU_328,4.61,0.11,0,0 2OJO.LYS 510.10.16.-0.62.0.0.28 1L2F,LYS_20,10.64,-0.34,0,0.49 3GYW,ARG 108,13.01,-0.66,0.52,0.65 1Z9L,ASP 116,4,2,-0.07,-0.15,0.62 3KEY,LYS_457,10.4,-0.12,0,0.03 3A7L,GLU_128,4.2,0.5,-0.38,-0.42 1NFN,ARG_145,10.87,-1.24,0,-0.39 3BWT,ARG 879,12.35,-0.56,0.05,0.37 2Z0M,CYS_191,10.73,0.6,0.22,0.91 2E3C,LYS_438,10.17,-0.48,0,0.15 1S7K,TYR_161,10.28,0,0.07,0.21 3PM2,GLU 113,4.83,0.33,0,0 1YTD,GLU_256,3.41,0.5,-0.97,-0.62 2PLQ,LYS_92,10.9,-0.3,0.33,0.37 3EGN,ARG_421,11.58,-0.84,0,-0.07 2B0J,GLU_70,4.51,0.14,0,-0.13 2H85,GLU 170,4.58,0.08,0,0 1KN3,TYR_176,11.29,0,0.04,1.26 3HVW,GLU_271,4.44,0.29,0,-0.36 1160,HIS_58,6.81,-0.6,0.7,0.22 2FI9,ASP_99,3.82,-0.4,-0.02,0.44 2Z84,TYR_209,10.22,-1.03,5.55E-17,1.25 2W2S,LYS_187,11.22,-0.65,0.42,0.95 2H85,HIS_242,6.58,-0.21,0,0.28 3B21,GLU_120,3.69,0.29,-0.71,-0.39 2H85,ASP_260,3.77,0,-0.31,0.29 2PLQ,LYS_268,10.41,-0.18,0,0.09 1R3D,ARG_40,12.3,-0.2,0,0 3ANJ,CYS_124,12.72,-0.7,0.36,4.07

3EVP.ARG 280,13,28,-0,31,0.62,0.47 1NAR,ARG_135,12.52,-0.42,0,0.44 1Y0K,ASP_28,3.18,-0.57,-0.5,0.46 2FD4,ASP_501,3.9,-0.13,-0.13,0.37 3CGW.ARG 62.12.58.-0.21.0.0.29 10XZ,LYS 198,10.4,-0.11,0.0.02 3IRA,LYS_142,11.52,-0.33,0.85,0.5 1C44,GLU_17,4.8,0.37,0,-0.07 2A1V,LYS_117,10.4,-0.46,0.25,0.11 1T3YLYS 118.8.34.-1.78.0.-0.38 1SIG,ARG_285,12.39,-0.09,0,-0.02 2R57, ASP_324, 3.55, -1.62, -0.11, 1.49 2DVK,GLU_132,4.13,0.58,-0.62,-0.34 3ZTALYS 117.11.15.-0.27.0.53.0.38 1M5I.TYR 133,10.39,0.0.18,0.21 3MEW,HIS_203,6.4,-0.85,0.24,0.51 3M7D,LYS_248,9.71,-0.52,0,-0.27 2BV9,ARG_244,12.23,-0.27,0,0 2G9D.ARG 39.11.7.-0.98.0.0.17 2OSA, ARG_428, 12.54, -1.17, 0.72, 0.49 2BDD,TYR_138,10.1,0,0.03,0.06 2RJD,CYS_403,12.01,0.51,0.6,1.89 3JSN,CYS 109,12.4,0,0.11,3.29 4E9E,TYR 523,12,42,-0,2,0,81,1,81 3HUE,GLU_7,3.73,0.49,-1.23,-0.04 1MML,LYS_257,10.32,-0.2,0,0.02 2OJQ,LYS_541,10.34,-0.16,0,0 3ONT,ARG 38,12.69,-0.29,0,0.49 1PVT,LYS_199,10.87,-0.2,0,0.57 4DIU,ARG_174,12.66,-0.37,0,0.52 2D59,ARG_114,12.95,-0.19,0.26,0.38 3EJG.ASP 29.3.11,-0.93,-0.17,0.41 1MD6.LYS 95,10.83,-0.26,0,0.6 2E3C,GLU_357,4.64,0.11,0,0.03 3RFY,ASP_171,3.81,0,-0.14,0.15 2AH5,HIS_150,5.71,-0.89,0,0.1 1Q46,GLU 37,5.71,3.16,-1.57,-0.38 3LPZ,ARG 230,12,28,-1,15,0,37,0,57 2VAN,GLU_129,4.55,0.26,0,-0.22 3DZ1,ASP_186,2.76,-1.45,-0.16,0.56 2AZP.GLU 270.4.2.0.72,-0.33,-0.69 2BLL/HIS 372.6.15.-0.46.0.0.1 3C38,ASP_241,3.22,-0.85,-0.32,0.59 4ANN,LYS_187,10.43,-0.19,0,0.12 2B0J,LYS_300,10.61,-0.24,0.04,0.31 1LTU,ASP_75,3.96,0,-0.06,0.22 3K8J.GLU 215.4.01.1.51.-1.51.-0.49 3AUF,ARG_46,11.63,-1.09,0,0.21 2PIM,ARG_108,12.38,-0.17,0,0.05 2BCF,CYS_102,10.64,-0.26,0.72,1.18 2CI3.CYS 273,13.26,-0.95,2.1,3.11 2WB8,LYS_584,10.33,-0.17,0,0 3EOD,TYR_125,10.48,0,0.1,0.37 4FZR,ARG_349,12.78,-0.21,0.03,0.45 105T,LYS 450,10.38,-0.11,0,-0.01 2H2Z,GLU_270,4.65,0.47,-0.31,-0.01 1EYH,ARG_139,13.37,-0.39,0.71,0.54 1P6F,GLU 87,4.52,0.33,0,-0.31 1UAJ,HIS_28,6.16,-0.25,0,-0.09 1XWM,TYR_123,13.96,-0.01,-0.09,4.07 3KT9,ARG_42,12.32,-0.18,0,0 1T07,TYR_31,9.95,-0.02,-0.37,0.34 1CBY,LYS_79,10.49,-0.34,0,0.34 1ES5,HIS_135,6.37,-0.18,0,0.05 3V55,ASP_645,3.96,0,-0.23,0.4 3F5D,LYS_146,11.32,-0.39,0.85,0.36 4EZB,LYS_134,10.41,-0.35,0,0.26 3I4T,ARG_153,11.01,-1.6,0,0.11 2RGY,HIS_189,3.07,-2.93,0.18,-0.67

2B61.ASP 205.4.66.0.0.09.0.78 1JKS,ASP_10,4.28,0,0.04,0.44 1ZBS,ASP_235,2.84,-1.13,-0.38,0.56 3N0K,TYR_56,9.94,-0.79,-0.15,0.88 1VSM,ARG 70,12,28,-0.56,0.0.34 2H30.ASP 106.3.27.-0.84.-0.05.0.36 2E3C,ARG_217,12.56,-0.17,0,0.23 3O48, ASP 57, 4, 72, -0.02, 0.3, 0.65 3UAH,ARG_448,11.96,-0.83,0,0.3 2PGE.HIS 235.6.09.-0.27.0.-0.14 1R9W.CYS 240.10.07.-0.15.-0.1.1.32 1J74,ARG_45,13.39,-0.34,0.34,0.9 1WRU,LYS_287,10.55,-0.3,0,0.35 2ZCO,LYS_13,10.16,-0.18,0,-0.17 3F6F,GLU 111,4.52,0.37,0,-0.35 3M16,ARG_308,12.66,-0.58,0.21,0.53 2ILR,LYS_525,10.46,-0.04,0,0 1LZL,ARG_314,12.22,-0.26,0,-0.03 1EDG,ARG_30,11.72,-0.79,0,0.01 3CBN,GLU_54,4.51,0.01,0,0 2P1W,ARG_227,12.57,-0.22,0,0.29 1DOV,ASP_143,3.52,-0.67,-0.21,0.61 2G5X,LYS_44,11.43,-0.3,0.85,0.38 1HF8.GLU 232.4.62.0.24.0.-0.12 2E3C,CYS_348,12.27,0,0.1,3.17 3BA1,ARG_92,13.12,-0.46,0.66,0.42 3BQW,ARG_19,13.38,-0.35,0.57,0.66 3U2R,GLU_102,4.46,0.29,0,-0.33 3CO1,ASP 123,3,91,0,0,0,11 3FNI,ARG_123,13.53,-0.33,0.8,0.56 2GYZ,ARG_8,11.71,-0.47,0,-0.32 4F8A,LYS_673,10.74,-0.22,0,0.46 1YB2.ARG 225,12.36,-0.14,0,0 10IS,HIS_196,5.73,-0.62,0,-0.15 1L2H,TYR_90,11.38,0.61,-0.02,0.79 1NJ4,GLU_318,4.56,0.27,0,-0.21 1HF8,GLU 51,4.09,0.22,-0.6,-0.02 2IXM,GLU_270,4.64,0.15,0,-0.02 3N0K,ASP_53,3.85,0,-0.1,0.16 2FXT,CYS_369,11.87,-0.01,0.07,2.81 3RFY,ASP_284,3.99,-0.61,-0.22,1.01 2EEY,HIS 77,6.48,-0.8,0.78,0 20GO.ASP 537,1.79,-2.48,-0.62,1.08 3ANJ,TYR_266,10.42,0,0,0.42 1R3F,LYS_33,10.25,-0.25,0,-0.01 3DTE,ARG_242,12.75,-0.41,0.1,0.57 2CWY,ARG_90,12.29,-0.23,0,0.03 1F2V,GLU_15,4.92,0.27,0,0.15 1YR6,TYR 221,12,25,0.05,0.14,2.05 2RFA,TYR_89,10.04,0,-0.26,0.31 3JRT,LYS 6,10.32,-0.19,0,0.01 2F4O,ASP 269,3,75,0,-0,39,0,35 1MTZ,HIS_255,6.21,-0.64,0.25,0.1 3DSH,ARG_301,13.27,-0.4,0.77,0.4 1WXQ,GLU_383,4.65,0.15,0,0 2CBE,GLU_236,4.1,0.3,-0.62,-0.07 2NMU,ARG_141,12.5,-0.93,0.55,0.38 1RI6,HIS_300,5.7,-0.66,0.08,-0.22 1TJE,ARG_110,13.47,-0.25,0.81,0.41 1YTQ,ASP_91,2.66,-1.03,-0.6,0.5 3LD1.ARG 228.12.36.-0.25.0.0.1 1BN6,GLU_109,4.58,0.11,0,-0.03 2XJ4,ARG_125,12.06,-0.84,0,0.4 30DJ,GLU_31,4.2,0.41,-0.82,0.12 2G2D,HIS_150,5.93,-0.4,0,-0.16 2A4D,GLU_144,4.83,0.42,0,-0.09 1RZ2,ASP_218,3.83,0,-0.09,0.13 2XWS,GLU_52,3.33,0.54,-1.32,-0.39 1YR6,TYR_28,12.06,0.84,0.54,0.67

1TJE,LYS_200,10.44,-0.06,0,0 3LJC.GLU 7.4.48.0.24.0.-0.25 2A6B,LYS_19,11.44,-0.24,0.79,0.38 3EUR.LYS 103,10,37,-0,15,0,0.02 3JSN,LYS_121,11.13,-0.5,0.49,0.64 2Q99,ARG 9,11.75,-2.47,0,1.72 2F9F,ARG_27,12.82,-0.83,0.68,0.46 1SIG.LYS 289,10.35,-0.17,0.0.02 1NWA, ASP_143, 3.22, -0.78, -0.53, 0.73 2A1V.TYR 83,10,3,0,0,08,0,22 3IL3,ARG 43,12,29,-0.84,0,0.63 2C2Y,ARG_281,12.53,-0.11,0,0.14 3HNX,ARG_81,12.31,-0.32,0,0.13 2FXT.TYR 338.10.48.0.0.1.0.38 1LN4,HIS 16,6.12,-0.13,0,-0.25 1XIP,HIS_95,6.05,-0.93,0.49,-0.01 3LJC,ASP_18,3.78,0,-0.3,0.28 3C38,LYS_80,10.47,-0.12,0,0.09 1VSM,TYR 194,10,27,0,0,13,0,15 3V46,LYS 304,10.91,-0.15,0.13,0.44 3RJZ,ARG_107,13.21,-0.3,0.59,0.41 3T8R,ARG_68,12.32,-0.19,0,0.01 2G5X,HIS_211,6.34,-0.91,0.57,0.18 2PIM,ARG 103,12.49,-0.53,0.27,0.23 4DNU.ASP 34.4.16.0.-0.01.0.37 4F8A,ARG_591,12.74,-0.27,0,0.52 2H8O,GLU_308,3.78,0.45,-0.61,-0.56 3FFM,ASP_68,2.4,-1.6,-0.43,0.64 4EVF,ARG 132,13.35,-0.32,0.75,0.42 1JT9,GLU_83,4.44,0.22,0,-0.28 3VJ8.GLU 83.6.72.2.83.-0.51.-0.11 3I47,GLU_83,4.72,0.2,0,0.03 1UXO,ASP 168,4.14,0,0.16,0.19 306L.GLU 110.4.88.0.34.0.0.05 3GFP,GLU_471,4.75,0.31,0,-0.05 4ETX,TYR_399,12.83,-0.24,0.28,2.79 3H8Y,ARG_62,12.34,-0.16,0,0 1MHN,ASP 117,3.55,-0.66,0,0.41 1R29,GLU_41,4.78,0.33,0,-0.06 105T,ARG_141,13.02,-1.27,0.92,0.88 3GA2,LYS_235,10.39,-0.11,0,0 2YWX,HIS 64,6.12,-0.38,0,0 3H04.GLU 226.4.35.0.43.-0.68.0.11 1MTZ,GLU_27,3.71,0.71,-0.77,-0.73 2JEO,GLU_41,5.01,0.52,0,-0.01 1CHD,LYS_157,9.47,-0.82,0,-0.21 1L2F,GLU_228,2.48,0.82,-2,-0.84 3U2R,ASP 75,3,42,-0.6,0,0,22 1R53,LYS_141,11,-0.78,0.85,0.43 3DHN,GLU_63,3.63,0.27,-0.76,-0.38 1VJG,GLU_174,3.95,1.2,-1.67,-0.08 1L2F,LYS 37,10.09,-0.18,0,-0.22 3I4T,LYS_44,10.55,-0.08,0,0.13 2QZQ,LYS_143,9.58,-0.63,0,-0.29 1MUF,ASP_194,2.92,-1.86,-0.5,1.49 2HRZ,TYR_173,11.62,0.41,0,1.21 1TWU.GLU 40,3.91,0.23,-0.55,-0.28 3RNV,GLU_403,4.64,0.12,0,0.02 20JQ,GLU_511,4.67,0.17,0,0 2P0Y,LYS_79,9.46,-0.85,0,-0.19 1ILW.GLU 56.3.05.0.48.-1.55.-0.38 2QK1,LYS_360,10.62,-0.2,0,0.32 1IDK,TYR_209,12.38,0.69,0.85,0.84 2CI3,GLU_22,5,0.27,0,0.23 3DSH,LYS_333,10.3,-0.14,0,-0.07 3FHF.GLU 76.4.1.0.23.-0.44.-0.18 3T57,GLU_203,5.42,0.79,0,0.15 2Q13,ARG_146,12.46,-0.14,0,0.1 4F8A,LYS_574,10.08,-0.19,0,-0.23

3HQX,GLU_51,4.55,0.17,0,-0.11 1X9G,ARG 3,12.43,-0.11,0,0.04 3N2T,ASP_35,3.82,-0.85,-0.43,1.3 3UPD,HIS_-21,5.61,-0.51,0,-0.38 2ZTY,LYS_156,10.29,-0.21,0,0 3GE9,GLU 115,4.1,0.29,-0.24,-0.46 2APL/TYR 75,11.1.0.0.4.0.7 1Q46,TYR_126,13.96,0,0.37,3.59 3BWT,HIS_688,5.37,-0.93,0,-0.2 3M7G,ARG_42,12.57,-0.1,0,0.17 1AKO,LYS 255,10.18,-0.2,0,-0.12 1WYC, ASP_150, 3.32, -0.8, 0, 0.33 1YTQ,ASP_126,4.07,0,0.03,0.22 4FCU,TYR_186,13.34,0,0.51,2.83 2H80,TYR 316,12,34,0,85,0,26,1,24 109G.HIS 23.4.22.-1.59.0.29.-0.96 2GQV,LYS_32,9.99,-0.51,0,0 2NRR,GLU_467,4.75,0.28,0,-0.03 3LJC,ARG_8,12.56,-0.1,0,0.17 3PU6,GLU 115,4.73,0.22,0,0.01 2CL3.HIS 164.6.38.-0.12.0.0 3KV0,HIS_147,5.28,-1.31,0,0.09 1T95,ARG_35,12.8,-0.84,0.3,0.85 1BKR.TYR 105.10.42.0.-0.09.0.5 2P4D.TYR 140.10.21.0.0.0.21 1Y2Q,TYR_102,9.8,-0.37,-0.62,0.79 2W0G,LYS 276,10.26,-0.24,0.0 4DNU,HIS_235,3.31,-3.21,0.02,0 3GV0,ARG_146,12.46,-0.24,0,0.2 102Y,LYS 139,10,76,-0,53,0,0,79 2EJX,TYR_74,13.32,0,0.19,3.14 3I0C,ARG_312,13.12,-0.56,0.73,0.46 1DTO,CYS 5.9.54,-0.02,-0.01,0.57 1UAJ,GLU_202,3.37,0.42,-0.9,-0.64 2OB5,LYS_60,10.45,-0.2,0,0.15 1XAW,LYS_496,10.5,-0.27,0,0.27 3GW3,ASP_327,3.8,-0.48,-0.21,0.68 3EGN,GLU_485,2.52,1.31,-2.33,-0.96 1QZN,LYS_171,10.45,-0.05,0,0 2R2Y,ASP_63,3.02,-1.3,-0.07,0.59 3M70,TYR_8,10.98,-0.85,0.29,1.54 1WXO,ARG 65,13.02,-0.62,0.46,0.69 3IL3.ASP 236.3.37.-0.83.-0.05.0.45 3H6Q,ASP_61,3.35,-0.52,-0.05,0.12 2PGE,CYS_194,10.77,0,0.01,1.77 3JSN,ARG_250,13.17,-1.53,1.21,0.98 1EYH,ARG_72,12.09,-0.52,0,0.12 3M66.GLU 268.5.29.0.97.0.-0.18 3ERF,TYR_22,11.26,0.51,0,0.74 3EJG,GLU_1,2.27,1.02,-2.54,-0.72 1XDZ,GLU_23,4.92,0.24,0,0.19 3BWT,ASP_707,4.02,-0.64,0.05,0.82 1MTZ,ASP_227,3.75,-0.15,-0.2,0.31 3I47, ASP_242, 3.91, 0, -0.01, 0.12 3C6B,ASP_239,2.18,-1.66,-0.5,0.54 2RH3,GLU_147,5.14,0.57,0,0.08 2H2W,GLU_129,3.47,0.55,-1.01,-0.57 3MIX,GLU_540,4.82,0.28,0,0.04 20JO,ARG 649,11.48,-1.57,0,0.55 1XDZ,HIS_125,6.73,-0.42,0.48,0.18 2CL3,LYS 50,9.52,-1.02,0,0.04 3M7D,ARG 288,12.68,-0.24,0.13,0.3 1PV5,HIS_193,5.64,-2.15,0.51,0.79 1AM2,ARG_26,12.44,-0.06,0,0 1W24,LYS_81,10.36,-0.47,0,0.32 1ZBS,LYS 258,10.42,-0.16,0.0.08 1W7B,GLU_156,3.73,0.6,-0.85,-0.53 3CNU,ASP_13,3.98,0,-0.12,0.3 2RFA,HIS_227,6.44,-0.06,0,0

2G2D,LYS 86,10,42,-0,08,0,0 3M7D,GLU_74,4.15,1.22,-0.69,-0.88 2B3M,LYS_7,10.46,-0.04,0,0 3EVZ,TYR 223,12.82,-0.01,0.04,2.78 1TD6.GLU 284.3.89.1.16.-0.85.-0.93 2B61.GLU 259.4.4.0.23.0.-0.33 3BPV,ARG_110,12.58,-0.36,0.06,0.39 1RL0,TYR_34,11.04,-0.9,0.15,1.8 4F85,HIS_156,5.99,-0.41,0,-0.09 2YT4.ASP 496.4.63.0.-0.17.0.99 3GOZ,HIS_300,6.16,-0.26,0,-0.09 1L3K.TYR 62.13.09.0.0.21.2.87 3RE9,LYS_108,11.45,-0.55,0.85,0.66 105T.LYS 369,10.05,-0.23,0,-0.23 1J33.GLU 195.4.49.0.18.0.-0.19 3GS3,GLU_47,4.55,0.23,0,-0.19 2ILR,ASP_338,3.34,-0.73,-0.3,0.56 1K95,ASP_102,2.82,-1.72,-0.31,1.06 3HUE.TYR 183.10.32.0.0.09.0.22 2EA9,GLU_67,4.31,0.7,-0.83,-0.06 3FRR,ASP_93,3.7,-0.49,-0.01,0.4 3R87, ASP_114, 2.02, -2.16, -0.38, 0.76 2BLL.ASP 384.3.28.-0.82.-0.68.0.98 1H09,ARG 172,13.06,-1.82,0.84,1.53 1NAR,TYR_44,13.42,0,0.84,2.59 1J74,GLU_75,4.68,0.29,0,-0.11 3K8J,LYS_157,10.3,-0.23,0,0.04 20EW,LYS 350,10.45,-0.06,0,0.01 3IDW,HIS_60,5.68,-0.67,0,-0.15 3VJ8,LYS_318,10.28,-0.21,0,-0.01 3R2E,GLU_73,3.85,0.32,-0.9,-0.08 20V2.LYS 45,11.42,-0.22,0.65,0.49 1SOH.GLU 264.4.42.2.78.-1.56.-1.3 3RNV,GLU_341,4.6,0.19,0,-0.09 3V3T,ARG_267,12.57,-0.34,0.17,0.24 2WB8,LYS_470,10.46,-0.04,0,0.01 3M70,LYS 277,10.46,-0.38,0,0.34 3PZ9.ARG 145.12.48.-0.73.0.22.0.5 1Q46,ARG_56,12.45,-0.11,0,0.06 1YR6,GLU_83,3.52,0.54,-0.85,-0.68 1EV8,ARG 126,12,49,-0.06,0.0.04 2EFK.GLU 285,4.64,0.14,0.0 2O4D,LYS_23,10.35,-0.15,0,0 2P65,ARG 40,12,2,-0,3,0,0 3HKX,LYS_140,10.32,-0.23,0,0.05 2B61,LYS_125,10.85,-0.94,0.85,0.44 1X8F,LYS 162,10.05,-0.45,0.0 4EUG,ASP_55,4.04,0,-0.12,0.37 1MUF,HIS_192,6.2,-0.5,0,0.19 1NWA.GLU 70.3.35.1.72.-2.13.-0.74 2CL3.HIS 89.6.63.-0.21.0.01.0.32 307K,GLU_166,4.75,0.31,0,-0.07 1GQE,ARG_159,11.12,-2.67,0.19,1.1 2EFK,GLU_142,4.05,0.26,0,-0.7 1DUP,GLU 42,4.71,0.18,0,0.03 3ERF,TYR_165,9.92,-0.69,-0.6,1.21 3ETV,GLU_148,4.55,0.09,0,-0.04 2QV2,ASP 258,3.29,-0.62,-0.31,0.42 3EVZ,CYS_105,11.68,0.23,0.45,2 1FQI,ARG 310,12.84,-0.88,0.76,0.45 3P28,HIS_217,6.25,-0.28,0,0.04 3H8Y,HIS_79,6.25,-0.25,0,0 2IN0, ARG_88, 12.33, -0.23, 0, 0.07 2IRM,LYS 49,10.38,-0.62,0,0.49 105T.CYS 309.13.19.0.0.47.3.72 1UCH,ASP_38,3.88,-0.19,-0.02,0.3 1L2F,LYS_82,10.43,-0.1,0,0.02 2Q12,ARG_121,13.94,-0.46,1.38,0.52 3D9H,ASP_32,3.87,0,0,0.07

1LTU.LYS 161.10.85.-0.24.0.31.0.28 3ZXY,ARG_107,12.07,-0.43,0,0 1FKM,LYS_452,10.29,-0.18,0,-0.03 1YM5,GLU_203,4.56,0.06,0,0 3A2Z,LYS 142,10.82,-0.4,0.73,0 1YG2.GLU 43.5.02.0.78.0.-0.26 4GCO,LYS_149,10.72,-0.25,0,0.47 1XTZ,ASP_250,2.53,-1.57,0,0.3 4ECC,GLU_101,3.47,0.3,-1.28,-0.05 3BOW.TYR 86.12.11.-0.92.0.28.2.75 2CVB,ARG_178,13.85,-0.87,0.84,1.38 3C6B,CYS_10,10.39,0,0.29,1.1 3M9A,TYR_81,12.21,0.77,0.45,0.98 1T3Y.GLU 119.5.15.0.38.0.0.27 30DJLYS 185.10.15.-0.2.0.-0.16 3B21,ASP_194,4.05,0,0.03,0.22 2FZ4,ASP_96,3.8,0,-0.21,0.21 1W24,HIS_86,7.21,-3.02,0.85,2.88 3M70,GLU_242,4.85,0.16,0,0.2 3C5V,GLU_59,4.52,0.1,0,-0.08 3LQE,ARG_523,12.5,-0.25,0,0.25 1QYI,GLU_303,4.71,0.23,0,-0.02 1TD6,HIS_46,5.99,-0.29,0,-0.21 3NBI,LYS 50,10.46,-0.14,0,0.1 3NBI,GLU_11,4.91,0.46,0,-0.05 2G7O,GLU_88,4.28,0.19,-0.26,-0.14 3ELI,HIS_73,5.83,-0.66,0,-0.01 1XAW,GLU 473,4.19,0.34,-0.65,0 3AUF,ARG 183,12,56,-0,54,0,17,0,44 1Z9L,CYS_41,10.35,0,-0.03,1.39 3FK5,ARG_28,12.72,-0.49,0.37,0.33 1EQ6,GLU_65,5.36,1.33,-0.78,0.3 1R5O.LYS 33,11.54,-0.21,0.74,0.51 200K,GLU_29,4.46,0.21,0,-0.25 2R51,HIS_150,3.47,-2.05,0,-0.98 2CL3,ASP_203,3.95,0,0,0.15 1PDB,GLU 62,4.49,0.12,0,-0.14 4F3J,LYS 222,10.47,-0.07,0.0.04 3BA1,CYS_120,9.78,-0.06,1.39E-17,0.84 1RZ2.GLU 80.4.84,1.23,-0.85,-0.04 1UXO,ASP_49,4.02,0,-0.07,0.29 1LN4,LYS 8,10.94,-0.34,0.19,0.6 1TXD.GLU 785.4.48.2.06.-1.49.-0.59 4E9E,ARG_497,12.79,-0.29,0.24,0.34 3Q9P,LYS_141,10.54,-0.13,0,0.17 1T3Y,ARG_91,12.09,-0.47,0,0.06 3T57,GLU_104,4.76,0.19,0,0.07 2IIA,HIS_44,6.37,-0.28,0,0.15 1ZP2,CYS_214,11.96,0,-0.12,3.09 20PJ,ARG_259,11.57,-1.25,0,0.31 1BYI,ARG 60,12.1,-0.43,0,0.04 1T95.GLU 52.4.99.0.2.0.0.28 2Q5X,HIS_776,5.96,-0.89,0.71,-0.36 2HNG,ASP_66,3.82,0,-0.13,0.15 2QDJ,GLU_53,4.68,1.09,-0.54,-0.37 3HNX,GLU_34,4.05,0.35,-0.54,-0.26 1RI5,CYS 56,11.83,-0.02,0.2,2.64 3CX2,LYS 246,10,43,-0,15,0,0.09 3CGW,GLU_157,4.58,0.23,0,-0.16 2BLL,ASP 631,2.29,-1.4,-0.48,0.37 1X7F,LYS 153,10.56,-0.12,0,0.18 3TMO,HIS_318,6.3,-0.2,0,0 1X91,ARG_148,12.37,-0.13,0,0 4HDE,ASP_121,2.65,-1.41,-0.24,0.49 1WNH,ASP_174,3.99,0,-0.02,0.2 2V5B,ASP_79,3.93,0,0,0.13 3SMD,ARG_11,12.27,-0.71,0,0.49 1SUU,GLU_599,4.07,0.69,-0.65,-0.46 2AH5,HIS_124,6.2,-0.41,0.03,0.08

4FZR.GLU 152,4.61,1.22,-0.47,-0.62 4FZR.GLU 332.4.95.0.76.0.-0.31 3CAX,GLU_308,3.67,0.25,-0.7,-0.38 4DNU.ARG 354,13.03,-0.62,0.69,0.46 1LPL.GLU 141.4.59.0.15.0.-0.06 2YX0,ARG_296,12.73,-0.37,0,0.59 2F8H,ARG_248,11.41,-1.05,0,-0.04 1SI7,ARG_321,13.03,-0.66,0.84,0.35 3JSN,TYR_18,11.86,0.85,0.6,0.41 1AD6,LYS 427,9.92,-0.55,0,-0.03 3CCY,ARG 19,12.84,-0.31,0.1,0.55 2CN1,HIS_57,4.21,-2.32,0.3,-0.27 2CN1.TYR 212.12.59.0.0.2.59 2P0L.GLU 39.5.07.1.2.-0.59.-0.04 3MTT,LYS 503,11.15,-0.19,0.49,0.35 3HVM,CYS_278,12.07,0,0.35,2.71 2P52.TYR 231.13.35.0.0.03.3.32 2G9D,ARG_333,12.4,-0.1,0,0 3UAH,LYS 279,10,43,-0,16,0,0.09 3LJC,LYS_89,10.26,-0.24,0,0 2X4L,LYS_203,10.99,-0.61,0.65,0.45 1NIJ.ASP 283,3.66,-0.44,0.06,0.24 3P28,ASP_69,3.22,-0.82,0,0.24 2IXM,HIS 248,6.98,-0.85,0.85,0.48 1017.GLU 64.4.54.0.15.0.-0.12 2R57,LYS_192,10.47,-0.14,0,0.1 3CNU,GLU_99,3.96,0.34,-0.85,-0.03 2PWQ,ASP_114,4.03,0,0,0.23 2Q13,GLU 364,3.73,0.4,-0.67,-0.5 3JRT,GLU_9,3.73,0.44,-0.85,-0.36 2PWQ,HIS_76,3.76,-3.33,0.6,0 2GEN,ARG_6,12.91,-0.3,0.26,0.45 3KEY,TYR 407,10.67,-0.07,-0.48,1.22 2R4O,ARG 257,12,79,-0,4,0,33,0,35 3HVM,HIS_319,6.77,-1.28,0.81,0.74 1YTD,ARG_242,12.39,-0.15,0,0.05 2CIU,ARG_173,12.66,-0.56,0.14,0.58 2P5D,ARG 30,12.76,-0.15,0.03,0.38 3A0X,LYS_673,11.27,-0.29,0.34,0.71 2H2W,GLU_51,5.68,3.55,-1.7,-0.67 2GZR,CYS_235,9.28,0,0,0.28 2PP6,ASP 37,3.66,-0.25,-0.21,0.32 1MIX.LYS 256,10.32,-0.18,0.0 3IBT,ASP_69,4.2,0,0.04,0.36 200K,GLU_255,5.36,2.5,-0.85,-0.79 2CN1,HIS_203,7.33,-0.37,0.85,0.34 3GFP,LYS_312,10.64,-0.1,0,0.24 3HVW,ASP 236,3.91,-0.05,-0.03,0.18 1UCH, ASP_109, 3.77, 0, -0.23, 0.2 2EEY,ASP_85,3.55,-0.5,-0.02,0.27 3V75,GLU_52,3.34,0.48,-0.98,-0.66 1046.HIS 4.6.52.-0.27.0.0.29 3G9T,GLU_15,4.4,0.2,0,-0.31 1L2F,LYS 300,10,42,-0,11,0,0,02 3EVN, ASP_161, 2.54, -1.38, -0.48, 0.59 3I0C,ARG_241,12.56,-0.3,0,0.34 4ANN.TYR 49.10.16.0.-0.14.0.3 1J74,GLU_59,4.07,0.34,-0.63,-0.14 2JEO,CYS_199,12.11,-0.02,-0.33,3.46 3GMS,ARG_81,12.22,-0.28,0,0 3K8U,HIS 5.6.03,-0.09,0,-0.38 2WB3,TYR_290,10.18,0,0.06,0.12 1EO6.LYS 101.11.47.-0.34.0.85.0.46 2BLL,CYS_536,12.27,0,0.1,3.18 2YYO,GLU_164,4.05,0.21,-0.67,0.01 1V6T.ASP 151.3.73.0.-0.39.0.33 1DVO,LYS_168,12.07,-0.47,1.7,0.34 3UPD,LYS_35,11.25,-0.87,0.85,0.77 2AHE,LYS_85,10.36,-0.37,0,0.23

3EZ7.CYS 220.10.94.0.0.01.1.93 2QEV,GLU_7,6.11,2.37,-0.5,-0.25 3DTE,ARG_226,12.4,-0.1,0,0.01 1QZN,LYS_42,10.13,-0.76,0,0.39 2CBE,ASP_72,4.02,-1.05,0.03,1.24 3LJC,ASP 245,3.83,0,0,0.03 307K.CYS 22.10.76.-0.08.-0.11.1.95 2QOP,GLU_67,5.77,2.97,-0.65,-1.04 3FK5,LYS_71,9.95,-0.71,0,0.16 2AXO,ASP_205,3.34,-0.95,-0.49,0.99 2H14,LYS 46,10.41,-0.15,0,0.06 2FL7.TYR 69,11.69,-0.67,0.67,1.7 1DTO,ASP_22,3.97,0,-0.05,0.22 3M7D,ASP_239,2.14,-1.73,-0.46,0.53 2DVK,LYS_162,10.45,-0.16,0,0.1 1UOH,ASP_37,2.52,-2.7,-0.29,1.69 1DUN,TYR_4,11.73,0.85,0.38,0.5 30DJ,LYS_188,10.33,-0.17,0,0 2AZL,ASP_110,3.88,0,-0.34,0.42 1WNH,GLU_177,4.28,0.9,-0.56,-0.55 2ZO5.HIS 334.6.16.-0.72.0.41.-0.03 1RHS,GLU_222,8.2,3.73,0,-0.03 1R53,ARG_165,12.33,-1.57,0.76,0.64 3D9H.TYR 156.10.36.0.0.36 30A7,ARG 462,12,92,-0.29,0,21,0,5 2QOP,LYS_188,10.46,-0.27,0,0.23 20RX,HIS 173,6,42,-0,16,0,0.08 1RL0,LYS_129,10.28,-0.14,0,-0.07 3QKY,GLU_266,4.63,0.34,0,-0.21 3DHN,LYS 51,9.63,-0.52,0,-0.35 3EVP,HIS_183,6.64,-0.29,0.32,0.11 2IIA,CYS_8,9.32,0,-0.08,0.4 300P.GLU 126.4.65.0.28.-0.13.0 3JSN,GLU 100,4.69,0.28,0,-0.09 3P2F,ARG_25,12.35,-0.44,0,0.3 1SQH,ARG_134,12.73,-0.65,0.44,0.45 1ES9,HIS_170,4.86,-1.09,0,-0.55 3A4C,ARG_481,12.5,-0.05,0,0.06 1AKO,LYS_24,12.12,-0.98,1.7,0.9 1WLY,LYS_22,11.45,-0.28,0.85,0.38 2DVK,GLU_48,4.76,0.35,0,-0.09 3EJC,TYR_160,13.41,0,0.62,2.78 3TMO,TYR 329,10.01,0,-0.23,0.25 2Q34,ARG_192,12.07,-0.8,0,0.37 2AHE,GLU_229,3.07,1.15,-2.07,-0.5 2FM9,LYS_68,10.43,-0.08,0,0.02 3V46,HIS_319,6.19,-0.26,0,-0.05 3H13,ARG 397,12,73,-0,21,0.06,0.39 2NSN,GLU_28,4.54,0.21,0,-0.17 2PPN,ASP_37,3.03,-1.6,-0.33,1.16 1ZBP,TYR_64,10.33,0,0.19,0.14 4DEZ,ARG 21,12.62,-0.32,0,0.43 2G3A,GLU_70,4.57,0.07,0,0 1D2K,CYS_189,12.37,-0.09,-0.11,3.57 2I88, ASP_350, 4.15, -0.03, 0.11, 0.27 2AH5,LYS_76,10.33,-0.46,0,0.29 2ZQ5,ASP_240,2.6,-1.68,-0.49,0.98 3EZ7,GLU_382,4.58,0.35,0,-0.27 3BB7,ASP 277,3.23,-1.32,-0.35,1.1 1X8F,ASP_123,3.95,0,-0.02,0.16 3RFY,GLU_381,7.02,2.37,0,0.15 3FS3,TYR_259,11,0,0.12,0.88 1N81,ARG_131,13.27,-0.8,0.7,0.88 3GS9,GLU_15,4.91,0.3,0,0.11 3V3T,LYS_44,10.46,-0.18,0,0.13 2WOZ,ASP_457,3.89,-0.13,-0.04,0.27 1R7J,GLU_15,2.79,0.8,-2,-0.5 1TXJ,LYS_100,10.48,-0.09,0,0.06 3L3P,CYS_337,8.19,-0.78,-0.44,0.42

1V43,ARG 122,12,41,-1,15,0,36,0,7 2P1W,LYS_142,9.89,-1.54,0.28,0.65 3P28.GLU 226.4.75.0.26.0.-0.01 3B7X,GLU_136,4.74,0.7,-0.22,-0.23 30KY.TYR 118.10.4.-0.09.-0.37.0.86 1WXO,ARG 237,12,39,-0,17,0,0.06 2H30,ASP_151,3.09,-1.08,-0.04,0.41 1XEU,ARG_130,12.29,-0.27,0,0.07 2DG7,TYR_44,13.21,0,0.35,2.85 2R57.ASP 356.4.48.-0.46.-0.06.1.21 1YTD,ARG_37,12.15,-0.28,0,-0.07 2E3I,ASP_93,2.44,-1.49,-0.42,0.55 3I47,ASP_66,3.24,-1.05,-0.18,0.66 2AD1.LYS 9,10.15,-0.35,0,0 2E3C,TYR 242,11,24,0,0,19,1,06 1LFP,LYS_71,9.76,-0.28,0,-0.45 208I,HIS_125,6.03,-0.22,0,-0.24 3RNV,ASP_384,4.19,-0.12,-0.05,0.55 1WPA.CYS 500.10.16.0.0.06.1.1 3PZ9,TYR_45,12.14,-0.85,0.78,2.2 3UPD,TYR_77,10.43,0,-0.2,0.63 2Z84,ARG_215,12.15,-0.47,0,0.12 3O48,LYS 111,10.44,-0.06,0,0 3CE7.LYS 34,10.5.0.0.0 3TMO,LYS_205,10.22,-0.27,0,-0.01 2CVB,ARG_22,13.61,-1.01,1.29,0.83 2D7U,GLU_291,4.95,0.19,0,0.26 1YOY,GLU 62,3.98,0.22,-0.72,-0.02 2NMU,GLU_135,3.85,0.35,-0.8,-0.19 2FGG,GLU_81,4.7,0.2,0,0 1RI6,HIS_18,4.71,-1.83,0,0.04 3PP8,LYS 244,10.98,-0.88,0.85,0.51 2AHE,HIS 111,7.09,-0.4,0.79,0.19 2A1V,GLU_69,4.48,0.22,0,-0.24 4F8A,CYS 619,12.08,-0.54,0.18,3.44 20KT,ASP_74,3.47,-0.64,-0.09,0.41 3LJN,GLU 170,4.98,1.39,-0.68,-0.24 3BA1,ARG 23,13,92,-0,49,1,06,0.86 2IF4,GLU_135,4.63,0.14,0,-0.01 3RKV,LYS_197,10.44,-0.15,0,0.09 1L2F,LYS 330,10.89,-0.59,0.77,0.21 3GMS,ARG 142,12.31,-0.19.0.0 2XJ4,GLU_200,3.95,0.36,-0.36,-0.55 2A6B,GLU 187,2.7,1.68,-3.21,-0.27 2BDV,ARG_175,12.07,-0.6,0,0.17 2EEY,LYS 149,9.99,-0.73,0,0.21 2R51.TYR 253.10.49.0.0.03.0.45 2YWX,TYR_137,11.31,0,0.62,0.69 3B7H,LYS_46,10.47,-0.03,0,0 1NIJ.CYS 118.9.7.0.0.09.0.61 1KCM.TYR 58.11.1.0.0.04.1.06 4EKU,TYR_118,12.9,0,0.79,2.11 3ONH,ASP_518,3.87,-0.05,0,0.12 2HRZ,ARG_307,11.34,-1.23,0,0.05 2B3M,CYS_49,9.7,0,-0.12,0.83 4EVF,ARG_151,13.84,-1.46,1.43,1.37 20KT,TYR_301,13.34,-0.03,1.07,2.29 4DEZ,GLU 168,4.28,0.68,-0.59,-0.3 3M9A,ASP_85,3.94,0,0,0.14 3SMD,GLU_131,4,0.2,-0.7,0 3LQE,ASP_440,4.06,0,0,0.26 3LOD,GLU_70,4.59,0.13,0,-0.04 3B21,HIS_110,6.1,-0.38,0,-0.03 1F2V,ASP 102,2.67,-1.35,-0.38,0.6 3ELI,CYS_106,10.23,0.4,0.34,0.49 1WXF,TYR_206,10.53,0,0.08,0.45 2B0J,ASP_310,2.84,-1.55,-0.03,0.63 1X9G,ARG_126,11.85,-0.92,0,0.28 2Q13,LYS_152,10.47,-0.03,0,0

4DBX.ASP 206.2.78.-1.24.-0.24.0.46 1AK1,TYR_271,10.23,0,0.03,0.2 3FS3,LYS_199,10.05,-0.14,0,-0.32 1J8B,GLU_32,4.02,0.48,-0.32,-0.65 10YI,LYS 189,10.6,-0.1,0,0.21 2IN0.ARG 26.12.25.-0.25.0.0 2FL4,CYS_91,11.67,0,-0.03,2.7 208P.TYR 39.10.35.0.0.12.0.23 3GE9,GLU_202,4.54,0.16,0,-0.11 1L2F,ASP_176,3.26,-0.81,-0.3,0.58 1ZYL,ARG 284,10.74,-3.5,0.7,1.05 1XIP,ARG_119,12.58,-0.11,0,0.19 2CVB,ARG_113,11.89,-0.69,0,0.09 3PP8.GLU 50.4.29.0.29.-0.47.-0.03 1EQ6,GLU 182,2.59,1.33,-2.68,-0.56 4ETX,ARG_435,12.43,-0.07,0,0 1S7K,HIS_167,6.99,-0.43,0.5,0.43 3K8J,TYR_225,12.08,0,0.06,2.02 2G3A,TYR_98,10.84,0,0.08,0.76 1Y2O.GLU 87.4.76.0.17.0.0.09 2P0Y,TYR_271,10.35,0,0,0.35 2IXM,GLU_117,4.66,0.42,0,-0.26 3BCY,GLU_26,4.68,0.15,0,0.02 2F9F.LYS 147,10.61,-0.24,0,0.35 1059,ARG_56,12.67,-0.27,0,0.44 3M3P,ARG_216,12.47,-0.21,0,0.19 1FHL,ASP_84,3.79,-1.56,0,1.55 2B0J,LYS 341,10.45,-0.21,0,0.15 2R57,ASP 204,3.93,0,-0.15,0.28 1SI7,GLU_252,3.8,0.38,-0.71,-0.36 1Y0K,ARG_12,12.32,-0.27,0,0.09 3I82,TYR_185,11.81,0,0.52,1.29 2B6P,HIS 61,6.73,-0.31,0.54,0 3CO1,ASP_26,4.04,0,-0.01,0.25 3CIV,LYS_89,10.32,-0.43,0,0.25 2VGY,ARG_146,12.53,-0.48,0.02,0.5 3UAH,LYS 287,10.31,-0.28,0,0.09 2Z61,ASP_238,3.91,-0.19,0.04,0.26 3RLE,ASP_51,4.14,0,0.03,0.31 2G9D,LYS 299,10,41,-0,13,0,0.03 2AZL,GLU_143,4.97,0.98,0,-0.5 1ZBS,GLU 110,3.21,0.41,-1.53,-0.17 2AH5.TYR 130.11.18.0.0.05.1.12 1YTD,LYS_317,10.18,-0.25,0,-0.08 2Z61,LYS_74,10.33,-0.45,0,0.27 2YX0,GLU_186,4.92,0.32,0,0.09 2P65,ARG_150,13.61,-0.34,1.07,0.38 208P,ASP_101,4.01,0,-0.1,0.31 2YWK, ARG 22, 12, 34, -0, 26, 0, 0, 1 1X8F,LYS 91,11.08,-0.7,0.51,0.76 2D7J,LYS 63,11.42,-0.31,0.8,0.43 2F4Q,ASP_208,2.59,-1.66,0,0.44 3C6B,LYS_200,12.35,-0.96,1.52,1.28 3RLN,ASP_709,2.24,-2.58,-0.11,1.12 2HRZ,LYS_101,11.06,-0.25,0.4,0.41 4EKU,CYS_246,11.69,-0.06,0.07,2.68 1TUL, ARG 38, 12.45, -0.05, 0, 0 2FL7,ARG_194,12.37,-0.3,0,0.17 3PU6,LYS_140,10.14,-0.36,0,0 3I4T,LYS_52,11.25,-0.21,0.59,0.38 3BPV.ARG 128,12.34,-0.17.0.0 2D0A,GLU_274,3.92,0.32,-0.33,-0.57 2CYG,TYR_218,12.22,0,0.15,2.08 1NAR,GLU_24,4.94,0.43,0,0 3LPZ,HIS_132,5.21,-2.09,0.81,-0.01 1FQI,TYR_404,12.16,-0.85,0.27,2.74 1WLY,GLU_208,4.82,0.28,0,0.04 2GEN,ARG_164,12.31,-0.36,0,0.17 3BB7,HIS_176,6.92,-0.88,0.85,0.45

2BQQ,ASP_135,4.08,0,0.06,0.23 1EO6,LYS 208,11.33,-0.37,0.85,0.35 1MN3,ARG_409,13.31,-0.33,0.71,0.43 2WB3.GLU 271.3.42.0.5.-1.58.0 1N81,ASP_111,4.06,0,-0.04,0.3 3VHJ,ASP 81,2.46,-1.64,-0.03,0.33 2FZ4.HIS 123.5.69.-0.69.0.06.-0.19 2ILR.GLU 430.4.71.0.14.0.0.07 3UAH,ASP_294,4.18,0,0,0.38 3N2T.HIS 130.2.65,-2.56,0,-1.29 3LJN.GLU 228,4.63,0.16,0,-0.03 2VC8,ARG_55,13.39,-0.16,0.66,0.39 1FQI,CYS_332,12.57,0,0.07,3.51 2CXA.ASP 54.3.48.-0.7.0.0.38 3RAZ,ARG 57,12.1,-0.42,0,0.02 1J33.GLU 4.4.63.0.13.0.0 3IU5,HIS_51,6.76,-0.43,0.58,0.1 1VSM,LYS_184,10.31,-0.26,0,0.07 10IS,ARG_279,12.89,-0.51,0.37,0.52 2013.GLU 125.4.85.0.52.0.-0.18 3GS9,HIS_170,7.3,-0.43,0.85,0.37 1GQE,HIS_214,6.8,-0.44,0.41,0.33 1MIX,HIS_228,4.36,-2.29,0,0.14 3RJZ,TYR 19,11.47,0.25,0.23,1 102Y.TYR 114.12.79.0.0.19.2.6 2PGX,ASP_7,2.44,-1.83,0,0.47 3B7X,ASP_54,4.01,0,0,0.21 106D,GLU_108,3.58,0.23,-0.75,-0.4 3M7G,GLU_202,4.23,0.4,-0.43,-0.24 2EYI,LYS_103,10.33,-0.54,0,0.36 2ORX.GLU 118.3.84.0.36.-0.81.-0.2 2X4J,LYS_136,11.39,-0.48,0.84,0.53 3CN5.LYS 33,10.54,-0.17,0,0.21 2R57.TYR 286.11.23.0.0.48.0.75 1XTD,TYR_100,9.94,-0.74,0.11,0.57 2AHE,GLU_20,4.51,0.84,-0.85,0.02 3HYQ,ARG_124,12.66,-0.74,0.02,0.87 3DTE,CYS_175,12.15,0,-0.07,3.22 1X8F,CYS_38,12.11,0,0.07,3.04 10TM,LYS_217,10.68,-0.16,0,0.34 1JB3,ASP_29,1.31,-2.5,-0.71,0.72 3U4K,TYR 29,10.33,0,0,0.33 3EX9,LYS_69,11.08,-0.14,0.34,0.37 2AZL,GLU_182,4.91,0.32,0,0.09 2Z0W,ARG_16,12.47,-0.03,0,0 1RAJ,TYR_313,10.82,-0.8,0.42,1.2 1SBX,CYS_150,10.17,-0.17,0.04,1.31 1F2V.HIS 43,5.25,-1.05,0,-0.2 1SUU,GLU_661,4.81,1.38,-0.9,-0.17 2FBQ,LYS_151,10.44,-0.06,0,0 4H4J,TYR_144,10.29,0,-0.04,0.32 2CBE,ARG 254,11.13,-1.96,0.0.6 3L7N,ASP_44,3.75,0,-0.3,0.25 1WXF.GLU 259,4,58,1.47,-0.41,-0.98 2YWJ,HIS_15,6.22,-2.25,0.49,1.49 3O48,HIS_106,6.01,-0.24,0,-0.25 4FZN,ARG 37,12,43,-0.07,0,0 3UAH,LYS_428,10.29,-0.35,0,0.14 2B6P,ARG_187,10.17,-3.21,0,0.87 3M7G,GLU_215,3.91,2.49,-0.93,-2.14 20ZO,ASP 88,3,48,-0,74,-0,15,0,56 2IRM,HIS_329,6.15,-0.26,0,-0.1 4E6S,ARG 4,12,49,-0,1,0,0,09 3CQ1,LYS_95,10.68,-0.14,0,0.32 3GE9,GLU_233,4.82,0.25,0,0.07 1R6Y,ARG 9,12.47,-0.25,0.0.23 1FKM,CYS_428,13.22,0,-0.04,4.26 4FZR,ASP_164,3.75,-0.6,-0.09,0.63 2X4L,ASP_193,3.96,0,-0.02,0.18

2F4Q,ASP_70,1.91,-2.28,-0.19,0.58 3RJX.GLU 93.3.88.0.21.-0.83.0 2Q99,GLU_263,4.51,0.11,0,-0.1 4FH3.TYR 178,13.21,-0.81,0.01,4 2B61,ARG_350,12.16,-1.19,0.08,0.77 3A7L,GLU 19,2.9,0.54,-1.41,-0.72 1XIP.CYS 93,12,81,0,0,64,3,17 1XKR,ASP_163,4.33,-0.28,0.01,0.78 3FS3,ARG_82,10.97,-2.11,0,0.58 3A0X,LYS_625,9.99,-0.59,0,0.08 3G9T,ARG 158,12.92,-0.9,0.75,0.56 1YM5,GLU_30,4.49,0.12,0,-0.13 2FC3,LYS_74,10.43,-0.07,0,0 3EX9,ARG_159,12.46,-0.04,0,0 1NAR.GLU 46.4.55.0.05.0.0 2FM9,ASP 64,3.94,0,-0.23,0.37 1SQW,GLU_8,2.36,0.92,-2.65,-0.4 2EFK,GLU_88,3.96,0.6,-0.73,-0.41 3Q1C,ASP_268,3.79,0,-0.14,0.13 1ZBS,TYR_64,11.29,0,0.22,1.06 3UAH,TYR_499,10.42,-0.01,0.08,0.35 105T,ASP_205,3.91,0,0,0.11 1ZBM,HIS_58,4.51,-2.23,0.69,-0.45 3H04, ASP 54, 2.97, -0.79, -0.38, 0.35 1NJ4,ARG 174,13,38,-0.87,0.8,0.94 1ZKZ,LYS_68,10.43,-0.07,0,0 3RLE,HIS 132,7.32,-0.38,0.85,0.35 2V81,ASP_19,2.82,-1.3,-0.02,0.34 1WYC,GLU_74,5.13,0.48,0,0.15 1RZ2,ASP 88,4,25,0,0,14,0,31 3RJX,ARG_304,11.8,-0.54,0,-0.16 2NRR,TYR_396,9.93,-0.83,-1.02,1.77 2W0G.LYS 224,10.4,-0.43,0.0.34 1J33,ARG 10,12.41,-0.25,0,0.17 3DB9,GLU_135,4.74,0.23,0,0.01 2IDC,ASP_77,4.38,0,0.33,0.25 2C2Y,CYS_91,11.17,-0.16,-0.43,2.77 2V5B,ARG_221,12.59,-0.22,0,0.32 105T.GLU 385.4.32.0.28.-0.45.-0.01 3I47,GLU_225,4.57,0.07,0,0 20JQ,GLU_453,4.65,0.33,0,-0.18 3BA1,ARG_249,13.94,-0.55,1.19,0.8 10QH,LYS 71,10.45,-0.26,0,0.22 2Q99,LYS_177,10.36,-0.09,0,-0.06 2D2S,ARG_551,12.31,-0.32,0,0.12 1RZ2,ARG_243,12.15,-1.3,0,0.95 2P0Y,CYS_227,12.37,-0.91,0.45,3.84 1UXO.ASP 147.3.18.-0.63.-0.41.0.42 1QQH,ARG_156,13.67,-0.44,1.2,0.42 1WXQ,LYS_375,10.42,-0.08,0,0 1XAW,LYS_462,10.85,-0.13,0.05,0.44 1MHN.CYS 98,11.17,0,0.26,1.91 1SJY,ASP_89,3.25,-0.93,0,0.38 3JV1,GLU_74,4.58,0.08,0,0 3G9B,LYS_123,10.9,-0.22,0,0.63 2YWX,GLU_139,3.24,0.33,-0.83,-0.76 2CN1,LYS_121,10.53,-0.11,0,0.15 3M7D,HIS_200,4.68,-2.57,0.85,-0.1 3CGW,ARG_155,12.49,-0.16,0,0.15 2Q12,ARG_20,12.31,-0.27,0,0.08 3EVP,ARG 81,13.03,-0.27,0.33,0.47 2NSN.GLU 81.4.03.0.23.-0.71.0.01 2CVB,LYS_176,10.21,-0.84,0.04,0.51 3U0V,CYS_98,11.16,-0.3,-0.1,2.56 2GKG,GLU_23,3.83,0.43,-0.83,-0.26 1R3D,ARG_142,12.86,-0.55,0.59,0.32 2B78,LYS_92,10.45,-0.07,0,0.01 3CAX,ASP_333,2.32,-1.49,-0.44,0.45 1MUF,GLU_254,4.77,0.25,0,0.02

2B0A.CYS 122.12.75.0.0.02.3.73 3QAV,ARG_177,11.81,-0.76,0,0.06 3LPZ,ARG_84,12.85,-0.29,0.39,0.25 3RFF,GLU_56,2.32,0.62,-2.08,-0.72 1UW7,GLU 3,4.63,0.13,0,0 2VGM,ASP_38,3.83,0,-0.24,0.26 10LR,ARG_97,12.11,-0.7,0.04,0.27 2AD1,GLU_84,6.32,4.33,-2.52,0 2R0S,HIS_265,4.56,-1.94,0,0 1X7F,TYR 289,11.92,0.3,0.29,1.34 10LR,TYR_132,9.95,0,-0.18,0.13 2BT8.CYS 182.9.52.-0.21.0.12.0.62 3N2T,ASP_322,2.93,-1.14,0,0.27 3JV1.GLU 100.4.87.0.54.0.-0.17 1R3F.GLU 300.5.13.0.26.-0.08.0.45 3E7P,LYS_142,10.67,-0.21,0,0.39 3F5D,GLU_30,4.6,0.08,0,0.03 3CAX,LYS_463,10.42,-0.09,0,0.02 3A4C.GLU 468.4.62.0.14.0.-0.02 1TXD,ASP_914,3.94,0,-0.08,0.22 3TMO,LYS_219,10.78,-0.32,0.41,0.2 3IDW,CYS_12,11.67,0,0.08,2.59 1TP6.LYS 52.9.85.-0.72.0.0.07 3HVW,ARG 265,12,4,-0,16,0,0.07 208P,GLU_93,4.63,0.13,0,0 4H86,GLU_129,4.11,0.62,-0.75,-0.26 2XHC,TYR_173,11.51,0,0.37,1.14 1ZYL,TYR 252,13.67,-0.09,0.23,3.53 2RIK,LYS_37,11.03,-0.76,0.76,0.53 3GE9,LYS_164,10.52,-0.12,0,0.14 1YTD,TYR_156,11.06,0,-0.35,1.42 1XTZ.HIS 222,4,59,-1,42,0,-0.5 3EJG.GLU 155.4.01.1.25.-1.68.-0.06 1PV5,HIS_90,6.37,-0.42,0,0.3 3M7D,ASP_75,3.21,-0.89,-0.15,0.45 1LTU,ASP_3,3.18,-0.89,0,0.26 1UOH,TYR 160,10.16,0,0.06,0.11 1SBX.ARG 132,12,47,-0,13,0,0,1 3IDW,GLU_33,4.68,0.29,0,-0.12 2VGM,GLU_302,5.38,0.82,-0.11,0.16 1ES5.TYR 258.10.44.0.0.04.0.39 3A0X,ARG 627,12,72,-0,23,0,0,45 3DB9,ASP_218,2.9,-1.43,0,0.53 4E6S,LYS 46,10.67,-0.09,0.0.26 1YB2,ARG_65,12.65,-0.59,0,0.73 2Q34,LYS 235,10.57,-0.18,0,0.24 1Y2O,LYS 16,10.63,-0,1,0,0.23 2CXC,GLU_73,3.6,0.67,-1.47,-0.09 1AK1,GLU_145,4.68,0.46,0,-0.28 1WJG,HIS 37,5,33,-1,85,0,52,0,17 2ATR.ARG 136.12.28.-0.22.0.0 3C5V,GLU_290,4.89,0.76,0,-0.37 2RIK,GLU_154,4.46,0.44,-0.09,-0.39 1W24,LYS_23,10.07,-0.47,0,0.04 2AD1,GLU 157,4.07,0.34,-0.82,0.05 2Z0M,GLU_19,2.96,1.25,-2.3,-0.49 4ACJ,ASP_749,4.24,0,0.23,0.21 3OBS,LYS 101,10.43,-0.11,0,0.03 1NFN,GLU_70,3.1,0.48,-1.37,-0.5 3MTT,GLU 555,4.51,0.21,0,-0.2 3DZ1,ASP_294,3.01,-1,-0.45,0.67 4DNU,GLU_170,3.96,0.17,-0.34,-0.37 3LJC,TYR_22,12.92,0,0.05,2.88 3DTE, ASP 132, 3.15, -0.57, -0.53, 0.44 2BDV,LYS_188,10.05,-0.57,0,0.12 2B02,GLU_390,2.89,0.52,-1.68,-0.45 1JB3,HIS_53,6.46,-0.21,0,0.17 2ZQ5,GLU_38,3.26,0.42,-1.52,-0.13 3NR5,GLU_55,4.57,0.61,0,-0.56

20EW.ARG 70.11.67.-0.97.0.0.14 301C.CYS 325,10.51,-0.03,-0.25,1.78 2D2S,ASP_677,2.47,-0.86,-0.69,0.23 2QOP,ARG_13,12.33,-0.54,0,0.37 2Z84,HIS 24,6,42,-0.08,0,0 1DZF,LYS 171,10,44,-0.06,0.0 1RHS,ARG_158,11.87,-0.65,0,0.02 3GA2,GLU_225,4.09,0.65,-0.55,-0.51 3BCH,LYS_166,10.31,-0.12,0,-0.07 2E3S,ARG_405,11.76,-1.08,0,0.34 3CS1.GLU 32.4.3.0.21,-0.1,-0.31 4GCO,LYS_171,10.32,-0.17,0,-0.01 1ES9,ARG_198,12.67,-0.37,0,0.54 3IO0,ARG_148,11.99,-0.7,0,0.2 3RNV.TYR 390.9.99.0.-0.14.0.14 3CGW,GLU_84,4.06,0.96,-1.03,-0.37 2CI3,GLU_265,3.67,2.58,-2.26,-1.15 4ETX,TYR_354,9.81,-0.01,-0.48,0.3 3CO1,HIS_18,6.55,-0.17,0,0.21 1RHS,ARG_205,12.36,-0.3,0,0.16 1TXJ,LYS_2,12.63,-0.39,1.32,1.2 10I7,GLU_97,4.84,0.23,0,0.11 1SJY,ARG_14,12.23,-0.38,0,0.11 1C3K,GLU 75,4.14,0.21,-0.71,0.14 1PGV,CYS_227,10.22,-0.07,-0.09,1.39 2BDV,GLU_77,3.74,0.23,-0.52,-0.47 1ZBS,GLU_129,4.71,0.16,0,0.04 3N0K, ASP_26, 3.75, -0.02, -0.19, 0.16 1SI7,ASP 314,2.65,-1.64,-0.08,0.57 1N81,LYS_200,10.47,-0.23,0,0.2 2QEV,GLU_114,5.57,2.79,-0.81,-0.91 3ZRI,ARG_3,12.53,-0.11,0,0.16 3IV4,TYR 53,10.21,-0.45,-0.2,0.85 2AZL,GLU_237,4.66,0.4,-0.22,-0.02 2CWC,ARG_133,11.49,-2.87,0.02,1.84 3M7G,ARG_172,12.67,-0.28,0,0.46 1RAJ,CYS 418,10.66,-0.8,0,2.46 1RSS,ARG_78,12.28,-0.22,0,0 2Q98,TYR_96,9.7,-0.52,0.06,0.17 3Q1C,ASP_46,3.68,0,-0.34,0.21 4DEZ,TYR_164,10.45,0,-0.07,0.53 1JSX,LYS 100,10.27,-0.11,0,-0.12 1X9G,LYS 143,10,19,-0,1,0,-0,22 3EVN,GLU_123,6.08,5.6,-2.01,-2.01 2FM9,LYS_228,10.64,-0.2,0,0.34 1LZL,ARG_52,12.21,-0.48,0,0.18 3ETU,GLU_297,4.58,0.18,0,-0.1 3M70,GLU_247,4.4,0.27,0,-0.37 3GG6.GLU 56.4.91.0.38.0.0.03 1SQW,CYS_153,10.63,0,-0.12,1.75 3GV0,ASP 222,3.77,-0.15,-0.04,0.17 1WP5.LYS 243.10.47.-0.03.0.0 3U0V,HIS_184,6.62,-0.71,0.42,0.42 2Q07,ARG_343,13.56,-0.3,0.76,0.61 3RJX,TYR_207,11.27,0,0.29,0.98 100X,ARG_178,12.4,-0.27,0,0.17 1TWU,TYR_112,10.24,0,0,0.24 2EYI,ARG_232,12.42,-0.34,0,0.26 3JV1,GLU_216,4.3,0.61,-0.79,-0.02 3S0A,GLU_20,4.94,0.4,0,0.04 2YX0.GLU 99.4.67.0.18.0.-0.01 1R53,GLU_171,4.89,0.13,0,0.27 1EW4,ARG_8,12.56,-0.12,0,0.18 3EAZ,TYR_145,10.98,0,0.37,0.61 4FH3,GLU_284,3.94,0.22,-0.32,-0.46 3QAV,GLU_79,4.88,2.59,-1.49,-0.72 1NWA, ASP_87, 4.16, -0.85, -0.13, 1.34 3KB5,LYS_389,10.27,-0.15,0,-0.09 1LPL,GLU_228,4.54,0.04,0,0

3P28.GLU 224,4.71,0.22,0.0 3N0K,GLU_116,4.67,0.11,0,0.06 3GA2,ASP_111,3.3,-1.42,-0.22,1.15 1T6L,ARG 28,12,36,-0,48,0,19,0,14 1NIJ,ASP_79,3.39,-2.02,-0.36,1.98 1ILW,GLU 161,4.46,0.19,-0.29,0.06 3LJN.GLU 121.4.52.0.02.0.0 1R53.LYS 212.10.44.-0.06.0.0 1NFN,ARG_158,13.32,-0.34,0.69,0.46 1YTD.LYS 202.10.4.-0.14.0.0.04 1RI6.ASP 263.1.98.-2.21.-0.05.0.44 3CAX,LYS_437,11.27,-0.31,0.43,0.65 2P65.GLU 109.4.5.0.0.0 2ILR.ARG 343.12.11.-0.4.0.0.01 1NWA,CYS 154,10.01,-0.54,0.21,1.34 3IO0,GLU_145,4.26,0.31,-0.52,-0.03 2IN0, ARG_7, 12.68, -0.34, 0.03, 0.49 1H09,LYS_250,10.48,-0.18,0,0.17 2ZO5,ARG 7,12,73,-0,14,0,0,37 3M16,GLU_78,4.5,0.62,-0.42,-0.2 1YB2,LYS_199,10.29,-0.21,0,0.01 3US6.GLU 54.4.6.0.28.0.-0.18 3LMO,LYS_91,10.5,-0.3,0.01,0.29 2YX0,LYS 259,10.31,-0.29,0,0.09 3LOD, ARG 102, 12, 59, -0, 4, 0, 0, 49 1SNT,ASP_131,1.18,-3.06,-0.31,0.76 4GA2,ARG_120,12.08,-0.6,0,0.18 1X91,LYS_65,9.98,-0.31,0,-0.21 1YTQ,GLU 62,3.36,0.54,-1.3,-0.38 1Q5Z,ASP_540,4.12,0,0.08,0.24 2EDM,LYS 198,10.4,-0.1,0.0 1EV8,HIS_255,6,-0.53,0.5,-0.47 3I4T,LYS 75,10.35,-0.23,0,0.08 1MJS.CYS 393,11.55,-0.67,-0.09,3.33 3EJC,HIS_164,6.76,-0.08,0,0.35 2D7J,ASP_7,3.86,-0.77,-0.13,0.97 2H30,LYS_42,10.41,-0.14,0,0.05 2GAU,GLU 24,4.69,0.11,0,0.08 1059, ARG_240, 12.19, -0.19, 0, -0.13 3BZT,ASP_344,4.58,0.23,0.34,0.21 1QQE,TYR_66,11.6,0,0.59,1.01 307K,HIS 42,6.29,-0.16,0,-0.05 2R4O,LYS 204,11.18,-0.62,0.85,0.45 2F8H,ARG_353,12.5,-0.18,0,0.18 1JSX,ASP_18,3.8,-0.13,0,0.13 2B2H,ARG_111,9.78,-3.38,0,0.67 3EVN,GLU_147,4.68,0.17,0,0.01 2VAN.GLU 329,4.54,0.27,0,-0.25 1HF8,ARG_139,12.27,-0.23,0,0 4FH3,TYR_366,10.17,-0.03,-0.09,0.29 3RE9,GLU_104,4.6,0.14,0,-0.05 2P65.ARG 17.12.27.-0.33.0.0.1 3A7L,ASP_68,4.38,0,0.26,0.32 3JZN.ARG 169.12.97.-0.42.0.16.0.74 3G9T,ASP_248,3.48,-1.31,-0.41,1.4 4ANN,GLU_43,3.82,0.38,-0.76,-0.31 3UPD.GLU 300.8.36.4.83,-1.51.0.54 3A4C,HIS_550,6.22,-0.21,0,-0.07 2E3H,LYS_277,10.15,-0.27,0,-0.08 3H13,HIS_287,6.38,-0.15,0,0.03 3CSR.ARG 147.12.69.-2.46.0.63.2.03 3JZ9,LYS_385,10.68,-0.08,0,0.26 2FZP,ARG_270,13.88,-0.17,1.17,0.38 2W2S,GLU_195,4.61,0.09,0,0.02 4F8A,TYR_666,10.16,0,0.04,0.12 3G9T.GLU 23.4.32.0.25.0.-0.43 2P5D,GLU_139,4.74,0.31,0,-0.07 3HVW,ARG_268,12.67,-0.16,0,0.33 2VAN,LYS_220,10.43,-0.1,0,0.03

2QZQ,HIS_110,4.61,-1.36,0.01,-0.54 3UPD,HIS -18,5.99,-0.14,0,-0.37 4FCU,ASP_89,3.44,-0.77,0.12,0.29 1MUF.TYR 123,11,79,0,0,14,1.65 20BI,ASP_165,2.16,-1.7,-0.6,0.66 3U4K,LYS 106,10.42,-0.08,0,0 2YX0.CYS 58.9.2.-1.82.-1.17.3.19 3QAV,ASP_65,3.83,0,-0.07,0.1 1RI6,GLU_197,3.78,2.55,-0.64,-2.64 1X1E,ASP_56,4.02,0,-0.22,0.44 3ASA,LYS 236,9.43,-0.75,0,-0.32 1SOW, ASP 87, 4, 29, 0, 0, 0, 49 20BI,LYS 127,10.32,-0.16,0,-0.02 3RLN,GLU_739,4.99,0.58,0,-0.09 20BI,ASP_30,3.53,-0.36,-0.32,0.41 1ZCU.TYR 186.12.58.0.83.0.52.1.24 3N0K,ASP_75,2.8,-1.72,-0.26,0.99 3H9W,ARG 63,11,45,-1,34,0,0,3 1DZF,LYS_24,10.11,-0.47,0,0.08 3GEC,HIS_493,3.12,-3.15,0,-0.22 1S7K,LYS 133,10,17,-0,41,0,0,07 1R9W,TYR_329,10.05,0,-0.2,0.25 3CS1,LYS_178,11.24,-0.24,0.59,0.38 2P4D.LYS 53,10.27,-0.24,0,0.01 3M7G,HIS_246,5.65,-1.67,0.83,-0.02 3TOW,LYS_144,11.4,-0.47,0.85,0.52 1ZYL,GLU_267,4.63,1.36,-0.62,-0.61 2AD1,ARG_289,12.45,-0.05,0,0 1Q5Z,LYS_586,10.3,-0.35,0,0.17 1XTD.GLU 144.4.79.0.27.0.0.03 100X,HIS_174,3.43,-2.43,0,-0.64 1V43,GLU_63,5.21,1.01,0,-0.31 2GZO.GLU 67.4.54.0.09.0.-0.06 1XEU.LYS 120.10.07.-0.27.0.-0.16 2GZR,ARG_97,12.05,-0.6,0,0.14 3T5B,ARG_337,12.95,-0.42,0.72,0.17 2H30,HIS_36,6.24,-0.15,0,-0.1 1I60,TYR_100,12.47,0,0.58,1.9 1DZF,ASP_182,3.52,-0.96,-0.24,0.91 20KT,ASP_227,3.44,-0.69,-0.02,0.34 4F85,GLU_150,4.51,0.29,0,-0.28 2YX0,GLU_138,2.55,0.87,-1.5,-1.33 4ETX,GLU 363,5.18,1.01,0,-0.34 1TD6,ASP_59,2.92,-1.25,-0.06,0.44 1PGV,ARG_230,13.93,-0.39,1.16,0.65 1R29,GLU_115,4.84,0.23,0,0.11 3GFP,LYS_454,10.57,-0.11,0,0.19 1WRU,ARG 330,12.96,-0.55,0.31,0.7 1RSS,LYS_138,10.14,-0.9,0,0.53 3MTT,ARG_539,12.32,-0.45,0,0.27 4EKU,LYS_334,10.73,-0.32,0.09,0.46 1MD6,GLU 86,4.67,0.23,0,-0.07 2QVT,TYR_42,9.66,-0.67,-0.11,0.43 1FO9,GLU_104,4.55,0.05,0,0 3BZT,LYS_254,10.53,-0.12,0,0.15 3PP8,HIS_267,6.56,-0.82,0.85,0.03 1AM2, ASP_158, 2.94, -1.17, -0.48, 0.78 3S0A, ASP_30, 3.7, -0.59, 0.05, 0.44 3IL3.GLU 218.4.56.0.86.-0.65.-0.16 1XFK,LYS_60,10.29,-0.1,0,-0.11 1T95,GLU 197,3.42,0.44,-1.52,0 3COU,HIS 133.6.11,-0.39.0.0 2B61,ARG_260,10.67,-1.66,0,-0.16 1UAJ,ASP_44,2.07,-2.09,-0.23,0.61 1Q46,HIS_139,4.66,-1.64,0,-0.19 1AIL.ARG 19.12.81.-0.76.0.64.0.42 1T3J,HIS_735,6.79,-0.19,0.49,0 3VJ8,TYR_139,12.87,0.83,0.49,1.56 3Q6L,GLU_117,4.16,0.43,-0.25,-0.52

1T3J.GLU 723.4.64.0.14.0.0 1GQE,LYS_302,10.61,-0.21,0,0.32 3RLE,ARG_21,12.26,-0.32,0,0.08 3BB7, ASP_261, 2.76, -1.29, -0.07, 0.32 2RGY.HIS 167,6.44,-1.16,1.04,0.06 3GFP.LYS 443,10,46,-0,04,0,0 2IRM,HIS_194,6.89,-0.16,0.51,0.04 1FO9,ARG_380,13.34,-0.26,0.77,0.33 3VHJ,LYS_63,11.32,-0.41,0.85,0.38 10YLCYS 18.12.66.-1.07.1.98.2.75 2IF4,ASP_87,3.02,-1.05,-1.13,1.41 2YWX.GLU 44,3.53,0.26,-0.85,-0.38 1ES9,GLU_60,4.56,0.15,0,-0.1 2RIK.HIS 171,6.1,-0.36,0,-0.05 2C2Y,ASP 68,4,13,0,-0,58,0,91 1SUU,GLU_590,4.54,0.25,0,-0.21 2GEN,GLU_140,4.81,0.31,0,0 3ULX,ARG_109,12.38,-0.14,0,0.02 4GA2.GLU 102.5.25.1.05.0.-0.29 10GL,ARG_267,14,-1.11,1.23,1.37 2Q34,HIS_240,4.51,-2.19,0.83,-0.63 3RLN,LYS_762,11.61,-0.47,0.83,0.76 3I47.ASP 84.4.49.-0.83.0.04.1.48 2B0J.GLU 83.4.86.0.17.0.0.2 3JSN,GLU_88,3.71,0.31,-0.85,-0.25 3CIV,ASP_271,3.83,0,-0.18,0.21 1SJY,ARG_75,12.59,-0.32,0,0.41 2RJD,GLU 429,4.77,0.17,0,0.11 1N81,ASP_59,3.29,-0.74,-0.37,0.6 2XHC,GLU_16,4.34,0.52,-0.15,-0.53 100X,LYS_59,10.08,-0.42,0,0 20JO.GLU 547.4.59.0.09.0.0 1MIX.LYS 295.10.41.-0.92.0.47.0.35 1XFK,HIS_288,5.77,-0.32,0,-0.42 2AZL.GLU 12.4.11.0.99,-0.79,-0.58 4DNU,LYS_225,10.79,-0.22,0,0.52 2JKF,ARG 108,12.32,-0.41,0,0.23 1RWZ,ASP 209,5.04,-0.58,0.17,1.65 2YX0,LYS_30,10.37,-0.39,0,0.26 3GEC,GLU_472,4.49,0.37,0,-0.39 2RJD,ASP 418,3,94,-0,18,0,0,32 1FO9.LYS 126.10.78.-0.29.0.0.57 1QQE,LYS_159,10.01,-0.89,0,0.4 2XHC,LYS 185,10.22,-0.17,0,-0.11 2NRK,ASP_64,2.01,-2.28,-0.45,0.94 1WXF,ARG_123,13.58,-0.29,0.89,0.48 2ZTY.GLU 93.4.75.0.14.0.0.12 1BKB,GLU_77,3.76,0.28,-0.74,-0.29 3FRR,TYR_173,10.4,0,-0.16,0.57 2R2Y,LYS 62,10.65,-0.25,0.0.4 1ILW.LYS 41,10.47,-0.19,0.0.16 2EFK,LYS_253,10.42,-0.08,0,0 30AV,LYS 42,10,28,-0,22,0,0 2GZR,ARG_225,13.14,-0.94,0.71,0.87 2RJD,CYS 390,11.43,-0.89,-0.42,3.73 2GEN, ARG_172, 12.46, -0.04, 0, 0 2CXA,ARG_161,12.31,-0.3,0,0.11 1WRU,GLU 34,4.38,0.56,-0.55,-0.13 3MTT,ARG_508,12.83,-0.35,0,0.68 1ANU,TYR 21,10.36,0,0.02,0.33 2P52,TYR_100,10.19,0,-0.02,0.22 1PBV,LYS_108,9.66,-0.89,0,0.05 1R9W,CYS_311,9.02,-0.37,-0.29,0.68 1SJY,GLU 32,2.88,1.1,-2.01,-0.71 4FZR,ARG_214,11.96,-1.07,0.02,0.51 2IRM,TYR_366,10.43,0,0.31,0.12 3LPZ,LYS_150,10.53,-0.14,0,0.17 1R7J,LYS_23,10.66,-0.43,0,0.59 3O16, ARG_59, 11.63, -1.01, 0, 0.14

3CRM.ARG 93.11.95.-0.22.0.-0.33 3EJC,ARG_118,13.31,-0.33,0.82,0.31 2GAU,ASP_30,2.9,-0.98,-0.52,0.6 1DTO,ASP_31,1.43,-2.08,-1.36,1.07 10YI.GLU 102,4.6.0.33,0,-0.23 20KT,LYS 65,12,3,-0,9,1,7,1,01 3H5T,GLU_342,4.62,0.18,0,-0.06 1JKS,ARG_263,12.36,-3.24,1.57,1.53 3GE9,GLU_33,5.44,2.12,-1.25,0.06 3G9T,LYS_11,10.5,-0.12,0,0.13 208P.ASP 66.4.12.0.-0.13.0.45 3DZ1,LYS_269,11.63,-0.4,0.74,0.78 3FFM,ASP_128,3.52,-0.58,0,0.3 10XZ.ARG 258.12.18.-0.37.0.0.04 100E.CYS 140.10.98.0.-0.63.2.61 4EZB,GLU_188,4.7,0.17,0,0.04 2ZTY,LYS_19,10.54,-0.12,0,0.16 3L7N,GLU_12,7.92,3.34,0,0.09 2W2S,CYS 62,9.81,0,0.12,0.69 3CIV.ARG 320,12.62,-0.09,0,0.21 4FZN,ASP_235,3.45,-0.71,-0.12,0.49 3V75,ASP_15,4.18,0,-0.02,0.4 3C2E,ARG_194,13.38,-0.54,0.75,0.66 2GS5,ASP 57,3.78,0,-0.18,0.16 2VGM,ASP_274,4.06,0,-0.09,0.35 3R2E,LYS_106,10.44,-0.1,0,0.05 3CIV,GLU_221,4.85,0.35,0,1.39E-17 1T3J,GLU_694,2.98,0.34,-1.19,-0.67 1RI6,ARG 318,13,77,-0,47,1,15,0,6 3LJN,GLU_111,4.15,0.19,-0.53,0 4DNU,GLU_158,4.84,0.13,0,0.21 1ES9,ARG_153,13.55,-0.35,0.88,0.51 1NAR.HIS 173,6.61,-1.09,0.89,0.3 3CCY,LYS_93,11.81,-0.44,0.98,0.76 20EW,GLU_119,5.01,4.29,-2.2,-1.59 1G5Z,LYS_115,9.93,-0.34,0,-0.23 2P0L,LYS 152,10.31,-0.19,0,0 2OJQ,LYS_699,10.47,-0.59,0,0.56 1YM5,TYR_278,11.97,-0.19,-0.43,2.59 3ZRI,HIS -3,6,26,-0,24,0,0 2X4G,GLU_256,3.79,0.44,-0.77,-0.37 2D0A,TYR 247,10.55,0,0.26,0.29 3CJW/HIS 306.6.2,-0.22,0,-0.08 3LD1,GLU_267,4.29,0.64,-0.13,-0.72 3N0K,ASP_54,2.91,-0.81,-0.39,0.32 1D2K.HIS 92.6.76.-0.78.0.77.0.27 4DIU,GLU_208,4.77,0.24,0,0.03 3RRQ,HIS_107,6.01,-0.55,0,0.06 3HKX,ARG 22,13.06,-0.68,0.84,0.4 2YYO,HIS_69,6.58,-0.53,0.34,0.26 2Q99,ASP 220,1.84,-1.7,-0.68,0.42 3ZRI,ARG 126,13.06,-0.3,0.45,0.41 3ULX,LYS_102,10.36,-0.25,0,0.11 2H2Z,GLU_55,4.67,0.11,0,0.06 2Q99,GLU_172,4.24,1.29,-1.35,-0.21 1BKR,ASP_81,3.34,-0.72,-0.14,0.39 2Q99,ARG 18,12.56,-2.7,1.23,1.53 1IAP,ASP_133,3.48,-0.19,-0.44,0.31 1G8P,ARG_296,12.02,-0.7,0,0.22 1UCH,LYS_21,10.42,-0.13,0,0.05 2YYO, ASP 49, 3.31, -0.82, 0.0.33 2WOZ,ARG_532,12.67,-2.2,1.65,0.72 2R57,ARG_236,13.03,-0.47,0.79,0.22 2FZ4,GLU_30,4.29,0.48,-0.15,-0.56 1TXJ,ASP 64,3.87,0,0,0.07 2X4L,ARG_174,11.81,-1.11,0,0.41 3AUF,GLU_159,3.53,0.19,-0.81,-0.34 2R0S,ASP_220,3.44,-0.63,0,0.26 2B0J,LYS_109,10.15,-0.11,0,-0.24

3I0C.GLU 322,5.68,3.96,-1.74,-1.05 2IXM,TYR 251,10,72,-0.63,-0.25,1.6 1MTZ,LYS_98,10.14,-0.4,0,0.04 3BWT.ARG 651,12,24,-0.68,0.0.42 1ANU,ARG_100,12.57,-0.27,0,0.35 3F6M,LYS 132,11.04,-0.79,0.85,0.47 2D0A,LYS_56,10.45,-0.05,0,0 1NIJ,GLU_205,3.3,0.69,-1.29,-0.58 3PBH,ARG_54,12.24,-0.32,0,0.07 3H5T,ASP 186,3.76,-0.38,-0.03,0.37 3MIX.ARG 628,12,29,-0,32,0,0,11 2H85,LYS_64,10.22,-0.35,0,0.06 2H2Z,ASP_263,3.57,-0.73,0,0.5 2CBE,LYS_257,11.2,-0.39,0.71,0.38 2FD5,GLU 81,3.67,0.26,-1.1,0.02 3T5B,ARG_11,11.56,-1.32,0,0.38 3ETU,CYS_80,11.78,0,0.1,2.68 1ZCU,GLU_51,4.67,0.32,0,-0.14 3EGN/LYS 466/10/37/-0/31/0/0.18 1H09.LYS 246.10.47,-0.31.0.0.29 2B0J,ARG_24,12.37,-1.76,0.47,1.15 2R0S,ASP 75,2.81,-0.75,-0.46,0.23 3MEW,GLU_173,3.96,0.41,-0.06,-0.89 1PVT,ASP 190,4.27,0,-0.18,0.65 2P5D,ARG 84,12,43,-0.07,0,0 3IBT,ARG_242,12.65,-0.36,0.04,0.47 1RAJ,GLU_247,4.43,0.25,0,-0.31 3PM2,LYS_7,10.32,-0.21,0,0.03 4DBX,ASP 7,3.91,0,-0.05,0.16 2H85,TYR_230,10.56,0,0.02,0.54 30KY,ARG 239,13,-0.74,0.77,0.46 3RE9,HIS_92,5.78,-0.69,0,-0.02 3RFY,LYS 202,11.75,-0.41,0.81,0.85 1TXD.CYS 784.10.11.0.38.0.12.0.6 1TP6,ASP_113,3.94,0,-0.03,0.16 3RVC,LYS_108,10.1,-0.22,0,-0.18 1MTZ,HIS_292,5.98,-0.73,0,0.21 3T5B,ARG_56,11.51,-1.25,0,0.27 1PVT,GLU_40,4.64,0.2,0,-0.06 3CXS,ARG_116,12.2,-0.82,0.27,0.25 2EJX,ARG_134,13.79,-1.01,1.4,0.9 1ES5,TYR 23,11.77,0,0.16,1.61 4FZN.LYS 215.10.05.-0.39.0.-0.07 1QQH,CYS_128,9.6,-0.24,-0.03,0.87 4DNU,ARG_346,13.4,-0.33,0.6,0.63 2D7J,CYS_148,13.23,-0.52,2,2.75 1ZKZ,LYS_78,10.63,-0.11,0,0.24 1G8PARG 231,13,-0.66,0.54,0.62 1UXO,HIS_59,6.22,-0.28,0,0 2VAN,HIS_135,5.12,-1.14,0,-0.24 4DEZ,ARG_178,12.25,-0.35,0,0.1 2098.GLU 118.3.66.0.5.-1.27.-0.07 1RL0,GLU_177,4.56,3.41,-1.18,-2.17 1YW5,LYS_59,10.39,-0.13,0,0.03 2YLF,HIS_206,6.59,-1.22,0.85,0.46 1XEU,ASP_111,3.01,-1.31,0,0.52 3EOD.GLU 89.4.58.0.08.0.0 4DVD,TYR_69,11.42,0,0.05,1.37 3MTT,LYS_564,10.75,-0.3,0,0.56 3CAX, ARG_193, 12.17, -0.77, 0, 0.44 1YOY.GLU 78.5.11.0.84.0.-0.23 1UAJ,GLU_188,4.57,0.07,0,0 3CRM,TYR 270,10.83,0,0.32,0.52 2CN1,LYS_73,10.7,-0.25,0,0.46 2F4Q,ARG_286,11.88,-0.69,0,0.07 3DZ1.TYR 295.9.75.-0.15.-0.29.0.19 2AD1,LYS_148,9.45,-0.62,0,-0.42 1CHD,HIS_248,6.55,-0.83,0.82,0.07 2X4G,HIS_132,5.74,-0.56,0,-0.2

3B4D,CYS_195,10.25,0,0,1.25 1SQH,ASP_19,3.14,-1.26,-0.41,1.02 2DG7,GLU_116,4.53,0.2,0,-0.18 3RFY,GLU_279,5.19,0.67,0,0.04 1LTU,ASP_154,4.54,0,0.07,0.66 4EZB,LYS 116,10.64,-0.16,0,0.3 1HF8.LYS 163.10.13.-0.39.0.0.02 3BA1,TYR_185,10.69,0,0.11,0.57 2NYC,LYS_279,10.32,-0.23,0,0.05 1J8B,GLU_19,4.75,0.25,0,0 1P4X,ASP 226,4.22,0,0.17,0.24 3GFP,GLU_353,3.84,0.24,-0.46,-0.45 3F5D,LYS 5,10.43,-0.28,0,0.21 3DSH,GLU_274,3.63,0.25,-1.12,0 3ON1,ARG_74,12.41,-0.09,0,0 1IDK.TYR 85,10.09,0.0.09 2GZQ,LYS_14,10.28,-0.17,0,-0.06 2AZL,HIS_80,6.81,-0.91,0.68,0.54 3MIX,GLU_328,3.75,0.22,-0.77,-0.2 1UAJ,HIS 200,6.39,-0.2,0,0.1 30DJ.TYR 43,10,47,0,0,37,0,1 3FK5,ARG_225,12.37,-0.15,0,0.02 1SJY,LYS_33,10.24,-0.42,0,0.17 3P28,LYS 158,10.37,-0.13,0.0 2XWS,LYS 45,10.25,-0.08,0,-0.17 2CWC,HIS_281,5.71,-0.88,0,0.09 3H5T.ASP 50.3.96.0.-0.16.0.31 2AH5,LYS_118,10.36,-0.15,0,0.01 10I7,ASP_66,2.12,-2.33,-0.39,1.04 3GOZ.LYS 246.10.5.0.0.0 2WB8.TYR 739.11.25.0.0.13.1.12 1EW4,TYR_69,10.37,-0.35,0.16,0.56 1WLY.ARG 34,13.11,-0.48,0.62,0.48 1PBV.ARG 212.12.44.-0.12.0.0.06 3A7L,GLU_34,4.45,0.21,-0.15,-0.11 1P6F,LYS_22,10.57,-0.14,0,0.2 1RZ2,TYR_104,10.26,0,-0.08,0.34 2BV9,GLU_21,3.46,0.19,-0.85,-0.38 2CWY,ARG_89,13.19,-0.6,0.73,0.56 3NJM,ASP_28,2.7,-1.67,0,0.57 1LPL,TYR_207,10.53,0,0.21,0.32 4F3J,ARG_127,12.6,-0.17,0,0.28 3LQE,HIS 270,5.71,-1.21,0,0.41 2R0S,TYR_225,11.76,0,0.18,1.58 3GEC,LYS_390,10.46,-0.07,0,0.04 2FM9,ASP_212,4.45,0,-0.06,0.71 3HVW,ASP_329,3.5,-0.6,0,0.3 4E9E.CYS 549,12,46,0,0.08,3,38 3BWT,HIS_648,5.65,-0.71,0,-0.14 3M7D,ARG_267,13.79,-0.39,0.81,0.87 3Q2C,GLU_34,4.72,0.27,0,-0.05 2G5X.LYS 98.10.03.-0.46.0.-0.02 4EUG,GLU_95,4.65,1.72,-1.56,-0.01 2X4G,ASP_78,3.44,-0.74,-0.13,0.5 2G3A, ASP_44, 3.87, 0, 0, 0.07 3M9A,GLU_16,4.1,0.18,-0.41,-0.17 3B79,GLU_90,4.56,0.43,-0.42,0.06 2GAU,GLU_207,3.38,0.55,-1.14,-0.52 4FZR.GLU 381,3.78,0.4,-0.74,-0.38 1ZKZ,ASP_19,4.17,-0.02,0.13,0.27 1FQI,GLU 294,4.71,0.26,0,-0.06 4H4J,LYS 175,10,18,-0,29,0,-0,02 2QVT,LYS_93,10.1,-0.19,0,-0.21 2GEN,LYS_7,10.3,-0.21,0,0 3E5T,ASP_151,2.79,-0.84,-0.49,0.31 3G9T,ASP_42,3.97,0,0.07,0.1 4FZN,GLU_115,4.22,0.41,-0.08,-0.61 1J85,TYR_150,10.37,0,-0.05,0.41 2CWC,ARG_85,12.51,-0.33,0,0.33

105Z,ARG 656,13,98,-0.56,1.6,0.44 105T,TYR_212,11.46,0,0.64,0.82 1L3K.HIS 119.6.46.-0.35.0.0.3 2PGX,TYR_245,11.78,0,0.13,1.66 307K.ARG 97.13.66.-0.32.1.1.0.38 2BDD.GLU 59,4.66.0.58.0.-0.42 2Z14,TYR_44,10.93,0,-0.06,1 1SQH,GLU_51,4.5,0.18,0,-0.18 1OXZ,LYS_210,11.41,-0.43,0.62,0.71 2Z0M.ARG 10.12.49.-0.35.0.0.34 3FS3,GLU_61,4.77,0.27,0,0 1L2F.GLU 202.4.41.0.59,-0.64,-0.04 1V8E,LYS_19,10.39,-0.22,0,0.12 109G.GLU 9,4.57,0.1,0,-0.03 2CXA.LYS 79.10.32.-0.21.0.0.03 2P0Y,HIS_244,4.9,-2.71,0.83,0.28 3PM2,GLU_148,4.85,0.29,0,0.07 2RJD,HIS_502,3.62,-3.87,0.85,0.15 4EUG.HIS 108.5.75.-1.43.0.68.0 1T95,LYS_56,12.51,-0.62,1.65,0.98 105T,GLU_455,4.19,0.28,-0.78,0.19 3FS3,ASP_55,3.43,-0.17,-0.59,0.4 2WZ9.GLU 23.4.73.0.24.0.1.04E-17 4AM1.GLU 147.3.83.0.27.-0.84.-0.11 2P5D,LYS_23,10.51,-0.25,0,0.26 1DOV,ASP_159,3.87,0,-0.24,0.3 2QV2,ARG_285,12.03,-0.65,0,0.18 2Q98,GLU 161,2.91,0.39,-1.48,-0.5 2CXA,TYR_87,10.8,0,-0.03,0.83 3T5B,ASP_123,3.93,0,0,0.13 1ZCU,LYS_228,10.59,-0.12,0,0.21 20JO.LYS 614,10,48,-0,2,0,0,18 4E6S.ASP 76.3.35.-0.71.-0.12.0.38 3RE9,HIS_228,6.27,-0.35,0,0.12 2R51,GLU_169,4.57,0.07,0,0 2JHY,GLU_109,4.85,0.19,0,0.16 4DNU,LYS_372,9.89,-0.33,0,-0.27 2F8H,HIS 212.6.37,-0.13.0.0 3MIX,ASP_363,3.87,0,-0.19,0.27 1U3Y,ASP_254,3.45,-0.97,-0.06,0.69 100E.GLU 6.3.86.0.32.-0.41.-0.55 4E6S.ARG 39.12.18.-0.32.0.0 2AZL,GLU_121,4.54,0.24,0,-0.2 2RFA,GLU_184,4.61,0.32,0,-0.21 3IBT,LYS_84,11.93,-0.68,1.23,0.88 1X6J,ASP_21,3.21,-0.83,-0.31,0.55 3M7G.GLU 194,3.76.0.25,-0.63,-0.36 1RZ2,LYS_129,11.26,-0.28,0.66,0.38 200K,LYS_70,10.63,-0.23,0.32,0.05 1BKR.LYS 93,10,46,-0.08,0,0.05 2D2S.GLU 541,3.93,0.38,-0.85,-0.1 2CBE,ARG_182,13.97,-0.3,1.24,0.54 2HNG,TYR_112,10.65,0,0.42,0.23 3JRT,TYR_71,11.89,0.85,0.4,0.63 105T,ARG 448,12.63,-0.47,0.07,0.53 2FBI,ASP 108,2.96,-0.68,-0.45,0.29 2GEN,ASP_161,3.94,0,-0.09,0.25 2IQT,GLU_93,4.77,0.22,0,0.04 2E3S,GLU_589,4.58,0.16,0,-0.08 2P0Y,ASP 237,3.95,-0.1,-0.06,0.32 3H13,ARG_432,12.18,-0.57,0,0.25 3ASA, ASP_87, 3.96, 0, -0.21, 0.38 2RFA,GLU_249,5.05,0.56,0,0 1UAJ,GLU_129,3.23,0.91,-1.63,-0.55 2CIU,LYS_190,10.32,-0.28,0,0.1 1NJ4,ASP_16,3.14,-0.65,-0.4,0.4 3B21,LYS_207,10.24,-0.24,0,-0.02 4FLE,GLU_135,4.12,0.54,-0.84,-0.07 3FFM,GLU_144,4.05,0.42,-0.58,-0.29

1R53.ARG 191.10.99.-1.88.0.23.0.13 1Q46,LYS_145,10.66,-0.19,0,0.35 2HP7,GLU_225,4.87,0.26,0,0.1 4ANN,HIS_73,6.28,-0.34,0,0.12 1H4U,ARG 580,12.59,-0.15,0.0.24 1TXD.GLU 878.4.41.0.27.0.-0.37 3LJC,GLU_118,4.5,0,0,0 3GMS,HIS_268,5.9,-0.43,0,-0.17 1A8Q,LYS_156,10.53,-0.21,0,0.24 2B0J.LYS 151.10.-0.42.0.-0.09 1JB3.GLU 13.3.94.0.34.-0.51.-0.39 1SI7,ARG_141,12.63,-0.45,0.09,0.5 3ZTA,GLU_49,4.79,0.26,0,0.04 2012.GLU 80.4.61.0.11.0.0 3N2T.TYR 59.11.29.-0.58.-0.77.2.64 1UOH,GLU_127,4.56,0.3,-0.22,-0.01 2W2S,GLU_149,4.36,0.47,-0.56,-0.04 3IU5,ASP_83,4.02,0,0,0.22 1RZ2,TYR_94,12.26,-0.72,0.16,2.83 1NRI,LYS 239,10.06,-0.2,0,-0.24 3RFY,ARG_108,12.1,-2.28,0.14,1.74 1Q2Y,LYS_88,10.29,-0.16,0,-0.04 1FOI.GLU 330.4.36.1.1.-0.76.-0.47 3MIX.TYR 418.10.22.0.0.11.0.11 3VJ8,LYS_358,10.5,-0.33,0,0.33 1MHN,ASP_140,3.59,-0.51,0,0.3 2R57,ASP_178,4.13,0,0.15,0.18 1Q8B,TYR_54,10.34,0,0.05,0.29 1GPP.LYS 53,11.06,-0.28,0.58,0.26 1XTZ,ARG_101,12.39,-0.11,0,0 2A4D,LYS_184,10.57,-0.13,0,0.2 1WYC,GLU_143,3.23,0.68,-1.39,-0.56 1PGV.LYS 388.10.45.-0.05.0.0 3FS3,LYS_70,10.59,-0.24,0.33,0 2YLF,CYS_203,12.64,-0.14,0.04,3.74 3COU,GLU_173,3.7,0.65,-0.81,-0.63 2B0J,ASP_77,3.67,-0.22,-0.11,0.2 3ONH, ASP_532, 3.98, -0.07, -0.07, 0.32 3C5V,GLU_75,4.57,0.12,0,-0.05 2GQV,GLU_58,4.01,0.27,-0.76,0 2B0A,TYR_90,11.36,0,0.51,0.85 1RL0,ASP 228,3.37,-0.22,-0.56,0.35 3DSH,HIS_233,6.21,-0.29,0,0 2E3C,ASP_433,3.8,0,-0.3,0.3 1LTU,ASP_252,4,0,-0.21,0.41 1DVO,LYS_176,9.84,-0.66,0,0 3CGW,LYS_291,11.38,-0.43,0.83,0.47 2V4X,GLU_94,4.85,0.32,0,0.03 1SI7.ASP 32.3.75,-0.48,-0.24,0.66 3BCY,LYS 110,10,27,-0,42,0,0,19 2FBQ,LYS 34,10.37,-0.32,0,0.19 1PSW,GLU_337,4.28,0.22,-0.39,-0.06 10GL,ASP_223,2.7,-1.17,-0.78,0.85 1V43,GLU_12,3.66,0.34,-0.76,-0.42 3CCY,CYS_74,11.54,-0.01,-0.09,2.64 1BGF,ARG_87,13.03,-0.37,0.59,0.31 1G5Z,LYS_122,10.59,-0.3,0,0.39 2WOZ,TYR_545,12.12,0,0.17,1.95 3M9A,ASP_71,4.25,0,0.09,0.36 1R3F,TYR_68,10.59,-0.43,-0.29,1.3 1ANU.GLU 115.4.79.0.14.0.0.14 2H14,TYR_252,12.71,0,0.07,2.64 1YDL,HIS_42,6.55,-0.38,0,0.43 2P0Y,CYS_296,11.16,-0.07,-0.03,2.26 1PVT,ARG_68,12.22,-0.26,0,-0.02 3AU3,ARG_657,13.06,-0.31,0.51,0.36 1ZBS,ARG_128,13.04,-0.25,0.2,0.6 2V1L,HIS_10,6.24,-0.26,0,0 2FZP,TYR 275,13.83,0,0.51,3.32

4FZR,LYS_247,11.46,-0.27,0.85,0.38 2PGX,LYS 213,10.31,-0.19,0.0.01 1WP5,GLU_227,4.61,0.11,0,0 1PDB.LYS 155,10.84,-0.3,0.17,0.48 3AU3.TYR 622.11.79.0.66.0.38.0.75 2APL.LYS 2.10.5.0.0.0 100X,LYS_69,10.34,-0.16,0,0 1FKM,TYR_412,12.32,0,0.08,2.24 3ULX,TYR_94,10.51,-0.01,-0.09,0.61 2P0Y,TYR 131,10,77,0,0,06,0,72 3HNX,ASP_91,3.95,0,-0.22,0.38 2CI3,ARG_44,12.35,-0.28,0,0.12 1TLV.LYS 143,10.83,-0.49,0.12,0.7 3AU3.ASP 459.2.64,-1.11,-0.49.0.44 4DNU,HIS 183,2.55,-3.07,0.16,-1.03 30NH,LYS_440,10.45,-0.1,0,0.05 3EVP.HIS 112,5,17,-2,08,0,84,-0,1 1A8Q,TYR_67,12.01,-0.85,0.35,2.51 3EVZ.LYS 215.11,-0.63.0.51.0.63 3ASA.GLU 323.4.18.0.53.0.-0.85 3ASA,TYR_301,12.02,0,0.49,1.54 4DIU,LYS 7,10,16,-0,34,0,0 4HDE,ASP_135,2.8,-1.36,-0.02,0.37 3H5T,HIS 307,6.42,-0.15,0,0.06 3LH5,ARG 690,12.68,-0,19,0,0.36 1SQH,GLU_108,3.49,0.39,-0.85,-0.54 3BCH,ARG_63,12.21,-0.29,0,0 1R53,GLU_182,4.62,0.1,0,0.01 1YTD,GLU_370,4.68,0.09,0,0.09 3OIP,HIS_208,6,-1.5,0.92,0.09 100E.GLU 101.4.46.1.08.-0.59.-0.54 3N2T,ASP_168,2.95,-0.83,-0.48,0.46 30IP,LYS 215,10.45,-0.11,0,0.05 1RI6.CYS 216.11.05.-0.73.0.9.1.88 2VGM,ASP_180,3.69,-0.48,0,0.37 2F4Q,GLU_257,4.82,0.33,0,0 1T95,TYR_32,11.68,0.85,0.37,0.46 3LMF,TYR 22,10.26,0,-0.04,0.3 3IL3,ASP_260,2.53,-1.54,0,0.27 1LZL,ASP_25,3.95,-0.36,0.13,0.38 1XFK,ARG_14,13.52,-0.17,0.75,0.43 2RFA,HIS 185,6.82,-0.53,0.8,0.06 1ZP2.LYS 210.10.32.-0.34.0.0.17 4AM1,HIS_227,3.91,-3.23,0.64,0 1ZCE,LYS_45,10.66,-0.2,0,0.36 2EFK,GLU_283,4.56,0.06,0,0 1QQE,GLU 262,4.57,0.22,0,-0.15 2NRR,LYS_397,10.98,-0.13,0.23,0.37 1T07,CYS_7,7.58,-3.05,-0.13,1.76 2D7U,LYS_111,12.01,-0.5,0.87,1.14 4H89,ASP_13,3.74,-0.11,-0.12,0.17 2P0Y,ARG 65,12,13,-0,37,0,0 20EW,ASP_328,4.12,0,0.09,0.23 1UW7,ASP_26,3.86,-0.38,0.04,0.4 3RVC,GLU_152,4.36,0.23,-0.34,-0.03 1WPA,ARG_429,12.96,-0.43,0.15,0.74 4H4J,HIS 111,4,2,-2,61,0,66,-0,35 2GEN,GLU_69,3.87,0.26,-0.57,-0.32 1R3F,GLU_157,3.74,0.29,-0.53,-0.52 2Q13,LYS_270,10.38,-0.12,0,0 1ES5.LYS 25.9.81.-0.72.0.0.02 2V81,CYS_81,11.16,-0.75,0.1,2.81 2G5X.ARG 56.12.26.-0.25.0.0.01 3BQW,GLU_152,3.96,0.61,-0.59,-0.55 2H2Z,ASP_153,4.08,-0.76,-0.2,1.24 3E7P.GLU 33.3.09.0.66,-1.62,-0.45 2FL7,ASP_60,2.69,-1.98,-0.01,0.89 2F4Q,CYS_270,12.14,0,-0.02,3.17 3GS9,GLU_34,5.02,0.52,0,0

1W7B,LYS_313,10.49,-0.24,0,0.23 3M7G,GLU 74,4.58,1.22,-0.3,-0.84 1TD6,LYS_254,11.31,-0.5,0.85,0.46 4H86,LYS 7,11.05,-0.36,0.53,0.38 3O48,ASP_5,2.77,-0.82,-0.38,0.18 4EVF,TYR 173,10.93,-0.35,-0.21,1.49 3TIR.LYS 196,10.66,-0.67,0.16,0.67 2QV2,CYS_212,10.74,-0.39,0.1,2.03 1R3F,GLU_61,4.37,0.57,-0.23,-0.47 3V55,HIS_681,6.06,-0.27,0,-0.17 3IV4,GLU 59,4.94,0.41,0,0.03 3G9T,GLU_34,3.65,0.92,-1.6,-0.17 3LJC,LYS 147,10.35,-0.12,0,-0.04 1JKS,CYS_30,11.16,-0.13,0.08,2.2 2CVB,LYS_78,10.78,-0.21,0,0.48 3RJX.TYR 69.11.93.0.0.56.1.35 1RHS,TYR_164,10.76,0,0.03,0.73 1H09,TYR_41,9.68,-0.85,-0.09,0.63 1YLN,HIS_214,6.32,-0.17,0,-0.01 2Z61,ASP_81,3.97,0,-0.17,0.34 3R2E,ARG_68,12.29,-0.21,0,0 3EVP,HIS_94,2.14,-3.6,0.71,-1.47 3FRR,ASP_42,3.8,-0.01,-0.37,0.38 3PP8.GLU 256.4.02.1.72.-1.54.-0.65 2G9D,LYS 171,10.23,-0.34,0,0.07 2FL7,LYS_42,10.31,-0.19,0,0 3UPD.TYR 255,11,44,0,0,27,1,17 2X5Y,HIS_734,6.25,-0.31,0,0.06 1DTO,GLU_142,3.81,0.13,-0.82,0 3TIR.HIS 90.5.9.-0.72.0.0.12 1JKS.LYS 86,10.29,-0.07,0,-0.14 3ERF,GLU_91,4.18,0.89,-0.94,-0.27 4D8L/ARG 242,11.54,-1.58,0,0.63 2WOZ.ASP 415.3.12.-1.16.-0.48.0.97 3DB9,ARG_163,12.79,-0.59,0.45,0.43 2Z61,LYS_53,10.85,-0.17,0,0.52 1BKR,ASP_47,1.91,-1.92,-0.48,0.51 30NH,ASP_493,4,-0.13,0.03,0.31 1ZKZ.LYS 53.10.45.-0.05.0.0 2W1R,ASP_92,3.83,0,-0.29,0.32 1ZCE,ARG_38,11.86,-0.6,0,-0.04 2G2D,GLU_152,4.61,0.11,0,0 3HQX,GLU 95,4.76,0.44,0,-0.18 1WXQ,ASP_202,2.86,-1.48,0,0.53 3GYW,LYS 81,10,36,-0,14,0,0 2G9D,ASP_243,5.36,-0.09,-0.23,1.89 2WOZ,GLU_559,4.59,0.09,0,0 1CBY.TYR 169.12.79.-0.31.0.04.3.06 1P6F,GLU_36,3.19,0.68,-1.29,-0.71 2Q98,ARG_192,11.95,-0.59,0,0.04 2OSA,TYR_346,13.73,0,0.28,3.45 1SJY,GLU 56,3.74,0.66,-1,-0.41 3ZTA,HIS_75,6.65,-0.17,0,0.33 2IF4,TYR 221,12.09,0.85,0.65,0.59 3GS9,GLU_282,4.5,0,0,0 3CO1,TYR_124,13.17,0.62,0.63,1.93 1W24,GLU_71,3.39,0.37,-0.91,-0.57 1WYC,ARG_182,13.42,-1.06,1.44,0.54 4EZB.GLU 11.4.55.0.13.0.-0.07 10XZ,GLU_275,4.58,0.08,0,0 1CHD,TYR 226,11.54,-0.84,0.14,2.23 2RIK.LYS 131,11.02,-0.76,0.66,0.62 2Z61,LYS_80,10.44,-0.51,0,0.45 1ZBP,CYS_42,12.64,0,0.16,3.47 2P0L,ASP_249,4.27,0,0,0.48 20JO.GLU 527.4.6.0.1.0.0 1RI6,ARG_250,9.87,-3.2,0.45,0.11 4FLE,GLU_35,3.76,0.34,-0.64,-0.44 1WXF,TYR_174,10.04,0,-0.28,0.32

3M7D,ARG 187,12.27,-0.34,0.0.12 2QZQ,CYS_122,12.44,0,-0.07,3.5 2AH5,ASP_109,3.4,-0.55,-0.5,0.65 2Z84,ARG_185,12.38,-0.42,0,0.3 204D.GLU 119.2.77.0.68.-1.93.-0.48 2R2Y,TYR 22,10.12,-0.15,-0.15,0.42 3B7X,ASP_69,3.6,-0.37,0,0.17 2CXC,ASP_113,4.05,-0.24,0.03,0.46 3GFP,LYS_341,10.33,-0.17,0,0 100E.GLU 146.5.44.0.66.0.0.28 2BLL,GLU_579,5.02,0.46,-0.07,0.13 1PGV.GLU 259.4.55.0.18.0.-0.13 1J33,GLU_43,4.13,0.28,0,-0.65 3KB5.GLU 407.4.19.0.25.-0.16.-0.39 3AU3.LYS 455,10.92,-0.17,0.1,0.48 1T95,ARG_106,12.11,-0.7,0,0.31 2PGE,ASP_144,2.75,-0.86,-0.5,0.32 1RHS,ARG_175,11.69,-0.97,0,0.16 2G2D.ARG 91.12.55.-0.98.0.55.0.48 3TIR,CYS_192,10.15,-0.22,-0.26,1.63 1X04,LYS_34,10.53,-0.2,0,0.23 2QZQ,LYS_40,10.59,-0.37,0,0.47 1JB3,ARG 43,12.41,-0.22,0,0.13 1SBX.ARG 96,12.71,-0.14,0.0.35 3EJG,LYS_54,10.5,-0.08,0,0.07 3LQE,GLU_338,4.59,0.35,0,-0.25 3RKV,HIS_260,6.85,-0.29,0,0.64 1ES9,HIS 28,6.12,-0.38,0,0 1NRI,GLU_120,5.29,0.73,0,0.06 4H89,GLU_129,3.81,0.32,-0.82,-0.19 3M7G,ARG_37,12.28,-0.6,0,0.38 1WP5.HIS 320.6.44,-0.11.0.0.05 1GOE.GLU 93,4.68,0.14,0.0.05 4ESS,GLU_102,4.68,0.37,0,-0.19 3ERF,ASP_157,3.32,-0.32,-0.52,0.36 1V43,ARG_182,12.91,-1.13,0.78,0.75 4F3J,GLU 112,4.06,0.26,-0.69,-0.02 3F5D,LYS 80,9.68,-0.44,0,-0.38 3IO0,GLU_197,5.33,3.76,-1.8,-1.14 1HUF,LYS_53,10.75,-0.22,0,0.47 20JO,LYS 640,10.37,-0.1,0,-0.03 1ZHV.GLU 43.4.69.0.31.0.-0.12 3C5V,ASP_65,4.03,-0.82,-0.37,1.42 10GL.LYS 109.10.84,-1.09.0.85.0.58 2RIK,LYS_226,10.48,-0.04,0,0.02 3AU3,GLU 538,3.13,0.81,-1.92,-0.25 1MD6.CYS 69,10.79,-0.85,0,2.64 2HRZ,LYS_127,10.56,-0.34,0,0.4 3V46,ARG_310,11.93,-1.09,0.03,0.49 2YT4.CYS 657.9.84.-0.85.0.02.1.67 1XIPLYS 48,10.26,-0.56,0.0.31 1GPP,TYR_179,10.02,-0.17,-0.2,0.39 1YIB,ASP_209,3.9,0,-0.16,0.26 3M7G,TYR_5,9.25,-0.78,-0.82,0.85 3CBN,GLU_74,4.56,0.22,0,-0.16 3COU,GLU_79,4.53,0.7,-0.39,-0.28 1X91,ASP_9,2.9,-0.89,-0.38,0.37 2R51,GLU_157,4.48,0.38,0,-0.39 10TM,HIS_151,6.62,-0.68,0,0.8 3G9T,ARG 14,12.19,-0.46,0,0.15 2P5D,ARG_93,11.41,-1.64,0,0.55 1WRU,TYR_150,10.9,0,-0.07,0.97 2QDJ,TYR_321,13.24,-0.79,1,3.03 3QAV,LYS_159,10.25,-0.25,0,0 3JRT,LYS_2,10.4,-0.17,0.06,0 20KT,LYS_140,10.38,-0.26,0,0.13 2B61,LYS_293,10.19,-0.37,0,0.06 2Z84,TYR_55,12.35,-0.79,0.27,2.87 3RJZ,TYR_150,10.2,0,0,0.2

1RSS.GLU 146.4.86.0.23.0.0.12 2AZP.HIS 217.6.43.-0.18.0.0.1 3MIX,LYS_579,10.5,-0.22,0,0.22 2IRM,ARG_104,12.65,-0.34,0.09,0.4 3KV0.GLU 176.4.66.0.14.0.0.02 1ZBM,TYR 152,10.68,-0.04,0.22,0.5 2GZQ,LYS_60,10.58,-0.26,0.01,0.33 4HDE,GLU_195,2.94,0.36,-1.36,-0.55 1Y0K,ARG_166,12.38,-0.2,0,0.08 2RIK.LYS 224.11.25.-0.79.0.85.0.69 3E5T,LYS 136,10.28,-0.3,0.0.08 3N2T,LYS_75,11.34,-0.39,0.85,0.38 3LJC,ARG_214,12.41,-0.26,0,0.17 1R50,HIS 57,4,97,-1,73,0,0,2 2Q13,GLU 10,4.63,0.16,0,-0.03 3QAV,TYR_118,11.47,0.55,0.39,0.53 2XWS,LYS_100,11.19,-0.35,0.55,0.49 2ZQ5,HIS_117,4.95,-2.52,0.78,0.19 3I4T,GLU 12,4.5,0.53,-0.69,0.16 3ERF,ARG_154,12.54,-0.11,0,0.14 3BB7,ASP_184,3.3,-0.79,-0.09,0.38 1UXO,HIS_128,5.22,-0.87,0,-0.41 3PZ9,TYR_332,12.28,-0.82,-0.62,3.72 2W0G.CYS 194,11.31,-0.94,0.03,3.22 1YM5,LYS_16,10.46,-0.09,0,0.04 3AUF,ARG_48,12.38,-0.35,0,0.23 100X,LYS_23,10.54,-0.27,0,0.3 3HYQ,ARG_83,13.11,-1.11,0.82,0.9 2FBI.GLU 48.4.8.0.3.0.0 3V75,HIS_57,5.7,-0.61,0,-0.18 1LPL,LYS_175,10.39,-0.15,0,0.04 2NRR,ARG_395,12.03,-0.74,0,0.26 2PGE.ARG 36,12.47,-0.51,0,0.49 1MML,TYR_146,11.15,0,0.23,0.92 3V3T,GLU_300,4.97,0.19,0,0.27 3M7G,ARG_76,13.7,-1.5,0.73,1.98 20EW,ASP 59,3.78,-0.24,-0.39,0.61 2V1L.GLU 27.4.68.0.21.0.-0.02 1AD6,TYR_446,13.69,0,0.2,3.48 3EZ7,LYS 375,9.97,-0.31,0,-0.22 2JHY,LYS_105,10.47,-0.2,0,0.17 3H6Q,GLU 14,4.7,0.29,0,-0.09 1M5I,LYS 167,10,39,-0,12,0,0.01 3AUF,GLU_74,4.57,0.15,0,-0.08 2YX0,ARG_56,12.59,-0.22,0,0.31 1YTQ,GLU_105,4.86,0.28,0,0.07 2H2Z,GLU_166,3.84,0.36,-0.69,-0.33 2B61,ARG_295,13.64,-0.5,0.78,0.86 4FZR,ARG_2,12.51,-0.45,0,0.46 1WLY,LYS_188,10.58,-0.16,0,0.23 1MIX,CYS 336,10.4,-0.69,0.37,1.72 3U0V.CYS 174.13.88.0.0.95.3.93 1MJS,TYR_296,11.6,0.85,0.13,0.61 4DIU,ASP_236,3.91,-1.04,-0.49,1.64 2RGY,ARG_238,12.49,-0.86,0.48,0.37 1RHS,GLU_285,4.07,0.28,-0.7,-0.01 3M9A,LYS 79,10.59,-0.32,0.26,0.15 1ZBM,GLU_135,4.03,0.39,-0.5,-0.37 2Z0W,ASP_53,2.57,-1.59,0,0.36 1UCH,ASP_198,2.92,-0.63,-0.7,0.45 1JSX.GLU 126.4.59.0.12.0.-0.04 1X04,GLU_97,4.41,0.2,0,-0.29 1Z9L,LYS_17,10.35,-0.51,0,0.36 1MTZ,LYS_157,11.06,-0.5,0.85,0.21 2R57,ARG_238,13.92,-0.49,1.42,0.48 1SUU,LYS_577,10.57,-0.14,0,0.21 3M16,LYS_71,10.12,-0.38,0,0 1OXZ,LYS_206,10.39,-0.32,0,0.22 2V5B,ARG_193,13.58,-0.34,1,0.42

2013.GLU 69.3.99.0.28.-0.58.-0.21 20GO.ASP 371,2.42,-1.08,-0.48,0.17 2FBI,ARG_89,12.91,-0.25,0,0.66 3CE7.GLU 68.4.38.0.67.-0.85.0.05 1X7F.ASP 291.3.72.0.-0.3.0.21 3JSN.GLU 238.4.49.1.25.-1.42.0.17 2A0J,GLU_141,3.23,0.42,-1.66,-0.03 3BPV,HIS_58,6.27,-0.26,0,0.03 2PPN,TYR_82,11.02,0,0.11,0.91 1FOLTYR 401,11.84,0.0.18,1.66 3BPP.GLU 134,4.67,0.31,0,-0.14 1L2F,GLU_124,4.7,0.18,0,0.02 3F6M,HIS 125,6.89,-0.19,0.13,0.45 2H2W.GLU 206,4,51,0.01,0,0 4AM1,GLU 335,5.31,3.15,-1.55,-0.79 105T.TYR 316.10.41.0.0.1.0.31 3C5V,GLU_124,3.82,0.44,-0.97,-0.14 2EA9,LYS_46,10.48,-0.07,0,0.05 3IVF,GLU_182,3.93,0.81,-1.17,-0.21 3BA1,LYS 25,10,29,-0,21,0,0 2PLQ,HIS_3,6.61,-0.73,0.83,0.01 2D2S.ASP 736.2.85,-0.96,-0.38,0.4 1SFE,HIS_147,4.31,-3.05,0.85,0.01 1TR9,GLU 19,4.66,0.13,0,0.03 1R6Y,HIS 80.5.45,-1.05.0.0 2EDM,LYS_119,10.15,-1.14,0.43,0.35 2Z0M,ASP_260,3.71,-0.17,-0.27,0.35 2FD5,GLU_57,3.44,0.85,-1.49,-0.42 3ETULYS 331.10.98.-0.15.0.25.0.38 105T,LYS_277,10.67,-0.38,0,0.55 2ZCO.TYR 131.11.76.-0.19.0.48.1.48 3H04,GLU_241,4.81,0.84,-0.14,-0.39 2E3H.LYS 238,10.46,-0.04,0,0 3ANJ,ARG 356,11,71,-0,99,0,0,2 3H04,GLU_80,4.96,0.38,0,0.07 3LH5,ARG_762,12.18,-0.46,0,0.14 3E0H,LYS_96,10.72,-0.24,0,0.45 100X,CYS 73,13.37,-0.94,1.57,3.74 2RJD,ARG_478,13.04,-0.97,0.41,1.11 1ZP2,CYS_87,11.53,0,0.22,2.31 1LN4,LYS_48,9.86,-0.62,0,-0.01 2QV2,GLU 153,4.76,0.26,0,0 3US6,ASP 35,3,3,-0.89,0,0.39 1SIG,ARG_436,12.61,-0.41,0.21,0.3 3NBI,TYR_151,9.91,0,-0.24,0.15 2OEW,LYS_239,10.75,-0.11,0,0.35 3LPZ,LYS 157,10.62,-0.15,0,0.28 2007.TYR 398.10.79.0.-0.08.0.88 2AHE,GLU_183,4.53,0.26,0,-0.24 2HRZ,GLU_320,3.41,0.52,-1.23,-0.38 2EFK,ASP_144,2.86,-0.85,-0.73,0.64 3GS3,ARG 174,12.85,-0.66,0.64,0.37 2BDV,GLU_53,3.9,0.39,-0.64,-0.35 1SOH.ASP 169.3.93.0.0.0.13 3DTE,LYS_190,10.31,-0.18,0,-0.01 2RGY,GLU_251,4.13,0.33,-0.91,0.21 1LN4,GLU 45,2.31,1.21,-3.13,-0.28 3DB9,CYS_65,12.24,0,0.13,3.11 3GYW,CYS_133,11.37,-0.01,-0.25,2.63 3N0K,ARG_135,12.16,-0.34,0,0 2F9F,ARG 60,13,42,-0,22,0,8,0,34 3PBH,TYR_177,10.58,0,0.26,0.31 3KB5,ARG 369,12,59,-0,49,0,0.58 3KB5,GLU_315,4.87,0.76,0,-0.39 3V55,LYS_648,10.41,-0.31,0,0.22 3UPD.LYS 43,10.47,-0.25,0.0.22 1DZF,ASP_84,4.24,0,-0.37,0.8 1YM5,GLU_142,3.54,0.99,-1.57,-0.38 2CVB,ARG_116,12.13,-0.57,0,0.19

1A80,ARG 151,12.08,-0.49,0.0.08 1EV8,HIS 32,5.36,-1.05,0,-0.08 2AHE,LYS_212,10.44,-0.06,0,0 3RKV.ASP 239,2.84,-1.69,-0.56,1.29 2FG1,LYS_7,10.44,-0.07,0,0.02 1YG2,ARG 161,11.95,-0.69,0,0.14 1JT9,ARG 2,13,2,-1,08,1,25,0,53 3ETU,GLU_146,4.46,0.23,0,-0.27 3G9G,ASP_145,3.99,0,-0.08,0.28 3R2E,GLU_77,3.23,0.51,-1.41,-0.37 3RFF,CYS 6,12.21,0,-0.03,3.24 2ZCO,ARG 158,13,57,-0.89,0.84,1.13 3IVF,LYS 256,10.39,-0.14,0,0.02 109G,ARG_158,12.49,-0.06,0,0.04 3PBH,LYS 62,10,43,-0.07,0,0 2B0J.HIS 88,5.24,-2.16,0.81,0.09 2YYO,CYS_109,13.12,0,0,4.12 1BKB,ARG_49,12.51,-0.25,0,0.27 2QEV,GLU_31,4.16,0.36,-0.69,0 1YLN,GLU 87,4.01,0.33,-0.63,-0.19 2X4L.GLU 188.4.77.0.3.0.-0.02 4HDE,ASP_54,3.53,-0.99,-0.24,0.95 3COU,ASP_132,4.5,-0.42,0.03,1.09 4H89,ASP 64,2.66,-1.57,-0.14,0.57 3EVZ,GLU 118,2.86,0.49,-1.47,-0.65 2OB5,ARG_114,12.99,-0.25,0.2,0.54 2CL3.LYS 73.10.56.-0.3.0.0.35 3DHN,ASP_54,2.67,-1.38,-0.07,0.32 1BKR,HIS 89,6.45,-0.2,0,0.16 3CS1,ARG 154,12,52,-0,33,0,0,35 1ZKZ,LYS_30,10.48,-0.06,0,0.04 1ES5,ARG_230,12.45,-0.56,0.07,0.44 2RGY,LYS 207,10.25,-0.15,0,-0.1 3FFM.GLU 109.4.59.0.09.0.0 2ZCX,ASP_99,3.83,0,-0.34,0.38 1TD6,LYS_187,11.16,-0.2,0.52,0.34 1DVO,ARG_165,13.14,-0.32,0.42,0.53 1XKR,GLU_175,4.45,0.23,0,-0.28 3GEC,ASP_529,3.46,0,-0.68,0.35 1SQW,HIS_112,5.7,-0.66,0,-0.14 2BDD,LYS_118,10.76,-0.21,0,0.47 10IS,GLU_274,4.01,0.27,-0.37,-0.39 1Y0K,GLU _3,4.53,0.17,0,-0.13 1VJG,GLU_190,4.09,0.83,-1.31,0.06 2BLL,GLU_576,4.3,0.3,-0.56,0.07 1UXO,ARG_87,12.54,-0.12,0,0.15 3H13,LYS_462,10.52,-0.28,0,0.29 1U3Y,ARG 332,11.82,-0.63,0,-0.05 3DHN,HIS_191,6.62,-0.68,0.47,0.34 3L7N,LYS_168,9.99,-1.01,0,0.5 1QQE,LYS_168,11.47,-1.02,0.77,1.23 3LH5,GLU 541,4.56,2.03,-1.37,-0.61 2AZP,CYS_88,13.14,-0.64,1.03,3.75 20KT,GLU_84,4.75,0.3,0,-0.06 1XEU,LYS_206,10.47,-0.09,0,0.06 3GYW,LYS_93,10.5,-0.08,0,0.08 1WXQ,GLU_135,3.55,2.19,-1.88,-1.27 2DVK,LYS_87,9.4,-1.01,0,-0.09 1FHL,ASP_125,3.68,0,-0.3,0.17 3ELI,ARG_64,12.32,-0.25,0,0.07 3GS3,GLU 267,4.69,0.13,0,0.06 1TR9.LYS 226.10.35.-0.21.0.0.06 1YB2,ARG_254,12.4,-0.2,0,0.1 1WP5,ARG_130,12.43,-0.08,0,0.01 3A2Z,TYR_52,11.3,0,0.23,1.08 3LH5.GLU 581.4.61.0.32.0.-0.21 3LMO,TYR_74,11.59,0.42,0.31,0.86 1AT0.HIS 329.3.7.-2.76.0.78.-0.82 2HRZ,ASP_172,3.08,-0.59,-0.51,0.37

4E6S.GLU 79.5.13.0.3.0.0.33 1H09,TYR_93,13.58,-0.05,0.95,2.67 3V3T,TYR_73,11.68,0,-0.05,1.73 2PWQ,TYR_129,10.9,0,0.1,0.8 1UW7.LYS 84.11.27.-0.36.0.75.0.38 1WRU,ARG 269,12.14,-0.52,0,0.17 2V4X,ASP_65,4.43,0,0.16,0.47 1T3Y,LYS_131,8.86,-1.78,0,0.13 1AKO,TYR_215,10.83,-0.83,-0.12,1.77 2JEO.GLU 147.4.5.0.2.0.-0.2 1R3D,GLU_82,4.6,0.11,0,-0.01 1Y0K,HIS_186,6.09,-0.4,0,-0.01 2l6l,GLU_27,2.52,0.39,-1.7,-0.67 3JRT.LYS 95,10.56,-0.17,0,0.23 1GVP.TYR 34,10.2.0,-0.04,0.24 3RJX,HIS_45,6,-1.68,0.85,0.33 3IPZ,LYS_159,10.53,-0.19,0,0.22 2A1V,ARG_72,12.39,-0.35,0,0.24 1ZCE.ASP 93.2.37.-1.52.-0.38.0.47 1R3F,GLU_120,4.58,0.08,0,0 2CXC,LYS_134,10.01,-0.58,0,0.09 2FZP,ARG_279,12.1,-0.67,0,0.26 3EZ7,GLU_393,4.74,0.19,0,0.04 1X1E.TYR 91,10.05.0.-0.18.0.23 1J74,GLU_20,4.25,0.3,-0.23,-0.33 1ES9,LYS_95,10.59,-0.18,0,0.26 3G9G,GLU_158,4.82,0.3,0,0.02 3IVF,ARG 35,12.43,-0.33,0.06,0.2 3VJ8,GLU_343,3.61,0.41,-0.85,-0.44 2GZQ,ARG_57,12.38,-0.12,0,0 2X5Y,TYR_740,11.09,0,0.06,1.02 2ZTY.TYR 113.11.43.0.0.1.43 1PVT.ASP 200.3.65,-0.8,-0.31,0.95 3I0C,GLU_203,3.82,0.31,-0.79,-0.19 1HF8,ASP 61,3.91,0,-0.2,0.31 2ZQ5,HIS_235,2.27,-3.67,0.23,-0.8 3CGW,ARG_281,12.26,-0.55,0,0.31 2RIK.ASP 165.4.21.0.0.15.0.25 1CHD,LYS_232,11.47,-0.31,0.85,0.43 2BT8,ARG_299,12.43,-0.32,0,0.24 4DBX,ARG 66,12,12,-0,38,0,0 3TOW, ASP 121, 3.61, -0.8, 0.17, 0.45 1LTU,ARG_231,12.23,-0.27,0,0 3TOW,HIS_194,6.11,-0.25,0,-0.15 3BA1,CYS_86,11.29,-0.01,0.23,2.07 2Q13,TYR 203,10.46,0,0,0.46 1YG2.ARG 123.13.07.-0.38.0.31.0.65 2C2Y,HIS_254,5.49,-1.02,0,0.01 2IXM,ARG_106,11.98,-0.52,0,0 4FLE.HIS 173.6.15.-1.66.0.85.0.47 3JZN.ARG 269,12.03,-0.47.0.0 2X4L,TYR_282,11.67,0.33,0.05,1.29 2F4Q,HIS_80,6.21,-1.03,0.23,0.51 1ZBM,LYS_258,11.28,-0.29,0.63,0.43 1YTD, TYR 105, 11.08, 0, 0, 1.08 3V46,TYR_307,9.79,-0.04,-0.46,0.27 3IL3,TYR_11,12.45,0.85,0.73,0.87 2GKG,LYS 76,11.13,-0.21,0.41,0.44 3LH5,ASP_678,3.95,0,0,0.15 1FO9,TYR 223,13.83,0,-0.39,4.21 3CIV,ARG 185,13.33,-1.1,0.76,1.17 2R57,ASP_341,4.02,0,0.08,0.15 3MEW,TYR_190,10.89,-0.82,-0.04,1.76 3PZ9,GLU_270,4.52,0.09,0,-0.07 2CIU,TYR_141,12.34,0.82,0.43,1.1 200K,ASP_296,4.09,0,-0.01,0.29 3BZT,GLU_307,3.58,0.32,-0.96,-0.28 2FL4,ARG_64,12.4,-0.24,0,0.14 2B3M,ASP_71,4.1,0,0.14,0.15

3JSN.HIS 150.3.7.-1.98.0.-0.82 1U3Y,GLU_265,4.76,0.32,0,-0.08 1MUF,ASP_101,4,-0.05,0.09,0.16 3QKY,GLU_126,4.62,0.18,0,-0.07 3EVN, HIS 51, 6.23, -0.2, 0, -0.07 3M66,LYS 211,10,27,-0,23,0,0 2ZQ5,TYR_307,12.37,0.83,0.47,1.07 20JQ,GLU_672,4.37,0.2,0,-0.33 3OA7,GLU_7,3.82,0.45,-0.81,-0.31 2CWY,ARG_91,13.81,-0.28,0.85,0.74 2IN0.HIS 17,5.68,-0.85,0.0.03 2V81,ASP_58,3.91,0,0,0.11 2WZ9,LYS_67,9.91,-0.86,0,0.27 3CSR.LYS 7.10.55.-0.15.0.0.19 30DJ,TYR_23,10.11,-0.65,0.09,0.67 2Q12,ARG_237,12.4,-0.1,0,0 2B6P,ARG_196,12.36,-0.14,0,0 2FC3,LYS_34,10.08,-0.34,0,-0.08 4DND,GLU_30,4.55,0.15,0,-0.09 2H14.TYR 75.10.69.-0.31.0.34.0.66 4EKU,GLU_325,4.27,0.17,-0.08,-0.32 3EZ7,ASP_383,4.14,0,-0.01,0.35 2FD5,CYS_104,10.31,-1.65,-1.01,3.97 3I4T,GLU 46,3.2,0.52,-1.44,-0.38 1T95,LYS_225,9.99,-0.22,0,-0.3 1DTO,ASP_124,3.12,-0.89,-0.15,0.35 3H9W,GLU_37,4.16,0.31,-0.33,-0.32 3ELI,ASP_41,3.81,-0.09,-0.06,0.16 2F8H,ASP_134,2.29,-1.27,-0.69,0.45 2A6B,HIS_71,6.34,-0.38,0.24,-0.01 1AD6,GLU_440,4.53,0.36,-0.45,0.13 2RIS.GLU 19.4.81.0.63.0.-0.33 1X04.GLU 184.4.72.0.19.0.0.03 3M3P,HIS_140,5.92,-2.94,1.59,0.77 1T3J,HIS_690,6.6,-0.25,0,0.34 3BA1,GLU_259,3.96,1.13,-1.24,-0.43 1XAW,GLU_470,3.68,0.31,-1.14,0 3UPD,ARG_6,12.36,-0.17,0,0.03 3DZ1,HIS_240,7.5,-0.61,0.88,0.71 3IVF.GLU 189.3.43.1.06.-1.51.-0.62 2B78,ASP_261,3.14,-0.83,-0.06,0.23 2Q34,ARG 38,12.46,-0.39,0,0.34 1BGF.LYS 13.10.63.-0.13.0.0.25 20YZ,GLU_74,4.64,0.16,0,-0.01 2CI3,LYS_246,11.3,-0.21,0.58,0.43 3B21,GLU_154,4.64,0.09,0,0.05 1T95,HIS 141,6.38,-0.25,0.0.14 3GMS,ARG_185,13.3,-0.14,0.62,0.32 1ZBS.GLU 93.4.99.0.83.0.-0.35 2EJB,ASP_68,2.56,-1.65,-0.1,0.51 208P,LYS 208,10.5,-0.09,0,0.09 1G8P.ARG 126.12.47.-0.29.0.0.26 1AT0,LYS_372,10.36,-0.16,0,0.02 2B6P,GLU_257,4.58,0.08,0,0 3DHN,ASP_86,2.31,-1.49,0,0 1WYC,CYS_332,12.22,-0.25,0.12,3.36 2Q34,GLU 90,3.7,0.5,-0.81,-0.48 3V55,LYS_404,10.63,-0.11,0,0.23 4FH3,ARG_137,12.45,-0.3,0,0.24 1RKA,GLU_29,3.81,0.34,-1.02,0 1W7B.CYS 335.11.76.-0.3.-0.4.3.47 1WJG,ARG_124,13.92,-0.37,1.16,0.62 1XEU,LYS_273,11.15,-0.76,0.85,0.56 4DVD,ASP_148,3.95,0,0,0.15 1ZBM,HIS_1,6.25,-0.3,0,0.05 2B3M,TYR_44,11.18,-0.02,-0.49,1.69 2VGM,GLU_149,4.66,0.16,0,0 3VHJ,LYS_159,9.9,-0.58,0,-0.02 2Z61,TYR_224,12.2,0,0.04,2.16

3KV0,ARG_75,13.85,-0.47,1.21,0.63 208I.GLU 6.4.06.0.31.-0.28.-0.47 10XZ,GLU_230,4.65,0.15,0,0 2NRK,ASP_147,3.95,0,-0.01,0.16 2VGM,HIS_235,6.34,-0.21,0,0.04 3Q9P,ASP 115,3.96,0,-0.05,0.21 2YX0,GLU_249,5.07,0.65,0,-0.08 3PZ9, ASP_135, 3.42, -0.77, -0.34, 0.73 3GW3,ARG_41,11.92,-0.39,0,-0.19 1TR9.HIS 207.6.8.-1.47.0.85.0.92 3F6F.GLU 195,4,74,0,3,0,-0.05 3ASA,LYS_331,10.21,-0.65,0,0.36 3M7G,ASP_49,4.16,0,0,0.36 2PP6,ARG 81,12,17,-0,33,0,0 2GS5,GLU 151,4.68,0.25,0,-0.06 1Z3X,ARG_169,12.01,-0.49,0,0 3VJ8,GLU_193,5.56,2.68,-1.65,0.03 2AD1,HIS_268,6.64,-0.64,0.5,0.28 4H86.GLU 82.4.41.0.13.0.-0.22 2O34,LYS 143,10,49,-0,42,0,0,42 1GXN,CYS_510,10.28,-2.64,0.24,3.67 2CE6,ARG 43,12,44,-0.06,0,0 3EOD, ASP_104, 3.67, -0.63, -0.26, 0.77 1XDZ,LYS 228,10.42,-0.08,0,0 10I7.ASP 223.3.63.0.-0.45.0.29 3JZ9,ASP_354,3.37,-0.77,-0.43,0.76 3EVN,ARG_232,12.29,-0.17,0,-0.04 2YYO,CYS_29,11.83,-0.03,0.06,2.79 1P4X,ASP 212,3.22,-0.64,-0.31,0.37 1H4U,ARG_411,12.36,-0.31,0,0.17 2OK0.GLU 85.3.87.0.32.-0.57.-0.38 2G5X,LYS_30,11.38,-0.43,0.85,0.45 2EYI,ARG 86,13.34,-0.45,0.75,0.53 3AUF.TYR 62,10,28,0,-0,08,0,37 2HRZ,GLU_310,4.71,0.25,0,-0.04 3DSH,ASP_294,3.77,0,-0.24,0.21 2HNG,GLU_29,4.67,0.13,0.04,0 1Q2Y,LYS 2,10.16,-0.29,0,-0.05 10IS,GLU_268,4.71,0.29,0,-0.08 4DBX,GLU_243,4.44,0.09,0,-0.16 1ES9,ASP_36,3.83,0,-0.32,0.35 2CXA, ARG 227, 12.63, -0.94, 0.61, 0.46 2R57.GLU 256.4.9.0.89.0.-0.5 3CAX,GLU_278,6.59,3.7,-0.54,-1.07 1Z9L,LYS_107,10.43,-0.07,0,0 3CCY,LYS_55,9.59,-1.03,0,0.12 2ZQ5,ARG 179,11.97,-2.65,0,2.12 1WRU,LYS_328,11.17,-0.44,0.51,0.6 20EW,GLU_14,4.47,0.21,0,-0.23 1QYI,GLU_15,6.18,1.3,0,0.39 2IN0, ARG_410, 12.33, -0.3, 0, 0.13 3A2Z,GLU 170,4.61,0.18,0,-0.06 1PBV,HIS_133,3.79,-2.64,0,-0.07 2Q12,TYR_68,10.41,0,0.14,0.27 3ZSL,HIS_208,6.88,-0.69,0.85,0.22 3ETU,GLU_283,4.49,0.47,-0.16,-0.32 2X4J.ARG 100.12.76.-0.37.0.0.62 2EFK,LYS_110,11.1,-0.79,0.85,0.54 2GZQ,ARG_131,13.22,-1.97,1.67,1.02 3ANJ,TYR_51,12.87,-0.94,0.27,3.53 2PGX,ARG 22,12,55,-0.31,0,0.36 3VJ8,ARG_185,12.61,-1.1,0.78,0.42 1V6T.ARG 195.11.53.-1.37.0.0.39 109G,HIS_6,5.95,-0.73,0.07,0.1 3ULX,GLU_29,4.49,0.45,0,-0.47 2Z0M,TYR 185,10.4,-0.23,-0.23,0.87 1PVT,TYR_205,13.17,0.31,0.64,2.22 4FZR,GLU_61,4.44,0.35,-0.39,-0.02 100X,TYR_116,11.6,0,-0.31,1.91

3EVP.ASP 275.3.94.0.0.0.14 200K,CYS 158,12.27,0,-0.06,3.33 3M7G,ARG_131,11.76,-1.44,0.24,0.47 3ZSL,LYS_226,10.35,-0.23,0,0.08 1YR6,TYR_129,11.67,-0.42,0,2.1 3RHE,CYS 120,9.78,0,0.18,0.6 3DSH,ASP_429,4.07,0,0.01,0.25 3UPD,LYS_288,10.45,-0.29,0,0.24 1EDG,LYS_64,11.36,-0.43,0.71,0.58 1WJG,HIS_14,6,-0.38,0,-0.12 3ADO,GLU 83,4.75,0.19,0,0.06 4EUG,ARG_195,12.42,-0.08,0,0 3K8J,GLU_122,4.72,0.22,0,0 4E9E,GLU_559,4.12,0.2,-0.22,-0.37 2WB8.LYS 575.10.37.-0.13.0.0 1RHS,HIS_2,5.08,-0.83,0,-0.58 2FD4,ASP_465,2.4,-1.9,-0.3,0.8 3QAV,CYS_223,9.53,0,0.23,0.31 3IL3,LYS_200,10.54,-0.18,0,0.22 3M3P,HIS 250,7.1,-0.25,0.85,0 2IXM,GLU_202,5.03,0.42,0,0.11 1FHL,ASP_322,4.67,0,-0.21,1.07 2G7O,TYR_102,10.22,0,-0.02,0.24 3U2R.GLU 144.4.62.0.12.0.0 2IF4,ASP 185,4,18,0,-0,15,0,54 1RZ2,TYR_175,12.98,0.85,0.5,1.64 2GAU,GLU_94,4.68,0.22,0,-0.04 3EVP,ASP_194,4.26,0,-0.09,0.55 3FRR,LYS 118,11.26,-0.32,0.68,0.39 2HXB.ARG 160.13.05.-0.51.0.6.0.46 1OXZ,ARG_191,12.61,-0.19,0.29,0 3FS3,LYS_40,10.12,-0.38,0,0 3MIX.HIS 496.6.48.-0.22.0.0.21 3IU5,ARG 146,13.3,-0.31,0.61,0.5 1XWM,ASP_156,4.24,0,-0.07,0.51 2F8H,ARG_91,12.14,-0.36,0,0 3FHF,GLU_107,3.87,0.83,-0.85,-0.61 2P65,LYS_108,10.5,0,0,0 2CBE,ASP 180,2.24,-2,-0.43,0.87 4HDE,TYR_163,10.84,-0.85,-0.12,1.81 1NIJ,ARG_172,11.63,-1.52,0.26,0.4 2P5D,LYS 77,10.24,-0.22,0,-0.05 2Q13,LYS 173,10.47,-0.14,0,0.1 3BB7,GLU_123,4.47,0.25,0,-0.28 3EJG,LYS_70,10.71,-0.12,0,0.32 1RHS,TYR_261,11.33,-0.09,-0.66,2.08 2ZCX,ARG_33,13.19,-1.06,0.79,0.96 1GXN.ARG 483.12.1.-0.51.0.0.11 2ZQ5,HIS_183,5.04,-2.77,0.81,0.48 2RJD,HIS_447,5.89,-1.54,0.84,0.1 2HRZ,LYS_123,10.56,-0.09,0,0.15 4FD6,LYS 110,11.36,-0.52,0.85,0.53 4GCO,TYR_234,11.79,0,0.42,1.37 1P1L,GLU_51,3.28,1.12,-2.26,-0.08 2ZQ5,ARG_62,12,-0.55,0,0.04 1XFK,LYS_66,11.2,-0.94,0.85,0.79 1T95,ARG_201,12.47,-0.03,0,0 3U0V,TYR_210,10.27,0,0.12,0.14 2CYG,TYR_116,13.33,0.57,0.04,2.72 2HP7,GLU_193,4.61,1.55,-1.44,0 3I82,ARG 67,14,-0.2,0.83,0.87 2CYG.TYR 284,13,28,-0.85,0.03,4,1 2BDD,LYS_49,10.42,-0.22,0,0.13 1MML,GLU_35,3,0.81,-2.14,-0.18 2P52,CYS_235,9.57,-1.7,-0.2,2.48 3R87,LYS 87,11.64,-0.39,0.8,0.74 1Q46,ARG_135,12.53,-0.35,0,0.38 1SIG,LYS_264,9.78,-0.92,0,0.21 1EV8,ASP_205,3.47,-0.4,-0.58,0.64

3ETV,LYS 242,10,45,-0.08,0,0.02 3EX9,GLU_47,3.74,0.35,-1.05,-0.05 2GZR,ARG_68,12.02,-0.52,0,0.04 1EV8,LYS_233,10.46,-0.36,0,0.32 1L3K.LYS 179.10.94.-0.65.0.58.0.52 3HZO,LYS 54,10,44,-0.06,0,0 2BDV,TYR_119,10.19,0,-0.2,0.39 3H5T,GLU_285,4.7,0.66,-0.03,-0.43 1FKM,CYS_579,12.92,0,0.17,3.75 2E3S.HIS 365,5.4,-0.7,0,-0.4 2IF4,LYS_79,10.35,-0.21,0,0.06 2V4X.CYS 77.12.58.0.-0.11.3.68 3R2E,LYS_27,10.34,-0.22,0,0.06 1NJ4.LYS 59,10.35,-0.29,0,0.15 1KCM.GLU 257.4.84.0.18.0.0.16 3P2F,ARG_136,12.78,-0.54,0.23,0.58 200K,TYR_237,10.85,0,0,0.85 2RJD,GLU_456,5.29,3.77,-2.92,-0.06 2R2Y.GLU 25.4.65.0.33.0.-0.19 2EJB,GLU_112,3.77,0.59,-0.85,-0.46 1P6F,LYS_7,10.44,-0.26,0,0.2 1PDB,GLU_123,5.58,1.1,-0.21,0.19 3M7D.GLU 266.5.19.0.26.0.06.0.36 1UOH,LYS 203,10,48,-0,1,0,0,08 3VHJ,HIS_108,6.81,-1.02,0.85,0.48 2XMZ, ASP_76, 3.13, -0.58, -0.42, 0.34 3JZ9, ASP_415, 4.04, 0, -0.16, 0.4 1V43,ASP 73,3.82,0,-0.12,0.13 4DND,LYS_103,11.33,-0.37,0.84,0.37 2ILR,ASP_432,3.97,0,0,0.17 3GOZ,ARG_146,12.98,-1.22,0.95,0.75 3VHJ.LYS 162.11.29.-0.33.0.85.0.26 1XTZ.HIS 182.6.28.-0.23.0.0.01 3LMO,LYS_54,10.53,-0.16,0,0.19 3I4T,HIS_158,5.34,-2.15,0.85,0.13 1W24,TYR_163,10.22,-0.14,-0.02,0.39 1LZL,HIS 290,6.27,-3.12,0.85,2.03 3KEY,LYS 370,11,23,-0,2,0,37,0,56 1TP6,HIS_10,6.27,-0.85,0.61,0.01 1EV8,CYS_161,12.6,0,0,3.6 3I0C,ASP 183,4.06.0,-0.02.0.28 1Q5Z,ASP_578,2.89,-1.09,-0.18,0.37 3GW3,ASP_29,3.7,0,-0.28,0.18 2H30,LYS_105,10.44,-0.16,0,0.1 1T6L,LYS_158,10.5,-0.16,0,0.16 4AM1,ASP 62,1.8,-2.08,-0.39,0.47 1XDZ.GLU 4.4.65.0.28.-0.3.0.17 1NAR,GLU_150,4.6,0.24,0,-0.15 3VJ8,GLU_202,4.97,0.22,0,0.25 1EV8,ASP 198,4.05,0,-0.35,0.6 2VGY.GLU 152,4.69,0.19,0.0 3RFY,ASP_292,3.03,-0.6,-0.77,0.61 1XDZ,HIS_93,5.81,-0.78,0.19,-0.1 2NYC,HIS_293,6.08,-0.34,0,-0.08 2J8A, ASP 257, 2.71, -0.95, -0.43, 0.29 1Q2Y,ARG_120,12.43,-0.1,0,0.03 1BKB,GLU_110,4.32,1,-0.72,-0.46 1RWZ,TYR_106,10.97,0,-0.04,1.01 1T07,GLU_12,4.57,0.27,0,-0.19 3A0X,LYS 701,10.17,-0.41,0,0.09 3BB7,TYR 168,9.58,-0.85,-0.31,0.74 2EYI,ASP_217,4.07,-0.12,-0.52,0.91 1MD6,ARG_131,12.82,-0.31,0.29,0.35 2OB5,ARG 40,12.29,-0.41,0,0.2 2B0J.GLU 137.4.06.0.37.-0.85.0.05 2YWX,GLU_128,4.61,0.07,0,0.04 3O16, ARG_222, 13.46, -0.31, 0.82, 0.45 3C38,TYR_187,11.15,-0.82,-0.31,2.28 2HXB,GLU_145,4.28,1.11,-0.8,-0.52

2PLQ,TYR_194,9.32,-0.85,-0.33,0.5 2V4U.GLU 408,4,48,2,72,-1,98,-0,75 4EUG,GLU_157,3.47,0.51,-1,-0.54 3OIP,TYR_139,11.26,0,0.16,1.1 3GMS.GLU 252,3.74,0.35,-0.73,-0.38 3OBS.TYR 32,10.98,0.0.0.98 2PGE,ARG_137,13.91,-0.33,1.22,0.53 2RGY,ASP_178,4.11,-0.01,0.13,0.19 2E3C,ASP_279,2.82,-1.34,0,0.36 4H4J,LYS_234,10.69,-0.18,0,0.38 2YX0.GLU 183.4.35.1.8.-1.16.-0.79 1YR6,CYS_207,11.22,0.15,0.47,1.6 1TD6,GLU_230,5.69,1.21,0,-0.02 3GYW,LYS 51,10.64,-0.12,0.0.27 1SIG.ARG 441.12.81.-0.25.0.0.55 3LJN,GLU_37,4.34,0.26,-0.13,-0.28 1PGV,CYS_262,11.45,-0.05,0.57,1.94 1XDZ,LYS_38,10.02,-0.57,0,0.1 3L3P,ASP 452,3.75,-0.5,-0.42,0.87 3LJC,LYS 82,10.62,-0.11,0.0.24 2XHC,LYS_150,10.13,-0.28,0,-0.09 1X1E,ARG_168,12.93,-0.8,0.82,0.41 2BLL,GLU_446,7.39,4.35,-1.67,0.2 1C3K.CYS 40.11.41.0.0.05.2.36 3ONT,ASP_18,4.05,0,0.02,0.22 3V55,GLU_704,4.75,0.19,0,0.06 3GW3,ARG_365,11.2,-1.51,0,0.22 4H86,LYS 102,10.18,-0.38,0,0.06 3ETU,LYS 286,10.75,-0.24,0.16,0.32 2YX0,LYS_304,10.25,-0.5,0,0.25 3EGN,LYS_481,10.15,-0.23,0,-0.13 3ZRI,HIS_33,5.99,-1.13,0.69,-0.06 2P1W.HIS 81,6.31,-0.42,0.05,0.19 4AE7,GLU_75,4.46,0.2,0,-0.24 3RNV,LYS_412,10.54,-0.06,0,0.11 3EJG,HIS_97,6.43,-0.14,0,0.07 1EQ6,LYS 119,10.43,-0.14,0,0.07 4E8B,ARG_146,12.39,-0.39,0,0.28 3JSN,ASP_13,3.97,0,-0.1,0.26 3CCY.GLU 18.4.5.0.19.0.-0.19 1D2K,TYR_93,12.92,-0.03,1.01,1.93 1RI6,TYR 8,12.95,-0.15,0.1,3.01 2P65,LYS_20,10.37,-0.12,0,-0.01 3BWT,HIS_732,5.51,-0.93,0,-0.06 4D8L,GLU_109,4.62,0.1,0,0.03 2WOZ,LYS_426,10.41,-0.13,0,0.03 4EKU,LYS_223,10.44,-0.06,0,0 1Q42,GLU_161,3.44,0.51,-0.85,-0.71 2R2Y,ASP_41,1.76,-2.21,-0.57,0.74 4E9E,GLU_483,4.3,0.32,-0.18,-0.34 2CBE,HIS 4,5.98,-0.45,0,-0.07 2D0A, ARG 164, 12, 35, -0, 23, 0, 0, 07 1S7K,HIS_54,6.03,-0.47,0,0 1AK1,TYR_196,13.48,0,0.11,3.38 3UC9,TYR_57,10.87,0,-0.2,1.08 3TMO,LYS_210,10.46,-0.11,0,0.07 1BKR,LYS 55,10.31,-0.16,0,-0.03 2CBE,HIS_107,5.67,-3.48,0.85,1.8 2IIA,GLU_46,4.65,0.32,0,-0.17 1Y0K,HIS 136,6.57,-0.9,0.87.0.09 2PGX.GLU 26.4.65.0.24.0.-0.08 3GMS,ASP_307,4.04,0,-0.03,0.27 4AF2,LYS_48,10.55,-1.41,0.85,0.61 3HUE,ASP_91,3.33,-0.66,-0.29,0.48 4F3J,ARG 103,12.44,-0.06,0,0 3BA1,ARG_215,13.05,-0.32,0.49,0.38 1RWZ,LYS_98,11.41,-0.34,0.49,0.77 1RAJ,TYR_195,10.41,0,0,0.41 3BCY,HIS_122,6.46,-0.95,0.57,0.34

4FD6.LYS 92.10.04.-0.47.0.0.02 1XIP.ASP 238.3.85,-0.19.0.0.23 4FCU,HIS_176,6.26,-0.85,0.42,0.18 3V46,GLU_386,5.29,1.29,0,-0.49 3A2Z,ASP_96,3.35,-0.44,-0.27,0.26 108B.GLU 60,4.51,0.19,0,-0.18 3V46,TYR_378,11.81,0.83,0.47,0.51 3PZ9,HIS_151,6.33,-0.51,0,0.34 2FD5,LYS_51,9.79,-1.02,0,0.32 1WYC,GLU_297,3.69,0.35,-0.77,-0.4 3ASA.ARG 186.13.11.-0.3.0.57.0.34 1ILW,ARG_38,12.46,-0.33,0,0.3 3OBS.GLU 24.5.46.1.97.-1.42.0.42 4AE7,LYS 78,10,59,-0,14,0,0,24 2B2H,LYS 173,10.21,-0.56,0,0.28 2QHT,GLU_40,4.7,1.25,-0.85,-0.2 2IXM,ARG_293,12.24,-0.26,0,0 3MTT,GLU_499,4.67,0.2,0,-0.03 3FNI,HIS_155,6.23,-0.2,0,-0.07 1R3F,TYR 156,10.83,0.0.38,0.46 2NRK,ARG_90,13.91,-0.34,1.19,0.55 2VGM,LYS 337,10.56,-0.16,0.0.22 1ZBP,ASP 225,3.87,0,-0.21,0.29 3HVM.CYS 324,13.45,-1.67,2.8,3.32 3I4T,GLU_32,5.47,2.42,-0.6,-0.86 1UJ8,ASP_42,3.24,-0.59,-0.38,0.41 2IXM,HIS_230,4.88,-1.41,0,-0.22 1QYI,GLU_100,4.19,0.51,-0.87,0.04 3F6M,GLU 137,4.62,0.12,0,0 3RLN,GLU_729,4.3,0.29,-0.38,-0.11 2X4G.ARG 131.12.05.-0.56.0.0.11 3FK5,HIS_18,7.26,-0.37,0.85,0.28 1WLY,GLU 101,4.47,0.82,-0.47,-0.39 1DZF,ARG 7,12,31,-0,19,0,0 4DND,ARG_11,12,-0.41,0,-0.09 3G9T,LYS_8,10.35,-0.2,0,0.05 2BDD,HIS_126,7.02,-0.44,0.85,0.09 106D, ASP 87, 2.97, -0.85, -0.38, 0.4 20EW,LYS_312,10.16,-0.41,0,0.07 3ZTA,HIS_99,6.57,-0.16,0.23,0 4FZR,ARG_106,12.46,-0.21,0,0.17 3EVP,TYR 95,10.27,0,-0.02,0.29 1CBY.GLU 78.4.69.0.19.0.0 2NRK,GLU_123,4.64,0.17,0,-0.03 4EKU,GLU_113,4.01,0.65,-1.12,-0.02 1SIG,ARG_150,12.41,-0.28,0,0.18 1ZCU,LYS 96,9.63,-0.92,0,0.05 3O6L,LYS 38,10.18,-0.23,0,-0.08 1WXQ,ASP_327,3.82,0,-0.17,0.2 3P2F,ASP_59,2.94,-1.4,-0.06,0.6 1R7J,LYS_55,10.46,-0.04,0,0 3GMS,LYS 10,10,41,-0.09,0,0 2AD1,LYS_198,10.57,-0.32,0,0.38 2O4D,GLU_6,4.65,0.15,0,0 3P51,ARG_22,13.02,-0.31,0.03,0.8 2YX0,GLU_26,3.72,0.34,-0.55,-0.57 10YI,LYS 62,10,42,-0,13,0,0,05 1ANU,TYR_88,10.71,0,0.4,0.3 3LH5,GLU_788,4.27,0.26,-0.46,-0.03 3BJV,TYR_54,10.05,0,-0.03,0.08 3BB7.GLU 214.4.1.0.14.-0.18.-0.35 2F4Q,ARG_97,12.46,-1.12,0.22,0.86 1SJY.GLU 115.4.77.0.17.0.0.1 3BQE,GLU_323,4.66,1.74,-1.3,-0.29 2ZCO,HIS_116,6.25,-0.27,0,0.02 2B61.TYR 329.10.44.-0.08.-0.14.0.66 2QDJ,LYS_153,10.36,-0.26,0,0.12 3CE7,ARG_48,12.55,-0.28,0,0.33 3G9B,CYS_58,9.93,-1.47,0.25,2.15

3EZ7,LYS_29,10.84,-0.34,0.68,0 2WB8,ASP 597,3.05,-0.65,-0.38,0.28 2D0A,ARG_27,12.43,-0.07,0,0 1A8Q,ASP_157,3.38,-0.72,-0.09,0.39 4ECC,LYS_188,10.67,-0.19,0,0.35 2OJQ,LYS 486,10.52,-0.14,0,0.16 1BN6,GLU_287,4.36,3.64,-2.49,-1.31 4EVF,ASP_167,3.92,0,-0.05,0.18 3ZXY,HIS_58,7.21,-2.18,0.85,2.03 2ATR,TYR_115,11.38,0,0,1.38 1R3F,ARG 306,13.28,-0.53,0.74,0.57 1AKO.CYS 177.12.17.0.47.0.05.2.64 20G0.GLU 555,3.68.0.35,-1.11,-0.06 2GAU,LYS_132,10.23,-0.12,0,-0.15 3H6O,LYS 48,10.38,-0.21,0,0,1 4EKU.CYS 120.9.28.0.0.05.0.23 3MIX,GLU_557,6.23,3.07,0,-1.33 3DB9,ASP_210,2.82,-1.2,0,0.23 2BCF,TYR_223,12.18,0.17,0.11,1.9 2PGX,ARG_188,13.23,-0.26,0.53,0.46 1LN4,LYS 19,10,45,-0.05,0,0 1SI7,LYS_67,10.5,0,0,0 3CIV,ASP_116,3.64,-0.33,0,0.18 4DVD.TYR 34.10.28.0.-0.1.0.38 1RZ2,ASP 38,3.76,-0.36,-0.1,0.43 3Q9P,HIS_124,6.85,-0.35,0.63,0.08 3L7N,TYR 36,10,42,0,0,0,42 3CAX,ARG_211,13.7,-1.68,1.56,1.31 1RAJ,LYS_395,10.72,-0.1,0,0.32 1K95,TYR 167,12,0,0,49,1,52 2CL3,LYS_189,10.4,-0.1,0,0 1ZP2,TYR_139,12.79,-1.14,0.08,3.86 1WYC.ASP 357.3.64.-0.84.-0.3.0.98 1C3K.ASP 52,4.25,0,0.27,0.18 2RGY,CYS_336,11.06,0,-0.14,2.2 3N2T,TYR_246,11.18,0,-0.16,1.35 1SQH,CYS_164,9.28,0,-0.08,0.35 1GVP,ARG_16,12.98,-0.15,0.17,0.45 1R3F,ARG_116,12.29,-0.67,0.21,0.25 2E3C,ARG_275,12.67,-0.66,0.41,0.42 1YTD,ARG_251,12.36,-0.31,0,0.16 1XTZ,LYS_40,10.33,-0.17,0,-6.94E-18 3CBN,HIS 165,6.31,-0.32,0,0.13 2RJD,TYR_396,12.36,0.69,-0.09,1.75 2H2Z,LYS_100,10.47,-0.18,0,0.14 1WYC,HIS_309,6.48,-0.37,0,0.35 1PSW,GLU_111,3.96,0.28,-0.74,-0.08 3RJX,ARG 295,11.86,-2.53,0.29,1.61 1YTQ,ARG_187,13.54,-0.35,0.78,0.61 2QHT,ARG_97,12.45,-0.05,0,0 1RI5,TYR_91,10.68,0,-0.26,0.94 2X5Y,LYS 829,10.3,-0.22,0,0.03 1KCM,HIS_60,5.1,-0.86,0,-0.54 1NFN,ARG_61,12.84,-0.32,0,0.67 20KT,LYS_78,10.19,-0.41,0,0.09 2WOZ,TYR_587,10.28,-0.15,0.05,0.38 3T5B,LYS_235,10.59,-0.12,0,0.21 3DHN,LYS_3,10.5,0,0,0 2G3A,GLU_14,4.23,0.17,-0.32,-0.13 1T3Y,ARG_11,12.33,-0.27,0,0.1 2E0T,ARG_196,12.33,-0.17,0,0 1AK1.LYS 81.10.71.-0.24.0.0.44 1WP5,ASP_143,2.8,-1.14,-0.11,0.26 2FM9,LYS_129,10.4,-0.1,0,0 1L2F,GLU_214,3.48,0.73,-1.45,-0.3 3JSN,TYR_22,10.2,0,0.13,0.07 3IRA,GLU_151,4.89,0.23,0,0.17 300P,ARG 87,12,47,-0.03,0,0 2XHC,ARG_338,11.85,-1.05,0,0.39

1CHD.HIS 190.5.07.-2.27.0.85.-0.01 4DNU,HIS_131,3.42,-3.14,0.2,-0.14 3ZXY,HIS 177.6.73,-0.16.0.0.4 2CN1,LYS_141,10.38,-0.39,0,0.27 3ANJLYS 142.11.25.-0.49.0.84.0.39 1TLV.GLU 135.4.99.0.44.0.0.05 1SI7,GLU_275,4.55,4.32,-2.74,-1.52 1YM5,TYR_141,12.2,-0.82,0.04,2.98 1T3Y,TYR_14,9.63,-1.33,-0.41,1.38 3EX9.ARG 160.12.35.-0.16.0.0.01 2WB3,ASP_300,3.83,-0.21,0,0.24 1TLV.ASP 65.4.02.0.0.22 1A8Q,TYR_103,11.59,-0.18,-0.29,2.06 2ZCX.GLU 92.4.57.0.13.0.-0.06 4F8A,ASP 642,4,18,-0.8,-0.02,1.2 3RJX,GLU_130,4.7,0.83,-0.67,0.05 2GAU,GLU_25,3.84,0.77,-1.42,-0.01 3CE7,LYS_37,10.48,-0.05,0,0.04 2VGM.TYR 374.10.24.0.-0.18.0.42 2H2W,LYS_99,10.49,-0.01,0,0 3BPV,LYS_129,10.2,-0.13,0,-0.18 3K9I,LYS_92,10.65,-0.26,0,0.41 2V5B.ASP 202.2.87.-1.24.-0.08.0.4 1M5I.GLU 225.3.78.0.36.-0.74.-0.35 2P0L,GLU_98,4.42,0.61,-0.71,0.03 1W24,GLU_120,5.33,1.34,-0.08,-0.43 3T5B,HIS_170,6.12,-0.4,0,0.02 2CVB,HIS 148,7.67,-0.56,0.85,0.88 1YG2,ASP_20,2.57,-1.53,-0.11,0.41 3EZ7,TYR_109,10.62,0,0.03,0.6 3FFM,ARG_94,12.18,-0.54,0,0.22 2X4G.TYR 127.9.91.-0.69.-0.88.1.48 2VAN,CYS_178,12.6,-0.48,0.31,3.76 1GXN,GLU_402,4.16,1,-0.76,-0.58 2B78,LYS_3,10.42,-0.78,0.18,0.53 1MD6,ARG_102,12.33,-0.25,0,0.07 3B21,ASP_59,3.8,-0.14,0,0.14 30KY,TYR 197,10,74,0,-0,33,1.07 2PGE,CYS_255,12.04,-0.02,0.06,3 3M66,LYS_321,10.16,-0.18,0,-0.15 1V6T,LYS 77,10.68,-0.16,0.0.35 1ZBM.LYS 2.10.71.-0.16.0.0.37 2B0A,HIS_44,2.93,-3.1,0.84,-1.31 3QKY,HIS_31,5.87,-0.46,0,-0.18 3V75,ASP_213,4.13,0,0.04,0.28 1SUU,ASP 660,3.32,-0.44,-0.34,0.3 1ZCU.TYR 223.11.15.0.0.29.0.86 3EJC,ASP_135,2.29,-2.11,-0.64,1.25 2ZTY,GLU_24,3.53,0.6,-1.49,-0.1 204D.ASP 13.3.91.0.0.0.11 3ADO.GLU 93,5.52,4.33,-2.52,-0.78 2PIM,GLU_34,4.54,0.05,0,-0.02 3H6Q,CYS_105,10.19,-0.81,-0.16,2.16 2ZQ5,TYR_36,11.34,-0.03,-0.73,2.1 1IDK, ARG 176, 12.24, -2.07, 0.28, 1.53 1XDZ,GLU_5,3.94,0.44,-0.84,-0.16 2IIA,ARG 61,12.61,-0.13,0,0.24 1VJG,TYR 43,11.3,0.56,0.38,0.36 1YR6,GLU_120,4.65,0.32,0,-0.17 10XZ,ARG 260,12.45,-0.36,0,0.3 1W7B,HIS_94,6.36,-0.65,0.06,0.46 2Q13,LYS_192,10.8,-0.88,0.59,0.58 3FRR,ARG_53,13.91,-0.79,0.76,1.45 2ZQ5,ASP_32,4.18,-0.82,-0.05,1.25 105T.GLU 151.4.05.0.75.-0.83.-0.38 2Z0M,ARG_70,12.78,-0.18,0,0.47 1LN4,GLU_36,4.75,0.26,0,-0.01 3BCH,LYS 52,10.35,-0.15,0.0.02 2E3C,ASP_414,3.8,0,-0.18,0.18

1SUU.ASP 543.3.8.0.0.0 3JSN,LYS_207,12.11,-0.45,1.31,0.76 2BAA, ASP_235, 3.9, -0.78, 0, 0.88 1SIG,LYS_236,10.36,-0.08,0,-0.06 3GS9.CYS 95.12.21.-0.13.0.19.3.15 3TIR.LYS 17.10.44.-0.06.0.0 1ZBS,LYS_21,10.41,-0.15,0,0.06 1SIG,GLU_219,4.7,0.16,0,0.04 1RI5,ARG_165,13.09,-0.27,0.22,0.64 1IDK,ARG_127,12.13,-0.52,0,0.15 3K1H.GLU 134,4.54,0.72,-0.22,-0.47 3N2T,LYS_307,10.61,-0.07,0,0.17 3GMS,GLU_99,4.54,1.08,-0.85,-0.2 2D7U,ASP 95,3.92,0,-0,16,0,28 1ZBPLYS 76.10.29.-0.19.0.-0.02 3M3P,TYR_141,12.85,0.85,0.65,1.34 3PZ9, ASP_360, 2.45, -1.7, -0.78, 1.13 2RIS,GLU_166,3.82,1.31,-1.92,-0.08 1DUN,HIS_108,6.3,-0.2,0,0 2P0L/HIS 69.6.2.-0.35.0.0.05 2X4J,LYS_80,10.49,-0.07,0,0.06 2OJQ,GLU_570,4.5,0.7,0,-0.7 2W0G,GLU_257,3.48,0.4,-0.85,-0.57 4DEZ,CYS 140,11.44,-0.01,-0.13,2.59 4EF5,TYR_164,10.55,0,-0.13,0.68 2IDC,GLU_121,4.6,0.1,0,0 1A8Q,ARG_233,13,-0.31,0.45,0.37 3BPV,HIS_28,6.22,-0.35,0.05,0.02 2V4U.GLU 438,3.73,1.47,-1.09,-1.14 1KCM,GLU_132,3.72,0.26,-0.85,-0.19 3KB5,ARG_404,12.43,-0.07,0,0 3RJX,LYS 266,10.7,-0.22,0.0.42 3FXH.GLU 39,4.84,0.39,0,-0.04 1V43,LYS_366,11.5,-0.29,0.85,0.44 3N0K,TYR_59,10.76,0,0.21,0.55 2YX0,HIS_83,3.38,-3.12,0,0 2WOZ,ASP_304,3.88,-0.12,-0.37,0.56 3PZ9,HIS_283,5.53,-0.86,0,-0.1 2H8O,CYS_119,13.8,0.04,1.32,3.46 1WXF,GLU_124,4.23,0.17,-0.42,-0.02 2EA9,GLU_30,4.06,0.25,-0.32,-0.37 1VSM,GLU 133,4.35,0.22,0,-0.38 3EUR.GLU 45.4.39.0.22.-0.35.0.02 1RKA,ASP_202,3.08,-0.85,-0.53,0.65 2P52,HIS_165,5.65,-0.67,0.39,-0.58 2H2W,ASP_97,3.98,0,0,0.18 4H4J,GLU_169,3.66,1.68,-2.45,-0.06 2GEN,HIS_53,4.51,-1.94,0,-0.04 3K1H,GLU_123,4.82,0.25,0,0.07 10I7,GLU_83,5,1.34,-0.82,-0.02 3ETU,LYS 99,10.42,-0.08,0,0 3PBH,TYR 94,10,51,0,0,21,0,3 1PSW,ASP_211,3.95,0,-0.03,0.18 2RFA,GLU_93,3.25,0.31,-1.56,0 1GVP,HIS_64,6.16,-0.3,0,-0.04 2G70,GLU_111,5.02,0.24,0,0.28 4DIU,LYS 143,12.41,-0.7,1.59,1.02 1C3K,TYR_56,11.84,0.85,0.58,0.4 3L3P,ARG_292,13.44,-0.29,0.78,0.45 2W0G,ASP_169,2.76,-0.85,-0.46,0.26 2CN1.ARG 253,13,21,-1.09,0.54,1.26 4FCU,CYS_128,11.62,0,0.05,2.57 3JZN,ASP_155,3,-1.23,-0.2,0.64 3LMO,ASP_6,3.28,-0.54,-0.32,0.34 3BWT,ASP_586,3.09,-0.6,-0.35,0.23 3GW3,GLU_48,4.65,0.12,0,0.03 10IS,GLU_264,4.18,0.36,-0.07,-0.62 1UAJ,GLU_185,4.74,0.24,0,0 1XEU,LYS_296,10.53,-0.1,0,0.13

3M7D,ARG_283,13.8,-0.29,1.2,0.38 3CJW.GLU 347.4.62.0.63.0.-0.51 2QEV,TYR_58,10.48,0,0.25,0.23 3I82,TYR 160,10.37,0.0.21,0.17 3GA2,LYS_75,11.19,-0.38,0.55,0.51 20PJ,ARG 15,12.38,-0.22,0,0.1 2OJQ,GLU_565,4.6,0.65,-0.33,-0.22 3COU, ASP_31, 3.49, -0.83, -0.23, 0.75 1FQI,ASP_306,1.41,-3.19,-0.67,1.46 2VGM.GLU 232.4.79.0.29.0.1.73E-18 3GE9,ARG 41,13,25,-0,51,0,66,0,6 2EFK,ARG_139,12.82,-0.29,0,0.6 1X7F,HIS_58,5.87,-0.78,0,0.14 3DSH,TYR 266,10,73,0,0.06,0.67 20YZ.LYS 4.10.59.-0.17.0.0.26 3E7P,LYS_212,10.38,-0.12,0,0 1GQE,CYS_274,11.1,-0.76,0.1,2.76 2D0A,ARG_246,11.83,-1.15,0.22,0.28 1MTZ.ARG 252,12.58,-0.35,0.0.43 1Q46,GLU_123,3.92,0.32,-0.19,-0.71 1WNH,ARG_115,12.46,-0.06,0,0.02 1LZL.GLU 187.6.91.2.38.0.0.04 3BA1,CYS_122,9.62,-0.02,-0.02,0.67 2GZQ,GLU 8,4.64,0.17,0,-0.03 1SBX,ARG 100,13.36,-0.36,0.71,0.51 2Q07,LYS_449,9.01,-1.5,0,0 3FS3,HIS_72,5.98,-0.76,0,0.24 3IL3,ASP_184,2.91,-1.67,0,0.78 3O7K,GLU 59,3.65,0.37,-1.2,-0.02 3ETV,LYS_213,10.6,-0.16,0,0.26 1LZL,ASP_231,2.36,-1.81,-0.16,0.54 1GQE,ASP_71,3.59,-0.85,-0.18,0.82 2H2W,TYR 151,11.97,0.85,0.24,0.88 301C.GLU 316.4.56.0.06.0.0 3S0A,LYS_99,10.07,-0.57,0,0.14 2B2H,LYS_243,10.4,-0.1,0,0 1U7U,TYR_207,9.97,0,-0.22,0.2 3N0K,CYS 60,11.57,-0.63,-0.52,3.73 3T57,GLU_300,4.84,0.16,0,0.17 2PPN,CYS_22,11.29,0,0.12,2.16 1XIP,ASP_6,3.92,0,-0.02,0.15 1PVT,TYR 57,10.07,-1.07,-0.03,1.17 1MD6,ASP 103,2.94,-0.81,-0.39,0.34 1TLV,ASP_261,2.57,-1.46,-0.27,0.51 2X4G,CYS_157,9.75,0,-0.26,1.01 1CHD,GLU_218,4.35,1.73,-1.56,-0.33 2XJ4,ARG 185,11.97,-1.34,0.09,0.73 3A0X,ARG 616,13.66,-0.23,0.92,0.47 2A4D,GLU_151,4.31,0.38,-0.51,-0.07 2Q13,GLU_223,4.63,0.13,0,0 3RKV,ARG_333,12.43,-0.07,0,0 3VHJ.ARG 69.12.47.-0.26.0.0.22 2GZQ,ASP_26,2.91,-0.78,-0.38,0.28 3C6B,TYR_78,10.28,-0.48,-0.15,0.91 1TXJ,GLU_12,5,0.56,0,-0.05 1Z9L,TYR_52,13.72,0.77,0.43,2.52 1WP5.GLU 174.4.22.0.66.-0.84.-0.1 3N0K,LYS_51,10.61,-0.28,0,0.38 3V55,LYS_661,10.46,-0.06,0,0.02 3IBT,ARG_146,11.62,-1.31,0,0.42 2G9D,ASP 272,3.85,0,-0,12,0,16 4E9E,HIS_561,6.03,-0.24,0,-0.23 2H14,LYS_78,9.08,-0.36,0,-1.07 3N2T,ASP_4,3.61,-0.72,-0.4,0.93 2B6P,GLU_3,4.55,0.16,0,-0.11 2013.GLU 53.4.65.0.15.0.0 2QOP,LYS_6,10.91,-0.25,0.66,0 3G9G,ARG_5,12.57,-0.43,0,0.51 1JYH,GLU_61,4.58,0.08,0,0

2BQQ,LYS_112,10.31,-0.35,0,0.16 4DEZ,GLU 102,3.75,1.09,-1.52,-0.33 1RAJ,GLU_254,4.66,0.17,0,-0.01 2012.LYS 130.11.35,-0.56,0.83,0.57 3US6,CYS_115,11.21,-0.02,0.14,2.1 1SI7,CYS 109,11.05,-0.36,0.1,2.3 1XEU.LYS 57.10.18.-0.35.0.0.04 1PV5,GLU_179,4.94,0.33,0,0.1 1UOH,HIS_144,4.94,-2.67,0.81,0.3 3V4G,ARG_110,12.45,-0.12,0,0.07 2H2W,GLU 122,4.63,0.12,0,0.01 1WPA,GLU_472,4.57,0.07,0,0 2RIK.GLU 93,3.84,0.28,-0.52,-0.42 3BQW,GLU_137,6.45,5.01,-3.06,0 3C5V.GLU 209.4.99.0.28.0.0.21 2IXM,LYS 63,11,47,-0,51,0,63,0.85 3AUF,GLU_174,7.28,2.8,0,-0.02 3M3P,GLU_126,3.89,0.49,-0.78,-0.32 2XMZ,GLU_35,4.64,0.13,0,0.01 2ZTY,LYS_176,9.79,-0.49,0,-0.22 3GV0.LYS 186.10.35.-0.22.0.0.07 2PLQ,ARG_176,11.38,-1.19,0,0.07 1RI5,LYS_75,10.88,-0.17,0.19,0.35 3KEY,ASP 397,4.08,-0.67,-0.16,1.12 1NFN.LYS 146.10.24.-0.13.0.-0.13 3G9G,GLU_117,4.47,0.4,-0.17,-0.26 1DVO.ASP 89.3.69.0.-0.3.0.18 3ILC,GLU_179,5.14,1.66,-0.98,-0.03 1G5Z,LYS_136,11.15,-0.76,0.57,0.85 3K1H.GLU 81.4.44.0.27.-0.27.-0.06 1D2K,HIS_54,4.4,-2.18,0,0.07 2OSA,ARG_445,12.14,-0.34,0,-0.02 1DOV.TYR 222.10.41.0.0.06.0.35 3EX9,GLU 103,3.6,0.32,-0.86,-0.35 2IF4,TYR_67,12.75,0,0.56,2.19 4AE7,TYR_215,10.42,0,-0.06,0.47 2D2S,LYS_740,11.01,-1.44,0.85,1.09 2YT4,GLU_502,4.69,0.18,0,0.01 1KW4,ASP 34,3.95,0,-0.05,0.2 1NAR,ASP_203,3.02,-0.69,-0.35,0.26 1RHS,LYS_223,9.99,-0.7,0,0.19 2EYI,LYS_121,10.44,-0.13,0,0.07 3HVW,GLU 257,4.63,0.13,0,0 3PAC, ARG_94, 12.5, -0.28, 0, 0.28 1FQI,ASP_386,3.75,-0.44,-0.38,0.76 2GZR,GLU_305,4.4,0.45,-0.63,0.08 3AU3,GLU_468,4.32,0.24,0,-0.42 2B61.TYR 171.12.32.0.36.0.52.1.45 3LH5,GLU_756,4.41,0.25,0,-0.33 2Q12,LYS_173,10.53,-0.18,0,0.21 2RIK,ARG_105,13.05,-1.08,0.77,0.86 1ZBP,ASP 115,3.32,-0.85,-0.03,0.4 2IQT,GLU_83,4.63,0.28,0,-0.14 3TIR,ARG_185,12.24,-0.41,0,0.16 3CO1,GLU_13,3.55,0.12,-1.06,-0.01 2DFL,ARG_284,13.42,-2.13,1.51,1.54 2QDJ,HIS_281,5.25,-1.33,0.45,-0.37 2BAA, ASP_135, 3.19, -0.98, -0.02, 0.4 1YLN,LYS_75,10.49,-0.11,0,0.09 1RAJ,LYS_220,10.2,-0.3,0,0 3HVM,HIS_202,11.69,-3.58,2.45,6.32 3DSH,ARG 432,12,41,-0.09,0,0 2VAN,LYS_206,10.48,-0.24,0,0.22 2HP7,ARG_119,12.19,-0.81,0,0.49 20EW,ASP_143,3.67,0,-0.43,0.3 1UXO.GLU 124,4,36,0.23,-0.34,-0.02 2FBQ,ARG_179,12.22,-0.32,0,0.05 1K95,ASP_104,3.93,0,-0.05,0.17 3V4G,ARG_48,12.23,-0.27,0,0

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2P0L/GLU 4,4.62,0.15,-0.21,0.18 3N2T,ASP_223,3.75,-0.29,0,0.24 3EJG,ASP_50,3.74,-0.74,-0.37,1.05 1T95,LYS_105,9.83,-1.34,0.26,0.4 3EVN.ASP 274.3.92.0.0.12 3LMF,GLU 89,4,45,0,31,0,-0.36 2P65,LYS_104,10.39,-0.22,0,0.11 3H5T,ASP_101,3.91,0,0,0.11 2X4G,ARG_237,11.19,-2.72,0.42,1 2X4J.TYR 123.10.51.0.0.17.0.34 2Z0M,LYS_97,10.41,-0.22,0,0.14 1LFP.LYS 220.9.95.-0.55.0.0 3CBN,HIS_40,6.27,-0.64,0.2,0.21 1V8E.ARG 114.12.54.-0.24.0.03.0.25 1X6J.LYS 40.10.36,-0.45,0.0.31 1SJY,ARG_24,12.77,-0.24,0.14,0.37 3IL3, ASP_72, 3.29, -0.64, -0.21, 0.34 3UC9,HIS_176,4.11,-2.52,0,0.13 2OSA.ASP 433.3.57.-0.43.0.0.2 1WYC,TYR_81,10.3,0,0.05,0.25 1L2F,GLU_46,4.96,0.47,0,-0.01 10IS,ASP_276,2.77,-1.52,-0.02,0.5 3N0K.LYS 32.10.01.-0.71.0.0.23 1SNT.CYS 125,12,18,0,0,39,2,8 3BQW,ASP_175,4.03,0,0,0.23 4ETX,ARG_256,12.52,-0.14,0,0.16 2XMZ,ARG_187,12.68,-0.79,0.46,0.51 1KW4,ASP 38,4.21,0,0.1,0.31 3TIR,ARG_141,12.69,-0.94,0.8,0.33 2Q98,GLU_131,4.87,0.84,-0.45,-0.03 10TM,LYS_89,10.55,-0.2,0,0.24 2BT8,ASP 259,2,79,-1,4,-0,08,0,47 1FKM,TYR 629,9.86,-0.04,-0.37,0.27 2D7J,HIS_82,3.51,-3.26,0.27,0 2G70.GLU 118.4.34.0.4.-0.56.0 10I7,GLU_259,4.6,0.33,0,-0.23 1WP5,HIS_323,6.39,-0.12,0,0.01 2Z0M,HIS 203,6.9,-0.42,0.52,0.29 4FZR,CYS_286,11.36,0,-0.09,2.44 4E8B,ARG_220,12.34,-0.16,0,0 1WNH,TYR 23,11.39,-0.8,0.27,1.92 3BPV.ASP 118.3.84.0.-0.11.0.14 1P4X,HIS_45,4.93,-1.38,0,-0.19 3RFY,LYS 138,10,43,-0.06,0,-0.01 3CIV,GLU_159,3.93,0.37,-0.56,-0.37 2EDM,ASP_86,2.85,-1.11,-0.12,0.29 1XFK.TYR 88,11.63,-0.04,0.31,1.35 1P4X,GLU_250,4.5,0.33,0,-0.34 1SQW,GLU_14,3.99,0.34,-0.37,-0.48 2RIK,LYS 32,10.39,-0.21,0,0.1 2PPN,LYS 44,10.31,-0.09,0,-0.1 1YLN,ARG_136,11.94,-0.24,0,-0.32 1TD6,LYS_110,10.51,-0.15,0,0.16 1GPP,TYR_101,10.35,0,0,0.35 1QYI,TYR 361,11.51,0,0.49,1.01 2X4G,ARG_33,12.22,-0.52,0,0.24 2IIA,LYS_70,10.14,-0.36,0,0 2BCF,LYS_262,10.43,-0.07,0,0 2JHY,LYS_135,9.97,-0.21,0,-0.31 1XFK,ARG 25,12.94,-0.46,0.76,0.15 2GS5,ASP 104,3.92,0,0,0.12 20EW,ASP_321,3.71,-0.54,-0.02,0.46 2ZCX,GLU_127,4.34,0.28,-0.44,0 2H2Z,ASP 48,2.82,-1.35,-0.1,0.47 1WOU,GLU_109,4.01,0.34,-0.8,-0.03 2BDD,TYR_83,12.83,0,0.86,1.98 1LPL,ASP_215,4.68,0,-0.03,0.91 3FHF,TYR_199,10.28,0,-0.07,0.36 1SNT,GLU_323,4.54,0.1,0,-0.06

3EGN,ARG 391,12.71,-0.2,0.09,0.32 2NSN,ARG 69,12.52,-0.33,0.08,0.27 3QAV,CYS_75,11.62,-0.07,-0.95,3.65 4DEZ,ASP_24,2.87,-1.03,-0.43,0.53 1ES5,TYR 63,13,58,0,8,0,39,2,38 4FZR.GLU 269.4.57.0.07.0.0 3DHN,ARG_123,12.02,-0.67,0,0.18 3ANJ.ASP 45.3.78.0.-0.26.0.24 3IRA,ASP_63,2.78,-1.35,-0.38,0.71 2EFK.CYS 248.9.64.-0.54.0.1.1.07 1XFK,LYS 290,10.34,-0.3,0.0.14 1SNT,CYS_164,11.43,-1.88,0.16,4.14 1MUF,CYS_318,12.22,-0.15,0.12,3.24 1X8F,LYS 154,9.42,-0.76,0,-0.31 3GW3.ASP 54.3.57.-0.5.-0.12.0.39 1D2K,ASP_301,3.71,-0.03,-0.27,0.22 2QRX,ARG_28,12.15,-0.26,0,-0.08 3I0C,HIS_301,6.25,-0.82,0,0.57 1U53.LYS 63.12.44.-0.55.1.61.0.88 3BWT.ASP 750.3.88,-0.03,-0.34,0.44 2B6P,CYS_144,10.62,-0.08,-0.05,1.75 3E5T,LYS_44,10.43,-0.14,0,0.07 3ANJ,LYS_287,9.64,-0.83,0,-0.03 2FC3.GLU 44.4.53.0.29.0.-0.26 3LQE,CYS_451,12.33,-0.95,0.04,4.23 3NJM,ASP_70,2.3,-2.43,0,0.92 4EZB,ARG_225,12.48,-0.53,0.03,0.49 3CGW,GLU_263,4.96,0.29,0,0.18 2IF4,LYS 50,11,22,-0,32,0,43,0,6 1T6L,HIS_131,6.4,-0.1,0,0 3ADO, ASP_170, 3.15, -0.64, -0.32, 0.31 1GXN,TYR_494,13.81,0,0.38,3.44 3C2E,ARG 166,10.96,-1.37,0,-0.17 1I60,GLU_21,4.68,0.25,0,-0.07 3G9G,ARG_90,12.4,-0.17,0,0.07 3FK5,ARG_319,13.28,-0.82,0.83,0.77 3V75,LYS 81,10.97,-0.75,0.64,0.59 1PSW,TYR_169,10.25,-0.04,0,0.29 1YTD,ASP_101,3.94,-0.5,-0.3,0.93 3BQW,LYS_88,10.69,-0.4,0.15,0.44 3R87,HIS_6,7.14,-0.4,0.85,0.19 1X1E,GLU 88,4.73,0.29,0,-0.06 3FNI.TYR 17,9.78,-0.41,-0.08,0.27 3RFY,LYS_315,10.42,-0.08,0,0 3FHF,ARG_136,13.51,-3.36,1.08,3.29 1SI7,ARG_136,13.83,-0.45,1.29,0.49 3T57,LYS_327,10.16,-0.55,0,0.2 1WPA,LYS_496,11.43,-0.3,0.47,0.75 3LPZ.GLU 18.4.5.0.21.0.-0.21 2FBI,ARG_5,12.46,-0.04,0,0 2EYI.LYS 214,11.03,-0.16,0.3,0.39 3IVF.CYS 286,11.17.0.-0.05,2.23 2R4Q,ASP_190,3.96,0,-0.1,0.26 2YLF,GLU_145,4.32,0.3,-0.5,0.01 3FS3,LYS_59,10.53,-0.23,0,0.26 1H09,TYR_176,12.43,0,0,2.43 3RLN,HIS_601,3.25,-2.94,0.78,-1.08 3P2F,GLU_29,4.04,0.42,-0.4,-0.48 3LH5,ARG_544,13.63,-0.31,0.75,0.69 200K,GLU_351,4.43,0.42,0,-0.49 1R3F.ASP 238.3.19.-1.55.-0.46.1.4 3K8J,LYS_74,9.79,-0.47,0,-0.24 1MD6,GLU_111,4.54,0.87,-0.82,-0.01 3DSH,GLU_222,3.86,0.39,-0.37,-0.65 1ZCE,CYS 68,10.42,-0.11,0.09,1.45 3G6S,CYS_31,10.78,-0.12,0.05,1.85 1SQW,LYS_78,10.35,-0.13,0,-0.03 2R51,ARG_294,12.96,-2.24,1.45,1.25 3RFY,ASP_242,3.36,-0.84,-0.41,0.8

3ERF,ARG_171,12.56,-0.16,0,0.22 3CGW.LYS 212,10.94,-0.28,0.04,0.68 2AHE,GLU_83,4.46,0.16,0,-0.2 3C6B.GLU 255.4.7.0.28.0.-0.08 3F5D,LYS_140,10.4,-0.12,0,0.02 3IU5,LYS 102,10.33,-0.17,0,0 2XHC,LYS_300,10.54,-0.05,0,0.09 2FXT,GLU_334,4.71,0.21,0,0 2EYI,GLU_142,3.27,0.38,-1.23,-0.38 1FO9.LYS 284,9.61,-0.74,0,-0.14 1PVT.LYS 96.10.19.-0.4.0.0.08 4DIU,GLU_109,4.59,0.99,-0.73,-0.16 1P2F,CYS 62,11.86,0,0.05,2.81 3V3T.TYR 72,10.25,0.0.0.25 2CIU,ASP 130,1.52,-2.43,-0.56,0.72 2ATR,ARG_80,12.35,-0.15,0,0 3EX9,ASP_88,4.14,0,0.12,0.22 2FB6,TYR_26,9.09,-1.36,-0.01,0.47 4FH3,ASP_59,3.59,0,-0.36,0.17 2RGY.ASP 229.3.71.0.-0.48.0.38 1G8P,LYS_130,10.45,-0.05,0,0 3I0C,ARG 161,12,37,-0,13,0,0 1Y2Q,GLU_12,3.61,0.36,-0.6,-0.65 2BLL,GLU 366,4.78,0.28,0,0 3IVF,CYS 243,12,43,0,0,17,3,26 1FKM,LYS_257,10.04,-0.26,0,-0.19 2CE6,TYR_69,11.96,0.67,0.24,1.05 109G,ARG 229,11.62,-0.88,0.0 2I88, ASP 408, 3, -1.1, -0.05, 0.35 2AXO,ASP_139,3.72,0,-0.4,0.32 1042.TYR 172.10.37.0.0.12.0.25 3MTT,GLU_512,4.46,0.35,0,-0.39 1NIJ.ARG 317,12.55,-0.32,0,0.37 3ETV.LYS 163,10,42,-0,12,0,0.03 2YT4,HIS_517,6.07,-0.32,0,-0.11 2NSN,GLU_84,4.69,0.33,0,-0.14 1R29,TYR_91,11.87,-0.74,-0.13,2.75 2P0Y,ASP 146,3.47,-0.36,-0.15,0.18 3CNU,CYS_51,10.21,-0.64,0.12,1.74 1PV5,GLU_185,4.69,0.53,0,-0.35 1BN6,GLU_154,4.51,0.13,0,-0.11 4DND,LYS 77,10.35,-0.15,0,0 2AXO,LYS 127,10.33,-0.17,0.0 2ILR,GLU_279,4.63,0.13,0,0 2H85,ASP_267,2.59,-1.61,-1.06,1.46 3ON1,ASP_54,3.4,-0.42,-0.24,0.27 2QEV,LYS 99,10.33,-0.19,0,0.02 1TR9,ARG 34,12,76,-0.92,0.59,0.58 2WOZ,GLU_572,3.66,0.38,-0.61,-0.61 2GYZ,HIS_43,6.63,-0.22,0.17,0.18 2G9D,GLU_71,5.78,2.07,-0.87,0.08 108B,LYS 89,10.57,-0.15,0,0.22 1ZBM,HIS_33,4.35,-1.53,0,-0.62 30KO,ASP 662,4.04,0.0.0.24 3QKY,ARG_168,13.01,-0.39,0.24,0.66 1QYI,GLU_28,5.66,3.65,-0.93,-1.57 108B.LYS 36.10.93.-0.61.0.62.0.42 4F8A,LYS_650,10.26,-0.26,0,0.02 2QV2,LYS_156,10.28,-0.22,0,0 106D,HIS_21,5.99,-0.37,0,-0.14 2WZ9.GLU 14.4.5.0.0.0 2PIM,ARG_93,12.26,-0.24,0,0 100X.GLU 123.4.08.0.34.-0.61.-0.15 1R7J,LYS_72,10.45,-0.12,0,0.07 3LH5,ARG_715,12.1,-0.43,0,0.03 2JHY,ARG 180,11.9,-1.02,0.0.41 2D8N,CYS_39,10.41,0,0.14,1.27 3GV0,ASP_157,3.94,0,0,0.14 3QKY,GLU_255,4.71,0.18,0,0.04

1J74,ARG 124,13,28,-0.42,0.69,0.51 3TOW.ARG 142.12.29.-0.21.0.0 3E7P,ASP_117,4.1,-0.75,-0.38,1.42 3ETU,LYS_59,10.49,-0.11,0,0.1 1EQ6,ASP_213,2.61,-1.56,0,0.37 2CWC, ARG_10, 12.15, -0.92, 0.01, 0.57 1ZBS.TYR 231,12.07,-1.18,0.77,2.48 3K9I,TYR_77,10.71,0,0.03,0.69 1NWA,HIS_155,4.47,-2.79,0.84,-0.08 3F5D,GLU_165,4.79,0.41,0,-0.11 1SQW,HIS_82,4.73,-1.23,0,-0.54 1XTD,ASP_122,3.67,-0.51,0.18,0.2 2B78,HIS 311,5.69,-0.77,0.6,-0.65 2DFL,LYS_81,10.2,-0.3,0,0 1X04,ASP_110,4.75,0,0.09,0.87 1Q46,LYS_77,10.52,-0.2,0,0.23 1H09,CYS_45,9.82,-0.21,0,1.03 2YX0,ARG_233,12.3,-0.31,0,0.11 1FKM,LYS_608,10.46,-0.17,0,0.12 2VGM,ASP 380,3.9,-0.41,0.09,0.41 1MJS.HIS 288.7.11.-0.3.0.83.0.07 2H2Z,CYS_117,12.17,0,0.07,3.11 1AKO,ARG_267,12.43,-0.07,0,0 1V6T.HIS 62.4.58.-3.55.0.78.0.85 3M7G,HIS 260,6.88,-0.94,0.77,0.56 2APL,TYR_127,11.39,-0.32,0.34,1.38 1UOH.GLU 204,4,48,0,19,0,-0,21 2YYO,TYR_65,11.15,-1.84,0.29,2.71 3GA2,HIS 237,6.63,-0.21,0,0.34 20DJ.LYS 80,10.54,-0.17,0.0.21 3MEW.CYS 243,10.09,-0.22,0.17,1.15 3FS3,ASP_119,3.16,-0.56,-0.28,0.2 1YTO, ARG 88, 12, 52, -0, 19, 0, 0, 21 4GCO.GLU 226.4.45.0.24.0.-0.29 1FHL,TYR_111,11.75,0.85,0.38,0.52 20KT,LYS_200,10.64,-0.26,0,0.39 3BZT,GLU_327,4.79,0.1,0,0.18 2E3I,GLU_79,4.61,0.11,0,0 1PBV.LYS 78,10.5,-0.19,0,0.2 1SNT,LYS_262,10.31,-0.19,0,0 1WLY,HIS_299,5.66,-0.59,0,-0.25 1YIB,ARG_222,12.47,-0.22,0,0.2 3C5V,GLU 140,4.67,0.19,0,-0.01 3F7M,HIS_176,4.01,-3.01,0.81,-0.28 1WJG.TYR 45,10.15,0,-0.02,0.16 1HUF,HIS_62,5.59,-0.86,0.1,-0.15 3LD1,LYS_66,10.16,-0.3,0,-0.04 1T95,ASP 67,3.81,0,-0.15,0.16 1X9G,ASP_141,3.72,0,-0.4,0.32 2ZCO,TYR_192,10.75,0,0.16,0.58 3M7G,ARG_14,12.88,-0.3,0.25,0.43 3AU3,GLU 418,4.69,0.21,0,-0.02 3NR5,TYR_144,12.66,0.11,1.05,1.49 2E3I,LYS_98,10.31,-0.19,0,0 1WLY,GLU_184,2.84,0.37,-1.39,-0.63 1RSS,LYS_36,10.35,-0.15,0,0 2YWX,LYS_85,10.46,-0.08,0,0.04 1ZBM,GLU_121,4.7,0.82,-0.21,-0.41 2OJQ,ASP_579,3.16,-0.85,-0.04,0.26 1QQL,ARG_88,13.24,-0.47,0.57,0.64 3ETV,ASP 12,3.7,0,-0.3,0.19 1MIX.CYS 243.12.49.0.0.14.3.35 3ERF,LYS_59,10.11,-0.68,0,0.29 1PBV,GLU_211,4.44,0.23,0,-0.29 1RWZ,TYR_59,12.39,-0.01,0.17,2.23 2IIA.GLU 31.4.01.1.29.-1.63.-0.16 3DZ1,HIS_254,5.24,-1.19,0,-0.07 3T5B,ASP_333,4.19,0,-0.06,0.45 1UAJ,ASP_69,3.58,-0.5,-0.55,0.83

1L3K.LYS 144.10.44.-0.06.0.0 1Y0K,HIS_127,6.24,-0.23,0,-0.02 1ILW,LYS_28,10.82,-0.15,0,0.47 3RAZ,ASP_150,2.94,-0.77,-0.45,0.36 4EKU.ASP 211.4.26.-0.29.-0.07.0.83 3CCY,ARG 105,12.05,-0.78,0.0.32 3A0X,HIS_729,5.82,-1.99,0.78,0.53 2YLF,ARG_79,12.66,-0.49,0,0.64 1EV8,HIS_51,6.11,-0.24,0,-0.14 1PNE.ASP 75.2.82.-1.98.-0.53.1.52 3TMO,ARG_331,12.64,-0.1,0,0.23 3LPZ,ARG_204,12.05,-0.64,0,0.2 2XJ4,ARG_46,12.43,-1.17,0,1.1 1TP6.LYS 62,10.2,-0.3,0,0 4ETX.TYR 327.10.29.-0.68.-1.31.2.27 3DTE,ASP_152,3.92,0,-0.28,0.39 3R87,TYR_23,10.25,0,0.03,0.21 3US6,TYR_123,12.75,0,0.45,2.3 208LGLU 53.4.37.0.41.-0.17.-0.36 4H4J,TYR_98,13.21,0.78,0.15,2.29 2JKF,LYS_73,11.09,-0.33,0.55,0.37 2E3I,LYS_127,10.45,-0.05,0,0 2Y2T,CYS_31,10.92,0.19,0.38,1.35 1XDZ.GLU 12.4.51.0.21.0.-0.2 1P1L,GLU_24,4.47,0.19,0,-0.23 1GXN,ARG_610,13.53,-0.39,1.17,0.24 2G9D,ARG_159,11.3,-1.29,0,0.08 3PBH, ASP 159, 3.62, -1.32, -0.08, 1.21 3Q1C,GLU_258,4.41,0.29,0,-0.39 3BJV,ASP_78,3.67,-1.18,-0.26,1.31 3G6S,LYS_1,10.35,-0.22,0,0.06 3KEY.GLU 409.5.51.1.08.0.-0.08 105T.GLU 451.4.75.0.22.0.0.03 2PWQ,GLU_10,5.19,3.33,-2.17,-0.47 3BQW,GLU_320,4.34,0.33,-0.32,-0.17 1WP5,GLU_192,4.55,0.05,0,0 4EKU,GLU 263,3.56,2.4,-1.27,-2.07 1RZ2,HIS 140.6.63,-2.06,1.59,0.61 3ELI,GLU_130,4.95,0.37,0,0.08 3LJI,ASP_132,3.85,0,-0.09,0.14 3GFP,ASP_374,4.21,0,0.13,0.29 2E0T,HIS_171,5.34,-1.02,0,-0.13 1V6T,ARG_15,12.44,-0.06,0,0 1MN3,ASP_444,4.11,0,-0.05,0.35 2WOZ, ASP_458, 2.64, -1.28, -0.34, 0.46 1UJ8,GLU 21,3.56,1.12,-1.5,-0.56 309P.GLU 160.4.4.0.22.-0.32.0 1SJ8,ASP_537,3.51,0,-0.6,0.31 3LE4,CYS_352,9.73,0.56,0,0.17 2B78,LYS 214,10.52,-0.17,0.0.2 3OBS.TYR 110.11.65.0.81.0.38.0.46 30IP,ASP_104,3.96,0,-0.01,0.16 3IVF,TYR_26,10.65,0.12,0.28,0.25 1JB3,TYR_94,10.28,0,0,0.28 208P,GLU_204,4.41,0.26,0,-0.36 1JT9,GLU_117,5.02,1.47,-0.84,-0.1 2D7U,ASP_137,3.33,-0.19,-0.67,0.39 3DB9,ARG_24,13.64,-0.36,0.79,0.72 2BAA,GLU_89,3.66,1.01,-1.69,-0.16 100E,CYS 260,11.3,-0.01,-0.04,2.35 3GV0,ARG_212,13.14,-0.3,0.59,0.34 3G6S,TYR_207,12.21,0.54,0.82,0.84 2XMZ,ARG_128,12.27,-0.37,0,0.14 3UV9,TYR 448,10.91,0,0.15,0.75 1RKA.GLU 147.4.01.0.35.-0.82.-0.02 3BWT,LYS_655,11.63,-0.46,0.69,0.89 2DG7,ARG 119,12.4,-0.27,0,0.17 2R57,ARG_352,12.48,-0.04,0,0.02 3EYE,HIS_111,6.25,-0.41,0.2,-0.04

3B79.LYS 35.10.58.-0.23.0.0.32 2D2S,LYS_669,10.57,-0.24,0,0.31 1YOY,GLU_147,4.55,0.37,0,-0.32 2W0G,GLU_255,4.68,0.27,0,-0.08 4FZR.GLU 244.3.53.0.26.-0.85.-0.38 3U4K,LYS 74,10.6,-0.3,0.04,0.36 200K,GLU_198,4.91,0.56,0,-0.14 3EGN,GLU_414,4.61,0.12,0,0 3MIX,GLU_475,4.36,0.44,-0.12,-0.47 2D0A.ARG 207.12.66.-0.63.0.34.0.43 1D2K,LYS 229,11,56,-0,33,0,85,0,54 2IXM,GLU_29,4.51,0.65,0,-0.64 1AKO,LYS_141,10.4,-0.16,0,0.07 3ULX.TYR 165.10.78.0.-0.06.0.84 1SJY.TYR 83.10.84.-0.68.-0.77.2.3 3RJX,TYR_209,10.3,0,0.02,0.27 1EDG,ARG 333,12,18,-1.67,0.62,0.72 3MTT,GLU_534,4.58,0.33,0,-0.25 3DZ1,ARG 270,13.21,-1.6,1.37,0.94 1SNT,ARG_208,11.47,-1.11,0,0.08 3Q1C,ARG_94,13.22,-1.05,1.1,0.66 1QQE,LYS_23,10.49,-0.08,0,0.07 2WOZ,CYS_324,10.83,0,0.06,1.78 3CX2,ARG 160,12.53,-0.36,0,0.4 1X8F,HIS_246,6.37,-0.13,0,0 3A7L,TYR_121,12.22,-0.85,0.41,2.66 3CAN, ARG_90, 13.04, -0.43, 0.52, 0.45 2VAN,LYS 131,10.85,-0.17,0.03,0.48 1RWZ.GLU 94.4.64.0.14.0.0.01 3HNX,GLU_68,2.96,0.58,-1.52,-0.59 10IS,GLU_228,4.08,0.27,-0.41,-0.29 3BB7.LYS 285.10.5.-0.19.0.0.2 1SBX.LYS 179.11.07.-0.51.0.58.0.5 1JT9,LYS_64,10.55,-0.14,0,0.19 3C5V,LYS_121,10.33,-0.2,0,0.03 3ETV,CYS_92,11.86,0,0.05,2.81 4ANN,ARG 67,12.45,-0.05,0,0 3H9W,ASP_125,2.84,-1.64,-0.09,0.78 1AKO,GLU_182,3.16,0.88,-1.8,-0.42 2P4D,ARG_160,12.52,-0.32,0.01,0.34 2P5D,ASP_2,3.75,0,-0.18,0.13 1YR6,LYS 138,10.69,-0.43,0.23,0.39 1KCM,HIS 64,7,2,-0,52,0,85,0,37 2WB3,HIS_281,6.48,-0.36,0.07,0.26 3M70,LYS_41,10.74,-0.14,0,0.39 1PNE,TYR_139,10.16,0,-0.06,0.21 1DTO,HIS_187,6.46,-0.47,0,0.43 2F8H,ASP_50,3.41,-0.67,-0.09,0.37 2VAN,HIS_197,6.64,-1.11,0.85,0.4 3COU, ARG_149, 12.39, -0.11, 0, 0 2R4Q,LYS 197,10.46,-0.06,0,0.03 1TJE,LYS 213,10,79,-0,23,0,0,53 3G9T,TYR_216,11.88,0.63,0.33,0.92 2WB8,ARG_644,12.86,-0.45,0.23,0.58 3MTT,ARG_554,12.34,-0.15,0,-0.01 1BKR,HIS_25,6.22,-0.28,0,0 1L2F,LYS_94,10.35,-0.37,0,0.22 3ANJ,ASP_192,3.26,-0.81,-0.14,0.41 2OB5,GLU_132,2.12,1.15,-3.12,-0.42 1RSS,LYS 48,10.53,-0.2,0,0.23 1042,ASP 153,3,16,-0,93,-0,39,0,69 20BI,LYS_31,10.39,-0.61,0,0.51 1R53,GLU_150,4.44,0.58,-0.19,-0.46 3PZ9,LYS_391,10.4,-0.11,0,0 3GW3,ARG_292,10.4,-1.84,0,-0.26 1RI6,GLU_79,3.82,0.34,-0.72,-0.3 1NIJ,TYR_183,10.24,0,-0.23,0.47 1Y0K,GLU_68,4.46,2.72,-1.7,-1.07 1XWM,ARG_78,12.34,-0.31,0.04,0.11

3F6F,GLU 203,3.55,0.33,-0.85,-0.43 3L3P.ASP 365.4.07.0.0.0.27 3F6F,ASP_173,3.47,-0.33,-0.37,0.36 20VO.TYR 35,11,17,0,27,0,38,0.53 1MML.TYR 109.10.89.0.0.19.0.7 3GYW,LYS 47,10.33,-0.17,0,0 2AD1,ARG_73,11.98,-1.12,0.18,0.42 4GA2,LYS 133,10,42,-0,28,0,0,2 1MIX,ASP_201,2.96,-0.82,-0.39,0.37 1L3K.ARG 82.12.35.-0.16.0.0 1A8Q,ASP_7,3.83,0,-0.36,0.39 2JEO,LYS_192,11.6,-0.29,0.82,0.56 10I7.CYS 123.11.93.-0.57.0.02.3.48 1UAJ,LYS_235,10.57,-0.12,0,0.2 1FQI,LYS 406,10.33,-0.12,0,-0.05 4EF5,TYR_240,10.08,0,0.03,0.04 1VJG,TYR_158,13.62,-0.99,0.83,3.8 1RI5,ARG_108,12.28,-0.22,0,0 2WOZ,ARG_586,12.82,-0.2,0.15,0.38 3C5V.GLU 54.4.52.0.25.0.-0.24 3C6B,HIS_19,4.88,-1.81,0,0.19 2CYG,GLU_45,3.6,0.33,-0.85,-0.38 2W1R,ASP_80,4.25,0,0.17,0.27 1RI6,GLU 171,4.79,0.55,-0.05,-0.22 2098,LYS 124,11.04,-0.28,0.13,0.69 2ZCX,GLU_77,4.38,1.3,-0.74,-0.69 1BN6,LYS_274,10.51,-0.19,0,0.19 3V4G,LYS_52,10.3,-0.21,0,0.01 4H86,ASP 3,3.1,-0.53,-0.38,0.21 2OSA,ARG_295,12.6,-1.25,0.79,0.56 2P1W,GLU_128,4.79,0.27,0,0.02 4EKU,CYS_352,11.93,0,0.26,2.66 2ILR,ARG 524,12.33,-0.17,0,0 2R2Y,LYS 123,10,75,-0,19,0,0,45 2HRZ,ARG_111,13.42,-0.24,0.48,0.68 2YWX,TYR_146,10.35,0,0.13,0.22 1ZBM,ARG_193,13.73,-0.37,0.91,0.69 3V75,ARG 144,13.18,-0.81,0.81,0.68 1DOV,ARG_98,13.49,-0.26,0.62,0.62 1GPP,GLU_422,3.75,0.68,-0.58,-0.85 1YB2,HIS_32,6.2,-0.33,0,0.02 1K95,LYS 165,10.16,-0.25,0,-0.1 2EFK.ASP 161.3.39.-0.81.0.04.0.35 3U4K,LYS_78,10.59,-0.17,0,0.26 1T6L,ASP_134,3.85,0,-0.14,0.19 2CW4,ASP_7,3.64,-0.27,-0.08,0.18 1UAJ,ASP 40,4.12,0,-0.1,0.43 1AK1.TYR 267,10.75,-0.25,0.31,0.69 2QK0,ARG_93,11.98,-0.52,0,0 3QKY,ARG_163,11.92,-0.88,0,0.29 3L3P,ASP_269,3.48,-0.62,-0.05,0.35 3K9I.CYS 76.9.95,-0.01.0.14.0.82 2CL3,TYR_40,10.75,0,0.27,0.49 2AHE,LYS_106,10.44,-0.17,0,0.11 2PIM,ARG_29,13.46,-0.19,0.77,0.39 3IL3,GLU_285,4.53,1.82,-1.27,-0.52 3EVPLYS 298,10.88,-0.34,0.25,0.47 2I88,GLU_361,4.62,0.16,0,-0.03 2BCF,ARG_247,13.69,-0.47,1,0.66 1YTQ,GLU_69,4.47,0.45,-0.44,-0.04 4FZR.GLU 115.4.54.4.1.-2.11.-1.95 2Z0W,TYR_61,9.62,-1.19,0,0.81 4FH3.HIS 170.4.89.-1.26.0.-0.36 1DOV,LYS_99,10.58,-0.14,0,0.22 1FKM,HIS_575,4.23,-2.99,0.72,0 3FHF.ARG 116,13.84,-2.31,1.69,1.95 3TIR,ARG_86,12.41,-0.09,0,0 2D2S,LYS_587,12.25,-0.56,1.7,0.61 2PLQ,HIS_26,6.82,-0.31,0,0.62

3CGW,LYS_293,11.43,-0.25,0.58,0.6 1BYI,TYR 187,10.39,0,0.13,0.27 3IDW,GLU_51,2.92,0.43,-1.62,-0.39 1VSM,CYS_125,11.11,-0.14,0.21,2.05 2QK1,TYR_492,10.21,0,-0.16,0.37 1R5Q,ASP 17,4.52,0,-0.11,0.83 4DVD,ARG 187,12.24,-0.47,0,0.21 3UV9,ASP_295,4.04,0,0,0.24 1VJG,GLU_102,4.02,0.3,-0.63,-0.16 3UPD,GLU_304,4.64,0.24,0,-0.1 2G9D,ARG 114,11.35,-1.4,0,0.24 2B78,LYS_384,10.25,-0.41,0,0.16 3CIV,TYR_65,11.14,0,0.2,0.94 2H85,ASP_39,3.1,-0.69,-0.38,0.37 1AM2.TYR 59.10.61.0.0.3.0.3 3ANJ.TYR 128.10.31.0.-0.05.0.36 1R3F,CYS_174,10.63,-0.8,-0.15,2.58 1ES5,ARG_117,13.11,-0.46,0.63,0.44 3CBN,LYS_134,11.73,-0.53,0.85,0.9 3BCY,HIS 48,6.05,-1.02,0.56,0.01 3GV0,ARG 239,12.23,-0.31,0,0.04 2OB5,CYS_138,12.64,-0.73,0.92,3.45 2EJX,LYS_6,11.5,-0.36,0.84,0.52 4EKU,ARG 287,12.07,-0.78,0,0.35 1ILW.GLU 164,5.35,0.38,0.29,0.18 2CWC,ASP_75,3.56,-0.78,-0.15,0.68 2BDD,LYS_134,10.29,-0.19,0,-0.01 2RH3,GLU_94,4.75,0.13,0,0.11 4ETX,GLU 186,4.63,0.13,0,0 2EDM.GLU 182.4.0.38.-0.14.-0.74 2V5B,GLU_112,5.01,0.54,0,-0.04 1KCM,HIS_127,5.35,-2.74,0.85,0.74 1IAP.ARG 189.12.19.-0.34.0.0.03 3HVW,ASP_295,4.14,-0.11,0.13,0.32 3H8Y,GLU_32,4.43,0.17,0,-0.24 1R29,ASP_33,3.57,-1.08,-0.53,1.39 3V55,CYS_539,7.74,-1.8,-0.17,0.71 3K1H,TYR_141,10.63,0.04,0.34,0.24 2PGE,ARG 276,11,48,-1,17,0,0,16 1L2F,ARG_326,13.7,-0.44,1.23,0.41 1RL0,LYS_201,10.06,-0.57,0,0.13 2F8H,TYR_59,10.79,-0.85,-0.17,1.8 1R3F,GLU 164,4.11,0.21,-0.4,-0.2 3F7M,ASP_148,3.99,-0.83,-0.03,1.06 3EZ7,ARG_74,12.35,-0.15,0,0 1FO9,ARG_300,12.61,-2.18,0.22,2.08 2CYG,TYR_204,11.31,0,0.1,1.21 2H2W/ARG 239,12.39,-0.38,0,0.27 2IRM,ARG_47,12.24,-0.82,0,0.56 2FBQ,GLU_69,4.75,0.25,0,0.01 1YR6,GLU_176,4.48,0.24,0,-0.26 1ZBS,HIS 279,5.95,-0.4,0,-0.15 2B2H,ASP_86,4.2,0,0,0.4 3EUR,ASP_107,1.42,-2.3,-0.55,0.47 4FCU,CYS_46,11.9,0,0.18,2.72 2V4U,GLU_322,4.67,0.34,0,-0.18 2P5D,LYS_54,10.48,-0.02,0,0 1XFK,ARG_285,12.57,-0.47,0.1,0.44 2ZCO.GLU 269.4.63.0.2.0.-0.06 2APL,GLU_26,5.04,1.48,-0.79,-0.16 3T5B,ASP 339,3.56,-0.53,0.12,0.17 1DOV,ASP_146,4.3,0,-0.33,0.84 2QEV,ARG_41,12.4,-0.45,0,0.34 1MD6,ASP_147,4.52,0,-0.05,0.77 3CAN,CYS_58,11.36,-0.36,0,2.73 3T5B,LYS 321,11.77,-0.58,0.65,1.21 3BZT,ASP_288,2.84,-0.89,-0.45,0.38 3GFP,CYS_311,11.29,0,0.07,2.22 2H2W,GLU_25,4.51,0.01,0,0

1X04,LYS 151,10,46,-0,11,0,0,06 4E9E,HIS_574,6.58,-0.49,0.59,-0.02 3V55.GLU 453,4.49,0.25,0,-0.25 4EKU,LYS_303,10.56,-0.1,0,0.16 1JT9.GLU 257.4.62.0.24.0.-0.12 4FZN.HIS 241.4.64.-1.99.0.0.12 1QQE,ASP_133,3.82,-0.23,-0.17,0.42 2BLL,TYR_463,13.82,-0.71,1.65,2.89 2PLQ,ASP_5,3,-1.01,-0.05,0.26 1N81.TYR 179.11.52.0.-0.17.1.69 1VSM,LYS_116,9.93,-0.39,0,-0.18 3Q1C,ASP_353,3.9,-0.03,-0.05,0.19 2CI3,GLU_36,4.27,0.26,-0.36,-0.14 2F8H.HIS 11.5.02.-1.59.0.0.11 2Y2T.GLU 51.4.41.0.31.0.-0.4 1X1E,ARG_203,13.76,-0.32,1.19,0.39 1AK1,ASP_149,4.17,-0.42,0,0.8 3EYE,HIS_17,6.13,-1.24,0.85,0.03 300P.GLU 140.4.75.0.25.0.0 1X7F,ARG_297,13.06,-1.41,1.21,0.77 3V75,GLU_160,3.31,0.25,-1.45,0 1NIJ,GLU_267,4.84,0.34,0,0 4F85,ASP_71,3.17,-0.81,-0.06,0.23 3ETV.LYS 15.10.47.-0.1.0.0.07 1BYI,ASP_67,3.98,0,0,0.18 4HDE,LYS_48,10.5,-0.12,0,0.12 3RFY,ASP_130,3.85,0,-0.2,0.26 2VAN, ARG 102, 13.85, -0.38, 1.35, 0.38 3CCY,TYR_171,11.32,0,0.15,1.18 2BT8,HIS_221,5.92,-0.4,0,-0.19 208I,GLU_34,4.62,0.12,0,0 2HNG,ARG 22,13.96,-0.56,1.56,0.46 2A0J,ARG 143,12,28,-0,28,0,0.07 3JV1,GLU_108,4.11,0.73,-0.63,-0.5 1S7K.TYR 172.10.78.-0.22.0.07.0.93 3L3P,ARG_534,12.49,-0.15,0,0.14 2DVK,GLU 125,4.53,0.05,0,-0.02 1EO6.ASP 62.3.85.-0.09.0.0.14 2R51,ARG_137,12.43,-0.08,0,0.01 3CAN,TYR_137,10.54,0,0.26,0.28 3US6.LYS 15.10.53.-0.16.0.0.19 3GG6.GLU 66.4.12.0.31.-0.51.-0.17 3CXS,TYR_177,10.76,0,0.56,0.2 1AKO.GLU 243.4.17.0.38.-0.34.-0.37 2YLF,GLU_56,3.21,1.3,-1.7,-0.89 2H01,LYS 53,10.33,-0.18,0,0.02 3MEW,LYS 230,10.4,-0.19,0.0.08 3RLE,GLU_147,4.73,0.19,0,0.05 1QYI,LYS_94,11.5,-0.55,0.85,0.71 3C5V,ARG 199,12.31,-0.24,0.0.05 3DTE,ASP 93,4,15,-0.01,0,17,0,19 4FZN,GLU_102,4.75,0.95,-0.44,-0.26 4EF5,HIS_185,6.48,-0.26,0.24,0 2RJD,ASP_227,3.95,-0.01,0,0.16 2ATR,ASP 14,3.78,0,-0.34,0.32 3EGN,LYS_429,9.92,-0.2,0,-0.38 1P4X,ASP_222,2.78,-0.85,-0.38,0.21 3B21,TYR 90,11.63,0,5.20E-18,1.64 2RGY,HIS_318,6.99,-0.95,0.85,0.6 1YB2.ASP 44,3.51,-1.69,-0.05,1.45 3EVP,LYS_210,10.46,-0.13,0,0.09 3QKY,TYR_82,12.23,0,0.82,1.41 1T95,GLU_136,4.41,0.25,0,-0.34 3S0A,CYS 47,12.59,-0.04,0.03,3.61 3AU3,ARG 401,12,43,-0.07,0,0 3Q1C,GLU_91,3.68,1.67,-1.94,-0.54 3M70,GLU_253,4.55,0.28,0,-0.22 2G3A,ASP_100,3.96,-0.85,0,1.01 2HP7,HIS_59,3,-3.5,0,0

3M7G.ARG 83.13.09.-0.65.0.7.0.54 2WB8,LYS_595,11.08,-0.2,0.19,0.59 1T95,GLU_230,4.91,0.24,0.28,-0.11 1H09,ASP_169,3.34,-0.69,0,0.23 3DTE,ARG 136,13,19,-0,16,0,57,0,29 20ZO,TYR 82,10.3,0,-0.23,0.53 1FHL,GLU_276,4.64,0.38,0,-0.24 1PGV.LYS 269,10.67,-0.18,0,0.35 2AZP,TYR_273,11.43,0,0.07,1.36 3HUE.TYR 167.10.57.-0.46.-0.08.1.1 3U2R.TYR 46.10.18,-0.65,-0.42,1.23 106D,HIS_126,6.42,-1.03,0.82,0.14 2Z61,GLU_27,3.55,0.31,-0.85,-0.41 3CE7,ASP 16,3,21,-0.92,-0.02,0.35 3C2E,ARG 107,12.34,-0.44,0,0.28 3BCY,LYS_90,10.29,-0.21,0,0 2FD4,TYR_506,10.38,-0.37,0.21,0.53 2RIK,LYS_7,10.67,-0.26,0,0.42 3Q1C,GLU_368,5.29,0.79,0,0 3IRA.CYS 95.10.86.0.-0.21.2.08 3H04,ASP_193,2.57,-1.65,0,0.42 2B78,TYR_166,12.26,0,-0.28,2.54 2FXT,GLU_245,4.09,0.41,-0.75,-0.06 1EO6.HIS 196,6.25,-0.28,0.03,0 1RHS,ARG_116,10.36,-2.83,0,0.68 3GS3,ARG_258,11.93,-1.96,0.66,0.73 1PV5,ARG_12,12.1,-0.42,0,0.02 3EIZ,LYS 10,10.44,-0.08,0,0.01 3PP8,HIS 7,4,4,-2,1,0,0 1XFK,HIS_310,6.33,-0.35,0,0.17 1GPP,ARG_414,11.68,-0.85,0,0.03 4EVF.GLU 124.4.73.0.18.0.0.06 2YT4,GLU 701,5.93,1.97,-0.34,-0.2 2JEO,ARG_175,12.27,-0.23,0,0 2CE6,TYR_89,11.79,0.85,0.47,0.46 3GA2,GLU_173,4.8,0.23,0,0.07 3RRQ,ARG 112,12.22,-0.21,0,-0.07 2WOZ,LYS_476,10.59,-0.25,0,0.34 2PP6,LYS_9,10.42,-0.13,0,0.05 3T5B.GLU 305.4.93.2.06.-1.46.-0.16 2J8A,TYR_275,11.45,-0.3,0.26,1.5 3LJC,TYR 229,10.14,-0.02,0,0.16 3E5T,LYS 120,10,39,-0,23,0,0,11 3CNU,TYR_42,10.69,0,0.19,0.5 1P2F,LYS_112,10.57,-0.26,0,0.32 1WXQ,HIS_48,4.44,-2.18,0.12,0 2FZ4,TYR 29,12,15,-0,16,0,11,2,2 10IS,HIS_165,6.09,-0.34,0,-0.07 2WOZ,TYR 348,11.92,0.0.43,1.49 3HVW.GLU 225.4.89.0.27.0.0.12 1P1L,GLU 87,4.57,0.07,0,0 3IDW.LYS 64,10,43,-0,23,0,0,15 3PBH,LYS_141,10.43,-0.57,0,0.5 3CQ1,ARG_97,12.2,-0.37,0,0.06 1NAR,ASP_202,3.67,-0.5,-0.04,0.41 1ES9,ASP_16,1.86,-2.35,-0.08,0.49 4ETX,GLU_409,4.71,0.21,0,0 1G5Z,ASP_152,1.9,-1.68,-0.69,0.47 2EFK,GLU_64,4.64,0.14,0,0 4H86,GLU_76,4.73,0.33,0,-0.1 3F1X.TYR 23.10.15.0.0.0.15 2D2S,LYS_680,10.64,-0.18,0.03,0.3 3MEW, ARG_207, 13.49, -0.55, 0.79, 0.75 3G9T,ARG_87,13.5,-1,1.39,0.61 2FXT,ASP 281,3.63,-0.73,-0.39,0.95 1AM2,ARG_62,11.83,-0.36,0,-0.32 3TIR,ARG_206,12.39,-0.11,0,0 3OA7,GLU_24,5.09,0.24,0,0.34 3P2F,HIS_98,6.34,-0.24,0.34,-0.26

2EFK,LYS 262,10,45,-0.05,0,0 3H6Q,ASP_32,4.3,0,-0.27,0.77 2FD4,ASP_489,3.99,0,0.04,0.15 2H2W,TYR_290,9.07,-0.95,-0.36,0.38 1CHD,ARG 257,13.08,-0.41,0.51,0.49 108BLYS 44.11.69.-0.29.0.85.0.63 1RI6,ASP_221,2.51,-2.12,-0.81,1.64 1WOU,TYR_99,10.78,0,0.12,0.66 3ONT,TYR_142,10.09,0,0,0.09 2EJB,HIS 181,7.26,-0.82,1,0.58 1FO9,ARG 122,13.01,-0.63,0.73,0.41 2RJD,LYS_405,10.37,-0.19,0,0.06 2V1L.GLU 127.4.35.2.43.-2.47.-0.12 1GPP.HIS 442,7.16,-0.55,0.84,0.37 4EKU.LYS 145,10.63,-0.17,0,0.32 1YR6,TYR_187,10.11,0,-0.22,0.34 2BAA,TYR_237,11.17,0,0.32,0.85 1EW4,LYS_74,10.44,-0.07,0,0.02 2F8H,ARG 90,12.89,-0.72,0.77,0.34 1SIG.CYS 295.11.01.0.0.09.1.91 3JSN,GLU_234,4.04,0.37,-0.78,-0.05 3FRR,ARG 16,12,48,-0,29,0,0,26 1FO9,GLU_382,2.98,0.38,-1.54,-0.37 3ELI,LYS 66,11.05,-0.62,0.83,0.33 3JZN,LYS 342,10.59,-0.08,0,0.16 2C2Y,ASP_220,2.78,-1.18,-0.21,0.37 1EW4,HIS_70,6.23,-0.85,0.5,0.08 1ZCE,GLU_28,2.84,0.76,-2.37,-0.05 2AD1.GLU 182.4.89.0.44.0.-0.06 2B02, ASP_404, 1.9, -2.03, -0.61, 0.74 4GCO.GLU 246.3.69.0.79.-0.85.-0.76 3F6M,HIS_44,6.31,-2.03,0.33,1.52 4FH3.LYS 60.10.66.-0.08.0.0.25 20ZO,ARG 149,12,96,-1,1,0,98,0,57 4FH3,GLU_353,5.47,1.31,0,-0.34 1KW4,GLU_54,4.78,0.34,0,-0.06 2O4D,LYS_9,10.43,-0.07,0,0 3U4K,TYR 92,11.06,0,0,1.06 3IL3,GLU_225,3.05,0.96,-1.56,-0.86 2OPJ,ARG_45,12.42,-0.08,0,0 3M7D,HIS_360,6.38,-0.24,0,0.12 1ZCU,ARG 47,12,-0.71,0,0.21 2JEO,ARG 55,12,52,-0,18,0,09,0,1 3R87,LYS_115,10.33,-0.22,0,0.05 2CW4,GLU_42,4.59,0.09,0,0 4F3J,LYS_187,10.53,-0.1,0,0.13 1U3Y,LYS 323,10.42,-0.08,0,0 3N0K.GLU 25.3.85.1.53.-1.12.-1.06 2IQT,TYR_40,10.63,0,0.06,0.58 2XJ4,GLU_165,4.49,0.31,0,-0.32 3GA2,LYS_12,11.24,-0.23,0.56,0.4 3IU5,ARG_78,12.35,-0.37,0,0.23 2ILR,ASP_325,4.18,0,-0.03,0.41 2CXC.LYS 67,11.14,-0.54,0.61,0.57 2IDC,GLU_124,4.57,0.07,0,0 1J8B,GLU_85,4.58,0.28,0,-0.19 1XDZ,ARG 134,13,98,-0.34,1.34,0.48 3RLE,HIS_114,5.38,-1.48,0.79,-0.43 2X5Y,TYR_857,10.53,0,0.19,0.35 2FG1,HIS_23,4.24,-3.07,0.81,0 208I,ASP 126,3.34,-0.83,-0.07,0.44 3BWT,LYS_692,10.41,-0.96,0.85,0.02 2A6B.TYR 6.11.88.0.0.21.1.67 1EV8,HIS_147,3.57,-2.93,0,0 3HZQ,ASP_16,3.97,0,0,0.17 1JYH,ARG 64,13.96,-0.33,1.3,0.48 3MIX,HIS_417,6.4,-0.23,0,0.13 1WPA,LYS_497,10.26,-0.17,0,-0.07 1PGV,HIS_368,6.5,-0.25,0,0.26

1WRU,HIS 145.6.63,-0.11.0.0.24 2G3A,CYS 94,10.01,-0.01,-0.1,1.12 1X7F,LYS_261,10.7,-0.29,0,0.49 3A4C.ASP 496.4.05.0.0.25 2O0K,HIS_129,5.91,-0.48,0,-0.12 1BKR.HIS 42.6.32.-0.78.0.5.0.09 301C.GLU 83.3.49.3.83.-1.74.-3.09 200K,ASP_327,4.19,0,0.07,0.32 2Z0W,HIS_49,6.24,-0.29,0.26,-0.23 1A8Q,GLU_138,4.66,0.13,0,0.03 2WOZ,TYR 420,11.37,0,0.07,1.3 1ZBP.ARG 81,13.53,-3.22,1,3.25 1WOU,GLU_14,4.05,0.33,-0.74,-0.04 2YX0,HIS_342,6.52,-0.18,0,0.2 2HXB,GLU_76,4.58,0.08,0,0 1UJ8.GLU 66.4.9.0.36.0.0.04 1N81,LYS_58,10.56,-0.13,0,0.19 1UW7,ASP_47,2.03,-1.62,-0.96,0.8 3JV1,ASP_109,3.2,-0.83,-0.16,0.39 1RI5,LYS 291,9.85,-0.91,0,0.26 4ETX.GLU 281.5.56.1.16.0.-0.11 3HVW,ARG_177,12.36,-0.32,0,0.18 2B0J,GLU_49,5.19,5.75,-1.93,-3.11 3HYO,ASP 138,3,48,-0.58,-0,1,0,36 20GO,ASP 558,4,0,-0.09,0.29 1IDK,ASP_88,3.9,-0.42,0.04,0.48 1YW5,LYS 52,10.27,-0.23,0.0 1TJE,HIS_194,5.95,-0.92,0.35,0.03 20EW,HIS_152,4.39,-1.87,0,-0.24 1PDB.LYS 122.9.63.-0.87.0.0 1TLV,GLU_167,5.69,1.17,0,0.03 2ZTY,HIS_167,6.36,-0.17,0.03,0 2IXM,GLU_255,4.21,1.65,-0.85,-1.08 1TR9.ARG 230.11.93.-1.24.0.14.0.53 3IU5,ASP_45,3.74,-0.36,-0.01,0.32 3H6Q,ARG_137,12.33,-0.99,0,0.81 3IV4,TYR_20,9.76,-0.27,-0.26,0.29 4EKU,TYR_351,13.52,-0.63,0.61,3.54 3H13.GLU 445.2.97.0.55.-1.31.-0.76 1A8Q,LYS_127,10.43,-0.18,0,0.12 3VHJ,LYS_14,10.39,-0.11,0,0 3PBH,HIS_97,6.59,-0.24,0,0.33 4D8L,ARG 20,12.54,-0.07,0,0.12 3GE9,GLU_30,4.66,0.16,0,0 1Z9L,ARG_120,13.08,-0.18,0.41,0.36 3TIR,ASP_111,3.78,-0.12,0,0.1 1N81,ASP_117,3.92,0,-0.03,0.15 1J33,ASP 109,2.77,-0.85,-0.38,0.2 3GS9,ARG_257,13.37,-1.29,1.49,0.67 1WXQ,GLU_254,6.5,2.97,-0.06,-0.92 1ZBP,TYR_155,12.72,0,0,2.72 2APL,LYS 114,11.42,-0.31,0.85,0.38 3CIV,ASP_174,2.89,-0.82,-0.38,0.29 2EYI,CYS_154,13,-0.09,0,4.08 1Z3X,TYR_197,11.43,-0.01,0.44,0.99 3CIV,CYS_234,12.83,0,0.42,3.41 1RAJ,GLU_399,4.52,0.31,0,-0.29 3IRA,LYS_33,11.63,-0.81,1.02,0.93 2H85,ASP 36,3,93,0,0,0,13 3N2T,ARG_101,12.24,-0.49,0,0.23 1KN3,GLU 35,4.39,0.22,0,-0.33 3U0V.HIS 211.6.07.-2.02.0.85.0.75 2OJQ,LYS_501,10.32,-0.18,0,0 3TMO,LYS_245,10.35,-0.2,0.01,0.04 1EDG,LYS_143,10.05,-0.37,0,-0.08 1TLV.GLU 193.4.28.0.22.0.-0.44 4E6S,ARG_2,12.22,-0.26,0,-0.02 2FM9.GLU 156.5.7.2.7.-0.81.-0.69 3JZ9,LYS_503,10.31,-0.09,0,-0.1

2R51,ARG 212,11.86,-0.81,0.0.17 1AM2,LYS_36,10.46,-0.36,0,0.32 1NJ4,ARG 302,12,11,-0.84,0,0.45 3V4G,LYS_45,9.63,-0.66,0,-0.21 3IPZ.LYS 72.10.64.-0.19.0.0.33 1SQH,ASP_218,2.53,-1.44,-0.31,0.49 2D2S,GLU_743,4.8,0.41,0,-0.11 2CBE,LYS_133,11.48,-0.25,0.85,0.38 2GEN,TYR_89,11.99,0,-0.12,2.11 3ULX.LYS 168.10.64.-0.06.0.0.21 3A2Z,LYS_122,10.62,-0.23,0,0.35 4ETX,ARG_402,12.13,-0.6,0,0.21 3VJ8,TYR_44,13.33,0.01,0.77,2.56 3LJN,TYR 67,10.64,-0.08,-0.05.0.78 4EVF.GLU 29.4.7.0.41.0.-0.21 3FXH,ARG_40,12.31,-0.35,0,0.16 2DG7,GLU_118,4.18,1.63,-0.63,-1.31 1ZCU,ARG_231,12.61,-0.26,0.01,0.35 2WOZ.TYR 325.11.74.0.85.0.53.0.36 2AZP,ARG_233,12.14,-1.69,0.04,1.3 2H2Z,TYR_237,10.16,0,-0.3,0.46 1PGV,ASP_279,3.5,-1.66,-0.16,1.52 1UOH.GLU 24.4.92.0.14.0.0.28 3H13.GLU 265.2.72.0.71,-1.63,-0.86 3RJZ,LYS_83,11.56,-0.43,0.85,0.64 1UAJ,LYS_93,11.47,-0.35,0.85,0.47 1EQ6,ASP_79,3.99,-0.82,-0.54,1.55 105T.GLU 459,4.57,0.32,0,-0.25 3RVC,ASP_120,2.74,-2.44,0,1.38 2Z61,LYS_341,11.47,-0.39,0.85,0.51 2CYG,ARG_290,12.28,-0.22,0,0 3BWT,TYR 854,9.58,-0.38,-0.34,0.3 2Z61,ASP 49,3.88,0,-0.32,0.4 3GMS,GLU_26,4.3,0.16,0,-0.37 3P2F,CYS_132,11.86,0.62,0.31,1.93 1YLN,LYS_148,11.45,-0.34,0.85,0.44 20GQ,ARG 557,12.23,-0.27,0,0 1R3F,LYS 290,10.39,-0.17,0.0.05 2ILR,LYS_475,9.33,-1.35,0,0.18 1X8F,GLU_261,2.72,0.41,-1.35,-0.84 2CBE,LYS 80,10.23,-0.37,0,0,1 2P5D.LYS 97.10.25.-0.42.0.0.17 3AUF,GLU_24,3.49,0.33,-0.89,-0.45 1GQE,ARG_240,12.46,-0.19,0,0.15 1V8E,CYS_161,9.17,0,-0.04,0.21 3IPZ,GLU_123,3.04,0.47,-1.48,-0.44 3M7G,LYS 244,10.54,-0.2,0,0.24 2P0L,ASP_226,3.93,0,0,0.13 2E3C,ARG_248,13.34,-0.4,0.77,0.47 3TRE,ASP 20,2,34,-1,56,-0,38,0,48 1V43.ARG 155.11.19.-0.9.0.-0.41 2YX0,ASP_234,3.86,0,-0.24,0.3 3FK5,HIS_265,3.92,-2.68,0.1,0 1YW5,TYR_58,10.25,0,-0.13,0.37 2P0L,CYS 183,9.88,0,0.06,0.84 2R51,TYR_155,10.27,0,-0.17,0.44 4GA2,GLU_71,3.37,1.19,-1.69,-0.63 2IDC,GLU_56,4.45,0.38,-0.19,-0.24 2EYI,LYS_174,9.92,-0.58,0,0 1QQH,HIS 155,6.22,-1.08,0.72,0.09 2D7J,GLU_157,4.34,0.18,0,-0.33 1KW4,HIS_56,5.72,-0.38,0,-0.41 1X04,GLU_73,4.49,0.33,0,-0.34 3LMO,LYS 59,10.57,-0.18,0,0.25 3DSH.GLU 285,4.04,0.31,-0.75,-0.01 1ZBM,GLU_166,4.72,0.21,0,0.01 2FZP,ARG_269,12.28,-0.23,0,0.02 2VAN,GLU_153,4.63,0.13,0,0 2E3C,LYS_286,10.43,-0.07,0,0

3Q1C,GLU_71,3.86,0.82,-1.04,-0.42 3D9H,GLU_176,5.14,1.02,0,-0.37 3GOZ,GLU_310,4.51,0.38,0,-0.37 3MIX,LYS_620,10.71,-0.18,0,0.4 1ZCU.HIS 211.5.96.-2.86.0.26.2.05 1JYH.HIS 17.6.21.-0.68.0.0.39 200K,GLU_109,3.56,0.94,-1.68,-0.2 2BT8,TYR 292,10,24,0,0,02,0,23 3HYQ,GLU_134,4.68,0.11,0,0.07 3T57.TYR 274.11.73.-0.01.0.15.1.59 3ERF.GLU 76.3.1.0.45.-1.45.-0.39 1WXF,ARG_186,11.69,-1.88,0.8,0.27 3DSH,CYS_262,12.36,0,0.09,3.28 2BLL/HIS 588.6.42,-1.03.0.85.0.1 3JSN.LYS 248.10.14.-0.76.0.13.0.28 2XMZ,ASP_132,4.34,0,-0.23,0.78 3GW3,ASP_326,2.87,-0.85,-0.48,0.4 3BCY,CYS_49,12.38,0,0.11,3.27 3IL3,GLU 210,4.45,0.23,0,-0.27 1XFK,HIS 159,8.04,-1.93,0.44,3.03 3NR5,GLU_94,4.67,0.08,0,0.09 3EVN,GLU_168,4.74,0.24,0,0 2VGM,ASP_378,4.33,-0.05,0.3,0.28 1ZCE, ASP 74, 1.69, -2.99, -0.41, 1.29 3ADO,ARG_231,12.38,-0.35,0,0.23 2D8N,LYS_154,11.95,-1.27,1.7,1.02 2CXC,GLU_92,3.99,0.54,-0.73,-0.32 3MTT,HIS_536,6.2,-0.28,0.12,-0.14 4H86,CYS 62.8.53,-2.63,-0.64,2.79 2BLL,ARG_337,12.77,-0.45,0.36,0.35 1GXN,LYS_369,10.24,-0.31,0,0.05 10TM.CYS 242.8.97.-0.85.0.37.0.45 1RI5,GLU 263,3.99,0.28,-0.54,-0.24 2GS5,CYS_70,10.35,0,-0.11,1.46 4AE7,LYS_76,10.39,-0.35,0,0.25 2Q07,ASP_438,1.99,-1.85,-0.75,0.79 1F2V,GLU_95,4.5,0.22,0,-0.23 3PU6,GLU_122,4.75,0.2,0,0.05 2YWK,LYS_58,10.42,-0.14,0,0.06 4ACJ,ARG_772,12.02,-0.95,0,0.47 2C2Y,ASP_43,2.74,-1.43,0,0.37 4D8L,CYS 78,11.56,-0.32,-0.01,2.88 4DND.GLU 72,3.88,0.28,-0.52,-0.38 2YX0,GLU_112,3.33,0.69,-1.36,-0.5 3LJN,GLU_116,4.55,0.88,-0.18,-0.65 2BDV,ARG_136,11.13,-1.4,0,0.03 4H89,TYR_35,11.99,0,0.37,1.62 1X7F,GLU_54,4.09,0.32,-0.37,-0.35 2098.GLU 128.3.85.0.7.-0.8.-0.55 1YB2,LYS_51,10,-1.29,0.29,0.5 3V75,GLU 141,4.55,0.3,0,-0.25 1H09.TYR 88.13.5.0.75.0.13.2.62 1R6Y,ASP_22,3.3,-0.83,-0.03,0.37 2CE6,LYS_6,10.22,-0.28,0,0 3JV1,GLU_77,4.59,0.09,0,0 4FCU,GLU_228,4.16,0.4,-0.74,0 2IRM,LYS_248,10.53,-0.31,0,0.34 3RJZ,LYS_113,10.41,-0.16,0,0.07 3BQW,ARG_224,12.33,-0.24,0,0.07 3IL3.ASP 48,3.58,-0.45,-0.03,0.26 3BOW.ASP 270.3.92.0.0.0.12 3AUF,HIS_109,5.58,-2.36,0.67,0.77 1ES9,HIS_27,4.37,-1.91,0.31,-0.54 1L2F,LYS_335,10.39,-0.11,0,0 1SQW,ASP 61,3.53,-0.1,-0.43,0.26 105T,GLU_429,3.73,0.34,-0.85,-0.27 3RLE,ARG_201,12.42,-0.48,0,0.41 1KCM,LYS_165,10.18,-0.32,0,0 2QRX,TYR_88,11.04,0.43,-0.2,0.8

1ZYL,ARG_51,12.19,-0.24,0,-0.07 2G9D,ASP 13,4.31,-0.35,-0.11,0.98 2GEN,TYR_137,10.1,-0.5,0.16,0.44 3BWT,ARG_720,12.31,-0.26,0,0.07 3FXH,ARG_19,13.03,-0.33,0.51,0.35 1PVT,LYS 10,10.24,-0.26,0,0 3C2E,LYS_41,10.49,-0.25,0,0.24 3ZRI,ARG_31,12.78,-0.52,0,0.8 3BA1,GLU_191,4.81,0.31,0,0 2RIK.TYR 270,10.09.0,-0.12.0.21 3T5B.GLU 385.4.59.0.25.0.-0.16 3LPZ,LYS_250,10.4,-0.11,0,0.01 2FB6,GLU_63,4.76,0.26,0,0 2BDD.LYS 135,10.35,-0.15,0.0 1UOH,ASP_39,4.65,0,0.51,0.35 2Z0M,LYS_15,10.3,-0.2,0,0 2007,LYS 386,10.94,-0.3,0.22,0.52 1XWM,GLU_191,5.59,1.02,0,0.06 2IOT,LYS 105,10.84,-1.08,0.85,0.57 3I82,ARG 97,12.32,-0.24,0,0.05 1AD6,GLU_398,4.57,0.07,0,0 3EGN.ASP 456.4.0.-0.28.0.49 1YTD,ARG_367,12.48,-0.83,0.24,0.57 1RSS,HIS 153,6.44,-0.06,0,0 4F85,ARG 237,12,21,-0.68,0,0.39 1JKS,GLU_197,5.27,1.51,-0.73,-0.02 3IVF,ASP_175,3.18,-0.78,-0.27,0.43 3VHJ,ASP_79,3.88,-0.32,0.04,0.36 1CBY,ASP 235,4.06,-0.05,0,0.31 1MUF,GLU_326,4.75,0.17,0,0.08 2YT4,ARG 700,12,71,-0,16,0,0,37 3A2Z,ASP_128,3.75,0,-0.24,0.19 2WB8,GLU 492,3.05,1.44,-2.36,-0.53 2E3S,ASP 460,3,91,0,0,0,11 3L3P,ARG_387,12.42,-0.15,0,0.06 3UAH,LYS_169,10.43,-0.17,0,0.1 3KB5,ASP_324,3.24,-0.81,-0.35,0.6 4ESS,GLU 161,4.46,0.29,0,-0.33 4DBX,LYS_171,10.64,-0.07,0,0.21 3ULX,GLU_48,3.51,0.33,-0.85,-0.48 2PGX,HIS_240,5.25,-1.01,0,-0.24 1RZ2,LYS 208,10.49,-0.13,0,0.12 3GA2.TYR 86.10.05.0.0.0.05 3FNI,ARG_51,12.22,-0.31,0,0.03 2ZCO,HIS_96,6.22,-0.32,0,0.04 2AZL,ARG_161,12.51,-0.3,0,0.3 2QHT,GLU_192,3.7,0.43,-0.81,-0.43 3FTT.HIS 37.6.92.-0.37.0.79.0 2FBQ,GLU_5,4.8,0.31,0,-0.01 2Z61,TYR_345,10.05,-0.76,0.1,0.71 4EF5,ARG_293,12.65,-0.17,0,0.31 3GW3.GLU 348.4.72.0.22.0.0.01 3G9G,GLU_63,4.43,0.18,0,-0.25 3GMS,ASP_16,3.49,-0.38,-0.23,0.3 2RIS,ASP_172,2.54,-1.47,-0.38,0.59 10LR,ARG_108,12.76,-0.12,0,0.38 3LOE.CYS 489.13.03.0.0.09.3.94 2AZP,LYS_229,10.03,-0.54,0,0.07 1L2H,HIS 30,7.41,-0.4,1,0.31 1R3F,ARG_282,12.06,-1.45,0.45,0.55 1K95,LYS 194,10,13,-0,33,0,-0,04 3I0C,GLU_197,4.35,0.38,-0.32,-0.21 3M70.HIS 66.6.25.-0.22.0.-0.04 1SUU,TYR_721,10.35,0,-0.32,0.68 2APL,GLU_133,2.98,0.56,-1.66,-0.42 1X04,HIS 134,5.89,-0.27,0,-0.33 3P28,HIS_33,4.33,-1.76,0,-0.42 3I4T,GLU_64,4.57,0.15,0,-0.08 2WB8,ASP_716,3.14,-1.47,-0.63,1.45

3CXS,LYS_108,10.66,-0.33,0.41,0.07 2VC8,GLU_66,4.6,0.16,0,-0.05 3M3P,ASP_63,4.14,0,0,0.33 2BLL/ARG 619/11.33/-2.29/0/1.11 2YWJ,ASP_119,3.97,0,-0.1,0.27 1059,HIS 164,4.79,-1.86,0,0.16 1V43,ARG_218,12.42,-0.13,0,0.05 3BQW,GLU_327,4.68,2.02,-1.23,-0.61 1WNH,GLU_102,4.37,0.57,-0.36,-0.34 1R53,ARG_368,12.98,-0.21,0.39,0.31 2RJD,ARG 324,12.44,-0.06,0,0 3HUE,LYS_58,10.29,-0.15,0,-0.05 3N2T,GLU_111,7.49,4.53,-0.84,-0.7 3M7G,ARG_109,11.99,-0.25,0,-0.27 3V55.TYR 615.11.07.0.0.16.0.91 1TR9,ASP 135,2.66,-1.53,-0.09,0.47 20EW,TYR_319,10.46,0,0.12,0.33 1TP6.CYS 3.7.16.-1.92.-0.44.0.52 1TR9,GLU_281,5,0.33,0,0.18 1160,LYS 25,11.44,-0.27,0.76.0.45 2FBI.LYS 124,10.41,-0.09.0.0 2AD1,LYS_199,10.44,-0.11,0,0.05 105J,HIS_-2,6.07,-0.14,0,-0.29 3LJC,TYR 141,12,36,0,58,0,45,1,32 2P65.TYR 164.11.71.-0.18.0.45.1.44 2FB6,LYS_110,10,-0.61,0,0.11 2099,ARG 130,12,4,-0,1,0,0 3TIR,TYR_221,10,-0.08,-0.39,0.47 2CXC,ARG 99,12.41,-0.09,0,0 2Z14,ARG 72,12.1,-0.83,0.0.43 1046.GLU 49.2.37.0.93.-2.25.-0.81 3IVF,ARG_207,13.82,-0.31,1.24,0.39 2B0J.LYS 298,10.38,-0.16,0,0.04 3P28.ASP 28.3.44.0.-0.59.0.23 2BLL,ARG_510,11.46,-2.15,0,1.12 1R53,ARG_47,12.61,-0.13,0,0.25 1JT9,HIS_65,6.02,-0.44,0,-0.04 1PBV,TYR_101,10.79,0,0.06,0.72 3P28,ARG_167,12.58,-0.35,0,0.42 2H2W,ARG_243,13.55,-0.6,0.66,0.99 4DVD,GLU_31,4.54,0.43,-0.04,-0.35 2AD1,LYS_215,10.56,-0.08,0,0.14 1AD6,GLU 551,4.49,0.34,0,-0.36 1AD6,GLU_545,4.52,0.17,0,-0.15 1PBV,ARG_232,12.77,-0.13,0,0.4 105T,GLU_217,4.16,0.75,-0.46,-0.64 1ZBS,ARG_25,13.8,-0.58,0.89,0.99 3BJV.GLU 52.3.97.0.31,-0.49,-0.35 3DTE,LYS_204,10.33,-0.17,0,0 3CSR,ASP_91,3.71,-0.85,-0.15,0.91 3B7H,HIS_11,5.56,-1.44,0.22,0.28 3CGW,LYS_78,10.66,-0.11,0,0.28 3V55,GLU_585,3.42,0.43,-0.7,-0.82 2B0A,GLU_24,4.69,0.19,0,0 1DOV,ASP_200,3.92,-0.11,-0.03,0.25 3BWT,GLU_623,4.5,0.42,-0.34,-0.08 1VSM.ARG 168.13.34.-0.32.0.64.0.52 1SI7,LYS_127,10.45,-0.29,0,0.24 3BB7,ASP_116,2.47,-1.54,-0.21,0.43 1FQI,ARG_361,13.03,-0.68,0.74,0.47 1X6J,LYS 6,11.27,-0.43,0.79,0.4 20KT.ASP 163.3.84.0.-0.18.0.23 1ZHV,ARG_108,13.63,-0.41,1.06,0.46 2Z61,ARG_131,12.21,-0.55,0.03,0.23 2VGM,ASP_73,3.15,-0.48,-0.55,0.37 1X6J.GLU 29.3.59.0.33.-0.73.-0.5 4EVF,LYS_267,10.43,-0.21,0,0.14 4FLE,GLU_149,4.63,0.09,0,0.04 2F4Q,ARG_216,11.44,-0.99,0,-0.07

3GV0.HIS 162.5.52.-1.88.0.75.0.15 3A4C,TYR_532,10.43,0,0.17,0.26 1PZC,LYS_38,10.44,-0.06,0,0 2OSA,CYS_288,12.75,-0.01,0.04,3.72 4F8A.ARG 693.12.24.-0.25.0.-0.01 3TMO.GLU 309.3.65.0.38.-0.85.-0.38 2E3C,HIS_369,5.98,-0.52,0,-1.56E-17 3EIZ,LYS_152,10.41,-0.16,0,0.06 4FZR,ASP_353,2.55,-1.62,-0.07,0.44 1HF8,TYR_96,10.1,-0.36,-0.04,0.5 1HF8,LYS_39,11.29,-0.25,0.62,0.42 30DJ,GLU_192,4.66,0.16,0,0 2X4J,TYR_130,11.62,-0.85,0,2.47 3CCY.CYS 43.8.56.-0.67.-0.31.0.54 1TXJ.ARG 30.12.87,-0.52,0.54,0.36 3G9G,ARG_28,13.64,-0.72,0.97,0.89 2X4G,GLU_58,3.17,0.6,-0.91,-1.01 109G,ARG_150,12.27,-0.23,0,0 2GEN,ASP_188,2.43,-1.5,-0.31,0.44 1GPP,LYS_124,10.17,-0.33,0,0 1QQH,CYS_196,9.88,-0.31,0.64,0.57 1R9W,ARG_231,12.07,-0.91,0.13,0.36 4DIU.TYR 43.13.08.0.57.0.46.2.05 2D7U,HIS 26,7.01,-0.44,0.59,0.35 1WNH,CYS_70,11.61,-0.06,-0.01,2.68 2EFK,LYS_171,10.51,-0.08,0,0.09 3EVP,GLU_85,4.78,0.33,0,-0.03 1SUU.LYS 696,10.1,-0.16,0,-0.25 1PSW,GLU_190,4.48,1.58,-1.55,-0.04 4D8L,LYS_46,10.46,-0.06,0,0.02 1W7B,GLU_125,5.14,0.65,-0.63,0.61 3CCY,ASP 68,3.09,-0.85,-0.44,0.58 1JKS,LYS 262,11.12,-0.19,0.47,0.34 2DVK,GLU_22,4.69,0.13,0,0.07 2D2S,ASP_692,4.13,0,-0.05,0.37 200K,ARG_279,12.34,-0.16,0,0 1ZCU,GLU_115,4.59,0.23,0,-0.14 2E3S.GLU 494,4.57,0.06,0.0.02 2BV9,LYS_100,10.32,-0.22,0,0.03 2D7J,GLU_177,4.45,0.4,0,-0.45 2H2W.GLU 126.4.93.0.34.0.0.09 4FH3.ASP 70.3.88.0.-0.26.0.34 1KCM,LYS_200,10.39,-0.38,0,0.28 2Z84,ARG 96,12,44,-0,11,0,0.05 3BJV,LYS_27,11.21,-0.27,0.5,0.48 2B2H,ASP_288,3.98,-0.5,-0.43,1.11 3PAC,ARG 172,12.35,-0.15,0.0 3MTT,GLU_517,4.56,0.32,0,-0.26 3GFP,LYS_349,11.19,-0.27,0.46,0.51 3I4T,ARG 126,12,73,-0.82,0.34,0.7 3HUE,TYR 23,12,89,-0.05,0,2,93 1J85,LYS_73,10.38,-0.12,0,0 30IP,LYS_73,9.6,-0.47,0,-0.43 1CHD,ARG_316,12.98,-0.25,0.49,0.25 3UC9,TYR 49,9.82,0,-0.35,0.18 1XFK.TYR 221,11.99,0.8,0.37,0.83 1H4U,GLU_491,3.44,0.4,-0.84,-0.62 4FCU,LYS_86,11.68,-0.64,0.85,0.97 1ES5,ASP_28,2.69,-1.25,-0.51,0.64 1SUU,ASP 611,3.84,0,-0.12,0.16 3C6B,GLU_99,4.73,0.23,0,1.39E-17 3F7M,LYS_191,10.27,-0.19,0,-0.04 1TD6,GLU_69,4.05,0.45,-0.38,-0.52 1EV8,HIS 108,6.12,-0.28,0,-0.1 3M7D,LYS 244,10,41,-0,14,0,0.05 2NRR,LYS_352,10.54,-0.28,0,0.32 2GZQ,LYS_110,10.5,-0.07,0,0.07 2XHC,CYS_145,9.86,-0.93,0.17,1.63 2R2Y,LYS_30,11.5,-1.13,1.22,0.91

105Z.LYS 617.11.21.-0.25.0.59.0.37 1T3Y,ARG_63,12.52,-1.03,0.66,0.39 2PGX,LYS_46,12.14,-0.57,1.7,0.51 3KV0,GLU_202,4.64,0.18,0,-0.04 3C38,ASP 65,4.31,-0.73,0,1.23 2H2W,TYR 153,11.85,0,-0.09,1.94 1K95,TYR_207,10.2,0,0.03,0.17 1EYH,ASP_136,3.56,-0.5,-0.13,0.39 1EYH,CYS_96,12.27,0,0,3.27 2CBELYS 111.10.69.-0.15.0.0.34 1XWM,LYS_209,10.34,-0.23,0,0.07 1LTU,ARG_76,12.84,-0.16,0.1,0.41 1XIP,GLU_63,5.11,0.75,-0.01,-0.12 3BCY,LYS 135,12,34,-0.86,1.66,1.04 3IBT.HIS 174.6.37.-0.33.0.0.2 3MEW,HIS_185,6.14,-0.3,0,-0.06 1R3F,LYS 64,10.4,-0.7,0.23,0.38 1UOH,GLU_139,4.69,0.29,0,-0.1 3RFY,ASP_90,4.45,-0.11,0.04,0.72 3NZL/CYS 42,10.3,-0.96,-6.94E-18,2.25 1QYI,ASP_49,3.61,-0.15,-0.45,0.42 4DND,ARG_22,12.38,-0.29,0,0.16 3FXH,ARG_29,13.61,-0.3,0.95,0.45 3DZ1.CYS 41,11.58,0,0.1,2.48 1WRU,ASP_92,4.79,0,0.12,0.87 3A2Z,ARG_88,11.95,-0.6,0,0.05 30IP,LYS_161,10.41,-0.09,0,0 3CAX,ARG 326,12.44,-0.06,0,0 1W7B.GLU 149.4.24.0.35.-0.17.-0.44 2F8H,HIS_81,6.36,-0.16,0,0.02 2HNG,GLU_127,4.67,0.13,0,0.04 1HF8,ASP_43,3.15,-0.62,-0.5,0.46 1S7K,LYS 30,11.87,-0.55,1.1,0.81 1AD6,ARG_552,12.21,-0.28,0,-0.01 3VJ8,GLU_64,3.7,0.29,-0.83,-0.27 2FD4,HIS_532,5.07,-1.47,0,0.05 2YWJ,ASP_140,2.66,-1.64,0.1,0.39 1L2F,GLU_63,4.72,0.22,0,0 2IF4,GLU_129,4.3,0.52,-0.43,-0.29 2R51.GLU 144.3.83.1.18.-1.07.-0.78 1NRI,TYR_159,9.65,-0.79,0,0.45 2AD1,GLU 60,4.25,1.3,-0.92,-0.63 4E9E,LYS 484,10.78,-0.25,0.0.53 1SIG,TYR_268,10.44,0,0.13,0.31 1KN3,LYS_129,10.46,-0.2,0,0.16 3T8R.TYR 122.10.09.0.0.09 1EDG,ASP_21,3.8,0,-0.17,0.17 1DVO,GLU_131,3.49,0.46,-1.12,-0.34 1RAJ,LYS_255,11.47,-0.28,0.79,0.45 1X91,ASP_73,4.06,0,-0.03,0.29 3FHF,LYS 189,10.74,-0.22,0,0.46 1X7F,LYS 18,10,42,-0,23,0,0,15 3UV9,ARG_297,12.28,-0.22,0,0 3R2E,ASP_49,3.95,-0.52,0.22,0.46 3U2A,GLU_80,4.58,0.08,0,0 3N2T,LYS_110,10.85,-0.51,0.85,-5.55E-17 3V75,GLU_271,4.61,0.33,0,-0.21 3CX2,TYR_237,12.09,0,0,2.09 2R0S,LYS 276,10.9,-0.53,0.2,0.73 1H09.TYR 124,13.9,-1.55,1.6,3.86 3EX9,ARG_121,12.7,-0.17,0.06,0.32 1LTU,ASP_61,3.92,0,-0.12,0.24

1RSS,GLU_139,4.53,0.34,0,-0.3

2Z0M,LYS_219,10.54,-0.05,0,0.1

3VHJ,ASP_92,3.32,-0.84,0,0.36

2RIK,ASP_38,2.25,-1.6,-0.4,0.46

2YX0,CYS_71,12.83,-0.07,0.85,3.05

2QDJ,GLU_313,4.3,0.53,-0.65,-0.08

3N2T,LYS_95,10.43,-0.07,0,0 1XDZ,CYS_159,13.02,0,0.21,3.8 2V4U,LYS_363,10.26,-0.29,0,0.05 4ETX,GLU_222,4.25,0.16,-0.26,-0.15 2ZCO.TYR 112,11.34,0,0,14,1,21 1XTZ,ASP_88,3.89,0,-0.2,0.3 1WLY,LYS_213,10.38,-0.08,0,-0.04 2GEN, ARG_191, 13.5, -0.24, 0.76, 0.48 1Y2Q,GLU 46,3.19,1.06,-1.69,-0.68 2GAU,ARG 156,11.39,-1.06,0,-0.05 3IPZ,CYS_172,9.3,0,0.06,0.24 3EZ7,LYS_386,11.44,-0.3,0.85,0.39 3FTT,LYS 47,11.28,-0.55,0.85,0.48 3TIR.GLU 142.3.31.0.63.-1.43.-0.4 1WRU,ASP_10,3.32,-0.43,-0.36,0.32 3CNU,ASP_37,4.26,0,0.11,0.35 2R51,LYS_295,10.49,-0.19,0,0.17 1RHS,GLU 233,4.61,0.13,0,-0.02 3CXS.HIS 111.6.14,-0.27.0,-0.09 1T95,GLU_100,3.84,0.26,-0.85,-0.07 1XEU,GLU_151,4.3,0.36,0,-0.56 3H6O,ASP 117,3.82,0,-0,14,0,16 2DFL.ASP 192,4.71,0.0.07,0.84 2WB8,HIS_579,6.29,-0.24,0,0.03 2CIU,GLU_177,3.96,0.51,-0.82,-0.23 2E3C,LYS_321,9.81,-0.66,0,-0.03 3FHF,LYS 171,11,-0.4,0.61,0.29 2ILR.LYS 532.10.45.-0.05.0.0 2F8H,ARG_144,12.9,-0.69,0.36,0.73 1PVT,GLU_69,3.49,0.35,-0.52,-0.84 1059,LYS 303,10.2,-0.26,0,-0.05 3PM2,TYR 81,13.19,0,0,3.19 1XWM,HIS_13,6.63,-1.23,0.85,0.51 1X1E,GLU_2,4.24,0.38,0,-0.64 1GPP,GLU_134,4.65,0.13,0,0.03 2OJQ,GLU_483,4.49,0.14,0,-0.16 2V5B.CYS 15.9.58.0.0.38.0.2 1PGV,GLU_365,4.01,0.27,-0.54,-0.22 3Q1C,HIS_148,6.06,-0.46,0,0.02 3F1X,GLU_16,4.42,0.16,-0.23,0 3ERF,HIS 161,6.28,-0.23,0,0.01 3KEY,ARG_379,12.09,-0.59,0,0.18 3KT9,TYR_55,9.96,0,-0.48,0.45 3HUE,GLU_295,4.69,0.68,-0.48,-0.01 20KT,ARG 279,13.17,-2.86,0.77,2.77 4EVF,LYS 199,10.25,-0.33,0,0.08 1ZBS,GLU_165,5.01,0.16,0.07,0.28 1TD6,GLU_175,4.78,0.28,0,0 1MIX,LYS_254,10.4,-0.1,0,0 4FLE,ARG 82,12.44,-0.22,0,0.16 3B21,ARG 119,12.6,-1.97,0.84,1.24 2EA9,GLU_93,4.09,0.82,-0.94,-0.27 2OJQ,LYS_620,10.61,-0.1,0,0.21 1BN6,GLU_151,4.79,0.28,0,0.02 1T95,ARG_133,12.54,-0.11,0,0.15 3H04,HIS_248,8.27,-3.35,0.85,4.27 2DFL,ARG 229,11.8,-0.67,0,-0.02 2P65,LYS 145,10.94,-0.92,0.85,0.51 1YDL, ASP 24, 2.97, -1.56, -0.22, 0.95 1S7K,TYR 98,11.09,-0.29,0.07,1.3 1NWA, ARG_45, 12.48, -0.06, 0, 0.04 1S7K,LYS_157,10.56,-0.07,0,0.13 4H4J,TYR_218,11.58,-0.37,0.26,1.68 2Q07,LYS_392,10.44,-0.09,0,0.04 3A7L,ASP_82,4.08,-0.03,0.01,0.3 2O34,GLU 167,2,22,0,48,-2,38,-0,38 3GS3,TYR_137,10.84,0,0.16,0.68

2E3C,ASP 365,3.57,-0.54,-0.19,0.5

2PPN,GLU 61,3.67,0.43,-0.83,-0.42

3RE9,GLU_140,3.54,1.4,-2.14,-0.22 2RFA,CYS 172,13.02,0,0,4.02 4ANN,GLU_185,3.01,1.09,-2.22,-0.37 1Q2Y,HIS_134,5.61,-2.18,0.79,0.5 2B2H,ARG_32,13.12,-1.55,1.37,0.81 1W7B,TYR 30,9,92,0,-0,33,0,25 2R0S.LYS 45.10.07.-0.43.0.0 3COU, ARG_96, 12.18, -0.94, 0, 0.63 3B7H,ARG_44,12.46,-0.04,0,0 1PBV,CYS_174,8.64,-1.34,-0.18,1.17 1X7F,ASP_160,3.92,0,-0.1,0.22 3P28,TYR_134,10.34,0,0.15,0.19 2Q13,ARG_279,12.21,-0.29,0,0 3A7L,TYR_24,10.64,0,-0.14,0.78 1WJG.GLU 40.4.79.0.36.0.-0.07 3LD1,LYS 107,10.06,-0.28,0,-0.16 1X04,GLU_140,3.14,0.53,-1.54,-0.34 1DCF,GLU_33,4.49,0.2,0,-0.21 1U53,TYR_158,13.75,-0.67,-0.08,4.49 2YLF.TYR 139,10.3,0,0.01,0.3 2AZL,LYS_15,11.46,-0.31,0.78,0.48 2FD5,GLU_68,4.46,0.2,0,-0.24 2W2S,ARG_118,12.06,-0.23,0,-0.21 1RKA,ARG_198,13.67,-0.22,0.74,0.64 4FCU,LYS 149,10.46,-0.04,0,0 2HRZ,ASP_329,3.03,-1.2,-0.76,1.18 4ESS,ARG_127,12.45,-0.3,0,0.25 1XFK,GLU_18,4.33,0.32,-0.75,0.26 1V43,GLU_103,4.84,0.34,0,0 4ETX,GLU_241,4.65,0.26,0,-0.11 3ETU,GLU_275,4.68,0.37,0,-0.18 3PAC,HIS_127,5.45,-0.77,0,-0.27 2Q98,LYS_53,10.17,-0.33,0,0 3CS1,GLU_167,4.51,0.11,0,-0.11 3IVF,LYS 316,10,29,-0,26,0,0.05 3GA2,ARG_94,11.87,-0.95,0,0.32 4E9E,HIS_535,5.66,-0.83,0.03,-0.04 2JKF,GLU_30,3.77,0.28,-1.06,0.05 3BQW,ARG 218,12.04,-0.37,0,-0.1 2Z61,ARG_273,12.61,-0.14,0,0.25 10IS.LYS 301.10.21.-0.28.0.-0.01 2FXT,ARG_342,12.42,-0.23,0,0.15 3K8U,LYS 59,10.25,-0.31,0,0.06 3ADO.GLU 211.4.58.0.3.-0.17.-0.04 4D8L,ASP_170,3.82,0,-0.21,0.22 3CBN,GLU_106,4.46,0.17,0,-0.21 3CAN,ASP_78,3.95,0,-0.01,0.16 1UOH,HIS 156,5.99,-0.5,0,-0.01 2OB5,GLU_89,4.24,0.37,-0.62,-0.01 2Q34,GLU_35,4.5,0.24,0,-0.24 1MJS,LYS_377,10.27,-0.29,0,0.05 3GEC,HIS_279,5.55,-0.79,0,-0.17 105J,LYS 49,10.53,-0.12,0,0.15 2R0S,TYR_284,11.57,0,0.04,1.54 3A2Z,TYR_18,10.25,0,0,0.25 1XIP,ASP_333,4.01,-0.52,0.01,0.72 3F6F,LYS 90,10.77,-0.19,0,0.46 3ONT,GLU_144,4.74,0.24,0,0 2FZ4,ARG_167,12.76,-0.42,0,0.68 2PGX,LYS_184,10.74,-0.32,0.17,0.38 1SJ8,ARG_532,12.16,-0.79,0,0.45 2R4O,LYS 214,10.22,-0.28,0,0 3QAV,GLU_133,4.58,0.19,0,-0.12 1JB3,GLU_102,5.33,2.57,-1.32,-0.43 1YW5,GLU_150,4.77,0.31,-0.04,0 1WRU,ARG_336,11.85,-0.74,0,0.09 2A6B.LYS 104.10.52.-0.14.0.0.16 1W24,GLU_175,4.64,0.3,-0.08,-0.08 1RI5,CYS_272,9.23,-0.02,0.06,0.19

1PDB.GLU 44.4.54.0.04.0.0 3CO1.CYS 39.10.73.-0.14.0.11.1.77 2OGQ,LYS_574,11.44,-0.21,0.76,0.38 3ULX,ASP_101,1.48,-1.97,-1.17,0.82 3M66, ASP_409, 3.73, -0.12, -0.24, 0.29 1T6L,LYS 101,10.55,-0.2,0.0.24 2EFK,TYR_105,10.81,0,-0.26,1.07 3JZN,ARG_420,12.02,-0.51,0,0.03 2P52,ARG_178,12.45,-0.11,0,0.05 3E5T,LYS_138,10.57,-0.16,0,0.22 1TLV,GLU_69,4.85,0.3,0,0.05 4FZN,ASP_214,4.11,0,0,0.31 3RJX,GLU_58,4.89,3.09,-2,-0.7 3JV1.ASP 197.4.18.0.0.01.0.37 3GMS.ARG 169.11.92.-0.58.0.0 1SQH,CYS_152,10.81,-0.15,-0.37,2.33 2G9D,ASP_280,4.01,-0.12,0.15,0.18 2ZQ5,ASP_27,3.96,-0.05,0.01,0.2 3COU,TYR_43,10.02,-0.06,-0.3,0.39 3ETV.ARG 21,13,55,-0.4,1.06,0.38 1MUF,ASP_99,3.24,-0.96,-0.23,0.61 1JB3,ARG_111,12.81,-0.37,0.24,0.45 1M5I,LYS_226,10.23,-0.41,0,0.15 1PBV,ARG 61,12.34,-0.28,0,0.12 3V3T,TYR_50,11.24,0,0.14,1.1 3B7H,ASP_4,3.24,-0.85,0,0.29 1UAJ,ARG_39,12.38,-0.44,0,0.32 4DND,ARG_27,12.58,-0.13,0,0.2 1WLY,GLU_19,3.79,0.52,-0.85,-0.38 3I0C, ARG_146, 12.37, -0.34, 0, 0.21 1WLY,CYS_191,11.82,-0.01,-0.05,2.87 1PZC,LYS_57,10.58,-0.24,0,0.32 4FH3,ARG 111,12.33,-0.17,0,0 1YTO,HIS 31,5.81,-0.61,0,-0.08 3RHE,ASP_27,3.79,0,-0.21,0.2 2A6B,ASP_91,4.11,-0.26,-0.03,0.59 3RFY,TYR 209,11.67,0.85,0.31,0.5 3ON1, ASP_100, 3.04, -0.82, -0.38, 0.44 2GQV,GLU_53,2.72,0.54,-2.28,-0.04 2007.TYR 460.11.67.0.0.46.1.21 2VAN,LYS 127,10,49,-0,14,0,04,0.09 4DVD.GLU 128,4.74,0.19,0,0.04 1U3Y,LYS 317,11.75,-0.34,0.75,0.84 3C6B,CYS_169,12.02,-0.47,-0.22,3.71 3L3P,GLU_529,4.54,0.18,0,-0.14 100H,CYS 109,10.62,-0.83,-0.56,3.01 1VJG.LYS 105.10.5.-0.1.0.0.1 2HRZ,ARG_286,12.08,-0.59,0,0.17 2EEY,ASP_93,2.99,-0.66,-0.38,0.23 10GL,ASP_40,3.29,-0.85,0.03,0.32 4AF2,ASP_158,3.83,-0.3,0,0.33 3H5T.GLU 230,4.63,0.56,0,-0.42 1XWM,ARG_154,12.86,-0.34,0.23,0.47 2XWS,GLU_56,3.45,0.26,-0.85,-0.47 3Q1C,ARG_382,13.17,-0.29,0.58,0.37 3P2F,TYR_54,13.01,0.44,-0.07,2.65 3DSH,HIS_344,6.25,-0.25,0,0 2IRM,HIS_172,5.2,-1.18,0,-0.13 1AK1,HIS_101,6.41,-0.37,0.27,0.02 1PBV,ASP 113,4.75,0,0.28,0.68 3TIR.ASP 191.3.82.-0.25.-0.14.0.41 2BQQ,GLU_121,4.03,0.33,-0.66,-0.13 200K,GLU_320,4,1.71,-1.21,-1 4AM1,LYS_296,10.3,-0.29,0,0.09 2ZQ5,ARG_299,13.94,-0.41,1.37,0.47 2QV2,LYS 289,11.19,-0.31,0.65,0.35 2G5X,ASP_179,4.41,0,0,0.6 2QVO,TYR_32,10.86,0,0.57,0.29 3BWT,ARG 555,12.53,-0.08,0,0.12

3EX9,HIS 123,6.91,-0.55,0.85,0.11 2BLL.HIS 359.5.73.-0.63.0.-0.13 2CVB,LYS_110,10.05,-0.56,0,0.11 3LQE,ARG_396,12.71,-0.25,0,0.46 2RIK.LYS 66.11.03.-0.32.0.52.0.33 2WOZ.LYS 521.10.45.-0.08.0.0.03 1ZYL,ARG 157,12,44,-0.9,0.04,0.8 2JEO,ASP_163,3.54,-0.48,-0.04,0.26 2RIK,LYS_100,10.37,-0.13,0,0 3FS3,TYR_127,10.47,0,-0.04,0.52 1S7K,GLU_12,3.82,0.42,-0.74,-0.36 2YT4,LYS_669,10.19,-0.18,0,-0.14 1WYC,TYR_97,11.73,0,0.56,1.18 1GXN,TYR_437,10.4,0,0,0.4 2V5B.ASP 37.3.12.-0.85.-0.29.0.46 1V8E,HIS 13,5.64,-2.52,0.85,0.82 1C3K,TYR_48,10.72,0,0.03,0.69 109G,GLU_228,2.89,1.27,-1.7,-1.19 3KT9,LYS_34,10.31,-0.14,0,-0.05 2HXB,TYR 43,11.84,0.32,0.73,0.79 106D,ARG_4,12.79,-0.75,0.66,0.38 2GAU,GLU_93,4.65,0.11,0,0.04 1DUN,LYS_88,10.47,-0.03,0,0 3T8R,ARG 8,12.5,-0.11,0,0.1 2H2Z,CYS 300,11.07,0,-0.05,2.11 3TRE,LYS_57,10.49,-0.11,0,0.1 2ZTY,LYS_65,10.29,-0.23,0,0.02 4EUG,ARG_31,11.17,-1.37,0,0.03 1WP5,GLU 207,4.97,1.76,-1.32,0.03 1Q8B,GLU_96,4.24,0.4,-0.16,-0.5 2EEY,GLU_50,4.54,0.19,0,-0.14 3AU3,HIS_427,6.45,-0.51,0.44,0.01 4FCU,ASP_92,2.48,-1.57,-0.75,1 1XTZ,ASP 103,2.8,-1.79,-0.58,1.36 2EYI,GLU_213,4.5,0.4,-0.17,-0.23 2PP6,ASP_65,3.86,-0.73,-0.13,0.93 1YLN,ARG_99,12.16,-0.34,0,0 2Q07,LYS 255,10.1,-0.65,0,0.26 2FC3,LYS_33,10.18,-0.24,0,-0.09 2VGM,LYS_226,10.68,-0.96,0.67,0.48 1DZF,GLU_133,3.93,3.34,-1.69,-2.22 1EV8.ASP 105.2.59.-1.73.0.0.51 2XMZ,LYS 184,10.91,-1.11,0.85,0.67 3C5V,LYS_296,10.63,-0.37,0.18,0.32 2J8A,GLU_363,4.67,0.33,-0.16,0 1W24,ASP_170,3.83,0,-0.13,0.15 3RRQ,ARG_143,13.49,-0.29,0.89,0.38 3U0V,GLU_180,4.7,0.15,0,0.04 2IXM,CYS_256,12.15,-0.51,-0.02,3.67 2BV9,TYR_131,13.86,0,-0.02,3.88 3C2E,LYS 100,10.36,-0.33,0,0.18 20EW.GLU 240.4.1.0.44,-0.69,-0.14 2G3A,ARG_28,13.03,-0.18,0.72,0 1FO9.LYS 287.10.46.-0.24.0.0.2 2Q5X,TYR_831,12.91,0,0.5,2.41 2B0J,LYS_154,10.49,-0.09,0,0.09 2B2H,GLU 386,4.6,0.09,0.0.01 3ON1,GLU_80,3.95,0.3,-0.69,-0.16 3PZ9,ARG_361,12.32,-0.14,0,-0.04 1XTZ,TYR_27,11.34,0.32,0.03,1.01 2AH5,GLU 52,4.07,0.49,-0.75,-0.16 2GZR,GLU_139,4.93,1.4,-0.71,-0.26 1ZP2,LYS_204,10.52,-0.09,0,0.11 1EQ6,ARG_162,13.12,-1.19,1.18,0.62 2G9D,LYS_75,10.46,-0.41,0,0.37 2YT4,HIS_491,6.04,-0.36,0,-0.09 2CBE,LYS_168,10.51,-0.37,0,0.38 3DB9,ASP 53,3.32,-1.01,-0.31,0.82 4FZN,ASP_194,3.63,-1.44,-0.11,1.38

3016.GLU 84.4.61.0.11.0.0 3IL3,HIS 243,4.62,-2.69,0.81,0 1P6F,HIS_142,5.71,-0.58,0,-0.21 3HYQ,GLU_74,2.61,0.75,-2.24,-0.41 3RLN,CYS_727,11.24,0,0.1,2.14 2H27 TYR 182 13 67 -0 7 1 07 3 3 3HVM,LYS_300,11.39,-0.36,0.85,0.39 1YB2,GLU_216,4.76,0.26,0,0 3ONT,HIS_120,6.25,-0.25,0,0 4DVD,ARG_115,12.74,-0.24,0.25,0.23 2FPN,HIS 134,7.58,-0.31,0.85,0.54 30KO,LYS 601,9,71,-0,4,0,-0,39 3EZ7,ARG_16,12.35,-0.15,0,0 3OA7,TYR_36,10.11,0,0,0.11 1MIX.HIS 283,4.45,-2.18,0.81,-0.67 3KB5.GLU 365.4.61.0.11.0.0 1J8B,LYS_23,10.46,-0.18,0,0.14 2EDM.LYS 165,9.99,-0.4,0,-0.11 1T95,GLU_88,4.36,0.38,0,-0.52 2A4D,ARG 137,12.81,-0.62,0.21,0.71 105T,TYR_201,10.22,0,0.06,0.17 3EX9,HIS_42,5.74,-0.72,0.11,-0.15 3LOD, ASP_22, 3.32, -0.68, -0.48, 0.68 1DZF.ARG 200.12.37,-0.13.0.0 1R3F,TYR 179,10.11,0,-0.03,0.14 3G9T,GLU_238,5.43,4.46,-2.51,-1.01 3IVF,TYR_270,11.45,-0.85,0.08,2.23 1XTD,GLU_125,4.76,0.1,0,0.16 1U3Y,TYR_283,10.71,0,-0.11,0.81 3QKY,ARG_40,13.01,-0.36,0.28,0.59 2B78,ARG_85,13.21,-2.64,1.19,2.16 3C38,ASP_92,3.88,-0.09,-0.18,0.35 1NAF,TYR_294,10.54,0,-0.1,0.64 2CXA.ASP 206.4.1.0.-0.05.0.35 2QK1,CYS_477,11.83,-0.61,0.37,3.08 2QK1,LYS_327,11.06,-0.44,0.55,0.45 2P65,TYR_8,9.66,-0.21,-0.58,0.45 1RI5,ARG 213,12.48,-0.25,0,0.23 3TOW,LYS 82,10,25,-0,16,0,-0,09 2JKF,ARG_152,13.49,-0.47,0.84,0.63 2GAU,ARG_216,13.4,-0.18,0.56,0.53 3RJX.GLU 68.4.57.0.28.0.-0.21 3FK5.HIS 271,5.34,-1.16,0,0 2QEV,LYS_76,11.34,-0.24,0.69,0.38 2ZCO,GLU_254,4.45,1.03,-0.85,-0.23 105T,ARG_122,12.32,-0.31,0,0.14 2PIM,LYS 125,10.31,-0.09,0,-0.11 2D7U,GLU_107,2.4,0.54,-1.64,-1 4FZR,GLU_105,4.77,0.32,0,-0.04 2H2Z,GLU_14,4,0.36,-0.85,-0.01 1YTQ,CYS_37,9.61,-0.69,0.18,1.13 3G9G,TYR 160,10.66,0,0.23,0.43 1NAF.GLU 173,4.62,0.12,0.0 1ZBS,LYS_56,10.19,-0.29,0,-0.02 3S0A,GLU_33,4.17,0.29,-0.41,-0.21 2XJ4,ARG_254,12.88,-0.64,0.59,0.42 1KCM,LYS_252,10.58,-0.14,0,0.22 20KT,HIS_337,6.2,-0.19,0,-0.11 4GA2,ARG 23,12,28,-0,25,0,0.03 3I0C,GLU_97,3.9,1.13,-0.71,-1.02 2EJX,LYS 60,11.52,-0.26,0.81,0.46 1XFK.HIS 235.5.58.-1.06.0.0.14 2FZP,GLU_198,4.09,0.51,-0.8,-0.12 3HUE,LYS_96,10.12,-0.49,0,0.1 3O16,LYS_50,10.84,-0.16,0.2,0.31 1L2H,CYS_8,11.53,0,-0.02,2.55 1WPA,LYS_521,10.6,-0.39,0.12,0.37 3COU, ARG_168, 12.45, -0.38, 0, 0.33 3C5V,ARG_303,13.34,-0.21,0.58,0.46

3F6M,GLU_30,4.62,0.35,-0.06,-0.17 1AK1,ASP_159,3.99,0,-0.31,0.49 1YOY.LYS 110.10.43.-0.07.0.0 2XMZ,HIS_3,5.46,-1.26,0.36,-0.14 1TD6,TYR_283,10.11,0,0,0.11 1SJ8.CYS 719.12.-0.06.-0.05.3.11 2H30.TYR 52.10.7.-0.01.-0.1.0.82 1T3J,GLU_701,4.63,0.35,0,-0.23 3PZ9,LYS_245,10.48,-0.16,0,0.13 1U7U,ASP_401,4.05,0,-0.27,0.52 3LJC.LYS 235.10.26.-0.24.0.0 1U7U,ARG_405,12.64,-0.17,0,0.32 3EYE, ASP_101, 3.26, -0.43, -0.4, 0.29 2P0L,ASP_203,3.75,0,-0.15,0.11 306L.GLU 23.4.6.0.29.0.-0.2 1V6T,ASP 202,3.92,0,-0.24,0.36 2YX0.HIS 144.3.61.-2.38.0.-0.51 4FD6,LYS_5,10.38,-0.12,0,0 20BI,ARG_12,12.58,-0.07,0,0.15 3JRT,ARG_46,13.27,-0.86,1.15,0.49 3V75,ARG 45,12,26,-0,46,0,17,0.05 10IS,GLU_182,4.88,2.2,-1.66,-0.16 20GQ,ARG_579,13.56,-1.05,0.81,1.3 1NRI.ARG 200,12.36,-0.15,0,0.01 4AM1,TYR 30,11.43,0.71,0.11,0.62 2QEV,ASP_33,3.3,-0.85,-0.8,1.16 3UV9,LYS_413,11.33,-0.22,0.67,0.38 3GS9,ASP_167,3.14,-0.81,-0.17,0.31 3OA7,GLU_42,4.63,0.28,0,-0.15 4EKU,LYS_206,10.49,-0.01,0,0 10LR,TYR_66,13.09,-0.05,0.9,2.25 3LOE,GLU 407,5,27,0,46,0,0,32 4GCO,LYS_156,10.64,-0.1,0,0.24 2F8H,ARG 294,11.85,-0.59,0,-0.07 1V43.HIS 201.6.69.-0.54.0.33.0.4 1KCM,GLU_218,6.22,1.9,0,-0.18 1TLV,GLU_150,3.67,0.46,-0.85,-0.44 3BA1,GLU_161,5,0.46,0,0.05 1TXD,HIS 842,5.32,-3.24,0.85,1.21 2Q07,ASP_482,3.07,-1.64,-0.21,1.12 1C3K.ARG 20.11.96.-0.54.0.0 1T3Y,TYR_31,12.71,0.47,0.05,2.19 3CAN,GLU 49,4.35,0.17,-0.16,-0.15 2RFA.TYR 115.10.46.0.0.02.0.45 3GA2,GLU_71,4.78,0.18,0,0.1 3ETV,ARG_281,11.41,-1.24,0,0.15 2Z61,ARG_347,12.4,-2.99,0.02,2.88 4DND,GLU_93,4.66,0.18,-0.02,0 1M5I,ARG_217,12.7,-0.8,0.34,0.66 3KEY,GLU_341,4.75,0.26,0,0 2CYG,ARG_102,12.55,-0.29,0.13,0.21 3F1X,ASP_257,4.25,0,0.1,0.35 3G9G.GLU 142.4.06.0.43.-0.85.-0.03 2G9D,GLU_89,7.37,4.01,-0.38,-0.75 2FBQ,GLU_132,4.07,0.22,-0.4,-0.24 3EVN,LYS_260,10.2,-0.38,0,0.08 1SJ8,GLU_694,4.75,0.28,0,-0.03 2BDV.HIS 46.4.56.-1.94.0.03.-0.03 30YB,LYS 875,10.36,-0.2,0,0.06 2FD5,ARG_160,11.51,-1.45,0,0.47 3C6B,CYS_219,12.55,-0.03,0.58,3 1FKM,ASP_264,3.9,0,0,0.1 3US6,GLU_106,4.64,0.14,0,0 2B78,ARG_154,12.83,-1.39,0,1.72 4EZB,GLU_259,4.64,0.14,0,0 3GV0,HIS_295,5.41,-1.3,0.24,-0.03 1WYC.GLU 20.3.8.0.44.-0.8.-0.34 2W2S,HIS_163,6.39,-0.11,0,0 1X04,GLU_101,4.92,0.31,0,0.12

2VGM.LYS 66.10.43.-0.77.0.0.71 2GAU,LYS_107,11.55,-0.29,0.85,0.48 3MIX,ARG_586,13.02,-0.14,0.23,0.43 3HQX,GLU_45,4.57,0.07,0,0 2D7J.CYS 61,12,28,-0.84,0.4,3,71 3EJG,ASP 161,4,13,-0.01,0,1,0.25 1SUU,ASP_747,1.26,-2.42,-0.86,0.74 3IRA,LYS_115,11.42,-0.31,0.85,0.38 3T57,ARG_258,12.3,-0.28,0,0.08 2FPN,ASP_51,4.02,0,0,0.22 3A0X,LYS_710,10.45,-0.05,0,0 3CSR,ARG_126,13.41,-0.34,0.72,0.53 1ZBS,ASP_42,3.78,0,-0.44,0.42 2B0J,GLU_69,4.66,0.32,0,-0.16 3EVP,GLU_273,3.61,0.29,-0.62,-0.56 3NZL,TYR_57,10.05,0,0,0.05 1NWA, ASP_109, 4.05, -0.15, 0.11, 0.29 1X1E,HIS_76,3.79,-2.92,0.81,-0.59 3LQE,ARG_478,12.96,-0.41,0.49,0.38 1K95,CYS 181,11.9,0,-0.01,2,91 3CGW,GLU_75,4.65,0.21,0,-0.07 2D7J,LYS_116,10.54,-0.11,0,0.14 1LZL,ARG_153,13.19,-0.67,0.78,0.57 105J.GLU 68.3.78.0.55.-0.85.-0.42 1XFK,HIS_140,4.69,-1.58,0,-0.24 2DFL,ASP_321,2.61,-2.15,-0.1,1.05 3Q2C,HIS_80,6.42,-0.1,0,0.02 3UC9,HIS 16,6.08,-0.38,0,-0.04 1WPA, ASP_492, 3.3, -0.47, -0.38, 0.36 3CS1,GLU_69,5.26,0.54,0,0.23 3MTT,LYS_489,10.73,-0.08,0,0.31 1Q46,GLU_42,5.53,1.19,-0.11,-0.04 3IV4,ASP 38,3.28,-0.63,-0.46,0.57 2YYO.HIS 151,5.99,-0.88,0.4,-0.05 1DUN,ASP_14,3.79,0,-0.13,0.11 1XDZ,ARG_216,13.25,-0.68,0.97,0.47 2V81,ARG_14,12.32,-0.18,0,0 2W2S,GLU_37,4.68,0.18,0,0 2YX0,LYS_11,10.47,-0.03,0,0 3PZ9.ARG 83.13.77.-0.21.0.83.0.65 3EUR,LYS_51,10.37,-0.41,0,0.29 2B6P,GLU_16,6.75,4.73,-2.47,-0.02 2RJD.GLU 430.4.02.0.51.-0.74.-0.26 1Q46,TYR_171,10.43,0,0.08,0.35 200K,GLU_108,4.44,0.29,0,-0.35 2R51,CYS_171,9.35,0,-1.39E-17,0.36 109G,GLU_91,4.62,0.13,0,-0.01 1WRU,ASP_323,4.04,0,0,0.24 208I,LYS_110,10.21,-0.47,0,0.18 2OSA,GLU_324,4.44,0.16,0,-0.22 2BCF,LYS 145,11.24,-0.49,0.85,0.38 2H14,HIS 86,4.85,-2.9,0.85,0.4 2AH5,ARG_72,12.32,-0.97,0,0.79 1SIG,GLU_378,3.85,0.41,-0.6,-0.46 1YTQ,GLU_46,3.68,0.3,-0.67,-0.45 3A2Z,TYR 71,10.78,0,0,0.78 1T6L,ARG_137,12.37,-0.45,0,0.32 1HF8,GLU_33,3.6,0.32,-0.59,-0.63 2CXC,ARG_127,11.61,-1.89,0.56,0.44 2C2Y,ARG 66,12.32,-0.62,0,0.44 100X,ARG 30,13.59,-0.35,0.76,0.68 2EDM,LYS_79,10.67,-0.17,0,0.34 2P4D,ARG_116,12.4,-1.03,0.17,0.76 1RZ2,HIS_163,6.61,-0.83,0.64,0.3 1NJ4,ARG_261,12.15,-0.35,0,0 1YTD,TYR_99,11.96,0,0.53,1.43 1QYI,GLU_179,3.58,1.45,-1.36,-1.01 2G3A,LYS_117,10.88,-0.26,0.26,0.37 2IRM,ASP_96,3.43,-0.41,-0.37,0.42

4F3J,ASP_213,3.99,0,0,0.19 1X7F.GLU 236.4.67.0.22.0.-0.04 2WZ9,HIS_115,6.23,-0.9,0.85,-0.22 1FQI,LYS_290,10.3,-0.4,0,0.2 4ESS,HIS_162,6.51,-0.34,0.27,0.07 2BCF,GLU _210,4.69,0.19,0,0 2B0J.GLU 338,3.81,0.24,-0.4,-0.53 3HUE,GLU_263,4.84,0.15,0,0.19 3F6F,LYS_175,10.52,-0.09,0,0.11 2QVT,LYS_70,10,-0.4,0,-0.09 3KEY,GLU_371,4.31,0.33,0,-0.52 1MIX,LYS_268,10.35,-0.11,0,-0.04 1N81,ASP_195,4.04,-0.13,-0.42,0.79 3ANJ,TYR_364,12.03,-0.77,0.66,2.14 2G2D.ARG 174.12.66.-0.72.0.53.0.36 3U4K,ARG 125,12.66,-0.22,0.16,0.22 2Q34,GLU_179,3.56,0.41,-0.91,-0.43 2WB3,GLU_378,5.15,0.3,0,0.35 2CL3,ASP_116,3.21,-0.87,-0.08,0.37 3K9I,ASP_159,4,0,0,0.2 1N81,TYR_21,10.29,0,0.04,0.25 2QK0,LYS_100,9.88,-0.65,0,0.02 3RFF,HIS_70,6.19,-0.31,0,0 2FI9,GLU 93,4.67,0.28,0,-0.12 208PLYS 80,10.27,-0.23,0,0 2FBI,GLU_130,4.7,0.2,0,0 30NT,CYS_12,7.86,-1.73,0.04,0.56 2V5B,LYS_154,10.23,-0.4,0,0.13 2RIK,LYS 22,10.37,-0.13,0,0 2R51,ARG_136,12.12,-0.43,0,0.04 3PAC,LYS_15,10.81,-0.4,0.28,0.43 1R3F,ASP_87,4.14,-0.01,0.04,0.31 1YR6,ASP 168,2.74,-1.34,-0.41,0.69 2VGY,HIS 56,5,29,-0,93,0,-0,29 3KEY,LYS_449,10.34,-0.37,0,0.21 4EZB,GLU_-7,4.97,0.33,0,0.14 4HDE,LYS_150,11.53,-0.52,0.85,0.71 1UAJ,GLU 34,3.94,0.59,-0.71,-0.44 307K,GLU_14,4.69,0.18,0,0.01 4E8B,ASP_214,3.85,-0.67,-0.21,0.94 1V43,GLU_351,4.58,0.25,0,-0.17 1TXJ.GLU 169.3.76.0.42.-0.85.-0.31 1KN3.HIS 159.6.24,-0.22.0,-0.05 3E7P,GLU_239,4.58,0.27,0,-0.19 2GAU,LYS_165,10.71,-0.36,0,0.57 3LJC,ASP_179,3.1,-1.01,-0.07,0.39 1ANU,GLU_81,2.37,0.91,-3.04,0 2EJX.GLU 121.4.77.0.23.0.0.04 200K,GLU_220,4.62,0.3,-0.16,-0.01 2B02,GLU_398,3.93,0.45,-0.83,-0.19 2013.GLU 155.4.59.0.09.0.0 4HDE,ARG 192,13,99,-0.33,1.36,0.46 4E9E,GLU_501,3.57,0.27,-0.85,-0.35 1RKA, ARG 171, 12, 17, -0, 39, 0, 0, 05 3D9H,HIS_204,5.86,-1.65,0.77,0.24 3C5V,ARG_102,13.08,-0.46,0.4,0.65 3MEW.GLU 197.4.6.0.06.0.0.04 105J,ASP_48,2.96,-1.4,0,0.56 1EV8,LYS_18,10.56,-0.18,0,0.24 3ZTA.ARG 38.12.94.-0.3.0.43.0.31 2D7U,TYR 187,10.54,0.0.33,0.21 3V3T,GLU_176,5.06,1.38,-0.34,-0.48 2BV9,ARG_234,13.1,-0.19,0.44,0.34 4DIU,GLU_141,4.25,0.82,-0.74,-0.34 2IF4,ASP_211,3.32,-0.59,-0.12,0.22 2CI3,HIS_231,5.84,-0.56,0,-0.11 1YB2,TYR_107,10.16,0,0.05,0.11 3AUF,HIS_-1,6.7,-0.5,0.23,0.47 2P65,GLU_114,4.65,0.1,0,0.06

1T6L.TYR 92.8.69,-1.01,-0.76,0.46 2YWX,GLU 150,4.15,0.2,-0.56,0 1RI6,HIS_93,6.21,-0.87,0.32,0.26 1R53,LYS 203,10.37,-0.13,0,-0.01 2EYI,LYS_220,11.91,-0.38,1.02,0.77 1PNE,LYS_37,10.11,-0.51,0,0.12 2CVB.GLU 161.4.07.0.2.-0.36.-0.27 2YX0,LYS_193,12.66,-0.48,1.68,0.96 4H4J,ASP_248,3.77,-0.08,-0.31,0.37 2F9F,LYS_123,11.03,-0.2,0.41,0.33 3K8U,TYR_101,13,0,0.01,2.99 2GZQ,TYR_71,12.39,0,0.34,2.05 3I4T,ASP_14,4.21,-0.98,0.29,1.11 1WRU,ASP_116,3.75,-0.93,-0.21,1.08 2012,HIS 175.6,-0.24,0,-0.26 1ILW,ARG 165,12.81,-0.2,0,0,5 1UAJ,ARG_52,12.55,-0.16,0,0.21 1BN6,GLU_110,4.63,0.32,0,-0.19 2Q12,LYS_66,10.33,-0.45,0,0.27 3ETV,LYS 298,10.38,-0.12,0,0 2YT4.LYS 667.9.94.-0.2.0.-0.36 1ILW,TYR_124,11.14,0,0.12,1.02 1J7G,GLU_36,4.37,0.13,0,-0.25 2R2Y,LYS 99,10.74,-0.26,0.0.49 3LMF.ARG 27.13.03.-0.24.0.37.0.4 2XMZ,HIS_42,5.97,-0.99,0.31,0.14 1P1L,GLU_65,4.16,0.31,-0.56,-0.08 3D9H,LYS_163,9.92,-0.64,0,0.07 3GE9,HIS 194,5.88,-0.49,0,-0.12 1MJS.ARG 267,12.82,-0.38,0.01,0.68 1BKR,GLU_71,3.99,0.41,-0.69,-0.24 1AD6,HIS_483,2.89,-3.08,0.32,-0.85 1F2V.GLU 147.4.94.0.54.0.-0.1 3R87, ARG 101, 12, 39, -0, 23, 0, 0, 13 1RL0,GLU_164,4.2,2.98,-2.81,-0.46 1RZ2,LYS_72,10.34,-0.16,0,0 3LJN,ARG_182,12.94,-0.45,0.32,0.56 3DHN,ARG_174,13.39,-0.14,0.69,0.34 3V55,GLU 355,3.6,0.4,-0.8,-0.5 1MUF,LYS_143,10.7,-0.13,0,0.33 1TWU,GLU_107,4.77,0.17,0,0.1 3PBH,HIS_111,5.65,-0.75,0,-0.1 1NRI,GLU 193,5.72,2.84,-1.39,-0.24 1V43,TYR_102,12.16,0.85,0.42,0.88 1PSW,ASP_124,3.49,-0.61,-0.02,0.32 1WRU,LYS_253,10.45,-0.05,0,0 1P4X,ARG 193,12.21,-0.29,0,0 1YIB,CYS_228,9.73,-0.04,0.13,0.66 1NFN,ARG_38,12.34,-0.28,0,0.12 1DTO.CYS 109.10.68.0.-0.53.2.21 1ZBM,ARG_227,12.11,-0.3,0,-0.09 4H4J,HIS_227,4.73,-1.86,0,0.09 1R3F,ASP_299,3.43,-0.62,0.1,0.14 3ANJ,GLU_395,4.97,0.79,0,-0.32 1YLN,HIS_38,6.43,-0.12,0,0.06 1YB2,LYS_182,11.56,-0.4,0.85,0.61 2R51,LYS 36,10,53,-0,11,0,0,14 4AM1,GLU_149,5.59,1.92,-0.74,-0.1 1EQ6,LYS_189,10.53,-0.05,0,0.08 3M7D,LYS 47,10,23,-0,79,0,85,-0,34 3QYB,LYS 897,10.69,-0.76,0.26,0.68 3VJ8,GLU 191,4,45,0,12,0,-0,18 1MUF,HIS_297,6.06,-0.44,0,0 3GS9,ASP_97,3.81,0,-0.51,0.52 3G9T,GLU_189,4.54,0.07,0,-0.03 1X7F,TYR_317,9.68,0,-0.54,0.21 3BCY,LYS_102,9.84,-0.86,0,0.21 2FC3,TYR_79,13.26,-0.62,0.73,3.16 3ANJ,GLU_28,1.48,0.89,-3.05,-0.84

2AZP,ARG_104,12.06,-0.43,0,-0.01 2R0S,LYS 106,11.16,-0.63,0.85,0.44 1UAJ,ARG_208,12.4,-0.29,0,0.19 3V55,GLU_388,4.41,0.83,-0.7,-0.22 3DSH,ARG_443,12.34,-0.16,0,0 3IO0,ARG 203,12.4,-0.15,0.0.05 3BOW.GLU 194.5.0.28.0.0.22 2HRZ,HIS_-3,6.34,-0.16,0,0 3HKX,ARG_89,12.23,-0.28,0,0.01 3EYE,LYS_103,11.14,-0.22,0.43,0.42 1R3F,ARG_40,12.56,-0.16,0,0.23 3GFP,GLU_473,4.95,0.3,0,0.16 1R29,ASP_119,3.59,-0.09,-0.53,0.4 2D0A,TYR_114,10.96,-0.66,0.52,1.1 2FI9,ASP 58,4,41,-0,93,0,04,1,5 1WP5,TYR_262,10.66,0,0.08,0.58 4ACJ,HIS_770,7.25,-0.5,0.82,0.42 2A6B,LYS_78,10.3,-0.21,0,0.02 2X5Y,LYS_779,10.39,-0.11,0,0 4DVD,ARG 58,11.33,-1.27,0.0.1 1X04,LYS_39,10.57,-0.18,0,0.24 2PLQ,CYS_189,13.19,0,0.2,3.99 3GFP,ARG_426,11.38,-0.8,0,-0.33 2|6|.TYR 16.10.26.0.0.12.0.14 2YT4.LYS 679.11.24.-0.76.0.79.0.7 20GQ,LYS_388,10.37,-0.22,0,0.09 1CBY,GLU_136,4.1,0.4,-0.09,-0.7 2B0J,GLU_110,4.57,0.26,0,-0.2 3F6M,LYS 89,10.22,-0.33,0,0.05 3ANJ,LYS 264,10,15,-0,35,0,0 3ASA,ASP_74,4.12,-0.06,0,0.39 3GW3.GLU 250.4.51.0.23.0.-0.21 3G6S,LYS_87,11.16,-0.87,0.81,0.74 3DB9,ARG 115,12.32,-0.48,0,0.29 3ETV,GLU_23,4.65,0.15,0,0 3LMO,LYS_78,10.45,-0.14,0,0.09 2YLF,TYR_63,11.18,0,-0.03,1.2 2CL3,ASP_142,4.04,0,-0.05,0.3 2HNG,GLU 87,4.12,0.2,-0.62,0.05 3ASA,LYS_12,11.45,-0.45,0.82,0.58 2JKF,GLU 29,4,22,0,5,-0,56,-0,23 2H01,LYS_73,10.98,-0.45,0.57,0.36 1ZP2,LYS 88,12.02,-0.66,1.25,0.92 1FOI,ARG 360,12.24,-0.21,0,-0.05 3G9G,LYS_200,10.5,-0.1,0,0.1 2P1W,ARG_177,13.84,-1.05,1.38,1.01 3V55,ASP_535,2.56,-1.27,-0.66,0.7 2FPN,ASP_108,3.19,-0.85,-0.04,0.28 2H8O,HIS_56,6.23,-0.24,0,-0.03 1WXQ,GLU_267,4.9,0.58,0,-0.18 2IXM,ARG_148,12.58,-0.69,0.26,0.5 1J7G,ARG_7,11.94,-0.86,0,0.3 1G5Z.GLU 87.4.73.0.23.0.0 1RI5,LYS_238,10.23,-0.31,0,0.04 3HVM,LYS_242,9.98,-0.5,0,-0.02 1Q2Y,GLU_37,4.72,0.11,0,0.1 2BLL,GLU_479,3.97,0.32,-0.64,-0.22 3V55.LYS 341.10.15.-0.62.0.0.27 1U53,LYS_172,10.23,-0.34,0,0.07 1YW5,ASP_42,3.2,-0.72,-0.28,0.4 3RKV,GLU_298,4.92,0.24,0,0.18 3CJW.CYS 213,9.63,0,-0.22,0.85 1X04,LYS_172,11.72,-0.66,0.97,0.91 4EVF,ASP_135,4.01,-0.88,-0.03,1.13 3E7P,ASP_107,3.55,-0.36,-0.21,0.31 1059,ARG_153,11.52,-1.05,0,0.07 3PZ9,TYR 179,11,49,0,54,0,27,0,68 2VC8,GLU_61,4.53,0.23,0,-0.2 3LH5,ARG_658,11.73,-2,0,1.23

2RGY.ARG 345.11.51.-1.29.0.0.3 1LFP,LYS 137,10.18,-0.91,0.12,0.46 100X,GLU_254,4.09,0.32,-0.42,-0.3 1AT0,LYS_340,10.35,-0.15,0,0 1X1E.ARG 156.12.2.-0.3.0.0 2XMZ.GLU 53.4.63.0.29.-0.11.-0.04 1ZP2,HIS_137,3.96,-2.58,0,0.04 2OGQ,TYR_552,11.4,-0.58,0.28,1.72 3LJC,GLU_203,4.47,0.55,-0.58,0 2EJB,HIS_64,6.23,-1.39,0.85,0.26 3PP8,LYS 21,10.35,-0.16,0.0.01 1FQI,TYR_383,9.83,-0.23,-0.21,0.26 3V4G,LYS_34,10.45,-0.21,0,0.16 2EHG,LYS_107,10.68,-0.21,0,0.38 3C5V.ARG 39.12.29.-0.27.0.0.07 3BB7,TYR_138,13.17,-0.14,0.3,3.02 1P4X,GLU_98,4.59,0.14,0,-0.05 2G9D,ASP_117,2.21,-2.05,-1.16,1.63 1V43,TYR_78,10.45,0,0.17,0.28 2BAA,TYR 112,10.05,-0.48,-0.34,0.86 3IVF,TYR_81,11.73,-0.15,-0.01,1.89 1RAJ,TYR_73,10.16,0,-0.05,0.21 4ETX,ARG_210,12.18,-0.42,0,0.09 2H2Z.LYS 180,10.19,-0.18,0,-0.13 3F1X,ARG_128,12.87,-0.25,0.34,0.28 2F4Q,GLU_312,4.71,0.17,0,0.04 4ESS,GLU_149,3.78,0.32,-0.69,-0.35 2WB8,CYS 679,9.8,-0.16,-0.1,1.07 4E6S,CYS_14,9.29,0,-0.01,0.3 2Z61,LYS_213,9.82,-0.9,0,0.22 3H6Q,GLU_142,4.7,0.21,0,-0.01 2GEN,ARG_138,11.82,-1.1,0,0.42 3RJX,HIS 127,4.63,-1.51,0,-0.36 3IL3.GLU 47.4.58.0.06.0.0.02 2ZCO,GLU_175,4.37,0.6,-0.57,-0.15 3F1X,ASP_256,3.29,-0.83,-0.09,0.4 3C5V,ARG 228,12.53,-0.5,0.0.54 1H09,ARG_73,13.54,-0.31,0.74,0.6 208I,ARG_56,12.18,-0.95,0.17,0.46 20ZO,ASP 60,2,91,-1.37,-0.12,0.6 1W7B,LYS_329,10.16,-0.45,0,0.12 2EFK.GLU 238,4.14,0.97,-0.84,-0.49 3EYE.GLU 114,4,55,0.05,0,0 3LJN,GLU_105,4.58,0.2,0,-0.12 3M66,CYS_399,10.96,0,0.34,1.62 3GS9,GLU_67,4.63,1.51,-1.06,-0.31 3A7L,GLU_30,4.96,0.68,-0.32,0.09 3ZXY,ASP_37,3.86,0,-0.34,0.4 2B6P,GLU_151,3.95,0.47,-0.78,-0.24 1FQI,GLU_333,3.13,1.07,-1.57,-0.87 3CO1,ARG_130,12.11,-0.62,0,0.23 1P6F.TYR 167,12.02.0.0.2.02 3CJW,LYS_303,9.54,-1.07,0,0.11 3JV1,HIS_150,5.89,-0.27,0,-0.33 10IS,TYR_169,9.22,-0.83,-0.37,0.42 3VHJ,GLU 94,4.61,0.12,0,-0.01 3F7M,TYR_340,11.68,-0.8,0.36,2.12 1PDB,LYS_184,10.3,-1.47,0.85,0.42 3H9W,HIS_86,5.95,-1.48,0.81,0.11 2CBE,GLU 239,5.11,0.51,0,0.11 1R3F,ASP 92,4.05,0.0.1.0.15 2Q07,CYS_253,9.58,-0.7,-0.69,1.97 2OYZ,TYR_89,11.99,0,0.53,1.46 1AK1,LYS_306,10.58,-0.22,0,0.3 1JYH,ASP_104,3.96,0,-0.01,0.17 1GQE,ASP 329,3.16,-0.8,-0.37,0.53 105J,GLU_34,4.48,0.23,0,-0.26 3UC9,ASP_129,3.81,-0.84,0.06,0.79 3H5T,ASP_116,2.41,-1.67,-0.1,0.37

2B61,ASP_197,2.77,-1.64,-0.07,0.69 3V3T.CYS 243.11.69.0.0.07.2.62 1T95,ASP_36,4.02,-0.3,-0.68,1.19 3ERF,LYS_118,10.47,-0.24,0,0.21 2IXM.LYS 111.10.61.-0.16.0.0.27 2FG1.LYS 90.11.22.-0.37.0.85.0.24 3V55,HIS_718,6.58,-0.18,0,0.26 2IF4,LYS_103,9.97,-0.7,0,0.17 3H5T,LYS_322,10.17,-0.36,0,0.03 2WB8,ASP_696,3.57,-0.41,-0.06,0.24 1T6L,ARG_243,11.65,-0.71,0,-0.15 1TP6,ARG_111,12.77,-0.31,0,0.58 2A4D,LYS 84,10.37,-0.13,0,0 1LN4,ASP_2,3.37,-0.19,-0.45,0.2 3ZSL.TYR 247.10.41.0.0.02.0.4 3PP8,LYS 127,10.31,-0.18,0,-0.01 2G9D,GLU_308,2.42,1.42,-2.53,-0.99 1X8F,LYS_47,11.27,-0.22,0.61,0.38 105J,ARG_25,12.66,-0.38,0.29,0.25 3I4T,CYS 134,10.1,0,0.38,0.72 1XWM,LYS_171,10.27,-0.23,0,0 2YX0,GLU_208,4.27,0.35,-0.69,0.12 1D2K,LYS_205,10.41,-0.14,0,0.05 1X04,ARG 152,12.71,-0.25,0,0.46 3O6L.LYS 59,10.52,-0.21,0.0.24 3R87,TYR_86,9.09,-0.85,-0.38,0.33 3FS3,GLU_41,4.67,0.17,0,0 3CIV,CYS_300,11.52,-1.66,0.15,4.03 4DNU,ASP 159,3.38,-1.63,-0.25,1.45 2DVK,ASP_157,3.37,-0.55,-0.29,0.41 1G8P,ARG_183,13.22,-0.29,0.47,0.55 3M70,LYS_286,10.53,-0.19,0,0.22 3LQE,ARG 392,12.02,-1.11,0,0.63 1K95,CYS 182,13,48,-0,38,0,91,3,94 3IVF,TYR_308,10.56,-0.08,-0.24,0.88 2P0L,TYR_148,12.05,-0.85,-0.16,3.05 1EV8,ASP_241,3.36,-0.66,-0.11,0.33 2PGE,LYS 229,10.35,-0.15,0,0 2E0T,ARG_186,12.32,-0.38,0,0.21 1RI6,ASP_123,3.3,-1.28,-0.2,0.98 1JKS,GLU_224,4.45,0.29,-0.61,0.27 3CRM,TYR 201,10.58,-0.57,0,1.15 3BOE,LYS 234,10,59,-0.08,0.0.18 3JSN,GLU_183,4.75,0.25,0,0 1BN6,GLU_27,4.73,0.19,0,0.04 3AU3,ARG_640,12.06,-0.6,0,0.16 1BKR,LYS 108,10.36,-0.21,0,0.07 2X4J.TYR 44,10.09.0.-0.04.0.14 3IRA,HIS_16,2.39,-2.6,0,-1.5 3ZTA,LYS_8,10.92,-0.87,0.46,0.83 2WB3.CYS 350.9.03.0.-0.32.0.35 3P2F,ASP 51,1.96,-2.17,-0.65,0.96 3C6B,ARG_13,13.85,-0.35,0.83,0.87 105Z.LYS 635,10.54,-0.16,0.0.2 3IBT,LYS_205,9.88,-0.89,0,0.26 3HKX,ARG_275,12.33,-0.17,0,0 3A2Z,ASP 40.4.16.0.0.06.0.3 1XWM,ARG_124,12.16,-0.55,0,0.21 307K,ARG_36,11.78,-0.72,0,0.01 2PGE,ARG_147,13.76,-0.33,0.93,0.66 3VHJ.CYS 86.11.54.-0.64.0.3.18 2NSN,ASP_95,3.97,0,0,0.17 3JV1,GLU_99,3.41,0.84,-1.2,-0.74 1R9W,HIS_270,4.36,-2.72,0.58,0 2Z0M,LYS_235,10.27,-0.17,0,-0.07 1ZBM,GLU_115,3.66,0.18,-0.63,-0.38 3GYW,GLU_41,4.66,0.16,0,0 2Q12,ARG_146,12.93,-0.36,0.29,0.51 4ESS,LYS_94,10.46,-0.24,0,0.2

4ETX.ASP 337.2.82.-1.35.-0.73.1.11 1X9G,LYS 131,9.91,-0.44,0,-0.15 3ADO,GLU_239,4.71,0.29,0,-0.09 200K,GLU_309,4.52,0.38,0,-0.36 100X,GLU_14,3.71,0.73,-0.94,-0.57 3IV4,ASP_64,3.73,0,-0.4,0.32 3N0K,ARG 35,11.42,-0.96,0,-0.12 2IF4,GLU_196,4.61,0.2,0,-0.09 1XTD,GLU_151,4.51,0.25,-0.31,0.06 2P52,ARG_245,12.28,-0.13,0,-0.09 1C44,LYS 98,10.4,-0.38,0,0.28 3IBT,GLU_176,4.57,0.13,0,-0.06 3LPZ,ARG_7,12.26,-0.22,0,-0.02 3EVP,ARG_231,12.1,-0.4,0,0 1DOV,LYS 163,10,48,-0,23,0,0,21 1EDG,LYS 27,10.18,-0.32,0,0 2RJD,LYS_509,10.3,-0.26,0,0.06 3PBH,LYS 19,10.45,-0.05,0.0 2FZ4,LYS_150,11.32,-0.61,0.7,0.74 2YLF,GLU 230,4.69,0.19,0,0 2A1V.LYS 43,10.87,-0.62,0.85,0.14 2CIU,ARG_167,12.62,-0.32,0,0.44 2FXT,LYS_311,10.48,-0.07,0,0.04 1XAW,LYS 521,11,59,-0.29,0.65,0.73 4F8A.GLU 627.4.05.0.51.-0.63.-0.33 3BQE,LYS_302,10.59,-0.17,0,0.26 2P52,ASP_278,3,-1.35,-0.72,1.27 3COU,ARG_78,11.74,-0.65,0,-0.12 2XMZ,HIS_246,1.72,-3.64,0,-1.14 2H85,ASP_219,3.78,-0.24,0,0.21 1J74,ARG_14,12.57,-0.56,0,0.63 3KEY,LYS_433,10.27,-0.12,0,-0.11 4EKU,GLU_66,3.86,0.4,-0.62,-0.42 4F85.HIS 58.2.06.-3.28.0.82.-1.98 20EW,GLU_165,4.54,0.28,0,-0.24 3IBT,ASP_158,3.32,-0.66,0,0.18 3EIZ,ASP_15,3.26,-0.69,-0.88,1.03 105J,LYS 84,10.41,-0.09,0,0 1ILW.GLU 87.4.63.0.09.0.0.04 3EVN,GLU_97,5.72,3.58,-1.19,-1.17 1MUF,GLU_330,4.13,1.3,-1.67,0 3CAN,HIS 128,6.54,-0.59,0.66,-0.03 10IS,ARG 296,12.4,-0.1,0,0 3DSH,GLU_241,3.33,0.68,-1.42,-0.43 1EDG,LYS_129,10.36,-0.25,0,0.11 1UOH,LYS_116,9.98,-0.22,0,-0.3 2YLF,GLU 44,3.91,0.93,-0.97,-0.56 1V6T,TYR_89,10.16,0,0,0.16 3NR5,ASP_128,4.24,-0.39,-0.09,0.92 2FPN,ASP_15,4.08,0,0.1,0.18 3HUE,CYS_105,9.12,-1.31,0,1.43 3HUE,CYS 204,10.17,-0.54,0.29,1.42 1IAP.LYS 106,10,49,-0.07,0,0.06 2Q13,TYR_41,10.3,0,-0.1,0.4 30IP,CYS_51,11.21,0,0.01,2.2 1R6Y,LYS_33,10.36,-0.14,0,0 3CIV,GLU_75,3.78,1.76,-2.25,-0.25 2RJD,ASP_384,3.44,-0.55,-0.56,0.75 1R7J.GLU 85.4.7.0.14.0.0.06 3FRR,ARG_55,13.26,-0.26,0.35,0.67 1R6Y,HIS 75,4.02,-2.27,0,-0.21 3JSN.GLU 180.4.5.0.17.0.-0.17 2QVT,LYS_149,10.62,-0.24,0,0.37 3ADO,CYS_125,9.86,-0.42,0.43,0.85 3B79,GLU_46,4.65,0.41,-0.2,-0.05 4EUG,ASP_9,2.7,-1.11,-0.33,0.34 1ZBS,GLU_169,4.04,0.29,-0.76,0 30KY,LYS 49,10.32,-0.18,0,0 1Y2Q,HIS_7,5.13,-1.2,0,-0.17

3GS3,ARG_122,12.33,-1.26,0.58,0.52 3F7M,TYR 375,10.27,0,0,0.27 3GT0.GLU 162.3.6.0.84,-1.44,-0.3 2B0A,GLU_1,4.42,0.17,0,-0.24 2R0S,LYS_74,11.1,-0.3,0.52,0.38 3ULX.GLU 136.5.41.3.31.-1.41.-0.98 3M7G.GLU 19.6.22.3.66.-2.1.0.14 1UJ8,ASP_18,2.59,-1.68,-0.76,1.23 3JV1,HIS_96,5.84,-0.42,0,-0.24 3F6F,TYR_113,12.8,0,0.45,2.35 1SIG,LYS 251,10.5,-0.1,0.0.11 1ZBP,GLU_177,5.23,0.3,0.24,0.19 3MTT,ASP_437,3.65,0,-0.31,0.16 1FHL,ARG 5,11.9,-0.81,0.0.2 208l,GLU_55,2.23,0.46,-2.35,-0.38 3GE9,GLU_145,4.62,0.12,0,0 2D0A.LYS 129.10.33.-0.15.0.-0.03 2WB8,HIS_794,5.12,-1.75,0,0.37 4DIU,GLU_39,4.78,0.49,0,-0.21 3IVF.GLU 80.4.89.0.61.0.-0.22 3BCY,LYS 154,10.42,-0.21,0.0.12 4H4J,LYS_194,10.16,-0.23,0,-0.11 1YOY.ASP 112.2.68.-1.22.-0.17.0.27 3U0V.HIS 28,4.88,-2.77,0.79,0.36 3H04,TYR 67,13.7,0,0.25,3.45 1J85.GLU 33.4.48.0.48.0.-0.5 3CJW,GLU_335,4.11,0.28,-0.71,0.04 30KQ,ARG_588,13.4,-0.19,0.71,0.38 2XHC,ARG_156,12.2,-0.29,0,-0.01 4ETX,ARG_367,11.66,-1.03,0,0.19 3DTE,TYR_25,11.83,0,0,1.83 10IS.LYS 173,10.44,-0.31,0.0.24 1TXJ,GLU_31,3.58,0.24,-0.76,-0.39 1PSW,LYS 167,10.76,-0.68,0.68,0.27 2NSN,HIS 17,6.27,-0.25,0,0.03 1MJS,ARG_367,12.41,-0.12,0,0.02 2X4J,ASP_107,3.22,-0.63,-0.31,0.36 1LN4,TYR_85,10.58,-0.63,-0.07,1.29 3EVZ,LYS 135,10.48,-0.53,0,0.5 2NYC,LYS_276,10.56,-0.12,0,0.17 2HRZ,ARG 253,12,47,-0,12,0,0.09 2FZ4,ASP_108,3.89,0,-0.16,0.25 3CBN,ASP 146,1.46,-2.69,-0.42,0.76 3GOZ,TYR 3,9.85,-0.58,0.06,0.37 4DVD,ARG_36,13.91,-0.28,1.3,0.38 3FHF,GLU_8,4,0.41,-0.52,-0.38 1ANU,GLU_4,3.68,0.42,-0.68,-0.57 2FC3,GLU 103,4.57,0.25,0,-0.18 2Z14,CYS_107,10.86,-0.01,0.07,1.8 3ASA,ARG_61,12.63,-0.33,0.06,0.4 3H5T,LYS_288,10.44,-0.09,0,0.03 3HVW,GLU 260,3.03,0.4,-1.51,-0.36 3FTT,LYS 165,10,45,-0.07,0,0.02 1OXZ,ARG_180,12.39,-0.24,0,0.13 2IRM,GLU_312,4.27,0.29,0,-0.52 3GMS,CYS_151,12.5,0,0,3.5 1IAP,GLU_155,4.57,0.17,0,-0.09 3CIV.ARG 260.13.86.-0.38.0.95.0.79 3EVZ,GLU_181,4.16,0.28,-0.31,-0.31 1V6T,ARG_237,11.93,-1.07,0.11,0.4 1XIP,ASP_180,3.09,-1.48,-0.01,0.78 1NAR.ASP 156.3.3.-0.6.-0.11.0.22 2Z14,GLU_56,4.64,0.16,0,-0.03 2AZL,ARG_243,12.42,-0.29,0,0.21 3UX2,GLU_75,4.55,0.08,0,-0.03 3I82,TYR_135,11.94,0,0.13,1.81 2EA9.TYR 36.10.62.0.0.05.0.57 2QDJ,LYS_96,10.06,-0.45,0,0.01 2FD5,GLU_60,5.31,0.76,0,0.04

2H2W.TYR 120.12.72.0.0.35.2.37 1J8B.LYS 20.10.29,-0.22,0.0.01 3GMS,LYS_15,10.67,-0.14,0,0.31 1MIX,LYS_278,11.48,-0.36,0.66,0.68 105Z,LYS 594,10,45,-0.05,0,0 2FXT.GLU 319.4.59.0.2.0.-0.11 1PVT,LYS_147,10.4,-0.1,0,0 3V3T,ASP_156,2.46,-1.45,-0.65,0.76 1EV8,GLU_86,4.51,0.2,-0.48,0.29 3ASA,GLU_253,4.01,0.93,-1.27,-0.15 1RI5,GLU_151,4.74,0.16,0,0.09 3I4T,ASP_11,3.73,-0.73,-0.23,0.89 2XJ4,ARG_55,13.55,-2.92,1.8,2.18 3SMD,GLU_108,3.76,0.32,-0.75,-0.31 4EKULYS 197.10.43.-0.07.0.0 4D8L,HIS_279,6.02,-0.5,0,0.02 1ZBM,LYS_250,10.47,-0.2,0,0.17 3UC9,LYS_163,10.93,-0.34,0.03,0.74 3ADO,CYS_285,9.16,-0.31,0.03,0.45 3L7N.GLU 84.4.61.0.11.0.-0.01 2QDJ,GLU_282,4.54,0.09,0,-0.05 2QZQ,LYS_114,10.43,-0.07,0,0 1RAJ,ARG_443,12.06,-0.33,0,-0.11 3HVW,ASP_221,2.96,-0.83,-0.37,0.36 3ADO,ARG_308,13.47,-0.19,0.78,0.38 2G9D,ARG_27,12.4,-0.1,0,0 3F5D,ASP_145,2.08,-1.64,-0.72,0.66 1YM5,ARG 260,12,-0.79,0,0.29 1GQE,HIS_199,4.1,-3.09,0.79,-0.11 2CIU,LYS_181,10.24,-0.37,0,0.11 1JB3,GLU_125,3.59,0.37,-0.69,-0.59 1EV8,ASP_81,4.06,0,-0.15,0.41 2D0A,ARG 117,13.28,-0.33,0.65.0.46 3I4T.TYR 145.13.26.0.0.55.2.73 1GQE,GLU_172,2.94,0.33,-1.51,-0.38 1LTU,GLU_157,4.09,0.93,-0.57,-0.77 3OKQ,ASP_616,3.14,-0.49,-0.57,0.4 3BOE.GLU 212.6.91.3.11.-1.07.0.37 3BB7,GLU_83,3.45,0.37,-0.85,-0.57 3C5V.TYR 49.12.65.0.85.0.43.1.37 1J74,LYS_72,10.44,-0.06,0,0 1X04,HIS 60,6.38,-0.18,0,0.06 2H30,ASP 84,2.27,-1.55,-0.47,0.49 1XAW,ARG_418,12.46,-0.04,0,0 1NAR,GLU_77,4.54,0.17,0,-0.13 2CWC,ARG 88,13,45,-0,34,0,81,0,48 1YTD,TYR_233,10.97,0,-0.01,0.97 3KT9,ARG_3,12.3,-0.37,0,0.17 1R3D,ARG_132,12.05,-1.72,0.37,0.9 3OA7,ARG_33,12.32,-0.18,0,0 1NAF, ARG 258, 12.27, -0.3, 0, 0.07 3N2T.GLU 65.5.29.4.-2.35.-0.86 1L2F,LYS_303,10.46,-0.16,0,0.12 3CRM,ARG_225,12.23,-0.3,0,0.03 3MIX,LYS_589,10.47,-0.32,0,0.29 3I4T,LYS 150,11.4,-0.35,0.85,0.4 1YR6,ARG_218,12.48,-0.22,0,0.2 1RHS,LYS_241,11.22,-0.51,0.85,0.38 1PNE,CYS_16,10.44,-0.41,-0.01,1.87 2NYC,LYS 200,10.2,-0.35,0,0.05 2XWS.LYS 26.11.61.-0.27.0.85.0.53 2P65,GLU_123,5.06,0.38,0,0.18 1IDK,TYR_268,10.7,0,0.35,0.36 1T6L,LYS_215,10.14,-0.36,0,0 3R2E,ASP_2,3.3,-0.72,-0.11,0.35 2EFK,ASP 159,3.48,-0.21,-0.38,0.27 1L2F,GLU_13,4.15,0.49,-0.85,0.02 3BB7,LYS 94,10.4,-0.21,0,0.11 4EVF,LYS_55,10.6,-0.13,0,0.23

20EV.ASP 71,3.35,-0.83,0.0.38 1RI6.HIS 244.5.42.-1.39.0.0.32 2P4D,LYS_98,10.77,-0.39,0,0.66 1ILW,HIS 144,5.61,-0.54,0,-0.34 1C3K,ASP_76,2.88,-0.86,-0.36,0.3 1SJ8.GLU 517.3.87.0.26.-0.52.-0.37 1BN6.GLU 211.3.83.1.44.-1.42.-0.69 4F8A,GLU_613,3.46,0.73,-1.51,-0.26 2OJQ,ARG_698,13.65,-1.2,0.95,1.39 1S7K,ASP_168,3.22,-0.82,-0.15,0.38 3GEC,LYS 374,10,17,-0,44,0,0,11 3RLN,GLU_728,3.83,0.32,-0.54,-0.45 2ZO5,ASP 198,2.97,-0.72,-0.44,0.32 2YYO,ARG_131,13.22,-0.54,0.73,0.53 3GG6.ARG 68.12.36.-0.21.0.0.06 1L2F,LYS 190,10.38,-0.08,0,-0.05 4H89,ASP_10,2.93,-0.81,-0.49,0.44 1RSS,ARG_119,12.11,-0.46,0,0.07 1RKA,GLU_190,6.45,2.98,-0.72,-0.31 2l88,LYS 455,10.43,-0.39,0,0.32 2CBE,LYS_172,11.4,-0.33,0.85,0.38 3IVF.ARG 131,13.05,-0.64,0.68,0.51 1LFP,LYS_189,10.55,-0.17,0,0.22 3GYW, ASP 189, 3.98, -0.13, 0, 0.31 1JSX.GLU 125.4.32.0.33.0.-0.52 2BDV,ASP_124,3.88,0,-0.09,0.17 3Q2C,ARG_39,12.95,-0.81,0.46,0.79 1SJ8,ASP_659,3.67,-0.26,-0.36,0.49 3RLE,GLU_34,5.26,1.69,-0.85,-0.07 3D9H,LYS_233,10.59,-0.17,0,0.26 2DVK,ARG_75,12.63,-0.27,0.06,0.34 2G9D,LYS_3,10.22,-0.34,0,0.07 2DVK,ASP_18,2.6,-1.28,-0.68,0.76 3CZC.ASP 76.4.0.-0.08.0.3 4H4J,GLU_73,4.29,1.15,-0.83,-0.54 2Z61,LYS_23,10.39,-0.14,0,0.03 2B0J,HIS_14,3.59,-2.83,0,-0.07 3GE9,ARG 168,12.38,-0.22,0,0.11 3CS1,GLU_118,5.9,2.02,-1.18,0.55 1J33,ASP_299,2.85,-0.92,-0.38,0.36 3A4C,ARG_462,11.99,-0.49,0,-0.03 3E7P,ASP 108,4,12,0,0,16,0,16 2Z84.LYS 200.10.41.-0.09.0.0 3VJ8,ARG_281,13.65,-0.17,0.84,0.48 3H5T,TYR_218,12.13,-0.9,0.1,2.92 1LFP,GLU_179,5.09,0.24,0,0.34 2YT4,CYS 666,9.13,-0.64,-0.07,0.83 4GA2,ARG 85,12,73,-0,34,0,25,0,32 2QOP,LYS_152,10.43,-0.07,0,0 1V43,ARG_84,10.94,-1.84,0,0.28 2NSN,LYS 67,10.37,-0.56,0,0.43 2X5Y,LYS 752,10.16,-0.33,0,-0.01 1JSX,ARG_68,11.76,-1,0,0.26 1D2K,LYS 91,10.23,-0.36,0,0.09 1MIX,ARG_328,13.01,-0.85,0.46,0.9 3PAC, ASP_49, 3.97, 0, -0.05, 0.21 3GFP.ARG 377,12.4,-0.19,0.0.09 4DNU,ASP_190,2.88,-1.05,-0.2,0.33 2D2S,GLU_546,4.34,0.64,-0.13,-0.67 20PJ.ARG 302.12.03.-1.32.0.18.0.68 3MIX.LYS 476.9.83.-0.68.0.0.01 2RGY,ARG_330,12.6,-1.13,0.73,0.5 2X5Y,GLU_766,3.83,0.33,-0.41,-0.59 2ZQ5,ASP_87,3.99,0,-0.05,0.24 2X4G,GLU_186,5.1,0.96,0,-0.35 4ACJ,TYR_680,13.07,-0.06,0.65,2.47 1TR9,GLU_92,4.74,0.21,0,0.03 3JZ9,ARG 342,12.47,-0.17,0,0.13 4DEZ,ARG_53,12.44,-1.15,0.26,0.83

208P.GLU 110.3.93.1.45.-1.29.-0.73 1WYC,TYR_215,12.77,-0.85,0.41,3.21 3SMD,TYR_39,10.11,0,-0.02,0.13 1WXF,LYS 241,10.96,-0.27,0.32,0.4 1NWA, ARG_88, 12.4, -0.11, 0, 0.01 2P0L LYS 74 10 48 -0 74 0 29 0 44 1YOY.GLU 117.5.18.0.9.0.-0.21 3CX2,ARG_177,12.29,-0.32,0,0.11 2D0A,LYS_122,10.14,-0.36,0,0 3SMD,LYS_123,10.38,-0.13,0,0.02 4E9E,HIS_557,6.19,-0.25,0,-0.06 2PLO,ASP 148,3.08,-0.93,-0.03,0.25 1IAP,GLU_171,3.76,0.89,-1.35,-0.3 3I47,ARG_157,12.44,-0.06,0,0 3BOW.GLU 92,5.0.33.0.0.18 2IOT.TYR 133,10.35,0.0.05,0.3 1SNT,GLU_225,4.08,0.32,-0.74,0 1TJE,ARG 39,13.33,-0.39,0.83,0.4 4EKU,ASP_278,2.47,-1.55,-0.38,0.61 1SNT,ARG_230,12.78,-0.39,0,0.67 3V75,ASP_101,3.47,-0.71,0,0.38 1RI5,TYR_284,13.26,0,0.5,2.76 1R3F,ARG_9,13.7,-0.91,1.55,0.57 3CAN, ASP 26, 2.96, -0.76, -0.45, 0.38 4EKU.GLU 245.3.9.0.37.-0.73.-0.25 2Q34,TYR_62,11.93,0.85,0.38,0.69 1NIJ,GLU_165,3.44,0.16,-0.84,-0.38 3CO1,LYS_66,10.47,-0.06,0,0.03 1Q8B,HIS 78,5.42,-2.3,0.85,0.37 1NJ4.TYR 159.10.03.-0.03.-0.36.0.42 2E0T,GLU_82,3.68,0.49,-0.84,-0.48 2EJX,LYS_133,10.94,-0.44,0.69,0.18 3I82,ARG 26,12,3,-0,2,0,0 1QQE,HIS_259,6.17,-0.96,0.2,0.42 1XTZ,HIS_39,5.31,-1.38,0,0.18 3R87,ASP_107,3.61,-0.58,-0.34,0.73 3PZ9,LYS_322,10.32,-0.3,0,0.11 2P4D,LYS 8,10.43,-0.07,0,0 2AXO,ARG 110,12,36,-0,42,0,0,27 3V55,LYS_360,10.18,-0.32,0,0 1WNH,GLU_101,4.67,0.09,0,0.08 2IXM,GLU_190,4.84,1.31,-0.5,-0.48 1PDB,LYS 18,10.5,-0.25,0,0.25 1RKA,HIS_279,4.52,-1.98,0.02,-0.02 1PZC,TYR_64,11.06,0,0.12,0.94 3IBT,ARG_112,12.15,-0.36,0,0.02 2A4D,TYR_139,11.84,-0.21,-0.29,2.35 2YLF,GLU_146,5,0.2,0,0.31 3G6S,ASP_70,4.32,0,-0.11,0.63 1WNH,LYS 42,10,45,-0,56,0,0,5 3KB5,HIS_345,7.56,-1.22,1.58,0.69 3BPP,GLU 175,3.89,0.37,-0.95,-0.03 2C2Y,HIS 123,5,43,-1,34,0,15,0,13 1XTZ,GLU_97,4.11,0.24,-0.64,0 3V75,ASP_16,3.9,0,-0.17,0.26 3C6B,TYR_216,11.86,-0.81,0.48,2.19 2NSN,TYR_49,10.44,0,0.08,0.36 2X5Y,LYS_822,11.42,-0.3,0.8,0.42 2X5Y,HIS 746,5,18,-1,31,0,-0.02 106D,TYR_103,10.04,0,-0.17,0.21 2QOP,LYS 146,10.3,-0.35,0,0.16 2IXM,HIS 271,5.25,-1.1,0,-0.15 3ZXY,ASP_287,3.5,-0.58,0,0.28 3C6B,ARG_45,12.46,-0.04,0,0 1FKM,LYS_630,10.78,-0.29,0,0.57 2P1W,ARG_213,12.31,-0.59,0,0.4 2Q07,ARG 335,12.26,-0.32,0,0.09 2G2D,ASP 98,3.36,-0.84,-0.02,0.42 3CQ1,ARG_42,12.59,-0.16,0,0.25

1GPP,ARG_90,12.28,-0.34,0,0.12 1F2V,ARG 65,11.37,-1.61,0,0.48 1RWZ,LYS_166,10.44,-0.2,0,0.14 1SBX,HIS_147,6.41,-0.13,0,0.04 3JV1,GLU_211,5,0.59,0,-0.08 2B2H.LYS 241,11.57,-0.3,0.58,0.8 2B78,CYS 114,12.31,-0.97,0.48.3.82 1RHS,ARG_64,13.19,-0.73,0.78,0.64 2VGM,ASP_90,2.53,-1.48,-0.38,0.58 3JV1,TYR_170,10.35,0,0.05,0.3 2X4G,HIS_243,5.54,-0.99,0,0.04 2FGG,ARG_23,12.53,-0.33,0.02,0.34 2XJ4,GLU_68,4.56,1.43,-0.73,-0.65 2YWJ.LYS 150.10.54.-0.32.0.0.36 2P0L,GLU_261,3.83,1.21,-1.15,-0.72 3GS3.CYS 247,11.47,0,0.01,2.47 3C2E.GLU 210.4.63.0.08.0.0.05 3BJV,ARG_14,12.84,-0.64,0.65,0.34 20BI,ASP_58,2.81,-1.28,-0.23,0.53 4DBX,LYS_253,10.16,-0.21,0,-0.13 1C44,LYS 87,10,4,-0,1,0,0 3G9T,GLU_119,4.66,0.52,-0.25,-0.11 1V43,ARG_290,11.01,-2.48,0,0.98 3L3P,ARG_436,13.15,-0.43,0.78,0.29 1X91,LYS 116,11.04,-0.24,0.42.0.36 2AD1.HIS 187.6.39.-0.71.0.6.0 3D9H,GLU_148,3.94,0.3,-0.65,-0.22 3GS9,GLU_58,4.05,0.69,-0.85,-0.28 1CBY,LYS_116,10.49,-0.12,0,0.11 3DTE, ARG_142, 12.42, -0.38, 0, 0.3 1YG2,ASP_169,3.71,-0.29,-0.39,0.59 2F4Q,ARG_310,12.44,-0.11,0,0.04 2QV2,ARG_133,12.57,-0.31,0,0.38 3TIR,GLU 162,2.7,0.78,-2.2,-0.39 3OKO,LYS 674,10.52,-0.23,0.25,0 2A0J,GLU_140,4.11,0.28,-0.69,0.02 2E3C,TYR_329,11.75,0.47,0.34,0.93 1JKS,ARG_156,12.03,-0.7,0,0.22 1Q42,HIS 83,5.14,-3.23,0.85,1.02 1ES5,TYR_102,11.01,0,-0.09,1.1 3ETV,TYR_215,11.84,-0.85,0.53,2.16 2HXB,ARG_117,12.01,-0.47,0,-0.02 3RNV,GLU 358,4.56,0.06,0,0 2AZP.ARG 3,12,36,-0,14,0,0 3GEC,GLU_518,4.6,0.1,0,0 2EYI,GLU_148,4.1,0.47,-0.72,-0.15 1RI5,GLU_199,4.75,0.39,-0.12,-0.02 2AZP,ARG_35,11.36,-1.18,0,0.04 2GEN,ARG_118,13.89,-0.68,1.36,0.71 1R3D,HIS_22,3.06,-3.32,0.37,-0.49 1JKS,GLU_115,2.93,0.68,-1.83,-0.4 2AH5,TYR_28,10.61,0,0.29,0.33 2EJB.TYR 16.11.14.0.-0.04.1.17 2VC8,TYR_21,10.9,0,0.29,0.62 3C2E,GLU_42,4.57,0.15,0,-0.08 3ETV,TYR_109,12.07,-0.08,-0.12,2.26 3R87,LYS_3,10.8,-0.21,0,0.51 2FD5.GLU 27.4.59.0.16.0.-0.07 3HYQ,ARG_82,13.72,-0.66,1.45,0.43 2CXA,GLU_125,4.11,0.23,-0.23,-0.38 1H4U,HIS_573,6.57,-0.22,0.12,0.17 3ERF.TYR 175.9.97.-0.1.-0.3.0.38 4ANN,ASP_195,3.58,-0.2,-0.22,0.2 3EUR.TYR 136.10.91.0.0.36.0.55 3V4G,CYS_149,11.56,0,0.4,2.17 1YR6,ASP_141,2.93,-1.58,-0.55,1.26 2FL7,TYR 66,12,61,0.83,-0.06,1.85 2H2W,GLU_73,5.11,0.26,0,0.35 2FM9,LYS_59,9.92,-0.4,0,-0.18

3T57.CYS 326.11.03.-0.64.0.14.2.52 2ZCO,ASP 225,2,7,-0.85,-0.63,0.39 1KCM,LYS_216,10.37,-0.13,0,0 1BYI,GLU_78,4.8,0.28,-0.04,0.06 2BAA.ASP 182,2.69,-1.65,-0.37,0.92 1JB3.LYS 129.11.04.-0.21.0.49.0.26 2QK1,LYS_540,10.43,-0.07,0,0 1BYI,LYS_27,10.31,-0.19,0,0 3FHF,ASP_181,3.95,-0.16,-0.04,0.35 1BN6,HIS_34,5.62,-2.15,0.85,0.42 3ETU,LYS 340,11.14,-0.38,0.47,0.55 2X4J,CYS_23,9.32,-0.01,-0.19,0.52 2D7U,ASP_165,4.4,0,0.22,0.38 4H4J,LYS_261,10.38,-0.18,0,0.06 4ANN.HIS 80.5.57.-1.07.0.0.13 3B79,GLU_54,5.02,0.79,0,-0.27 1IAP,GLU_91,4.44,0.19,-0.21,-0.05 2WB3,LYS_303,10.34,-0.16,0,0 10IS,LYS 257,10.31,-0.19,0,0 3VHJ.LYS 103.11.41.-0.35.0.71.0.55 1ZBM,TYR_216,10.65,-0.05,-0.02,0.72 2HRZ,GLU_328,4.67,0.16,0,0 4FLE,LYS 127,10.2,-0.25,0,-0.04 2WOZ, ASP 573, 2.65, -1.06, -1.26, 1.18 3IL3,GLU_31,4.66,0.11,0,0.05 3HUE,TYR_93,11.46,0,0.47,0.99 2JEO,ARG_212,12.38,-0.27,0,0.15 2Z0W,TYR 68,10.34,0,0,0.33 3GV0,HIS_106,5.11,-1.21,0,-0.18 1QQE,ARG_48,13.39,-0.68,0.85,0.72 2WB8,LYS_754,11.49,-0.32,0.85,0.46 3OA7, ARG_506, 12.29, -0.21, 0, 0 1HUF,ASP 89,3.09,-0.9,-0.38,0.57 3G6S,LYS 126,10.29,-0.39,0.0.17 3BPP,GLU_59,6.41,2.19,0,-0.27 2P1W,LYS_34,10.3,-0.23,0,0.03 2FXT,GLU_384,4.56,0.12,0,-0.05 2VGM,TYR_335,12.91,0.33,0.65,1.94 10XZ,LYS_226,10.45,-0.14,0,0.09 30IP.ARG 60.12.55.-0.1.0.0.15 1WYC,ASP_165,4.03,0,0.01,0.22 20PJ.HIS 262,5.84,-0.36,0,-0.3 1PDB.GLU 81.4.75.0.25.0.0 2RIK,HIS_247,6.04,-0.41,0,-0.05 3JSN,TYR_126,10.26,-0.06,0.01,0.3 3CO1,ARG 17,12,35,-0,18,0,0.03 2PGX,ASP_13,2.89,-1.42,0.12,0.4 2FC3,ARG_45,12.41,-0.27,0,0.18 3Q1C,ASP_232,4.13,0,0.06,0.27 3ETV,ASP_169,4.49,0,0.15,0.55 2YYO, ASP_142, 3.99, 0, -0.09, 0.28 3JSN.TYR 262.13.99.0.0.92.3.06 3M7D,CYS_297,11.53,0,-0.22,2.75 2QOP,ARG_161,12.85,-0.31,0,0.65 1W7B,LYS_80,10.39,-0.09,0,-0.02 1U7U,ASP 365,3.48,-0.16,-0.33,0.18 1WPA,LYS_511,10.36,-0.12,0,-0.02 3GA2,TYR_202,10.92,0,0.12,0.81 1UOH,ASP_86,4.82,0,0.29,0.73 2IDC,ARG 123,13,-0.4,0.34,0.56 3C6B,ARG 179,12.23,-1.68,0.02,1.39 1059,LYS_310,10.23,-0.27,0,0 200K,TYR_323,13.77,0,0.32,3.45 3ANJ,ASP_213,3.93,-0.01,-0.09,0.23 1R53,LYS_253,10.16,-0.14,0,-0.19 3LQE,ASP 272,2.52,-1.66,-0.3,0.68 1059,HIS_268,6.04,-0.49,0.37,-0.34 1J7G,ARG_90,12.45,-0.05,0,0 2HRZ,LYS_195,10.19,-0.15,0,-0.16

3EVP,ASP_103,3.75,-0.14,0,0.1 2CBE,ASP 75,3.06,-0.85,-0.46,0.57 1MJS,GLU_245,4.55,0.09,0,-0.05 307K,GLU_161,4.79,0.62,0,-0.33 3L7N.LYS 32.10.33.-0.24.0.0.07 4DIU.TYR 181.10.65.0.0.36.0.29 3B79,LYS_122,10.42,-0.14,0,0.07 2GEN,ARG_76,12.59,-0.07,0,0.15 3ADO, ARG_299, 12.14, -0.27, 0, -0.08 1ZKZ,HIS_7,5.89,-0.6,0.23,-0.25 2W2S,ARG 156,12,49,-0.53,0,12,0,39 3RKV,LYS_271,11.53,-0.32,0.85,0.51 3LJN.ARG 249,12.24,-0.97,0.04,0.66 2DG7,ARG_159,12.88,-0.49,0.21,0.66 20DJ.LYS 327.10.33.-0.11.0.-0.06 3G9B,ARG_32,12.24,-0.29,0,0.02 3NBI,ARG_62,12.48,-1,0,0.98 2QK0,ARG_99,13.26,-0.48,0.75,0.48 1U53,LYS_56,10.51,-0.16,0,0.17 3BJV,HIS 68,4.73,-2.06,0.81,-0.52 1DVO,ARG_174,12.23,-0.27,0,0 2F4O,TYR 250,11,2,0,0,5,0,7 1YR6,LYS_193,10.56,-0.07,0,0.14 2OJQ,LYS 675,10.8,-0.14,0,0.43 2X4G.GLU 140.5.67.3.23.-1.61.-0.45 1MTZ,GLU_262,4.77,0.72,0,-0.45 3K8J,GLU_177,3.25,1.53,-1.98,-0.78 20EW,ASP_330,3.67,-0.12,-0.18,0.17 2FC3,LYS 124,10.51,-0.07,0,0.09 3CRM,LYS_108,10.3,-0.47,0,0.27 1DZF,LYS_45,10.4,-0.18,0,0.07 10IS,HIS_150,4.25,-2.93,0.74,-0.06 1ES5,ASP_54,2.91,-0.82,-0.35,0.27 3FK5,LYS 205,9.85,-0.96,0.42,-0.11 3L7N,TYR_226,10.93,0,-0.09,1.03 3U4K,GLU_30,4.01,0.24,-0.4,-0.33 2H01,GLU_158,4.6,1.06,-0.85,-0.12 2IDC,LYS 17,10.67,-0.12,0,0.28 2EJX,GLU_130,3.16,1.02,-1.5,-0.85 3LJN,GLU_73,3.97,0.34,-0.18,-0.69 1QQL,ASP_9,3,-0.52,-0.49,0.2 300P,ASP 96.3.82.0.-0.11.0.13 2l6l.LYS 7.10.94,-0.53,0.85,0.12 3LJN,CYS_132,9.81,-0.86,0.02,1.65 2Z0M,GLU_264,4.64,0.13,0,0.02 1FQI,TYR_351,10.38,0,-0.01,0.38 2Q5X,TYR 725,11.07,-0.01,0.17,0.91 2APL.TYR 19.11.44.0.0.39.1.05 3LD1,CYS_331,12.65,-0.19,0.2,3.65 2B61,TYR_29,10.83,0,0,0.83 1WP5.GLU 312.5.03.0.24.0.0.29 2AZP,ARG_141,12.53,-0.28,0,0.32 1W7B,TYR_151,11.53,0,0.07,1.47 1EV8,CYS_167,9.76,0,-0.15,0.91 3FK5,LYS_315,10.39,-0.18,0,0.07 2H85,ASP_106,3.76,-1.5,-0.12,1.59 1PSW.GLU 238,4,11,0,26,-0,65,0 1V43,LYS_337,10.41,-0.45,0,0.36 2HXB,CYS_68,11.25,0,0.1,2.14 1KW4,ASP 45,3.22,-0.97,0.0.39 3BOE,HIS 245,6.59,-0.22,0.35,-0.05 4GA2,LYS_135,10.42,-0.3,0,0.22 1YG2,TYR_31,10.75,-0.6,0.24,1.11 1L2F,LYS_280,10.5,-0.22,0,0.22 4DIU,GLU_85,4.46,0.22,0,-0.26 2OBI,LYS_135,9.47,-0.71,0,-0.32 3US6,GLU_2,4.42,0.15,0,-0.24 1VJG,TYR_128,11.2,0,0.22,0.99 2DFL,LYS_60,10.51,-0.15,0,0.17

2YYO.TYR 64,10.06,0.0.0.06 1VJG,LYS_62,10.59,-0.16,0,0.24 3D9H,CYS_175,12.3,-0.07,0.12,3.26 2V4U,HIS_526,4.83,-1.61,0,-0.06 1YTQ,GLU_32,4.51,0.33,0,-0.32 3ANLLYS 38.10.54-0.22.0.0.26 1PSW.GLU 166.2.22.0.58.-2.4.-0.46 3P28,GLU_124,4.93,0.29,0,0.13 2XWS,GLU_109,4.71,0.15,0,0.06 1JSX,GLU_178,5,0.2,0,0.31 1XTD,ASP_121,2.85,-1.46,-0.03,0.53 3GFP,ASP_316,3.69,-0.29,-0.22,0.4 3GS3,CYS_211,9.5,-0.9,-0.12,1.52 1WLY,ASP_201,2.17,-1.82,-0.39,0.58 2FXT,ASP 340,4.05,0,-0.58,0.83 1PSW.TYR 323,11.05,-0.81,0.14,1.72 1SQH,ARG_77,13.26,-0.46,0.69,0.53 1TUL,LYS_46,10.59,-0.15,0,0.23 208I,GLU_109,4.6,0.1,0,0 1Q46,TYR 81,10.03,0,-0.08,0.12 3BCH,LYS_57,9.97,-0.57,0,0.05 1RSS,GLU_67,3.55,0.44,-0.67,-0.72 1DVO,CYS_142,9.24,-0.21,0,0.46 2R2Y,ASP 72,3.93,-0.13,-0.37,0.64 2W0G.ARG 262.12.18.-0.47.0.0.14 4FZR,ARG_87,12.21,-0.65,0,0.36 1SIG,ASP_445,3.79,0,-0.26,0.25 2H2W,HIS_79,6.61,-0.28,0.07,0.32 1BN6,GLU 141,4.73,4.98,-3.24,-1.51 4EZB,TYR 131,10,15,0,-0,01,0,16 3H04,LYS_184,11.55,-0.34,0.75,0.64 2PWQ,HIS_25,6.91,-0.58,0.82,0.17 2EJB,TYR 86,13,16,0,-0,08,3,23 200PLYS 116.10.53.-0.59.0.2.0.42 3US6,ASP_75,2.7,-1.48,-0.59,0.97 3F7M,LYS_158,10.24,-0.15,0,-0.11 1F2V,ARG_207,12.43,-0.26,0,0.2 3B21,LYS_26,10.38,-0.12,0,0 3ELI,ARG 117,12,36,-0.66,0,0.53 1I60,HIS_79,7.38,-0.47,0.85,0.5 2RFA,GLU_232,5.09,1.98,-0.85,-0.54 1V8E.HIS 155.6.44,-0.31.0.0.25 3BA1.GLU 121,5.01,0.91,0,-0.41 2EFK,TYR_190,10.18,0,-0.26,0.44 1ES9,ARG 132,11.85,-0.48,0,-0.17 2B0J,LYS_209,10.4,-0.39,0,0.29 3G6S,ARG 148,13.19,-0.19,0.29,0.61 3G9G,ARG_239,13.67,-0.72,1.12,0.77 1ILW,GLU_163,4.61,0.92,-0.76,-0.05 2CIU.ASP 148.3.95.0.0.0.15 4DBX,LYS_139,10.35,-0.08,0,-0.07 1L3K,LYS 166,10.4,-0.1,0,0 2QDJ,GLU_352,4.69,0.31,0,-0.12 2H01,LYS_102,10.13,-0.54,0,0.17 20KT,ASP_326,3.04,-1.19,0,0.44 3QKY,LYS_134,10.73,-0.25,0,0.47 1FQI,GLU_412,4.43,0.22,0,-0.3 3ADO,GLU_163,4.53,0.27,0,-0.25 2FL4.TYR 59.10.55.-0.85.-0.16.1.56 100X,LYS_144,10.37,-0.13,0,0 1Z3X,LYS 103,10.23,-0.51,0,0.24 1SOH.HIS 86.3.53.-2.46.0.73.-1.23 1WRU,GLU_189,4.88,0.26,0,0.13 1RHS,ARG_50,12.2,-0.48,0,0.18 1MD6,GLU_72,4.65,0.15,0,0 2HXB,TYR_86,9.81,-0.3,-0.2,0.3 4E8B,ASP_241,4.58,-0.25,0.05,0.99 2P52,ARG_279,12.69,-1.08,0.8,0.47 1MUF,HIS_283,6.19,-0.33,0,0.02

3CNU,GLU_80,4.63,0.3,0,-0.18 2QVT,ARG 98,11.93,-0.62,0,0.05 2PLQ,ASP_265,3.42,-0.55,-0.09,0.26 2EDM,ARG_136,12.37,-0.2,0,0.07 3EUR,LYS_1,10.17,-0.2,0,-0.13 1SJ8,LYS 529,10.53,-0.36,0.37,0.03 3RJZ.LYS 106.11.1.-0.3.0.73.0.17 1WYC,CYS_271,12.99,-0.01,0.3,3.7 3DHN,GLU_143,4.83,0.31,0,0.02 4ANN,HIS_44,5.95,-0.48,0,-0.08 3BA1,ARG 128,12.33,-0.32,0,0.15 3ELI,ASP_90,3.94,0,0.03,0.11 2A0J,GLU_28,5.32,0.94,0,-0.13 307K.GLU 128,4.05,0.42,-0.23,-0.63 1SBX,ASP_181,4.07,-0.45,-0.12,0.84 2AD1,LYS 266,10.57,-0.19,0,0.26 3EIZ.ARG 51.12.38.-0.32.0.0.19 1R3F,HIS_163,6.21,-0.87,0.56,0.02 2FBQ,HIS_45,5.97,-0.53,0,0 1WOULYS 58,11.37,-0.23,0.71,0.39 1Y0K,ASP_19,4.08,0,0,0.28 1RAJ,LYS_75,10.79,-0.17,0.06,0.39 2B0A,LYS 26,10,45,-0.05,0,0 3M70,LYS 246,10,24,-0,3,0,0.05 3GEC,ARG_319,12.05,-0.33,0,-0.11 1QZN,ASP_44,3.27,-0.79,-0.3,0.56 1SI7,ASP_38,2.67,-1,-0.8,0.67 3RKV,ARG_283,12.86,-1.58,1.49,0.47 1DOV,ARG_204,12.28,-0.3,0,0.08 1FO9,GLU_148,4.61,0.24,-0.06,-0.06 3GV0,GLU_218,4.25,1.61,-1.25,-0.61 3EGN.GLU 476.4.81.0.25.0.0.05 3GS3,ASP_192,2.77,-1.51,-0.09,0.56 3KV0,GLU 31,4.55,0.05,0,0 2IRM,ARG_39,12.46,-0.06,0,0.02 3T5B,LYS_172,9.78,-0.81,0,0.08 2CBE,GLU_205,3.9,1.36,-1.56,-0.4 1P6F,TYR_147,9.94,-0.18,-0.38,0.5 3V55,HIS 584,6.07,-0.76,0.45,-0.12 4FZR,GLU_208,3.9,0.19,-0.79,0 1PSW,GLU_204,4.82,0.6,0,-0.27 2V5B,GLU_27,4.6,0.26,-0.04,-0.12 2AH5.GLU 66,4.56,0.33,-0.3,0.03 1ZCE.LYS 22.11.4.-0.48.0.85.0.53 3LD1,ARG_122,11.78,-0.85,0,0.13 3ILC,GLU_158,4.65,0.13,0,0.03 2H2Z,ARG_88,12.58,-0.66,0,0.72 3JZN,LYS 83,10.53,-0.1,0,0.12 4ESS,GLU_48,4.06,0.59,-0.81,-0.21 4H89,GLU_38,4.58,0.08,0,0 2I88, ASP_450, 3.52, -1.01, -0.37, 1.1 1AKO,TYR 56,10.88,0,0.28,0.61 2B6P.HIS 66.3.35.-3.4.0.35.-0.1 2Y2T,ARG_76,12.6,-0.08,0,0.18 3Q1C,HIS_280,6.14,-0.66,0.03,0.27 3HKX,CYS_165,13.39,-1.03,1.96,3.46 3Q9P,ASP_107,3.8,0,-0.23,0.23 3ANJ,TYR 41,12,75,0.83,0.45,1.47 3JZN,ASP_421,2.64,-2.02,-0.05,0.91 1SI7,CYS_53,9.72,0,-0.13,0.85 3U2A, ARG_92, 12.11, -0.35, 0, -0.04 20GO.HIS 524,4.32,-2.16,0.52,-0.53 3V3T,GLU_189,4.56,0.46,0,-0.4 3FRR,LYS_28,10.28,-0.13,0,-0.09 1YLN,LYS_137,10.74,-0.1,0,0.34 3H13,CYS_298,9.3,0,0,0.3 2V4X.TYR 10.10.43.0.0.11.0.32 1L2F,GLU_67,4.8,0.17,0,0.13 2RJD,ASP_491,3,-1.72,-1.13,2.05

1P4X,ASP 243,3.93,-0.1,-0.1,0.33 3PP8.GLU 30.4.22.0.46.-0.36.-0.38 1YR6,CYS_143,10.12,-0.15,-0.07,1.34 1PBV,LYS_207,9.94,-0.59,0,0.04 2P1W,ASP_129,3.09,-0.82,-0.49,0.61 2CL3.GLU 88,4.25,0.29,-0.01,-0.52 2WB8,HIS_778,5.28,-1.28,0,0.06 1P2F,LYS 206,10,16,-0,49,0,0,14 2IF4,LYS_134,9.65,-0.56,0,-0.29 2OJQ,GLU_449,4.74,0.21,0,0.03 1XFK,ARG 272,12,48,-0.28,0.0.26 1V6T,ARG_148,13.38,-0.28,0.49,0.67 2GZR,ARG_152,12.27,-0.36,0,0.13 1NFN,ARG_150,12.33,-0.29,0,0.12 1Z3X.ARG 219.12.12.-0.39.0.0.02 3DZ1,LYS_23,10.93,-0.2,0.21,0.43 2YWX.LYS 133.10.19.-0.46.0.0.15 3V55,GLU_652,4.11,0.38,-0.74,-0.03 3TOW,HIS_193,6.17,-0.31,0,-0.02 2FD5.GLU 166.4.58.0.06.0.0.02 1YTQ,GLU_74,4.68,0.18,0,0 3EVZ,ARG_79,12.24,-0.35,0,0.09 2HP7,ASP_85,3.87,-0.49,0.07,0.48 4F3J.HIS 156.6.01.-0.49.0.0 3CAN, ASP_69, 3.09, -0.98, -0.11, 0.37 4ESS.ARG 156,13.97,-0.4,1.09,0.78 3FTT,LYS_45,11.17,-0.28,0.39,0.56 1WNH,ASP_124,2.65,-1.75,-0.04,0.62 1G5Z,ASP_147,3.91,0,-0.04,0.15 3H9W,ASP_112,3.89,0,0,0.09 3H5T,ASP_145,4.4,0,-0.23,0.84 2EDM,LYS_174,10.56,-0.14,0,0.2 4ACJ,LYS 745,10.69,-0.62,0.38,0.43 20EW,LYS 110,10,35,-0,15,0,0 2AZL,TYR_100,11.81,0.85,0.38,0.58 3F1X,ASP_15,4.08,0,0,0.28 2EYI,ARG_76,12.59,-0.11,0,0.19 2B0J,ASP_319,3.71,-0.45,0,0.36 3FK5,GLU_24,4.21,0.43,-0.37,-0.35 1DZF,LYS 103,10.57,-0.13,0.0.2 3P51,ASP_135,3.16,-1.58,-0.07,1.02 1TUL, ASP_10, 3.93, 0, -0.21, 0.34 3CRM,ARG 287,11.89,-0.61,0.0 3CBN,TYR_102,9.86,-0.13,-0.2,0.19 1PV5,GLU_151,5.3,3.5,-1.68,-1.02 1MIX,GLU_384,4.88,0.39,0,0 2B61,TYR_219,11.43,-0.07,-0.71,2.21 1G5Z,LYS_174,10.77,-0.15,0,0.42 3G9T,HIS_137,5.72,-0.41,0,-0.36 2IQT,GLU_196,5.25,1.19,0,-0.43 3H9W,GLU_87,4.77,0.26,0,-2.78E-17 30A7,ARG 25,12,23,-0.31,0.0.04 2CE6,ARG_1,12.37,-0.29,0,0.16 3MIX,GLU_325,4.61,0.1,0,0.01 3C6B,ASP_97,2.26,-2.03,-0.4,0.9 3UPD,LYS 293,10.61,-0.38,0.06,0.43 1YDL, ASP_13, 3.65, -0.42, 0, 0.27 2YWX,GLU_113,4.99,0.51,0,-0.03 1PVT,GLU_3,4.33,0.15,0,-0.32 1U53,LYS 167,10.34,-0.17,0,0 3NBI,HIS 66,5,7,-0,83,0,0,03 1BKB,GLU_103,4.71,0.21,0,0 4DBX,LYS_275,11.85,-1.03,1.37,1.01 3FRR,TYR_132,13.34,0.31,0.87,2.16 1X04,GLU_112,4.95,0.37,0,0.07 3BWT,ARG 579,12.39,-0.2,0,0.09 3A2Z,GLU_83,4.03,0.39,-0.84,-0.02 2AHE,LYS_150,10.61,-0.16,0,0.27 2A4D,GLU_94,5.53,3.32,-1.97,-0.3

2Q13,GLU_358,5.4,0.79,0,0.11 3M66,LYS 361,9.61,-0.65,0,-0.23 2E3C,ARG_439,11.48,-1.55,0.17,0.37 2AD1,ASP_287,3.94,0,-0.07,0.2 2F4Q,ARG_129,11.5,-1.2,0,0.2 20VT.HIS 88.4.91.-1.09.0.-0.5 1LTU,ARG 15,13,95,-0.38,1.38,0.45 2GZQ,TYR_158,10.14,0,0,0.14 3RNV,GLU_363,4.05,0.23,-0.57,-0.12 4EKU,ARG_159,12.17,-3.25,0.01,2.92 2QVT,GLU_62,4.6,0.1,0,0 1DTO,GLU_176,4.63,0.3,0,-0.16 2FZ4,LYS 169,10.07,-0.46,0,0.03 30IP,HIS_119,4.14,-2.61,0,0.25 2BDV.ASP 142.2.53.-1.34.-0.45.0.53 3NR5.GLU 30.4.44.2.54.-2.14.-0.46 1AD6,CYS_553,12.63,-0.14,0.78,3 1LFP,ARG_21,12.25,-0.25,0,0 1XKR,LYS_173,10.33,-0.44,0,0.25 3GOZ,LYS 314,10.5,0,0,0 2GZR,ARG_182,12.21,-0.72,0.06,0.36 2HXB,LYS_151,10.7,-0.1,0,0.29 4DIU,LYS_41,10.51,-0.3,0,0.31 1LZL.ARG 317,12.4,-0.15,0,0.05 2E3S.GLU 397.4.47.0.28.0.-0.32 1R29,LYS_126,10.45,-0.05,0,0 2F9F,GLU_106,5.82,1.97,-0.71,0.05 1WXQ,ASP_77,3.55,-0.81,-0.51,1.07 2FZP,ASP 299,4.07,-0.23,0.13,0.37 2Q07,ASP_379,3.86,0,-0.09,0.15 1NFN,GLU_49,4.73,0.15,0,0.08 2RH3,ASP_171,3.29,-0.99,-0.2,0.69 2Q12,ARG 154,12.45,-0.05,0,0 3GEC.GLU 336.4.66.0.91,-0.22,-0.53 3UPD,CYS_227,11.83,-0.03,-0.31,3.17 4FZN,GLU_15,4.41,0.8,-0.36,-0.51 1WYC,ARG_62,12.63,-0.16,0,0.3 3IBT,GLU 155,2.95,0.58,-1.74,-0.38 2E3C,TYR_447,10.72,0,0.02,0.7 1WLY,CYS_288,11.03,0,0.06,1.95 1JKS,GLU_239,4.62,0.12,0,0 1AK1,HIS 65.6.29,-0.49.0.0.28 205X,CYS 743,9.49,-0.6,-0.04,1.13 4FZN,ASP_28,3.92,0,-0.1,0.22 2V1L,GLU_89,4.61,0.11,0,0 1DOV,GLU_89,3.9,0.35,-0.69,-0.26 3V55,ARG 392,12.87,-1.02,0.7,0.69 2HXB,ASP 109,2,13,-1,72,-0.67,0.73 2Q13,LYS_360,10.61,-0.09,0,0.21 1QYI,TYR_191,12.54,-0.18,0.76,1.96 4E8B,ASP_23,3.33,-0.4,-0.4,0.33 3CNU,LYS_90,10.5,-0.21,0,0.21 3AU3,GLU_574,4.58,0.29,0,-0.23 3IV4,ARG 91,12,36,-0,34,0,0,19 3IVF,GLU_187,4.7,0.83,0,-0.64 3EZ7,GLU_107,4.48,0.21,0,-0.22 1RHS,LYS 153,9.92,-0.67,0,0.08 3AU3,GLU_650,3.9,0.29,-0.51,-0.39 3C5V,LYS_203,10.35,-0.15,0,0 4FZR.CYS 301.13.1.-0.1.0.94.3.26 3I0C.GLU 297,4.66,1.41,-0.8,-0.44 3BCY,ARG_82,12.37,-0.13,0,0 2Q07,LYS_457,10.78,-0.17,0,0.45 3IO0,LYS_301,10.41,-0.09,0,0 3I0C,HIS_313,6.1,-0.71,0.27,0.04 4ANN,TYR_57,10.65,0,0.2,0.45 2IF4,ARG_269,10.99,-1.95,0,0.45 3LD1,ARG_103,12.32,-0.35,0,0.17 1ZYL,CYS_202,13.94,0,1.55,3.4

3D9H,HIS 48,6.07,-0.33,0,-0.1 2ZCX,GLU 206,4.91,0.38,0,0.03 1H09,ASP_133,3.88,0,-0.23,0.32 1R3D,HIS_7,5.17,-1.33,0,0 1PV5,LYS_24,10.3,-0.23,0,0.04 20HTTYR 117.12.41.0.8-0.06.1.67 1TXJ.ASP 22.3.43.-0.54.-0.27.0.44 1SI7,LYS_64,10.14,-0.39,0,0.03 1TLV,LYS_88,10.02,-0.51,0,0.03 1IDK,ASP_37,2.64,-1.45,-0.88,1.16 1SJ8,GLU_738,4.29,1.04,-0.84,-0.42 1J74,TYR_58,12.89,-0.1,0.28,2.71 2P0Y,ARG_297,12.28,-0.39,0,0.16 3RKV,ASP_222,4.2,0,0.01,0.38 2EYI.TYR 161.11.15.0.-0.25.1.4 3EYE, LYS 68, 10, 15, -0, 31, 0, -0, 04 2FM9,LYS_173,11.09,-0.26,0.85,0 3DHN.LYS 6.10.45,-0.23,0.0.18 3Q1C,GLU_113,3.82,1.08,-1.15,-0.61 2FD5,GLU_140,3.58,0.35,-1.4,0.13 3L3P,HIS 279.6.45,-0.12.0.0.07 3MTT,LYS_456,10.75,-0.29,0.11,0.43 2CL3,GLU_154,4.7,0.25,0,-0.05 1NRI.GLU 117.4.68.0.11.0.0.07 3T5B,GLU 66,5.32,1.35,-0.52,0 3BPV,GLU_45,3.67,0.42,-0.69,-0.55 3L7N,HIS_26,5.28,-0.89,0,-0.33 2F8H,GLU_10,4.58,0.19,0,-0.11 3GOZ,GLU_215,3.64,0.43,-0.99,-0.31 2EJX,ASP_13,2.8,-1.2,-0.16,0.37 10I7,ASP_180,3.68,-0.77,-0.04,0.7 2PLQ,ARG_188,10.9,-3.46,0,1.87 3MTT,ARG_531,12.58,-0.17,0,0.25 2CYG,TYR 33,12.51,0,0.03,2.48 4F85,TYR_55,10.77,-0.13,-0.39,1.29 3I47,ARG_131,12.11,-0.4,0,0.01 3LJI,ASP_170,3.16,-0.97,0,0.32 1R3F,ASP 71,3.78,0,-0.37,0.35 1CHD.CYS 309.11.31.0.0.05.2.26 2PPN,HIS_94,6.29,-0.24,0,0.03 3EYE,GLU_154,4.13,0.41,-0.83,0.06 3VHJ.LYS 111.9.93.-0.61.0.0.04 2NYC,ASP_300,3.94,0,-0.01,0.15 3CAX,TYR_190,13.15,0,0.37,2.79 2OB5,TYR_136,10.35,0,0.08,0.27 1R6Y,ARG_11,12.31,-0.23,0,0.04 3LOD, ARG 53, 12.82, -0.47, 0.29, 0.5 3NJM,LYS_92,10.43,-0.17,0,0.1 3V55,ASP_634,4,-0.02,-0.07,0.29 2CN1,GLU_162,3.67,0.78,-1.14,-0.47 2Q12,ASP_141,3.9,0,-0.19,0.3 2R2Y,ASP_117,3.78,-1.36,-0.5,1.83 1TXJ.ASP 108.3.59.-0.38.-0.14.0.31 3L3P,GLU_477,4.64,0.14,0,0 105J,GLU_59,4.69,0.29,0,-0.09 2D7U,ARG_315,12.48,-0.34,0,0.31 1BKR.LYS 56.10.42.-0.22.0.0.14 3CAX,ARG_224,12.94,-0.94,0.55,0.83 3RLE,LYS 162,11.82,-0.32,0.69,0.95 3Q9P,HIS_103,6.23,-0.12,0,-0.15 1EW4,LYS 48,10.36,-0.15,0,0 204D.HIS 105.6.42.-0.08.0.0 1Q46,CYS_114,11.04,-0.08,0.12,2.01 1WOU,TYR_76,11.17,-0.1,0.37,0.9 1WJG,ASP_101,2.68,-1.24,-0.33,0.44 3PM2,ASP_2,3.86,0,-0.03,0.09 2G2D,ASP_30,2.78,-0.99,-0.5,0.48 3RFF,LYS 41,10,44,-0.06,0,0 3RFY,LYS_329,10.24,-0.26,0,0

1RI6,ASP_160,2.89,-0.84,-0.28,0.21 2D59,ASP_73,4.08,-0.07,-0.04,0.4 3CGW,ARG_93,12.44,-0.87,0.18,0.64 2F4Q,ARG_44,12.33,-0.17,0,0 2FG1,ARG_51,13.25,-0.51,0.76,0.5 3NR5,ASP 98,3,99,0,0,0,19 3ILC.HIS 177.7.22.-0.83.0.85.0.7 2BV9,TYR_59,13.43,-0.84,0.44,3.82 2Q99,ARG_270,10.7,-1.65,0,-0.14 3F1X,TYR_43,10.78,0,0.52,0.27 2PLQ,HIS_275,5.08,-1.17,0,-0.25 3IVF,ASP_375,3.9,0,0,0.1 2A6B,LYS_120,11.51,-0.23,0.85,0.38 1J7G,ASP_84,3.07,-0.74,-0.3,0.31 2X4G,ARG_213,12.76,-1.29,0.69,0.86 20EW,LYS 81,11.62,-0.72,0.85,0.98 2EFK,GLU_79,3.73,0.49,-1.16,-0.1 2B78,LYS_347,10.16,-0.28,0,-0.05 3ON1,ARG_93,12.27,-0.27,0,0.04 1A8Q,CYS_3,11.22,0.1,0.62,1.49 1SI7.ARG 164.10.46.-1.93.0.-0.11 3H04,LYS_198,11.08,-0.73,0.58,0.73 3K1H,LYS 55,10.15,-0.29,0,-0.06 2O34,LYS 208,10.36,-0.1,0,-0.04 3GV0,ARG 306,12.93,-0.41,0.19,0.66 1G8P,GLU_214,4.89,0.38,0,0.01 3NBI,LYS_21,10.19,-0.31,0,0 4EVF,TYR_46,9.92,-0.7,-0.07,0.69 3NR5,CYS_86,9.26,0,-0.03,0.29 3R2E,ASP_55,3.85,-0.23,-0.02,0.3 3BJV,ASP_126,3.68,0,-0.28,0.16 3M66.HIS 366.4.64,-1.86.0.0 3M66,ASP_219,3.39,-0.75,-0.11,0.45 2CWC,ARG 283,12.54,-0.48,0,0.53 4FZN,ASP 52,2.87,-0.83,-0.31,0.2 3V3T,ARG_62,12.47,-1.35,0.47,0.85 3BPP,LYS_227,10.44,-0.08,0,0.02 3JZN,ARG_302,12.34,-0.3,0,0.15 1NFN,GLU 27,5.28,0.95,0,-0.17 1MML,TYR_268,13.13,0,0.43,2.7 2E3C,GLU 240,3.48,0.32,-0.77,-0.57 2RJD,LYS_426,10.58,-0.21,0,0.29 1NKD,ARG_13,13.25,-0.33,0.7,0.38 3HOX.GLU 76.4.85.0.35.0.0 307K,GLU_127,3.42,0.41,-1.1,-0.39 2QV2,GLU_178,5.73,3.5,-1.51,-0.76 2YWJ,LYS_122,11.69,-0.22,0.85,0.56 2RFA,CYS_213,10.05,0,-0.18,1.23 1PVT,GLU_89,4.88,0.62,0,-0.25 3JRT,LYS_128,11.21,-0.25,0.35,0.61 1XKR,LYS_2,10.41,-0.08,0,0 105J,GLU_67,4.82,0.24,0,0.09 2FXT.GLU 350.4.63.0.21.0.-0.08 3OBS,LYS_9,10.64,-0.46,0.22,0.38 1RAJ,LYS_314,10.5,-0.04,0,0.05 3ERF,LYS_158,10.58,-0.31,0,0.38 1J8B,ARG 83,13.23,-0.28,0.52,0.48 3ADO.LYS 188,10.43,-0.07,0.0 1YG2,TYR_69,10.84,0,0.39,0.45 4D8L,ASP_138,3.06,-0.84,-0.24,0.34 3CRM,TYR_42,11.7,0,0.03,1.67 1KCM,LYS 135,11.14,-0.21,0.85,0 3M9A,CYS_66,9.33,0,0.03,0.29 1D2K,LYS_384,10.04,-0.92,0,0.47 1AD6,TYR_424,9.54,-0.31,-0.43,0.28 1JT9,LYS_14,10.6,-0.24,0,0.34 4EKU.GLU 207.4.68.0.18.0.0 1UXO,ASP_35,2.81,-1.65,-0.19,0.86 3LPZ,ASP_174,2.61,-1.55,-0.11,0.46

1RHS.LYS 235.9.85.-0.65.0.0 2P4D.ASP 17.3.95.0.-0.12.0.26 3GMS,LYS_178,10.42,-0.16,0,0.08 3RLN,CYS_637,9.27,0,-0.25,0.53 3LJC.GLU 108,4.39,0.23,-0.01,-0.32 1Y2O.GLU 36.4.53.0.19.0.-0.16 3M3P,ASP_77,4.16,0,0.02,0.34 4E8B.CYS 139,12.01.0.0.04,2.98 3EVN,GLU_322,4.85,0.23,0,0.13 3C5V,GLU_61,4.56,0.12,0,-0.06 3HVM,TYR_330,13.61,-0.81,0.67,3.75 3CAN, ASP_95, 3.25, -0.51, -0.28, 0.24 3FRR,LYS_35,10.4,-0.13,0,0.03 1GPP,ARG_87,12.16,-0.89,0,0.55 2FD5.ARG 93.12.53.-0.16.0.0.19 1XIP,ASP_318,3.68,0,-0.36,0.24 1XTZ,LYS_174,10.33,-0.35,0,0.18 1L3K,LYS_145,11.43,-0.58,0.85,0.66 1KCM,HIS_215,4.72,-2.29,0.8,-0.29 3ASA.GLU 318.4.16.0.5.-0.58.-0.26 1GVP,LYS_7,11.37,-0.36,0.77,0.45 2FI9,ARG_88,12.37,-0.36,0,0.23 3HYQ,LYS_145,10.32,-0.22,0,0.04 1WRU,TYR 32,12.08,0.55,0.54,0.98 2D7U,GLU_314,4.57,0.19,0,-0.12 3M7G,ASP_201,3.21,-0.54,-0.4,0.34 2AD1,TYR_227,10.38,0.12,0.05,0.22 3HVM,GLU 62,4.38,0.26,0,-0.38 3IRA,GLU_146,3.63,0.36,-0.85,-0.39 1YR6,ASP_96,2.26,-1.86,-0.35,0.68 3BJV.LYS 95.10.28.-0.37.0.0.16 3EVN,ARG_269,12.74,-0.39,0.25,0.38 1JB3,ARG 9,13.23,-0.11,0.51,0.34 3IL3,LYS 133,10.39,-0.68,0,0.57 1D2K,LYS_148,10.94,-0.78,0.85,0.36 4FH3,GLU_257,4.05,0.28,-0.73,-0.01 3BPV.HIS 43.6.18,-0.44,0.0.12 1WLY,LYS 287,11.57,-0.26,0.85,0.49 1WRU,ARG_201,13.87,-0.18,0.9,0.65 1NJ4,ASP 204,2.28,-1.89,-0.38,0.75 2RFA,HIS_264,6.44,-0.11,0.07,-0.01 2QRX,LYS 39,10.27,-0.2,0,-0.03 3P28.GLU 47.4.41.0.53.-0.33.-0.29 1TJE,ASP_133,3.33,-0.85,-0.04,0.43 2CWC,ARG_111,12.74,-0.39,0.3,0.33 1YLN,ARG_169,12.29,-0.57,0.08,0.3 1Q5Z,ASP_652,2.5,-1.7,0.02,0.38 2CYG,TYR_182,10.38,0,0.05,0.34 1WNH,TYR_107,11.24,0,0.36,0.88 1RHS,GLU_62,4.76,0.33,0,-0.07 1UOH,ASP_71,4.32,-0.1,0.22,0.4 3PAC, ARG 179, 12, 98, -0.1, 0.22, 0.36 4GCO,TYR_153,10.08,0,-0.08,0.17 3I47,GLU_80,3.8,0.31,-1,0 2RIK,ARG_43,12.57,-0.26,0,0.33 1SUU,GLU 525,4.64,0.18,0,-0.04 3NR5,TYR_141,11.82,0,0.41,1.41 3MEW,GLU_265,4.09,0.58,-0.61,-0.39 20BI,CYS_148,10.16,0,0.38,0.77 1P2F,LYS 140,10.8,-0.13,0,0.43 1PGV.GLU 352.4.3.0.2.0.-0.41 3GA2,GLU_109,3.46,0.19,-0.85,-0.38 2CXC,TYR_27,9.87,-0.33,-0.17,0.37 2O4D,ASP_117,3.08,-0.65,-0.38,0.31 3ETU,GLU_118,5.04,0.87,0,-0.33 2V81,GLU 160,4.44,0.3,-0.36,0 4EF5,TYR_199,13.96,-0.04,1.1,2.92 2FBI,TYR_52,10.03,0,-0.13,0.16 2B0J,ARG_136,13.29,-0.37,0.7,0.47

1Y0K,LYS 26,11,55,-0.68,0,78,0.95 3JRT,LYS 118,10.63,-0.07,0.0.2 1YR6,GLU_19,3.51,0.82,-1.08,-0.73 2OJQ,ARG_566,11.34,-1.32,0,0.16 3R87,TYR_13,10.11,0,0,0.11 3N2T.TYR 197.11.94.0.2.0.04.1.68 3GOZ,LYS_182,10.07,-0.77,0,0.35 1ANU,ASP_53,3.58,-0.25,-0.29,0.3 1Q2Y,GLU_20,3.89,0.35,-0.58,-0.38 1X04,ASP_30,2.33,-1.56,-0.41,0.49 3CJW.GLU 346.3.45.0.63.-1.26.-0.41 2WB3,TYR_375,10.05,0,-0.18,0.23 1PGV.GLU 252.4.43.0.11.0.-0.18 20GQ,ASP_554,1.28,-2.63,-0.8,0.9 10YI.HIS 98.6.59.-0.37.0.0.46 2IF4,LYS 292,10.34,-0.17,0.0.01 4EUG,GLU_112,4.26,0.67,-0.83,-0.09 2OSA,GLU_410,4.61,0.17,0,-0.06 3FTT,ARG_121,12.18,-0.32,0,0 1SUU,GLU 506,4.49,0,-0.01,0 4FH3,LYS_227,10.16,-0.36,0,0.02 1YM5,LYS_96,10.45,-0.07,0,0.02 1V43,GLU_118,4.52,0.29,0,-0.27 1YB2,ARG 148,12.5,-0.25,0,0.25 1XWM.GLU 32.4.7.0.25.0.-0.05 3HVW,ASP_298,3.29,-1.68,0,1.17 3U4K,ARG_105,11.78,-1.58,0.1,0.76 4DIU,ASP_245,3.98,0,0.02,0.15 4DIU,TYR 238,11.07,0.23,0.43,0.41 3F5D,TYR_180,10.43,0,-0.03,0.46 2RH3,TYR_139,12.58,-0.09,0.01,2.66 4EZB,ASP_57,4.02,0,-0.02,0.24 2JEO,TYR 144,10.58,0,0.17,0.41 1KN3,HIS 145,6,45,-0,25,0,0,2 2AZP,TYR_231,10.48,-0.04,-0.42,0.95 1FO9,TYR_204,10.92,0,0,0.92 1J7G,LYS_25,9.95,-0.54,0,-0.02 2CXC,LYS 120,10.47,-0.03,0,0 4FH3,ARG_184,13.53,-1.3,1.64,0.69 3IBT,CYS_98,12.61,-1.45,0.11,4.95 2IF4,GLU_49,4.68,0.1,0,0.08 3GA2.GLU 51.4.59.0.09.0.0 2YT4.HIS 687.5.8.-0.81.0.0.11 2E3C,LYS_375,10.46,-0.08,0,0.04 3CAN, ARG 56, 12, 94, -0, 29, 0, 29, 0, 44 3BWT,GLU_627,4.18,0.24,-0.47,-0.08 1WXQ,ARG 136,13.12,-0.33,0.37,0.59 2V4X.ARG 79.12.18.-0.34.0.0.03 1T3Y,ARG_57,11.88,-1.23,0.01,0.61 3DSH,ARG_399,12.08,-0.69,0,0.27 3HUE,ASP 200,3.68,-0.32,-0.15,0.35 4HDE.GLU 89,4.65,0.1,0,0.05 1YDL,GLU_48,3.93,0.27,-0.77,-0.07 1ILW,GLU_97,4.54,0.23,0,-0.18 1ZHV,HIS_130,6.01,-0.55,0.28,-0.21 2D59,LYS_99,10.43,-0.1,0,0.03 1XTD,ASP 110,3.66,-0.45,0.0.31 2W2S,ARG_88,12.76,-0.33,0.21,0.38 2IIA,TYR_50,10.38,0,0.07,0.32 306L/ARG 131/11.91/-0.45/0.-0.14 20K1,LYS 437,10.6,-0.21,0.0.31 2H01,GLU_9,3.85,0.29,-0.57,-0.37 1YTD,LYS_389,10.58,-0.06,0,0.14 3DSH,ASP_395,1.89,-1.7,-0.82,0.6 3EIZ,ASP_125,3.86,-0.03,-0.14,0.23 2RIS,GLU_171,4.02,0.28,-0.74,-0.02 2PGX,ARG_146,11.51,-1.05,0,0.06 2IF4,ARG_181,12.57,-1.65,0.78,0.95 3CCY,GLU_130,4.53,0.35,0,-0.32

2VGM,GLU 280,5.05,2.03,-0.86,-0.62 1ZBS,ARG_61,12.58,-0.33,0,0.41 1C44,LYS_110,10.3,-0.2,0,0 4H86,LYS_124,10.69,-0.31,0,0.5 10I7,ARG_106,12.37,-0.24,0,0.12 3FTV1YS 71.10.27-0.26.0.0.03 3M66,ASP_259,3.04,-0.85,-0.26,0.34 1YB2,GLU_14,4.63,0.19,0,-0.06 2EJX,ARG_71,13.75,-0.35,0.96,0.63 2B2H,TYR_59,12.46,0,0.58,1.89 3LH5,ASP_517,3.79,-0.13,0,0.13 2NSN,ARG_101,12.39,-0.11,0,0 3ZRI,HIS_-7,6.24,-0.26,0,0 1WLY,GLU_281,3.44,0.68,-1.69,-0.05 2HNG,ASP 81,2.89,-0.85,-0.4,0.34 3CX2.TYR 220.10.8.0.0.25.0.56 2IF4,GLU_58,4.29,0.28,-0.13,-0.35 2D7U,TYR_298,11.6,0,0.45,1.14 4ECC,LYS_132,10.55,-0.39,0,0.44 3M66, ASP_187, 2.28, -1.7, -0.38, 0.56 3ZSL/ARG 144,12,-0,7,0,0,2 3LD1,LYS_32,10.3,-0.14,0,-0.06 2ZQ5,TYR_160,10.1,0,-0.03,0.12 2CBE,HIS 94,1.33,-2.73,0.21,-2.65 1MHN.LYS 119.10.46.-0.04.0.0 2OSA,GLU_392,3.02,1.21,-1.81,-0.88 3LQE,GLU_336,4.11,0.78,-0.85,-0.33 2QEV,LYS_56,11.64,-0.44,0.85,0.73 3GA2,HIS 7,4.76,-1.77,0,0.03 1NIJ.GLU 250.4.58.0.14.0.-0.07 3ADO,LYS_286,10.42,-0.08,0,0 3P51,TYR_89,10.46,0,0.26,0.21 1ZHV,HIS 104,4,7,-1,7,0,-0,1 1Q8B,GLU_40,4.59,0.17,0,-0.07 1SQW,GLU_171,5.12,1.08,-0.56,0.09 2CN1,TYR_81,11.57,0.73,0.07,0.77 1T07,GLU_28,4.64,0.14,0,0 3C2E,TYR_275,10.8,-0.8,0.71,0.88 1YM5,LYS 269,10.67,-0.21,0.0.39 3IRA, ASP_154, 3.09, -0.81, -0.38, 0.48 1CBY,GLU_214,4.64,0.58,-0.19,-0.24 1MUF,GLU 90,5.07,0.28,0.03,0.26 2PLQ,TYR 214,13.53,-0.11,0.23,3.42 1G8P,LYS_248,10.32,-0.26,0,0.07 3E7P,ARG_132,13.53,-0.35,0.79,0.59 1YDL,ASP_37,2.73,-1.17,-0.38,0.48 3F7M,ARG_293,11.63,-1.03,0,0.16 20KT,ARG_317,12.05,-0.55,0,0.1 3M7D,ARG_252,12.21,-0.23,0,-0.05 4FCU,ASP_25,3.91,0,-0.04,0.15 2R57,ASP_176,3.51,-0.57,-0.01,0.29 2V1L,CYS 93,11.11,0.16,0.64,1.31 3GV0,HIS_200,6.2,-1.2,0.76,0.13 2H30,LYS_57,10.08,-0.35,0,-0.07 3FRR,HIS_150,6.06,-0.32,0,-0.13 2J8A,LYS_356,10.51,-0.11,0,0.12 1EYH, HIS 73, 5.87, -1.1, 0.84, -0.37 3F1X,ARG_109,13.13,-0.33,0.54,0.43 2DG7,ARG 182,13,42,-0.25,0.85,0.32 2QHT,HIS_151,2.93,-2.84,0,-0.74 3ZSL,GLU 165,2.31,0.48,-2,-0.67 3FHF,ASP 104,3.38,-0.74,-0.06,0.38 3HUE,ASP_261,4.1,0,0.09,0.22 3EAZ,GLU_127,4.47,0.31,0,-0.35 2EYI,GLU_113,4.03,0.32,-0.73,-0.06 3V4G,GLU_39,4.49,0.09,0,-0.11 2B78,GLU_11,4.42,0.42,-0.44,-0.06 3JRT.HIS 109.6.29.-0.21.0.0 2P0L,ASP_185,3.37,-0.65,-0.19,0.42

2D2S,ASP_699,4.3,0,-0.49,0.98 2P5D,LYS 121,9.89,-0.71,0,0.1 2Q12,TYR_203,10.34,0,0,0.34 2CN1,GLU_94,3.34,0.36,-1.47,-0.05 3IVF,HIS_188,6.49,-0.28,0,0.28 2FPN.TYR 67,10.65.0.0.32.0.33 1RI5.GLU 89.3.54.0.52.-0.85.-0.63 4DIU,GLU_145,4.53,0.08,0,-0.04 1L2H,TYR_121,11.1,0,0.43,0.67 4F85,LYS_221,10.42,-0.19,0,0.11 1WNH,ASP_173,3.04,-0.98,-0.42,0.64 2VAN.TYR 327,11,47,0,19,-0,09,1,36 3G9G,LYS_33,10.17,-0.32,0,-0.01 1DVO,ASP_74,4.09,-0.12,0.14,0.27 3CO1,LYS_100,9.88,-0.36,0,-0.27 3CXS,GLU 69,4.3,0.36,-0.56,0 3M66,GLU_174,4.59,0.13,0,-0.05 3E5T,GLU_204,4.61,0.69,-0.56,-0.01 300P,ARG_25,12.24,-0.26,0,0 3F1X.ARG 297.12.45.-0.05.0.0 2B6PLYS 259.10.46.-0.09.0.0.05 10IS,GLU_350,2.59,1.08,-2.69,-0.31 1ES9,ARG_59,12.4,-0.17,0,0.07 2WB8,TYR_464,11.98,0,0.71,1.27 2P52,TYR 217,11.52,0,0.05,1.48 2AZP,ARG 260,12,55,-0,14,0,0,19 1YLN,GLU_159,4.12,0.66,-0.7,-0.36 1PNE,HIS_133,6.04,-0.29,0,-0.17 1ZP2.GLU 102.4.58.0.51.-0.18.-0.25 3VJ8,LYS 242,10.92,-0.32,0.69,0.05 1KN3,HIS_118,6.71,-2.56,0.98,1.79 1ZBS,ARG 46,12.62,-0.26,0.0.38 3IVF,TYR_395,10.3,0,-0.12,0.42 2B3M,GLU 50,3.94,0.32,-0.72,-0.16 1WOU.GLU 117.4.51.0.3.0.-0.3 20KT,HIS_341,6.29,-0.21,0,0 2F4Q,ARG_323,13.77,-0.18,0.96,0.49 3LOD,TYR_2,10.67,0,0.07,0.6 2Q13,GLU 198,4.81,0.32,0,-0.01 2QV2,TYR_257,10.23,0,-0.18,0.41 1NJ4,ASP_218,3.73,0,-0.22,0.15 3H5T,TYR_9,10.05,0,0,0.05 3T8R,LYS 19,10.16,-0.31,0,-0.04 2DG7,ARG 41,12,22,-0.31,0.0.02 1IDK,HIS_259,6.48,-1.72,0.85,0.85 3M16,LYS_151,10.34,-0.17,0,0.01 1SUU,ASP_545,3.01,-2.15,-0.24,1.6 2RJD,GLU_297,4.6,0.18,0,-0.08 3BA1,ARG_47,13.32,-0.56,0.95,0.44 3MTT,ARG_547,12.46,-0.23,0,0.19 105T,ARG_417,13.69,-0.36,0.81,0.73 2E3C,ASP_281,3.93,0,0.01,0.12 2X4L.TYR 248.11.56.0.0.02.1.54 3GMS,GLU_73,4.42,0.77,-0.47,-0.37 2Q07,LYS_270,10.8,-0.27,0,0.58 1P6F,ASP_49,4.79,0,-0.02,1.01 3AU3,ARG_623,12.44,-0.06,0,0 1RHS.GLU 226,4.56,0.1,0,-0.04 20EW,LYS_23,10.23,-0.16,0,-0.1 2A4D,GLU_215,4.56,0.31,0,-0.25 2FM9,HIS_193,6.36,-0.36,0,0.22 1XDZ.TYR 29.10.97.-0.03.0.16.0.85 2OSA,GLU_416,4.57,0.17,0,-0.1 3GS3,HIS_238,6.36,-0.14,0,0 2R0S,LYS_87,10.36,-0.14,0,0 3CGW,ARG_76,12.5,-0.31,0.31,0 3PU6,ASP 55,3,14,-0.66,-0.44,0.45 3HVM,GLU_226,3.94,0.6,-0.46,-0.7 2D7U,TYR_250,10.19,0,-0.04,0.23

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3MEW.HIS 250.5.94.-0.35.0.-0.21 3F6F.TYR 177,11.56,-0.28,0.4,1.44 3RLN,LYS_732,10.51,-0.19,0,0.2 2Q99,GLU_81,4.66,0.16,0,0 3AU3.GLU 565.4.26.0.38.0.-0.62 1C44,CYS 71,11,19,-0.01,0.06,2.14 3ETV,GLU_214,4.01,1.1,-1.24,-0.35 1LPL,ASP_220,3.9,0,-0.07,0.17 3GE9,ARG_163,12.38,-0.12,0,0 1V6T,LYS_159,10.59,-0.47,0,0.56 100L.GLU 70.4.38.0.2.0.-0.32 3CQ1,GLU_62,3.63,0.3,-0.84,-0.33 3ELI,GLU_118,4.59,0.12,0,-0.04 2B6P,ARG_226,12.75,-1.42,0.49,1.18 3K1H.CYS 86.10.89.0.-0.06.1.95 1MUF,ASP_112,3.7,-0.03,-0.32,0.26 3PZ9, ASP_204, 1.37, -2.98, -0.21, 0.76 4E9E,GLU_489,4.1,0.38,-0.73,-0.05 2FPN,GLU_176,4.46,0.21,-0.31,0.05 3B7X.GLU 138.3.76.0.43.-0.62.-0.55 1MML,TYR_64,10.08,0,0,0.08 3GA2,LYS_151,11.03,-0.16,0.1,0.6 2BT8, ASP_178, 3, -1.06, -0.49, 0.75 2YWJ.ARG 146,12.21,-0.31,0,0.02 1J33,ARG_21,12.52,-0.08,0,0.1 1D2K,LYS_348,10.46,-0.27,0,0.23 3ELI,HIS_128,4.38,-1.74,0,-0.38 2CI3,CYS 73,10.93,-0.92,0.14,2.7 1FKM,TYR_440,13.93,0,0.63,3.3 1EV8,ARG_127,12.41,-0.1,0,0.01 2CW4.TYR 98,10.32,0,0.0.32 3M7D,ARG_270,12.46,-0.04,0,0 3FXH,CYS 18,9.59,0,0.05,0.55 1P4X.GLU 89.4.63.0.13.0.0 4EKU,LYS_169,10.36,-0.2,0,0.06 1AK1,ASP_237,4.25,0,-0.01,0.47 3LJN,LYS_92,10.55,-0.11,0,0.16 1WYC.GLU 78.4.81.0.31.0.0 1P4X,ASP_31,3.9,0,-0.03,0.14 3HZO,LYS 11,10,44,-0.06,0,0 1GPP,ARG_91,11.95,-0.53,0,-0.03 3HVM,LYS 10,10.47,-0.11,0,0.08 3N2T.TYR 208,11.77,0.0.05,1.72 105T,ARG_119,13.93,-0.71,1.37,0.77 3RLE, ARG_174, 13.4, -1.26, 1.55, 0.61 2V5B,LYS_53,10.31,-0.53,0,0.34 1ZBS,HIS_282,6.39,-0.26,0,0.15 2H2W,ARG_171,13.92,-0.32,1.08,0.66 4FLE.HIS 30.6.05,-0.45.0.0 3CAN,HIS_20,7.12,-0.3,0.65,0.27 2FL7,LYS 183,10.65,-0.15,0,0.3 3PAC,LYS 41,10.8,-0.36,0,0.66 2PP6,LYS_85,10.64,-0.75,0.48,0.41 1MUF,ARG_320,12.67,-1.16,0.09,1.24 1U53,LYS_94,10.57,-0.21,0,0.29 2I88, ASP 423, 3.5, -0.53, -0.22, 0.45 2F8H,HIS_272,7.07,-0.36,0.85,0.08 2JEO,GLU_138,3.97,2.61,-1.21,-1.93 3LH5,HIS_766,5.96,-0.79,0.15,0.1 2AZL,ARG 130,12.02,-0.28,0,-0.2 1PZC.LYS 109.10.59.-0.18.0.0.27 2l6l,LYS_48,11.79,-0.36,0.85,0.79 3UX2,GLU 60,4.6,0.1,0,0 1WRU,GLU_337,5.03,0.59,0,-0.05 2D7U,GLU_176,6.75,4.37,-0.98,-1.14 1NIJ,GLU_74,4.76,0.42,0,-0.16 1ILW,TYR_132,10.66,0,0.15,0.52 1UJ8,HIS_9,7.48,-0.35,0.85,0.49 3HYQ,TYR_104,11.28,0,0.2,1.07

1X91,LYS_51,10.5,-0.26,0,0.25 4DIU.ARG 36,12.35,-0.36,0.0.21 4DBX,TYR_240,13.93,0,0.27,3.66 3048.CYS 87.12.22.0.26.0.44.2.52 2AH5.GLU 172.4.79.0.34.0.-0.05 3G9G.ASP 238.3.39.-0.53.-0.27.0.39 1UAJ.TYR 86,12,29,-0.08,0.32,2.04 1V43,LYS_330,10.62,-0.16,0,0.28 2QHT,TYR_71,10.94,0,0.41,0.53 3F7M,GLU_278,4.99,1.25,-0.76,0 30KQ,GLU_645,3.65,0.26,-0.73,-0.38 1RHS,TYR_83,12.53,-0.84,0.92,2.46 2FPN.HIS 161.6.31.-0.28.0.0.09 20EW,ARG_173,12.43,-0.07,0,0 1TWU, ARG 17, 11.61, -1.74, 0, 0.85 3I0C,ASP 326,3.71,-1.07,0.06,0.92 3C38,ASP_233,3.39,-0.36,-0.32,0.27 105J,LYS_24,11.28,-0.58,0.85,0.5 1WYC,ASP_252,3.89,0,-0.16,0.24 2HXB,TYR 11,9.55,-0.88,-0.34,0.77 3EVZ,LYS_45,10.4,-0.44,0.1,0.23 3OA7,GLU_27,4.66,0.2,0,-0.04 3BWT,TYR_775,10.4,-0.14,0.06,0.48 2E3C.ASP 230,4.5,-0.16,-0.42,1.28 1AKO,LYS 218,10,47,-0,11,0,0.07 3KB5,LYS_460,10.42,-0.11,0,0.03 1LZL,ASP_175,2.98,-1.35,-0.41,0.94 3U2A,LYS_119,10.48,-0.25,0,0.23 2GAU,LYS 40,10.06,-0.2,0,-0.24 4H4J,ASP_232,3.76,-0.02,-0.32,0.29 1RAJ,ARG_306,9.74,-3.5,0,0.74 1L2F,GLU_141,4.58,0.23,0,-0.15 109G,GLU_180,5.6,0.95,0,0.14 1AT0.GLU 361.4.57.0.07.0.0 3LE4,ARG_325,12.37,-0.13,0,0 1WP5,GLU_319,4.54,0.15,0,-0.11 3CGW,LYS_154,10.51,-0.25,0,0.25 1NIJ,ASP 47,3.41,-0.61,0,0.21 1D2K,TYR_133,10.64,-0.39,0.25,0.78 2RIK,LYS_233,10.46,-0.04,0,0 1YM5,HIS_82,7.06,-3.09,1.12,2.52 2CBE,LYS 24,10.23,-0.25,0,-0.02 1NAR, ASP 119, 3.88, -0.16, 0.04, 0.21 4EZB,LYS_78,10.35,-0.17,0,0.01 208P,ASP_214,3.9,0,0,0.1 4FCU,TYR_196,13.6,-0.13,1.06,2.66 3ASA,LYS 310,9.96,-0.42,0,-0.12 1J74,ARG 11,11.71,-1.03,0.0.24 3M7G,HIS_200,4.72,-2.4,0.85,-0.24 3FWU,LYS_33,9.72,-0.95,0,0.17 4DEZ.GLU 54.4.69.0.15.0.0.04 4GCO.CYS 203,11.02,-0.24,0.06,2.21 4DVD,ARG_127,12.62,-0.11,0,0.23 2H2Z,ASP_33,4.33,0,0.11,0.42 3CQ1,TYR_44,9.93,-0.71,0.14,0.51 1XDZ,ARG_138,11.53,-1.31,0,0.34 1WLY.GLU 74.3.04.0.47,-1.62,-0.31 1RI5,ARG_259,12.99,-0.25,0.34,0.4 4H86,ASP_134,3.89,0,0,0.09 1XIP.ARG 274,12.57,-3,18,0,72,2.54 3RE9, HIS 182, 6.02, -1.09, 0.78, -0.17 2BQQ,GLU_120,4.58,0.23,0,-0.13 1T07,ARG_36,12.62,-0.26,0,0.38 2VAN,HIS_252,5.98,-1.41,0.54,0.36 2Q5X,ARG_825,13.1,-0.33,0.62,0.31 3GA2,CYS_153,9.55,0,0.03,0.52 1YTD,GLU_309,5.22,0.98,0,-0.26 4FCU,ARG_78,10.94,-1.39,0,-0.18 1X8F,HIS_67,6.41,-0.09,0,0

3LPZ.CYS 96.11.-1.14.0.3.15 3C2E,LYS 202,10.43,-0.31,0,0.24 2RGY,ARG_359,12.37,-0.29,0,0.16 2BV9,ASP_56,3.35,-0.79,-0.28,0.62 1K95,ASP_132,5.29,-0.48,0.21,1.76 2CVB1YS 86.10.55-0.14.0.0.19 3LOD,ARG 126,12,35,-0,33,0,0,19 1ILW,LYS_159,10.83,-0.17,0,0.5 1MTZ,TYR_44,12.92,-1.52,0.56,3.88 1PV5,GLU_188,4.81,0.26,0,0.05 3CNU,TYR 91,11.28,0,0.08,1.19 3BCY,LYS 97,9.74,-0.61,0,-0.15 2E3C,LYS_205,10.43,-0.08,0,0.01 10GL,LYS_210,10.46,-0.04,0,0 2161,ASP 124,4,1,0,-0.02,0.33 3UAH, ARG 404, 12, 19, -0, 55, 0, 0, 24 10LR,LYS_62,8.63,-1.91,0,0.04 2YYO.ASP 68.1.63.-1.84.-0.69.0.37 3GS3,CYS_139,10.97,-0.29,0.36,1.89 1ZBM,LYS 169,10.3,-0.27,0,0.07 3CO1.GLU 68.4.56.0.31.0.-0.25 1TLV.TYR 254,10.68,-0.46,-0.14,1.29 3MIX,TYR_558,10.42,0,0.04,0.37 1XIPLYS 58,10.48,-0.58,0.16,0.39 20G0.GLU 568.4.49.0.86.-0.82.-0.05 106D,HIS_41,7.25,-0.52,0.85,0.42 1YDL,ASP_62,3.86,0,0,0.06 3CXS,LYS_135,10.04,-0.46,0,0 2RGY,HIS_203,5.85,-0.52,0,-0.13 1XAW,LYS 485,10,74,-0.32,0,0.56 1MUF,TYR_86,10.07,0,0.01,0.05 3V3T,TYR_273,9.43,-0.65,-0.36,0.44 2E3C,LYS_214,10.57,-0.15,0,0.22 106D,GLU 80,4.16,0.3,-0.83,0.19 1YW5,GLU_32,4.79,0.29,0,0 2B0A,GLU_108,4.62,0.12,0,0 1DUN,CYS_22,9.72,-0.03,-0.48,1.23 1XEU,GLU 276,4.92,0.37,0,0.05 1AM2,TYR 162,11,18,0,0,41,0,78 1RI6,ARG_181,11.69,-3.24,0.19,2.25 3C2E,GLU_24,4.75,0.19,0,0.05 1ZP2.ASP 226.4.07.0.0.0.27 3COU.TYR 146,10.63,0,0,0.63 3M3P,HIS_88,4.83,-2.79,0,1.12 1FHL,ASP_17,4.1,0,0.09,0.21 2P5D,GLU_103,4.5,0.29,0,-0.29 3H9W,TYR_99,10.46,0,-0.02,0.48 3GS9,GLU_234,4.5,0,0,0 3EZ7,ARG_13,12.15,-0.25,0,-0.09 3LH5.GLU 640.4.66.0.16.0.0 1X7F,LYS_237,11.13,-0.38,0.29,0.71 3LH5,GLU 659,4.79,0.49,0,-0.19 4FZR,ARG 351,13.65,-0.41,1.15,0.41 3CS1,LYS_108,10.55,-0.07,0,0.12 4FH3,GLU_54,4.61,0.18,0,-0.08 3I47,ARG_50,11.8,-0.93,0,0.23 1TXJ,GLU_21,4.1,0.57,-0.44,-0.53 2RIK,GLU_17,4.73,0.23,0,0 1CBY,TYR_48,10.34,-0.85,0.27,0.92 1TD6,GLU_156,5.62,3.89,-1.78,-0.99 30NT, ARG 19, 12.4, -0.1, 0, 0 106D,TYR 22,11.87,0.85,0.39,0.62 3MTT,LYS_590,11.96,-0.39,1.08,0.76 2C2Y,GLU_80,4.73,0.2,0,0.03 3EJG,GLU_63,3.99,0.35,-0.48,-0.38 3D9H,ASP_68,4.14,0,0.1,0.24 2B0A,GLU_34,4.67,0.17,0,0 2R57.GLU 310.4.56.0.07.0.-0.01 2FBQ,LYS_101,10.45,-0.05,0,0

3ULX,ASP_55,3.42,-1.43,0,1.05 2H2W,GLU 226,4.99,1.58,-0.98,-0.1 2YYO,ARG_95,12.39,-0.11,0,0 1H09,TYR_238,10.74,0.06,0.06,0.61 1YM5,GLU_223,4.96,2.56,-1.14,-0.97 2R51,LYS 49,11,28,-0,28,0,68,0,38 4EKU.GLU 202.4.56.0.17.0.-0.12 1T95,GLU_90,4.1,0.29,-0.42,-0.26 2BAA,GLU_56,7.04,4.07,-1.53,0 2X4G,ASP_145,3.93,0,0,0.13 10LR/ARG 3,12,27,-0,23,0,0 1L3K,ARG_14,12.26,-0.58,0,0.34 3RLN,ASP_656,3.91,0,-0.01,0.12 10I7.LYS 284,10.53,-0.29,0.0.31 2QV2,ASP_195,3.99,0,-0.11,0.3 3A0X,ARG 738,12.89,-0.39,0.39,0.39 2BV9,TYR_74,10.66,0,0.15,0.51 3FHF,TYR_159,11.37,0,0.11,1.26 2OSA,ARG_304,12.26,-0.31,0,0.07 3O6L.LYS 32,10,29,-0,29,0,0.08 1U53,LYS 184,10,26,-0,24,0,0 2YWK,GLU_23,4.09,0.48,-0.76,-0.12 4F85,LYS_171,10.28,-0.09,0,-0.13 1NAF.GLU 275.4.58.0.08.0.0 3DHN.GLU 44.4.56.0.06.0.0 2Q07,LYS_344,10.89,-0.83,0.76,0.46 3CS1,ARG_120,13.6,-1.94,1.6,1.45 1QQE,ARG_192,12.45,-0.05,0,0 1ZKZ,HIS_98,6.28,-0.34,0,0.12 1T95.CYS 207.11.13.0.0.12.2 1XKR,TYR_28,10.06,0,0,0.06 3G9G,TYR 53,12,29,0,71,0,91,0.68 1YR6,ARG_51,13.56,-0.81,1.09,0.79 2NSN,ASP 66,3.12,-0.73,-0.28,0.33 3V55,GLU 390,3.83,2.5,-2.42,-0.75 3GW3,ARG_179,12.29,-0.16,0,-0.04 2IRM,LYS_190,10.49,-0.44,0,0.43 2QDJ,GLU_72,4.5,0.21,0,-0.22 2Z0M,GLU 315,4.14,0.77,-0.59,-0.54 2C2Y,CYS_57,12.25,-0.03,0.06,3.22 3BOW.GLU 234.4.75.0.13.0.0.12 1FKM,ARG_286,13.22,-2.51,1.41,1.83 1SNT,ARG 189,12.5,-0.1,0,0.09 2C2Y,ASP 153,3.89,0,-0.08,0.17 1R3F,HIS_196,5.29,-1.5,0.36,-0.06 3RKV,LYS_241,10.28,-0.28,0,0.05 2D59,LYS_24,12.38,-0.74,1.5,1.13 2CWC,ARG 203,12.45,-0.33,0,0.27 3C6B,LYS_249,10.81,-0.36,0,0.67 3RLN,LYS_598,10.33,-0.17,0,0 1DUN,HIS_107,6.11,-0.44,0,0.05 3EZ7,LYS_234,11.41,-0.65,0.44,1.12 1T3Y,GLU 128,4.64,0.32,0,-0.18 2OPJ,ARG_13,11.99,-0.51,0,0 3E7P,GLU_215,4.61,0.11,0,0 2D8N,LYS_180,9.94,-0.64,0,0.07 3GW3,GLU_119,4.75,0.19,0,0.06 100E,ASP 179,4,14,-0.22,-0.26,0.81 2AZL,HIS_118,6.35,-0.43,0,0.29 1RAJ,TYR_384,10.17,0,-0.09,0.26 2A6B,HIS_172,3.77,-3.52,0.79,0 3CCY,ASP 14,3,94,-0.11,-0.21,0.46 2X4G,GLU_236,3.65,0.76,-0.78,-0.83 2X5Y,GLU_745,4.68,0.18,0,0 4D8L,LYS_137,10.26,-0.53,0,0.3 1ZKZ,ASP_88,4.16,0,0,0.36 2X4G.GLU 220.3.28.1.56.-2.7.-0.09 2CXA,GLU_163,4.67,0.19,0,-0.02 1GPP,GLU_100,4.72,0.22,0,0

1SQH,ASP_101,3.91,0,0,0.11 3CGW.HIS 146.5.6.-1.08.0.0.18 1R53,LYS_6,10.66,-0.18,0,0.33 2HRZ,GLU_40,4.78,0.28,-0.03,0.04 3AUF,GLU 127,3.98,0.37,-0.6,-0.29 2B0J.CYS 253,9.8,-0.29,0.3,0.8 1AD6,LYS_432,10.38,-0.13,0,0 1EV8,ASP_139,3.92,-0.02,0,0.13 3I0C, ARG_248, 11.8, -1.25, 0, 0.55 2RH3,HIS_183,5.58,-0.81,0.21,-0.33 3KB5,HIS 299,4.8,-1.77,0.04,0.03 3E0H,ASP_114,3.9,0,-0.1,0.2 3RHE,ARG_117,12.82,-2.68,1.58,1.42 2QRX,GLU_25,4.6,0.32,0,-0.22 2ZTY.ASP 66.3.97.0.0.01.0.16 3DZ1,ARG_91,12.56,-0.11,0,0.17 4DBX,GLU_77,4.5,0.28,0,-0.28 2Q07,ASP_466,3.33,-0.68,-0.11,0.32 1R29.TYR 58.9.92.-0.19.-0.02.0.13 1GXN.LYS 411.11.31.-0.42.0.85.0.38 1W7B,GLU_242,4.49,0.36,-0.1,-0.27 20YZ,LYS_49,10.44,-0.06,0,0 2FZ4.GLU 99.5.43.0.91.-0.08.0.1 3GV0.CYS 183.10.27.0.0.19.1.08 3JV1,ARG_110,12.58,-0.08,0,0.16 2IIA,HIS_85,6.66,-0.39,0.53,0.02 2F4Q,LYS_22,9.4,-0.84,0,-0.26 3LPZ,TYR 124,10.29,0,0.14,0.15 3CS1,ARG 35,12.66,-0.36,0.1,0.41 2VGM,GLU_72,4,1.01,-0.85,-0.66 2H85,TYR 32,10.86,0.05,0.44,0.37 1A8Q,HIS_57,3.43,-3.2,1.11,-0.97 1R3D,HIS 37,5.94,-0.43,0,-0.13 1YIB,LYS_204,10.38,-0.12,0,0 2F8H,HIS_165,2.92,-3.64,0.07,-0.01 3GOZ,GLU_128,3.58,0.45,-1.01,-0.35 2CXC,GLU_139,3.86,0.35,-0.84,-0.15 1ZBPLYS 82.10.16.-0.61.0.0.28 4D8L,ASP_256,3.97,0,0,0.17 1YB2,ARG 123,12.69,-0.58,0.0.77 3PAC,GLU_156,4.63,0.17,0,-0.04 4H89.ARG 100,12.37,-0.21,0,0.09 2H85,HIS 337,6.82,-0.38,0.4,0.31 1YB2,GLU_125,4.53,0.12,0,-0.1 4GA2,GLU_81,3.89,0.42,-0.68,-0.34 3L3P,ARG 323,13.32,-1.09,1.47,0.43 3O16,LYS_102,10.42,-0.08,0,0 3H6Q,GLU 85,4.68,0.18,0,0 2HRZ,GLU_51,4.57,0.11,0,-0.04 2P5D,TYR_60,10.56,0,0,0.56 3BWT, ASP 602, 3.94, 0, -0.14, 0.28 2O34.GLU 173.4.61.0.19.0.-0.07 2Z0M,ASP_207,1.22,-2.19,-1.65,1.26 3HVW,ARG_179,13.08,-0.25,0,0.83 2VGM,LYS_297,10.05,-0.69,0,0.25 3L7N,ASP_135,3.34,-0.38,-0.38,0.3 3DHN,LYS_101,10.58,-0.12,0,0.19 1ZBS,GLU_174,4.63,0.48,-0.25,-0.1 3HKX,ARG_85,13.58,-0.71,1.07,0.73 1GXN,GLU 529,3.26,1.04,-1.66,-0.62 2EA9,ARG 78,12.5,-0.09,0.0.09 1PVT,GLU_137,4.98,0.34,0,0.14 2C2Y,ASP_238,3.96,0,-0.04,0.21 3M7G,GLU_50,4.83,0.32,0,0.01 4FLE,HIS_180,6.44,-0.25,0,0.18 1XEU,HIS_106,6.1,-0.27,0,-0.13 2G7O,LYS_83,10.36,-0.16,0,0.02 3PAC,GLU_18,4.13,0.26,-0.28,-0.34 3PU6,ASP_15,3.59,-1.46,0,1.24

20V2.ARG 274.11.97.-0.4.0.-0.13 3JSN.GLU 264.4.77.0.16.0.0.1 1GPP,LYS_26,10.53,-0.3,0,0.33 3ANJ,TYR_347,12.97,0.75,0.3,1.92 2XJ4,ARG_5,13.06,-0.63,0.72,0.47 4DIU.CYS 45,12.83,0,0.14,3.7 1WXQ,LYS_74,11.22,-0.34,0.65,0.41 1XFK,ARG_213,11.56,-0.91,0,-0.02 100X,ASP_44,2.94,-1.26,-0.3,0.7 3PP8,GLU_284,4.66,0.24,0,-0.08 1NAF,GLU_251,4.79,0.31,0,-0.02 3H5T,ARG_201,12.23,-0.72,0,0.45 2G3A,ARG_73,12.13,-0.37,0,0 3TMO,HIS_330,6.61,-1.25,0.79,0.57 3U2A.GLU 54.4.58.0.4.0.-0.33 2G2D,ASP 181,3,58,-0.86,-0.47,1.1 2NRK,TYR_77,13.17,0.73,0.18,2.27 3GEC,ARG_317,12.66,-0.53,0.22,0.47 3U2R,CYS_123,10.55,0,0.14,1.41 2B6P,ARG 113,12.26,-0.63,0.02,0.37 2Q13,HIS_45,6.47,-0.37,0,0.34 1J8B,LYS 91,10.63,-0.17,0.0.29 1HF8,LYS_112,10.94,-0.21,0.65,0 2RGY,GLU_162,4.69,0.24,0,-0.03 3E5T,ASP 165,3.85,0,-0.3,0.36 1EQ6,TYR_39,13.73,0,0.62,3.11 3C2E,GLU_215,3.78,0.57,-1.27,-0.02 20KT,TYR_273,11.79,0,0.07,1.71 1WNH,LYS_55,10.29,-0.29,0,0.07 2AD1,ARG_188,12.06,-0.52,0,0.08 3EX9,GLU_12,4.94,0.14,0,0.3 2CXA,ARG_84,12.35,-0.15,0,0 2WZ9,GLU_24,3.57,0.37,-0.92,-0.38 2WOZ.ASP 398.4.26.0.0.08.0.38 3RJZ,LYS_198,10.37,-0.45,0,0.33 1WXQ,TYR_43,10.72,0,0.21,0.52 3H04,GLU_247,4.78,0.57,0,-0.27 1D2K,ARG 407,12.12,-1.29,0,0.92 3ZRI,LYS_12,10.23,-0.27,0,0 3M3P,ARG_76,12.23,-0.33,0,0.06 1SQH,ARG_258,11.79,-0.39,0,-0.32 1LZL.HIS 86.4.01.-3.28.0.79.0 1X6J.TYR 32.12.23.0.0.24.1.98 3UPD,LYS_42,10.4,-0.18,0,0.08 3P2F,GLU_150,3.1,1.12,-1.65,-0.87 3HKX,CYS_73,9.52,0,-0.03,0.55 3R87,HIS 24,6.17,-0.38,0,0.05 3U2R.ARG 98,12.33,-0.17,0.0 10IS,ARG_349,12.21,-0.37,0,0.08 1ANU,LYS_73,10.38,-0.16,0,0.05 3PM2.GLU 48.4.56.0.06.0.0 2GKG,ASP 73,3.27,-0.41,-0.28,0.17 1RAJ,ASP_319,2.83,-0.7,-0.57,0.3 3ELI,ASP_46,3.51,-1.57,-0.3,1.58 2Q98,ARG_176,11.86,-0.84,0,0.2 2B3M,ARG_135,12.42,-0.28,0,0.19 2CXC.GLU 44,4.37,0.22,-0.1,-0.25 2AH5,LYS_31,10.65,-0.11,0,0.26 1W7B,ASP_209,3.56,-0.36,-0.32,0.44 1ILW,LYS 143,11.46,-0.38,0.81,0.52 2XHC,ARG 222,12,41,-1.06,0.13,0.83 1TJE,ARG_207,12.07,-0.82,0,0.38 1V43,ASP_316,3.76,0,-0.36,0.33 3M70,LYS_102,12.87,-0.81,1.7,1.49 4F8A,CYS_667,9.71,-0.85,0.1,1.46 3COU,LYS_131,11.25,-0.25,0.46,0.54 2IRM,HIS_206,3.43,-2.62,0,-0.43 2E3S,LYS 425,10.5,-0.18,0,0.18 3QAV,GLU_48,4.49,0.31,-0.06,-0.26

4DBX,ARG 296,12.55,-0.4,0,0.45 1X1E.ARG 83.11.68.-0.98.0.0.16 3BPP,LYS_21,11.29,-0.45,0.85,0.39 2B3M.GLU 43.4.96.0.3.0.0.16 1UJ8,CYS_48,10.44,-0.01,0.15,1.3 3EVZ.TYR 203.9.87.-0.96.-1.47.2.29 3L7N,LYS 85,10,13,-0,55,0,0,18 4H86,HIS_111,6.72,-0.66,0.83,0.05 3RKV,GLU_228,4.9,0.29,0,0.11 1UAJ,TYR_115,11.15,0,0.11,1.04 208P,GLU_86,4.24,0.24,-0.49,0 1AK1,LYS 4,10,44,-0,15,0,0,08 3JZ9,GLU_392,4.74,0.27,0,-0.03 2JEO,ARG_99,13.66,-0.18,0.95,0.39 1LFP.CYS 129,10.03,-0.21,0.26,0.98 1KCM.CYS 188,10,75,0,-0,24,2 1RSS,ASP_20,3.04,-1.4,-0.17,0.82 3GV0,GLU_285,4.6,0.41,-0.35,0.05 3IVF,TYR_127,10.44,0,0.01,0.43 3V3T,ASP_172,3.6,-0.17,-0.37,0.35 1YR6,ASP 232,4,39,0,-0.02,0.61 3V55,ARG_671,13.4,-2.22,1.68,1.45 2H01,LYS_59,10.55,-0.26,0,0.3 3RHE,HIS 83,5.9,-0.71,0,0.11 2H14.LYS 109.10.38.-0.19.0.0.07 3CAN,TYR_177,11.58,0.85,0.26,0.46 3ETV,ASP_186,3.88,-0.28,-0.01,0.36 3A0X,ASP_632,2.91,-0.8,-0.38,0.29 2CBE,GLU_187,4.83,0.1,0,0.22 2B3M.GLU 14.4.64.0.14.0.0 3HQX,ASP_101,4.41,0,0,0.6 2QZQ,CYS_49,10.9,-0.02,-0.24,2.17 2EFK.ARG 122,12,43,-0.23,0,0,15 1NFN,ARG 103,13.52,-0.58,0.67,0.93 2EJB,CYS_97,9.98,-0.09,-0.09,1.16 2RIS,GLU_9,3.85,0.2,-0.85,0 2IXM,ASP_176,3.95,-1.6,0.25,1.49 1AM2,ARG_107,12.12,-0.54,0,0.16 2VC8.LYS 63.10.56.-0.14.0.0.2 1YOY,LYS_63,11.66,-0.37,0.85,0.68 3FK5,CYS_185,11.16,-1.57,0.11,3.62 1NWA,ARG_165,12.46,-0.04,0,0 2DFL,ARG 154,12.61,-0.34,0,0.45 1L2F,GLU_28,4.83,1.41,-0.79,-0.29 3A7L,LYS_64,10.36,-0.2,0,0.06 1T6L,LYS_97,10.29,-0.11,0,-0.1 2IN0, ARG 60, 11.98, -0.42, 0, -0.1 3F6F,ASP_152,3.78,0,-0.25,0.23 3M7G,GLU_17,4.59,0.3,0,-0.21 3KEY,LYS 389,11.55,-0.3,0.7,0.65 2QK1,TYR_498,11.03,0.34,0.01,0.68 3H6Q,GLU 41,3.71,1.19,-1.68,-0.29 1C3K.LYS 36.9.78.-0.41.0.-0.31 2P52,GLU_168,3.75,0.53,-0.65,-0.64 2EFK,GLU_149,4.68,0.18,0,0 1WYC,ASP_193,1.89,-2.25,-0.77,1.1 2PLQ,HIS_110,5.9,-0.77,0.42,-0.26 1TXJ,LYS_37,10.66,-0.93,0.85,0.24 1046.GLU 14.4.77.0.19.0.0.08 2P4D,ASP 90,3.03,-0.72,-0.38,0.34 3JRT,CYS 53,10.74,-0.03,0.03,1.75 4DEZ,ASP_79,4.04,-0.02,-0.09,0.35 1TR9,GLU_277,4.56,0.11,0,-0.04 3M70,ARG_201,12.5,-0.35,0,0.35 30IP,CYS_128,12.95,0,0.08,3.87 1UCH,TYR_181,10.6,-0.86,0.2,1.25 2H2W,TYR_262,12.52,-0.67,0.18,3.01 3AU3.GLU 411.4.09.0.32,-0.43,-0.3 3RLN,ARG_699,12.72,-0.45,0.03,0.64 307K,ARG_159,12.1,-0.51,0,0.11 1R5Q,GLU 34,4.74,0.25,0,-0.01 2NYC,ARG_303,13.63,-0.28,0.77,0.65 3PP8,ARG_112,12.42,-0.2,0,0.12 3IU5,LYS_135,10.42,-0.23,0,0.14 3GS9,ARG 87,13,12,-0,27,0,52,0,38 2EJB.ASP 164.2.89.-1.3.-0.01.0.4 1QQE,CYS_40,11.43,-0.15,-0.13,2.72 109G,CYS_18,10.5,-0.01,-0.01,1.53 1C44,LYS_18,10.85,-0.13,0,0.48 1NAR.LYS 67,10.06,-1.0.0.56 2CI3.LYS 143.10.13.-0.15.0.-0.22 1NAR,ASP_240,3.98,0,-0.04,0.21 3RNV.LYS 442,10.21,-0.38,0,0.09 2D8N,HIS_91,5.25,-1.19,0,-0.07 3OA7,GLU 537,4.36,0.18,0,-0.32 20ZO,TYR 111,10,43,-0.03,0.04,0.42 1ZBS,TYR_175,11.73,0.25,0.39,1.09 3NZL,LYS_40,10.43,-0.07,0,0.01 2E3I,LYS_70,9.84,-0.56,0,-0.1 3CS1.LYS 28.10.54.-0.16.0.0.19 1NAR,ASP_274,2.44,-1.41,-0.58,0.63 2C2Y,ARG 172,12,34,-0,16,0,0 2EFK.GLU 147.4.15.0.3.-0.02.-0.63 2FZ4.LYS 172.10.36.-0.5.0.0.36 1RI5,LYS_200,10.42,-0.08,0,0 2CW4,LYS_21,10.69,-0.33,0,0.53 1WYC,TYR_242,10.76,-0.16,0.13,0.78 2XJ4,ARG 221,12.69,-0.56,0.12,0.63 3CE7,GLU_78,4.13,0.27,-0.79,0.15 2WZ9,GLU_51,4.72,0.15,0,0.07 1T07.LYS 26.10.65.-0.13.0.0.28 1WNH,LYS_51,11.53,-0.47,0.85,0.64 3JZ9,GLU 374,3.78,0.36,-0.7,-0.39 1SI7,ARG 298,12.35,-3.23,1.5,1.57 2QV2,GLU_247,4.08,0.5,-0.81,-0.1 3GS9,GLU_28,4.51,1.83,-1.67,-0.15 3HKX,ARG_175,11.6,-0.86,0,-0.05 2WZ9,ASP 130,3.84,0,0,0.04 3P51,ARG_70,12.23,-0.59,0,0.32 4DEZ,ASP_234,4.17,0,-0.17,0.53 3LJC,ASP_47,3.61,0,-0.36,0.18 1JT9,GLU 217,2.53,0.75,-2.51,-0.2 1PVT.LYS 184,9.98,-0.52,0,0 3US6,GLU_20,4.14,0.32,-0.33,-0.35 1MJS,GLU_301,3.47,0.82,-1.47,-0.39 2O4D,GLU_110,4.7,0.2,0,0 2F8H,ASP 254,3.39,-0.89,0.15,0.33 3ADO,LYS_313,9.96,-0.58,0,0.04 2GAU,ARG_224,13.34,-0.38,0.79,0.42 2FC3,LYS_119,11.27,-0.48,0.85,0.39 2V4X,ASP_106,3.99,0,0,0.19 2098, ARG 164, 12, 39, -0, 44, 0, 0, 33 2Z14,ASP_47,2.22,-1.79,-0.44,0.66 3BCY,LYS_23,10.56,-0.32,0,0.38 1ZCE,TYR_4,10.31,-1.03,0.25,1.09 3RFY,CYS_256,10.6,-0.17,0.2,1.58 3CXS.GLU 62.4.59.0.09.0.0 4ECC,ARG_35,12.5,-0.34,0.02,0.31 2WOZ,LYS_482,10.29,-0.46,0,0.25 1SNT,ARG_140,11.74,-0.8,0,0.03 3KB5,ARG 412,13.87,-0.72,1.03,1.06 2J8A,LYS_349,11.55,-0.36,0.85,0.56 3CIV.ASP 129,3.37,-0.81,-0.35,0.72 1YOY,LYS_12,10.53,-0.08,0,0.11 2X4L,TYR_85,13.57,-0.78,1.06,3.29 1Z9L,LYS 87,9.88,-0.45,0,-0.18 1WXQ,HIS_359,6.58,-0.23,0.04,0.27 3F6F,ARG_182,11.99,-0.59,0,0.08

1P6F.GLU 98.4.97.0.75.0.-0.27 1YB2.GLU 12.4.63.0.69.0.-0.55 2B3M,TYR_143,10.52,0,0.02,0.5 3ZRI,LYS_131,10.38,-0.12,0,0 3V55.GLU 500.4.63.0.48.0.-0.35 1WRU,LYS 81,10.1,-0.34,0,-0.06 3L3P,ASP_470,3.92,0,-0.01,0.13 4FCU,ARG_221,12.48,-0.2,0,0.18 3EJG,ASP_20,4.33,0,0.23,0.3 2D59,GLU_61,4.73,0.17,0,0.05 2FZ4,GLU_151,4.77,0.12,0,0.16 1SUU,LYS_534,10.38,-0.27,0,0.16 1WXQ,TYR_62,12.47,0,0.24,2.23 1LTU,ARG_177,11.25,-1.22,0,-0.03 20DJ.CYS 61.11.74.-0.02.0.09.2.68 1EYH,ASP_45,3.56,-0.46,-0.44,0.66 3GV0,GLU_266,4,0.81,-0.85,-0.47 2FG1,LYS_115,10.42,-0.08,0,0 2P65,GLU_175,3.92,0.42,-0.82,-0.17 1AD6.ASP 479.3.73.-0.6.-0.13.0.66 2CN1,LYS_190,10.71,-0.16,0,0.37 1R3D,LYS_195,10.05,-0.46,0,0.01 2B6P,CYS_14,9.39,-0.05,-0.06,0.49 1YOY.GLU 150.4.46.0.18.0.-0.22 2XMZ,ARG_127,12.58,-1.71,0.69,1.1 3A2Z,GLU_51,4.08,0.6,-0.77,-0.26 3ANJ,ASP_87,2.3,-1.67,-0.42,0.59 1NJ4,GLU 264,4.21,0.79,-0.62,-0.46 2OJQ,ARG_489,13.62,-1.01,1.17,0.97 3DHN,ASP_69,2.47,-1.49,-0.29,0.44 1DZF,TYR_211,10.94,0,0.11,0.83 1GPP,GLU_160,4.72,1.15,-0.79,-0.13 2H2W,LYS 270,10.6,-0.16,0,0.25 3OBS, ASP 19, 3, 74, 0, -0, 29, 0, 23 3JZ9,HIS_488,6.06,-0.82,0.34,0.04 2F9F,CYS_160,12.16,0,0.12,3.04 3U0V,LYS 115,10,72,-0,93,0,52,0.63 1R3D, ASP_154, 3.21, -0.59, -0.36, 0.36 1SFE,GLU_175,4.67,0.28,-0.01,-0.1 4F8A,HIS 610,7.2,-0.33,0.77,0.26 3O48,GLU_121,4.3,0.45,-0.4,-0.26 1BKB,ARG 31,12.48,-0.5,0,0.48 1ZYL.TYR 277,11.53,0.0.05,1.48 3MIX,ASP_342,3.33,-0.42,-0.61,0.57 3P51,LYS_35,10.25,-0.32,0,0.07 3Q1C,GLU_125,4.78,0.14,0,0.14 3A0X,ASP_641,3.92,0,-0.28,0.4 1DZF,ASP_48,1.34,-2.76,-0.38,0.68 3ERF,LYS_214,10.03,-0.28,0,-0.19 1P4X,LYS_215,10.6,-0.15,0,0.25 3LPZ,LYS_262,10.31,-0.19,0,0 3CO1,ASP 26,3,28,-2,23,-0,11,1.81 1C44,LYS_19,11.34,-0.79,0.97,0.66 2D7J,ASP_110,3.68,-0.37,-0.34,0.59 2CXC,GLU_10,4.33,0.36,-0.6,0.07 3LJC,GLU_115,4.45,0.35,0,-0.4 1P2F,TYR_56,10.47,0,0.25,0.21 2QRX,LYS_127,10.44,-0.19,0,0.13 2QK0,LYS_96,10.33,-0.13,0,-0.05 1RKA, ASP 83, 2.61, -1.62, -0.29, 0.72 3P28,ASP 142,3,91,0,0,0,11 4ACJ,GLU_648,4.52,0.22,0,-0.19 4FD6,ARG_162,12.09,-0.51,0,0.1 3EJC,ASP_41,3.88,0,0,0.08 3BJV,GLU_146,3.83,0.32,-0.55,-0.44 3UAH,LYS 167,10.56,-0.1,0,0.16 2IN0,GLU_427,3.58,0.29,-0.74,-0.47 1Z3X,HIS_230,5.43,-1.72,0.63,0.02 3NR5,TYR 119,10.45,-0.56,-0.36,1.36 2QDJ,ASP_68,3.71,-0.01,-0.28,0.2 3G9T,LYS 250,10,76,-0.65,0.51,0.4 3B4D,TYR_175,9.87,-0.34,-0.42,0.63 1Z3X,TYR_38,10.75,-0.04,0.08,0.71 1AKO,GLU_86,4.73,0.78,-0.1,-0.44 3KB5.GLU 290.4.64.0.11.0.0.03 2XWS.CYS 104.10.55.-0.01.0.05.1.51 3I47,GLU_79,4.33,0.23,-0.4,0 3KV0,ASP_175,3.67,-0.37,0,0.24 3DZ1,LYS_280,10.41,-0.09,0,0 3KEY,LYS_453,10.12,-0.32,0,-0.05 3UAH,ASP_283,3.92,0,-0.17,0.29 10IS.ARG 360.12.27,-0.28.0.0.06 2FL7,ARG_210,12.47,-0.38,0,0.35 1D2K.HIS 200.6.69.-0.52.0.39.0.32 200K,TYR 119,12,22,0.66,0.74,0.82 3V55,ASP_403,4.31,0,-0.54,1.06 3HYQ,ARG_85,13.44,-0.3,0.82,0.42 1YOY,HIS_42,6.65,-2.23,0.85,1.54 1UOH,CYS 180,11.61,-0.04,0,2.65 3L7N,GLU_181,5.57,4.6,-1.51,-2.03 3LD1.LYS 55.10.31.-0.16.0.-0.03 1YTD,ARG_380,11.56,-1.78,0,0.83 2FM9,CYS_225,10.44,0,0.12,1.31 3FK5,TYR 144,10,51,0,-0,15,0,65 4DND,GLU_62,4.98,0.32,0,0.16 2EDM,GLU_200,4.58,0.08,0,0 1DOV,ASP_102,3.66,-0.1,-0.3,0.26 2PWQ,LYS 138,10.38,-0.1,0,-0.02 2Q98,GLU_140,3.52,0.44,-0.77,-0.66 3K9I,TYR_147,10.07,0,0,0.07 1XIP,LYS_179,10.29,-0.21,0,0 3GV0,HIS 202,5.04,-1.54,0,0.07 3DHN.GLU 87.4.5.0.0.0 1L2F,LYS_263,10.34,-0.16,0,-0.01 3FWU,TYR_23,12.52,-0.85,0.19,3.18 2EJB,LYS_3,10.29,-0.21,0,-5.20E-18 3FHF,ARG 170,12.47,-0.24,0,0.2 2YT4,GLU_593,5.06,0.41,-0.18,0.32 3U0V,ASP_79,2.39,-2.23,-0.57,1.4 3AU3,LYS_398,10.4,-0.05,0,-0.05 2XMZ.GLU 264,5.23,0.62,0.0.12 1Y0K.ARG 149,13.1,-0.28,0.28,0.61 2APL,HIS_129,6.49,-0.22,0,0.22 3C2E,LYS_89,10.54,-0.37,0,0.41 3C5V,TYR_143,11.89,0,-0.21,2.1 2JHY,GLU 95,3.75,0.32,-0.85,-0.22 2B0A.CYS 84,11.41,-0.01,-0.06,2.48 3ZXY,ARG_94,13.03,-0.18,0.38,0.32 1J33,GLU_153,3.49,0.48,-1.17,-0.32 2EFK.GLU 236,4.84,0.34,0,-0.01 3IOC,HIS 148,4,93,-1.63,0,0.07 3N2T,ARG_117,13.17,-0.34,0.49,0.52 3CIV,LYS_139,11.25,-0.25,0.62,0.39 1NJ4,GLU_185,4.31,1.65,-1.17,-0.68 1X7F,GLU_90,4.5,0.16,0,-0.16 3LJI.GLU 57.4.86.1.44.-0.85.-0.22 3C2E,GLU_218,4.71,0.19,-0.03,0.04 3FRR,LYS_90,10.39,-0.11,0,0 1O5J,HIS_-1,6.6,-0.42,0.5,0.03 3SMD.TYR 44,10.11.0.0.0.11 1NWA,ASP_82,4.08,0,-0.21,0.49 3I0C,GLU_303,6.04,3.08,-1.69,0.17 2B0A,TYR_69,10.44,0,0.07,0.37 2G5X,LYS_132,10.39,-0.22,0,0.11 2ZCO,GLU_65,3.9,0.26,-0.84,-0.01 3T5B,LYS_395,10.64,-0.27,0,0.41 2W0G,HIS_161,5.96,-0.55,0,0.01 1W7B,TYR_333,10.24,-0.09,0,0.33

3ONT.ASP 51,3.92,-0.05,0.04,0.13 3Q9P,TYR 142,10.44,-0.1,-0.38,0.92 3B21,LYS_165,10.29,-0.51,0,0.31 2P0Y.ASP 243,3.6,-0.88,-0.34,1.02 2Q07,HIS_494,5.42,-1.28,0.02,0.19 3HKX ARG 158 11 74 -0 86 0.0 1 1L2H,LYS 63,11.5,-0.3,0.6,0.7 3M9A,ASP_21,4.1,-0.18,0.08,0.39 2RJD,TYR_266,10.9,-0.72,0,1.63 2XJ4,ARG_99,13.21,-0.29,0.67,0.34 1YLN,LYS 53,10.25,-0.25,0,0 2G9D,ARG 149,11.56,-1.33,0,0.39 3VJ8,TYR_346,10.17,0,-0.1,0.27 1WXF,ASP_28,3.41,-0.35,-0.44,0.39 3ELI,GLU 34,3.46,0.52,-0.96,-0.61 1UAJ,ASP 50,3.89,-0.33,-0.08,0.49 2A6B,ASP_124,2.94,-0.85,-0.38,0.38 10IS,ARG_260,12.57,-0.13,0,0.19 3LH5,ARG_639,12.25,-0.3,0,0.05 4DNU,ASP 65,3.37,-0.84,-0.09,0.5 2YWX,LYS 51,10.32,-0.12,0,-0.06 3ASA,HIS_6,6.15,-0.35,0,0 4GA2,CYS_50,10.09,0,-0.09,1.18 3GG6.GLU 134.4.73.0.28.0.-0.05 3FTT.TYR 110.10.63.0.0.08.0.56 3HYQ,TYR_139,10.34,0,0.05,0.29 2AZP,CYS_65,11.4,-0.08,-0.33,2.82 2CL3,GLU_115,2.56,0.71,-2.15,-0.49 4EUG,LYS 42,10.99,-0.42,0.84,0.06 3TIR,TYR_66,11.04,0,-0.14,1.18 1L3K,HIS_173,5.79,-0.52,0,-0.19 3CCY,GLU_118,4.53,0.36,0,-0.33 2YX0.GLU 255,3.8,0.47,-0.67,-0.5 3Q2C,LYS 56,10.51,-0.16,0,0.17 4FH3,LYS_77,10.32,-0.28,0,0.1 4AF2,ASP_142,3,-0.85,-0.71,0.76 1RZ2,LYS_153,10.15,-0.35,0,0 2H2Z,GLU 47,4.66,0.08,0,0.08 3HKX,ARG 87,13,1,-0,73,0,72,0,61 3A4C,ASP_530,4.09,0,0,0.29 3RE9,HIS_106,6,-0.37,0,-0.13 2IXM.CYS 299,12.24,-0.94,0.54,3.64 2012.LYS 192,10.5,-0.27,0,0.26 2PP6,ASP_13,3.31,-0.48,-0.46,0.45 3COU,TYR_28,10.85,0,-0.11,0.96 1KCM,GLU_106,4.43,0.19,0,-0.27 4HDE,ASP_36,2.79,-0.85,-0.38,0.22 2B02.HIS 378.6.37.-0.21.0.0.09 4EKU,GLU_244,4.86,0.85,-0.1,-0.4 205X.GLU 742.4.0.3.-0.79.0 2EJX,ASP_89,2.17,-1.7,-0.42,0.49 1FHL,TYR 238,11.89,-0.02,0.22,1.69 2P65.LYS 170.10.32.-0.44.0.0.26 3TIR,LYS_173,10.02,-0.26,0,-0.22 2NRR,GLU_440,4.75,0.27,0,-0.02 3V46,TYR_326,12.33,-0.83,0.06,3.1 3JRT,ASP 140,4,37,0,-0.02,0.6 1G5Z,ASP_70,4.26,-0.02,-0.42,0.89 1RWZ.ASP 170.4.08.-0.09.0.0.37 2CBE,LYS 154,9,91,-0.68,0,0.08 1LN4,LYS 12,10.33,-0.17,0,0 2JKF.TYR 144,10.72,-0.84,-0.13,1.69 2Z0M,LYS_313,10.47,-0.19,0,0.16 1X04,ASP_85,3.48,-0.52,0,0.19 3COU,HIS_24,4.24,-2.36,0.27,-0.17 3L3P,ARG_516,12.32,-0.28,0,0.11 3GFP,ASP_302,4.08,0,0.05,0.23 2EA9,GLU_51,4.06,0.47,-0.88,-0.04 3DZ1,HIS_246,5.14,-1.59,0,0.22

2CXA,ARG_122,12.06,-0.61,0,0.17 1PZC,GLU 19,4.19,0.48,-0.69,-0.09 2WB3,ASP_363,3.23,-0.85,-0.04,0.32 1UOH,HIS_111,4.76,-2.3,0.69,-0.14 2W2S,ASP_80,2.32,-1.27,-1.09,0.89 3I0C,ARG 110,12,15,-0,3,0,-0.05 3GV0.GLU 77.4.54.0.46.-0.43.0.02 2H14,GLU_80,4.67,0.31,0,-0.14 1UW7,TYR_87,10.35,0,-0.12,0.47 3GE9,ASP_237,3.06,-0.88,-0.24,0.38 2BLL/ARG 400,12.86,-0.24,0.32,0.28 2BV9.HIS 257.4.44.-2.66.0.84.-0.24 4D8L,ARG_52,12.44,-0.44,0,0.37 1UAJ,LYS 47,10,43,-0,14,0,0.07 3GYW,TYR_191,10.36,0,0.03,0.33 4DIU,GLU 66,4.61,0.11,0,0 1TD6.HIS 18.5.34,-1.54.0.7,-0.33 1HF8,GLU_133,5.54,1.2,0,-0.16 2F4Q,GLU_11,5.38,0.79,0,0.09 3LPZ.LYS 40.10.36.-0.09.0.-0.05 1GPP.GLU 137,3.9.0.24,-0.8,-0.05 3UPD,HIS_-19,6.14,-1.38,0.85,0.17 1X7F,ARG_304,12.57,-0.87,0.53,0.42 3CO1.ASP 58.4.07.-0.71.0.04.0.94 3FS3.LYS 137.10.5.-0.06.0.0.06 20EW,LYS_229,10.3,-0.51,0,0.31 3HUE,GLU_245,4.49,0.31,0,-0.31 2IRM,GLU_305,4.65,0.35,0,-0.21 1LZL,TYR_226,13.62,0.85,0.68,2.1 1DZF,TYR_28,11.24,-0.43,-0.39,2.06 3A0X,LYS_671,11.49,-0.28,0.8,0.47 3GYW,LYS 44,10,39,-0,11,0,0 3LQE,TYR_295,11.86,-0.15,0.15,1.86 3U2R,HIS 137,6.34,-0.26,0,0.11 1WLY,LYS 108,9,28,-1,49,0,0,27 3F7M,ARG_301,12.46,-0.07,0,0.03 1ZCU,ARG_179,12.47,-0.2,0,0.17 3V46,ARG_286,12.72,-0.12,0,0.33 2CI3,GLU 136,4.31,1.53,-1.61,-0.1 3GS9,TYR_249,11.06,-0.78,-0.24,2.07 3CX2,ASP 248,3.02,-1.31,-0.3,0.82 3M3P,GLU_15,6.04,2.02,0,-0.49 2EJX,LYS 88,11.33,-0.56,0.85,0.54 2FZ4,ASP 81,3.77,0,-0.42,0.39 1SQW,TYR_134,12.05,0,0.17,1.88 3V3T,TYR_116,10.32,0,-0.04,0.35 1YTQ,ARG_188,11.94,-0.63,0,0.07 2YWJ,TYR_159,11.15,0,-0.03,1.18 1SUU,LYS_515,10.46,-0.25,0,0.21 1C44,GLU_47,4.03,0.34,-0.44,-0.37 2ZCX,HIS_56,6.4,-0.1,0,0 2YX0,GLU_34,4.85,1.73,-0.79,-0.59 2EFK,ARG 47,13.22,-0.5,0.73,0.49 1WXQ,ASP_229,2.84,-0.74,-0.51,0.29 1WNH,HIS_53,5.85,-0.86,0.02,0.18 1NWA,HIS_141,5.44,-1.5,0,0.44 1SI7,GLU 270,4.98,0.36,0,0.12 1P6F.TYR 100.10.17.0.0.01.0.15 2GS5,GLU_30,4.78,0.08,0,0.19 3M7D,ARG_205,13.14,-0.55,0.68,0.52 1H4U,GLU_398,4.81,0.27,0,0.05 1GOE,ARG 245,12,15,-0,3,0,-0,05 2ZQ5,GLU_274,4.56,0.26,0,-0.2 2BLL,TYR_419,11.15,-0.02,-0.04,1.21 2CYG,ARG_299,12.35,-1.05,0.5,0.4 2A1V,LYS_87,10.06,-0.43,0,-0.02 1KCM.GLU 130.4.62.0.12.0.0 3JZN,CYS_361,11.18,0,-0.74,2.91 2Z14,LYS_13,10.77,-0.18,0,0.44

200P.CYS 148.11.17.0.0.1.2.07 3LOD.GLU 74,5.06,1.96,-0.74,-0.66 1NIJ,ASP_92,3.82,0,-0.55,0.57 3CXS,GLU_174,4.55,0.05,0,0 3IV4,HIS 93,7.5,-0.4,0.85,0.55 1XEU.GLU 262.4.07.0.42.-0.85.0 3BZT,ASP_328,3.99,0,0,0.19 3JRT,HIS_82,6.05,-0.44,0,-0.01 3TIR,GLU_41,3.91,0.54,-0.8,-0.33 1YM5.LYS 151.10.25.-0.25.0.0 1G8P.ARG 246.11.9.-1.0.04.0.36 2WZ9,GLU_15,4.39,0.97,-0.81,-0.27 1A8Q,ASP_197,2.23,-1.69,-0.8,0.92 1NAF,ARG_265,12.36,-0.23,0,0.09 30A7.GLU 6.4.57.0.07.0.0 1XAW,LYS_506,10.66,-0.44,0,0.6 1JSX,HIS_32,6.14,-0.2,0,-0.16 2XHC,LYS_201,10.51,-0.19,0,0.2 2BT8,ARG_205,13.41,-0.31,0.76,0.45 106D,LYS 31,10,27,-0.32,0,0.08 3F5D,CYS_190,9.63,-0.01,0,0.64 3LH5,GLU_802,4.51,0.33,0,-0.33 2R51,TYR_37,11.5,0.08,0.54,0.88 1R3F,GLU 169,3.12,0.71,-1.45,-0.64 3GOZ,GLU_271,3.84,0.28,-0.78,-0.16 2EFK,LYS_104,10.48,-0.09,0,0.07 3N2T,ASP_251,4.35,0,-0.15,0.71 1G5Z,GLU 118,4.76,0.25,0,0.01 1GPP,GLU_19,3.1,0.71,-1.86,-0.26 1H09,TYR_314,10.4,0,0.01,0.39 3PP8,ARG_113,13.76,-1.01,0.81,1.45 3N2T,ARG_285,12.43,-0.22,0,0.15 2DFL,ASP_185,3.9,-0.19,0.04,0.25 1UXO,LYS 3,10.22,-0.31,0.0.03 3IBT, ARG_35, 13.04, -1.11, 0.51, 1.15 2ATR,TYR_19,13.18,0.49,0.29,2.41 2JKF,LYS_148,10.74,-0.24,0,0.47 2G5X,TYR_176,10.6,0,0.18,0.42 3EVN,ASP_57,3.85,-0.14,-0.16,0.35 3PU6.GLU 141.4.48.0.39.-0.11.-0.29 2D7U,CYS_103,13.14,-0.18,0.33,3.99 1DTO,GLU 100,4.66,0.16,0,0 3LOD,ASP_38,3.85,0,-0.2,0.25 1SFE,ASP_44,3.5,-0.59,-0.21,0.5 1IAP,GLU_187,4.31,0.31,0,-0.51 3H5T,ARG_43,12.41,-0.14,0,0.05 3D9H,LYS_197,10.49,-0.42,0,0.41 3M66,ASP_148,2.72,-1.07,-0.16,0.15 3RFY,HIS_281,6.67,-0.25,0.15,0.27 3I0C,TYR_264,13.93,0,1.08,2.84 2J8A,LYS 274,10.33,-0.17,0,0 3CS1.LYS 158.10.34.-0.21.0.0.05 1NJ4,TYR_136,10.86,0,0.03,0.83 2P65,GLU_6,4.5,0,0,0 1DVO,GLU_152,3.26,0.58,-1.73,-0.1 2X4G,ARG_334,12.43,-0.32,0,0.24 2IF4,GLU_91,4.58,0.19,0,-0.12 1Q8B,ASP_27,2.92,-1.15,-0.15,0.42 30DJ,GLU_44,4.72,0.07,0,0.15 1KCM,ARG 227,11.52,-1.77,0.03,0.77 4ANN,ASP 78,3,13,-0,79,-0,03,0,15 1P6F,GLU_42,3.94,0.34,-0.84,-0.06 2EYI,GLU_56,3.92,0.34,-0.66,-0.27 3E0H,GLU_110,5.02,0.25,0,0.26 1YTQ,TYR_153,9.93,-0.78,-0.36,1.08 1TR9,GLU_231,4.77,0.28,0,0 1U7U,ARG_281,12.19,-0.48,0,0.17 2D7U,ARG_303,12.64,-0.09,0,0.24 2JEO,LYS 203,10.89,-0.43,0.36,0.47

1RAJ,GLU_428,4.61,0.3,0,-0.21 1P6F.ASP 126.3.58.-0.48.-0.01.0.26 3P28,ASP_107,2.75,-1.02,-0.59,0.55 4E6S,GLU_55,2.24,0.98,-2.43,-0.8 1RI6.HIS 163.6.78.-0.35.0.0.63 1YTO.GLU 112.3.94.0.38.-0.81.-0.13 3E7P,TYR_248,13.48,0,0.42,3.07 1XWM.TYR 189,10.27.0.-0.39.0.66 2YT4,LYS_561,10.28,-0.22,0,0 1IAP,HIS_65,5.82,-1.58,0.85,0.06 3IO0,ASP_149,2.68,-1.29,-0.51,0.69 3DB9,ASP_116,4.06,0,0.13,0.13 3TMO,TYR_301,10.61,0,0.05,0.56 2FGG,GLU_19,5.46,0.29,0.19,0.47 30A7.LYS 456.10.45.-0.05.0.0 3BWT,TYR_856,11.09,-0.34,0.24,1.19 3B4D,ARG_240,12.32,-0.37,0,0.19 1SUU,LYS_644,10.4,-0.1,0,0 3GG6,ASP_136,1.95,-1.96,-0.41,0.52 3FWU,LYS 86,10.49,-0.25,0,0.24 3UC9,GLU_122,4.44,0.12,0,-0.19 1WYC,TYR_170,12.08,0.37,0.26,1.46 3B7H,GLU_75,4.64,0.14,0,0 1AKO, ARG 89, 12.39, -0.57, 0, 0.45 1XAW.CYS 500.9.9.0.-0.11.1.01 3GA2,ARG_214,11.46,-1.13,0,0.09 1V43,TYR_280,11.64,0.65,0.51,0.48 2D7U,ARG_256,12.19,-0.22,0,-0.09 2RGY,CYS 258,9.42,-0.11,-0.15,0.68 2QDJ,LYS_289,10.63,-0.21,0,0.35 1FKM,LYS_459,10.59,-0.16,0,0.25 1TWU,LYS_3,10.85,-0.59,0.31,0.63 1ZP2,GLU 122,4.48,1.16,-0.68,-0.48 3RVC,ASP_125,3.92,0,-0.13,0.24 1ZBM,HIS_7,3.55,-2.95,0,0 3CIV,GLU_110,4.48,0.11,0,-0.13 3LJI,ARG_179,12.23,-0.63,0,0.36 2Z84,GLU 163,3.65,0.72,-1.44,-0.13 3MEW,GLU_225,4.37,0.4,-0.77,0.24 3LOD,GLU_112,5.35,1.38,-0.7,0.17 3F6M,GLU_120,4.6,0.21,0,-0.12 3GG6,ARG 170,13.63,-1.08,1.57,0.64 3CSR.TYR 8,10.54,0,0,0.54 2Q99,ASP_83,3.82,0,-0.61,0.64 2QK1,ASP_401,2.54,-1.16,-0.96,0.87 3HUE,ASP_32,1.92,-2.06,-0.39,0.57 1VJG,ASP 155,3.99,0,0.03,0.17 2OSA,ASP_358,3.97,0,0,0.17 2D7U,ARG_67,12.77,-1,0.66,0.61 1YG2,TYR_19,10,0,0,0 2RIK, HIS 207, 6, 98, -0, 68, 0, 85, 0, 31 4EKU.GLU 126.3.6.0.45.-0.65.-0.71 2YT4,LYS_650,10.33,-0.2,0,0.03 3TMO.HIS 201.6.01.-0.25.0.-0.24 1MML,LYS_75,10.66,-0.41,0.03,0.55 3UX2,LYS_36,11.08,-0.44,0.27,0.74 300P,ASP 70,3.72,-0.13,-0.3,0.35 2IQT,GLU_223,2.76,0.38,-1.62,-0.5 1ZYL, ARG_273, 13.02, -1.77, 0.62, 1.67 3RJX,GLU_334,3.64,1.19,-1.82,-0.23 1YW5,HIS 171,2.23,-3.05,0,-1.21 1RKA,GLU_71,4.52,0.15,0,-0.13 1YTD,LYS_360,11.31,-0.44,0.28,0.97 3CZC,ASP_65,3.92,0,-0.05,0.17 1LTU,GLU_68,4.64,0.13,0,0.01 3BQE,ASP_339,3.67,-0.53,-0.13,0.52 2GZR,GLU_173,4.69,2.42,-1.29,-0.93 2QDJ,ASP_139,3.76,0,-0.18,0.14 1ZBS,ARG_188,12.39,-0.24,0,0.12

2AH5.GLU 121.4.58.0.12.0.-0.05 2NRK,GLU 29,4.14,0.16,-0.39,-0.13 4EZB,ARG_27,12.4,-0.1,0,0 3BPV,ARG_86,12.4,-0.16,0,0.06 3GS3,GLU_149,4.89,0.19,0,0.2 3FS3,TYR 151,10.22,-0.61,-0.07,0.9 2GS5,ARG 55,12,52,-0.34,0,0.35 2X5Y,LYS_726,10.41,-0.26,0,0.17 3HKX,HIS_279,5.92,-0.38,0,-0.2 2RIK,ARG_192,12.42,-0.24,0,0.16 1IAP,ARG 227,12.27,-0.32,0,0.08 2RIS,GLU_30,4.64,0.11,0,0.03 3CO1,ASP_88,3.31,-1.03,-0.03,0.56 1BN6,HIS_95,3.1,-3.16,0,-0.24 3M3P,HIS 158,6,42,-0,59,0,0,51 3LJI,HIS 19.6.31,-0.15.0,-0.04 3Q1C,GLU_305,4.33,0.13,0,-0.3 3PP8,GLU_176,3.92,0.28,-0.52,-0.34 3M66,LYS_412,10.64,-0.14,0,0.28 1X91,LYS 19,10.4,-0.1,0,0 2JHY,LYS 138,10.08,-0.68,0.0.26 2Z84,GLU_83,3.63,0.47,-1.27,-0.08 4H89,ARG_104,12.21,-0.34,0,0.05 3FS3.ASP 189.4.06.-0.05.0.0.31 2FXT.TYR 325.12.49.-0.01.0.46.2.04 3PZ9,HIS_278,0.87,-4.11,0,-1.52 3RJX,ARG_211,13.16,-0.23,0.24,0.65 2NRK,HIS_101,5.52,-2.67,0.84,0.85 1NAF,GLU_199,4.55,0.25,0,-0.2 3M7D,GLU_255,3.51,0.69,-0.85,-0.83 2G5X,ASP_90,3.25,-1.99,0.05,1.4 1G5Z,LYS_79,10.34,-0.29,0,0.12 3GYW,ASP_55,3.76,0,-0.39,0.35 3MTT,GLU 459,4.65,0.2,0,-0.04 3ANJ,ASP_297,3.52,-0.84,-0.1,0.66 4H89,ASP_41,3.02,-0.85,-0.28,0.35 2D59,GLU_95,3.67,0.3,-0.72,-0.41 1NAR,ASP_118,2.51,-1.1,-0.75,0.56 1PDB.ASP 95.2.86.-1.17.-0.33.0.58 3FHF,TYR_140,11.9,0,0.49,1.42 2XMZ,GLU_12,4.45,0.1,0,-0.15 1YG2.CYS 103.9.69.0.-0.02.0.71 1UCH,ARG 136,12.53,-0.08,0,0.11 4DVD,ARG_179,12.26,-0.24,0,0 2B2H,TYR_180,10.55,0,0.28,0.27 2Q99,ARG_192,12.39,-0.08,0,-0.02 1TR9,LYS 54,10.26,-0.21,0,-0.03 1PDB,GLU_180,3.87,1.57,-1.46,-0.73 1AM2,ASP_154,3.97,0,-0.01,0.18 2CL3,TYR_160,10.3,0,0,0.3 1XIP,GLU_125,4.62,0.13,0,-0.01 2E3S,GLU 372,4.59,0.35,0,-0.25 10LR.GLU 53,4,76,0,27,0,-0.01 2OJQ,ARG_448,12.5,-0.19,0,0.19 2R0S,LYS_189,11.39,-0.39,0.85,0.43 2HRZ,LYS_274,11.16,-0.24,0.46,0.44 1H4U,GLU 587,4.08,0.79,-1.2,0 3IRA,GLU_28,4.42,0.1,0,-0.18 1PVT.ASP 74,3.53,-0.52,-0.23,0.47 2G2D,ASP_105,4.04,0,0,0.24 2F9F,ASP 97,3.17,-1.04,-0.52,0.94 3048,ASP 122,4.03,0,-0,13,0,35 2QOP,LYS_189,10.69,-0.1,0,0.29 105J,GLU_12,4.04,0.32,-0.79,0.01 1ZBS,TYR_139,10.71,0,0,0.71 3KB5,GLU_312,3.45,0.91,-1.52,-0.44 1XTZ,GLU 19,2.37,0.34,-1.72,-0.74 3L3PLYS 389,10.68,-0.25,0.0.43 3G9G,GLU_132,4.77,0.44,-0.07,-0.11

2VGM,GLU_79,4.13,0.31,-0.54,-0.15 2R4Q,LYS_244,9.84,-0.79,0,0.14 1NU/HIS 29,5.96,-1.19,0.67,-0.03 3P2F,ASP_192,3.73,-0.42,-0.04,0.39 3EAZ,ARG_107,11.87,-0.94,0,0.31 3M70,LYS 250,10.81,-0.15,0.0.47 2V1L.ARG 46.12.45.-0.38.0.0.34 3BA1,LYS_289,12.54,-0.37,1.55,0.85 2EHG,ARG_30,12.52,-0.26,0.05,0.24 2EFK,GLU_39,3.02,1.42,-1.96,-0.94 3A7L,ASP_43,4.12,0,0,0.32 2FZ4,GLU_91,4.59,0.15,0,-0.06 2P1W,TYR_209,11.3,0,0.21,1.1 100X,TYR_189,10.35,0,-0.09,0.44 1VJG,ARG_138,12.3,-0.21,0,-2.78E-17 4D8L,LYS 139,10.64,-0.13,0,0.27 1HUF,GLU_71,4.4,0.27,-0.15,-0.23 2CXA,ASP_62,2.61,-1.23,-0.64,0.69 1IAP,TYR_225,12.66,0,0.44,2.22 1J74,ARG 61,12.62,-0.63,0.17,0.58 2DVK,ASP_126,2.99,-0.8,-0.45,0.44 1ES5,ARG_114,13.55,-0.5,0.58,0.97 1H09,LYS_222,10.81,-0.77,0.85,0.23 2GEN.GLU 20.3.46.0.26.-0.64.-0.66 3LE4,ASP 344,3.86,0,-0.07,0.13 208P,GLU_51,3.74,0.22,-0.85,-0.14 2I6I,LYS_83,10.34,-0.15,0,-0.01 1IDK,ARG_41,13.63,-0.48,0.63,0.98 1YB2,ASP_19,3.6,-0.53,-0.03,0.37 1XKR,TYR_184,11.18,0,0.35,0.83 3IVF,LYS_357,10.65,-0.16,0,0.31 2FG1.GLU 2.4.56.0.11.0.-0.05 2G2D,CYS_104,11.11,-0.02,0.4,1.72 3U4K,LYS_53,10.28,-0.22,0,0 2G7O,ASP_125,3.34,-0.58,0,0.12 2CXA,ARG_215,12.15,-0.35,0,0 2Q13,GLU_245,4.63,0.13,0,0 3BQE,GLU_334,3.21,1.24,-2.25,-0.28 3A0X,ARG 650,12.51,-0.31,0,0.32 20KT,GLU_81,4.15,0.18,-0.16,-0.38 2IXM,ASP_85,3.27,-1.02,-0.55,1.06 2D7U,LYS_50,10.81,-0.49,0.38,0.43 2V1L,GLU 53,4.57,0.07,0,0 2ZTY,ARG 134,13,43,-0,78,0.6,1.1 1GPP,LYS_72,10.4,-0.16,0,0.07 3LD1,LYS_85,10.41,-0.17,0,0.09 3CS1,GLU_188,4.18,0.83,-0.59,-0.57 20BI,LYS 80,10.44,-0.06,0,0 1YLN,GLU_101,4.66,0.27,0,-0.11 3GV0,GLU_161,4.4,0.25,-0.45,0.1 2FPN,ARG_48,12.44,-0.1,0,0.03 3UPD,HIS_322,4.52,-2.49,0.85,-0.33 1TXJ,LYS 151,10,43,-0,28,0,0,22 1YTQ,ARG_80,13.13,-0.25,0.36,0.52 1Z3X,GLU_43,4.11,0.62,-0.59,-0.42 1OXZ,LYS_176,10.28,-0.22,0,0 1XFK,HIS_82,6.13,-0.28,0,-0.09 2YWK.CYS 42.9.65,-0.14.0.02.0.78 1P4X,ASP_179,4.02,0,-0.18,0.4 1NRI,LYS_161,10.85,-0.35,0.42,0.28 1X8F,GLU_39,4.46,0.37,-0.32,-0.1 2YWK.TYR 27.10.2.0.-0.07.0.27 10GL,LYS_247,10.44,-0.1,0,0.03 2X4L,GLU_247,5.38,1.46,-0.84,0.25 2GEN,GLU_114,4.59,0.1,0,-0.02 4DBX,LYS_166,10.34,-0.09,0,-0.07 3ZXY,ASP 91,3.05,-2.05,0.02,1.29 3BZT,LYS_273,10.58,-0.13,0,0.21 3KV0,ASP_25,4.08,0,0,0.28

1TP6.ARG 6.12.57.-0.36.0.0.43 20KT,ARG_178,13.08,-0.25,0.34,0.49 3JV1,ASP_49,3.35,-0.69,0,0.23 1XDZ,ASP_126,3.08,-1.51,-0.49,1.28 3GE9,HIS 203,6,24,-0,26,0,-0.01 2F4O,LYS 302,11.32,-0.34,0.59,0.58 1AKO, ARG_90, 11.97, -2.65, 0.21, 1.91 1YOY.GLU 165.4.79.0.29.0.0 1UAJ,ARG_219,11.81,-0.28,0,-0.41 1YLN,GLU 37,4.65,0.21,0,-0.06 3R87.CYS 112.11.31.0.0.03.2.28 3QAV,GLU_141,4.74,1.85,-1.52,-0.08 2CN1,GLU_242,3.39,0.26,-0.83,-0.54 1NKD,GLU_35,4.66,0.11,0,0.04 3P51.HIS 96.5.83.-1.15.0.54.-0.07 4EUG,TYR_38,10.58,0,0,0.58 3T5B,CYS_68,12.75,-0.17,0.36,3.57 20PJ,TYR_251,11.03,0,0.14,0.9 1RL0,ARG_68,12.61,-0.93,0.52,0.52 2B2H.LYS 270,10.55,-0.07,0.0.12 1NIJ,HIS_23,6.82,-0.35,0,0.67 2EHG,LYS_139,10.38,-0.12,0,0 4FZR,GLU_11,4.69,0.4,-0.14,-0.07 2YWX.GLU 121,4.92,0.63,0,-0.2 3N0K,GLU_95,4.56,0.08,0,-0.02 3F6F,LYS_130,10.61,-0.23,0,0.34 2D0A,LYS_140,11.72,-0.31,0.76,0.76 1X6J,LYS 63,10.84,-0.19,0.24,0.28 2IF4,ARG_270,12.33,-1.19,0.26,0.76 2XHC,LYS_330,10.88,-0.4,0.5,0.27 1H4U,ARG_393,12.61,-0.22,0,0.33 1RL0,ASP_241,3.87,0,-0.26,0.33 2XJ4,GLU 103,3.37,0.37,-0.9,-0.6 1WLY,ARG 237,12,33,-0.09,0,-0.07 1ZBM,GLU_89,4.36,0.28,-0.1,-0.33 2H01,TYR_30,11.23,0.1,0.11,1.02 1IAP,GLU_202,4.89,0.22,0,0.16 1TP6,HIS_13,5.23,-2.92,0,1.65 2D8N,LYS_11,10.43,-0.27,0,0.21 3G9G,ASP_10,4.06,0,-0.08,0.34 1TXJ,TYR_149,13.63,0.81,0.6,2.23 2EHG.LYS 74,10.74,-0.32,0.01,0.54 3BA1.CYS 168.10.66.-0.46.0.07.2.05 1X1E,GLU_37,4.86,0.39,-0.01,-0.01 1VJG,ASP_199,3.75,-0.34,0,0.29 4FD6,LYS_129,10.13,-0.45,0,0.08 2P0Y,ASP_287,3.37,-0.49,-0.41,0.47 2IF4,LYS_242,10.28,-0.23,0,0.01 3NJM,TYR_26,11.97,-0.48,0.04,2.41 1XKR,GLU_178,4.84,0.14,0,0.2 2BCF,TYR_268,12.63,-0.26,-0.03,2.92 3JRT,ASP 136,3.39,-0.57,-0.08,0.25 3DB9,CYS_233,9.92,-0.36,-0.31,1.6 2l88,LYS_453,10.78,-0.21,0.16,0.34 1VSM,LYS_178,10.41,-0.06,0,-0.04 1XDZ,LYS 185,10.29,-0.24,0,0.03 3EVP,GLU_300,4.94,0.32,0,0.13 2W1R,LYS_91,10.54,-0.04,0,0.08 3EGN,ASP_435,3.34,-0.85,-0.34,0.73 2B6P,ARG 33,11.8,-0.7,0,0 1BGF.ASP 24.3.94.0.-0.07.0.21 2Q99,TYR_292,13.43,0.02,1.16,2.25 2BLL,HIS_592,6.29,-0.33,0.15,-0.04 3V75,HIS_27,5.68,-1.05,0.02,0.22 3LJC,LYS_56,10.5,-0.36,0,0.37 1EV8,GLU_237,4.5,0,0,0 2AD1,LYS_267,10.59,-0.14,0,0.23 3AUF,ARG_195,12.25,-0.31,0,0.05 2IRM,ASP_298,3.6,-0.41,0,0.21

1NIJ,ASP_75,4.13,0,-0.05,0.38 4E8B,LYS 98,11.3,-0.33,0.75,0.39 2CVB,HIS_32,6.26,-0.25,0.02,-0.01 3GEC,LYS_437,10.71,-0.27,0,0.48 1RWZ,ARG_190,13.18,-0.61,0.44,0.85 1XDZ.ARG 127.12.55.-0.37.0.0.42 3T5B,HIS_208,5.26,-1.24,0,0 3LJN,ARG_314,12.57,-0.21,0,0.28 2Q34,GLU_92,4.59,0.11,0,-0.02 2RJD,TYR_309,10.6,0,0.11,0.49 2ILR,ASP_354,3.28,-0.45,-0.42,0.35 1PSW,GLU_179,4.6,0.12,0,-0.02 1J8B.GLU 70.3.99.0.32.-0.82.0 4DBX,GLU_148,5.12,0.24,0,0.37 1059.ARG 337.10.21.-2.41.0.0.11 2EA9,ASP 39,3,77,-0.09,-0.36,0.41 3RKV,TYR_246,11.19,0,0.17,1.03 3RFY,LYS_170,10.46,-0.18,0,0.14 1X1E,GLU_66,4.49,0.23,0,-0.23 1XKR,ASP 159,4.13,0,0.02,0.31 2ZCX,ARG_89,13.28,-0.25,0.76,0.26 2RIS,GLU_40,4.99,1.26,-0.75,-0.02 3M70,GLU_256,4.05,0.33,-0.8,0.03 2FBQ,CYS 65,11.56,0,0.05,2.51 10GL.CYS 230,11,22,0,0,15,2,07 2Z84,HIS_16,4.75,-1.91,0,0.16 2QHT,GLU_2,4.4,0.25,-0.07,-0.27 3C2E,CYS_197,9.44,-0.2,-0.23,0.87 3IVF.LYS 234,11.02,-0.41,0.39,0.54 2CN1,LYS_105,10.46,-0.29,0,0.26 2EHG,TYR_99,10.46,0,-0.02,0.48 1WPA,TYR_443,10.16,-0.01,-0.2,0.38 1DTO,HIS 161,6.89,-0.61,0.45,0.55 2AHE, HIS 74, 6.25, -0.23, 0.16, -0.19 2PWQ,TYR_63,9.92,0,-0.26,0.17 1LTU,ASP_213,3.82,0,-0.3,0.33 1WYC,ARG_189,12.25,-0.56,0,0.32 1RHS,TYR 47,11.36,-0.51,0.04,1.83 2O4D,HIS_114,6.54,-0.5,0.36,0.18 3M3P,ASP_132,3.8,-0.23,0.01,0.22 1FQI,LYS_411,10.22,-0.31,0,0.02 2CIU.ARG 154,12.51,-0.26,0.0.27 2B0A.CYS 128.11.16.-0.16.0.06.2.27 2XWS,ASP_51,4.35,-0.7,0.21,1.05 4F3J,ARG_114,12.4,-0.05,0,-0.05 4AM1,TYR_323,10.22,0,-0.18,0.4 3B7H,ARG 54,12.28,-0.23,0,0.01 3P28,GLU_198,4.72,0.22,0,-0.01 4DVD,ARG_156,12.28,-0.34,0,0.11 3JZN,LYS_211,10.66,-0.18,0,0.34 2R51,ARG_24,12.11,-0.4,0,0.02 2B0A,GLU_152,4.25,0.5,-0.76,0.01 3H5T,GLU_214,4.4,0.17,0,-0.27 4EF5,LYS_224,9.99,-0.48,0,-0.03 3JSN,LYS_53,11.13,-0.72,0.79,0.57 1Y2Q,GLU_134,4.68,0.18,0,0 1P1L.GLU 14,3,49,1.05,-1.59,-0.47 3UX2,GLU_150,4.67,0.17,0,0 2Q07,ARG_279,11.84,-0.36,0,-0.3 2AXO,GLU 40,3.65,0.22,-0.7,-0.37 10TM,LYS 58,11.34,-0.43,0.85,0.41 2YX0,CYS_45,11.21,-0.26,-0.1,2.57 3G9B,TYR_37,10.56,0,0.03,0.54 2BLL,ASP_441,2.83,-1.36,0.01,0.38 2RIS,HIS_128,7.27,-0.49,0.85,0.41 1UAJ,ARG_234,12.48,-0.14,0,0.12 2PLQ,ARG_282,12.23,-0.41,0,0.14 3BPV,ASP 60,2.41,-1.83,0,0.44 1Q46,GLU_92,4.29,0.14,-0.47,0.11

2098,HIS 27.6.28,-0.3.0.0.08 2RGY,ARG 354,13.17,-0.8,0.69,0.77 3P28,ASP_54,2.89,-0.68,-0.52,0.29 1SJY,CYS 67.9.38.-0.13.-0.27.0.79 20BI,GLU_91,4.93,0.19,0,0.24 2YX0,LYS 49,10.18,-0.2,0,-0.11 3M7D,ARG 14,12.66,-0.09,0.03,0.22 3KT9,LYS_48,10.03,-0.27,0,-0.19 1PSW,GLU_50,5.18,1.6,-0.72,-0.2 4FZR,ARG_361,12.3,-0.21,0,0.01 3TMO,TYR 335,10.25,0,0.08,0.17 4ETX.ARG 336.14.-0.29.1.35.0.43 2F9F,GLU_25,4.36,0.59,-0.82,0.09 2R51,TYR_271,10.64,-0.03,-0.35,1.03 1T95.GLU 132.4.77.0.27.0.0.01 20ZO,GLU 79,4,39,0,37,0,-0,48 1PSW,ARG_180,11.91,-0.63,0,0.05 1YOY,LYS 21,10,41,-0.09,0,0 3K1H,LYS_56,10.21,-0.23,0,-0.06 2D0A,LYS 301,10.88,-0.19,0.23,0.34 3NJM,ASP 52,2,97,-2,3,0,1,48 2G5X,LYS_79,10.52,-0.04,0,0.06 2RIK,ARG_114,13.52,-0.35,0.85,0.53 2PLO.CYS 139,10.12,-0.03,0.21,0.94 2B61.ASP 78.4.31.0.0.24.0.28 3US6,ASP_24,4.04,-0.85,-0.15,1.23 4DBX,LYS_159,10.4,-0.09,0,-0.01 3BJV,GLU_140,3.94,0.39,-0.82,-0.14 2CI3,ARG_18,12.03,-1.54,0,1.07 1SJ8,LYS 685,9,94,-0,43,0,-0,12 3PM2,LYS_105,10.54,-0.08,0,0.13 2CXC,GLU_98,4.52,0.29,0,-0.27 1RWZ,ARG 73,12.85,-0.16,0,0.51 3GEC,LYS 387,10.37,-0.11,0,-0.01 3CBN,TYR_161,10.56,0,0.11,0.45 3CBN,ASP_110,3.02,-1.09,-0.12,0.43 1SUU,ARG_724,12.28,-1.25,0.28,0.75 2D59,HIS 137,4.8,-1.29,0,-0.42 1T95,LYS 60,10,74,-0.08,0,0.32 1T95,LYS_175,10.54,-0.21,0,0.25 1FKM,HIS_468,6.37,-0.51,0.03,0.34 1X7F.GLU 107.4.17.2.17.-2.6.0.09 3AU3.TYR 493.10.99.-0.84.0.44.1.4 1WLY,ARG_207,11.96,-0.83,0,0.28 3MIX,HIS_472,5.5,-0.86,0,-0.13 2H2W,GLU_111,5.77,1.96,-0.38,-0.3 2BDD,GLU_116,4.47,0.93,-0.85,-0.11 1NJ4,HIS_320,6.84,-0.4,0.53,0.21 1U7U,GLU_395,5.15,1.07,-0.01,-0.4 3C5V.ARG 113.13.79.-1.77.1.58.1.45 3CIV,ARG_208,12.92,-0.18,0.1,0.51 2D8N,CYS 29,9.76,-0.04,0.12,0.67 1J7G.LYS 22,10,42,-0.09,0,0.01 1H09,ARG_213,13.44,-0.66,1.12,0.48 3ZTA,GLU_59,4.73,0.68,-0.51,0.08 10I7,ASP_79,4.25,0,0.15,0.3 2Z14,ASP_28,3.98,0,0,0.18 2X4L,GLU_272,3.76,1.35,-1.66,-0.42 2XWS.GLU 77,4,74,0.32,0,-0.07 3AUF.GLU 173.3.89.0.45,-0.71,-0.35 3EAZ,ARG 166,12.31,-0.23,0,0.04 1BKB,LYS 100,12.38,-0.64,1.7,0.82 3ULX,HIS_21,6.33,-0.18,0,0 2FZ4,GLU_159,4.73,0.28,0,-0.05 3ASA,ARG_385,12.29,-0.34,0,0.13 3AU3,ARG_564,13.44,-0.36,0.57,0.73 1RZ2,ASP_176,3.88,-0.62,-0.18,0.87 30KO,ARG 595,12,46,-0.04,0,0 2ZQ5,ASP_204,3.03,-1.52,-0.02,0.78

2WZ9,LYS_29,10.24,-0.26,0,0 2CXC,CYS 29,12.76,0,0.24,3.53 3TRE,LYS_42,10.62,-0.17,0,0.29 3CXS,LYS_79,10.22,-0.31,0,0.03 3VHJ,LYS_160,9.9,-0.23,0,-0.37 2EJX,ARG 131,13.87,-0.41,1.25,0.52 1V43.GLU 184.5.36.1.3.0.-0.45 1I60,LYS_77,10.77,-0.1,0,0.37 2XHC,LYS_158,9.7,-0.73,0,-0.06 2HRZ,GLU_96,4.02,0.36,-0.84,0 2P1W,ARG 45,12,28,-0.25,0.0.03 1DCF,HIS 73,5.91,-0.97,0.51,-0.12 4E6S,ARG_68,12.52,-0.24,0,0.26 10I7,GLU_110,3.79,0.36,-0.8,-0.26 3BQW,LYS_221,11.09,-0.18,0.45,0.33 3GS9,ASP_85,4.19,0,0.11,0.28 1ZHV,ASP_103,3.97,-0.83,-0.05,1.05 3AUF,ARG_38,12.44,-0.29,0,0.23 20BI,ASP_112,3.99,0,0.04,0.15 3LE4,ASP_305,3.83,-0.08,-0.01,0.12 1H4U,HIS 575,5,46,-0,73,0,-0,31 3GYW,ASP_80,2.97,-0.56,-0.68,0.41 2FB6,GLU_60,5.37,0.58,0,0.29 2FXT,LYS_315,10.63,-0.73,0.08,0.78 2NRR,TYR 494,9.73,-0.23,-0.4,0.36 4DVD.LYS 136.10.37.-0.13.0.0 2D2S,CYS_694,12.09,-0.07,0.13,3.03 3FFM,ASP_53,3.38,-0.84,0,0.42 1YTQ,ASP_125,2.3,-1.56,-0.49,0.54 3EZ7,HIS_33,6.42,-0.27,0.13,0.05 1DOV, ARG_165, 13.21, -0.5, 0.67, 0.54 3R2E,TYR_53,10.31,0,0.05,0.26 2E0T,ARG_85,13.5,-0.28,0.84,0.44 3A2Z,TYR 26,10.73,0,-0.09,0.81 3ZTA,LYS 85,11.26,-0.37,0.32,0.8 3M70,TYR_257,12.52,0.39,0.52,1.62 1V43,ASP_257,3.61,-0.32,-0.03,0.16 3ASA,ASP_94,3.2,-0.83,-0.32,0.55 3U2R,GLU 33,4.36,0.2,0,-0.34 2YX0,TYR_315,10.54,0,-0.09,0.63 2P0L,GLU_34,4.14,1.63,-0.62,-1.36 3M7G,ARG_205,12.75,-0.27,0.08,0.44 3M66,ASP 183,3.26,-0.93,-0.03,0.41 3CO1.GLU 84.4.59.0.09.0.0 1J7G,ASP_43,3.25,-0.85,-0.24,0.55 3M7D,ASP_49,2.92,-1.68,0,0.81 1L3K,TYR_128,12.89,0.77,0.57,1.54 1V43,LYS 339,10.65,-0.45,0,0.6 2ZCO,ARG_84,13.28,-0.38,0.78,0.38 1RKA,GLU_105,4.9,0.15,0,0.25 10LR,TYR_9,10.67,0,0.02,0.65 2JEO,ASP_234,4.25,0,0.23,0.22 4F85.GLU 283.4.67.0.31.0.-0.14 3BQW,ARG_135,11.73,-1.02,0,0.25 3UPD,ARG_108,10.61,-1.91,0,0.02 4EF5,ARG_169,12.4,-0.25,0,0.16 2CE6,ASP_11,2.3,-1.57,-0.38,0.45 2BDD.HIS 23,6.96,-0.34,0.5,0.3 2D7J,TYR_12,10.19,-0.75,-0.08,1.02 3IPZ,LYS_83,10.8,-0.32,0.22,0.4 3UC9,TYR_160,10.13,0,0.09,0.04 1LPL.ASP 185.2.99.-1.59.-0.49.1.27 3EVZ,LYS_220,10.4,-0.15,0,0.06 3TIR,ARG_32,12.06,-0.41,0,-0.02 3QKY,TYR_237,11.18,0,0.24,0.94 2AZL,GLU_158,4.12,0.72,-0.85,-0.25 1SOH, ARG 87, 13, 21, -0, 76, 1, 01, 0, 47 3O48,LYS_11,11.18,-0.14,0.38,0.44 2G9D,HIS_289,6.32,-0.24,0.07,0

1RI6.HIS 299.6.03.-0.54.0.0.07 1R3D,ASP 263,4,1,0,0,21,0,09 2CIU,ASP_199,3.85,-0.1,-0.27,0.42 1Q5Z,GLU_637,4.61,0.11,0,0 1Z3X.GLU 72.4.5.0.38.-0.39.0 1JB3.CYS 37.11.41.-0.23.0.04.2.59 1AKO,CYS_240,9.54,0,0.04,0.49 3LPZ,LYS 108,10.32,-0.21,0.0.03 1AIL,ASP_12,3.57,-0.65,-0.35,0.77 3LJI,GLU_34,4.54,0.27,0,-0.23 1YR6.GLU 107.4.73.0.23.0.0 1QQE,GLU_52,4.8,0.5,0,-0.21 1W7B,LYS_281,10.48,-0.02,0,0 3RJZ,LYS 26,10.62,-0.2,0,0.32 1P4X.ARG 107.12.61.-0.96.0.42.0.64 1P4X,GLU_36,4.02,1.41,-1.4,-0.49 2CN1,GLU_256,3.9,0.4,-0.48,-0.51 2QV2,ARG_260,12.61,-0.16,0,0.27 2CN1,GLU_195,4.39,0.21,0,-0.32 3C5V,LYS 328,10,47,-0.06,0.0.04 2QV2,ASP_82,3.89,0,-0.17,0.27 3HKX,ARG_274,12.05,-0.49,0,0.04 3ERF,ARG 32,13,54,-3,03,0.66,3,41 2W0G.GLU 153.4.78.0.26.0.0.02 3GS9,ASP_297,4.26,0,0.01,0.45 3MTT,ARG_520,12.62,-0.14,0,0.27 3LJI,LYS_206,10.19,-0.4,0,0.08 2GEN,GLU_117,4.09,0.16,-0.54,-0.03 1TJE,LYS_33,10.16,-0.13,0,-0.21 1PVT,GLU_34,4.98,0.23,0.23,0.01 2OKT,GLU_334,3.61,0.5,-0.85,-0.54 1RAJ,GLU_72,4.34,0.17,-0.06,-0.26 1WPA,LYS 433,10.6,-0.18,0,0.28 2YWJ.GLU 13.4.17.0.28.-0.68.0.07 3BPV,ARG_69,12.42,-0.14,0,0.07 3M7G,HIS_56,4.12,-2.16,0.28,-0.49 3BQE,GLU_239,4.5,0.36,-0.57,0.21 2YWX,LYS_153,11.56,-0.34,1.41,0 3ERF,LYS_224,10.19,-0.29,0,-0.01 1Q46,LYS_162,11.05,-0.2,0.31,0.44 1JB3,TYR_35,10.78,-1.1,0.4,1.47 20EW,CYS 122,11.76,-0.89,-0.82.4.47 1DCF.GLU 134,4,59,0.09,0.0 1NAR,LYS_214,10.44,-0.15,0,0.09 3L7N,GLU_194,4.72,1.08,-0.74,-0.12 3CIV,GLU_272,3.41,0.49,-1.26,-0.32 1XKR,GLU_13,4.87,0.29,0,0.08 2V81,LYS_6,10.51,-0.07,0,0.08 2EEY,LYS_133,10.63,-0.17,0,0.3 3M3P,GLU_186,4.6,0.27,0,-0.17 3H5T,HIS_352,6.9,-0.57,0.67,0.3 1D2K.LYS 247.10.47.-0.07.0.0.04 4ANN,LYS_102,10.67,-0.46,0.2,0.43 1WXQ,LYS_293,9.26,-1.3,0,0.06 1JYH,GLU_57,4.78,0.18,0,0.1 3M70, ARG 77, 12.63, -0.53, 0.15, 0.5 2RGY,ARG_165,12.49,-0.14,0,0.13 2Cl3,CYS_83,11.68,-0.02,0.46,2.24 3HZQ,GLU_94,4.54,0.04,0,0 100X,LYS_141,10.52,-0.12,0,0.14 3ETU,ASP 157,4.13,-0.2,-0.14,0.67 1ZP2,GLU_69,4,0.27,-0.38,-0.4 20EW,GLU_197,5.32,3.7,-0.85,-2.03 2Q12,TYR_161,10.24,0,0.17,0.07 3HQX,GLU_107,4.56,0.32,0,-0.25 1WP5,LYS 133,10.42,-0.08,0,0 2R57,TYR_180,13.72,1.27,1.27,1.18 2R4Q,GLU_194,4.71,0.13,0,0.08 1UCH,ASP_204,3.37,-1.4,-0.04,1.02

2WB3,ASP_287,3.44,-0.69,0,0.33 3R87,LYS 85,11.3,-0.43,0.85,0.38 2X4G,GLU_167,4.96,0.5,0,-0.03 2l6l,ARG_102,13.82,-1.95,1.48,1.8 1W7B,TYR_199,10.37,0,-0.01,0.38 3LPZ.TYR 38.10.1.0.-0.39.0.48 3ERF,HIS 133.6.04,-1.79.0.85.0.47 2F4Q,LYS_272,10.51,-0.14,0,0.15 2AZL,HIS_74,2.13,-2.26,0,-2.11 1Q8B,GLU_34,3.31,0.48,-1.28,-0.39 4ANN,GLU_62,5.8,0.6,0.29,0.42 2QVO,CYS_62,10.16,-0.15,-0.21,1.52 1UW7, ARG 74, 12, 48, -0, 19, 0, 0, 16 2EEY,CYS 132,10.83,0.0.02,1.81 3EAZ.GLU 174.4.58.0.12.0.-0.04 3GS9.TYR 266.11.46.0.0.84.0.62 3FS3,HIS_168,7.16,-0.5,0.85,0.31 2B02,GLU_370,3.89,0.2,-0.81,0 3ETV,ASP_162,3.98,0,0,0.18 1RWZ,ASP 93,1.59,-2.48,-0.16,0.43 1YM5,GLU_106,3.92,1.26,-1.65,-0.19 3FS3,LYS_194,10.38,-0.29,0,0.17 1X7F,GLU_2,4.49,0.31,0,-0.32 2IDC,HIS 134,8,-0.4,0.85,1.05 3M70,TYR 174,10.95,-0.84,0.08,1.71 1JKS,GLU_114,4.71,0.17,0,0.04 1N81,ASP_181,3.98,0,-0.42,0.6 1DZF,GLU_137,4.68,2.39,-1.41,-0.81 3MIX,GLU 499,4.52,0.19,0,-0.18 2EFK,LYS_33,10.68,-0.38,0,0.55 208P,GLU_162,4.6,0.25,0,-0.16 3GW3,GLU_271,4.46,0.64,-0.67,0 1W7B,LYS 88,10.42,-0.23,0,0.14 2X4L.LYS 129.10.22.-0.28.0.0 1SUU,LYS_729,10.44,-0.31,0,0.25 2PGX,CYS_4,9.86,-0.03,0.02,0.86 2BQQ,ARG_89,12.52,-0.07,0,0.09 1SBX,GLU 102,3.76,0.28,-0.71,-0.31 1MHN,CYS_123,10.67,-0.06,0.08,1.65 1EDG,LYS_313,8.85,-1.65,0,0 1J7G,ASP_60,3.97,0,0.03,0.14 3GG6.ARG 174.12.42.-0.17.0.0.09 2BV9.TYR 171.13.65.0.8.0.51.2.35 1J7G,TYR_106,11.94,-0.43,0.34,2.02 2HRZ,TYR_126,13.54,0,0.07,3.46 3IL3,LYS_235,10.64,-0.06,0,0.2 3VHJ,LYS 157,10.35,-0.12,0,-0.03 1R9W,LYS 277,10.34,-0.25,0.0.09 1RI6,ARG_61,13.19,-0.78,0.72,0.75 2AXO,ASP_164,3.58,-0.49,-0.09,0.36 3UX2,GLU_71,3.96,0.37,-0.82,-0.1 1GPP.ASP 439.3.99.0.0.03.0.16 3P51,LYS_3,10.4,-0.14,0,0.04 3M3PLYS 4,10.35,-0.32,0,0.16 1X1E,GLU_221,3.05,0.71,-1.73,-0.43 3B7H,ARG_25,12.28,-0.22,0,0 1R50,ASP 75,3.25,-0.66,-0.52,0.63 3RLN,GLU_749,4.27,1.38,-0.75,-0.87 1EYH,GLU_98,4.71,0.25,0,-0.03 1KN3,LYS 78,10,44,-0.06,0,0 2DG7,ASP 179,2.96,-0.85,-0.3,0.31 3CAN,GLU_16,4.49,0.26,0,-0.27 1SUU,GLU_764,4.06,0.45,-0.61,-0.27 2C2Y,ARG_51,12.22,-0.21,0,-0.07 2B0J,LYS_185,11.29,-0.19,0.6,0.38 3O16,LYS_38,10.41,-0.09,0,0 3G6S,ARG_29,11.64,-0.88,0,0.02 2E3S,ARG_478,11.79,-0.75,0,0.04 3G9B,GLU_113,4.31,0.2,-0.2,-0.19

1SI7.HIS 43.5.51.-1.17.0.43.-0.26 2HNG,ARG 9,11.53,-1.08,0,0.12 2EYI,ASP_223,3.34,-0.77,-0.31,0.61 1P4X,GLU_99,4.6,0.1,0,0 1WJG,TYR_39,11.41,0.42,0.41,0.58 2H2Z,HIS 134,5.69,-0.77,0,-0.03 2RIK.ASP 132,2.36,-1.49,-0.39,0.44 3BA1,LYS_22,11.39,-0.29,0.85,0.34 2D7U,LYS_150,10.69,-0.08,0,0.26 1JYH,LYS_27,10.63,-0.15,0,0.29 1WJG,ARG 56,12.42,-0.27,0,0.18 3FHF.GLU 36.4.67.0.47.0.-0.31 2XHC,ARG_98,12.8,-1.05,0.86,0.49 1TWU,ASP_48,3.4,-0.82,0,0.43 3AU3.CYS 599.9.15,-0.98,-0.01,1.13 10ZN,LYS 13,11,48,-0,48,0,85,0,61 2X4L,ASP_144,2.74,-1.87,-0.02,0.83 3HVM,GLU_34,4.71,0.23,0,-0.02 3CQ1,GLU_39,3.98,0.25,-0.42,-0.36 2R0S,TYR 112,10.19,-0.85,0.29,0.74 2R4Q,GLU_239,4.4,0.22,-0.35,0.03 3HVW,ARG_212,12.35,-0.15,0,0 2W1R,ASP_57,3.28,-0.49,-0.42,0.39 30AV.TYR 77.12.3.0.85.0.44.1.02 3PBH.TYR 31.10.66.0.0.03.0.64 2V1L,ASP_97,4.2,-0.67,-0.14,1.21 103X.ARG 214.12.14.-0.64.0.0.27 2FC3,LYS_41,10.38,-0.22,0,0.11 1PVT,GLU 136,4.52,0.08,0,-0.06 3EAZ,LYS 86,10,57,-0,17,0,0,25 1X7F,ASP_191,3.36,-0.65,0,0.22 2VAN,ARG_213,12.52,-0.34,0,0.37 1GPP,ASP_441,2.76,-1.38,-0.91,1.24 2B0A,GLU 101,3.83,0.35,-0.52,-0.5 1LTU,ASP_280,2.66,-2.27,-0.54,1.68 3C0C,GLU_318,4.36,0.28,-0.4,-0.03 3IL3,HIS_15,6.12,-0.36,0,-0.02 1N81,ASP_177,4.13,0,0.17,0.17 3LOE,LYS 345,10.93,-0.18,0.61,0 1WP5,LYS_313,11.65,-0.41,0.85,0.71 2Q98,GLU_110,4.75,0.2,0,0.05 1WP5.LYS 267.10.44.-0.35.0.0.29 2JHYLYS 167.10.55.-0.11.0.0.15 3UV9,ASP_386,4.18,-0.83,0,1.21 3IV4,LYS_69,11.62,-0.56,0.9,0.79 3GT0,LYS_84,10.24,-0.32,0,0.07 1DOV,ASP_233,3.81,0,-0.12,0.13 4H86,ASP_75,3.69,0,-0.35,0.25 3M7D,ARG_293,11.91,-1.98,0.09,1.3 4AE7,CYS_119,9.71,-0.18,-0.07,0.95 3QAV,HIS_209,5.56,-0.73,0,-0.21 3CAX,LYS 235,11.41,-0.32,0.85,0.38 20KT.CYS 48.11.02.-1.64.0.11.3.55 307K,GLU_96,3.93,0.19,-0.76,0 1L2F,LYS_320,10.25,-0.18,0,-0.07 1P2F,ARG_192,11.61,-1.3,0,0.41 3TMO,ASP_249,3.67,0,-0.37,0.25 4HDE,LYS_107,10.35,-0.38,0,0.24 30DJ,ASP 33,4.09,0.0.01,0.28 1UCH,ARG_145,12.3,-0.25,0,0.05 1L2F,LYS 111,10.3,-0.2,0,0 4FD6,LYS_96,9.69,-0.83,0,0.02 2H85,ASP_212,3.01,-1.1,-0.29,0.6 4DNU,ASP_327,3.76,0,-0.3,0.26 3M16,LYS_29,10.64,-0.2,0,0.34 2R57,ARG_217,12.78,-0.38,0.21,0.45 1X04,LYS_106,11.93,-1.27,1.7,1 3S0A, HIS 97, 6, 22, -0, 54, 0, 0, 25 2P0Y,GLU_265,4.42,0.29,-0.29,-0.07

3BQW,LYS_274,10.63,-0.22,0,0.35 3JSN,LYS 72,10.52,-0.19,0,0.22 2AZL,GLU_58,4.62,0.11,0,0.01 2AHE,LYS_110,10.61,-0.12,0,0.24 2FBI,ARG_88,12.44,-0.06,0,0 3B79.TYR 11.11.17.0.0.29.0.88 1TD6.TYR 206.12.57.0.0.16.2.41 2WZ9,LYS_128,10.5,0,0,0 1VJG,LYS_176,9.9,-0.69,0,0.09 1SQH,ARG_285,12.39,-0.11,0,0 2AHE,ARG_133,13.6,-0.16,1.27,0 1XKR,GLU_151,4.85,0.2,0,0.14 1NAR,LYS_110,12.15,-0.57,1.45,0.77 1G8P,ARG_101,12.5,-0.32,0,0.33 2AHE,GLU_135,2.84,0.37,-2.03,0 10GL,ARG_75,11.96,-0.7,0,0.17 1Z9L.LYS 43,9.91,-0.44,0,-0.15 4FZR,ASP_66,2.87,-1.32,-0.18,0.58 1BKR,ASP_50,2.88,-0.9,-0.42,0.4 1NAF,LYS 213,10.35,-0.11,0,-0.04 3RE9.LYS 174.10.44,-0.13.0.0.07 2D59,LYS_100,9.66,-0.83,0,-0.01 2FG1,ARG_101,13.89,-0.44,1.22,0.62 1YG2,ARG_156,12.15,-0.39,0,0.04 1YTD,GLU 10,4.64,0.15,0,-0.02 2BOO,LYS 53,10.28,-0.62,0.0.39 1FKM,LYS_585,10.38,-0.34,0,0.21 2NRK,HIS_36,3.8,-2.59,0,-0.1 3M7G.GLU 51,3.68,0.67,-0.87,-0.61 3P51,ARG_146,12.41,-0.09,0,0 1GXN,ARG_329,13.47,-0.32,0.82,0.49 3M70, ASP_17, 3.91, 0, -0.07, 0.18 2CL3,LYS_192,10.34,-0.16,0,0 4FH3,ARG 364,12.49,-0.13,0.03,0.09 1MML.ARG 211,11.33,-1.2,0,0.03 4E8B,GLU_101,3.84,0.48,-0.75,-0.38 3KB5,HIS_373,6.19,-0.23,0,-0.08 3N2T,LYS_135,10.53,-0.08,0,0.11 1JT9,ASP 32,3.89,0,-0.03,0.12 3TMO,CYS_224,9.61,-0.27,0.19,0.7 3F5D,TYR 55,10.38,0,-0.06,0.43 3TMO,GLU_321,4.6,0.08,0,0.02 1ES9,ARG 168,12.21,-0.29,0,0 1DTO.TYR 159,11.18,-0.1,0.39,0.89 1TD6,GLU_178,3.3,0.37,-1.23,-0.34 3ZXY,LYS_12,10.41,-0.18,0,0.08 1AK1,LYS_18,11.27,-0.34,0.68,0.43 1J74,ARG_55,12.56,-0.07,0,0.12 3JRT,ARG_164,13.43,-0.45,0.63,0.74 1V43,ASP_367,4.08,0,0.06,0.21 3JZN,ASP_109,4,0,-0.06,0.26 3ELI,HIS_116,2.89,-2.88,0,-0.72 2H30,LYS 86,11,59,-0,36,0,77,0,68 300P,CYS_113,9.57,0,0.21,0.36 1JB3,ASP_70,3.9,-0.76,-0.01,0.86 1MHN,TYR_130,10.47,0,0.18,0.3 3BQW,TYR_196,12.84,0,0.57,2.27 3ZXY,ARG 238,12,34,-0,35,0,0,19 3EJG,GLU_98,4.05,0.47,-0.76,-0.17 4FD6,LYS_154,11.05,-0.46,0.46,0.55 2ZCO,HIS_18,3.27,-1.76,0,-1.47 1DUN.LYS 98,10.69,-0.33,0.03,0.48 2CXA,ARG_136,12.57,-0.3,0,0.37 3JRT,LYS_70,10.59,-0.21,0,0.3 1DTO,HIS_35,6.86,-0.91,1.16,0.11 1QYI,GLU_211,6.13,4.24,-1.34,-1.28 3HOX,TYR 85,10.61,0.0.23,0.37 3H5T,GLU_84,4.73,0.22,0,0.01 3HUE,GLU_95,4.75,0.42,-0.16,-0.01

2E3I.ASP 100.1.3.-2.59.-0.38.0.47 2NYC.GLU 259.3.51.0.35.-1.34.0 2O4D,GLU_113,4.71,0.21,0,1.39E-17 10GL,HIS_269,6.51,-0.18,0,0.19 3N0K, ARG 21, 13, 09, -1, 52, 1, 12, 0, 99 2Z0M,TYR 82,10.97,0.38,0.14,0.45 2QZQ,LYS_100,10.5,0,0,0 1WXF,ARG_68,13.04,-0.82,0.83,0.54 3LH5,ASP_682,3.54,-0.32,-0.06,0.12 1PVT,HIS_1,7.17,-0.33,0.57,0.43 3CN5,ASP_184,2.61,-1.28,-0.44,0.53 2E3C,GLU_341,4.42,0.63,-0.47,-0.24 2VGM,LYS_373,10.27,-0.44,0,0.2 3EJC,ASP_163,3.89,-0.02,-0.34,0.44 3F1X.CYS 108,7.96,-1.99,0.5,0.44 1XDZ,LYS_111,10.45,-0.39,0,0.34 2GZR,GLU_243,6.53,1.98,0,0.05 1GQE,LYS_303,10.7,-0.11,0,0.31 1P1L,GLU_47,3.88,0.44,-0.67,-0.38 2DG7.ARG 160.12.55.-0.28.0.06.0.27 3BWT,ASP_558,3.88,0,-0.04,0.13 3ETV,ASP_274,3.91,0,-0.6,0.71 3VHJ,ASP_117,3.83,0,-0.15,0.18 1MJS.TYR 363,10.2,0,0.05,0.16 2P0L,GLU_27,4.25,0.74,-0.7,-0.3 1XIP,GLU_328,4.59,0.08,0,0.02 1SIG,ARG_225,12.13,-0.45,0,0.07 3UV9,TYR 414,12.77,0.67,0.54,1.57 1G8P,HIS_184,4.89,-2.54,0.87,0.06 3JZN,LYS_284,10.45,-0.05,0,0 2JKF.GLU 43.4.55.0.07.0.-0.02 1AKO,ARG_268,12.62,-0.06,0,0.18 3M70,HIS 212,6.72,-0.7,0.87,0.04 1FOLASP 334,2.97,-0.85,-0.42,0.44 2F4Q,GLU_319,4.64,0.14,0,0 3PZ9,GLU_382,3.63,1.35,-1.52,-0.71 2CVB,ARG_130,13.06,-0.67,0.18,1.06 2OGQ,ARG_516,13,-0.59,0.74,0.34 2RJD,GLU_277,4.56,0.14,0,-0.08 3ASA.GLU 230.7.03.4.88.-2.67.0.31 2CI3,LYS_210,10.06,-0.42,0,-0.02 3V4G,HIS 99,5.99,-1.09,0,0.57 1X6J.GLU 82.4.58.0.22.0.-0.14 3FRR,ARG_82,12.33,-0.2,0,0.02 1MTZ,ARG_201,12.7,-0.27,0,0.47 1059,ARG_321,12.6,-0.18,0,0.28 1WLY,GLU_181,4.63,0.17,0,-0.05 4EUG,ASP_176,2.56,-1.48,-0.37,0.61 2NRR,TYR_393,13.1,0.85,0.44,1.8 3ERF,LYS_105,10.56,-0.13,0,0.19 2ZQ5,LYS 59,10.31,-0.13,0,-0.06 2Z84,HIS 40,4.93,-2.46,0.95,-0.06 2GZQ,GLU_142,4.46,0.18,0,-0.22 1X7F,ARG_286,11.96,-0.71,0,0.18 1T07, ARG_8, 13.92, -0.78, 1.64, 0.56 2DFL,ARG 217,11.27,-1.4,0,0.16 3CX2,ARG_215,12.43,-0.07,0,0 3EJG,LYS_144,9.25,-1.55,0,0.3 1R53,TYR_276,9.34,-0.85,-0.27,0.46 3G9T,LYS 35,10.16,-0.19,0,-0.15 3CBN,ARG 81,12,17,-0.59,0,0.26 4AE7,ARG_114,12.36,-0.33,0,0.18 3UC9,ASP_159,3.33,-0.6,-0.03,0.17 2HXB,LYS_24,10.33,-0.25,0,0.09 3CIV,ARG_248,12.8,-0.19,0.04,0.45 4EVF,ASP 157,3.6,-0.25,-0.19,0.24 2PGE,ASP_108,3.31,-0.74,-0.74,1 1SIG,GLU_254,3.97,0.5,-0.55,-0.47 3CS1,GLU_41,4.08,0.8,-0.66,-0.56

100L,LYS 27,10.38,-0.19,0.0.07 1AT0,ARG 348,12,41,-0,29,0,0,2 2PGE,ARG_82,13.89,-0.41,1.28,0.52 1OXZ,ASP_189,3.18,-0.95,-0.13,0.46 3BCH,LYS 11,10,17,-0,36,0,0.02 2BDD.ASP 151.3.74.0.-0.36.0.3 4DEZ.LYS 192.10.44.-0.12.0.0.06 2AD1,LYS_167,10.55,-0.11,0,0.16 3H13,HIS_334,5.85,-0.41,0,-0.24 3RLE,TYR_196,11.05,0,0.23,0.81 2EYI,TYR_241,13.94,0,0.19,3.75 1RI6,LYS_208,10.42,-0.09,0,0.01 2FZ4,ARG_95,13.15,-0.19,0.5,0.35 2C2Y,ARG_181,12.43,-0.07,0,0 1ZCE.GLU 110.4.65.0.15.0.0 3ANJ,ASP_393,3.78,0,-0.21,0.19 2FL4,TYR_62,12.48,0.67,0.59,1.22 1R6Y,GLU_73,4.73,0.23,0,0 3A2Z,ARG_110,12.28,-0.4,0,0.18 3V3T,LYS 276,10.68,-0.15,0,0.33 2P0L,ARG_169,12.43,-0.27,0,0.2 4FH3.LYS 255,10.84,-0.12.0.0.47 1W24,TYR_179,12.12,0,0.57,1.55 2IF4,CYS 232,12.03,0,-0.44,3.48 2R57,TYR 361,10.67,-0.15,0.15,0.67 3CRM,ARG_282,12.06,-0.44,0,0 2HNG,LYS_36,10.81,-0.13,0.15,0.29 2X4G,ARG_72,12.46,-0.14,0,0.1 2E0T,HIS 185,6.87,-0.35,0.79,-0.06 2RH3,HIS_143,6.24,-0.23,0,-0.03 3I0C,TYR_149,13.5,0.44,-0.21,3.27 3UPD,HIS_-22,6.06,-0.12,0,-0.32 20GQ,LYS_420,10.65,-0.09,0,0.24 2JKF,LYS 100,10.15,-0.31,0,-0.04 3UPD,ARG_61,13.6,-0.49,0.78,0.8 2H2Z,HIS_41,4.46,-2.39,0,0.34 2EDM,GLU_66,4.48,0.31,0,-0.33 3JSN,ARG 230,12.63,-0.1,0,0.23 3GS3,CYS_252,9.46,-0.03,-0.15,0.64 105J,GLU_86,4.58,0.17,0,-0.09 1H4U,GLU_512,4.64,0.08,0,0.06 3C2E,CYS 269,9,5,-0.04,0.02,0.52 108B.GLU 73,4.42,0.31,-0.39,0.01 1TR9,ARG_86,12.28,-0.44,0,0.22 1HF8.LYS 238.10.43.-0.14.0.0.07 1WRU,ARG_71,11.61,-0.55,0,-0.35 3UAH, ASP_465, 3.54, -0.64, -0.25, 0.63 2D0A, ASP 208, 3.9, 0, -0.08, 0, 17 2IDC,TYR_44,12.44,-0.45,-0.17,3.06 4DND,LYS_89,11.04,-0.37,0.52,0.38 3UX2.GLU 115.3.78.0.15.-0.85.-0.02 2IXM,ASP_240,3.17,-0.82,-0.28,0.48 2Z0W,GLU_46,4.64,0.2,0,-0.06 3GS9.TYR 191.10.07.0.0.0.07 4ETX,ARG_410,13.14,-0.36,0.73,0.26 3GOZ,LYS_4,10.57,-0.11,0,0.18 2BAA,HIS 169,5,31,-1,42,0,23,0 2PGE,GLU_149,4.75,0.31,-0.07,0 1LZL,ARG_30,13.54,-1,1.48,0.57 3ILC.GLU 7.4.45.0.27.-0.03.-0.29 1WPA.GLU 463.4.91.0.34.0.0.07 2BAA,HIS_66,5.9,-2.23,0.85,0.78 3L7N,ASP_27,3.95,0,-0.09,0.24 3BCY,GLU_89,3.93,0.88,-0.82,-0.63 2CL3,ARG_78,12.12,-0.65,0,0.27 3GS9,LYS_84,9.78,-1.07,0,0.34 2P5D,TYR_92,9.81,-0.35,-0.36,0.53 3M3P,ASP_168,3.94,-0.11,-0.17,0.43 1BN6,LYS_206,10.56,-0.12,0,0.18

1G8P,GLU_152,5.1,0.36,0,0.24 2IDC,ARG 171,12.24,-0.1,0,-0.16 1EYH,LYS_97,10.62,-0.5,0.26,0.35 1BN6.ARG 71.13.37.-1.1.46.0.42 1EV8.HIS 217.6.35.-0.26.0.0.11 1RALLYS 435.9.94-0.57.0.0.01 3H04,ARG 172,12,79,-2,09,1,44,0,94 1JYH,GLU_88,3.74,0.35,-0.73,-0.38 4FZN,ASP_161,3.39,-0.47,-0.34,0.41 3IRA,GLU_169,4.81,0.19,0,0.12 1YTD,LYS 266,11.69,-0.44,0.85,0.77 2E0T,ARG_100,12.49,-0.21,0,0.2 2FBI,ARG_74,12.55,-0.26,0,0.31 10I7,LYS_33,9.91,-0.52,0,-0.06 2ILR.GLU 418,4.68,0.25,-0.07,0 4ANN,LYS 94,9,28,-1,21,0,-0.01 2R51,ARG_199,12.32,-0.25,0,0.08 1R7J,ASP_69,4.03,0,-0.04,0.27 4F85,ARG_126,13.66,-0.74,1.17,0.73 1SUU,ASP_647,3.89,0,0,0.09 4AE7.GLU 151.4.11.0.44.-0.84.0 3TOW, ARG_59, 12.61, -0.16, 0, 0.27 3RLN,ARG_657,13.34,-0.44,0.7,0.57 2BLL,ARG 460,12,49,-1,19,0,34,0,83 3K1H.GLU 137.4.58.0.21.-0.04.-0.09 2AZP,ARG_221,13.19,-0.49,0.78,0.4 2FL7,LYS_111,10.34,-0.28,0,0.12 3K8U,LYS_46,10.3,-0.07,0,-0.13 3JSN,ASP_205,2.54,-1.32,-0.38,0.44 1WXF,LYS 112,10.54,-0.17,0.0.21 3FS3,GLU_63,4.65,0.15,0,0 1QQE,LYS_68,11.42,-0.85,0.85,0.93 3IBT,HIS_244,3.51,-3.31,0,0.32 1AKOLYS 2.9.64.-1.15.0.0.29 1XTZ,GLU_179,4.86,0.26,0,0.1 3E0H,TYR_132,12.02,0,-0.13,2.15 3EJG,HIS_41,4.72,-1.99,0,0.21 2XJ4,ARG_170,11.32,-1.04,0,-0.14 1JKS.GLU 143,4.12,0.85,-0.85,-0.38 3P28,HIS_191,5.94,-0.23,0,-0.33 3LQE,GLU_471,3.28,0.38,-1.42,-0.17 20DJ.ARG 71.13.12.-0.42.0.1.04 3TMO,GLU_220,4.55,0.1,0,-0.05 3O16,LYS_116,10.59,-0.08,0,0.16 1ES5,LYS_233,10.47,-0.24,0,0.2 4GA2,TYR_36,11.79,0.09,0.67,1.02 1U7U,GLU 383,4.93,0.45,0,-0.01 2WB8,CYS_550,9.15,-0.1,0.05,0.21 2F8H,ASP_94,3.87,-0.06,-0.18,0.32 2VAN.GLU 232.4.6.0.35.0.-0.25 2FL4,ASP 52,3.22,-0.85,0.0.27 3HVM,LYS 317,11.09,-0.32,0,0.91 3GW3,ARG 21,12.66,-0.46,0.01,0.62 1QZN,GLU_124,4.68,0.31,0,-0.12 1UAJ,TYR_54,10.1,0,0.02,0.07 1RZ2,CYS_233,12.68,-0.11,0.26,3.53 3PBH,LYS_18,10.13,-0.36,0,0 3GE9,LYS_153,10.44,-0.06,0,0 2GAU,LYS 218,10.56,-0.2,0,0.25 1RL0,ARG_24,10.39,-2.12,0,5.55E-17 1R9W,GLU 345,3.49,0.19,-0.85,-0.35 2AH5,ARG_171,12.43,-0.1,0,0.03 1MJS,ARG_322,12.49,-0.07,0,0.06 2FG1,LYS_41,10.41,-0.13,0,0.04 3BB7,TYR_256,10.87,0,0.14,0.73 2JEO,GLU_181,4.6,0.1,0,0 3RKV,TYR_214,11.56,-0.84,0.28,2.12 4DND.GLU 42.4.61.0.18.0.-0.06 2D7U,ASP_299,3.77,0,-0.26,0.23

3EZ7,CYS_352,9.42,0,0.04,0.38 1WLY,CYS 240,12.57,0,0.49,3.09 3RE9,ARG_165,12.99,-0.29,0.21,0.57 2DVK,ARG_149,12.77,-0.44,0.47,0.23 106D,GLU_36,3.14,0.68,-1.5,-0.54 3PBH.TYR 136.11.54.-0.1.0.51.1.12 3T57.ARG 250.12.58.-0.31.0.0.4 1NJ4,GLU_187,4.45,0.46,-0.12,-0.38 2PGX,ARG_47,12.89,-0.37,0.03,0.72 3U0V,GLU_107,4.12,0.89,-0.77,-0.5 4DEZ,LYS_3,10.7,-0.13,0,0.34 2WB8,TYR_580,11.57,0,0.58,0.99 2CYG,ARG_57,12.4,-1.35,0,1.26 2Z61,ARG 318,12.83,-0.49,0,0.82 2JKF.GLU 87.4.71.0.24.0.-0.02 3KB5,TYR 450,10.32,-0.07,-0.3,0.68 2RIK,ASP_12,4.08,0,0,0.28 4H86,TYR_18,11.56,0,0.05,1.51 2H01,CYS_164,9.16,-0.03,0,0.18 1YTO,TYR 158,11,3,0,0,29,1,01 4FD6.LYS 149,10.48,-0.22,0.0.2 2Z14,ASP_108,2.16,-2.31,-0.21,0.87 1RI6,HIS_333,5.66,-1.04,0.16,0.02 1UXO,ARG 26,13.66,-0.48,0.78,0.86 4EVE.ASP 52.3.94.0.-0.17.0.31 3O16,ASP_64,3.93,0,0,0.13 2P52,ARG_206,12.44,-0.15,0,0.09 3HYQ,ASP_94,3.34,-0.41,-0.51,0.47 2GZO,LYS 192,10,54,-0,15,0,0,19 1XDZ,GLU_179,3.85,0.41,-1.06,0 3V46,GLU_333,4.69,0.33,0,-0.14 100H,TYR 87,12.1,-0.09,0.88,1.32 1X1E,ARG_123,10.59,-2.31,0,0.39 1Z9L, ASP 79, 3.49, -0.91, 0.16, 0.44 1JT9.HIS 232,5.96,-1.46,0.88,0.05 1XEU,TYR_225,10.74,0,0.01,0.73 1T6L,GLU_140,4.5,0,0,0 2WB8,GLU_708,4.75,0.1,0,0.15 3COU,GLU 136,4.85,0.27,0,0.07 1GPP,GLU_36,4.54,0.23,0,-0.19 3RLN,HIS 757,5.59,-1.9,0.72,0.28 1TJE,ARG_151,12.09,-1.56,0,1.14 1X9G,ASP 98,2.32,-1.2,-0.75,0.47 3PAC.GLU 160.4.5.0.25.0.-0.25 105T,ARG_326,12.28,-0.3,0,0.09 1XKR,GLU_162,4.16,0.48,-0.82,-0.01 3NZL,TYR_58,10.1,0,0,0.1 2X5Y,GLU_892,3.75,1.4,-1.57,-0.57 1QQH,TYR_120,10.85,0.21,0.19,0.45 2PGE,LYS_184,10.41,-0.2,0,0.12 2P4D,LYS_22,10.08,-0.28,0,-0.14 3EIZ, ASP 34, 3.24, -0.89, -0.1, 0.43 2BLL/ARG 651,13,16,-0.36,0.64,0.38 3N2T,LYS_153,11.45,-0.37,0.8,0.52 3KEY,ARG_343,13.44,-0.39,0.49,0.85 3ETV,ASP_312,3.92,0,-0.12,0.25 1WXQ,GLU_170,4.46,0.16,0,-0.2 3V55.TYR 657.10.32.0.0.02.0.29 1X1E,TYR_176,11.96,0,-0.17,2.13 200K, ASP_10, 2.98, -0.84, -0.4, 0.42 1AM2, ARG_160, 12.46, -0.27, 0, 0.23 20BLLYS 145,10.53,-0.11,0.0.14 2B0J,ASP_189,3.16,-0.6,-0.47,0.43 4E9E,LYS_504,11.72,-0.49,0.85,0.86 1YM5,LYS_62,10.63,-0.14,0.26,0.01 1F2V,GLU_32,4.54,0.09,0,-0.06 1P6F,HIS 163,5.89,-0.77,0.32,-0.15 1TXJ,LYS_97,10.36,-0.38,0,0.25 3C5V,GLU_184,4.34,1.24,-1.56,0.18

2H85.HIS 234.5.6.-1.13.0.0.22 1NKD,LYS 6,10.28,-0.25,0.0.02 3ULX,LYS_96,10.65,-0.3,0,0.45 1ZBP,LYS_262,10.16,-0.67,0,0.32 2H2W.GLU 195.5.26.1.21.0.-0.45 3GMS.GLU 21,2.68,0.8,-2.24,-0.37 1RL0, ARG_137, 12.61, -2.29, 0.64, 1.75 1R53,ASP_213,3.21,-0.69,-0.24,0.34 1OXZ,HIS_235,6.73,-0.36,0.08,0.52 2V1L,HIS 18,5.27,-1.15,0,-0.08 3B79,ARG_43,12.14,-0.32,0,-0.05 4DEZ,ASP_114,3.57,0,-0.54,0.31 3OA7,LYS_514,10.7,-0.18,0,0.38 2GEN.GLU 29.3.92.0.28.-0.74.-0.12 2YYO.HIS 10.6.31.-0.47.0.08.0.21 3RNV,HIS_417,6.24,-0.81,0,0.54 2G2D,HIS_54,6.32,-0.18,0,0 2GKG,ASP_48,3.01,-0.84,-0.49,0.54 3CCY,HIS_66,4.6,-1.78,0,-0.12 3IVF,ASP 77,3.33,-0.77,-0.21,0.5 1T3Y,ASP_54,3.22,-0.62,-0.28,0.32 2PPN,LYS_17,10.4,-0.1,0,0 3NBI,ASP_94,2.85,-1.37,-0.21,0.63 2l6l.GLU 40,3.32,1.73,-2.27,-0.63 1X9G,ASP_100,3.73,-0.4,-0.22,0.55 2R57, ASP_342, 3.29, -0.62, -0.28, 0.38 3A7L,GLU_109,4.53,0.2,0,-0.17 2ZCX,ARG 39,12.59,-0.28,0,0.37 3F6F,LYS_107,10.39,-0.28,0,0.17 3DSH,CYS_332,12.55,0,0.75,2.8 2VGM,GLU_233,4.58,0.52,-0.27,-0.17 1QQH,LYS_148,10.83,-1.27,0.85,0.75 3AUF, ARG 198, 13.2, -0.28, 0.61, 0.37 4E9E.TYR 545.11.84.0.0.55.1.29 2H14,TYR_284,12.54,0.85,0.52,1.18 1GQE,LYS_362,10.33,-0.39,0,0.22 1YW5,LYS 22,10,48,-0,12,0,0,11 1UAJ,GLU_232,2.93,0.48,-1.51,-0.54 1P2F,LYS_119,10.13,-0.56,0,0.19 2Z61.LYS 200.10.56,-0.09.0.0.14 2I88,LYS_512,10.6,-0.5,0,0.6 4FCU,ARG 31,11.73,-0.95,0,0.19 3M3P.GLU 110.4.08.3.25.-2.53.-1.15 3B79,GLU_112,4.43,0.18,-0.19,-0.05 3M3P,ASP_22,3.09,-0.84,-0.24,0.38 3PP8, ARG_163, 12.72, -1.14, 0.59, 0.77 3H5T,ASP_238,4.05,-0.02,-0.01,0.28 3FK5,LYS_82,10.71,-0.19,0,0.4 2JHY,ASP_89,2.54,-1.61,-0.01,0.37 1T3J,GLU_706,4.56,0.22,-0.2,0.04 3Q1C,ARG 262,12.42,-0.3,0,0.22 1H09,TYR 273,12.63,-0.36,0.93,2.05 30KQ,CYS_677,9.24,0,0,0.24 3LJC,ARG_226,12.46,-0.15,0,0.11 3NJM,LYS_59,10.4,-0.15,0,0.05 106D,ARG 42,12.44,-0.06,0,0 3JV1,ASP_138,3.94,0,0,0.14 3LD1,ARG_183,12.19,-0.31,0,0 1QZN,ASP_81,4.02,0,0.01,0.21 2W1R,ARG 104,12.61,-0.24,0.06,0.3 1SOW,TYR 35,11.69,0.85,0.36,0.49 1FO9,GLU_385,3.03,1.56,-1.66,-1.37 1G5Z,ASP_166,2.38,-1.12,-0.75,0.44 2H2Z,ARG_222,12.3,-0.2,0,0.01 3OA7,GLU_469,4.64,0.32,-0.11,-0.07 2QK1,LYS 467,10.44,-0.18,0,0.12 3ILC,GLU_96,3.76,0.45,-0.81,-0.38 1SJ8,LYS_535,10.41,-0.28,0,0.18 1ZYL,ARG_131,12.24,-0.55,0,0.29

3RNV,ARG_406,12.02,-0.51,0,0.03 1JKS,ASP 149,3.32,-0.82,-0.03,0.37 1AM2,LYS_165,10.72,-0.37,0.14,0.45 2X4G,ARG_311,12.13,-0.4,0,0.03 1X1E.TYR 99.10.97.0.0.24.0.74 3GA2.CYS 61.12.21.0.0.4.2.82 2FM9,ASP_72,3.36,-0.76,0,0.32 1TWU,ASP_58,3.63,0,-0.45,0.28 3P2F,TYR_77,12.7,0,0.33,2.37 1MTZ,LYS_123,11.3,-0.58,0.85,0.53 2G9D,ASP_296,4.35,0,-0.09,0.64 3V4G,GLU_31,3.77,0.26,-0.83,-0.16 2CI3.GLU 68.3.42.0.65.-1.79.0.06 1V6T,TYR_16,10.1,0,0,0.1 1D2K.ARG 147.12.67.-1.08.0.58.0.66 4EKU,ARG 85,12.57,-0.21,0.0.29 2BAA,ARG_90,12.34,-0.17,0,0.01 2F8H,ARG_62,11.21,-1.49,0,0.2 2WOZ,TYR_367,10.38,0,0.01,0.36 3JZ9,LYS 438,10.11,-0.25,0,-0.14 3CBN,LYS_154,9.79,-0.41,0,-0.29 3V46,ARG_268,12.45,-0.05,0,0 2B0J,LYS_273,10.57,-0.13,0,0.19 2EFK.TYR 205,10.35,0,0.04,0.31 1FOI.GLU 320.3.7.0.53.-0.9.-0.43 2FXT,GLU_303,4.8,0.57,0,-0.26 2QHT,ARG_104,12.22,-0.29,0,0.01 3FTT,TYR_82,10.29,-0.15,0.02,0.43 4EZB,ASP 66,3.52,-0.83,-0.44,0.98 2P4D,LYS_165,11.24,-0.37,0.72,0.38 2RJD,GLU_262,4.09,0.63,-0.64,-0.41 1YB2,ASP_93,3.17,-0.85,-0.18,0.4 3MIX,GLU_333,4.37,0.21,-0.34,0 3RFY,ARG 152,12,42,-0.08,0.0 1SFE,GLU_32,4.52,0.17,0,-0.15 3RHE,LYS_122,10.45,-0.22,0,0.18 3Q1C,ARG_208,12.38,-0.29,0,0.17 1AK1,CYS 273,13.28,0,0.84,3.44 3RLE,HIS_156,6.54,-0.52,0.7,-0.14 1BN6,ARG_299,12.49,-0.16,0,0.14 1H09,TYR_252,11.13,0,0.36,0.78 2PIM.ARG 111,12,46,-0.04,0.0 3H8Y,HIS 85.6.35,-0.16.0.0.01 1Q5Z,ARG_565,12.33,-0.17,0,0 1SQH,ASP_189,3.65,0,-0.32,0.17 1EV8,ASP_156,3.83,0,-0.09,0.12 2CE6,GLU 30,3.89,1.34,-1.58,-0.36 1XTZ.LYS 226.10.49.-0.4.0.0.4 2D7U,LYS_304,10.34,-0.33,0,0.17 3CS1,GLU_150,4.8,0.11,0,0.2 105J.LYS 71.10.5.0.0.0 4ECC.TYR 7,11.82,-0.82,-0.24,2.87 4EVF,ARG_229,12.01,-0.73,0,0.23 2CIU,ARG_111,11.54,-1.04,0,0.08 2AXO,LYS_95,11.03,-0.3,0,0.84 1NJ4,ARG_194,12.51,-0.51,0.12,0.4 4ECC,LYS 77,10.59,-0.23,0.02,0.3 2Z61,LYS_84,10.47,-0.04,0,0.01 2CI3,ARG_135,12.41,-0.28,0,0.18 3IRA,HIS 149,6.24,-0.71,0.31,0.15 2RGY,ASP 295,2.82,-1.3,0.0.32 3LJC,GLU_57,4.38,0.2,-0.17,-0.16 2OJQ,GLU_529,5.39,0.84,0,0.05 1I60,CYS_93,11.43,-0.04,0,2.46 3H8Y,ASP_25,3.35,-0.5,-0.38,0.44 4D8L, ASP_64, 3.48, -0.54, -0.43, 0.65 1TJE,ARG_145,13.93,-0.37,1.42,0.38 2CN1,CYS_53,10.38,0,-0.04,1.41 3ETU,LYS_90,10.26,-0.31,0,0.06

2JKF,LYS 156,10.8,-0.88,0.76,0.42 2IXM.LYS 286.10.31.-0.19.0.0 1R5Q,GLU_4,4.12,0.18,-0.56,0 3M16,LYS 32,10,44,-0,11,0,0,05 3MIX,TYR_545,10.61,0,0.32,0.29 1UOH.GLU 183.4.58.0.25.0.-0.17 3IL3,ARG 196,12,45,-0.05,0,0 1X91,TYR_68,10.83,-0.72,0.31,1.25 4EVF,GLU_185,3.46,0.59,-1.54,-0.08 2NSN,TYR_88,10.36,0,0.21,0.15 2W2S,ASP_146,4.03,0,-0.06,0.29 3UPD,LYS 297,10.99,-0.16,0.28,0.36 1JYH,ASP_141,3.38,-0.83,0.04,0.38 1WLY,TYR_135,13.04,0,0.4,2.64 2B78,TYR 26,12,76,0,0,15,2,6 1R29.GLU 77.4.78.0.11.0.0.17 1BYI,ARG_91,12.78,-0.2,0.23,0.25 3PM2,GLU_58,5.28,1.48,-0.55,-0.14 1ZCU,ARG_33,12.84,-0.27,0,0.61 1MTZ,GLU_87,3.95,2.02,-1.62,-0.94 1P6F.GLU 153.4.75.0.25.0.0 2P1W,GLU_181,4.83,1.43,-0.58,-0.53 2R0S,ASP_184,3.01,-0.73,-0.48,0.43 3M7D.GLU 309.4.81.0.18.0.0.13 1TLV.LYS 82.11.38.-0.6.0.85.0.62 3UPD,HIS_310,6.36,-0.83,0.76,-0.06 2B6P,ARG_11,12.42,-0.13,0,0.06 3GA2,HIS_125,4.21,-2.04,0,-0.26 3UAH,GLU 272,4.45,0.17,0,-0.22 2P65.LYS 172.10.53.-0.09.0.0.11 1TUL,TYR_33,10.4,-0.85,0.08,1.17 1ES9,HIS_108,6.08,-0.95,0.74,-0.21 1W7B,ARG 205,12,37,-0,34,0,0,21 2E3H.GLU 211.4.39.0.11.0.-0.22 30NH,ASP_460,3.84,0,-0.27,0.31 1YTD,TYR_387,10.27,0,-8.67E-18,0.26 1YW5,LYS_76,9.42,-1.2,0,0.13 3MIX,ASP_464,3.33,-0.62,-0.21,0.37 3CAN, ARG 47, 12.5, -0.36, 0.16, 0.19 3T57,ARG_323,12.7,-0.57,0.25,0.52 3ETU,LYS_320,9.79,-0.5,0,-0.21 1WLY,GLU 67,6,74,4,36,-1,64,-0,48 3HQX,HIS 26,6.17,-0.38,0.13,-0.07 3MTT,LYS_516,10.46,-0.04,0,0 2EJB,ASP_175,3.12,-0.85,-0.57,0.74 1JSX,GLU_183,3.57,0.71,-0.96,-0.69 2HRZ,TYR_159,12.05,0,-0.03,2.08 4FLE,GLU_98,3.88,0.4,-0.61,-0.41 1DZF,GLU_203,4.71,0.22,0,0 3LMO.ASP 48,4,73,-0,72,-0,24,1.88 1SUU,GLU_718,3.85,0.79,-1.1,-0.34 1JYH,CYS 65,10.88,-0.68,0.24,2.33 1Y2O.TYR 120.10.22.0.0.04.0.18 1WP5,GLU_46,4.45,1.19,-0.85,-0.4 3G9G,LYS_109,11.47,-0.36,0.81,0.53 2W2S,ARG_70,12.38,-0.29,0,0.16 3G6S.TYR 62.12.33.0.0.16.2.16 1UW7,GLU_70,4.77,0.72,-0.06,-0.39 3DZ1,ARG 31,12,29,-0,44,0,0,23 2E0T,LYS 180,11,48,-0,25,0,85,0,38 10LR,ARG 193,12.58,-0.09,0,0.17 2B6P,HIS_40,5.01,-1.06,0,-0.43 3DTE.ARG 238.12.18.-0.32.0.0 1NIJ,LYS_211,11.02,-0.84,0.82,0.53 3RRQ,ASP_105,2.31,-1.66,-0.33,0.5 3K8U,ARG_15,12.37,-0.27,0,0.14 3E7P,ASP_157,3.59,-0.32,-0.09,0.21 2R51.LYS 203.10.69.-0.19.0.0.38 3B7H,GLU_10,3.63,0.36,-0.85,-0.38

1WOU,GLU_62,4.48,0.06,0,-0.08 4E9E,LYS 576,10.41,-0.25,0,0.16 3P51,CYS_37,10.5,-0.09,-0.34,1.93 2VGM,LYS_190,10.48,-0.1,0,0.09 1Y0K,GLU_163,3.07,0.5,-1.47,-0.46 2V4X.LYS 20.10.4.-0.12.0.0.02 3H5T.LYS 260.10.64.-0.33.0.0.47 2FPN,LYS_185,10.47,-0.06,0,0.02 208P,CYS_26,9.1,-0.34,0.07,0.37 2OB5,LYS_46,11.31,-0.28,0.72,0.37 2H14,ASP_76,3.1,-1.11,0,0.41 2RIK,TYR_115,11.8,0,-0.35,2.15 1SQW,ASP_138,3.13,-0.84,-0.19,0.36 200P.HIS 115.6.18.-0.93.0.18.0.44 3GV0,ASP_111,3.2,-0.32,-0.73,0.44 2FM9,LYS 71,10.4,-0.1,0,0 2E3H,LYS_268,10.43,-0.16,0,0.09 2XMZ,ASP_65,3.69,-0.42,-0.05,0.35 3F6F,LYS_206,11.51,-0.27,0.85,0.43 1SNT.TYR 310.12.69.0.1.04E-17.2.69 2BOO,ASP 62,2,26,-2,2,-0,27,0,94 3L3P,GLU_380,5.78,1.11,-0.1,0.26 3M66,LYS_224,11.46,-0.34,0.85,0.45 1U7U,ARG 226,12.11,-0.32,0,-0.08 1SBX,ARG 184,12.48,-0.15,0,0.13 3HKX,ASP_273,4.2,0,0.17,0.23 3BZT,GLU_284,3.27,1.73,-2.01,-0.93 2GAU,ARG_88,10.78,-1.88,0,0.16 2B0J,GLU_193,4.56,0.22,0,-0.16 2GEN,GLU_79,4.85,0.37,0,-0.03 2PGX,LYS_69,10.42,-0.08,0,0 1PZC,LYS 107,9.06,-1.52,0.0.08 2R2Y,GLU_118,4.03,0.45,-0.72,-0.2 2R4Q,LYS 195,11.39,-0.39,0.85,0.43 3M9A.GLU 89.4.82.0.23.0.0.09 2O4D,LYS_27,10.34,-0.16,0,0 1ES5,GLU_219,4.54,0.19,0,-0.14 1YOY,LYS_66,11.11,-0.55,0.76,0.4 3Q6L,TYR 129,11.12,-0.24,-1.05,2.42 1LN4,LYS_6,10.84,-0.22,0.56,0 105Z.LYS 551,10.3,-0.18,0,-0.02 3D9H,LYS_185,10.54,-0.31,0,0.35 2OKT,ARG 29,13.05,-3.43,0,3.99 3EGN,ARG 401,12,42,-0.08,0,0 1O6D,LYS_51,10.01,-0.51,0,0.02 2R4Q,GLU_198,3.52,0.25,-0.85,-0.38 3G6S,LYS_124,11.01,-0.25,0.38,0.38 3AUF,HIS 56,6.64,-0.64,0.5,0.28 1YM5,TYR_130,11.24,0,0.11,1.13 3I47,LYS_138,10.55,-0.37,0,0.42 2PPN,HIS_25,5.59,-0.7,0,-0.21 1R3F,TYR_263,10.09,0,0,0.09 20GO.HIS 468.6.3.-0.19.0.-0.01 2IRM,CYS_277,8.26,-1.7,-0.43,1.39 1XKR,GLU_112,4.73,0.67,-0.39,-0.05 3FHF,GLU_53,3.59,0.34,-0.85,-0.4 3UV9,CYS_438,8.73,-0.79,0.06,0.45 1NFN.GLU 121.3.73.0.32.-0.84.-0.26 2NRR,TYR_361,10.86,0,0.57,0.3 4EKU,HIS_96,6.52,-0.7,0.5,0.21 1PDB,LYS_55,9.9,-0.57,0,-0.03 2AXO.GLU 182.4.69.0.37.-0.13.-0.05 3HUE,ASP_146,3.88,0,-0.06,0.13 1ZBP.GLU 186.3.54.0.87,-1.42,-0.42 3B4D,GLU_187,3.48,0.53,-1.28,-0.27 1O5T,TYR_240,12.47,-0.85,0,3.32 2X4L.GLU 121,3.8.0.28,-0.63,-0.35 3G6S,GLU_144,4.73,0.16,0,0.07 3GE9,GLU_214,4.83,0.84,0,-0.52

3FRR.HIS 58.6.08.-0.58.0.0.17 1GOE,CYS 128,12.61,0,-0.19,3.8 3CIV,HIS_188,6.61,-0.44,0.45,0.1 3ADO,HIS_161,5.69,-1.21,0,0.4 3KV0,ARG 184,12.28,-0.27,0,0.05 208P.GLU 168.3.47.0.9.-1.55.-0.39 4EF5,GLU_339,4,0.35,-0.32,-0.52 4ETX,ARG_312,12.19,-0.42,0,0.11 103X,GLU_275,4.4,0.23,-0.32,-0.01 3HUE,ARG_143,12.43,-0.27,0,0.2 2HNG,GLU_94,4.71,0.1,0,0.11 4ESS,GLU_87,4.49,0.29,0,-0.31 2V1L,CYS_73,9.77,0,0.29,0.48 1BN6.GLU 104.3.92.0.52.-0.77.-0.33 3EJG.GLU 131.3.78.0.57.-0.75.-0.54 4E9E,ASP_521,3.82,0,-0.38,0.39 2QOP,GLU_72,4.68,0.15,0,0.03 1UOH,GLU_182,4.93,0.51,0,-0.08 2RGY,GLU_346,4.77,0.23,0,0.04 4FCU,ARG 9,11.87,-1.32,0.0.69 1PVT,ARG_220,12.42,-0.1,0,0.02 3LJC,GLU_34,4.34,0.1,0,-0.27 1HUF,GLU_124,4.76,0.25,0,0.01 300P,ARG 88,12.45,-0.05,0,0 2Z84, ASP_204, 3.16, -0.84, -0.12, 0.32 1RWZ,HIS_28,6.33,-1.29,0.85,0.27 2CXY,GLU_56,4.59,0.25,0,-0.16 1ILW,LYS 156,10.21,-0.6,0,0.32 3GV0,HIS_100,6.33,-0.17,0,0 2CW4,GLU_81,4.84,0.09,0,0.25 4EVF,LYS 282,10.48,-0.05,0.0.02 2R2Y,ARG_64,12.03,-0.3,0,-0.18 2W0G,LYS 260,11.56,-1.02,1.52,0.56 1X8F.GLU 126.4.73.0.18.0.0.04 1SIG,ASP_118,3.82,-0.02,-0.19,0.23 3M3P,ARG_38,12.5,-0.11,0,0.11 2J8A.TYR 253,11.1.0.0.18.0.91 3TIR,LYS_220,11.44,-0.23,0.85,0.32 3GFP,GLU_323,4.85,0.26,0,0.09 1R53.LYS 366.11.21.-0.53.0.85.0.38 3RRQ,ASP_48,3.92,0,-0.17,0.29 2Z84,CYS 53,7.77,-3.39,-0.37,2.53 1TUL.GLU 80.3.76.0.51.-0.57.-0.67 3U0V,ASP_48,2.38,-1.44,-0.68,0.7 1T95,GLU_46,4.71,0.16,0,0.06 3GOZ,CYS_233,11.97,-0.06,0.7,2.31 1CHD,ARG_197,12.69,-0.11,0,0.29 2FBQ,ARG_140,12.98,-0.61,0.61,0.47 2CE6,LYS 33,10,21,-0,29,0,0 2V5B,LYS_251,11.13,-0.23,0.11,0.75 1DUN,LYS 56,11.29,-0.63,0.85,0.57 3ANJ,LYS 146,9,51,-0.82,0,-0.16 2GEN,HIS_105,5.72,-0.51,0.01,-0.27 2HP7,ASP_128,4.1,0,0,0.3 2P0L,ARG_87,11.49,-1.55,0,0.54 1JKS,GLU 32,4.02,0.59,-0.94,-0.15 3GS9,ARG_188,12.92,-0.25,0.37,0.31 30IP,ARG_79,12.49,-0.05,0,0.04 3ANJ,ARG_247,11.29,-3.56,0.12,2.22 1RAJ,GLU 369,4.46,0.12,0,-0.16 2B0A,LYS 137,10,38,-0,24,0,0,11 3HUE,GLU_313,4.46,0.46,-0.11,-0.38 1SQH,ARG_178,12.03,-0.57,0,0.1 2XJ4,ARG_258,12.43,-0.15,0,0.07 1WYC, ASP_169, 4.33, 0, 0.18, 0.35 2P5D,LYS 57,9.62,-2.11,0.73,0.49 3F5D,LYS_132,10.24,-0.2,0,-0.05 3O48,CYS_79,11.2,-0.06,0.04,2.22 3D9H,ARG_234,13.24,-0.36,0.49,0.61 1DZF,ARG_26,13.72,-3.1,1.69,2.63 1A80.ASP 267.2.95.-1.49.-0.62.1.26 1NAF,CYS_256,10.58,-0.01,-0.04,1.63 3KV0.GLU 115.5.46.0.86.0.0.1 2CN1,ARG 233,13,44,-0,22,0,75,0,4 3FFM.CYS 38.10.42.-0.11.0.04.1.49 1U3Y,ASP 336,1.82,-2,18,-0,4,0.59 3M70,TYR_185,11.35,-0.21,0.05,1.51 2JEO,GLU_45,3.71,0.31,-0.72,-0.38 3RFF,GLU_96,4.26,0.2,-0.61,0.17 3M70,GLU_160,3.79,0.2,-0.52,-0.38 1DTO,TYR_167,11.59,0.15,0.41,1.04 2QOP,ARG_162,12.26,-0.24,0,0 1Z9L,CYS_53,9.15,0,-0.15,0.3 2E3S.TYR 466.11.7.0.16.0.38.1.16 1RAJ,ARG 376,11.25,-1.68,0,0.43 1WRU,ASP_251,3.68,-0.39,-0.08,0.35 2P4D,ARG_19,12.36,-0.11,0,-0.02 3N2T,GLU_92,4.35,0.14,-0.38,0.09 3GG6,CYS 67,9.38,-0.48,-0.18,1.04 1M5I,ARG_194,12.43,-0.24,0,0.16 2WB8,LYS 456,11,23,-0,56,0,53,0,76 2HRZ,GLU_321,4.25,0.45,-0.9,0.2 1WRU,LYS 308,10.12,-0.89,0,0.5 2Z61,LYS 29,11.34,-0.39,0.85,0.38 1FO9,GLU_373,4.65,0.18,0,-0.03 2B61,TYR_32,12.77,-0.59,0.49,2.86 2CXA,GLU_133,4.89,3.9,-3.37,-0.13 3DHN,LYS 100,12.2,-0.76,1.39,1.07 2D7U,GLU_108,4.84,0.3,-0.02,0.05 2F8H,ASP_78,2.65,-1.25,-0.45,0.55 1YIB,LYS_212,10.57,-0.16,0,0.22 2CE6,HIS 84,7.12,-0.31,0.85,0.08 3PM2,LYS 111,10.65,-0.21,0.0.36 3E5T,GLU_141,3.4,0.35,-1.38,-0.07 2F8H,TYR_36,10.89,-0.6,0.07,1.41 1A8Q,HIS_252,3.05,-3.45,0,0 3GW3,TYR 342,11.54,0.2,0.6,0.73 2EJB,GLU_25,4.37,0.71,-0.63,-0.21 3M7G,ARG_93,12.58,-0.13,0,0.21 1XKR,GLU_72,3.45,0.48,-1.5,-0.03 3JZN,LYS 275,10.52,-0.24,0.0.26 1L2F,GLU 216,4,55,0,3,0,-0,25 1ZBM,TYR_252,13.58,0,0.41,3.17 2E3S,HIS_469,5.36,-1.84,0.29,0.4 3FS3,TYR_75,10.46,0,0.16,0.29 3O7K,ARG_103,13,-0.27,0.76,0 4ESS,GLU_47,4.76,0.26,0,0 1XDZ,CYS_124,10.56,0,0.09,1.47 3RKV,GLU_263,3,1.2,-1.54,-1.16 2WB8.ASP 459.3.35.-0.21.-0.87.0.63 3FHF,ARG_71,12.76,-0.5,0.2,0.55 4FZR,HIS_291,3.86,-2.84,0.71,-0.51 1X7F,TYR_244,9.8,-0.66,-0.09,0.54 2FXT,ARG_404,11.92,-1.54,0.39,0.57 3KEY,GLU_369,3.97,0.67,-0.96,-0.24 3ETU.TYR 111,9.29,-0.85,-0.3,0.44 3ERF,TYR_213,11.91,0,0.02,1.89 10IS,LYS_249,10.34,-0.16,0,0 3G6S.TYR 25.10.18.0.0.0.18 2PWO.ASP 119.4.15.0.0.1.0.24 1AD6,LYS_420,11.07,-0.16,0.31,0.42 2PGX,ARG_214,11.72,-0.94,0,0.16 3M70,ASP_186,2.98,-1.4,-0.1,0.67 3I47,ARG_152,12.1,-0.62,0,0.23 1TUL,GLU_22,4.6,0.15,0,-0.04 2CBE,HIS_36,6.74,-0.18,0,0.42 2FXT,ARG 378,12.67,-0.31,0,0.48 1059,ARG_254,12.82,-0.4,0.4,0.33

3P28,ARG 120,12,25,-0,25,0,0 1V43,HIS_304,6.28,-0.15,0,-0.07 3F7M,ASP_201,1.54,-2.65,-0.15,0.54 3M66,GLU_364,5.45,0.92,0,0.04 3NBI,ARG_107,12.44,-0.09,0,0.02 3IVELYS 7.10.31 -0.19.0.0.01 3HNX,HIS 65,6,26,-0,4,0,0,16 1FKM,HIS_321,6.61,-0.24,0,0.35 3GT0,LYS_3,11.23,-0.93,0.85,0.81 1TUL,GLU_32,4.74,0.24,0,0 3V1Q,TYR 586,10.15,-1,-0.16,1.31 4FLE,HIS 197.6.25,-0.25,0.0 1DCF,ARG_20,12.29,-0.44,0,0.24 1SBX,CYS_186,11.31,-0.02,0.3,2.05 4ETX,ARG 311,12,74,-0.22,0,14,0,32 2EJB.ARG 78.12.32.-0.18.0.0 3M7G,GLU_183,4.58,0.08,0,0 2YYO,GLU_112,4.04,0.64,-0.73,-0.36 1F2V,ARG_116,12.23,-0.2,0,-0.07 2OB5,ASP 86,3.84,0,-0.09,0.13 3P28/HIS 151/5.08/-2.56/0.83/0.31 10I7,ARG_6,12.44,-0.29,0,0.22 1R9W,TYR_327,12.18,-0.12,0,2.3 1DCF.CYS 59,10.07,-0.44,0.19,1.32 3ZXY.ARG 18.11.6.-0.73.0.-0.16 3H6Q,ASP_4,3.43,-0.82,-0.11,0.56 2H85,GLU_304,3.94,0.29,-0.85,0 2EFK,HIS_272,6.24,-0.28,0.04,-0.01 1YR6,GLU 25,4.58,0.67,-0.54,-0.05 1SQW,TYR_172,10.8,0,0.27,0.52 1RSS,ASP_15,2.75,-2.58,-0.03,1.57 3OA7,GLU_451,4.6,0.15,0,-0.05 3NBI,ARG_9,12.22,-0.28,0,0 2A4D,CYS_218,9.4,-0.22,-0.01,0.62 1XFK,ARG_119,10.93,-1.57,0,0 2AZL,ARG_91,11.93,-0.54,0,-0.04 208I,ARG_10,12.63,-0.32,0.21,0.24 2R0S,ASP_52,3.82,0,-0.22,0.24 2GAU.TYR 129,12.6.0.0.59,2.01 1KN3,GLU_31,4.65,0.15,0,0 1R3F,ARG_181,12.65,-1.52,0.51,1.16 1DZF.TYR 112,10.65,-0.02,0.0.68 1ZYL.GLU 312.4.54.0.29.0.-0.25 2HNG,HIS_46,6.87,-0.45,0.83,0 2AZP,HIS_90,4.98,-3.21,0.01,1.68 3GV0,HIS_165,4.62,-1.97,0,0.09 1X8F,ARG 63,10.76,-1.82,0,0.08 2B61,GLU_247,3.45,0.48,-1.64,0.12 2JEO,GLU_125,4.65,0.11,0,0.04 2P52,ARG_277,12.84,-0.22,0,0.56 2YYO,ARG_53,12.52,-0.25,0,0.26 1YLN,GLU 153,4.57,0.07,0,0 3O16.GLU 136.3.8.0.67.-1.08.-0.3 1G5Z,LYS_195,9.97,-0.25,0,-0.28 2ILR,GLU_299,4.1,0.46,-0.75,-0.12 1NRI,GLU_59,4.74,0.24,0,0 4EZB,ARG_47,12.53,-0.19,0,0.23 2D2S,ASP_728,3.99,0,-0.24,0.42 3IBT.ASP 47.2.41,-1.3,-0.64,0.55 2V4X.GLU 99.3.65.0.85.-0.85.-0.85 3HVW,GLU 233,4.64,0.28,0,-0.14 1SNT.GLU 10.4.6.0.98.-0.7.-0.18 1S7K,HIS_120,5.61,-0.9,0,0.02 3UX2,ARG_31,12.87,-0.23,0.6,0 4DVD,ARG_47,12.75,-0.31,0.15,0.41 3T5B,GLU_348,4.78,0.15,0,0.13 4AE7,HIS_94,5.88,-0.51,0,-0.12 2ZCO.GLU 162.6.7.2.16.0.0.05 3EVP,ASP_86,3.11,-0.93,-0.05,0.29

3QAV,LYS_132,11.11,-0.22,0.43,0.4 1RZ2,TYR_215,11.31,0,0.32,0.99 3LD1,LYS_161,10.19,-0.71,0,0.4 2ZCX,CYS_87,10.38,-0.47,0.06,1.8 3UC9,CYS_181,10.76,-0.13,-0.06,1.96 3CIV.GLU 187.3.06.1.5.-1.9.-1.05 2CBE.LYS 261.10.67.-0.14.0.0.3 3AU3,LYS_560,10.29,-0.27,0,0.06 30KQ,GLU_661,4.66,0.16,0,0 3A2Z,ASP_9,3.89,0,-0.29,0.38 3CSR.TYR 24.11.17.0.0.31.0.86 3GS3.GLU 69.4.61.0.11.0.0 2Q12,LYS_193,10.39,-0.13,0,0.02 3HQX,GLU_74,4.51,0.07,0,-0.06 2H85,LYS_344,10.45,-0.19,0,0.14 3FHF,GLU_40,5.08,3.18,-1.68,-0.9 3LJN,LYS 58,10,15,-0,45,0,0,1 1X8F,CYS_249,9.43,-0.02,0.14,0.31 3CGW,LYS_215,10.68,-0.23,0,0.41 2E0T.HIS 90.4.98.-1.4.0.-0.12 2AZL,LYS 214,10,46,-0.04,0,0 1BGF,ASP_65,3.27,-0.59,-0.34,0.4 2B2H,GLU_179,4.59,0.09,0,0 2P1W.ARG 148.12.34.-0.16.0.0 1YTD,ARG 235,11.6,-2.18,0,1.27 2HXB,ARG_122,12.31,-0.19,0,0 1DTO,HIS_18,6.16,-1.19,0.85,0 1SNT,CYS_196,13.56,0,1,3.57 10IS,LYS_245,9.71,-0.67,0,-0.12 20EW,ASP_16,3.4,-0.71,-0.21,0.52 3MTT,LYS_584,10.28,-0.44,0,0.22 1WYC.GLU 212.3.95.0.22.-0.79.0.02 1XIP,HIS_381,7.15,-0.2,0.3,0.56 1BGF,ARG 113,12.07,-0.52,0,0.09 1T95.GLU 80.4.85.0.27.0.0.07 1JKS,GLU_118,4.29,0.44,0,-0.65 3O48, ARG_98, 12.37, -0.2, 0, 0.07 2PPN,TYR_26,11.78,0.01,0.17,1.61 3HVW,ARG 253,12.36,-0.21,0,0.07 3I4T,GLU_199,5.12,0.46,0.03,0.13 3EUR.GLU 134.4.18.0.51.-0.83.0 3TIR,LYS_5,10.3,-0.2,0,0 2D7U,ASP 337,4.26,0,0.39,0.06 2RIK.ASP 5,3.64,-0.38,-0.37,0.6 3E0H,ARG_150,11.82,-0.83,0,0.15 3TRE,LYS_14,10.03,-0.61,0,0.14 1LZL,ARG_272,11.81,-0.95,0,0.26 3EVZ,ARG 217,12.46,-0.28,0,0.24 3H04,LYS_24,11.35,-0.39,0.79,0.44 2PIM,ARG_101,13.11,-0.49,0.61,0.49 2H2W,TYR_247,10.39,0,-0.08,0.47 2HNG,HIS_18,6.41,-0.3,0,0.2 2RIK.LYS 262,10.35,-0.15,0.0 3CRM,GLU_32,4.31,1.07,-0.35,-0.91 3CZC,ARG_67,12.3,-0.24,0,0.04 3ADO,GLU_38,4.87,0.28,0,0.09 3CCY,ASP_61,4.15,-0.17,-0.48,1 2R51,TYR 231,10.46,-0.07,-0.01,0.53 3NJM,ASP_37,4.11,-0.35,0.01,0.66 1A8Q,ASP_212,3.2,-0.96,-0.02,0.38 2WB8,LYS_726,10.18,-0.4,0,0.08 2C2Y,HIS 54,4.54,-1.7.0,-0.25 3GE9,ARG_209,11.87,-0.85,0,0.22 2RIS,GLU_64,4.85,0.55,0,-0.2 2FBI,ARG_80,13.44,-0.63,1.16,0.41 2ZCO,ASP_210,4.06,0,-0.07,0.33 10GL.GLU 49.5.72.0.8.0.0.43 3ZXY,GLU_134,4.8,0.26,0,0.04 2FL7,ASP_188,3.68,-0.58,-0.05,0.52

1DUN,ASP_20,3.45,-0.85,-0.43,0.93 3EVP.HIS 130.6.25,-0.89.0.75,-0.13 1CBY,HIS_158,5.46,-1.15,0,0.1 3IU5,LYS_124,10.88,-0.43,0.1,0.72 2IDC,GLU_29,4.78,0.28,0,0 3GE9.TYR 81.9.87,-0.05,-0.51,0.44 4EVF,TYR_42,13.48,0.85,0.76,1.86 3LPZ,LYS 172,10.92,-0.24,0.0.66 3LD1,LYS_211,10.18,-0.43,0,0.11 1DTO,GLU_80,4.2,0.77,-0.74,-0.32 30NT/HIS 72.7.18.-0.21.0.79.0.1 1UOH,GLU_187,4.87,1.12,-0.69,-0.07 1WRU,LYS_132,10.6,-0.12,0,0.22 1HF8,ASP_180,2.33,-1.58,-0.97,1.07 1U7ULYS 215.10.51.-0.33.0.0.33 2QZQ,GLU_107,5.19,2.21,-0.85,-0.67 3EZ7,HIS 131,5,18,-1,32,0,0 4FH3,TYR_122,10.63,0,0.04,0.59 2IXM,ASP_89,2.89,-0.85,-0.44,0.38 2Z14,ARG 116,12,25,-0,25,0,0 2FC3,LYS_18,11.43,-0.41,0.85,0.48 3TRE,TYR_90,10.11,0,0.02,0.09 1YR6,LYS 175,10,48,-0,47,0,0,45 3UAH.LYS 456.10.73.-0.12.0.0.35 1ZCE, ASP_84, 2.85, -1.34, -0.62, 1.02 1R3F,GLU_97,4.6,0.38,0,-0.28 2B2H,CYS_283,12.64,0,0.04,3.61 3MIX,GLU_649,4.39,0.33,0,-0.46 3FRR,LYS_159,10.64,-0.14,0,0.27 2EJB,LYS_104,10.28,-0.12,0,-0.1 1ILW,ASP_162,3.85,0,-0.31,0.35 4DVD,GLU_26,4.03,1.35,-0.83,-1.01 1Z3X,ARG 65,10.59,-2.48,0,0.57 3P28,LYS 195,10,42,-0,19,0,0,11 3BWT,LYS_601,11.56,-0.35,0.85,0.56 3NR5,CYS_116,12.11,0,0.4,2.71 3IL3,LYS 185,10,44,-0.06,0,0 1H4U,LYS 409,10.6,-0.14,0.0.24 1ES9,GLU_5,3.89,0.15,-0.44,-0.33 2HP7,TYR 124,11.05,-0.48,-0.04,1.57 3FXH,GLU_16,3,1.52,-2.19,-0.83 2OB5,ARG 57,13.91,-0.59,1.51,0.5 3CS1,ARG 33,12.68,-0.98,0.63,0.52 2IIA,ARG_67,12.75,-0.2,0.4,0.04 1TLV,GLU_152,7.51,2.98,0,0.03 3RLE, ARG_205, 13.83, -0.2, 1.47, 0.06 2IDC,GLU_119,5.03,0.36,0,0.17 3H13,CYS_254,13.62,0,0.52,4.1 3IRA,HIS_51,6.12,-0.29,0,-0.09 2Z0M,ASP_149,4.94,0,0.09,1.05 1PNE,LYS_126,10.99,-0.65,0.46,0.67 4H86,TYR 14,10,12,-0,25,0,07,0,3 3EYE, ASP_43, 3.28, -0.82, 0, 0.31 1TJE,ASP_15,2.57,-1.11,-0.33,0.21 1ZCE,LYS_108,11.15,-0.36,0.72,0.29 1RI6,ASP 35,4.01,0,-0.04,0.25 1TP6,ARG_100,13.01,-0.31,0.62,0.19 1A8Q,ARG_55,12.68,-1.7,0.6,1.28 3CRM,ASP_265,3.86,-0.03,-0.4,0.49 2FM9,ARG 204,12.37,-0.3,0,0.17 2GEN.ARG 144.12.39.-0.11.0.0 3LE4,ARG_331,12.35,-0.56,0.16,0.25 1Q5Z,LYS_520,11.48,-0.32,0.85,0.44 3GG6,TYR_44,9.11,-1.22,-0.34,0.66 1R7J,TYR_34,9.89,0,-0.36,0.26 1SJ8,ARG 624,12.52,-0.38,0,0.4 3OKQ,GLU_636,4.56,0.25,0,-0.18 2BT8, ASP_212, 2.48, -2.19, 0, 0.88 2XJ4,GLU_226,4.81,0.35,0,-0.04

2EJX.ARG 62,12.97,-0.31,0.15,0.63 20HT.GLU 69.5.22.0.69.0.0.04 3U2R,LYS_29,11.07,-0.23,0,0.81 1CBY,ASP_69,2.92,-1.32,-0.06,0.5 208P,LYS 103,9.98,-0.32,0,-0.2 2W0G,ASP_245,3.29,-0.79,0,0.28 1YM5.GLU 254,10.41,5.38,-0.84,1.37 3JZN,ARG_306,12.53,-0.09,0,0.11 1WNH,LYS_210,10.29,-0.25,0,0.04 1JYH,GLU_79,4.51,0.06,0,-0.05 1X91,LYS_50,10.4,-0.11,0,0.01 1PNE,LYS_107,10.55,-0.18,0,0.24 3BWT,ARG_858,12.86,-0.44,0.38,0.42 2PGE,ASP_102,3.55,-0.73,-0.47,0.95 2WB8.HIS 737.7.63.-1.22.1.55.0.8 1R53.GLU 128.4.79.0.79.-0.14.-0.36 2FM9,TYR_186,13.79,0.35,0.86,2.58 1WXQ,LYS_161,10.35,-0.14,0,-0.01 3ON1,LYS_55,10.34,-0.21,0,0.05 2VAN,GLU 295,5,0.75,0,-0.25 3KB5,GLU_387,4.55,0.19,0,-0.14 3ASA,TYR_14,9.09,-0.82,-0.33,0.25 3N2T,LYS_286,10.11,-0.14,0,-0.25 2ZTY,ARG 39,13.44,-0.51,0.76,0.69 1R53,ASP 273,4,1,0,-0,01,0,31 2BLL,ASP_529,4.06,0,0,0.26 2V5B,LYS_177,10.25,-0.44,0,0.19 1ZCU,LYS_26,10.2,-0.57,0,0.27 3Q1C,ARG 72,12.03,-0.37,0,-0.1 1RL0,ASP_197,3.91,0,-0.04,0.16 1O3X,LYS_295,10.19,-0.25,0,-0.05 3HVM,LYS_243,11.22,-0.57,0.54,0.75 1MUF, ARG 115, 13.01, -1.29, 0.7, 1.1 3016.GLU 76.3.85.0.36.-0.53.-0.48 208P,ASP_111,3.32,-0.43,-0.39,0.34 3RKV,LYS_205,10.66,-0.09,0,0.25 1RI5,TYR_169,10.13,-0.05,-0.4,0.59 2QZQ,ASP_71,3.53,-0.85,-0.48,1.05 2F4Q,ARG_4,11.12,-2.72,0,1.33 1NFN,LYS_157,10.83,-0.16,0.04,0.45 4FLE,GLU_50,4.77,0.25,0,0.02 2E3C,CYS 354,11.02,-0.23,0.09,2.16 3I47,ARG 229,12,35,-0,15,0,0 1P4X,LYS_27,10.38,-0.12,0,0 1AD6.LYS 524,11.17,-0.26,0.71,0.23 3TIR,ASP_224,2.83,-0.85,-0.51,0.39 3CS1,GLU 61,4.74,0.14,0,0.09 1X1E.ARG 3,13.9,-1.03,1.36,1.08 3CAX,ARG_374,12.47,-0.27,0,0.24 3EVP,GLU_175,4.84,1.02,-0.79,0.11 2XMZ,ARG_134,11.57,-1.47,0.39,0.16 3B79.TYR 16.10.76.0.0.1.0.66 2Q5X,ASP_732,3.06,-0.76,-0.27,0.28 3UX2,ASP_49,1.85,-2.42,-0.3,0.77 2I88,LYS_436,10.39,-0.11,0,0 3RNV,TYR_429,10.34,0,0,0.34 1YOY,LYS 157,10.69,-0.22,0.0.41 1ZKZ,TYR_99,10.54,0,0.02,0.52 3BCY,GLU_40,3.51,0.16,-0.84,-0.32 3HVW,ASP 183,3.53,-0.85,-0.37,0.95 3HYO,ARG 51,11.91,-1.44,0.05,0.79 3A2Z,ARG_144,13.11,-0.55,0.84,0.32 10GL,ARG_161,12.62,-0.4,0.04,0.48 3BWT,GLU_791,3.98,0.45,-0.54,-0.42 2H2W,LYS_174,11.35,-0.35,0.6,0.6 1XDZ,GLU_110,4.63,0.38,0,-0.25 3M7D,ASP_178,3.93,0,0,0.13 2CWC, ARG 7, 13.12, -0.15, 0.36, 0.41 1NAR,HIS_217,5.88,-0.34,0,-0.28

2BAA, ASP 224, 3, 45, -0.8, -0.18, 0.63 1YIB,ARG 214,13.66,-0.24,0.81,0.58 4FLE,LYS_59,11.19,-0.29,0.5,0.48 1TXJ,LYS_5,11.79,-0.5,0.85,0.94 2H2Z,CYS_128,12.56,0,0.39,3.17 2Y2T.ARG 39.12.34.-0.27.0.0.11 3LPZ,ARG 37,12.3,-0.23,0.0.04 4EUG,ASP_219,3.93,-0.6,0,0.73 1MML,HIS_204,5.18,-1.11,0,-0.21 3H04,GLU_205,4.81,0.37,0,-0.06 3I4T,LYS 100,10.33,-0.12,0,-0.05 20V2.TYR 249.10.76.-0.71.0.21.1.26 2E3C,ASP_256,3.66,-0.11,-0.45,0.42 3HUE, ARG_307, 12.19, -0.38, 0, 0.07 1L2H,LYS 109,9,52,-1,32,0,0,35 1NIJ.CYS 98,12.31,-0.13,-0.04,3.47 1Q8B,GLU_91,4.62,0.12,0,0 1X7F,HIS_269,4.92,-2.62,0.81,0.22 2NYC,ASP_278,3.75,-0.77,-0.03,0.76 3IDW,ASP_27,4.21,0,-0.01,0.43 3DSH.GLU 450.4.73.0.21.0.0.02 3UC9,ARG_110,11.7,-0.8,0,0 2PWQ,ASP_23,4.2,-0.6,-0.19,1.18 3H6O,ARG 50,12,19,-0,43,0,0,13 20RX.GLU 20.3.12.0.57.-1.29.-0.66 2H85,LYS_34,11.32,-0.25,0.69,0.38 2H2Z,LYS_12,10.98,-0.27,0.43,0.32 1MTZ,ARG_184,11.97,-1.24,0,0.71 3F6M,ARG_26,12.28,-0.22,0,0 2PGX,HIS_41,6.3,-1.32,0.76,0.37 1X04, ARG_130, 12.72, -0.24, 0.23, 0.22 1AD6,TYR_498,10.95,-0.44,0.68,0.73 2XMZ.GLU 252.5.01.0.32.0.0.19 2R0S,LYS 291,10.36,-0.16,0,0.02 2V5B,LYS_240,10.51,-0.17,0,0.18 2EJB,TYR_82,12.59,0.51,0.22,1.85 3ELI,GLU_129,4.73,0.28,0,-0.05 1X8F,TYR_41,13.35,-0.59,0.32,3.62 10XZ.GLU 209.4.02.0.16.-0.6.-0.03 3CQ1,TYR_19,10.36,0,0.15,0.21 10IS,GLU_193,4.77,0.24,0,0.03 3H6Q,GLU_68,4.68,2.17,-1.43,-0.57 1X1E,ARG 28,12.23,-0.27,0,0 1RI6,GLU_315,4.85,0.35,0,-6.94E-18 2BLL,GLU_633,4.45,0.18,0,-0.23 2FBI,ARG_71,12.27,-0.25,0,0.02 2AZL,GLU 122,4.42,0.22,0,-0.3 3EIZ,ARG 87,13,19,-0,41,0,69,0,4 1QYI,HIS_380,7.16,-0.2,0.46,0.4 2G9D,ASP 79,4,3,-0,34,-0,39,1,22 1AD6,ARG_451,12.85,-0.77,0.69,0.43 3RFF,TYR 97,10.27,0,0.07,0.2 1TXJ.GLU 154,2.06,0.64,-2.07,-1.02 1DVO,GLU_147,5.07,0.27,0,0.29 1UAJ,LYS_210,11.99,-0.82,1.55,0.77 1H4U,ARG_438,12.41,-0.88,0.34,0.45 3BOE,HIS 350,5,43,-2,12,0,76,0,29 1TJE,ASP_99,3.89,0,-0.03,0.12 2OB5,ASP 36,3.82,0,-0.25,0.27 4ECC,ASP_184,4.1,0,0,0.3 1YW5,ARG 109,13.07,-0.31,0.52,0.36 2GEN.GLU 145.4.56.0.06.0.0 3NJM,GLU_18,4.7,0.2,0,0 1XWM,GLU_24,6.28,2.16,-0.47,0.08 2AZL,ARG_19,11.6,-1.02,0,0.13 3SMD,GLU_106,4.11,0.73,-0.22,-0.89 3RLE,GLU_175,3.87,0.35,-0.69,-0.28 3ERF.TYR 146.9.51.-0.82.0.01.0.32 1ZP2,TYR_223,10.39,0,0.23,0.16

4GCO,ASP_207,3.58,-0.56,-0.07,0.41 1WYC,ASP_298,2.5,-0.98,-0.75,0.44 2CXY,LYS_90,10.09,-0.41,0,0 3SMD,GLU_68,4.48,0.54,-0.31,-0.25 1MML,ARG_110,12.29,-0.21,0,0 2CBE,ARG 27,11.35,-1.66,0,0.51 3LMF.GLU 79.4.66.0.13.0.0.03 2NRK,GLU_35,3.97,1.17,-0.71,-0.98 2VGM,LYS_183,10.45,-0.05,0,0 1XWM,GLU_57,4.89,0.13,0,0.26 1AT0,ARG 358,12.31,-0.5,0.0.31 2YLF,GLU_143,3.57,0.17,-1.1,0 1PDB,GLU_101,4.71,0.29,0,-0.07 1GQE,TYR_123,12.28,0.19,0.86,1.22 1ES9,ARG_149,11.63,-1.01,0,0.15 3DB9,ARG 159,12.28,-0.23,0,0.01 3T5B,ARG 259,10.86,-2.33,0.14,0.55 4DVD,LYS_180,10.41,-0.33,0,0.24 3QKY,LYS_169,10.2,-0.41,0,0.11 1TXJ.GLU 168.4.57.0.56.-0.17.-0.32 2QK1,ASP_411,3.95,0,-0.01,0.17 3BZT,GLU_276,3.64,0.45,-0.85,-0.46 1NIJ.TYR 151.13.49.0.0.58.2.92 3FRR,TYR_43,9.01,-0.85,-0.62,0.49 3ETV,CYS 269,12.77,-0.08,0.28,3.56 3RAZ,GLU_24,4.41,0.3,-0.14,-0.25 3A7L, ASP_117, 3.1, -0.88, -0.16, 0.35 2EDM,LYS_157,10.51,-0.3,0,0.31 2RH3,ARG_118,12.68,-0.15,0,0.34 3OA7,CYS_470,9.84,0,0.16,0.69 3BCY,GLU_113,4.52,0.15,0,-0.13 3GS3,GLU_217,4.61,0.11,0,0 1XAW,LYS_455,10.59,-0.1,0,0.19 2PGE,ASP 67,3.28,-0.85,-0.12,0.45 2X4L.LYS 99,10.45,-0.05,0,0 2IN0, ARG_92, 13.37, -0.3, 0.66, 0.51 3KB5,LYS_398,10.42,-0.08,0,0 3B7H,ASP_66,3.87,-0.1,-0.08,0.25 1WLY,ARG 87,12.7,-1.19,0.55,0.84 2FC3,ARG_112,12.57,-0.32,0,0.38 2F9F,GLU_41,4.18,1.22,-1.15,-0.39 1Q5Z,HIS_538,6.34,-0.2,0,0.04 2H2W,HIS 133,6.22,-0.28,0.06,-0.05 3V55,LYS 679,11.38,-0.18,0.39,0.67 1RAJ,LYS_375,11.08,-0.32,0.44,0.46 2X5Y,TYR_833,11.45,0.13,0.57,0.75 1EV8,ASP_66,3.42,-0.83,0,0.45 1JB3,ARG_115,12.62,-0.08,0,0.21 2JEO,LYS_108,10.53,-0.12,0,0.15 2CXY,CYS_101,8.93,-0.91,0.03,0.82 2V5B,ARG_100,10.65,-2.61,0,0.76 3L3P,HIS 275,6.61,-0.31,0,0.42 3ETU.TYR 203,12,0,0,46,1,54 1ZP2,LYS_37,10.43,-0.29,0,0.22 1HF8,ASP_260,3.21,-0.78,-0.04,0.23 4GCO,GLU_141,4.99,0.16,0.2,0.13 2GQV,TYR 46,10.49,-0.17,0,0.66 1J33,ASP 93,2.93,-0.68,-0.56,0.37 1PBV,GLU_120,4.61,0.09,0,0.02 4H89,ARG_98,12.2,-0.49,0,0.19 307K,GLU_143,3.41,0.34,-1.16,-0.26 3RJX.GLU 75.4.54.0.12.0.-0.08 1BKB,ASP_89,3.94,0,0,0.14 2Q99,ASP_127,3.15,-0.64,-0.31,0.29 1MJS,ASP_261,3.88,0,-0.24,0.33 2EEY,GLU_22,4.6,0.08,0,0.02 3V55,ASP 629,4,54,0,0,03,0,71 1RZ2,ARG_164,11.91,-0.98,0,0.39 1DTO,CYS_11,11.22,-0.04,0.27,1.99

2P65.TYR 95.9.73.-0.49.0.07.0.15 20K1.LYS 425,10.18,-0.3,0,-0.02 3C5V,CYS_312,10.84,-0.09,-0.23,2.16 3BCH,LYS_42,9.98,-0.2,0,-0.32 3ADO.GLU 47.3.38.0.2.-0.76.-0.56 200P.HIS 147.6.34,-0.4,0.05.0.19 1ZYL,ARG_49,12.48,-0.11,0,0.09 4DVD,GLU_41,4.53,0.03,0,0 3IRA,GLU_1,4.63,0.13,0,0 2QK1,ARG_423,12.57,-1.37,0.85,0.59 1JKS,LYS 167,11.51,-0.54,0.85,0.7 1MUF,GLU_272,4.67,0.1,0,0.07 2FBQ,LYS_49,9.61,-0.93,0,0.04 2E3S,GLU 398,4.53,0.27,0,-0.24 4AM1.ARG 229.13.59.-2.47.0.07.3.49 2Q99,ASP_238,3.78,0,-0.26,0.24 1GXN,TYR_428,11.8,0,0.38,1.42 2R2Y,ARG_122,13.49,-0.3,0.66,0.63 3MTT,TYR_449,9.4,-0.87,0,0.26 1IAP.HIS 192.6.39.-0.2.0.0.09 3G9T,GLU_92,4.41,1.57,-0.79,-0.87 2Q13,TYR_340,9.93,-0.1,-0.42,0.44 1PSW/TYR 140/10.93/-0.05/-0.33/1.31 1ILW,GLU 3,3.36,0.27,-0.71,-0.71 1PVT,HIS_87,6.81,-0.36,0.59,0.08 1EDG,HIS_87,3.41,-3.39,0.47,-0.17 4GA2,ASP_7,1.65,-2.01,-0.51,0.37 3RE9,GLU_98,2.78,0.97,-2.1,-0.58 3K8U.GLU 125.4.64.0.14.0.0 1J33,GLU_106,3.81,0.18,-0.62,-0.24 3ODJ,TYR_36,10.26,-0.07,0.12,0.21 1PSW,GLU_321,4.54,0.04,0,0 1XKR,LYS 190,11.25,-0.66,0.46,0.93 3EJG,ASP 153,3.12,-0.84,-0.03,0.19 1MUF,ASP_136,4,0,0,0.2 1L3K,LYS_106,10.53,-0.33,0,0.36 1BKB.LYS 138.10.15.-0.14.0.-0.2 3NR5,ARG 28,13,-0.64,0.52,0.62 2ZTY,LYS_133,10.69,-0.22,0,0.41 2PLO,CYS 91,12,28,-0.03,-0.04,3.34 1RAJ,TYR_454,13.05,0.85,1.08,1.12 3P28.HIS 192,7.09,-1.25,1.69,0.14 3MIX.GLU 607.3.89.0.18.-0.76.-0.02 1LPL,LYS_190,10.2,-0.15,0,-0.14 1WRU,ASP_44,2.81,-1.16,-0.22,0.39 3IPZ,LYS_169,10.76,-0.15,0.02,0.38 3FRR,ARG_51,13,-0.27,0.5,0.27 2F4Q,GLU_317,4.44,0.26,0,-0.32 3E7P,TYR_247,10.24,0,0,0.24 1P4X,ASP_241,3.76,-0.01,-0.15,0.13 1Q5Z,ARG 633,12.29,-0.21,0,0 1RHS.HIS 138.6.-0.79.0.08.0.21 3ZTA,GLU_32,5.12,0.72,0,-0.11 2Z0W,ARG_79,12.37,-0.13,0,0 2V4U,ARG_465,12.19,-0.44,0,0.13 2FL4,GLU 46,4.06,0.44,-0.67,-0.21 3BPP,ASP_42,3.13,-0.96,-0.43,0.71 4DND,HIS_105,6.47,-0.26,0,0.23 2IRM,ASP_17,4.05,0,0.07,0.19 2H14,TYR 260,9.83,-0.71,0.08,0.47 3EVN,LYS 206,10,46,-0,04,0,0 1LZL,ARG_174,12.99,-1.07,0.5,1.06 3V55,ASP_517,4.02,0,-0.21,0.42 2IQT,GLU_149,3.95,0.23,-0.2,-0.58 1059,LYS_284,10.18,-0.59,0,0.28 1X6J,HIS 61,6.45,-0.14,0.09,0 2X4J,GLU_41,3.64,0.5,-0.85,-0.51 1LPL,GLU_165,4.68,0.42,0,-0.25 1UCH,CYS 50,12.32,-0.06,-0.38,3.75

2H85,GLU_201,5.03,0.17,0,0.37 2B78,TYR 73,11,95,0,0,1,95 2IXM,ASP_175,3.56,-0.3,-0.26,0.32 2WOZ,GLU_411,4.39,0.15,0,-0.27 2NRR.HIS 469.6.26.-0.24.0.0 1MUETYR 211.12.48.-0.01.-0.16.2.64 3ZTA,GLU_96,4.63,0.22,0,-0.1 3GE9,GLU_66,4.4,0.16,0,-0.27 3EIZ,LYS_174,10.31,-0.19,0,0 3BB7.LYS 147.10.71.-0.09.0.0.29 3GA2,ARG_230,12.04,-0.55,0,0.1 1BN6,HIS_125,4.08,-1.73,0,-0.68 208P.ARG 17.12.15.-0.38.0.0.03 2AH5,LYS_201,10.45,-0.11,0,0.05 2G3A.ARG 136.12.75.-0.25.0.14.0.36 4EZB.LYS 269,10.65,-0.11,0.0.26 2IXM,GLU_246,3.66,0.27,-0.79,-0.31 3T5B,HIS_346,6.62,-0.4,0.02,0.5 2APL,LYS_6,10.43,-0.07,0,0 3EGN,ARG_458,12.65,-0.11,0,0.26 3F5D,HIS_35,5.81,-0.79,0,0.1 2HRZ,GLU_74,4.12,0.35,-0.74,0.02 2ZCO,ASP_228,4.14,0,0.09,0.26 1L2F,GLU 69,4.79,0.14,0,0.15 2012,LYS 91,10.57,-0.11,0,0.18 1ZBM,ARG_96,12.56,-0.3,0,0.36 3H8Y,ARG_51,12.31,-0.96,0.39,0.38 1P4X,TYR_62,12.95,0,0.13,2.81 1SJ8,GLU 586,4.79,0.39,0,-0.1 2FB6,TYR_104,11.85,0.4,0.37,1.08 2X4L,LYS_197,10.44,-0.06,0,0 3C6B,ASP_138,3.44,-0.84,0.06,0.42 2H8O,HIS 118,1.81,-2.51,0.3,-2.46 1JKS.ARG 53,12.3,-0.2.0.0 4DIU,HIS_222,6.1,-2.55,0.85,1.3 3EVZ,HIS_91,4.22,-2,0,-0.27 1JB3,HIS_33,6.37,-0.14,0,0.01 1RI6,GLU 309,4.58,0.07,0,0.01 1SIG,GLU_155,4.8,0.35,0,-0.05 1TLV,LYS_123,11.33,-0.46,0.85,0.44 2EYI,ARG_60,12.55,-0.4,0,0.46 20JO,ASP 518,3.84,0,-0,13,0,17 1WP5.GLU 241.3.21.0.76.-1.55.-0.49 2G7O,LYS_76,10.42,-0.08,0,0 3U0V,GLU_212,4.14,0.48,-0.85,0.01 1R53,ARG_224,11.71,-1.4,0.19,0.42 3EJC,CYS 114,10.77,0,0.08,1.69 3JV1,ARG_64,12.43,-0.3,0,0.23 1FHL,LYS_23,10.37,-0.41,0,0.28 4ECC,HIS_228,6.47,-0.25,0,0.21 3NJM,LYS 98,10.62,-0.13,0,0.25 3JSN,GLU_163,4.85,2.27,-1.44,-0.47 1QQL,ARG_14,12.07,-0.61,0,0.17 10XZ,GLU_188,4.61,0.34,-0.29,0.06 3KV0,GLU_43,4.74,0.17,0,0.08 3NBI,ASP_63,4.69,0,0.23,0.67 2A4D.LYS 209,10.37,-0.13,0.0 3FK5,HIS_293,4.37,-1.65,0,-0.47 1V43,LYS_191,10.57,-0.28,0,0.36 2GAU,ARG_208,12.39,-0.09,0,-0.03 2PPN, HIS 87, 6.25, -0.25, 0.0 2FG1,CYS_103,11.55,-0.33,0.14,2.74 3CRM,GLU_112,4.5,0.27,0,-0.27 2P65,GLU_163,3.5,0.64,-1.09,-0.54 3O16,ASP_192,3.94,0,-0.07,0.21 2YX0,ARG_338,13.11,-1.76,1.27,1.1 1JT9,HIS_143,6.52,-1.26,0.88,0.4 3EVN,TYR_50,11,0.23,0.3,0.46 2JHY,TYR_110,12.21,0,0.38,1.83

3ZRI,HIS -4,7.03,-0.23,0.76,0 4EZB,CYS 258,8.75,-0.89,-0.04,0.68 2CIU,ASP_105,2.95,-1.34,-0.37,0.85 2NMU,CYS_105,10.49,-0.84,0.23,2.1 4F85,ASP_154,3.77,-0.49,0.06,0.39 3I4T,GLU_203,4.53,0.35,-0.03,-0.29 4F8A,ASP_606,3.31,-0.84,0,0.34 3Q6L,LYS_113,11.29,-0.3,0.54,0.56 3HKX,ARG_31,12.39,-0.27,0,0.15 4DBX,LYS_11,10.32,-0.25,0,0.07 1RKA,ARG_244,12.44,-0.06,0,0 2IN0.ARG 416.11.76.-0.79.0.0.05 1TLV,LYS_58,10.38,-0.12,0,0 3K8J,HIS_253,6.55,-0.21,0,0.25 2HRZ.ARG 185.13.19.-2.36.1.6.1.45 2FPN.GLU 179.4.48.0.34,-0.36.0 2V81,ARG_78,12.46,-0.04,0,0 1AT0,ASP_359,2.34,-1.54,-0.37,0.44 1SFE,ASP_153,2.32,-1.61,-0.38,0.52 2FXT,ASP_309,4.32,0,-0.13,0.66 2H2Z,ARG_188,12.19,-0.34,0,0.04 1XTD,HIS_62,6.43,-0.07,0,0 2FBQ,LYS_70,10.45,-0.07,0,0.02 307K, HIS 139, 6.97, -0.69, 0.73, 0.43 2D7J.CYS 79.8.97.-1.78.-0.87.2.62 1A8Q,LYS_209,11.48,-0.28,0.85,0.41 1PVT,LYS_18,11.32,-0.57,0.85,0.54 1M5I,ARG_230,12.4,-0.11,0,0.01 1ZP2,CYS 92,9.09,-0.07,-0.34,0.52 2D59,LYS 43,10.6,-0.14,0,0.24 2OB5,TYR_125,10.66,0,0.24,0.42 2IQT,ASP_218,3.91,-0.03,-0.22,0.37 2BV9,LYS_260,10.59,-0.23,0,0.31 1SI7,ARG 119,12.51,-0.14,0,0.15 3ILC,GLU_129,4.22,0.54,-0.79,-0.03 4ANN,GLU_203,4.8,0.27,0,0.02 2P4D,ARG_149,10.78,-1.81,0,0.09 3AU3,TYR_500,10.67,0.15,0.24,0.28 1NJ4.LYS 270.10.29.-0.21.0.0 3NBI,ASP_160,3.81,0,-0.17,0.18 2Q07,LYS_374,10.64,-0.06,0,0.2 1KN3,TYR_181,11.69,0,0.15,1.54 2OJQ,TYR 513,10.31,-0.05,-0.06,0.42 2H14,GLU_313,3.6,0.26,-0.63,-0.53 3CAX,LYS_416,11.23,-1.11,0.85,0.99 2A1V,LYS_88,10.25,-0.25,0,0 1WNH,GLU 118,4.42,0.18,0,-0.26 3P28,ARG_32,11.85,-0.51,0,-0.15 1SI7,LYS_154,10.45,-0.16,0,0.11 1G5Z.TYR 101.10.57.0.-0.07.0.64 3GT0,CYS_10,10.46,-0.59,0.39,1.66 1PNE,LYS 25,10.31,-0.24,0,0.06 20V2.ARG 171.12.44.-0.06.0.0 3GG6,GLU_103,3.23,0.96,-1.57,-0.66 2PGX,TYR_222,10.23,0,0.16,0.07 1MML,ARG_241,12.36,-0.37,0,0.23 2G3A.GLU 87.3.95.0.14.-0.39.-0.29 2H85,LYS_316,10.37,-0.23,0,0.1 20JO.GLU 665,4,56,0,79,-0.67,-0.06 3C5V.GLU 213.3.53.0.41,-0.85,-0.53 1J85,ARG 45,11.98,-0.91,0.05,0.34 3IVF,ARG_91,12.41,-0.29,0,0.2 1YM5,GLU_93,3.59,1.48,-1.7,-0.69 3LH5,ASP_731,2.64,-1.99,-0.01,0.85 3RLN,GLU_715,5.32,0.85,0,-0.03 10GL,ASP_140,3.88,0,-0.05,0.13 3C5V,CYS_238,9.37,-0.18,-0.05,0.59 1K95,LYS 108,10,75,-0,14,0,0,4 1SQH,ARG_32,12.42,-0.46,0,0.39

3UC9,LYS_96,10.5,-0.23,0,0.23 2H2W,ASP_244,3.84,-0.65,-0.42,1.11 3M3P,ARG_221,12.76,-1.18,0.76,0.67 1PZC,TYR_22,10.93,0,0.17,0.75 4GCO,GLU_146,3.98,0.74,-0.85,-0.41 20PJ.CYS 220.9.5.-0.89.-0.1.1.48 1X7F,TYR_278,10.06,0,-0.11,0.17 1ZBP,LYS_133,10.41,-0.41,0,0.33 1UW7,ARG_99,12.65,-0.34,0.03,0.45 1X7F,ARG_3,11.64,-1.18,0,0.33 2H2Z,ASP_229,3.61,-0.27,-0.18,0.26 3GV0,ARG_315,12.12,-0.5,0,0.12 4DBX,GLU_274,4.88,2.29,-0.75,-1.17 1DTO.TYR 19,10.4,-0.85,0.07,1.18 1L2F,LYS 209,10.31,-0.45,0.0.25 3IL3,ARG 315,12.99,-0.68,0.57,0.61 2Z0M,TYR_324,10.35,0,0.11,0.25 1T95,ARG_83,12.27,-0.36,0,0.14 2Z84,LYS_183,10.67,-0.09,0,0.25 2YT4,ASP_636,3.92,0,0,0.12 1MN3.LYS 436.10.46.-0.05.0.0 3H13,ARG_315,11.76,-0.86,0,0.13 2R4Q,TYR_273,10.88,0.28,0.38,0.21 3P2F.ASP 180.3.57.-0.81.-0.64.1.21 1J33,GLU 229,8.72,5.05,-1.1,0.28 3L7N,GLU 64,4.19,0.39,-0.7,0 1AKO,GLU_239,4.72,0.25,0,-0.02 2GAU,LYS_215,10.44,-0.23,0,0.16 1JT9,LYS 234,10,49,-0,3,0,0,29 3M70,LYS_36,10.77,-0.27,0.06,0.48 2B0J,GLU_140,4.5,0.17,0,-0.17 3K8U,LYS_92,10.47,-0.03,0,0 2RGY,GLU_342,4.62,0.12,0,0 200K,HIS 37,7.23,-0.5,0.86,0.36 2|88,LYS 382,10,41,-0,23,0,0,14 3N2T,GLU_113,3.77,0.42,-0.8,-0.36 3GS9,GLU_16,5.06,0.49,0,0.07 2Q07,LYS_417,10.4,-0.1,0,0 2Z0M,GLU 173,4.12,0.43,-0.74,-0.08 1RAJ,ASP_459,4.03,0,0.02,0.21 3F1X.TYR 138.10.39.0.0.18.0.2 1EV8,ARG_21,12.42,-0.21,0,0.13 1JT9,HIS 222,6.24,-0.26,0,0 3A7L,GLU 14.8.29.4.42,-0.79.0.16 3CBN,ARG_126,13.18,-0.32,0.25,0.77 1YB2,ASP_13,3.1,-0.6,-0.51,0.41 3H9W,LYS_28,11.12,-0.29,0.33,0.59 3LJC,ASP_45,3.81,0,-0.17,0.18 3HUE,LYS_99,10.57,-0.12,0,0.19 2FXT,TYR_377,10.64,0,-0.15,0.79 3JZN,CYS_330,11.68,0,0,2.68 3PU6,TYR 84,10.13,0,0,0.13 3PU6,ARG 50,13.07,-0.31,0.49,0.39 4EKU,LYS_42,10.27,-0.3,0,0.07 3FHF,LYS_165,10.36,-0.1,0,-0.05 2AZL,ARG_44,10.86,-2.74,0,1.1 1G8P,GLU_86,4.02,0.25,-0.73,0 1Z3X.ARG 162.11.65.-0.69.0.-0.16 3F5D,GLU_18,6.72,3.33,-1.14,0.04 1MUF,CYS_288,10.14,0,0.04,1.1 1CBY,TYR_168,11.22,0,0.39,0.82 4FD6.GLU 212.4.43.0.17.0.-0.23 1LTU,GLU_124,2.89,0.73,-1.38,-0.97 1UCH,CYS_209,12.5,-0.07,0.09,3.47 1L2H,ARG_98,13.34,-0.68,0.63,0.89 10IS,GLU_262,4.69,0.19,0,0 1R53.GLU 204.4.0.68.-0.81.-0.35 3ADO,GLU_300,4.69,0.15,0,0.05 1SI7,ARG_191,12.54,-0.54,0.25,0.33

1XDZ.GLU 194.4.76.0.22.0.0.05 3LJI,CYS_109,10.02,-0.01,-0.03,1.05 1Z3X,GLU_111,4.77,0.47,0,-0.2 3E5T,GLU_86,3.94,0.5,-0.74,-0.32 2F4O,TYR 12,12.3,-0.65,0.32,2.64 2EEY,LYS 67,10.29,-0.18,0,-0.03 1JYH,GLU_147,5.28,1.18,-0.55,0.15 106D,GLU_23,5.55,1.41,0,-0.35 3IL3,ARG_288,13.06,-1,0.78,0.78 2W0G,ARG_167,12.73,-0.12,0,0.35 2ZCX.ASP 30.3.98,-0.05,-0.34,0.58 2YWK,GLU_24,4.63,0.11,0,0.02 2BDV,ARG_94,10.82,-1.76,0,0.08 1MUF,TYR_156,10.54,0,-0.22,0.76 2D0A.HIS 119.5.95.-0.39.0.-0.17 1P1L,ASP_98,3,-0.74,-0.77,0.7 2188,GLU_388,3.98,0.23,-0.8,0.06 3UX2,LYS_131,10.39,-0.11,0,0 2B2H,HIS_385,6.2,-1.35,0.66,0.4 1LZL.GLU 104.5.84.1.25.0.0.09 1ZBS,ASP_181,4.2,-0.11,0.15,0.36 1MD6,LYS_16,10.54,-1.42,0.85,0.61 1QQL,TYR_63,10.29,0,-0.08,0.37 2AHE,ASP 58,3.27,-0.76,-0.29,0.53 1VSM,ARG_74,12.09,-0.41,0,0 3N2T,GLU_172,4.63,0.15,0,-0.02 3BQW,GLU_160,5.31,1.62,-0.27,-0.54 4AM1,HIS_261,5.24,-1.21,0,-0.07 3RFF,ASP 48,4,18,0,0,18,0,19 2GZR,ASP_281,4.05,-0.2,-0.08,0.54 2E0T,HIS_96,6.17,-0.77,0.33,0.12 1N81,HIS_25,6.27,-0.23,0,0 1YLN,GLU 225,4.79,0.29,0,0 3EVN,ASP 61,4,24,0,0.03,0,41 1BN6,ASP_87,4.01,0,0.05,0.16 1LTU,TYR_48,12.28,0.48,0.74,1.06 3CSR.TYR 20.12.1.0.85.0.59.0.67 1KW4.CYS 32.9.93.0.-0.22.1.15 3UC9,ASP_42,3.13,-0.71,-0.25,0.29 1N81.TYR 84,11.26,-0.04,0.06,1.24 2OJQ,ARG_517,12.85,-0.21,0.05,0.51 1FO9,ASP 125,3.51,-0.79,-0.23,0.72 2FZP.GLU 273,3.33,0.38,-1.17,-0.39 105T,LYS_220,11.02,-0.54,0.46,0.61 2D7J,HIS_14,6.2,-0.27,0,-0.04 2GAU,ASP_16,3.44,-0.46,-0.39,0.49 1WLY,LYS_111,10.92,-1.11,0.85,0.68 1X7F,TYR_159,10.96,-0.85,0.33,1.47 2FD5,ARG_82,12.6,-0.61,0.37,0.35 3K8J,ASP_45,3.51,-0.9,-0.22,0.83 2B61,LYS 106,10.48,-0.22,0,0.2 4F3J,ARG 161,12,74,-0.3,0.03,0.51 1RAJ,ASP_79,2.95,-0.79,-0.42,0.36 3ZXY,ARG_95,12.81,-0.35,0.14,0.52 3EJG,CYS_81,10.92,0,0.03,1.87 3R2E,GLU 58,4.82,0.29,0,0.04 3N2T,GLU_48,4.79,0.52,0,-0.23 1DCF,GLU_74,4.63,0.19,0,-0.07 1WP5,ARG_283,12.12,-0.54,0,0.15 2YX0,HIS 67,5.7,-0.8,0,0.01 1PVT.LYS 213,10.48,-0.14,0.0.12 3COU, ARG_142, 13.98, -0.83, 1.57, 0.75 1DVO,HIS_153,6.3,-0.22,0,0.03 1T95,GLU_53,4.18,0.5,-0.48,-0.34 2PGE,ARG_88,13.43,-0.4,0.73,0.6 1J7G,LYS 12,11.19,-0.27,0.57,0.38 3IVF,GLU_291,4.02,0.63,-0.64,-0.45 1BKR,HIS_104,5.81,-0.37,0,-0.32 1UAJ,ARG_-3,12.47,-0.03,0,0

2CN1.GLU 273,4,44,2,18,-1,5,-0,74 1FKM,HIS 371,5.65,-1.66,0.75,0.06 1TWU,HIS_100,6.23,-0.22,0,-0.06 3B4D,LYS_247,11.27,-0.49,0.52,0.74 3PZ9,LYS 215,10,29,-0,23,0,0.02 1H4U.ARG 631.12.45.-0.23.0.0.18 1AKO.GLU 19,4,79,0,24,0,0.06 3CNU,LYS_23,11.11,-0.24,0.85,0 2RGY,LYS_105,10.37,-0.13,0,0 2Q98,ASP_68,2.34,-1.76,-0.11,0.42 1RKA,LYS 207,11.26,-0.28,0.43,0.6 20EW,ASP_314,3.82,0,-0.3,0.32 2ZCO,ARG_265,13,-0.79,0.57,0.72 1JKS,ARG_48,12.31,-0.23,0,0.04 2ZCX.GLU 25.4.23.0.61.-0.2.-0.69 2IOT.GLU 178,5.59,2.05,-0.6,-0.36 1LZL,GLU_145,4.58,0.08,0,0 1H4U,TYR_546,11.25,0.34,0.41,0.5 3ETU,LYS_237,10.45,-0.05,0,0 1ZBS,HIS 278,3.41,-2.73,0,-0.36 3CGW,GLU_67,4.74,0.24,0,0 3V55,ASP 640,4,0,0.02,0,17 1NWA,ASP_100,3.6,-0.89,0,0.69 3FS3,TYR 56,10.25,0,0.15,0.09 1KCM.TYR 18,13.82,0.0.33,3.49 1CHD,GLU_215,3.45,0.21,-0.85,-0.41 1EDG,LYS_71,9.33,-0.92,0,-0.25 1MTZ,ARG_49,12.17,-0.38,0,0.05 1W7B,LYS 28,10.03,-0.48,0,0.01 3T8R,GLU_94,4.02,0.21,-0.69,0 3FTT,LYS_11,10.36,-0.1,0,-0.04 2B2H,HIS_185,5.92,-1.39,0.74,0.07 1ZBM,ARG 180,13.45,-0.94,0.68,1.2 2YWX.ARG 38,12,28,-0.23,0.0.01 3ADO,ARG_171,11.6,-0.87,0,-0.03 3EZ7,TYR_287,12.31,-0.85,-0.11,3.27 1I60,LYS_235,10.29,-0.24,0,0.02 2CN1,LYS 64,11.89,-0.37,0.93,0.82 3ANJ,GLU_385,4.38,4.99,-3.72,-1.39 3JZ9,ASP_477,2.66,-0.85,-0.73,0.44 1RI5,ARG_104,12.14,-0.37,0,0.01 4GA2.ASP 140.4.04.0.0.0.24 1RI5,LYS 63,11.65,-0.39,0.81,0.72 4EKU,TYR_166,9.96,-0.21,-0.37,0.55 3T57,ARG_322,12.54,-1.62,0.66,1 1RWZ,LYS_140,10.52,-0.12,0,0.13 2CYG,ARG_298,12.74,-0.87,0,1.1 1T95,ASP 119,3.21,-0.63,-0.54,0.59 3FWU,GLU_17,3.87,0.33,-0.72,-0.24 3N2T,HIS_316,6.89,-0.57,0.85,0.11 2B0J.LYS 82,10.64,-0.13,0.0.28 3MEW, ASP 271, 3, 29, -0.82, 0, 0, 32 4F85,TYR_216,9.5,-0.53,-0.32,0.34 1T6L.TYR 69.10.0.-0.11.0.11 1IAP,LYS_160,10.98,-0.39,0.5,0.38 2Z61,HIS_61,6.37,-0.13,0,0 3T57.GLU 320.4.56.0.06.0.0 3MIX,LYS_410,10.81,-0.18,0.13,0.35 3LD1,LYS_178,10.33,-0.17,0,0 2CXY,ARG 70,12,25,-0,25,0,0 2l6l,TYR_158,10.36,0,-0.07,0.43 1DUP,LYS_3,11.38,-0.24,0.74,0.38 3B21,ARG_97,13.07,-0.32,0.54,0.35 3V75,GLU_4,3.23,0.5,-1.3,-0.46 4FLE,GLU_196,4.68,0.18,0,0 2G3A,TYR_62,12.36,0.85,0.68,0.84 3L3P,ARG_443,12.18,-0.5,0.04,0.13 2XHC,TYR_286,11,0,0.05,0.95 4FCU,LYS_203,10.53,-0.14,0,0.17

3HVW,ARG 190,12.36,-0.17,0.0.02 109G,CYS 147,10.51,0,0,1.51 3AUF,TYR_79,11.66,0.85,0.27,0.54 3U4K,ASP_115,3.24,-0.48,-0.37,0.28 2IF4,LYS_84,10.14,-0.52,0,0.17 1TR9.GLU 134,4.82,0.24,0,0.07 2Z61.CYS 140.11.29.0.0.1.2.19 2QK1,LYS_402,10.79,-0.36,0.33,0.33 2IDC,CYS_30,10.05,-0.46,0.1,1.41 3HVM,LYS 223,10.69,-0.09,0,0.29 3FK5,GLU 97,4.58,0.08,0,0 2VGM,HIS 356,5,44,-1,0,-0.06 3NR5,ARG_58,12.67,-0.16,0,0.34 2FD5,GLU_32,3.06,0.4,-1.42,-0.43 2EYI,LYS 64,10.27,-0.53,0,0.3 3ILC.ASP 107.3.68,-0.13,-0.19,0.2 2CXA,CYS_154,13.17,-0.44,1.2,3.41 1R3D,LYS 10,10,42,-0,08,0,0 1NAR,ARG_248,13.7,-0.36,0.86,0.7 1WNH,HIS 29,6.59,-1.63,0.85,0.86 1SOH.GLU 280.4.45.0.4.0.-0.45 10YI.GLU 250.4.74.0.24.0.0 3GFP,LYS_351,11.52,-0.25,0.85,0.42 4EKU,TYR 46,12,28,-0,29,0,11,2,47 2P0YASP 35.3.65.-0.1.-0.69.0.64 1R53,CYS_192,11.91,-0.36,0.31,2.95 2D2S,TYR_656,10.75,0,0.02,0.73 2BAA,LYS_152,10.1,-0.47,0,0.07 3F6F,ARG 205,12.52,-0.18,0,0.19 4FZR.GLU 99.4.65.0.21.0.-0.07 1T6L,TYR_227,10.48,0,0.02,0.46 1EQ6,ARG_207,12.27,-0.37,0,0.13 1C44.LYS 55.10.61.-0.2.0.0.32 2ZQ5,GLU 173,4.36,2.68,-1.06,-1.75 3I0C, ASP_83, 1.7, -2.04, -0.65, 0.59 1H4U,HIS_515,6.07,-0.39,0.03,-0.06 1ZYL,TYR_102,10.42,0,0.1,0.32 1TLV,ASP 128,4.42,0,0.12,0.5 3RVC,LYS 126,10,49,-0.25,0,0.24 1QQE,LYS_9,10.62,-0.19,0,0.31 1XEU,TYR_272,10.9,-2,0.29,2.61 2HRZ,ARG 129,11.16,-1.58,0,0.24 2BLL.GLU 569.4.76.0.16.0.0.1 1XTD,LYS_66,10.28,-0.22,0,0.01 4EKU,ARG_353,13.28,-2.4,0.32,2.86 2B3M,GLU_107,4.35,0.26,0,-0.41 1Q8B,HIS 83,6.83,-0.93,0.85,0.41 3AU3,LYS_580,10.57,-0.09,0,0.16 2GAU,ARG_66,12.13,-0.52,0,0.15 3GFP,GLU_378,4.63,0.27,-0.34,0.2 1XIP,LYS_158,10.7,-0.21,0,0.41 3AUF,HIS 138,4.95,-2.55,0.92,0.08 1GPP.GLU 45.3.9.1.16.-1.61.-0.14 1LN4,ARG_56,12.27,-0.24,0,0.01 2RFA,HIS_165,5.09,-1.65,0,0.23 2DFL,TYR_278,12.84,-0.78,0.77,2.85 3OKQ,LYS_633,10.38,-0.21,0,0.09 3LPZ,ARG_79,13.79,-1.04,1.31,1.03 30KY/HIS 149.5.86.-0.73.0.0.1 2CVB,LYS_140,10.43,-0.47,0,0.39 1Q5Z,LYS 606,10.34,-0.5,0,0.34 2DFL.CYS 124,13,72,-0,47,1,33,3.86 3H6Q,GLU_3,4.59,0.12,0,-0.03 3BQW,GLU_154,4.27,0.37,-0.15,-0.46 2C2Y,GLU_111,4.32,0.24,-0.37,-0.05 3MTT,TYR_453,10.16,-0.03,-0.21,0.41 1M5I,LYS_155,10.88,-0.41,0,0.8 3US6,GLU_137,6.28,2.49,-0.78,0.07 1W7B,CYS_133,13.43,0,0.81,3.63

2HXB,ASP_174,3.9,0,0,0.1 4DBX,TYR 4,12.93,0.4,0.75,1.78 1UCH,GLU_114,4.49,0.32,0,-0.34 3BWT,TYR_836,10.31,0,-0.25,0.56 4EF5,ARG_334,13.19,-0.39,0.67,0.41 2JHY.GLU 164,4.65,0.17,0,-0.02 2FB6.HIS 38.6.17.-0.31.0.14.-0.15 2NMU,HIS_84,5.53,-0.58,0,-0.39 1P4X,LYS_172,11.56,-0.38,0.85,0.59 2B0J,TYR_261,10.05,0,-0.09,0.14 3RJX,TYR_138,9.45,-0.72,-0.19,0.36 1KN3,GLU_83,6.68,4.34,-1.97,-0.19 1U53,LYS_46,11.3,-0.55,0.79,0.57 3LJI.ASP 161.2.97,-0.85,-0.67,0.69 2E0T,ASP_120,3.15,-0.81,-0.23,0.39 2RH3,ASP 129,2.34,-1.84,-0.04,0.42 1EYH,ARG 144,12.21,-1.15,0.3,0.55 1VJG,ARG_33,13.72,-1.16,1.48,0.9 3NBI,ARG_176,12.28,-0.22,0,0 4EZB,ASP 103,3.23,-1.37,-0.01,0.8 2Z14,ASP 48,4,48,0,-0,33,1 3LOD, ARG_85, 11.97, -0.86, 0, 0.33 3EX9,GLU_107,4.36,0.34,-0.23,-0.25 1JKS,ARG 253,12,41,-0,49,0,0,4 1ZHV,HIS 131,6.37,-0.12,0,-0.01 1TWU,HIS 60.6.29,-0.82,0.82,-0.22 2A6B,GLU_146,7.38,3.68,-0.79,-0.01 3KV0,GLU_84,4.54,0.23,0,-0.2 1GQE,ARG_154,12.25,-0.3,0,0.05 2H85,LYS_226,10.52,-0.08,0,0.1 3I4T,ASP_212,3.17,-0.41,-0.57,0.34 204D.LYS 61.10.7.-0.14.0.0.34 1PSW.GLU 68,4.8,0.2,0,0.1 4DND,ARG 88,11.62,-0.93,0,0.05 1WYC.GLU 92,4.62,0.22,0,-0.09 2XHC,LYS_186,10.34,-0.25,0,0.09 4GA2,LYS_94,10.32,-0.19,0,0.01 3M66,LYS_158,10.52,-0.22,0,0.24 2CW4,ARG 69,12.44,-0.21,0,0.15 2G5X,ARG_173,13.52,-2.78,0.58,3.23 2ZQ5,ARG_211,8.45,-3.3,0,-0.75 3V75,ASP_171,2.19,-1.52,-0.61,0.52 3EVZ,LYS_49,10.53,-0.09,0,0.12 3CO1,LYS 113,9.94,-0.57,0,0.01 2HNG,ARG_83,13.44,-0.36,0.75,0.55 3LJN,ARG_180,12.19,-0.38,0,0.06 4DVD,LYS_17,10.15,-0.39,0,0.05 208P,CYS 91,9.54,-0.06,0.03,0.57 3BQW,GLU_55,4.57,0.07,0,0 1WYC,ARG_107,11.57,-0.77,0,-0.16 3C2E,LYS_125,9.98,-0.52,0,0 1RL0,ARG_87,13.41,-0.32,0.72,0.51 2R57.GLU 264.4.62.0.12.0.0 1PVT,GLU_182,4.61,0.17,0,-0.07 2Q99,LYS_348,10.33,-0.07,0,-0.1 3Q6L,ARG_79,12.95,-2.21,1.23,1.43 2CE6,ASP_55,4.23,0,0.06,0.37 2GEN/ARG 51/13.08/-0.45/0.8/0.23 2B61,TYR_344,10.35,-1.04,0.16,1.24 3C6B,ARG_48,12.27,-0.23,0,0 3F6M,TYR_29,11.04,0.06,0.26,0.71 1X91.GLU 83.4.85.0.26.0.0.09 1WRU,GLU_147,4.68,1.61,-1.32,-0.13 2WOZ, ASP_318, 3.77, -0.83, -0.43, 1.24 2CBE,ASP_130,2.46,-1.37,-0.38,0.41 3ANJ,ARG_236,11.94,-1.43,0.39,0.48 3V75,ASP 211,3,47,-0,73,0,0,4 2Q13,GLU_365,2.44,1.57,-2.52,-1.11 2FD5,GLU_112,4.66,1.26,-0.97,-0.13

3EVN.LYS 49.10.36.-0.14.0.0 3FS3,ASP 73,3.88,0,-0.19,0.27 3F6M,CYS_124,10.74,0,0.26,1.48 2GZQ,ASP_109,3.16,-1.36,-0.13,0.85 3HVM.GLU 306.4.66.0.28.0.-0.12 3EJC.GLU 42,3.02,0.53,-1.69,-0.31 3IO0, ARG_171, 12.28, -0.38, 0, 0.16 3HNX,ASP_38,3.48,-1.7,-0.13,1.51 3KV0,CYS_118,11.19,-0.55,0.45,2.28 1TJE,TYR_205,10.23,0,0.02,0.21 2BDV.GLU 208,4,78,0,17,0,0,1 1AK1,ARG_173,12.35,-0.33,0,0.18 3K9I,GLU_61,4.72,0.31,0,-0.09 2B0A.LYS 121.10.41,-0.29.0.0.2 3IVELYS 300.10.05.-0.5.0.0.04 2B02,TYR_450,10.06,0,0,0.06 1WPA,TYR_493,11,-0.09,0.18,0.9 1U7U,ASP_210,5.53,0,0,1.72 2CN1,GLU_101,3.56,0.37,-0.85,-0.46 20GO,ASP 376,3.97,0,-0.13,0.3 3A2Z,LYS_56,9.9,-0.68,0,0.08 1MTZ,ASP_50,3.59,-0.66,-0.71,1.16 3FHF.GLU 75,4,44,0,41,-0,2,-0,27 3GS3.ASP 228.4.39.0.0.0.59 1BGF,ASP_23,2.99,-1.36,-0.32,0.87 2AHE,LYS_146,10.13,-0.1,0,-0.27 1RZ2,LYS_143,10.32,-0.12,0,-0.05 2QV2,LYS_27,10.41,-0.3,0,0.2 1T6L, ASP_155, 2.9, -0.79, -0.48, 0.37 3KV0,ASP_167,4.05,0,0.05,0.2 1L3K,HIS 77.5.35,-1.88,0.83,-0.1 2D2S,GLU_567,4.72,0.13,0,0.1 3KB5.HIS 442.6.2.-0.3.0.0 10IS.LYS 357,10.83,-0.69,0.32,0.7 3N0K,GLU_148,4.61,0.11,0,0 3RLN,GLU_579,3.9,0.49,-0.7,-0.38 3V4G,LYS 6,10.33,-0.27,0,0.11 2CWY,TYR 27,10.26.0.0.02.0.23 3LOD,CYS_106,10.35,-0.47,0.04,1.78 1SFE,ARG 15,13,24,-0.67,0.43,0.98 2ILR,CYS_399,11.95,-0.12,-0.01,3.08 3QKY,GLU_68,4.74,0.24,0,0 2Z0M,ASP_107,3.61,-0.81,-0.12,0.74 3F6M,LYS_92,10.47,-0.18,0,0.14 2HRZ,LYS_249,10.51,-0.1,0,0.11 2X4L,LYS_114,10.78,-0.15,0,0.44 2A4D,LYS_161,10.21,-0.3,0,0.01 3P28,HIS 187,6.36,-0.11,0,-0.03 2V4U,TYR_307,9.53,-0.47,-0.33,0.33 3FHF,TYR_172,13.34,-1.68,0.63,4.39 3UC9,GLU_121,4.55,0.22,0,-0.17 1XDZ.ASP 66.3.08.-1.14.-0.04.0.46 1ILW,GLU_101,4.67,0.28,0,-0.12 1WRU,LYS_52,11.03,-0.29,0.43,0.38 3I4T,LYS_232,10.46,-0.24,0,0.21 2H2W,GLU_199,4.36,0.2,-0.12,-0.23 2OBI,CYS_10,9.43,0,0.23,0.2 3BPV,LYS_8,10.25,-0.15,0,-0.1 3JRT,GLU_32,2.81,1.42,-2.29,-0.84 3M66,LYS_233,10.34,-0.39,0,0.24 4FH3.ASP 115.3.7.-0.43.0.0.33 3LQE,LYS_351,10.31,-0.48,0,0.3 4F85,ARG_160,12.48,-0.79,0.6,0.17 1RI5,CYS_73,13.15,-0.33,1.56,2.93 1LTU,CYS_211,13.17,-0.03,0.39,3.82 2EFK,ASP_260,3.67,-0.61,0.1,0.37 3ZTA,GLU_10,4.13,0.3,-0.43,-0.24 2AXO,ASP_130,3.31,-0.74,-0.08,0.33 3U2R,ARG_91,12.97,-0.89,0.68,0.69

4E9E,LYS 437,10,43,-0.07,0.0 2F8H,ARG 289,12.02,-0.5,0.0.02 1XKR,LYS_12,10.65,-0.24,0,0.4 3FK5,LYS_285,10.63,-0.31,0,0.44 4EVF.GLU 134.4.15.0.51,-0.75,-0.11 3G9G.ARG 51.13.34.-0.65.0.85.0.64 1PV5.GLU 161.6.13.1.73.-0.65.0.55 1XKR,ASP_9,3.83,0,-0.24,0.27 2IQT,HIS_51,5.42,-0.97,0,-0.1 2CBE,LYS_228,10.23,-0.16,0,-0.11 2QRX,HIS_91,6.12,-0.81,0.47,-0.03 1JSX,ARG_103,12.25,-0.25,0,0 1U53.LYS 110.11.22.-0.22.0.54.0.4 3LJN,HIS_212,4.79,-1.99,0,0.27 3A0X.ARG 684.13.28.-0.76.0.77.0.78 1T07.GLU 77.4.75.0.23.-0.01.0.02 4ESS,LYS_99,10.52,-0.46,0,0.47 2JEO,GLU_74,4.48,0.11,0,-0.13 1TR9,GLU_196,4.59,0.29,0,-0.21 3RJX,GLU 38,4.08,0.38,-0.23,-0.58 2XMZ,LYS_234,10.61,-0.16,0,0.27 2IOT.GLU 226,4.02,0.35,-0.52,-0.32 2CWC,ASP_237,3.79,-0.84,0.19,0.65 2Z84,TYR 39,12.82,0,0.49,2.33 2FBO.GLU 71.2.03.0.53.-2.2.-0.8 3GE9,ARG_217,12.41,-0.5,0,0.41 3T57,GLU_88,4.73,0.61,0,-0.38 3GE9,GLU_92,3.37,0.48,-0.67,-0.92 2CN1,ARG 165,13.22,-0.49,0.4,0.81 2GZQ,CYS_112,11.65,0.12,0.48,2.05 2FL7,ARG_106,13.87,-0.42,1.03,0.76 3ANJ,GLU_149,3.83,0.34,-0.49,-0.52 1RKA,GLU 299,4.74,0.15,0,0.09 1WPA, ASP 426, 3, 24, -0, 38, -0, 52, 0, 35 3TIR,ASP_71,4.04,0,-0.03,0.26 3C5V,GLU_117,4.24,0.76,0,-1.02 4EZB,ARG_255,13.91,-0.37,1.07,0.72 1RKA,TYR 36,10.46,0,0,0.46 2JKF,TYR_59,13.34,0.85,0.61,1.88 1ZBP,ARG_34,11.85,-0.65,0,0 2F8H,ARG_198,12.4,-0.1,0,0 3CAX,LYS 133,10.32,-0.1,0,-0.08 20JO.GLU 701.4.13.0.51.-0.31.-0.58 1BKB,ASP_26,3.92,0,-0.08,0.2 2CIU,GLU_117,4.64,0.39,0,-0.24 3GW3,ASP_344,3.11,-1.18,0,0.49 307K,ASP_142,3.98,0,0.03,0.16 2FG1.ASP 98.3.41,-0.59,-0.08.0.29 1X04,GLU_131,3.69,0.26,-0.74,-0.33 1M5I,GLU_154,4.88,0.53,0,-0.15 3H04,LYS 22,11.05,-0.8,0.72,0.63 4EUG.HIS 155,5.92,-0.46,0,-0.13 2H2W,LYS_198,10.49,-0.01,0,0 1M5LARG 186,12,46,-0.32,0.0.29 2ZCX,LYS_57,10.21,-0.29,0,0 2CVB,GLU_151,4.91,0.48,0,-0.08 4DBX.ASP 236.4.12.0.0.1.0.22 3GMS,ASP_144,4.48,-0.85,0.28,1.25 2Z0M,GLU_172,4.36,0.33,-0.12,-0.35 1EDG.LYS 295,9.88,-0.68,0,0.06 3V3T,TYR 265,10,13,-0,33,0,14,0,32 2Q5X,ARG_752,12.71,-0.55,0.14,0.61 1X6J,ARG_79,12.96,-0.45,0.4,0.51 3JRT,ARG_51,12.91,-0.43,0.26,0.58 2D7J,GLU_66,3.32,0.32,-0.8,-0.69 3RAZ,HIS 156,6,24,-0,53,0,24,0,03 3GEC,CYS_369,9.39,-0.18,0,0.57 3EVN,GLU_109,3.48,0.44,-1.08,-0.38 2QHT,GLU_146,4.36,0.29,0,-0.44

2GZQ,ASP_178,3.9,0,-0.03,0.14 2FL7,LYS_144,11.36,-0.31,0.79,0.38 2CN1,ARG_208,12.72,-0.42,0,0.63 3IPZ,GLU 166,4,55,0,42,-0.02,-0.35 3LPZ,GLU_175,4.54,0.17,0,-0.13 2B0LASP 80.3 52 -0.63 -0.19.0 54 3DZ1,ARG 279,13.86,-0.78,1.53,0.61 2A0J,LYS_22,10.86,-1.76,1.16,0.96 3VHJ,ASP_102,2.94,-1.52,-0.44,1.1 3N2T,ASP_139,3.5,-0.58,-0.1,0.37 20JQ,CYS 512,9.68,0,0.05,0.63 2IRM.GLU 212,4.63,0.13,0.0 3A7L,LYS_18,10.75,-0.17,0,0.42 3EVZ,LYS_177,11.07,-0.24,0.37,0.43 2D2S.GLU 697.5.54.2.26.-0.73.-0.49 1T95,ARG 99,12.38,-0.28,0.11,0.06 2EFK,TYR_42,10.44,0,0.02,0.42 1Z9L,LYS_39,10.57,-0.2,0,0.28 2BDD,ASP_30,4.35,-0.68,-0.53,1.77 3JZN,GLU 276,4.59,0.26,0,-0.17 3HUE,GLU_5,4.98,0.74,-0.55,0.29 1SJY,LYS 41,10.36,-0.17,0.02,0 1KW4,ARG_11,12.54,-0.33,0,0.37 1J85.GLU 113.4.69.0.19.0.0 1FO9.TYB 157.12.58.0.77.0.25.1.56 2FG1,GLU_147,4.61,0.11,0,0 3GYW,LYS_40,10.29,-0.21,0,0 1BKB,LYS_4,10.61,-0.08,0,0.19 2GEN,LYS_49,9.95,-0.68,0,0.13 1JKS.GLU 192,4.84,0.44,0,-0.09 2BLL,HIS_448,6.6,-0.28,0,0.39 1JKS,HIS_131,3.99,-3.19,0.53,0.15 1ZCE,LYS 104,10,29,-0,21,0,0 1HF8,TYR 211,12.94,0,-0.1,3.05 3I4T,GLU_195,4.8,0.32,0,-0.02 2QDJ,LYS_279,10.56,-0.13,0,0.2 1Y2Q,GLU_54,4.55,0.16,0,-0.1 2D2S,ASP_642,4.07,0,0,0.27 3CIV.ASP 9.3.52,-0.36,-0.12,0.19 3N0K,LYS_61,9.69,-1.12,0,0.31 2R0S,LYS_181,11.65,-0.73,0.85,1.03 2W2S,ARG_51,11.94,-0.71,0,0.16 2XHC,GLU 141,4.64,0.14,0,0 1TXJ,LYS_85,10.39,-0.11,0,0 1QZN,GLU_108,4.36,1.45,-1.58,-0.01 3DSH,ASP_312,3.83,-1.04,-0.06,1.15 20BI,ARG_9,12.38,-0.31,0,0.19 2YWX,HIS_37,5.82,-0.38,0,-0.3 2X4L,LYS_64,10.35,-0.15,0,0 2|88,LYS 395,10.32,-0.19,0.0.02 2IF4,GLU_154,4.79,0.79,0,-0.5 2B78, ASP 32, 3.99, -0.52, -0.26, 0.96 1Y0K,ARG_199,12.2,-0.3,0,0 3DSH,LYS_374,10.95,-0.3,0.37,0.38 3ODJ,CYS_19,11.76,-0.06,0,2.82 3NJM,ASP_81,2.29,-1.9,-0.05,0.45 30N1.HIS 47.6.37.-0.15.0.0.03 1V6T,LYS_53,10.46,-0.26,0,0.21 3V75,TYR_-3,10.17,0,-0.09,0.26 2YT4,GLU_610,4.7,0.28,0,-0.07 1EV8.LYS 2.10.5.0.0.0 20VO.GLU 63.3.7.0.21.-0.7.-0.3 2IN0,TYR_406,10.77,0,-0.03,0.81 208P,GLU_209,4.7,0.21,0,-0.01 4F85,GLU_84,2.85,1.3,-2.46,-0.5 3PP8,ARG_291,13.41,-0.4,0.84,0.47 3V75,ARG_254,11.99,-0.28,0,-0.23 2D59.CYS 67.11.11.-0.07.0.01.2.17 3Q1C,GLU_379,3.25,0.51,-1.28,-0.47

2G5X,ARG_84,13.51,-1.47,1.41,1.07 2EFK,GLU 221,4.89,0.22,0,0.17 1UJ8.GLU 75.4.62.0.45.-0.5.0.17 2IXM,LYS_60,10.7,-0.21,0,0.4 1OTM,LYS_63,11.45,-0.4,0.85,0.5 3OBS,ASP 137,3.91,0,-0.05,0.16 1KW4.LYS 64.10.63.-0.06.0.0.2 3QYB,ASP_911,4.07,0,-0.02,0.29 3EZ7,GLU_185,3.93,0.38,-0.72,-0.24 1F2V,GLU_111,4.63,0.17,0,-0.03 1XTD.GLU 123.4.77.0.09.0.0.18 1SIG,ARG_279,13.46,-0.78,1.06,0.68 1TXJ,TYR_18,11.87,-0.04,0.43,1.48 20DJ.GLU 204.4.82.0.48.0.-0.17 3EVN,LYS_214,10.35,-0.23,0,0.08 1ZYL, ARG 137, 12.06, -1.12, 0.09, 0.6 3P28,ARG_61,13.24,-0.33,0.49,0.59 2DG7,ASP_131,3.36,-0.35,-0.52,0.42 3LMO,ARG_83,13.9,-0.77,1.59,0.58 2AHE,LYS 249,10,28,-0,24,0,0.02 2ZTY,ARG 87,13.68,-0.64,0.97,0.86 1JT9,LYS_264,10.33,-0.18,0.02,0 2YWX,GLU_30,4.74,0.25,0,0 1RI5.GLU 83.4.08.0.79.-0.81.-0.41 1WXOLYS 148.10.36.-0.14.0.0.01 4ACJ,GLU_759,4.4,0.28,0,-0.37 3M7G,ARG 250,10.81,-2.99,0,1.3 10GL,ASP_41,2.69,-1.28,-0.49,0.66 2FL4,ASP_113,3.81,-0.01,-0.35,0.37 3ULX,LYS_115,10.17,-1.17,0.85,-0.01 2D7U,GLU_151,3.88,0.42,-0.78,-0.26 3V55.HIS 666.6.29.-0.16.0.-0.05 2HP7,ARG_64,12.33,-0.29,0,0.12 3IV4,GLU 86,4.6,0.11,0,-0.01 20RX.TYR 13.10.17.0.0.01.0.16 3M9A,ARG_74,12.4,-0.17,0,0.07 4DNU,LYS_175,10.36,-0.48,0,0.34 3BJV,HIS_127,6.73,-0.2,0,0.43 20PJ,ARG_307,12.53,-0.39,0,0.43 2CL3,ARG_131,13.08,-0.3,0.54,0.34 2JEO, ASP_133, 3.91, -0.12, -0.54, 0.78 3FFM,GLU_127,4.62,0.07,0,0.05 3A2Z,CYS 59,11.58,-0.86,0.19,3.25 3FRR,ASP 49,4,26,-0.01,-0.21,0.68 2Q07,HIS_320,6.47,-0.13,0,0.11 1X1E,GLU_223,3.4,0.34,-0.82,-0.62 2D59,LYS_58,10.45,-0.16,0,0.11 4FD6,TYR 196,12.91,0.68,0.57,1.66 3M9A,GLU_37,4.62,0.12,0,0 1O5T,CYS_305,12.77,-0.64,0,4.42 2OPJ,TYR_42,11.02,0,0.24,0.77 1XDZ,LYS_165,10.37,-0.19,0,0.05 4DEZ.GLU 51.4.12.0.95.-1.31.-0.02 3K8U,ARG_121,12.25,-0.33,0,0.07 4EF5,GLU_174,4.52,0.25,0,-0.23 1Y2Q,TYR_119,10.74,0,0.05,0.69 3A0X,CYS_634,9.85,0.12,0.14,0.59 1NRLARG 243,12,19,-0,28,0,-0.03 2PGE,TYR_178,11.28,0,0.23,1.05 3T8R,GLU_96,4.05,0.59,-0.86,-0.18 1GXN,GLU_571,4.69,0.3,0,-0.11 2EFK.GLU 128,4.7.0.33,0,-0.12 3O48, ARG_59, 12.51, -0.28, 0.01, 0.28 2EYI,ARG_46,12.43,-0.67,0.12,0.48 1J33,GLU_69,4.61,0.21,-0.04,-0.06 3JRT,LYS_113,10.52,-0.23,0,0.25 1WOU.GLU 55.3.64.0.29.-0.71.-0.44 3MEW, ASP_193, 2.6, -1.22, -0.65, 0.67 2D8N,ARG_151,10.42,-2.98,0,0.9

2012.LYS 153.10.63.-0.33.0.11.0.34 1MML,ASP 114,3,47,-0.65,-0.08,0.4 2W1R,ARG_109,12.38,-0.33,0,0.21 3LPZ,ARG_109,12.94,-0.26,0.35,0.36 3O1C,LYS 126,10.38,-0.18,0,0.05 3UV9.TYR 299.10.4.0.0.25.0.15 2X5Y,ARG_742,12.6,-0.31,0,0.4 3EJG,LYS 72,10.22,-0.13,0,-0.15 3RLN,LYS_759,10.33,-0.23,0,0.06 2IRM,CYS_184,12.38,-1.86,1.34,3.9 2NRK,HIS 142.6.2,-0.42.0.0.13 2OSA, ASP_314, 3.34, -0.82, -0.05, 0.41 2FGG,GLU_5,4.56,0.06,0,0 3A4C,GLU_480,2.54,0.47,-1.83,-0.6 1ILW.LYS 113.10.23.-0.12.0.-0.16 3E5T,LYS_74,10.51,-0.15,0,0.16 3C2E,ASP_177,3.25,-0.8,-0.18,0.43 3GT0,GLU_85,4.5,0.07,0,-0.08 1SQW,HIS_175,6.37,-0.13,0,0 3M3PARG 185,12,41,-0.3,0,0,21 2OJQ,TYR_608,11.92,0,0.4,1.52 2YWJ,LYS_185,10.45,-0.29,0,0.25 3TMO.ASP 192.3.7.-0.47.0.0.37 4DNU,ARG 55,13.21,-0.49,0.78,0.42 3MIX,GLU_506,4.59,0.17,0,-0.08 2C2Y,ARG_235,12.31,-0.19,0,0 3H6Q,TYR_166,10.18,0,0.08,0.1 1A8Q,LYS 144,11.4,-0.53,0.85,0.58 2YT4,TYR_653,10.43,-0.79,-0.33,1.55 1FKM,TYR_395,11.98,0,0.24,1.74 2Z0M, ASP_268, 3.4, -0.62, -0.28, 0.5 1G8P,ARG_289,11.3,-1.08,0,-0.12 1WRU,ARG 8,12.85,-0.33,0.29,0.38 3V75,CYS 21,11.69,-0.8,-0.42,3.91 1T95,LYS_146,10.64,-0.18,0,0.31 2EHG,TYR_26,11.66,0,0.43,1.24 1R3F,ARG_99,13.81,-0.54,1.02,0.84 3P28,TYR 152,10,27,0,0,0,27 2P4D,TYR_137,10.76,0,0.12,0.64 3GOZ.LYS 291.10.5.0.0.0 3EX9,ASP_83,3.12,-1.07,-0.15,0.54 1X8F,LYS 248,10.5,-0.15,0,0.14 108B.LYS 37,11.18,-0.22,0.44,0.45 2CXC,LYS_140,10.17,-0.13,0,-0.19 3RHE,ASP_112,4.04,0,0.06,0.18 3EVZ.LYS 142.10.44,-0.48.0.0.42 2RH3,LYS 97,10.58,-0.18,0,0.27 1WRU,GLU_57,4.28,0.46,-0.29,-0.38 1UJ8,HIS_6,7.52,-0.38,0.85,0.55 3BCH,ARG_117,12.01,-0.49,0,0 3RJZ,TYR 176,9.04,-0.85,-0.38,0.27 1XIP.ASP 290.3.93.0.0.0.13 1X6J,ARG_14,12.86,-0.26,0.22,0.41 3IDW,ASP_62,4.16,0,-0.09,0.44 2P4D,GLU_49,4.44,0.09,0,-0.15 2C2Y,ARG 280,11.52,-1.26,0.02,0.26 20EW,LYS_357,10.54,-0.08,0,0.12 2FBQ,LYS_136,10.19,-0.19,0,-0.13 4GA2,ARG_3,13.48,-0.34,0.8,0.51 1UXO,TYR 66,11.36,0,0.12,1.23 3O1C,ASP 378,4.03,0.0.03,0.19 20BI,GLU_157,4.27,0.87,-0.83,-0.27 3CNU,LYS_10,11.32,-0.23,0.62,0.42 1XWM,ARG_192,11.86,-0.61,0,-0.03 2P0L,GLU_71,4.06,0.32,-0.29,-0.48 3CX2,LYS 202,10.35,-0.15,0,0 1SQH,HIS_71,6.63,-1.06,0.89,0.29 4DBX,LYS_172,10.47,-0.11,0,0.08 1HUF,LYS_35,10.51,-0.23,0,0.24

3H9W,HIS_130,6.02,-0.63,0,0.15 1YTD.ASP 35,3.95,0,-0.05,0.2 4F85,ARG_299,12.2,-0.62,0.25,0.07 2YX0,GLU_93,4.55,0.19,0,-0.13 3AUF.ARG 91,12,79,-0,79,0,29,0,79 2IDC.GLU 23.4.2.0.37.-0.66.0 1WOU.GLU 6.3.81.0.83.-1.04.-0.47 1EYH,TYR_111,10.49,0,0.02,0.46 3GEC,GLU_438,4.7,0.14,0,0.07 1LTU,ARG_195,12.16,-0.46,0,0.13 2OJQ,TYR_677,13.4,0.85,0.57,1.98 3M16,LYS_45,10.24,-0.36,0,0.1 1U3Y,TYR 347,13.29,0,0,11,3,17 1NAR,LYS_2,10.45,-0.29,0,0.24 1NU.GLU 245.4.55.0.17.0.-0.13 3LH5.TYR 533,10.07,0.0.0.07 1QQE,LYS_32,10.72,-0.77,0.68,0.31 2B6P,ARG_233,12.03,-0.68,0,0.21 3EUR,LYS_88,10.66,-0.07,0,0.24 1MUF,ARG 179,12.53,-0.15,0,0.18 1C3K,LYS_126,10.83,-0.2,0,0.52 3ADO,LYS 260,10,41,-0,12,0,0.04 1JSX,GLU_111,4.52,0.2,0,-0.18 1WNH, ASP 179, 4.48, -0.53, -0.09, 1.31 3OAV,LYS 97,9.89,-0.35,0,-0.26 1WYC,ARG_302,13.46,-0.23,0.8,0.39 1MTZ,LYS_283,10.58,-0.12,0,0.2 10LR,TYR_17,11.4,-0.79,0.24,1.94 2RIS,ARG 169,13.82,-0.36,0.64,1.04 1I60,LYS_111,10.46,-0.04,0,0 2H01,ASP_152,3.31,-0.62,-0.46,0.6 2EA9,ASP_49,3.91,0,0,0.11 2E3C,TYR_308,10.39,0,0.09,0.29 301C.TYR 339,11.79,-0.02,-0.54,2.34 105J,GLU_11,5.01,0.3,0,0.21 2QK1,ARG_344,13.75,-0.77,1.5,0.52 1WNH,HIS_202,5.83,-0.83,0,0.16 1Y0K,ASP_5,3.56,-0.43,-0.06,0.26 1N81,LYS_157,10.43,-0.16,0,0.1 1059,CYS_202,10.08,-0.64,0,1.73 2E3S,TYR_482,11.78,-0.38,-1.06,3.23 1L2F,ASP 245,2,7,-1,23,-0,39,0,53 3CS1.TYR 125.12.67.0.-0.23.2.9 208I,ARG_91,12.64,-0.05,0,0.19 3JSN,GLU_34,3.83,0.18,-0.85,0 3FK5,CYS_331,11.52,-0.85,-0.01,3.38 3M66,ARG 358,12.37,-0.13,0,0 2BOO,TYR 105,11,17,0,0,26,0,91 3QAV,HIS_139,6.54,-0.93,0.7,0.27 1ZCU,LYS_226,10.47,-0.03,0,0 3GW3.GLU 26.4.75.0.33.0.-0.08 3UAH,ARG 383,11.45,-1.92,0.01,0.85 3Q6L,LYS_106,10.38,-0.21,0,0.09 2CN1.LYS 49.10.41.-0.08.0.-0.01 2B78,LYS_76,10.36,-0.14,0,0 1PNE,ASP_26,3.85,0,-0.11,0.16 2H14.GLU 258.3.81.0.23.-0.84.-0.08 1WOU,LYS_25,11.17,-0.4,0.69,0.38 10I7,GLU_46,4.7,0.2,0,0 1RKA.CYS 63.11.29.0.0.2.29 2Z14,LYS 117,10,18,-0,17,0,-0,15 2F9F,LYS_151,10.42,-0.06,0,-0.02 2WB3,GLU_282,4.56,0.1,0,-0.04 2QEV,ARG_51,12.77,-0.41,0,0.68 1U7U,GLU_200,5.65,1.97,-0.82,-0.01 2HRZ,ASP_100,4.1,0,0.11,0.19 1MUF,HIS_293,3.09,-2.85,0,-0.57 2AH5,ASP_115,3.88,0,-0.22,0.31 3U0V,ASP_86,3.47,-0.39,-0.16,0.23

3O2C,GLU 53,3.87,0.24,-0.69,-0.18 3ZTA,TYR 98,10.02,0,-0.3,0.33 3MEW,LYS_167,10.48,-0.12,0,0.1 100X,HIS_239,4.24,-2.23,0,-0.02 3N2T,LYS_306,10.53,-0.48,0,0.52 1L2F,LYS 163,10.39,-0.39,0.0.27 3I47,ASP 170,3.27,-0.85,-0.04,0.36 3C6B,TYR_265,10.47,0,0.21,0.27 3BWT,LYS_774,10.4,-0.07,0,-0.03 3LPZ,LYS_120,11.38,-0.29,0.85,0.31 3BA1,GLU 17,4.08,0.69,-0.83,-0.27 3V46.GLU 384.4.21.0.91.-0.79.-0.41 2DFL,ASP_168,4.27,-0.18,0.27,0.38 3US6,LYS_94,10.41,-0.23,0,0.15 1YB2.LYS 247.9.87.-0.63.0.0 2VGM,HIS 153,4,98,-1,38,0.03,-0.17 3CIV,GLU_151,5.77,2.78,-1.47,-0.04 1R3D,CYS_214,11.38,-0.02,0.23,2.17 2D2S,ASP_750,3.64,-0.26,-0.05,0.15 2H85,GLU 210,3.5,2.67,-2.7,-0.96 2RFA,HIS 84,3.82,-2.9,0.53,-0.3 4E8B,LYS_59,10.27,-0.12,0,-0.11 3RJZ,LYS_68,11.07,-0.55,0.73,0.39 1FKM,HIS 347,5.83,-0.79,0.0.11 3N2T.GLU 140.4.74.0.26.0.-0.03 2JHY,ASP_184,3.72,-0.68,0.19,0.41 2Z0M,ASP_206,1.72,-2.3,-0.4,0.61 3H9W,ASP_59,2.77,-1.3,-0.34,0.61 3U2A,GLU_95,5.21,0.57,0,0.14 3FTT,ASP 185,3,94,0,0,0,14 3IBT,ARG_180,11.46,-1.3,0,0.25 2V1L,GLU_91,4.83,0.29,0,0.04 2FB6,ASP_54,2.17,-1.83,-0.38,0.58 1J85,LYS 71,10.4,-0.11,0,0.02 4D8L,ARG_270,12.7,-0.64,0.48,0.35 3ANJ,ARG_282,13.85,-1.75,1.63,1.48 30NH,GLU_515,5.38,0.67,-0.01,0.22 3V1Q,GLU_645,5.07,0.57,0,0 2FBI.LYS 137,10.33,-0.15,0,-0.02 2OB5,ARG_78,12.08,-0.66,0,0.24 2D8N,LYS_192,10.66,-0.17,0,0.33 4FD6.ARG 27.13.93.-0.48.1.18.0.73 3UX2.ARG 45.13.9.-0.28.0.94.0.74 105T,LYS_465,10.24,-0.1,0,-0.16 1U3Y,TYR_316,11.73,0.69,0.15,0.9 3PZ9,GLU_92,5.26,0.67,0,0.09 1V43,ARG 21,12.4,-0.26,0,0.16 1QQL,LYS_101,10.88,-0.28,0.19,0.48 2I6I,GLU_42,5.15,0.34,0,0.31 2G7O.GLU 101.4.7.0.2.0.0 3B7H,CYS_57,10.93,-0.01,0.01,1.92 3AU3,GLU 658,4.1,0.28,-0.64,-0.04 1ZBS.LYS 131.10.72.-0.11.0.0.33 1J33,HIS_213,7.08,-0.3,0.8,0.08 3T5B,ARG_197,12.49,-0.17,0,0.17 1T6L,LYS_21,10.07,-0.5,0,0.07 1T3Y,ASP_68,3.59,-0.35,0,0.14 2CE6,ASP_22,3.22,-0.61,-0.35,0.39 2GAU,LYS_151,10.91,-0.95,0.85,0.5 1L3K,GLU_85,4.14,0.32,-0.14,-0.53 1SJ8,ARG 606,12.59,-0.37,0,0.45 1Q46,LYS_174,10.5,-0.22,0,0.22 1N81,ARG_160,13.38,-1.04,0.7,1.23 1N81,LYS_79,10.48,-0.15,0,0.13 1QQE,ASP_29,2.13,-1.73,-0.45,0.51 3CIV,HIS_158,5.36,-1.47,0.3,0.02 3Q1C,ASP_101,1.87,-3.03,-0.05,1.15 1MIX.LYS 357.10.54.-0.12.0.0.16 2CXA,ARG_80,12.4,-0.1,0,0

2D7U,LYS_94,10.76,-0.14,0,0.41 3DZ1,TYR 36,13.56,0,0.34,3.21 1TR9.HIS 23.5.7.-0.85.0.0.05 1TXJLYS 40.10.36.-0.14.0.0 2CWC,ARG_236,13.63,-0.17,0.8,0.5 4AM1.LYS 16,10.25,-0.59,0.0.34 1R9W.LYS 210.10.56.-0.23.0.0.29 3GW3,GLU_278,4.48,2.66,-2.01,-0.68 4FH3,GLU_375,4.72,0.24,0,-0.03 1TXD,GLU_776,4.51,0.17,-0.15,0 2AHE,LYS 238,10,53,-0.07,0,0,1 1AK1,ASP_45,4.16,0,0.06,0.3 1AK1,TYR_156,12.63,-0.23,0.19,2.68 2FL4,ASP 67,3.82,0,-0.13,0.16 2CN1,ASP_204,3.67,0,-0.44,0.32 2ZCO,CYS 44,13.07,-0.03,0.61,3.49 2DVK,ARG_171,11.26,-1.36,0,0.12 2Z14,TYR_42,10.22,0,-0.12,0.33 3HNX,ARG_79,13.53,-0.39,0.78,0.65 4FLE,ASP 179,3.65,-0.38,-0.08,0.31 2VAN,LYS 230,10.31,-0.24,0,0.05 3I4T,GLU_259,2.51,1.76,-2.83,-0.91 2BDD,TYR_122,9.91,-0.33,0.09,0.15 1PSW,LYS 71,10.42,-0.08,0.0 3EZ7,TYR 93,12.25,0,0.13,2.12 1BN6,ARG_41,13.74,-0.57,1.22,0.6 2CXC,HIS_19,6.17,-0.28,0,-0.05 3TMO,TYR_292,11.61,0,0.38,1.24 1U53,ASP_183,2.91,-1.06,-0.38,0.55 2Z61,ASP_153,3.88,0,-0.03,0.11 3US6,LYS_127,10.71,-0.36,0,0.57 1NIJ,GLU_137,4.7,0.38,0,-0.17 1FHL,TYR_218,12.33,0,0.46,1.87 2FI9,ARG 82,12.06,-0.19,0,-0.26 3P28,ASP_211,3.52,-0.61,0.02,0.3 2Q99,LYS_225,11.16,-0.58,0.85,0.38 2H8O,LYS_301,10.15,-0.53,0,0.17 3CO1,LYS_62,10.45,-0.24,0,0.19 4FCU,ASP 166,4.07,0,0.12,0.15 3IVF,LYS_278,11.66,-0.48,0.85,0.79 300P,TYR_30,10.66,0,0.25,0.41 2FPN,TYR_110,11.13,-0.05,0.24,0.94 1VJG,TYR 47,11.06,-1.69,0.45,2.31 3O16.LYS 73.11.15.-0.26.0.53.0.38 2VGM,GLU_169,4.54,0.39,0,-0.35 2EJX,LYS_65,11.13,-0.58,0.78,0.43 3BZT,ASP_308,3.67,-0.66,0,0.52 3RFY,ASP_414,3.38,-1.8,-0.56,1.95 3IVF,LYS_324,10.45,-0.05,0,0 2CXY,GLU_104,4.11,0.87,-0.85,-0.41 3CO1,ASP_103,3.62,-0.15,-0.52,0.49 3IU5,LYS_100,11.32,-0.73,0.85,0.7 1WXF.GLU 91.3.73.0.33.-0.72.-0.38 3F6F,ARG_13,11.83,-3.29,0.08,2.54 2CI3,LYS_33,10.2,-0.23,0,-0.07 2P1W,GLU_141,4.67,0.25,0,-0.09 1HUF,ARG_91,12.22,-0.28,0,0 1MHN.CYS 146.9.45.-0.09.0.12.0.42 3FK5,ARG_175,12.37,-0.29,0,0.16 3LMO,GLU_72,3.5,0.25,-1.14,-0.1 3AU3,ASP_700,3.82,0,0,0.02 1L3K.ASP 27.3.44,-0.79,-0.19,0.62 1NWA, ARG_158, 11.15, -1.71, 0, 0.36 2ZQ5,HIS_108,2.67,-2.91,0,-0.92 1GPP,ARG_172,11.3,-1.67,0,0.47 1UAJ,ARG_24,12.22,-0.28,0,0 3RKV.TYR 207.10.13.-0.19.-0.13.0.44 4H4J,LYS_239,10.42,-0.11,0,0.03 1XTD,ASP_147,3.64,-0.16,-0.38,0.37

20GO.HIS 489.7.1.-0.59.0.8.0.38 2WB8.CYS 702.11.06.0.0.02.2.05 1XFK,LYS_292,10.27,-1.01,0,0.78 1XWM,GLU_58,3.97,0.25,-0.44,-0.34 1IAP.ASP 128.3.87.0.-0.11.0.17 3BOW, ASP 50, 3, 17, -1, 06, 0, 0, 43 1AKO,LYS_169,10.36,-0.17,0,0.03 3A4C,ARG_452,12.56,-0.38,0,0.45 1IDK,TYR_202,10.52,0,0.26,0.27 3VJ8,GLU_91,4.58,0.09,0,-0.01 200K, ARG_57, 12.51, -0.14, 0, 0.15 3HKX,GLU_117,4.24,2.36,-1.96,-0.67 2P0Y,ASP_273,4.01,0,0,0.21 2HRZ,ARG 254,11.55,-1.34,0,0,4 4EZB.GLU 133.4.13.0.74.-0.58.-0.53 1ZHV,ARG_52,12.48,-0.59,0,0.56 2P0L,HIS_141,5.62,-0.62,0.03,-0.3 1FQI,ASP_339,1.36,-2.32,-0.52,0.41 1U7U,CYS_351,12.38,0,0,3.38 2YX0.TYR 125.11.23.0.0.1.23 3ANJ,TYR_290,10.61,-0.25,0.03,0.83 3BCY,LYS_79,10.49,-0.23,0,0.22 20EW.LYS 209,10.45,-0.09,0.0.04 1J7G,ARG 39,12.68,-0.33,0,0.52 4E6S,ASP_20,4.01,-0.14,0,0.35 3ANJ,ASP_265,3.4,-1.56,-0.07,1.23 1ZBP,GLU_263,4.41,0.14,0,-0.23 2B61,LYS 227,11.47,-0.29,0.85,0.4 1RAJ,LYS_405,10.48,-0.02,0,0 1YOY,TYR_135,11.51,-0.6,0.55,1.55 2012,HIS 59,6,28,-0,25,0,0.02 2CN1,LYS_80,10.79,-0.31,0.12,0.48 20KT,HIS 154,6.09,-0.24,0,-0.17 3V46.LYS 256.10.17.-0.33.0.0.01 10GL,GLU_152,4.74,0.24,0,0.01 3DSH,CYS_347,9.17,-0.48,0.31,0.34 3E7P.GLU 162.3.67.0.35.-0.85.-0.33 2D2S,ASP_544,3.43,-0.86,-0.5,0.99 2G9D,LYS_119,10.49,-0.46,0.26,0.19 1DOV.ARG 121.12.39.-0.11.0.0 3M16,ARG_327,13.58,-0.43,0.83,0.68 1Z3X.TYR 83,10.38,-0.42,-0.44,1.24 1NRI,LYS_256,10.33,-0.15,0,-0.02 1DOV,TYR_177,10.73,0,-0.17,0.89 3H5T,ASP_268,2.87,-0.85,-0.48,0.39 2JEO,TYR_130,10.21,0,-0.06,0.28 3DSH,CYS_330,11.26,-0.48,-0.72,3.47 1ZKZ,LYS_10,10.48,-0.39,0,0.37 2BV9,LYS_83,10.56,-0.13,0,0.19 1WNH,ASP_100,4.09,0,-0.05,0.33 3AUF,LYS 131,11.43,-0.28,0.81,0.39 1YM5.LYS 67.11.21.-0.91.0.85.0.77 3PBH,ARG_20,13.33,-0.28,0.73,0.39 1JB3,GLU_54,4.83,0.34,0,-0.02 1PSW,HIS_324,6.1,-0.39,0,0 4DBX,GLU_10,5.15,0.46,0,0.19 2G5X,LYS_205,10.58,-0.11,0,0.19 3NZL,HIS_7,6.2,-0.27,0,-0.03 3JZ9,HIS_338,6.2,-0.09,0,-0.2 3COU,GLU 118,4.65,0.15,0,0 3EJG,ASP 18,2.61,-1.59,0,0.39 2Q5X,LYS_735,10.63,-0.13,0,0.27 3LH5,ARG_757,11.75,-0.75,0,0 2CWY,GLU_87,3.37,0.89,-1.65,-0.37 3JV1,ASP_184,4.34,0,0.23,0.32 1KCM,ASP 243,2.97,-1.06,-0.17,0.41 2ZQ5,GLU_126,4.31,1.95,-0.67,-1.48 20EW,LYS_339,10.42,-0.08,0,0 2JHY,ASP_188,3.46,-0.85,-0.19,0.7

3HUE,ARG_155,12.61,-0.61,0.05,0.66 3UPD,LYS 153,11,15,-0,53,0,61,0,58 3ZXY,ARG_268,12.28,-0.35,0,0.14 3UC9,GLU_130,4.79,0.15,0,0.14 3V46.GLU 285.4.56.0.16.0.-0.12 3V55.ARG 435.12.33.-0.34.0.0.17 1KN3,ARG_146,10.21,-2.43,0,0.14 3E0H,HIS_40,6.37,-0.22,0,0.09 3CIV,ARG_14,11.24,-1.26,0,0 2C2Y,ASP_205,2.94,-1.06,-0.45,0.67 1JT9,GLU_80,4.03,0.25,-0.61,-0.11 2AH5,TYR_208,11.03,0,0.33,0.71 1WXF,LYS_173,10.21,-0.52,0,0.23 3ETU,GLU_229,4.59,0.09,0,0 2GZO.LYS 36.10.17.-0.32.0.-0.01 3BPP,ARG_208,12.44,-0.06,0,0 1N81,LYS_150,10.39,-0.11,0,0 2YX0,LYS_168,11.27,-0.52,0.85,0.45 1V6T,ASP_138,4.01,0,0,0.21 1RSS,GLU 52,4.59,0.1,0,-0.01 3QKY,ARG_223,13.38,-0.37,0.81,0.45 30NH,LYS 455,10.82,-0.33,0.16,0.5 2BLL,GLU_545,3.08,1.09,-1.34,-1.15 2RFA,HIS 73,6.39,-0.66,0.1,0.45 20VO.TYR 22,10,29,-0,1,-0,14,0.53 2XMZ,GLU_120,4.39,0.27,-0.31,-0.08 3A7L,TYR_9,13.13,0,0.71,2.43 3L3P,GLU_449,4.23,0.73,-0.65,-0.35 2CVB,ARG 25,13.11,-0.39,0.61,0.38 1J33,HIS_283,4.23,-3.2,1.25,-0.32 3R87,LYS_29,10.39,-0.23,0,0.13 3M66,GLU_401,4.55,0.2,0,-0.15 3JSN,ARG 177,12.36,-0.29,0,0.14 2BT8,ASP 310,3.83,-0.14,-0.07,0.23 2NYC,TYR_231,10.26,0,0,0.26 1T3J,LYS_718,10.4,-0.1,0,0 3MTT,CYS_501,9.33,0,0.09,0.24 2CIU,LYS 160,10.47,-0.16,0,0.14 3I82,ARG_131,12.37,-0.17,0,0.04 3V55,ASP_642,3.32,-0.59,-0.22,0.34 2FZ4,TYR_54,10.46,0,0.05,0.41 2ZCO.ARG 159,13.13,-0.78,0.6,0.81 3ELI,LYS 138,10.37,-0.42,0,0.29 2QOP,ARG_131,12.32,-0.21,0,0.03 4F85,ARG_158,13.53,-0.49,0.97,0.55 1T3J,LYS_689,10.73,-0.15,0.38,0 1ZP2,ARG 45,12.66,-0.51,0.18,0.49 3EVP.GLU 248,4.08,0.33,-0.79,0.03 1BGF,LYS_75,10.45,-0.05,0,0 3KB5,HIS_394,5.24,-1.71,0.13,0.32 3N0K,LYS 84,11.2,-0.36,0.16,0.9 3RLN.LYS 628.11.11.-0.7.0.74.0.56 2W2S,GLU_137,4.68,0.41,0,-0.23 3GYW, ASP_134, 4.36, 0, -0.27, 0.85 3LJC,GLU_128,4.59,0.25,0,-0.16 2DG7,ASP_109,3.53,-0.21,-0.8,0.75 3F1X.ARG 118,12.33,-0.17,0.0 4EKU,ASP_293,3.37,-0.76,0,0.32 2OB5,GLU_94,3.08,0.45,-1.67,-0.19 1Q2Y,ARG_19,12.82,-2.81,1.39,1.74 3F7M,HIS 150,5.89,-1.47,0.4,0.46 1G5Z,GLU_121,4.4,0.18,0,-0.28 1T6L,ASP_249,3.19,-0.81,-0.06,0.26 3IVF,ARG_178,12.78,-0.36,0.16,0.48 4FZR,GLU_143,4.57,0.13,0,-0.06 2WB8,GLU_482,3.88,0.23,-0.69,-0.16 20KT,ARG_143,13.35,-2.28,0.09,3.04 4GCO,LYS 147,9.96,-0.55,0,0.01 1RZ2,TYR_138,13.67,0.47,0.52,2.68

3M7D,GLU_21,4.9,0.49,0,-0.1 2W0G,ARG_246,12.43,-0.07,0,0 1SUU,ASP_540,3.57,-0.41,-0.05,0.22 3JSN.ASP 291.4.44.0.0.17.0.47 4E8B,LYS_133,11.09,-0.28,0.4,0.47 1DZF,GLU_163,4.66,0.17,0,-0.02 1ZCE.ASP 48.4.63.-0.74.-0.33.1.9 2V4U,LYS_392,10.2,-0.33,0,0.03 2PLQ,CYS_300,8.53,-0.8,-0.21,0.54 1EDG,ASP_112,4.07,0,-0.13,0.4 1SI7,LYS 96,10.14,-0.3,0,-0.06 20VT.GLU 75.4.6.0.08.0.0.02 1KCM, ARG_246, 12.69, -0.2, 0, 0.39 2BLL,CYS_558,11.57,-0.14,0.19,2.53 2BLL.GLU 644.5.55.1.01.-0.07.0.1 3ZSL,ARG 183,12,39,-0.07,0,-0.04 4DND,ARG_94,12.22,-0.24,0,-0.04 1Q46,LYS_103,11.46,-0.37,0.68,0.65 2E3C,LYS_429,10.18,-0.68,0,0.36 3F7M,TYR 241,10.3,0,0.05,0.25 2EJX,LYS_109,10.33,-0.17,0,0 3TOW,CYS_95,11.29,-0.16,0.1,2.34 4DND,TYR_25,11.43,0.28,0.64,0.51 30NH,LYS 468,11,16,-0,37,0,65,0,38 1JT9.GLU 54.4.53.0.31.0.-0.29 1AD6,LYS_530,11.37,-0.45,0.85,0.48 3EX9,ARG_129,12.4,-0.48,0,0.38 3EIZ,TYR_31,10.33,0,0.03,0.3 1EV8,ASP 85,2.73,-1.63,0,0.56 2V81.TYR 137.10.68.0.0.14.0.54 2Q13,LYS_130,10.47,-0.48,0,0.45 2ZCO,LYS_17,10.41,-0.09,0,0 1XEU,ARG 144,13.42,-0.28,0.58,0.63 2CXA, ARG 37, 13.15, -0.99, 1.21, 0.43 3GOZ,LYS_253,10.42,-0.25,0,0.18 1VJG,LYS_41,10.44,-0.23,0,0.16 2D2S,ARG_591,13.33,-0.76,0.86,0.72 1LTU,ARG_35,12.24,-0.44,0,0.18 1ZCU,ARG 32,12,14,-0,79,0,0,43 2Z0M,ARG_115,12.47,-0.52,0,0.49 1D2K,LYS_159,11.11,-0.98,0.85,0.74 3V4G,HIS_91,6.45,-0.56,0.07,0.43 4DIU,HIS 191,6.29,-0.24,0,0.02 2VGM,ASP_295,3.04,-0.76,-0.65,0.65 3I4T,LYS_267,10.91,-0.43,0.46,0.38 10GL,LYS_275,10.76,-0.5,0.53,0.24 2CIU,LYS 219,10.45,-0.06,0,0 1RKA, ARG 227, 13.64, -0.61, 1.04, 0.72 20BI,HIS_168,6.34,-0.22,0,0.05 1P6F,HIS 40.6.55,-0.8,0.85,0 2A4D,ARG_131,12.59,-0.07,0,0.16 1YTD,CYS 114,10.73,-0.76,0.15,2.34 3LD1,ASP 338,3,76,0,-0,16,0,12 3M16,GLU_254,4.11,0.23,-0.62,0 1FHL,TYR_209,10.81,-0.85,-0.03,1.68 2OJQ, ASP_465, 2.47, -1.89, -0.68, 1.24 1RZ2,ASP_195,3.78,-0.33,-0.11,0.42 3ADO,ARG_208,12.56,-0.6,0.32,0.33 3NJM,TYR_48,13.39,0,0.33,3.06 1DOV.LYS 238,10.42,-0.23,0.0.15 2CVB,TYR 112,13.31,-0.36,0.13,3.54 3LQE,TYR_328,13.85,0,0.01,3.84 3LD1,TYR_332,12.16,0,0.11,2.06 2FM9,LYS_147,10.43,-0.07,0,0 3IVF,ARG_82,11.92,-0.89,0,0.3 1DVO,ASP_102,3.8,0,-0.21,0.21 2CI3,ARG_41,12.87,-0.27,0,0.64 3M70,LYS 9,10.27,-0.18,0,-0.05 2X4G,ARG_253,12.46,-0.52,0.09,0.39 1UCH,HIS_175,6.21,-1.16,0.64,0.24 1WJG,GLU 20,4.6,0.14,0,-0.04 3DSH,GLU_446,3.95,0.31,-0.54,-0.32 1BN6,ARG_170,13.9,-0.72,1.42,0.71 3CAN,TYR_99,10.55,0,0.19,0.35 2H85,ARG 138,12.68,-0.27,0.14,0.32 4E8B.ASP 73.2.54.-1.59.-0.14.0.46 1XEU,ASP_154,3.83,-0.78,-0.01,0.82 3P2F,ARG_172,12.37,-0.25,0,0.12 3ETU,LYS_201,10.52,-0.15,0,0.17 3V46,HIS_381,6.06,-0.29,0,-0.13 1IAP.LYS 214,10.06,-0.89,0.0.46 3M3P,ARG_242,12.22,-0.32,0,0.04 2ZCX,ARG_112,13.56,-1.15,1.36,0.85 4DND,ARG 51,12.6,-0.2,0.03,0.28 1KW4,TYR 35,10.49,0,0.1,0.4 3F1X,LYS_44,10.29,-0.16,0,-0.05 2AD1,ARG_104,13.32,-1.51,1.54,0.79 4D8L,ARG_146,12.68,-0.49,0.32,0.36 3LPZ.TYR 263.11.14.0.0.1.14 2NYC,ASP_285,2.84,-0.82,-0.45,0.3 3F6M,TYR_91,9.12,-0.9,-0.49,0.5 3EGN,LYS_477,10.4,-0.09,0,-0.01 30KY,LYS 158,11.19,-0.82,0.59,0.92 4E9E,ASP_498,4.23,0,0.17,0.27 20KT,TYR_235,10.59,0,0.26,0.32 2CIU,ASP_206,3,-1.32,-0.54,1.05 1JSX,ARG_139,12.12,-0.54,0,0.17 3G9T,GLU_293,4.33,0.43,-0.29,-0.31 1EDG,ARG_237,12.35,-0.15,0,0 2Q98,ARG_21,12.5,-0.15,0,0.15 1KCM,GLU_79,4.56,0.07,0,-0.02 4DNU,GLU_182,4.2,1.4,-0.76,-0.94 1KCM,TYR 103,10.18,0,0.01,0.17 2CYG.TYR 108.10.58.0.-0.19.0.77 2V4U,GLU_483,8.15,4.35,-0.61,-0.09 3I4T,HIS_246,4.72,-2.06,0.43,-0.15 2BAA,ARG_187,12.3,-1.04,0.49,0.34 106D,GLU 79,3.87,0.24,-0.8,-0.06 3GYW,TYR_54,10.29,0,0.12,0.17 3U0V.ARG 136,13.14,-1.3,0.68,1.26 1PBV,ARG_69,12.21,-0.6,0,0.3 2BV9,ASP 94,4.66,0,-0.07,0.93 1V8E,ARG 113,12.38,-0.33,0.0.2 4DIU,LYS_138,11.78,-1.29,1.7,0.87 3Q9P,LYS_112,11.26,-0.26,0.58,0.43 1XAW,HIS_499,6.13,-0.43,0,0.06 2XJ4,HIS_123,4.46,-2.84,0.81,0 106D,HIS_145,6.48,-0.43,0.07,0.34 2V4U,GLU_460,4.5,0,0,0 3DZ1,HIS_19,6.47,-0.48,0,0.44 2WB8,HIS 666,6.02,-0.32,0,-0.15 1W7B,LYS 152,10,34,-0,28,0,0,12 1U7U,GLU_386,3.9,0.5,-0.81,-0.27 2H85,TYR_342,10.38,-0.11,-0.15,0.63 2FG1,LYS_131,10.55,-0.23,0,0.28 2YWX,LYS_157,10.36,-0.14,0,0 1LPL,ASP 136,3,55,-0,48,-0,15,0,38 2FD5,ASP_101,3.83,0,-0.09,0.12 1RWZ,ASP_40,2.7,-2.52,-0.06,1.49 2ZQ5,LYS_378,10.63,-0.21,0,0.34 1RZ2,ASP 144,2.33,-2.44,-0.29,1.26 3GFP,ARG_392,12.46,-0.23,0,0.2 2D59,GLU_13,4.51,0.18,0,-0.17 3ETU,LYS_66,10.33,-0.13,0,-0.04 2R0S,TYR_287,10.78,0.16,0.21,0.4 1ZP2.LYS 71.10.85,-0.35,0.09,0.61 1V6T,ARG_46,13.28,-0.36,0.84,0.3 2R57,GLU_311,4.64,0.16,0,-0.03

4FLE,TYR_159,12.47,0,0.39,2.08 1D2K.ASP 337.3.75.-0.48.-0.04.0.46 2A0J,GLU_34,4.47,0.48,-0.04,-0.46 1XEU,ASP_117,2.89,-0.85,-0.43,0.38 20K1.CYS 400.12.42.0.0.22.3.2 1AK1,LYS 246,10,59,-0,12,0,0,2 2A1V,ARG_125,12.17,-0.49,0,0.16 1RSS,LYS_29,9.63,-0.67,0,-0.21 3ETU,GLU_45,4.66,0.2,-0.03,0 3CRM,TYR_106,12.79,0,0.51,2.27 1ZBS,ARG_91,12.77,-0.26,0,0.54 2RIK, ARG_96, 12.31, -0.23, 0, 0.04 1UAJ,HIS_180,6.3,-0.28,0,0.09 200P,ARG 192,12.86,-0.34,0.14,0.57 2GZQ,LYS_144,11.32,-0.64,0.64,0.82 3BB7,ASP_67,3.4,-0.85,0,0.45 3ERF,LYS_55,10.45,-0.08,0,0.03 2B0J,LYS_105,10.41,-0.12,0,0.03 2QK1,TYR_445,12.09,0.64,0.4,1.06 1NIJ.ARG 154,11.81,-1.2,0,0,51 3DTE,CYS_116,12.12,-0.04,0.48,2.68 1GXN,LYS_522,11.25,-0.57,0.85,0.47 1UCH,ASP 33,4,41,-0.24,0,0.85 1CHD,ARG 172,12.29,-0.28,0,0.07 1MUF,GLU_212,7.75,4.87,-2.45,0.82 3GW3,HIS_223,5.74,-1.12,0.42,-0.07 3TRE,ARG_50,12.42,-0.08,0,0 2QDJ,HIS 339,7.38,-0.47,0.85,0.5 2FC3,ASP_14,3.54,-0.32,-0.19,0.24 2P0L,GLU_140,4.68,0.26,0,-0.08 1LPL,TYR_184,11.88,-0.02,-0.4,2.3 2Q12,TYR_36,10.14,0,-0.02,0.16 4FCU,LYS 37,10.38,-0.28,0,0.16 2ZCX.ARG 148,13.02,-0.3.0.12.0.7 2YX0,GLU_187,4.68,0.92,-0.32,-0.4 2FZP,ASP_298,3.74,-0.22,0,0.16 1GPP,TYR_176,11.22,-0.01,0.16,1.08 2OSA, ARG_281, 13.7, -1.11, 1.31, 1.01 1PSW,GLU_230,4.49,0.46,0,-0.47 1JT9.GLU 123.4.51.0.35.-0.01.-0.33 1WP5,GLU_294,4.76,0.08,0,0.17 3M70.LYS 43,10.38,-0.15,0,0.02 1I60.GLU 91.3.67.0.29.-0.85.-0.26 3UAH,ASP_194,2.82,-0.85,-0.57,0.44 2IRM,GLU_313,4.61,0.59,-0.28,-0.2 2XMZ,GLU_121,4.71,0.17,0,0.04 1DUP,LYS_4,10.49,-0.05,0,0.04 1L2F,LYS_95,10.27,-0.2,0,-0.04 1MD6,TYR_88,9.43,-0.83,-0.35,0.6 2E3S,LYS_573,10.06,-0.25,0,-0.19 2E3H,HIS_276,5.85,-0.32,0,-0.34 2FGG.ARG 29.12.59.-0.17.0.01.0.26 3BPV,ARG_16,12.12,-0.29,0,-0.1 3I82,CYS_197,10.65,-0.05,0,1.7 2P4D,TYR_35,10.3,-0.06,-0.42,0.77 1DTO,HIS 29,5.6,-2.01,0.85,0.27 2NRK,TYR_131,12.36,-0.6,0.23,2.73 2V4X,ARG_124,12.67,-0.84,0.59,0.42 2PPN,ARG_57,13.74,-0.38,0.87,0.74 3JRT,GLU 161,3.93,0.72,-0.85,-0.44 1MTZ.GLU 85.8.27.4.47.-0.7.0 2J8A,LYS_360,10.34,-0.16,0,0 1GPP,ASP_430,4.17,0,0.15,0.23 1JKS,TYR_39,11.08,0,0.41,0.68 2X5Y,ASP_769,4.09,0,0,0.28 2CVB,GLU 33,4.36,0.54,-0.49,-0.18 3FS3,ARG_108,13.34,-0.76,0.81,0.78 2Z61,CYS_125,10.22,-0.78,-0.16,2.17 2EHG,TYR_5,10.42,-0.01,-0.3,0.73

1AM2.HIS 144.6.04.-0.34.0.-0.12 1ANU,LYS 92,10,46,-0,26,0,0.23 2W1R,GLU_128,4.09,1.65,-1.62,-0.45 2YX0,GLU_314,3.58,0.68,-0.85,-0.74 4DIU,ARG_190,13.73,-0.52,1.37,0.38 2BT8,ASP 277,3.96,0,-0.13,0.29 3OBS,LYS_98,10.51,-0.17,0,0.18 3EGN,HIS_430,6.26,-0.31,0,0.07 3RE9,GLU_205,3.66,0.41,-0.8,-0.46 3UX2,ARG 138,12,23,-0,27,0,0 3CAN,GLU_106,4.63,0.34,0,-0.2 3RFY,LYS_195,10.53,-0.2,0,0.23 2WB8.GLU 488.4.81.0.36.0.-0.05 3K8J,LYS_31,10.43,-0.07,0,0 3CZC.LYS 85.10.6.-0.16.0.0.26 3U0V,ASP_219,3.97,0,-0.25,0.43 2AD1,ASP_40,3.55,-0.48,-0.29,0.52 3K8J,TYR_103,9.91,-0.1,-0.27,0.28 3H13,HIS_469,5.57,-0.93,0,0 4ETX,ASP 430,4.06,-0.04,0,0.29 2Z0W,ARG_28,13.27,-0.31,0.73,0.35 2VGM,GLU_334,4.47,0.32,-0.22,-0.12 2ZTY,ARG_84,11.39,-0.92,0,-0.19 2A1V,TYR 112,12.41,0,0,2.41 2PGX.GLU 138.4.1.0.24,-0.49,-0.15 1X1E,ARG_186,11.89,-0.81,0,0.2 2WOZ,LYS_605,10.45,-0.05,0,0.01 3KEY,GLU_488,3.69,0.38,-0.81,-0.37 3GW3,ARG 120,12.5,-0.65,0.23,0.42 2GS5,ASP_121,3.37,-0.78,0,0.35 1EYH,ASP_118,2.69,-1.31,-0.35,0.56 2D2S,LYS_707,10.36,-0.15,0,0.01 3K8J,ASP_71,3.79,0,-0.51,0.5 1TXJ.LYS 43,10,41,-0.09,0,0 1YG2,ASP_84,4.04,0,0,0.24 4DNU,GLU_262,4.93,0.18,0,0.25 3JZ9,LYS_351,10.41,-0.21,0,0.12 1Y0K,GLU 30,5.07,1.96,-0.78,-0.6 3EVP,TYR_64,9.97,-0.38,-0.01,0.36 3BA1,ARG_162,13.58,-0.61,0.95,0.73 1WXQ,ARG_376,12.39,-0.11,0,0 2YYO,LYS 9,11,16,-0,26,0,52,0,4 3K9I.GLU 75.4.48.0.34.0.-0.35 1JYH,LYS_10,11.42,-0.21,0.73,0.41 2G2D,TYR_36,10.46,0,0.25,0.2 1KN3,HIS_23,6.25,-0.41,0,0.16 20EW,TYR_291,10.76,0,-0.05,0.81 1PDB.LYS 68,10,-0.32,0,-0.18 1PZC,LYS_10,10.26,-0.3,0,0.06 3IRA,LYS_114,10.03,-0.46,0,-0.01 2GS5.GLU 44.4.6.0.1.0.0 1YTD.ASP 31.3.89.-0.1.0.0.18 3EVZ,GLU_111,5.38,2.21,-1.46,0.14 1DUN,ASP_16,3.02,-0.75,-0.42,0.39 3RKV,LYS_208,10.51,-0.09,0,0.1 1X6J,CYS_13,12.01,0,-0.09,3.09 1RI5.LYS 111.10.41.-0.09.0.-6.94E-18 1ES5,TYR_179,11.47,0,0.12,1.35 2B61,HIS_181,6.03,-0.26,0,-0.22 2CXY,LYS 102,10,38,-0,25,0,0,13 4DNU.HIS 264.5.18.-1.14.0.-0.18 3S0A, ASP_24, 3.69, 0, -0.33, 0.22 4AF2,GLU_160,4.14,0.31,-0.82,0.15 3DTE,ASP_92,3.14,-0.87,-0.29,0.51 2CYG,ASP_128,3.9,0,-0.02,0.12 3RFY,ARG_148,12.92,-0.28,0.37,0.33 2XHC,LYS_320,10.48,-0.21,0,0.19 2GS5,GLU_140,4.73,0.37,0,-0.15 109G,ARG_235,11.22,-1.48,0,0.2

2A1V,GLU_106,3.38,0.92,-1.56,-0.48 2HNG,TYR_17,11.31,-0.85,0,2.16 3F1X,TYR_6,10.39,0,0,0.39 1ZBP.ARG 49.12.36.-0.33.0.0.18 10GL,GLU_219,4.57,0.07,0,0 3G9G,ASP_38,4.13,0,-0.02,0.35 2PGX,GLU_40,4.55,0.17,0,-0.13 2EYI,ASP_58,3.2,-1.36,-0.16,0.93 1J85,ASP_40,3.86,0,-0.14,0.19 3E5T,LYS_6,10.4,-0.1,0,0.01 2QK1,LYS 330,10.5,-0.04,0,0.04 3N2T,ASP_303,3.73,0,-0.23,0.16 1RSS,ASP_33,3.96,0,0,0.16 4EF5,TYR_261,11.71,-0.8,0.36,2.15 1PVT.HIS 149.5.89,-0.68,0.0.07 2CI3.ARG 207,12.55,-0.08,0,0.13 3ETU,LYS_151,10.49,-0.11,0,0.1 2WB8,GLU_606,4.98,0.56,0,-0.08 3ELI,TYR_65,10.17,0,-0.09,0.26 1MTZ,TYR 18,13.4,0.85,0.65,1.91 1TXJ,LYS 114,10,49,-0,11,0,0,09 2CXY,GLU_2,4.27,0.2,0,-0.43 4FD6,HIS_25,4.26,-2.44,0,0.21 2RIK.GLU 116.3.37.0.33.-0.85.-0.62 1RHS.HIS 203.5.36.-1.92.0.74.0.05 3OKQ,ASP_582,4.04,0,0.03,0.21 1PVT,GLU_117,4.48,0.18,0,-0.2 1VJG,GLU_196,5.73,1.48,0,-0.23 3BPP,ASP_51,2.51,-1.23,-0.66,0.6 20ZO,HIS 94.6.41,-0.59,0.41,0.1 2E3H,GLU_245,4.47,0.57,-0.34,-0.26 2OSA,ARG_348,11.92,-0.74,0,0.16 2|88.GLU 365.4.52.0.21.0.-0.19 1Q2Y,LYS_75,10.34,-0.2,0,0.03 3N0K,LYS_4,10.37,-0.13,0,0 1MTZ,GLU_140,3.82,0.98,-0.99,-0.67 1R3D,HIS_120,3.58,-2.09,0,-0.82 3FRR,ASP_146,3.98,0,-0.06,0.23 3HNX,ARG 90,12,16,-0.52,0,0,19 3N2T,GLU_144,4.87,1.24,-0.55,-0.32 3JZN,TYR_278,13.56,0.85,0.66,2.05 1NFN.TYR 162,10.05,-0.32,-0.07,0.45 2PLO.LYS 28.10.77.-0.74.0.24.0.76 2B78,LYS_353,10.5,-0.05,0,0.05 1UAJ,LYS_107,10.13,-0.38,0,0.01 4ACJ,GLU_796,5.11,2.52,-2.25,0.34 1L2F,LYS 43,10.28,-0.22,0,0 2Q99,ARG_131,11.24,-1.78,0,0.52 1M5I,GLU_211,4.49,0.23,0,-0.24 2BLL/ARG 624,13,54,-0.26,0.74,0.56 3GG6,LYS_40,10.45,-0.05,0,0 3FWU,GLU 87,3.78,0.58,-0.83,-0.48 1TUL.TYR 34,10.04,-0.55,0.02,0.57 1YTQ,LYS_139,10.42,-0.37,0,0.29 3M7D,ARG_317,12.99,-0.29,0.4,0.38 2FD4,ASP_513,3.96,0,0,0.16 2H8O,TYR_120,11.51,0,0.17,1.34 2B0J,LYS_130,11.13,-0.26,0.42,0.47 3GYW, ASP_119, 3.61, -0.14, -0.22, 0.17 3BCY,TYR_54,10.6,0,0.25,0.35 3B7H,ARG 47,12.2,-0.3,0,0 3EJC.GLU 55.4.59.0.09.0.0 1WJG,GLU_25,4.04,0.44,-0.54,-0.36 2PGX,GLU_29,3.46,0.25,-0.85,-0.43 2IQT,GLU_157,3.38,0.31,-1.01,-0.43 2CBE,LYS_170,9.85,-0.73,0,0.08 2QZQ,ARG_93,12.1,-0.42,0,0.01 2B78,ASP 133,3.82,0,-0.22,0.24 2D7J,ASP_69,3.62,-0.42,-0.14,0.38

2NRR,GLU_348,4.58,0.32,0,-0.25 3CSR,LYS 123,10.62,-0.18,0,0.3 1WOU,HIS_22,7.11,-0.55,1.19,-0.04 3T57,HIS_215,6.16,-0.61,0.74,-0.46 2E3C,GLU_283,3.83,0.33,-1.03,0.02 1JKS.GLU 7,2.94,0.4,-1.68,-0.28 3G9T.HIS 214.5.64.-0.96.0.0.1 1R5Q,CYS_93,9.32,-0.03,0.07,0.28 106D,LYS_86,10.46,-0.13,0,0.1 2CYG,TYR_207,10.68,0,0.21,0.47 1X7F.ARG 203,13,75,-1,56,1,5,1,31 1HUF,GLU_19,4.61,0.08,0,0.03 2ZQ5,ARG_227,11.22,-1.4,0,0.12 3K9I,TYR_114,11,-0.08,0.15,0.92 2H2Z,ARG 4,12,42,-0.08,0,0 3CRM,ARG 314,12.36,-0.14,0,0 1MJS,GLU_283,4.38,0.29,0,-0.4 2CI3,GLU_121,4.56,0.08,0,-0.02 1EV8,ASP_214,3.86,0,-0.11,0.17 2OK0,ARG 32,12,52,-0.09,0,0,1 1J85.HIS 60.4.75.-1.57.0.-0.18 1UXO,GLU_158,4.6,0.4,0,-0.3 2XHC,LYS_17,10.88,-0.22,0,0.6 1TJE.TYR 155,12,75,0.85,0.54,1.36 1YB2,GLU 122,4.11,1.19,-1.57,-0.01 2D2S,ARG_664,11.27,-2.29,0.44,0.63 2CI3,HIS_206,6.08,-0.53,0.33,-0.22 2D0A, ARG_167, 13.22, -0.3, 0.7, 0.31 3HUE,LYS_14,10.46,-0.16,0,0.13 2FBI,TYR_113,10.72,0,-0.35,1.07 1EW4,ASP_27,4.24,0,0.31,0.14 3EX9.ARG 24,13.53,-0.43,0.93,0.54 2O4D, ASP_58, 3.61, 0, -0.72, 0.53 3M3P,HIS_28,6.38,-0.16,0,0.04 3CN5.TYR 159,10.28,0.0.0.28 3LQE,ASP_512,3.39,-0.52,-0.29,0.4 1R5Q,LYS_15,12.01,-0.83,1.59,0.76 3ETV,LYS_32,10.39,-0.3,0,0.19 3K1H,GLU 42,3.8,0.48,-0.85,-0.33 3EVP,GLU_269,3.55,0.38,-0.72,-0.62 2DFL,LYS 232,10.66,-0.24,0.0.4 3ZXY,ASP_125,4.26,0,0.28,0.19 3ETV,TYR 238,11.8,0,0.33,1.48 3FHF,LYS 79,10.93,-0.16,0.0.58 2JHY,GLU_163,4.71,0.92,-0.81,0.09 1CHD,ARG_255,12.23,-0.3,0,0.03 1XEU,TYR_246,9.37,-0.85,-0.28,0.51 3CGW,LYS_234,9.75,-0.78,0,0.03 3LJC,ASP_123,3.69,-0.45,0,0.34 2RIS,ARG_111,11.57,-0.95,0,0.02 2V4X,LYS_17,10.5,0,0,0 1EQ6,ARG 72,13.21,-0.21,0.78,0.14 1YTO, ARG 97, 13.34, -0.36, 0.63, 0.57 4E6S,HIS_43,6.32,-0.6,0.77,-0.36 1YTQ,HIS_132,6.11,-0.42,0,0.04 2F4Q,ARG_137,11.55,-1.28,0,0.33 2W0G,ARG_231,12.53,-0.58,0,0.61 1NWA.GLU 138,2.76,1.13,-2.47,-0.39 1ZCE,TYR_35,9.11,-0.75,-0.45,0.31 2Q12,ASP_122,2.4,-2.23,-0.87,1.7 2QEV,ARG_89,12.7,-0.54,0.26,0.48 2CBE,HIS 17,5.58,-0.39,0,-0.52 2RGY,HIS_156,6.45,-0.39,0.37,2.78E-17 1AIL,ARG_38,13.4,-0.18,0.66,0.41 3GG6,CYS_43,9.45,-0.04,-0.39,0.88 2B3M,CYS_142,11.57,0,0,2.58 3IO0,ARG 290,12,35,-0,31,0,0,16 3HUE,GLU_315,4.61,0.2,0,-0.1 2FBQ,GLU_147,4.7,0.31,0,-0.1

3M7D.GLU 256.5.06.0.75.0.-0.2 3CNU/GLU 3/3/83/0/26/-0.63/-0.3 1Z3X,ARG_196,12.42,-0.12,0,0.04 1Y0K,TYR_6,10.36,0,-0.01,0.38 2WOZ.CYS 419,10.55,-0.52,-0.17,2.24 1KCM,HIS 136,6,18,-0,31,0,-0,01 20GQ,GLU_460,4.75,0.6,-0.3,-0.06 1W7B,LYS_148,10.46,-0.26,0,0.22 3JSN,ARG_165,11.39,-2.25,0.22,0.93 3T5B,HIS_182,5.22,-1.36,0,0.08 1Y2Q,GLU_37,3.64,0.32,-0.85,-0.33 2G3A,TYR_24,9.55,-0.72,0,0.27 3OA7,LYS_503,10.38,-0.12,0,0 3Q1C,ASP_162,3.85,-0.37,0.06,0.37 3O2C.TYR 77.10.73.0.0.11.0.63 2RJD,GLU_313,3.87,0.34,-0.71,-0.26 3E5T,CYS_172,11.79,-0.17,0.01,2.96 3QKY,GLU_235,4.62,0.79,-0.22,-0.45 2YX0,ASP_132,2.91,-0.9,-0.47,0.48 100X.ARG 33.12.48.-0.29.0.0.27 1IAP,ARG_54,12.6,-0.25,0.05,0.31 3GYW,HIS_168,6.65,-0.36,0.29,0.22 3F1X,ARG_179,13.21,-0.43,0.58,0.55 3D9H,ASP 220,3.95,0,-0.17,0.33 2Z0M,LYS_328,10.51,-0.06,0,0.08 1WP5,TYR_126,13.24,-0.85,0.29,3.8 3IDW,ASP_15,3.87,-0.18,0.01,0.23 3I4T,CYS 223,10.66,-0.3,0.27,1.69 102Y,GLU 43,4,31,0.89,-0.81,-0.27 1PVT,LYS_42,10.42,-0.08,0,0 2YYO,LYS_38,10.57,-0.16,0,0.23 2QEV,LYS_136,10.37,-0.16,0,0.03 1J33,GLU 145,3.87,0.76,-0.84,-0.56 1C3K.GLU 77.2.59.0.86.-2.48.-0.29 1FO9,GLU_309,3.82,3.43,-2.33,-1.77 3V1Q,ARG_506,12.89,-1.25,1.16,0.48 2PGX.LYS 85,10.24,-0.13,0,-0.13 2RFA,GLU 80,4.37,1.35,-1.27,-0.2 2H85,ASP_335,3.87,0,-0.16,0.23 2FPN,HIS 87,6,41,-0.09,0,0 1SIG,LYS_300,10.43,-0.07,0,0 2CXC,ARG 49,12.96,-0.31,0.38,0.38 2IOT,LYS 81,10.42,-0.12,0.0.04 3CBN,ARG_151,13.28,-0.42,0.5,0.7 3RLN,LYS_623,10.37,-0.31,0,0.18 2W1R,LYS_153,10.89,-1.05,0.77,0.68 2Q34,ARG_176,12.74,-0.31,0.08,0.46 2DFL,HIS 275,6.31,-0.13,0,-0.05 4DBX,LYS_247,9.83,-0.42,0,-0.24 1XWM,ASP_150,4.01,-0.02,-0.13,0.36 2XMZ,GLU 248,5.43,2.49,-1.64,0.08 3JZN.ASP 317.4.51.0.0.08.0.64 20PJ,GLU_153,4.59,2.79,-0.72,-1.97 1YM5,TYR_222,10.2,0,0,0.2 3GEC,ASP_267,3.74,-0.12,-0.23,0.29 4DVD,GLU_50,4.47,0.35,0,-0.38 10I7,ASP_54,2.83,-1.35,-0.01,0.39 3EYE, ASP_151, 3.99, -0.33, 0.12, 0.4 20PJ,ARG_192,12.26,-0.25,0,0.01 1F2V,GLU 49,4.29,0.16,-0.07,-0.31 1SFE,CYS 36,11,71,-0.23,0.12,2.81 1SJ8,GLU_650,4.8,0.34,0,-0.05 3VHJ,GLU_146,3.42,0.37,-0.96,-0.49 1WXQ,GLU_132,4.21,0.47,-0.37,-0.4 3QKY,ARG_225,12.51,-0.23,0,0.24 3CRM,ASP_20,4.33,0,-0.03,0.57 1Z3X,CYS_175,9.44,0,-0.33,0.77 3PM2,ASP_108,3.75,0,-0.28,0.23 2GKG,ASP_34,3.4,-0.64,-0.07,0.3

3BOW,LYS 344,10,72,-0,44,0,09,0,58 1PSW.GLU 212.5.15.1.12.-0.54.0.06 3D9H,CYS_117,10.61,-0.85,0.2,2.27 2QEV,TYR_138,11.41,0,0.41,0.98 4F85,ARG_200,12.79,-0.43,0.36,0.36 3LE4.ARG 322.12.35.-0.14.0.-0.01 2H85,TYR_7,10.17,0,-0.05,0.21 3BWT,LYS_661,10.07,-0.29,0,-0.14 3JSN,ARG_97,11.74,-0.66,0,-0.11 1KCM,GLU_158,3.96,0.27,-0.7,-0.12 1Q46,GLU_142,3.45,0.41,-0.68,-0.78 2FG1,HIS_83,7.29,-0.29,0.85,0.23 1H09,TYR_164,11.25,0.51,0.42,0.32 2GEN,HIS_126,5.73,-1.01,0,0.24 3LD1.ASP 69.3.92.0.-0.22.0.33 3KV0.ARG 199,12,28,-0.28,0.0.06 1X8F,HIS_40,5.73,-0.9,0,0.13 2RJD,ARG_460,11.32,-1.22,0,0.03 3BCH,HIS_131,6.57,-0.36,0.38,0.06 3CO1,LYS 34,10.46,-0.14,0,0.1 3IVF,LYS_196,10.23,-0.5,0,0.23 2Q34,TYR_198,10.23,0,-0.11,0.35 3JSN,ASP_89,3.86,-0.14,-0.11,0.31 1MD6,GLU 125,4.61,0.14,0,-0.02 3CAX,LYS 421,10,44,-0.08,0.0.02 307K,GLU_94,4.95,0.61,0,-0.16 4H86,LYS_48,10.56,-0.7,0,0.75 1HF8,ASP_119,4.11,0,0,0.31 1R53,TYR 305,12.41,-0.82,0.15,3.08 3GE9,ARG_62,12.47,-0.1,0,0.07 3GA2,HIS_77,5.59,-0.73,0,-0.18 2XWS,ASP_78,4.16,0,-0.35,0.71 2B3M,LYS 31,9.68,-0.82,0,0 2ZO5.GLU 50.4.07.1.46.-1.68.-0.22 3CRM,ASP_82,3.75,-0.85,-0.11,0.91 2CVB,ARG_61,12.78,-0.15,0,0.43 3M9A,LYS_43,9.95,-0.63,0,0.09 1GPP,HIS 79,4.56,-3.09,0,1.16 3K1H,ASP_116,3.99,-0.11,0.08,0.22 1L2F,LYS_193,9.8,-0.66,0,-0.05 1DZF,HIS_146,6.18,-0.84,0,0.52 2098.GLU 67.4.16.0.31.0.-0.65 1G8P.GLU 261.4.57.0.18.0.-0.1 1EDG,HIS_162,6.91,-1.07,0.78,0.69 3FRR,TYR 177,12,98,0,48,0,35,2,13 2VGM,LYS_187,10.51,-0.18,0,0.19 3F5D,LYS 126,11.09,-0.26,0.85,0 2013.GLU 67.3.65.0.33.-0.7.-0.48 2F8H,LYS_233,10.45,-0.05,0,0 3EAZ,TYR_116,11.87,0,0.76,1.11 1WNH,TYR_76,13.37,0,0.23,3.14 1NRI,ASP_232,4.02,0,-0.18,0.39 1DCF,ASP_121,4.36,0,0.26,0.3 3CS1,GLU_76,3.95,0.24,-0.45,-0.34 3U0V,LYS_42,10.44,-0.19,0,0.13 1L2F,ASP_299,2.99,-1.19,-0.04,0.43 20BI.GLU 82.6.27.3.31.-1.33.-0.21 1L2F,ARG_51,14,-0.44,1.22,0.72 2B0J,GLU_307,4.43,0.2,-0.04,-0.22 2B0A,LYS 49,11.2,-0.37,0.59,0.48 2Z61.GLU 177.4.06.0.58.-0.8.-0.2 1GQE,LYS_31,10.67,-0.16,0,0.33 3FTT,LYS_79,10.74,-0.11,0,0.35 2BCF,LYS_149,11.21,-0.58,0.85,0.43 2PWQ,HIS_50,6.02,-0.5,0,0.02 3GOZ,LYS_294,10.53,-0.14,0,0.17 2X5Y,TYR_893,12.97,0,0.27,2.7 2QHT,GLU 65,4.65,0.15,0,0 3RKV,GLU_323,4.43,0.3,0,-0.37

2FBO,ARG 103,12,13,-1.61,0,49,0,75 300P,GLU_53,4.57,0.27,0,-0.19 1UJ8,HIS_10,6.4,-0.07,0,-0.03 30KY/CYS 117,12,18,-0.09,-0.03,3,31 1RSS,LYS_137,10.17,-0.38,0,0.05 1BGF,ARG_70,13.14,-0.17,0.52,0.29 3VHJ.LYS 3.10.18.-0.18.0.-0.14 2D7J,GLU_156,4.63,0.33,0,-0.2 2CWY,GLU_70,4.35,0.16,-0.12,-0.19 2RFA,LYS_244,10.36,-0.14,0,0 3IBT,HIS 49,6.63,-1.05,0.98,0.19 20GO.HIS 373.6.17,-0.4,0.0.07 3IO0,GLU_262,3.28,3.58,-0.85,-3.96 1D2K,LYS_223,9.83,-0.88,0,0.21 10LR.ASP 111.4.09.0.0.03.0.25 1EW4,ASP_25,3.92,0,0.02,0.11 2E3S,LYS_578,10.35,-0.28,0,0.13 3ADO,GLU_304,2.55,0.48,-1.63,-0.81 1XDZ,ASP_142,1.78,-2.75,-0.48,1.2 3IRA,LYS 39,9.97,-0.69,0,0.16 3GV0.ARG 117.12.35.-0.17.0.0.03 4DNU,ARG_121,13.15,-0.13,0.46,0.32 1JSX,GLU_170,4.73,0.14,0,0.09 2F8H,ARG 214,12,39,-0.11,0,0 1SJ8.ASP 695.3.9.0.0.0.1 1RI6,ASP_151,3.2,-1.69,0,1.09 2P1W,GLU_92,4.56,0.1,0,-0.03 3I4T,LYS_24,10.29,-0.22,0,0 2R51,HIS 184,5.66,-0.91,0,0.07 4ETX,GLU_178,4.81,0.3,0,0.01 1X7F,GLU_277,4.36,0.18,0,-0.32 3M7D,ARG_151,13.03,-2.15,1.39,1.3 3CNU,LYS_77,11.24,-0.27,0.63,0.38 2EHG,LYS 101,10.49,-0.24,0,0.24 2FD5,ARG_11,12.18,-0.32,0,0 2ZQ5,ARG_333,13.88,-0.32,1.17,0.53 1PNE,LYS_53,10.52,-0.09,0,0.1 1J33,ARG_293,12.64,-0.4,0.24,0.3 2Z14.HIS 88.5.77.-0.9.0.13.0.05 3F6F,GLU_132,4.21,0.55,-0.48,-0.36 1RL0,TYR_183,11.88,0.73,0.43,0.72 2CN1,LYS_32,11.4,-0.35,0.83,0.41 10TM.GLU 167,4.53,0.43,-0.2,-0.21 3ANJ,LYS_96,10.37,-0.29,0,0.16 1C44,ASP_5,3.37,-0.52,-0.09,0.19 2FD5,LYS_5,10.39,-0.09,0,-0.02 3RKV,ASP_216,3.47,-0.38,-0.28,0.33 1RSS,ARG_32,12.39,-0.11,0,0 2ZCO,LYS_275,10.37,-0.13,0,0 1T95,GLU_171,3.09,0.45,-1.2,-0.65 3RLE,CYS_173,12,0,-0.08,3.08 2X5Y,TYR 819,11.57,-1.39,0.48.2.48 2CN1.HIS 107.3.1.-2.58.0.-0.82 2Q99,HIS_91,2.14,-3.09,0,-1.27 1RWZ,ARG_162,12.78,-0.49,0.12,0.64 3I82,ASP_23,3.97,0,0,0.17 1AM2.HIS 41.6.84,-0.86,0.33,0.87 3ETU,TYR_343,10.85,0,0.26,0.6 1WRU,LYS 210,10,28,-0,29,0,0.07 3GA2,HIS_35,6.55,-0.19,0,0.25 105T,LYS_331,9.8,-0.56,0,-0.14 2CXA.GLU 156.7.87.4.01.-0.85.0.2 2Z61,ARG_72,11.38,-1.54,0,0.41 3DHN,TYR_197,13.73,-0.05,0,3.78 2YT4,CYS_627,11.24,-0.85,0.19,2.9 4H86,LYS_15,10.63,-0.17,0,0.29 1HF8,ASP_266,3.29,-0.81,0,0.31 1TLV.ARG 272,12,21,-0.31,0.0.03 2B61,LYS_92,10.47,-0.45,0,0.43

2JHY,ARG_172,13.9,-0.53,1.46,0.46 1PV5,GLU 113,4.1,0.37,-0.4,-0.37 3D9H,LYS_86,10.36,-0.15,0,0.01 3UX2,GLU_144,4.61,0.11,0,0 2X5Y,ASP_896,4.38,0.27,0.06,0.24 1ZP2.HIS 95.5.63,-0.34,0,-0.53 3EAZ,LYS 171,10,41,-0,27,0,0,18 2EYI,GLU_225,4.9,0.13,0,0.27 106D,ARG_50,13.07,-0.25,0.14,0.69 3JV1,LYS_84,10.62,-0.17,0,0.28 1N81.GLU 24.3.71.0.31.-0.74.-0.36 1NAR,TYR_174,13.94,-0.7,0.67,3.96 2GS5,HIS_138,6.25,-0.88,0.48,0.15 30AV,LYS 35,10.7,-0.22,0,0.41 1ZYL,ARG_283,11.92,-1.71,0.03,1.11 3MIX,LYS 547,10.42,-0.34,0,0.25 2BDV,ASP_13,4.46,0,0.33,0.33 2E3S,GLU_575,3.92,0.64,-0.6,-0.62 1W7B,GLU_306,3.61,0.71,-1.24,-0.36 2GZR/ARG 180,13.03,-0.25,0.16,0.62 1WRU,ASP_325,3.08,-0.68,-0.42,0.39 20EW,GLU_272,4.22,1.02,-0.71,-0.6 1Q8B,GLU_72,3.9,0.21,-0.25,-0.56 3LPZ,ARG 60,12,25,-0,25,0,0 2R57,LYS 206,10.45,-0.2,0,0.15 2P65,ARG 33,11.92,-0.51,0,-0.07 2D8N,LYS_139,10.36,-0.14,0,0 3HVM,CYS_52,12.33,0,0.06,3.27 1QYI,GLU_192,4.11,0.35,-0.8,0.06 1SFE, TYR_16, 10.82, 0, 0.19, 0.64 1RI6,ASP_48,2.08,-2.36,-0.49,1.13 2R2Y,ASP 115,3,47,-0.51,-0.02,0,2 1CHD,ASP_231,3.1,-0.51,-0.51,0.31 3CAX,GLU 155,4.38,0.27,0,-0.38 1PGV.ARG 382.13.37.-0.28.0.69.0.46 3OBS,ARG_18,12.37,-0.22,0,0.09 3E5T,GLU_29,3.06,0.54,-1.41,-0.58 4F85,HIS_229,5.92,-0.6,0,0.02 3DZ1,TYR 252,11.97,0.85,0.35,0.78 2CL3,LYS_173,11.56,-0.58,0.85,0.79 20JQ,GLU_462,4.4,0.84,-0.74,-0.21 3KT9,TYR_96,11.58,-0.69,-0.34,2.61 1QYI,TYR 106,11.01,-0.24,0.48,0.77 2EA9.CYS 52.9.66.-0.02.0.29.0.39 2H8O,CYS_230,12.47,-0.14,0.02,3.59 2RFA,ARG_155,12.13,-0.39,0,0.03 3C38,TYR_230,11.53,-0.68,0.67,1.54 1KCM,LYS_87,10.14,-0.44,0,0.08 3BJV,ASP_93,3.51,-0.98,-0.16,0.84 1NWA,HIS_50,5.76,-1.43,0.84,-0.16 2VGM,TYR_316,11.27,0,0.17,1.09 2HRZ,GLU 248,4.69,0.17,0,0.03 1XIPASP 239,3.89,0,-0.04,0.13 1DCF,ARG_45,12.45,-0.15,0,0.1 1V43,LYS_176,10.46,-0.04,0,0 2B61,ASP_62,4.09,0,0,0.29 3ANJ,ASP_224,3.03,-1.18,0,0.4 2RIS,ARG 143,12,25,-0.36,0.0.1 2CIU,LYS_135,10.24,-0.28,0,0.02 3RKV,GLU_317,4.09,1.15,-0.71,-0.87 1RAJ,ASP_317,3.37,-0.73,-0.13,0.45 3MIX.ASP 390,3.73,-0.4,-0.07,0.39 3EUR,LYS_20,9.97,-0.5,0,-0.03 2NYC,HIS_182,6.23,-0.18,0,-0.09 3ETV,GLU_90,5.15,0.59,0,0.06 1ANU,TYR_39,11.35,0,0.1,1.25 2012.HIS 45.7.15.-0.32.0.6.0.38 2H8O,HIS_124,6.18,-1.51,0.75,0.44 3TIR,GLU_7,4.01,0.25,-0.74,0

3ILC.ASP 156.3.41.-0.85.0.0.46 2Y2T.ASP 15.4.14.0.0.06.0.28 2P4D,TYR_166,11.9,-0.07,0.22,1.75 3I82,LYS_57,10.78,-1.04,0.69,0.64 1G8P,ARG 54,12,55,-0,1,0,0,15 1PSW/HIS 104.6.09,-0.3.0,-0.12 2G3A,ARG_108,13.08,-0.26,0.52,0.33 1CBY.GLU 198,4.47,0.23,0,-0.26 1EW4,ARG_53,12.43,-1.23,0.56,0.6 1C3K,HIS_26,6.32,-0.34,0,0.16 1W7B,TYR 232,11,36,-1,7,0,35,2,72 2P52,ASP_256,2.19,-2.22,-0.01,0.62 1MTZ,ARG_267,12.47,-0.18,0,0.15 1SQW,ARG_120,12.24,-0.35,0,0.09 4FD6.HIS 55.4.55.-1.47.0.-0.49 1YTQ,HIS_134,6.32,-0.33,0.13,0.02 4FCU,GLU_205,3.94,2.05,-2.24,-0.38 2IQT,ARG_76,12.7,-0.42,0.28,0.33 3KB5,ARG_282,13.2,-1.02,0.75,0.97 10TM,ASP 233,4.06,0,0,0.26 3BJV,LYS_23,11.28,-0.29,0.49,0.59 1TWU, ARG_37, 13.87, -0.56, 1.21, 0.72 3C0C,CYS 311,11,53,0,0,2,53 3RFYLYS 244.11.32.-0.35.0.44.0.73 3SMD,GLU_60,4.09,0.27,-0.79,0.11 1KCM,LYS_209,10.43,-0.07,0,0 2YYO, ARG_106, 13.17, -0.42, 0.33, 0.76 1W24,HIS_13,6.23,-0.18,0,-0.09 10LR,TYR_119,11.19,0,0.23,0.96 3M3P,GLU_27,4.75,0.33,0,-0.08 3D9H,ARG_143,12.79,-0.66,0.46,0.5 3LJC,ASP_188,2.81,-1.42,-0.06,0.49 3TOW, ARG 92, 11.31, -1.5, 0, 0.3 3F1X,TYR 163,12,58,-0,2,-0,56,3,35 4EF5,CYS_206,11.16,0,-0.22,2.38 3KB5,CYS_456,13.47,0.42,1.15,2.9 3ETU,HIS 153,7.48,-0.35,0.85,0.48 3G9T,GLU_47,3.96,0.33,-0.55,-0.33 1DUN, ARG_112, 12.45, -0.05, 0, 0 1H4U,TYR 540,13.09.0.0.38,2.71 1GQE,LYS_307,10.42,-0.17,0,0.09 2EDM, ASP 84, 3.16, -0.43, -0.77, 0.58 2W0G,LYS 157,10.56,-0.17,0,0.23 3DSH,GLU_423,4.67,0.17,0,0 2PGE,TYR_96,11.09,-0.66,0.13,1.6 306L.TYR 20,12,29,-0.85,0.59,2.55 1XAW,ASP_437,3.87,0,-0.28,0.36 3LJN,GLU_124,4.52,0.02,0,0 1NJ4,LYS_62,10.34,-0.16,0,0 1WP5,GLU_157,3.71,0.88,-1.36,-0.32 2PGX,ARG 132,12.37,-1.66,0.65,0.88 3L7N.GLU 212,3.87,0.36,-0.99,0 3CAX,LYS_319,10.49,-0.08,0,0.07 3FXH,ASP_30,3.83,0,-0.14,0.17 1YR6,LYS_137,10.76,-0.16,0,0.42 3AU3,GLU 633,4.7,0.95.-0.76.0 3GV0,LYS_291,10.8,-0.97,0.85,0.43 2CW4,CYS_75,10.81,-0.85,-0.32,2.98 2XHC,LYS_60,10.41,-0.09,0,0 3A2Z,ASP 50,3.99,0,0.06,0.13 3U2R,GLU_117,4.34,0.26,-0.13,-0.29 2D59,GLU_136,4.54,1.94,-1.24,-0.66 3GW3,HIS_331,6.95,-0.43,0.85,0.02 3FS3,TYR_135,10.89,0,0.09,0.79 3OA7,GLU_492,4.69,0.19,0,0 1EYH,ARG 63,10.88,-1.39,0,-0.24 2B6P,CYS_88,9.85,-0.03,-0.04,0.93 3H13,GLU_398,4.55,0.18,0,-0.14 1XEU,GLU_228,4.87,0.17,0,0.2

1J33.GLU 304.6.94.2.53.-0.59.0.49 1LPL,LYS 137,10.33,-0.17,0,0 1YTD,LYS_375,10.38,-0.16,0,0.04 2A0J,LYS_95,10.63,-0.19,0,0.32 3EX9.HIS 73,4.85,-1.41,0,-0.24 3RNV.CYS 389.12.52.-0.04.0.3.55 3IRA,TYR_24,10.24,-0.88,-0.22,1.34 2FC3,HIS_65,5.65,-0.93,0,0.09 1DVO,LYS_56,10.46,-0.16,0,0.11 3JSN,LYS_182,9.99,-0.62,0,0.12 3I47,GLU_35,5.29,0.79,0,0.01 1BYI,ARG_183,12.47,-0.13,0.08,0.02 2H14,HIS_255,4.27,-2.43,0,0.2 1GXN,TYR_598,13.77,-0.82,0.43,4.16 2IRM.GLU 45,4.13,0.34,-0.4,-0.31 2F9F,ASP 159,2,92,-0,79,-0,48,0,38 4FH3,ARG_294,13.44,-0.35,0.69,0.58 3Q1C,ARG_147,13.05,-1.19,1.15,0.59 10I7,LYS_188,10.49,-0.23,0,0.22 2DFL,LYS 288,10.34,-0.33,0,0.17 3BB7,LYS_144,10.03,-0.29,0,-0.18 3ETU,LYS_125,10.34,-0.17,0,0.01 3M66,ARG_277,12.32,-0.42,0,0.25 3GFP,ASP 470,3.95,0,0,0.15 3ADO,LYS 311,9,73,-0.52,0,-0.24 3C5V,LYS_64,11.33,-0.18,0.54,0.47 2H2W,GLU_116,3.44,0.53,-1.56,-0.03 3GG6,GLU_95,8.83,4.13,-0.62,0.83 1K95,CYS 94,12.21,-0.03,0.3,2.94 2PGE,LYS_192,10.54,-0.32,0,0.37 3S0A,HIS_11,6.87,-0.43,0.44,0.35 1GXN,HIS_446,5.18,-1.33,0,0.01 4EF5,ARG 331,13.16,-0.27,0.52,0.4 1SNT.HIS 82.6.76.-0.6.0.82.0.04 3ZRI,ARG_141,11.51,-1.07,0,0.08 1X7F,CYS_359,12.16,0,0.01,3.15 1MD6,GLU_137,4.57,0.07,0,0 3CAX,LYS 356,10.36,-0.17,0,0.03 1DCF,LYS_100,10.18,-0.44,0,0.11 1YTQ,TYR_155,10.3,0,0,0.3 2AZL,GLU_71,6.45,2.64,0,-0.69 1RI5,ARG 290,12.59,-0.37,0.05,0.41 1YM5.ARG 236.13.5.-1.44.1.08.1.35 1XIP,LYS_310,11.61,-0.57,0.82,0.86 2FPN,ARG_77,12.39,-0.72,0,0.61 1PDB,LYS_54,10.38,-0.58,0.24,0.21 3R2E,ARG 93,13.66,-0.39,0.83,0.72 3CO1,LYS 89,9,73,-0.81,0,0.05 2CXA,GLU_22,4.68,0.19,0,-0.01 2BLL,ARG_549,12.87,-0.85,0.75,0.48 3IU5.LYS 128.10.4.-0.11.0.0.01 4GA2,ASP 108,3,48,-0.82,0,13,0,36 1H4U,TYR_452,10.51,-0.18,0.03,0.66 1RI6.TYR 319,10.33,-0.78,-0.03,1.15 3CSR,ARG_96,12.63,-1.95,0.77,1.31 2OJQ,LYS_671,10.32,-0.18,0,0 3BCY,LYS 68,10.33,-0.17,0.0 2IF4,HIS_60,6.31,-0.26,0.15,-0.08 1NJ4,GLU_351,4.76,0.2,0,0.06 4FLE,ASP 125,4.06,0,-0.25,0.5 1ES9,ARG_214,12.24,-0.27,0,0 2Q5X,GLU_848,4.04,0.47,-0.67,-0.26 4FZR,ARG_97,12.67,-0.59,0,0.76 3ANJ,GLU_13,4.71,0.23,0,-0.03 2JKF,TYR_115,10.49,0,0.02,0.46 3V1Q,LYS_612,10.43,-0.39,0,0.32 2IQT,GLU_243,4.8,0.19,0,0.12 1P1L,ASP_68,2.47,-1.34,-0.43,0.44 3ADO,TYR_232,10.58,0,-0.1,0.68

3LMF,LYS 110,10.61,-0.22,0.1,0.24 2VAN, ARG 149, 12.23, -0.33, 0, 0.05 1G5Z,GLU_180,3.47,0.43,-0.79,-0.66 3M7D,GLU_259,4.74,0.17,0,0.07 2I88, ASP_422, 4.02, 0, 0.04, 0.18 1FO9,LYS 180,10,43,-0.07,0,0 3FHF.GLU 112,5.94,2.03,-0.56,-0.03 1L2H,LYS_77,10.42,-0.08,0,0 3QKY,GLU_86,4.56,0.57,-0.66,0.16 3NR5,ARG_67,12.66,-0.11,0,0.27 4EKU,TYR 265,12.94,0.17,0.28,2.49 1A80,ASP 87,3.65,-0.12,-0.56,0.54 2APL,LYS_104,10.29,-0.21,0,0 3M16,HIS_167,5.6,-1.41,0,0.52 100X.GLU 127.4.56.0.37.0.-0.32 3GOZ,ASP 263,4.09,0.0.04,0.25 1NWA,GLU_115,3.95,0.47,-0.78,-0.24 1W7B,ARG_196,13.74,-0.25,0.77,0.71 2VGM,TYR_268,10.21,-0.75,0.1,0.86 1NAF, ASP 189, 2.86, -1.46, 0, 0.51 2GKG,ARG_44,12.49,-0.29,0,0.27 2ILR.LYS 447.10.31.-0.34.0.0.15 1XKR,TYR_193,10.29,0,-0.07,0.37 3CRM,TYR 60,11.37,0.77,0.0.6 3MTTLYS 598.10.46.-0.04.0.0 4ANN,ASP_31,3.92,0,-0.34,0.46 1XDZ,LYS_186,10.44,-0.2,0,0.14 3VJ8,ASP_85,2.05,-2.72,-0.31,1.29 1WPA,LYS 501,9.77,-0.43,0,-0.29 1K95.TYR 57.10.17.0.0.0.17 2XJ4,GLU_86,4.01,0.32,-0.84,0.03 1V8E,HIS_171,6.63,-0.97,0.77,0.34 1SBX.TYR 149.10.18.0.0.02.0.15 4AE7,ARG 118,11.74,-3.48,0.28,2.44 1LZL,GLU_123,2.5,0.67,-2.22,-0.45 1G5Z,LYS_75,11.4,-0.23,0.68,0.45 4EUG,TYR_19,13.37,0.85,0.54,1.97 3CJW,GLU_300,4.51,0.4,-0.14,-0.25 4FZN.TYR 189,13,0.85,0.56,1.59 3C38,GLU_161,4.63,0.13,0,0 3DHN,HIS_37,6.39,-0.26,0.28,-0.13 3UAH,ASP_173,4.86,0,0.2,0.87 3HZO.CYS 32.9.44.-0.09.0.07.0.45 2GS5,GLU_149,3.42,1.31,-2.4,0 10IS,ARG_278,12.56,-0.06,0,0.12 1X04,GLU_202,4.51,0.24,0,-0.23 3V75,TYR_109,10.25,0,-0.02,0.27 2EEY,ARG_12,12.33,-0.17,0,0 1YB2,LYS_176,10.11,-0.45,0,0.05 1G5Z.GLU 196.4.65.0.42.0.-0.27 2FL4,LYS 97,10.53,-0.2,0,0.23 1GQE,LYS 204,10.36,-0.19,0,0.05 3LD1.GLU 90.3.58.0.79.-1.13.-0.58 1Q46,LYS_11,10.4,-0.12,0,0.03 20GQ,ASP_419,4.06,0,0.1,0.15 3GFP,ARG_371,12.47,-0.18,0,0.15 1P4X.HIS 186.4.48.-1.93.0.-0.09 1JT9,ASP_115,4.03,-0.02,0.04,0.21 3BQW,ASP_300,2.81,-1.41,-1.04,1.46 2F4Q,TYR_289,9.24,-0.52,-1.29,1.04 1UOH,GLU_205,4.5,0.1,0,-0.1 2B0J,GLU_36,4.41,0.78,-0.5,-0.39 2X4G,HIS_37,5.93,-0.81,0,0.26 3EZ7,ARG_391,12.67,-0.3,0.19,0.27 1WYC,ASP_207,2.4,-1.76,0,0.35 4ESS,LYS_135,11.25,-0.32,0.7,0.38 2RIK,ARG_227,12.43,-0.08,0,0.01 4ETX.ARG 234,12.65,-0.15,0,0.31 1SNT,GLU_257,4.6,0.1,0,0

3GA2,LYS_70,10.28,-0.42,0,0.21 1T95,ASP 57,3.33,-0.6,-0.33,0.47 3BWT,ASP_715,2.83,-1.25,-0.44,0.73 4GCO,LYS_209,10.53,-0.05,0,0.07 1H09,TYR_232,10.92,0,0.22,0.7 2YT4,ARG 663,12.82,-0.28,0.21,0.4 2AD1.LYS 282.10.54.-0.25.0.0.29 2FBI,ARG_38,11.5,-0.99,0,-0.01 2QZQ,LYS_148,10.48,-0.15,0,0.13 1XAW,ASP_466,3.65,-0.05,-0.38,0.28 1YW5,ARG 18,12,44,-0.06,0,0 2G5X.GLU 23.4.65.0.63.-0.01.-0.48 2DG7,GLU_113,4.68,0.38,0,-0.19 3GMS,GLU_82,4.51,0.1,0,-0.09 3GW3,HIS_358,6.42,-1.93,0.85,1 1R5Q,GLU 52,4.86,0.34,0,0.02 10TM,LYS 133,10.09,-0.17,0,-0.24 2F4Q,ARG_135,13.35,-1.85,1.55,1.15 2G3A,ARG_42,12.17,-0.33,0,0 2FL7,TYR 119,10.18,-0.79,0.13,0.85 4ESS.ARG 90.13.16.-0.38.0.49.0.56 3OA7, ASP_550, 3.46, -0.68, -0.09, 0.43 2CW4,ARG_92,12.45,-0.39,0,0.35 1GXN,ARG_626,11.93,-0.69,0,0.12 4FLE,TYR 181,12.29,0.85,0.41,1.03 3GW3,HIS_266,6.18,-0.53,0,0.2 2D2S,ARG_724,13.39,-0.48,0.8,0.56 4DVD,LYS_24,11.1,-0.74,0.85,0.49 1NJ4,ARG_39,12.56,-0.41,0.03,0.44 3RFF,LYS_106,11.21,-0.28,0.62,0.37 1X8F,ASP_175,3.96,0,0,0.16 1R3F,TYR_36,13.25,0,0.12,3.12 1V43,ASP_75,2.05,-2.28,-0.35,0.88 2AZL,GLU 260,4.68,0.33,0,-0.14 2R51,LYS 33,10,42,-0.07,0,-0.01 2H85,ARG_224,13.39,-0.32,0.47,0.74 1WOU,GLU_13,4.61,0.17,0,-0.06 3M70,ARG_133,11,-1.74,0,0.24 1Q46,LYS 60,9.96,-0.21,0,-0.32 3N2T,GLU_305,3.62,1.45,-1.86,-0.48 1X9G,LYS_138,10.4,-0.13,0,0.03 3LMF,CYS_33,10.06,-0.09,0.21,0.95 1NAR,GLU 42,6.07,3.65,-2.13,0.04 4D8L,ASP 226,3.39,-0.48,-0.26,0.33 2E3C,ARG_227,12.81,-1.51,0.92,0.9 3GMS,ARG_36,13.05,-0.52,0.47,0.6 1PNE,ASP_13,2.1,-1.7,-0.46,0.46 2X4L,LYS_195,10.53,-0.06,0,0.09 1SJY,GLU_2,3.4,0.2,-1.3,0 3BB7,ASP_85,3.84,0,-0.17,0.2 2H8O,LYS_86,10.19,-0.19,0,-0.12 200K,HIS_352,4.6,-1.79,0,-0.11 1L2F.ASP 151.3.83.-0.15.-0.42.0.6 3DSH,LYS_397,10.62,-0.24,0.06,0.31 1MML,LYS_53,10.12,-0.38,0,5.55E-17 3CXS,LYS_152,10.27,-0.3,0,0.07 3FNI,ARG_151,12.47,-0.46,0.14,0.3 1XAW.TYR 420.9.91.-0.68.-0.22.0.8 1LN4,GLU 54,3.3,0.13,-0.85,-0.48 1160,LYS_195,11.03,-0.54,0.27,0.8 4EKU,ARG_309,12.26,-0.31,0,0.07 3RLE.GLU 8.4.54.0.08.0.-0.03 1NRI,CYS_90,11.44,-0.18,0.59,2.03 2H30,LYS_54,10.21,-0.28,0,-0.01 3FWU,TYR_99,11.48,-0.86,0,2.34 3M66,TYR_384,11.08,0,0.17,0.91 2V4X,ARG 58,12,47,-0.56,0.19,0.34 4EZB,HIS_265,6.63,-0.7,0.94,-0.1 1O3X,ARG_299,12.51,-0.13,0,0.14

1MTZ.LYS 76.10.39.-0.26.0.0.15 1W24.TYR 69.12.08.-0.17.0.75.1.5 1PV5,GLU_103,3.2,0.32,-1.24,-0.38 2WOZ,ARG_335,12.59,-0.26,0.07,0.28 1WRU.GLU 198.4.81.0.31.0.0 2ZCO,ASP 52,3.98,0,-0.02,0.2 3IL3,HIS_180,7.14,-0.75,0.83,0.56 1PBV,ASP_206,3.89,0,-0.05,0.13 2ZCO,TYR_54,10.16,0,0.04,0.12 3GOZ,HIS_22,6.3,-0.2,0,0 3CRM,ARG 43,12,49,-0.34,0,0.33 109G,TYR_28,11.34,0,0.43,0.91 3G9G,LYS_149,10.21,-0.32,0,0.03 2W1R,GLU_166,3.01,0.39,-1.27,-0.6 4ANN.ARG 33.11.51.-1.79.0.13.0.67 1YTQ,ASP_175,3.78,-0.55,0.15,0.39 2Cl3,GLU_151,4.29,0.26,-0.4,-0.07 2HRZ,GLU_278,4.32,0.24,-0.24,-0.19 2EFK,GLU_34,3.89,0.18,-0.45,-0.34 3LMO,ASP 66,4,08,0,0,0,28 3NZL,LYS_77,10.93,-0.34,0.05,0.72 3FS3,HIS_232,5.6,-0.93,0,0.02 1RKA, ARG 218, 12, 23, -0, 31, 0, 0, 03 1YTD.ASP 175,3.97,0,0,0.17 1Q2Y,ASP_49,3.61,0,-0.42,0.23 3GS9,TYR 298,11,99,-0.85,0.16,2.68 2XWS,ARG_2,13.02,-0.27,0.03,0.76 3U0V.GLU 170,4.19,1.12,-0.68,-0.75 1UAJ,ASP_95,3.15,-0.89,-0.2,0.44 1EQ6,ASP_110,4.49,0,-0.11,0.81 2W0G,CYS_233,9.87,-0.12,-0.01,1 3CIV,HIS_57,6.76,-0.29,0.05,0.5 3Q2C,CYS 74,10.31,-0.02,0.23,1.09 2E3S.GLU 410.4.72.0.22.0.-0.01 1YW5,GLU_124,3.81,0.7,-0.85,-0.55 2P0Y,GLU_321,4.95,0.5,0,-0.05 2AXO,ASP_173,4.28,0,0,0.47 3CS1.CYS 124,12.58,-0.15,0.63,3.09 2FZ4,ASP_39,2.92,-1.57,-0.22,0.91 1ILW,ASP_27,3.46,-0.48,-0.27,0.4 1LN4,GLU_57,4.61,0.11,0,0 3LQE,TYR 496,13.14,0,0.46,2.68 3UX2.CYS 90.9.55.0.0.07.0.49 3IVF,ASP_94,2.35,-1.73,-0.11,0.39 2HXB,LYS_20,10.44,-0.14,0,0.08 3PU6,GLU_27,4.84,0.35,0,-0.01 3O48, TYR_131, 11.59, 0.85, 0.43, 0.31 2JHY,ARG_120,12.44,-0.25,0,0.2 2FXT,GLU_415,5.23,0.83,0,-0.11 1X7F,TYR_82,10.05,0,0,0.05 3GOZ,GLU 243,4.65,0.15,0,0 2WB8,ASP_714,3.89,0,-0.07,0.16 2CL3,GLU_117,3.71,0.75,-0.85,-0.68 3OBS,TYR_82,10.5,0,0.17,0.33 3CJW,ARG_187,12.46,-0.12,0,0.08 2Q98,HIS_138,5.92,-0.72,0,0.14 2B0A,TYR_47,12.15,0,0.18,1.99 2A1V,ASP_55,3.97,0,0,0.17 1GPP,ASP_438,2.88,-0.84,-0.29,0.2 1JKS,LYS 261,10.58,-0.1,0,0.18 4EUG,LYS 177,10.37,-0.18,0.0.05 2QZQ,TYR_161,10.34,0,0.1,0.23 1QZN,CYS_37,11.89,0,-0.3,3.19 3P51,GLU_120,4.91,0.22,0,0.19 2l88,LYS_461,10.48,-0.13,0,0.11 2F9F,GLU_29,3.96,1.16,-1.59,-0.1 10TM,HIS_162,5.71,-0.37,0,-0.43 2WOZ,GLU_331,4.62,0.12,0,0 1XAW,HIS_509,5.38,-0.84,0,-0.29

3E7P,GLU_122,5.77,3.48,-1.57,-0.63 1MUF.CYS 200.9.19,-0.3.0.16.0.34 1SUU,ASP_612,4.07,-0.14,0.04,0.38 1H4U.GLU 615.4.11.0.27.-0.53.-0.13 1ZBM,LYS_155,10.66,-0.18,0,0.33 208LGLU 16.3.97.1.03.-0.59.-0.98 3K8J,TYR_47,11.55,-0.8,0.06,2.3 4FH3,TYR_298,10.13,0,-0.14,0.27 3EOD,LYS_68,10.61,-0.13,0.09,0.14 1X7F,GLU_344,4.96,2.86,-1.64,-0.75 2YWK,LYS_50,10.54,-0.2,0,0.24 2CWC,TYR_87,10.33,0,-0.1,0.43 3GFP.GLU 460,3.89,0.19,-0.76,-0.03 1Z3X,ARG_132,13.62,-0.61,1.02,0.72 1Y2O,LYS 47,11.32,-0.41,0.85,0.38 3G9G,GLU 129,3.85,0.5,-0.49,-0.67 1W24,ASP_55,1.87,-1.67,-1.01,0.76 2A6B,ARG_32,13.69,-0.39,0.8,0.77 3ADO,ASP_110,3.16,-1.55,-0.32,1.23 2QDJ,HIS 129,6.19,-1.8,0.85,0.64 2GAU,GLU_59,3.58,0.31,-0.85,-0.38 3BWT,LYS_878,10.3,-0.2,0,0 1QZN,ASP_132,3.53,-0.66,0,0.4 3F1X,GLU 110,4.64,0.11,0,0.03 3F5D.LYS 81,10.35,-0.15,0,0.01 3H5T,ARG_210,12.61,-0.09,0,0.2 3RJZ,HIS_179,6.48,-1.12,0.53,0.56 2E3H,ARG_297,12.48,-0.02,0,0 3TRE,LYS 104,9.58,-0.56,0,-0.36 10GL,ARG_13,12.81,-0.27,0,0.58 2D7J,ARG_18,12.19,-0.22,0,-0.09 3ETU,TYR_344,9.5,-0.47,-0.34,0.31 3G9G,ASP_123,3.94,-0.85,-0.46,1.45 3IL3.GLU 224.3.71.0.26.-0.43.-0.61 1WJG,ARG_32,13.52,-0.47,0.74,0.75 1SQH,GLU_17,3.12,0.73,-1.57,-0.55 1SJY,GLU_5,4.55,0.05,0,0 1MUF,GLU 132,4.54,0.18,0,-0.14 1X7F,TYR_229,12.58,0,0.65,1.93 1X04,ASP_84,3.42,-0.52,-0.01,0.15 1FKM,CYS_486,12.39,0.09,0.61,2.69 2IF4.GLU 174.3.92.0.74.-1.43.0.1 2BDD.TYR 38.9.73.-0.45.-0.18.0.36 2FPN,HIS_24,5.62,-0.95,0,0.07 3GW3,ARG 47,12,11,-0,42,0,0.03 3JSN,GLU_10,4.04,0.26,-0.5,-0.22 1EYH,GLU_137,4.05,0.16,-0.26,-0.36 3ZTA.ASP 100.3.52.-0.58.0.0.3 3IPZ,CYS_97,8.06,-1.4,-0.26,0.72 1NAR,GLU_7,12.98,4.95,1.5,2.03 2VGM,ASP 206,3,56,0,-0,52,0,28 3UX2.GLU 120.4.6.0.1.0.0 3PM2,LYS_36,10.24,-0.26,0,0 2IRM,CYS_237,11.03,-0.34,-0.8,3.17 2QEV,ARG_104,12.65,-0.22,0,0.36 2NMU,TYR_133,10.16,0,0.07,0.09 2EDM.TYR 153,10.46,-0.01,0.1,0.37 3KT9,GLU_92,4.59,0.22,0,-0.14 2B0A,CYS_70,12.61,0,0.24,3.36 4FZN.GLU 264.4.77.0.27.0.0 3P2F,GLU_7,3.9,0.63,-0.85,-0.38 1SNT,ARG_170,12.46,-0.04,0,0 2E3S,LYS_522,10.31,-0.34,0,0.15 3IRA,TYR_122,12.56,0.85,0.26,1.44 1G8P,GLU_172,4.03,0.42,-0.47,-0.42 3M70, ARG_273, 12.53, -0.37, 0.04, 0.36 3LD1,ARG_46,12.25,-0.26,0,0.01 2PLQ,TYR 255,12.71,-0.11,0.61,2.21 3R87,GLU_69,4.79,0.23,0,0.06

1L2F,CYS 250,11,11,0,0,09,2,01 2D2S,ARG_592,12.61,-0.84,0.19,0.75 1WJG,LYS_99,10.45,-0.09,0,0.04 3GG6,LYS 93,10,16,-0,35,0,0,01 1WP5,ARG_40,10.78,-2.01,0,0.29 4FUG IYS 147.10.4 -0.39.0.0.29 3ETV,LYS_226,10.41,-0.23,0,0.14 1IDK,GLU_265,4.6,0.09,0,0.01 1SQH,LYS_166,10.45,-0.05,0,0 1X9G,GLU_162,4.68,0.27,0,-0.08 2E3I,ARG 63,13.88,-0.5,1.49,0.38 3GE9.ARG 140.11.73.-0.77.0.0 2YWJ,ASP_171,2.77,-1.39,-0.39,0.76 1ZBM,HIS_-2,5.88,-0.42,0,-0.19 1PV5.GLU 121.4.56.0.2.0.-0.13 3RKV,ARG 195,12.37,-0.49,0.03,0.34 1BN6,LYS_186,10.38,-0.13,0,0.01 4DEZ,ARG_150,12.58,-1.78,0.83,1.03 1T3Y,GLU_111,3.03,1.16,-1.7,-0.93 2EFK,HIS 116,6.53,-0.89,0.72,0.21 1Z9L,LYS_3,11.47,-0.33,0.63,0.67 3EUR,LYS_64,11.59,-0.39,0.85,0.63 3CZC,LYS_21,10.74,-0.25,0.1,0.38 2ILR.GLU 506.3.01.0.46,-1.57,-0.38 1X7F.HIS 13.6.79.-0.62.0.7.0.21 2CVB,GLU_81,4.4,0.25,0,-0.35 2RFA,HIS_157,6.41,-0.09,0,0 3JRT,HIS_84,6.29,-0.21,0,0 4D8L,ARG_200,12.86,-0.3,0.38,0.28 2099,LYS 173,10,44,-0,06,0,0 2WOZ,CYS_389,10.51,-0.01,-0.12,1.64 1SQH,LYS_284,10.58,-0.17,0,0.25 20JO,ASP 605,4,12,0,0,01,0,3 2QDJ,LYS 95,11.22,-0.32,0.59,0.45 3ASA,ASP_18,3.98,-0.03,-0.2,0.41 3IO0, ASP_88, 2.79, -0.85, -0.46, 0.31 3ADO,ASP_8,2.68,-1.1,-0.95,0.94 3IU5,TYR_144,12.27,-0.85,0.17,2.95 100E,LYS 85,11,15,-0,26,0,51,0,42 1DTO,LYS_91,10.46,-0.16,0,0.12 2GAU,ASP_49,3.4,-0.83,0,0.43 2F9F,LYS 64,10.02,-0.21,0,-0.26 1LZL,HIS 143,7.21,-0.44,0.76,0.38 2IXM,LYS_40,11.73,-0.36,0.85,0.75 1XEU,TYR_266,10.94,0,0.33,0.61 3GT0,LYS_43,10.8,-0.19,0.48,0 3GS3,ARG 198,12.64,-0.14,0,0.28 2RFA,HIS_122,3.83,-3.29,0.82,-0.19 3ZTA,HIS_114,6.5,-1.32,0.97,0.34 3PBH,ARG 235,11.66,-1.64,0.2,0.59 3ERF,GLU_39,4.14,1.95,-1.66,-0.65 1WNH,HIS 50,7.07,-0.66,0.85,0.38 2EYI,ASP_226,4.39,0,0.09,0.51 2FM9,ASP_200,2,-2.27,-0.02,0.49 3R87,TYR_5,10.64,0,-0.09,0.74 1JB3,ASP_49,3.4,-0.6,-0.13,0.33 2IIA.HIS 71.6.16,-0.28.0,-0.06 2D0A, ARG_219, 13.7, -0.31, 1.13, 0.39 1ZBS.ARG 249.12.53.-0.35.0.0.38 1ZBP,ASP_46,3.63,-0.57,-0.25,0.65 2R4O.LYS 216,10.39,-0.17,0,0.06 2QEV,GLU_65,4.2,0.28,0,-0.58 3LH5,TYR_718,10.11,0,-0.1,0.21 2Q34,TYR_137,12.07,-1.21,-0.1,3.38 2Q5X,ASP_824,3.94,0,0,0.14 3CIV,TYR_278,13.83,0,0,3.83 4ANN,ASP_126,3.83,0,-0.13,0.16 3GA2.TYR 175.10.99.0.0.29.0.7 2ZCO,HIS_278,6.36,-0.17,0,0.04

1G8P,GLU_226,3.66,0.31,-0.8,-0.35 3K1H,TYR 127,10.56,-0.79,-0.06,1.43 3R87,ASP 15,3.24,-1.68,-0.3,1.42 1SUU,LYS_662,10.87,-0.22,0.26,0.33 3ELI,ASP_122,3.16,-0.44,-0.36,0.16 3G9G,LYS 59,10.56,-0.19,0,0.25 2FBO.GLU 87.2.22.0.48.-2.33.-0.43 3BCY,HIS_76,6.91,-0.55,0.81,0.14 10GL,GLU_144,3.49,0.29,-0.85,-0.45 3CO1,GLU_106,4.8,0.25,-0.03,0.07 1V6T,ARG 73,12.09,-1.01,0.0.61 3GW3.GLU 110.4.83.0.33.0.0.01 3JV1,LYS_166,9.35,-1.35,0,0.21 3G9B,TYR_109,13.91,0,0.28,3.64 1XTZ.HIS 62.6.24,-0.23,0,-0.03 2BCF,HIS_134,7.58,-0.6,0.85,0.82 1DOV,ASP_113,3.91,0,-0.1,0.21 1X7F,ASP_84,3.97,0,0,0.17 1YLN,ASP_79,4.07,0,0.08,0.19 1ES9,ASP 189,4,45,0,-0,23,0.87 3CBN,ASP 133,3.66,-1.12,-0.22,1.18 3PAC,TYR_166,10.12,0,-0.03,0.15 3K8J,HIS 255,7,15,-0,37,0,52,0,5 3IVF.CYS 116,10,46,-0.07,0.02,1.5 2Z84,GLU 131,3.96,1.21,-1.81,0.07 2HRZ,ARG_27,12.98,-0.59,0.66,0.41 3D9H,GLU_242,4.61,0.11,0,0 3G6S,LYS_159,10.36,-0.24,0,0.1 1EYH,TYR_48,10.07,-0.3,-0.2,0.58 307K,TYR_109,12.94,0.74,-0.21,2.42 3QYB,LYS_954,10.64,-0.09,0,0.23 1RKA,GLU_176,3.7,0.23,-0.65,-0.38 2QK1,LYS_500,10.09,-0.42,0,0 2A6B,GLU_167,5.59,1.04,0,0.05 3CIV.HIS 133.6.54,-1.33.0.85.0.52 2P0Y,ARG_10,12.68,-0.37,0.1,0.44 2CXA,HIS_193,5.83,-0.46,0,-0.21 2D59,TYR_22,10.51,0,0.01,0.5 1HF8,CYS 230,10.23,-0.05,0.33,0.96 1OGL,ASP_185,4.23,-0.84,0.06,1.19 3RFF,ARG 150,12.83,-0.33,0.46,0.21 1VJG,CYS_151,11.41,0,-0.02,2.42 1SQH,CYS 109,12.26,-0.03,0.43,2.86 1J8B.GLU 36.4.19.0.37.-0.67.-0.01 1X04,LYS_137,10.41,-0.09,0,0 3E7P,LYS_220,10.42,-0.2,0,0.13 2D2S,GLU_538,4.8,0.24,0,0.05 3PBH,HIS 45,4.73,-1.88,0.66,-0.55 1ZCU,TYR_221,10.85,0,0.06,0.79 4GA2,LYS_46,11.24,-0.61,0.41,0.94 3BQE,LYS_310,10.23,-0.16,0,-0.11 3RE9,LYS 209,9.59,-0.97,0,0.07 3GT0.LYS 163.10.44,-0.06.0.0 3EZ7,GLU_235,4.59,0.72,-0.54,-0.09 1T07,ARG_3,12.31,-0.63,0.02,0.42 3NR5,GLU_115,2.5,0.52,-2.14,-0.38 3MEW,ASP_196,3.76,-0.28,0,0.24 2PPN.LYS 52,11,47,-0.25,0.84,0.38 1HF8,ARG_66,12.11,-0.86,0,0.46 3RE9,ASP_193,3.18,-1.34,-0.86,1.58 2PGX,ARG_68,12.78,-0.58,0.49,0.36 2AXO,LYS 228,10.7,-1.14,0.83,0.5 2FZ4,GLU_131,4.76,0.28,0,-0.01 1WP5,GLU_69,3.79,0.45,-0.85,-0.32 3ZXY,ASP_182,3.85,0,-0.12,0.18 1YM5,HIS_192,4.68,-1.9,0,0.08 1WOU.TYR 4.10.48.0.0.08.0.39 3COU, ARG_20, 12.22, -0.3, 0, 0.02 2AZP,ARG_41,12.27,-0.25,0,0.01

1SUU.TYR 743.12.36.-0.72.0.13.2.96 4EF5,LYS 289,10.49,-0.25,0.0.25 2QEV,GLU_48,4.46,0.09,0,-0.13 2B78,GLU_256,4.52,0.16,0,-0.14 4FH3.GLU 287.4.65.0.23.0.-0.07 2E3C,ASP 389,3.95,-0.23,0,0.38 2IDC,GLU_82,3.97,0.26,-0.8,0 1HF8.LYS 202,10.44,-0.38,0.0.32 3IBT,ARG_259,12.35,-0.55,0.48,-0.08 3V75,ARG_99,12.86,-1.13,0.7,0.78 2YT4,HIS 660,5.85,-0.82,0.27,-0.1 2YT4,ARG_630,13.35,-0.81,0.34,1.32 1SNT,CYS_219,12.43,-0.18,-0.07,3.68 3HOX,LYS 35,10,28,-0,22,0,0 1WYC, ASP 127, 4.16, 0, -0.18, 0.55 1LTU,HIS_22,6.09,-0.5,0,0.09 3LJI,ARG_96,11.74,-0.59,0,-0.17 2QV2,LYS_19,10.72,-0.94,0.85,0.32 1NIJ,CYS 67,12.45,0,0.12,3.33 1RKA, ASP 204, 2.77, -1.28, -0.28, 0.53 3F1X,LYS_300,10.48,-0.02,0,0 2HXB,ASP_38,3.18,-0.51,-0.6,0.5 1RI6,GLU_262,4.54,0.07,0,-0.03 3M7G,ARG 144,13.15,-2.59,0.67,2.57 3OBS,GLU_51,4.67,0.2,0,-0.04 2EEY,LYS 68,10.61,-0.11,0,0.22 1QYI,LYS_308,10.38,-0.14,0,0.02 10IS,ASP 176,2.93,-0.85,-0.4,0.37 2YX0,GLU_300,4.43,0.23,0,-0.3 3CRM,HIS_297,6.3,-0.2,0,0 1RI6,TYR_290,11.17,-0.15,0.23,1.09 1ZP2,GLU_157,4.69,0.22,0,-0.03 2NRR,ARG 394,12.37,-0.48,0.1,0.25 4DNU,TYR 253,10.06,-0.1,-0.65,0.81 3B79, ARG_117, 12.23, -0.34, 0, 0.06 2NYC,ASP_210,4.15,0,0,0.35 2WZ9,GLU_71,4.02,0.32,-0.8,0 3BB7.LYS 90.9.98.-0.84.0.0.32 2EFK,ASP_168,2.56,-1.45,-0.09,0.3 1SI7,TYR_159,13.72,-0.01,-0.11,3.85 3EYE,LYS_117,10.47,-0.08,0,0.05 3V1Q,ARG 585,12.17,-0.34,0,0.01 2PGX.LYS 177,10.3,-0.2,0.0 3O16,GLU_60,4,2.08,-2.48,-0.09 1QYI,TYR_209,10.55,0,-0.05,0.6 3BWT,ASP_743,3.34,-0.77,-0.2,0.5 1K95,ARG_103,12.62,-0.12,0,0.24 3L7N,GLU_204,4.26,0.33,-0.09,-0.48 3F6M,HIS 110,5,95,-0,55,0,0 1XIP,GLU_314,4.92,0.49,0,-0.08 1YR6,LYS_180,10.57,-0.26,0,0.33 3OKO,ASP 609,3.94,0,-0.23,0.38 3BPV,ASP_122,3.94,0,0,0.14 3B79,ARG_47,12.08,-0.45,0,0.03 3EVN,TYR_56,11.61,0.39,0.45,0.77 3JSN,GLU 181,4.29,0.33,0,-0.53 1DUN,TYR_25,10.36,0,0,0.36 1U53,ASP_91,3.04,-1.01,-0.09,0.34 3Q1C,GLU_282,3.84,1.27,-1.6,-0.33 1NKD,ARG 57,12.44,-0.07,0,0.02 1UCH.ARG 221,12.68,-0.18,0,0.36 2FI9,ARG_15,11.65,-0.95,0,0.1 2D8N,LYS_101,10.39,-0.2,0,0.09 2O0K,TYR_55,12.33,0,0.45,1.88 1DVO,ARG_171,13.13,-0.24,0.44,0.43 3ETU,ASP_262,4.14,0,-0.52,0.87 1SUU,TYR_574,10.43,0,0.14,0.29 3CAX,GLU_353,4.65,0.12,0,0.03 3QAV,ASP_184,3.8,0,-0.26,0.26

3H5T,GLU_344,4.64,0.23,0,-0.09 2RJD.LYS 239.10.33.-0.17.0.0 3U2R,ASP_85,4.28,0,0.21,0.27 1PNE,LYS_115,10.33,-0.25,0,0.08 1RI5,GLU_182,4.39,0.23,-0.11,-0.22 3EVN.TYR 189.11.6.-0.12.0.15.1.57 4EVF,LYS_48,11.31,-0.48,0.78,0.51 1RL0,ASP_38,3.59,-0.32,-0.12,0.24 3L7N,ARG_2,14,-0.41,1.32,0.58 3JZN.ARG 120.13.72.-0.85.1.23.0.86 4FCU,LYS_206,10.04,-0.39,0,-0.07 3GS3,LYS_270,10.42,-0.08,0,0 3EGN/TYR 423,11,45,0,0,28,1,18 3IL3,HIS_83,5.06,-1.81,0.23,0.14 3GA2.GLU 95.6.58.3.01.-0.85.-0.09 4ETX.GLU 416.4.69.0.22.0.-0.02 2FL7,TYR_102,11.78,0,0.21,1.58 1NAF,LYS_250,10.89,-0.17,0,0.56 2NRR,GLU_407,4.93,0.18,0,0.24 2EJB,GLU 45,4.64,0.13,0,0.02 2A6B,GLU_107,4.5,0,0,0 3GW3.TYR 30.12.08.-0.52.0.77.1.83 2Q99,ARG_110,11.14,-1.63,0,0.26 2H2Z,ARG 60,13.32,-0.19,0.61,0.39 2EA9.HIS 35.6.9.-0.36.0.32.0.43 3CIV,HIS_24,6.36,-0.39,0,0.25 2YYO,ASP_16,3.82,0,-0.23,0.24 3IVF,ASP_46,3.98,0,-0.22,0.41 2P0Y,HIS 160,6.4,-0.1,0,0 1HF8,ARG_129,13.3,-0.69,0.85,0.63 1GQE,LYS_284,10.33,-0.3,0,0.14 3GMS,HIS_179,5.32,-1.1,0,-0.07 2B3M,ARG_123,13.69,-0.56,0.82,0.94 4DVD,ASP 146,3,39,-1.07,-0.31,0.99 2GEN,GLU_180,2.9,0.38,-1.49,-0.5 20BI,ASP_21,2.14,-2,-0.44,0.77 105J,ARG_70,12.24,-0.36,0,0.11 2G7O,GLU 65,4.17,0.26,-0.6,0 1DZF,ARG_212,12.32,-0.25,0,0.07 4FH3,ARG_277,12.23,-0.56,0,0.29 1MTZ,TYR_281,13.11,-0.85,0.3,3.65 3EAZ,ASP 115,2.5,-1.57,-0.5,0.77 1WXO,ARG 234,13.1,-0.42,0.2,0.81 1BKB,TYR_108,9.4,-0.65,-0.54,0.6 1NRI,CYS_50,10.54,-0.17,0.1,1.61 3H6Q,TYR_7,11.76,0,0.48,1.29 105T,TYR 150,12.5,0.58,0.48,1.44 1DUPASP 90.4.1.-0.15.0.18.0.26 3ERF,ARG_34,13.13,-1.47,1.4,0.7 3EVP,LYS_265,10.37,-0.14,0,0 4ACJ.ASP 765,2.42,-2.52,-0.34,1.48 2Z0M,ARG 278,12.05,-0.5,0.0.04 2VGM,LYS_128,10.43,-0.23,0,0.16 2099.TYR 37.9.77.-0.06.-0.57.0.39 2JEO,GLU_106,3.74,0.27,-0.45,-0.58 3LD1,ARG_266,12.92,-0.92,0.06,1.27 2FD5.GLU 141.3.12.0.5.-1.58.-0.3 1MUF,GLU_97,5.05,1.26,-0.22,-0.49 1YOY,LYS_167,10.25,-0.35,0,0.09 2ZO5.GLU 188.5.89.3.46.-1.5.-0.56 2W2S.GLU 202,4,26,2,08,-1,5,-0.84 3P28,TYR_95,12.21,-0.05,0.07,2.19 1ES9,LYS_118,10.29,-0.21,0,0 1XIP,ASP_331,3.97,0,0,0.17 3ETV,ARG_220,12.21,-0.44,0,0.15 3IBT,ARG_221,12.01,-0.55,0,0.05 3BCY,GLU_20,4.62,0.12,0,0 3EJC,CYS_119,10.25,-0.17,0.06,1.36 2RGY,TYR_254,10.11,-0.29,-0.04,0.45 200K.LYS 148,10.5,-0.29,0.0.3 3E5T,GLU 16,4.27,0.3,0,-0.53 1Q8B,LYS_62,11.08,-0.38,0.16,0.8 1RKA,GLU_143,5.45,2.61,-1.52,-0.14 1KCM,GLU_159,5.12,1.25,-0.51,-0.13 3FXH GLU 47 4 67 0 14 0 0 04 3BPV.TYR 89,9,93,0,-0,3,0,24 3CAN,LYS_113,10.59,-0.11,0,0.2 1WRU,ARG_268,11.3,-1.38,0,0.18 3L3P,GLU_447,4.59,0.11,0,-0.02 3CJW,TYR 181,12.63,-0.85,0.35,3.13 2WB8,HIS_651,7.08,-2.34,0,2.92 4FZN,CYS_55,11.31,0,-0.15,2.46 1K95,GLU_140,3.32,0.94,-1.48,-0.65 3M16,LYS 6,10.6,-0.13,0,0.23 1J85,ARG 74,13,54,-1.12,1.63,0.53 4EZB,ARG_142,12.38,-0.1,0,-0.02 1XIP.HIS 252,5.53,-1.03,0,0.05 2FC3,ARG_27,12.25,-0.56,0,0.32 2FZ4,HIS 41,6.51,-0.2,0,0.22 1W7B.TYR 75.11.44.0.0.05.1.4 2V4U.ASP 507.4.42.0.0.28.0.33 1CHD,HIS_173,6.03,-0.41,0,-0.07 1T6L,ARG 54,11.36,-1.46,0.0.32 3FS3,CYS 133,11.08,0,-0.28,2.36 1GQE,ARG_256,12.39,-0.11,0,0 2W1R,ASP_107,4,0,-0.09,0.29 4GA2,LYS_123,10.45,-0.11,0,0.05 2VGM,TYR_277,11.72,-0.09,0.22,1.59 3DB9,ASP 69,3.29,-1.67,0,1.16 3BQW,CYS_202,9.9,0,-0.17,1.07 2X4L,LYS_313,10.26,-0.24,0,0 3LJI.GLU 286.3.49.0.47.-0.87.-0.61 3GYW,GLU 84,4.56,0.19,0,-0.13 1WJG,HIS_29,6.66,-0.42,0.54,0.04 1PNE, ARG 74, 13, 22, -0, 31, 0, 69, 0, 34 2V1L,ASP_102,4.06,0,-0.17,0.42 106D,LYS_24,10.18,-0.21,0,-0.11 4EKU,ASP 189,3.91,0,-0.21,0.32 3M7G,TYR_258,12.49,0,0.51,1.98 2PLQ,ARG_316,12.73,-0.18,0,0.41 3ADO,GLU_86,4.43,0.13,0,-0.2 3EJC,LYS 81,10.04,-0.47,0,0 3A2Z,HIS_139,5.68,-0.41,0,-0.4 3BA1,GLU_2,4.45,0.04,-0.09,0 3ULX,GLU_69,4.63,1.61,-0.71,-0.77 2APL,LYS 106,10.25,-0.25,0,0 3BPP,GLU_174,4.58,0.38,-0.31,0.02 2H2Z,LYS_137,10.32,-0.46,0,0.27 1WP5,TYR 16,9.67,-0.58,-0.09,0.34 1DZF,GLU_36,3.84,0.27,-0.7,-0.23 1T07,TYR 22,10.85,0,0.08,0.78 2W2S.GLU 193.4.79.0.08.0.0.21 2R51,ARG_283,13.04,-0.35,0.58,0.31 3US6,GLU_105,4.76,0.18,0,0.07 2R2Y,ARG_92,13.57,-0.91,1.35,0.63 3I4T.GLU 264,4.06,0.4,-0.46,-0.38 4DEZ,TYR_50,11.73,-0.07,0.05,1.75 1J74,LYS 108,10,48,-0.09,0,0.07 4ETX.GLU 379.4.72.0.14.0.0.08 1SJ8,ASP 666,3.79,0,-0.32,0.31 4DVD,GLU_138,4.78,0.28,0,0 1RI6,ARG_57,11.76,-0.74,0,0 3ERF,ARG_119,13.25,-0.45,0.69,0.51 2Q34,ASP_102,4.05,0,-0.13,0.38 2IN0,CYS_1,9.28,-0.92,-0.42,1.61 3RFY,ARG_194,12.35,-0.3,0,0.15 2DFL,LYS 80,10.38,-0.12,0,0 3N2T,ASP_151,3.46,-0.32,-0.48,0.46

3JZ9,GLU_505,3.14,0.63,-1.59,-0.4 3FK5,ARG 139,13.46,-0.18,0.79,0.35 1J33,GLU_184,3.98,0.39,-0.68,-0.23 2IN0,GLU_102,3.94,0.19,-0.85,0.09 2XMZ,LYS_152,10.52,-0.15,0,0.18 3LOE, ASP 443, 4.04, 0.0, 0.24 1J8B.ASP 71.4.18.0.0.11.0.27 2H2Z,ARG_279,12.31,-0.36,0,0.17 2YWJ,ASP_139,3.96,0,0.07,0.1 3PZ9,CYS_82,11.9,-1.21,0.55,3.57 2B0J,GLU_344,4.74,0.11,0,0.14 2GZQ,LYS_102,10.45,-0.19,0,0.13 3V4G,ARG_12,12.43,-0.08,0,0.01 2PPN,LYS_34,10.63,-0.1,0,0.23 2X4J,LYS_59,10.75,-1.01,0.85,0.41 1WRU,ARG 12,12.38,-0.35,0,0.23 3CXS,ASP_18,3.72,-0.34,-0.1,0.37 2YLF,ARG_83,12.15,-0.25,0,-0.1 1PGV,ARG_356,13.22,-0.5,0.84,0.38 3H6O,ARG 108,11.67,-0.88,0,0.05 1AT0.GLU 262.4.51.0.67.-0.6.-0.06 1P6F,LYS_149,10.46,-0.04,0,0 1C44,ASP_79,4.4,0,-0.25,0.85 1YB2,ARG_38,12.84,-0.18,0.08,0.43 4DVD,TYR 107,9.91,-0.25,-0.22,0.38 2BQQ,ARG_76,12.35,-0.24,0,0.08 3CCY,ASP_137,3.84,-0.34,-0.38,0.76 3RVC,LYS_131,10.69,-0.64,0.31,0.52 3N2T.GLU 191.4.76.1.67.-0.95.-0.47 3CIV,GLU_307,3.73,1.7,-1.99,-0.47 3NJM,ASP_74,3.83,-0.44,-0.08,0.55 2RGY.GLU 126.4.54.0.04.0.0 2EEY,ASP_17,2.42,-1.62,-0.09,0.34 2B0A,CYS 181,13.36,0,0.5,3.85 2D7U,ASP 243,3.88,0,-0.32,0,4 1NIJ,ASP_219,4.58,0,-0.37,1.15 1Q8B,LYS_100,10.03,-0.65,0,0.18 1JYH,ASP_38,4.11,0,0,0.31 1ZBP,GLU 233,5.32,0.86,0,-0.04 3RKV,GLU_261,4.89,0.47,0,-0.08 3LD1,ASP_127,3.13,-0.66,-0.38,0.38 3M16,CYS_90,10.17,0,0.03,1.14 1HF8,LYS 166,10.56,-0.12,0,0.17 3DSH,ARG 288,12,79,-0.61,0.45,0.45 1FO9,CYS_123,13.01,-0.06,0.73,3.35 1DVO,LYS_81,10.63,-0.39,0.15,0.37 1XEU,ASP_239,4.16,0,0.11,0.25 3RE9,TYR 99,13.64,-0.04,0.5,3.17 3P2F,TYR_24,10.3,0,0.07,0.24 2JEO,ASP_229,4.06,-0.07,-0.12,0.45 3N0K,ASP_40,3.9,-0.12,0,0.22 1NFN,ARG_142,12.22,-0.28,0,0 3ZXY.GLU 212.4.47.0.28.0.-0.31 2AD1,GLU_95,3.23,0.22,-1.04,-0.46 2EEY,ARG_159,12.61,-0.32,0,0.43 20JQ,ARG_686,12.47,-0.24,0,0.22 3K8J,GLU_257,3.91,0.22,-0.52,-0.29 1T95,LYS 107,10.54,-0.1,0.0.13 1ZCU,TYR_14,11.07,0,0.04,1.03 3M70, ASP_268, 3.45, -0.82, 0, 0.47 20EW,ASP_141,2.92,-0.92,-0.18,0.21 3UPD.LYS 92,10.4,-0.14,0,0.05 3ADO,GLU_157,3.79,2.14,-2.32,-0.51 2YWX,GLU_45,4.69,0.18,0,-3.47E-18 1MUF,ASP_328,3.25,-0.85,0,0.3 3BQE,ASP_332,4.33,-0.02,-0.15,0.69 1LFP.GLU 243.5.21.0.42.0.0.29 2Q13,ARG_237,12.38,-0.12,0,0 2RFA,HIS_201,4.74,-2.52,0.63,0.13

2CI3.ARG 30.11.84.-0.98.0.0.32 1TR9.GLU 175.4.67.0.14.0.0.03 3BB7,LYS_314,10.66,-0.12,0,0.28 1J85,ARG_20,13.97,-0.32,1.35,0.43 2RIK.GLU 258,3.97.0.31,-0.72,-0.12 30NH.CYS 540.11.51.0.24.0.49.1.78 3M7D,HIS_271,6.18,-0.2,0,-0.12 1MIX,LYS_306,11.24,-0.46,0.55,0.64 3LQE,GLU_311,5.52,1.96,-0.72,-0.22 1P1L,TYR 6,10.77,0,0.24,0.52 3BWT,LYS 780,10.88,-0.27,0.0.65 3CIV,GLU_224,4.58,0.11,0,-0.03 2X4G,HIS_139,6.15,-0.56,0,0.22 3F6F,GLU 125,4,92,0,38,0,0,04 2Q12,GLU_95,4.78,0.4,0,-0.13 2WB8,HIS_505,6.49,-0.11,0,0.1 1ZBM,GLU_39,6.21,3.06,-1.48,0.13 4H4J,HIS_212,3.89,-1.9,0,-0.71 3AU3,LYS 561,10.61,-0.12,0,0.23 1ZBS.ASP 222.4.63.0.0.04.0.79 3MIX,GLU_412,4.72,0.27,0,-0.05 1EV8,GLU_14,3.6,0.35,-0.83,-0.42 109G,GLU_111,3.41,0.55,-0.59,-1.06 1ZKZ,ASP 23,3.83,-0.39,0,0.42 1EDG,ARG_357,10.64,-2.95,0,1.08 3HQX,GLU_59,4.31,0.57,0,-0.76 1ZBP,GLU_223,4.77,0.28,-0.16,0.16 1RKA,GLU 192,3.85,0.5,-0.74,-0.41 1S7K,ARG_128,13.36,-0.32,0.84,0.34 1MTZ,ARG_90,13.18,-1.4,1,1.07 2W0G,ARG_266,12.16,-0.26,0,-0.09 208P,LYS_29,10.5,0,0,0 1H4U,LYS 504,10.44,-0.24,0,0.18 3V3T,LYS 47,10.33,-0.2,0,0.03 3CS1,GLU_82,4.02,0.6,-0.63,-0.46 3FK5,ASP_143,3.2,-0.69,-0.41,0.5 1L2F,LYS 16,10,41,-0,25,0,0,16 1JSX,GLU_172,3.8,1.12,-1.39,-0.42 3S0A,LYS_41,10.38,-0.25,0,0.14 1XKR,GLU_177,3.71,0.45,-0.75,-0.49 1G5Z,ASP_151,3.42,-1.15,-0.1,0.86 20BI,CYS 46,8.76,-1.62,-0.29,1.68 1RAJ.GLU 427.4.48.0.1.0.-0.13 2BAA,TYR_111,10.78,-0.83,0.1,1.52 3JSN,LYS_37,10.46,-0.06,0,0.02 1QQE,GLU_176,3.76,0.45,-0.77,-0.44 3COU, ASP_71, 3.59, -0.45, -0.1, 0.34 3C2E,ASP_222,3.14,-1.28,-0.52,1.15 1ZBM,GLU_197,4.77,0.37,0,-0.08 2CWC,HIS_199,6.27,-0.54,0,0.31 2P1W,LYS 53,10.64,-0.1,0,0.24 4E9E.LYS 529.10.48.-0.13.0.0.11 4GA2,ARG_58,12.23,-0.19,0,-0.07 1J33,ARG_200,12.24,-0.34,0,0.08 3BWT,ARG_728,12.21,-0.84,0,0.55 2FXT,ARG_291,12.76,-0.14,0,0.4 4H89,GLU_151,4.66,0.16,0,0 2P5D,ASP_140,3.89,-1.54,-0.28,1.91 1U7U,ASP_185,2.33,-1.55,-0.76,0.83 2EYI,TYR 246,10.83,0,0,0.83 2PLO.TYR 20.12.26.0.0.02.2.24 4ANN,HIS_179,7.02,-0.65,0.85,0.31 1GPP,ARG_138,12.77,-0.11,0,0.38 4D8L,ARG_124,12.79,-2.61,0.72,2.18 3BCH,LYS_17,9.98,-0.64,0,0.12 1ZBM,LYS 226,12.46,-0.43,1.64,0.75 3MIX,LYS_330,10.2,-0.5,0,0.21 1Q5Z,ASP_593,3.15,-0.5,-0.35,0.2 20YZ,ASP_61,3.91,0,-0.06,0.16

3RJX,TYR_325,11.21,0,0.26,0.95 2ZO5,ASP 330,1.81,-2.02,-0.48,0.51 1T07, ARG_19, 12.57, -0.17, 0, 0.24 2B0J.CYS 322.9.79.0.0.1.0.68 4EF5,LYS 338,10.43,-0.1,0,0.03 2CXA.ARG 88.12.29.-0.53.0.0.32 1U7U,LYS_247,10.11,-0.39,0,0 3M16,LYS_67,10.08,-0.4,0,-0.02 1TLV,TYR_240,9.86,-0.09,-0.38,0.34 1NIJ,ARG_242,12.5,-0.12,0,0.13 2Q99,TYR_183,11.64,0,0,1.64 2A4D,TYR_219,10.67,-0.84,0.01,1.5 208P,GLU_211,4.5,0,0,0 2NSN,ARG_35,12.27,-0.14,0,-0.09 2IOT.ASP 154.4.37.0.-0.02.0.59 3GYW.ARG 82,10.82,-2,11,0,0,43 3UAH,HIS_320,8.46,-1.38,1.7,1.64 2AH5,GLU_95,4.9,0.21,0,0.19 1QYI,GLU_130,3.7,0.92,-1.19,-0.54 3ERF,LYS 60,10.34,-0.17,0,0.01 3G9G,ARG_195,12.35,-1.2,0.81,0.24 1U7U.TYR 337,10.33,0.0.0.34 2JEO,ASP_116,3.17,-0.96,-0.06,0.38 1HF8,ASP 224,3.9,0,-0.02,0.12 3TMO.GLU 189.4.58.0.08.0.0 1G8P,LYS_316,12.17,-0.59,1.44,0.82 1U53,LYS_186,11.48,-0.32,0.8,0.5 2V4U,ARG_481,13.05,-0.33,0.47,0.41 2Q12,GLU 14,4.11,0.15,-0.54,0 2A6B,LYS 48,10.54,-0.29,0,0.33 2VGY,ASP_100,3.99,-0.16,-0.05,0.41 2JKF,GLU_57,4.64,0.1,0,0.04 3IV4,ASP 61,3.6,-0.44,0.01,0.22 10YI.GLU 112,4,4,1,44,-1,05,-0,5 2OSA,LYS_402,10.22,-0.44,0,0.16 3RJZ,LYS_175,11.34,-0.4,0.85,0.38 3KEY,HIS_429,6.13,-0.32,0,-0.05 3BQW,ASP_256,3.8,-0.3,0,0.3 20PJ,ARG_280,12.27,-0.83,0,0.59 100X,ASP_222,2.02,-2.5,-0.25,0.96 2H2W,TYR_293,10.22,0,0,0.22 100E.GLU 125,5.06,1.09,-0.06,-0.48 3RJX,ARG 86,11.35,-1.63,0.0.49 3UV9,ARG_441,13.53,-0.34,0.43,0.94 3PZ9,LYS_311,9.29,-1.42,0,0.21 1UCH,ASP_167,3.92,0,-0.14,0.26 3JZN, ARG 216, 11.42, -1.38, 0, 0.3 3RVC,ASP 101,3.86,0,-0.09,0.15 3AU3,ASP_610,3.88,0,-0.06,0.14 2F9F,LYS_96,10.18,-0.2,0,-0.12 2G2D,ARG 164,12,86,-0,49,0,36,0,49 2EJX.GLU 47.4.14.0.34.-0.13.-0.55 3LJI,GLU_201,4.92,0.14,0,0.28 1ZP2.GLU 228.4.8.0.38.0.-0.07 3ZXY,LYS_284,10.3,-0.18,0,-0.01 1VJG,ASP_142,3.96,0,-0.19,0.35 3JZN,CYS 126,11,66,0,-0,28,2,93 2R57,LYS_195,11.93,-0.8,1.66,0.58 2ZQ5,ARG_202,13.28,-0.35,0.72,0.42 3F6F.TYR 128.10.13.-0.73.0.16.0.69 1W24,ARG 176,13.63,-0.34,0.96,0.51 3GS9,ASP_20,4.11,-0.32,-0.06,0.69 2W1R,GLU_161,3.29,1.2,-2.07,-0.34 2Z0W,ASP_82,4,0,0,0.2 2DG7,HIS_167,6.48,-0.14,0,0.12 1YR6,ASP_132,3.63,-0.73,-0.35,0.91 3E0H,CYS_9,9.72,-0.22,-0.21,1.15 2VGY,HIS_109,5.82,-2.04,0.85,0.51 3Q9P,ARG_94,12.18,-0.23,0,-0.09

3N2T,ASP 311,3,99,0,-0,16,0,35 2V81,TYR 180,12.39,0.26,0.45,1.69 4ANN,ARG_111,12.43,-0.29,0,0.22 100E.LYS 51,10.45,-0.05,0,0 3Q2C,GLU_86,4.5,0.19,0,-0.19 3CRM,ARG 68,13,2,-0,46,0,18,0.98 2W2S,ASP_194,4.04,0,0,0.24 1QQL,ARG_122,12.28,-0.22,0,0 3H6Q,LYS_21,10.45,-0.05,0,0 1ZBP,ARG_151,13.26,-2.3,0.46,2.6 2FXT,LYS 314,10.39,-0.14,0,0.03 1KCM,LYS 5,9.83,-0.92,0.05,0.21 3BB7,GLU_78,4.64,0.14,0,0 3ON1,ARG_17,12.45,-0.05,0,0 2F4O,ARG 170,12,24,-0,26,0,0 3ETU,LYS 313,12,31,-1.07,1.51,1.37 1WP5,TYR_108,10.53,0,0.22,0.31 20KT.HIS 7.6.19.-0.66.0.0.35 1H09,LYS_197,10.43,-0.07,0,0 1PGV,ASP_329,3.4,-1.08,-0.17,0.85 2YYO,LYS 86,10,51,-0,24,0,0,25 3GT0,LYS_100,10.29,-0.31,0,0.1 3GE9,ASP_205,4.04,-0.25,0.05,0.45 1MIX.LYS 322,10.39,-0.11,0.0 30BS.LYS 33.10.41.-0.12.0.0.03 2GAU,ARG_77,11.17,-2.43,0,1.1 3F6M,ASP_67,3.84,-0.31,-0.03,0.38 1FQI,TYR_393,10.92,0,-0.16,1.08 3GW3,GLU_115,4.65,0.23,0,-0.08 3ADO,ASP 291,2.23,-1.8,-0.38,0.61 1R53,HIS_244,6.01,-0.46,0,-0.03 2FZP,GLU_195,3.4,1.06,-1.8,-0.37 2HP7.GLU 206.4.55.0.05.0.0 1WXQ,LYS 233,10.33,-0.18,0,0.01 1YB2,HIS_173,6.14,-0.95,0.06,0.51 2Z61,TYR_62,10.15,0,0,0.15 1PSW,GLU_226,4.63,0.15,0,-0.02 3RJZ,LYS_208,10.4,-0.42,0,0.32 3CIV.ASP 246.3.42,-0.76,-0.35,0.72 1MJS,LYS_332,10.33,-0.2,0,0.03 3C6B,GLU_246,4.45,0.27,0,-0.32 3CBN.ARG 145,12,78,-0.25,0.08,0.45 1TD6,GLU 194,4.86,0.38,-0.02,0 3TIR,ASP_155,3.89,0,-0.1,0.19 1YTQ,LYS_167,10.39,-0.11,0,0 1UCH,TYR_141,11.86,0,0.41,1.44 2QZQ,ARG 77,12.24,-0.31,0,0.05 3A2Z,ASP_182,3.35,-0.94,0.05,0.43 1ILW,ARG_13,12.65,-0.33,0.06,0.42 3CNU,TYR 34,13,53,0,1,21,2,33 3LD1,LYS_101,10.94,-1.17,0.85,0.77 4FCU,CYS 122,10.47,-0.42,-0.15,2.05 1R3F.HIS 173.6.46.-1.04.0.85.0.15 1MTZ,GLU_26,3.75,0.2,-0.57,-0.38 1MML,LYS_120,10.84,-0.28,0.57,0.04 1PVT,ARG_31,10.85,-1.71,0,0.06 4DEZ,ASP_204,3.72,-0.38,0,0.3 1PBV,ARG_63,12.41,-0.09,0,0 200P.GLU 122.4.81.0.17.0.0.15 1TJE,ARG_12,12.93,-0.36,0.23,0.55 3ETV,LYS 78,10.19,-0.31,0,0 2B78.GLU 319.4.81.0.66.0.-0.35 1YB2,ASP_150,2.95,-0.83,-0.55,0.53 3EGN,GLU_449,4.6,0.1,0,0 3KT9,CYS_51,9.99,-0.06,1.39E-17,1.04 1RKA,GLU_130,4.58,0.12,0,-0.04 3GW3,ASP_306,4.36,-0.47,0,1.04 3C2E,HIS_179,5.73,-0.67,0,-0.1 1O5T,HIS_257,5.72,-0.42,0,-0.36

1W7B,TYR_275,10.02,-0.22,-0.07,0.31 2YWJ,GLU 47,2.65,0.89,-2.34,-0.39 1NWA, ASP_19, 4.25, -0.42, -0.16, 1.03 3Q1C,ASP_123,2.82,-1.35,-0.03,0.4 3OKQ,GLU_565,4.96,0.31,0,0.15 1W24,HIS 57.6.01,-1.13.0.82,-0.18 2AH5,ASP_127,4.21,0,-0.1,0.51 1BYI,TYR_218,10.09,0,-0.26,0.35 3C5V,CYS_178,12.82,0,0,3.82 3JV1,LYS_72,10.11,-0.29,0,-0.1 4ECC,ASP 227,3.66,-0.03,-0.43,0.32 106D.LYS 142.10.41.-0.35.0.0.27 1RAJ,HIS_336,6.28,-0.23,0,0 3RE9,HIS 235,6,7,-0.62,0,33,0,49 2FL4,GLU_24,4.79,0.29,0,0 1J85,GLU 8,4.08,0.96,-1.09,-0.28 105T.HIS 336.3.86.-2.77.0.03.0.09 3LJI,TYR_262,11.3,-0.24,0.45,1.09 2Q99,ARG_362,12.23,-0.27,0,0 1EO6,ARG 71,12.38,-1.77,0.82,0.82 2D7U,LYS 300,10,47,-0,15,0,0,11 1R7J,LYS_18,10.41,-0.24,0,0.14 4H4J,GLU_60,3.95,0.27,-0.83,0 1V43.LYS 193.10.29.-0.64.0.0.43 2YYO,TYR 20,11.26,-0.02,0.31,0.98 2E3C,GLU 274,4.93,0.28,0,0.15 3ANJ,TYR_46,10.65,0,0,0.65 4DIU,GLU_136,4.21,0.37,-0.06,-0.6 2FXT,ASP_389,4.04,0,0,0.24 2P65,ASP_139,4.08,-0.77,0,1.05 2WOZ, ASP_477, 3.2, -1.35, -0.46, 1.21 100E,TYR 31,10,18,0,0,12,0,06 3CAX,LYS_371,10.51,-0.2,0,0.21 1QQL,TYR 41,10.22,0,-0.13,0.35 2PGX,LYS 185,10.08,-0.2,0,-0.22 3O48,TYR_81,11.95,0,0.06,1.88 2JKF,ASP_118,3.49,-0.73,-0.36,0.78 3TOW,LYS_102,10.4,-0.12,0,0.02 2OB5,LYS 120,10.05,-0.48,0,0.04 1X9G,GLU_186,4.89,0.81,0,-0.43 2G3A,ARG_92,12.97,-0.77,0.77,0.46 2CBE,GLU_221,3.8,0.21,-0.89,-0.03 2D8N,LYS 166,10.49,-0.28,0,0.28 1RL0,ASP 163,3.84,0,-0.51,0.55 3GA2,TYR_57,10.53,0,0.22,0.31 1G8P,TYR_274,10.08,0,0,0.08 3FHF,GLU_9,4.34,0.22,0,-0.38 3FHF,GLU_156,3.99,0.38,-0.66,-0.22 3GT0,TYR_76,12,-0.31,-0.02,2.33 2Q13,CYS_99,9.99,-0.23,0.14,1.07 2E3S, ASP_479, 2.41, -2.5, -0.63, 1.73 1J74,ASP_28,2.23,-1.75,-0.22,0.4 4F3J.ASP 167.3.25.-1.7.0.1.15 1YM5,HIS_157,6.81,-0.69,0.12,0.89 2V4X,GLU_12,4.62,0.19,0,-0.07 2QDJ,LYS_228,10.55,-0.45,0,0.49 1VJG,ARG_108,12.76,-0.35,0.35,0.26 1TP6,HIS 110.6.46,-0.36,0.0.31 3OIP,LYS_214,10.27,-0.25,0,0.03 2B61,TYR_156,12.5,0,0.62,1.89 3RFF,GLU_142,4.74,0.11,0,0.13 1SIG,ARG 364,13.26,-0.72,0.62,0.86 3V75,HIS_166,6.56,-0.37,0,0.43 1ZHV,ASP_101,3.94,0,-0.04,0.18 1W24,HIS_115,5.43,-1.07,0,0.01 2BQQ,GLU_118,3.07,0.45,-1.65,-0.23 4F8A,HIS 689,6,11,-0,25,0,-0,14 3GA2,ASP_154,3.81,-0.21,-0.15,0.37 2ZCO,ASP_155,3.04,-0.6,-0.8,0.64

2B02.GLU 455.4.24.0.48.-0.69.-0.05 20EV.HIS 37,5.35,-1.26,0.66,-0.55 3U4K,ASP_169,3.97,0,0,0.18 1DUN,ASP_40,1.84,-2.75,0,0.8 4DIU,ASP_231,3.07,-0.42,-0.57,0.26 3L3P.GLU 281,4.07,0.22,-0.28,-0.36 3LJN,CYS_141,11.6,-0.23,0,2.83 2F8H,LYS_66,10.72,-0.26,0,0.48 3EGN,CYS_388,9.36,0,-0.28,0.64 3US6,ASP_52,3.64,-0.6,-0.28,0.72 2R57.GLU 212.4.91.2.31,-1.6,-0.3 3HVW,CYS_276,10.48,0,0.15,1.34 2JHY,ASP_201,3.75,0,-0.36,0.31 2Z0M,ARG 232,13.04,-1.7,1.42,0.81 1R3F.ASP 298.2.71.-1.41.-0.34.0.65 3P28,HIS_133,2.31,-3.38,0.74,-1.53 1YW5,LYS_84,10.14,-0.13,0,-0.23 3E7P,ASP_114,2.7,-0.85,-0.76,0.51 2GZQ,ASP_30,3.95,0,-0.53,0.69 10LR.TYR 183,10.69,-0.37,-0.07,1.13 3GYW,TYR_135,10.38,0,-0.3,0.68 3Q6L,ASP_72,2.83,-0.85,-0.38,0.26 3ERF,GLU_144,3.61,1.99,-1.69,-1.19 3EVN.HIS 252.5.04.-0.99.0.-0.47 3PAC, ARG_114, 12.48, -0.27, 0, 0.26 105T,ASP_239,4.5,0,-0.04,0.74 2BAA, ASP_146, 3.36, -1.06, -0.07, 0.69 1H4U,GLU 485,4.85,1.2,-0.59,-0.26 3GG6.GLU 94.5.48.0.89.-0.22.0.31 1UXO,GLU_63,4.07,0.28,-0.37,-0.34 3V4G.GLU 21.4.79.0.29.0.0 2BV9,LYS_151,10.52,-0.52,0,0.53 3D9H,GLU_237,3.06,0.45,-1.22,-0.67 3BPPASP 68.3.18,-0.6,-0.38,0.37 3BQW,TYR_16,10.39,-0.72,-0.64,1.75 1G8P,ARG_219,12.5,-0.08,0,0.08 2A1V,ASP_64,3.51,-0.61,-0.06,0.38 4E9E.GLU 450.4.47.2.63.-2.33.-0.33 2DFL,HIS_236,4.14,-2.63,0.27,0 1H09,TYR 253,10,79,-0,19,0,11,0.87 1M5I,TYR_191,10.19,0,0.01,0.18 1BKB,ARG 116,12.28,-0.22,0,0 2B2H.GLU 178.4.32.0.35.0.-0.53 2Cl3,GLU_240,4.28,2.38,-1.86,-0.72 3GS9,GLU_32,5.22,2.07,-0.55,-0.81 3DTE,ARG_179,12.39,-0.15,0,0.04 3B7X,ARG_70,12.45,-0.1,0,0.04 2QK1,TYR_412,10.2,-0.97,0.03,1.15 1WP5,GLU_172,5.88,2.2,-0.85,0.02 3DTE,GLU_20,4.13,0.24,-0.35,-0.26 1U7U,TYR 400,10.88,-0.04,0.07,0.84 30KY,TYR 125,10.6,-0.02,0.2,0.42 3RKV,GLU_264,4.65,0.47,0,-0.33 4AM1,LYS_94,11.21,-0.28,0.66,0.32 1XIP,LYS_19,10.39,-0.12,0,0.02 1PSW,GLU_338,4.95,0.62,0,-0.16 3PZ9,LYS_307,10.27,-0.37,0,0.14 30IP,ARG_195,12.55,-0.33,0,0.38 4EF5,TYR_245,11.25,-0.15,0.04,1.36 3M70,CYS 87,11.08,0,0.02,2.06 3SMD.GLU 56,2.81,0.9,-2.17,-0.43 2F9F,GLU_33,4.06,0.29,-0.32,-0.41 2AHE,ARG_176,11.22,-1.58,0,0.3 1V43,ARG_350,12.29,-0.25,0,0.04 3Q1C,ASP_249,2.17,-1.27,-0.85,0.49 4F8A,GLU 633,4.72,0.19,0,0.03 2EDM,LYS_160,9.07,-0.98,0,-0.46 1FKM,HIS_285,5.72,-1.75,0.81,0.16 3Q2C,ARG_49,12.24,-0.28,0,0.02

2JEO,ASP 95,2,75,-0,95,-0,47,0,37 4F85.HIS 66.6.36.-0.28.0.0.15 2YWJ,ASP_147,2.58,-1.62,-0.57,0.96 2V4U,CYS_413,10.42,-0.02,-0.16,1.61 1CBY.TYR 245,10.3,0,-0,1,0,4 2H85.TYR 193.12.5.0.85.0.63.1.02 3C5V,ARG_201,9.77,-2.75,0,0.03 2E3C,ASP_394,3.73,-0.12,-0.09,0.15 10GL,ARG_218,13.24,-0.29,0.61,0.42 2EJX,GLU_69,3.59,0.71,-0.96,-0.67 3JSN,LYS_93,11.47,-0.32,0.73,0.55 3DZ1,ASP_25,2.61,-1.89,-0.68,1.39 2CI3,HIS_14,5.66,-0.71,0,-0.13 3PM2,LYS_162,10.68,-0.19,0,0.37 3CBN.ARG 87.12.1.-0.45.0.0.05 3G9G,GLU 106,4,79,0,42,0,-0,15 3U2A,ARG_44,12.43,-0.07,0,0 4H4J,LYS_95,10.23,-0.41,0,0.13 3RKV,ARG_324,12.31,-0.41,0,0.21 2QDJ,GLU 125,4.47,0.16,0,-0.19 1JT9,LYS_57,10.28,-0.28,0,0.06 2B3M,LYS_155,10.5,-0.26,0,0.25 2X5Y,GLU_757,3.67,0.34,-0.83,-0.33 3M66,LYS 308,10.59,-0.1,0,0.19 3ADO,ARG 302,13.19,-0.54,0.79,0.43 2E3S,GLU_456,2.65,0.55,-1.69,-0.7 1C44,ASP_70,3.18,-0.78,-0.36,0.51 3HUE,LYS_299,10.39,-0.17,0,0.06 3F1X,HIS_186,6.94,-0.59,0.26,0.76 1RSS,ARG_114,12.46,-0.04,0,0 1R3D,GLU_117,8.8,5.1,-0.89,0.09 1RZ2,GLU_193,5.32,0.75,0,0.07 1MD6,HIS 31,6.43,-0.11,0,0.04 301C.GLU 276.3.29.0.32,-1.01,-0.52 3EJG,GLU_112,4.92,0.65,0,-0.24 3RJZ,TYR_11,13.89,-0.5,0,4.4 3PZ9,TYR_88,10.83,0,0.1,0.73 2CI3,ARG 91,12.19,-0.48,0,0.17 3GOZ,GLU_295,4.75,0.41,0,-0.16 3UX2,GLU_39,4.59,0.21,0,-0.13 3JRT,GLU_66,4.2,0.59,-0.33,-0.54 2G5X,LYS 212,10,35,-0,22,0,0.07 3B4D,ASP 222,3.98,0,-0.05,0.23 2YT4,CYS_514,8.52,-0.71,-0.09,0.31 3ADO,ASP_115,3.46,-0.56,0.02,0.2 4FZR,CYS_347,11.74,-0.06,-0.03,2.83 2X4J,LYS 85,11,-0.27,0.39,0.38 3LOD,ARG 104,12,23,-0.32,0,0.05 2NMU,GLU_83,5.13,1.01,0,-0.38 1FQI,LYS_336,11.71,-0.83,0.75,1.29 1PBV.TYR 171.12.56.0.0.44.2.13 2D8N,LYS 157,10.52,-0.14,0,0.15 30NH,LYS_447,10.59,-0.18,0,0.27 1YM5,TYR_242,10.91,0,0.02,0.89 1UW7,TYR_66,10.28,-0.01,-0.19,0.48 3RHE,LYS_43,10.47,-0.03,0,0 2V1L,ASP 140,2.32,-2.22,0.24,0.49 2QVT,ASP_127,3.93,0,-0.04,0.18 3EX9,ASP_48,1.62,-2.3,-0.44,0.56 3V55,ARG 354,12.66,-0.28,0,0.43 3JSN.TYR 219,12,93,0,0,43,2,5 1EV8,ARG_222,11.96,-0.52,0,-0.03 2CN1,HIS_171,6.76,-0.72,0.73,0.25 3EZ7,HIS_230,5.85,-1.66,0.85,0.15 3NBI,GLU_185,3.9,0.38,-0.76,-0.23 2X4J,GLU_37,4.82,0.22,0,0.1 3EJG,LYS_2,10.45,-0.05,0,0 3GOZ,CYS_236,9.39,0,0.08,0.31 1J8B,ASP_79,2.38,-1.33,-0.62,0.53

2G5X,LYS 38,9.16,-1.35,0.0 3M7D,GLU 262,5.04,0.41,0,0.13 3RJX,LYS_300,9.62,-0.44,0,-0.43 1TD6.LYS 50.10.35,-0.21.0.0.06 3LOD,GLU_148,4.42,0.8,-0.23,-0.64 3CCY,ARG 129,12,27,-0.23,0,0 2R57,ASP_243,2.27,-1.7,-0.32,0.5 1UOH,LYS_90,10.39,-0.13,0,0.01 1K95,ASP_209,2.4,-1.56,-0.43,0.59 3H13,TYR_479,9.98,0,-0.13,0.11 3EIZ,ASP 157,3.27,-0.61,-0.24,0.33 1NRI.GLU 109.4.77.0.27.0.0 1Q2Y,GLU_34,6.32,1.82,0,0.01 1SQW,TYR_88,9.88,-0.85,0.14,0.59 1J7G,LYS 16,10,48,-0.08,0.0.07 1MUFLYS 111,10,72,-0,14,0,0,35 3ODJ,TYR_102,10.16,0,0.05,0.11 3P28,ASP_168,3.05,-0.99,-0.81,1.05 3LQE,GLU_488,4.42,0.84,-0.81,-0.11 1YLN,LYS 197,10.5,-0.1,0,0.1 2P5D.LYS 43,10.66,-0.92,0.53,0.55 1PGV.ARG 283,12.3,-0.28,0.0.09 3M16,GLU_26,4.73,0.28,0,-0.05 2B78,TYR 278,10,16,0,-0,06,0,23 4AM1.LYS 151.10.77.-0.34.0.4.0.21 2I88,ASP_446,4.71,-0.14,0.07,0.98 1MIX,LYS 300,12.11,-0.66,1.56,0.7 3ONH,GLU_546,4.58,0.09,0,-0.01 3AUF,ASP_161,1.9,-2.28,-0.39,0.77 2G3A,GLU_86,2.52,1.15,-2.34,-0.78 1VJG,ARG_54,12.65,-0.27,0.08,0.33 2VGM,CYS_134,10.03,-0.13,-0.2,1.37 105T,ASP_148,3.45,-0.54,-0.34,0.53 3IRA,GLU 143,4.68,0.22,0,-0.03 3ANJ,ARG_108,13.03,-0.25,0.49,0.3 3GS9,GLU_177,2.75,1.02,-2.24,-0.53 3V55,LYS_523,11.45,-0.33,0.79,0.5 2B02,GLU 362,3.82,0.41,-0.85,-0.23 3IVF.GLU 293,4.68,1.32,-0.63,-0.51 2IRM,HIS_346,6.42,-0.08,0,0 2ILR,TYR_489,12.01,0,0.23,1.78 1DZF.LYS 43.10.5.-0.33.0.0.33 4ANN,GLU 105,5.68,1.26,-0.02,-0.04 1NKD,ASP_34,3.48,-0.58,0,0.26 2D8N,LYS_37,10.09,-0.42,0,0.01 1UOH,LYS_221,10.67,-0.14,0,0.31 1NAF,GLU 230,4.63,0.17,0,-0.04 3M9A,LYS_54,10.42,-0.24,0,0.16 1PVT,LYS_86,10.6,-0.11,0,0.2 100L,ARG 18,12,56,-0,31,0,02,0,35 10I7,LYS_57,10.34,-0.22,0,0.06 3CN5,ARG 112,12.53,-0.09,0,0.12 3ETU,HIS 355.6.4,-0.1.0.0 2A1V,ASP_31,2.72,-1.56,-0.04,0.51 2XJ4,LYS_208,10.23,-0.26,0,-0.01 1X1E,ARG_12,11.63,-1.03,0,0.17 3DB9,ARG_60,12.1,-0.35,0,-0.04 2P1W,HIS_174,6.65,-0.6,0.72,0.03 1ZBM.GLU 32.4.49.0.31.0.-0.32 1UOH,ASP_29,3.2,-0.69,-0.3,0.39 1YG2,GLU 170,4.76,0.18,0,0.07 3P51,ASP_77,2.32,-2.45,-0.31,1.28 3ONT,GLU_28,4.68,0.41,0,-0.22 1SJ8,ARG_634,10.61,-2.16,0,0.27 1R3D,HIS_244,4.29,-2.19,0,-0.02 3CJW,HIS_265,6.51,-0.3,0.14,0.17 1EYH,LYS 23,11.6,-0.4,0.7,0.8 4ACJ,LYS 671,11.29,-0.44,0.76,0.46 3T5B,CYS_246,10.65,-0.28,0.11,1.82

2G9D,ARG_315,12.62,-0.12,0,0.24 4GA2,GLU 38,3.54,0.34,-0.8,-0.49 2P0Y,CYS_217,9.94,0,-0.01,0.95 3F6F,GLU_65,4.83,0.56,0,-0.23 2GYZ,ASP_91,3.93,-0.01,-0.04,0.17 1MJS.ARG 294,12.17,-0.69,0.0.36 3ULX.ARG 68.12.43.-0.16.0.0.09 3IBT,ASP_18,3.54,-0.36,-0.19,0.29 1ZYL,LYS_158,10.36,-0.16,0,0.02 1JSX,TYR_162,11.29,-0.85,-0.25,2.39 2FL7,TYR 175,10.55,-0.06,-0.15,0.76 2012.CYS 183.9.27.0.0.05.0.23 4FH3,LYS_56,10.19,-0.45,0,0.13 1160.TYR 158.10.58.-0.8.0.01.1.36 1WXQ,GLU_307,5.56,1.2,0,-0.14 3I82, TYR 176, 10.06, -0.38, 0, 0.45 1GQE,GLU_170,4.91,0.19,0,0.23 1D2K,ASP_419,3.13,-0.71,-0.3,0.34 3EVN,ARG_167,13.48,-0.82,1.38,0.43 1WP5,ARG 231,12,11,-0,5,0,0,11 3U2R,ASP_115,2.96,-0.85,-0.39,0.41 1MN3,LYS_403,10.61,-0.19,0,0.31 30KY,ARG 259,12.22,-0.28,0,2,78E-17 2AH5,LYS 78,10,56,-0,22,0,0,28 3I82,HIS 33,6.35,-0.39,0.02,0.22 2X5Y,LYS_775,11.26,-0.49,0.85,0.4 2HXB,GLU_39,4.07,0.29,-0.34,-0.38 2V5B,HIS_36,5.87,-1.14,0.01,0.5 3A4C.ASP 540.3.29,-0.68,-0.12.0.29 3OBS,ASP_78,2.6,-1.32,-0.44,0.56 2CN1,GLU_126,4.44,0.43,-0.25,-0.23 1MTZ.GLU 84.3.26.0.82,-1.67,-0.39 1SNT,ASP_80,3.83,0,-0.09,0.13 3CAN, ARG_89, 12.37, -0.34, 0, 0.21 2D59.GLU 143.4.56.0.06.0.0 3US6,LYS_73,10.4,-0.39,0,0.28 3CAX,ARG_469,12.57,-0.08,0.15,0 3EYE,ASP_127,3.87,0,-0.1,0.16 3CAX,LYS 287,10.24,-0.29,0,0.02 1RHS,ARG_131,12.38,-0.4,0,0.28 2BLL,HIS_330,4.63,-2.62,0.85,-0.1 20PJ,ARG_171,12.95,-0.33,0.19,0.6 3EX9,ARG 34,12.21,-0.29,0,0 4FH3,ARG 166,12,26,-0,55,0,0,32 1OXZ,HIS_186,6.34,-0.16,0,0 1DVO,ASP_91,3.54,-0.15,-0.33,0.22 1TUL,CYS_66,10.49,0,0.1,1.39 10IS,ARG 337,13.99,-0.51,1.5,0.5 2XMZ,GLU_112,8.97,5.29,-0.89,0.07 3QKY,GLU_181,4.66,0.16,0,0 1R7J,ARG_25,12.21,-0.29,0,0.01 3ZSL,LYS_196,10.99,-0.21,0.42,0.28 3ASA.CYS 170.12.82.-1.41.1.49.3.74 2Q99,TYR_251,10.52,-0.29,0.27,0.53 3JV1,GLU_217,4.85,0.28,0,0.06 3EZ7,TYR_69,12.38,0.29,0.51,1.57 2FXT,GLU_287,4.47,0.13,0,-0.15 1UAJ.GLU 101.4.33.0.38.-0.29.-0.26 2BDV,HIS_122,6.57,-0.74,0.82,-0.02 2FL7,ASP_170,3.44,-0.83,-0.01,0.48 1R53,CYS_18,8.59,-1.28,0.31,0.57 2CBE,ASP 32,3.31,-1.65,-0.15,1.3 2R4Q,GLU_202,4.37,0.16,0,-0.28 1T3J,GLU_692,4.75,0.21,0,0.05 2RJD,CYS_278,8.53,-0.94,0.07,0.41 3B21,HIS_191,5.49,-0.96,0,-0.05 20VO.GLU 65.4.94.0.23.0.0.22 2FGG,LYS_27,10.13,-0.21,0,-0.16 1SQW,ASP_42,3.81,0,-0.25,0.25

1X9G.GLU 50.3.67.0.41.-1.15.-0.09 1AD6.ASP 394.2.65,-1.01,-0.84,0.69 3CX2,LYS_193,9.51,-0.97,0,-0.02 2EFK,LYS_273,10.35,-0.15,0,0 3EYE,LYS_75,10.31,-0.19,0,0 3BB7,ASP 200,3.5,-0.83,-0.01,0.54 1PZC,LYS_46,10.71,-0.11,0,0.32 1R5Q,ARG_19,13.21,-0.47,0.85,0.34 3C6B,CYS_183,13.06,0,0.02,4.04 1SIG,LYS_329,10.43,-0.14,0,0.07 3E0H,ASP_137,1.69,-2.33,-0.38,0.61 1S7K,LYS_53,10.44,-0.06,0,0 3FRR,CYS_76,12.57,-0.03,0.14,3.47 3PAC,CYS 38,9.22,-0.4,-0.17,0.8 1ZBM,ASP_137,3.15,-0.86,-0.32,0.53 300P,ARG_74,12.36,-0.23,0,0.1 3IBT, ARG_190, 12.87, -0.35, 0.3, 0.42 3L7N,HIS_179,9.15,-3.13,2.45,3.32 3OBS,LYS_118,10.43,-0.15,0,0.07 1X7F.GLU 167.4.77.0.33.0.-0.06 3EUR,LYS_119,10.53,-0.09,0,0.12 3IU5,GLU_52,4.63,0.25,0,-0.12 3KB5,TYR 416,10,75,-0.62,0.55,0.81 3I0C,ARG 282,12.74,-0.36,0.32,0.27 1LZL,ARG_119,13.94,-1.02,1.44,1.02 3L3P,ASP_295,4,0,-0.03,0.24 1R9W,TYR_288,12.72,0,0.01,2.72 10GL,GLU 89,7.29,3.86,-0.83,-0.23 1N81,ASP_124,4.61,0,-0.13,0.94 20EW,ARG_205,12.56,-0.34,0,0.4 3VJ8,CYS_258,13.31,0,0.27,4.04 1SJY,ARG_86,12.31,-0.28,0,0.09 1R29,LYS 47,9.91,-0.85,0,0.27 2RJD,CYS_423,8.41,-1.08,0.12,0.37 3ASA,ASP_165,3,-1.61,-0.53,1.33 1SQW,CYS_36,10.55,-0.02,-0.4,1.97 3GE9,ARG_182,13.04,-0.37,0,0.92 3FK5,ARG_313,12.25,-0.25,0,0 3CBN,GLU_98,4.27,0.48,-0.05,-0.67 1I60,HIS_177,4.7,-3.26,0,1.45 3PP8,ARG_56,12.46,-0.12,0,0.07 3K1H,GLU 84,4.54,0.29,0,-0.25 3BCY.GLU 61.4.77.0.66.0.-0.4 2R0S,GLU_170,4.65,0.33,0,-0.17 2XWS,ARG_46,11.81,-0.53,0,-0.17 2Z61,ARG_5,12.42,-0.2,0,0.11 1DVO,TYR_67,10.39,0,0,0.39 2CI3,GLU_109,4.22,0.35,-0.35,-0.27 2H01,LYS_81,10.25,-0.25,0,0 2A4D,ARG_199,11.64,-1.08,0,0.23 2CWC, ARG 194, 12.32, -0.3, 0, 0.12 1PSW.LYS 207.10.36.-0.37.0.0.23 2Z61,GLU_25,3.7,0.36,-0.76,-0.4 2RH3,ARG_167,12.07,-0.61,0,0.17 1MHN,CYS_107,10.27,0.45,0.48,0.35 1ZBS,TYR 213,10.11,-0.45,0.01,0.55 2PGX,GLU_43,3.46,1.14,-1.57,-0.6 3N2T,ARG_171,13.31,-0.55,0.63,0.74 3L3P,GLU_335,5.07,0.22,0,0.35 3LD1,HIS_29,6.16,-0.69,0,0.35 1TXJ.ASP 142.4.14.0.0.1.0.24 2AHE,ASP_65,3.64,-0.49,-0.01,0.34 2X4L,LYS_346,10.41,-0.09,0,0 3T57,ARG_187,12.71,-0.35,0,0.56 3FFM,ASP_71,3.64,-0.52,-0.05,0.41 3JSN,GLU 140,3.28,0.57,-1.06,-0.73 2F9F,LYS_157,10.06,-0.48,0,0.05 2A4D,LYS_148,10.42,-0.08,0,0 10TM,ARG 224,12.46,-0.09,0,0.05

2CIU,LYS_164,10.47,-0.04,0,0 1DUN,LYS 61,10.37,-0.13,0,0 3UV9,LYS_362,10.65,-0.13,0,0.28 2VAN,TYR_266,11.1,0,0.08,1.02 2VGM,LYS 200,11.13,-0.63,0.85,0.41 3MEW.GLU 179.4.81.0.43.0.-0.12 1BKB.GLU 124,4.04,0.6,-0.78,-0.27 1RHS,GLU_148,3.94,0.46,-0.71,-0.3 1MTZ,HIS_121,5.89,-0.7,0,0.09 3F1X,GLU_286,4.4,0.18,-0.22,-0.06 3CRM,LYS 89,10,12,-0,12,0,-0,26 2P0Y,ARG_250,12.18,-0.75,0.18,0.25 3SMD.GLU 34,4.21,0.45,-0.83,0.09 3B4D,CYS_205,9.75,0,0.15,0.6 20K1.LYS 404.10.42.-0.55.0.0.47 2RGY,ASP 159,2.22,-2.19,-0.76,1.36 3GW3,LYS_290,10.51,-0.09,0,0.1 3M70,CYS_129,13.58,-0.31,1.75,3.15 1I60,TYR_30,11.01,0,0.32,0.69 2GKG,ASP 87,3.96,0,0,0.16 1L2H,LYS_65,10.37,-0.14,0,0.01 1RZ2,GLU_113,4.18,0.3,-0.46,-0.16 20GQ,LYS_413,9.53,-0.87,0,-0.09 1X7F,LYS 60,10.58,-0.19,0,0.26 3H8Y,GLU 13,4,55,0,45,-0,39,-0.02 3PBH,ARG_3,12.14,-0.36,0,0 4ETX,ARG_291,12.36,-0.14,0,0 3JSN,TYR_20,9.44,-0.69,-0.45,0.58 1RZ2,GLU 60,4.59,0.25,0,-0.15 2XJ4,GLU_192,3.6,0.31,-0.82,-0.39 1PSW,ARG_113,10.61,-1.94,0,0.05 4DBX,LYS_121,10.31,-0.25,0,0.05 3BQW,CYS_241,11.63,0,0.02,2.62 2VAN, ASP 91, 3.01, -0.85, 0.0.06 2AH5,GLU_204,3.2,0.51,-1.42,-0.39 3LJI,HIS_102,6.1,-0.86,0,0.44 1J85,ARG_121,12.34,-0.29,0,0.13 1BKR,ASP_91,2.55,-1.57,-0.05,0.36 200K,ASP_325,3.6,-0.48,0,0.29 3GW3,LYS_322,11.44,-0.3,0.85,0.39 20GQ,ARG_518,12.46,-0.04,0,0 4ACJ.TYR 661.10.39.0.0.27.0.13 1KCM.GLU 49.4.73.0.19.0.0.04 1DCF,LYS_9,10.47,-0.41,0,0.39 105J,TYR_66,10.36,-0.85,0.26,0.95 3H6Q,TYR_91,11.08,0,0.33,0.75 2IDC,ASP 58,3.51,-0.74,0,0.45 1J33,HIS 285,6,1,-0,58,0,0,18 3IVF,ARG_297,13.07,-0.57,0.63,0.52 3ZXY,GLU_234,4.16,0.71,-0.52,-0.54 20GO.CYS 573.9.19.-1.48.0.15.1.53 1V43.TYR 139.10.22.0.0.03.0.19 3I4T,ASP_27,3.69,-0.27,-0.2,0.35 2AZP,HIS_42,5.8,-0.63,0,-0.07 2HRZ,TYR_5,10.17,0,0,0.17 2Q13,LYS_124,10.35,-0.15,0,0 3H13,ASP 409,2,13,-1,99,-0,25,0,58 3MIX,GLU_489,4.76,1.58,-0.98,-0.33 3CZC,GLU_89,4.43,0.31,0,-0.38 2Z61.LYS 365.10.74.-0.2.0.0.44 1L2F,LYS 29,10.39,-0.17,0,0.06 1NJ4,ASP_284,3.37,-0.8,0,0.37 30IP,ARG_83,12.39,-0.14,0,0.04 2V5B,GLU_242,3.76,0.55,-0.82,-0.48 20KT,ARG_189,12.41,-0.11,0,0.02 3CGW,GLU_250,4.97,0.32,0,0.15 1GPP,LYS_112,10.06,-0.36,0,-0.08 1RHS,CYS_63,12.16,0,-0.08,3.23 1QYI,ARG_280,12.16,-0.34,0,0

3PU6.GLU 45.4.26.0.9.-0.81.-0.32 1Z9L,LYS 110,10.92,-0.2,0.34,0.28 1YR6,GLU_173,4.57,0.09,0,-0.03 1J33,ARG_284,12.49,-0.23,0,0.23 2P0Y,HIS_286,7.17,-0.77,0.85,0.58 1MIX,TYR_308,10.21,-0.3,-0.32,0.84 2CI3.GLU 106.4.62.0.22.0.-0.1 4ANN,GLU_120,5.33,2.87,-1.68,-0.36 30KQ,ARG_594,13.07,-0.16,0.45,0.28 2CXA,ASP_105,3.97,0,-0.05,0.22 2H2Z,CYS 265,12.06,0,-0.03,3.08 2X4L.LYS 162.10.5.-0.09.0.0.09 2IRM,GLU_28,4.9,0.98,0,-0.58 1W7B,LYS_324,10.38,-0.13,0,0.01 2EJX,ARG 86,12,49,-0,53,0,0,53 3AUF.GLU 120.3.8.0.26,-0.54,-0.41 3LPZ,LYS_215,10.64,-0.09,0,0.23 3RJX,GLU_293,4.54,0.16,0,-0.12 2OB5,TYR_-3,10.04,0,0,0.04 2OGQ,GLU_391,4.35,0.23,0,-0.39 3E7P,LYS 48,10,45,-0,05,0,0 1R53,ASP 38,2.8,-1.6,-0.43,1.04 1PBV,ARG_118,12.5,-0.06,0,0.06 4GA2.TYR 31.9.93.0.-0.22.0.15 3RE9.GLU 113.3.65.0.68.-0.78.-0.75 1ZYL,GLU_257,4.92,0.13,0,0.29 3U0V,GLU_188,4.2,0.56,-0.42,-0.45 3M3P,ASP_167,3.98,0,-0.4,0.58 4ECC,GLU_26,3.85,0.63,-0.85,-0.43 3ZSL,LYS 176,10.3,-0.31,0.0.1 2A6B,CYS_68,12.35,0,0.04,3.31 2QDJ,GLU_119,4.07,1.22,-1.22,-0.43 3H5T.GLU 211.4.66.0.1.0.0.05 10XZ.ARG 255.12.8.-0.41.0.34.0.38 2P1W,GLU_241,3.94,0.55,-0.78,-0.32 2H85,HIS_-1,5.94,-0.14,0,-0.42 4EZB,ASP_214,2.95,-1.14,-0.12,0.42 3TMO, ARG_208, 12.64, -0.26, 0, 0.41 2AH5.GLU 135.4.83.0.32.0.0.01 3A4C,ARG_547,12.23,-0.36,0,0.08 1SFE,ARG_171,12.24,-0.26,0,0 3RE9.GLU 204,4.94.0.27.0.0.17 1EV8.HIS 207.6.65.-1.32.0.77.0.7 2QV2,HIS_273,5.94,-2.09,0.94,0.57 3CAX,GLU_467,4.48,0.12,-0.15,0 2Z0M,TYR_267,10.44,0,0.17,0.27 3I0C,HIS_219,6.4,-1.78,0.85,0.84 1J85,ARG_59,11.74,-0.91,0,0.15 2OSA,GLU_365,3.94,0.38,-0.53,-0.41 1LTU.ASP 279.4.04.0.0.06.0.18 3RJX,LYS_101,11.52,-0.21,0.85,0.38 4DNU,LYS 123,10.12,-0.54,0,0.15 3ETU.TYR 124,10.35,-0.41,0.13,0.62 2CBE,TYR_191,12.11,0,0.08,2.03 3I4T,TYR_230,11.55,0,0.1,1.46 4ACJ,ASP_685,3.9,0,0,0.1 2FL4,HIS_4,7.29,-0.17,0.96,0 3IO0,LYS_103,10.32,-0.18,0,0 3MEW.ASP 160.4.17.-0.77.-0.16.1.3 3QKY,GLU_137,4.63,0.19,0,-0.07 1ZBS,ASP 37,3.33,-0.82,-0.06,0.42 1P2F,ARG 69,12.38,-0.24,0.0.13 3CAX,LYS_263,10.25,-0.25,0,0 3BA1,GLU_164,4.1,0.45,-0.85,0 1ZBM,TYR_212,9.34,-0.79,-0.37,0.5 3F5D,ARG_29,13.03,-0.53,0.51,0.55 3LJC,ARG_33,12.44,-0.7,0.23,0.42 3MEW.CYS 145,11,28,0,0,26,2,02 3H6Q,TYR_146,12.86,0.56,0.67,1.64

3F6FLYS 120.10.3.-0.3.0.0.1 1KN3,ASP_128,3.72,0,-0.3,0.22 3F1X.HIS 71.6.43.-0.35.0.27.0 4DBX,GLU_268,5.56,0.97,0,0.09 3GW3,HIS_220,4.04,-2.05,0,-0.42 3HUE, TYR 60, 11, 65, -0, 75, 0, 29, 2, 11 1SUULYS 567.10.73.-0.27.0.0.5 2X4L,GLU_222,3.97,0.48,-0.79,-0.22 3CBN,ARG_131,12.5,-0.4,0.13,0.27 3EJG,ASP_27,3.88,0,-0.12,0.21 2CWY,CYS 74,9.65,-0.41,0.21,0.84 1X04,LYS_138,9.69,-0.42,0,-0.39 3ULX,TYR_71,12.67,-0.05,-0.04,2.76 4EVF,GLU_245,6.14,0.89,0,0.76 3QKY,TYR_183,10.98,0,0.55,0.42 3CAX,ASP 372,4.12,0,0.06,0.26 3ZXY,ARG_248,10.79,-1.71,0,0 2PLQ,TYR_305,11.93,0.85,0.44,0.63 1KN3,CYS_133,10.54,-0.39,0.28,1.65 2VGM,LYS 68,10,58,-0,2,0,0,28 3F5D,ASP_16,2.49,-2.05,0,0.74 1SNT,ARG_152,12.45,-0.14,0,0.08 1R53,TYR_208,10.42,-0.16,0.22,0.36 1V6T,TYR_27,9.61,-0.69,-0.05,0.34 2PGX,GLU 8,3.22,0.48,-1.38,-0.38 3UC9,GLU_70,4.88,0.26,0,0.12 1A8Q,ASP_78,3.46,-1.48,-0.37,1.51 3GE9,GLU_124,4.91,0.26,0,0.15 3RLN.TYR 645.11.39.0.03.0.31.1.05 3CNU,LYS_46,11.37,-0.24,0.51,0.6 1SBX,ARG_120,12.19,-0.58,0,0.27 3C2E,GLU_67,4.55,0.13,0,-0.08 30NH,ASP_490,4.2,0,0.22,0.18 1RHS,GLU 49,4.43,0.22,0,-0.3 2Z61,LYS_294,10.25,-0.11,0,-0.15 3GS9,HIS_116,6.31,-1.11,0.8,0.12 10TM,TYR_214,10.66,0,0.23,0.42 3VJ8,LYS_335,10.69,-0.27,0,0.46 1YLN, ASP 31, 3.36, -0.72, 0, 0.28 2E3H,ARG_229,12.82,-0.49,0.34,0.47 3P2F,HIS 85,6.22,-0.32,0.04,0 1W24,LYS_24,10.34,-0.08,0,-0.08 1DTO,GLU 185,4.67,0.28,0,-0.11 4ACJ,HIS_774,7.33,-0.38,0.83,0.38 4EUG,TYR_110,12.32,0.83,0.45,1.04 1OXZ,LYS_183,10.39,-0.11,0,0 4FH3,ASP_296,3,-1.04,-0.16,0.41 1AD6,LYS 447,10.79,-0.25,0.32,0.22 2I88,ASP_376,4.38,-0.06,-0.26,0.91 1PDB,LYS_157,10.39,-0.11,0,0 2QK0,CYS_84,10.51,0,0.09,1.42 1W7B,TYR_318,11.23,0.22,0.55,0.46 2CBE,ASP 162,3.52,-0.41,-0.23,0.37 4FLE,CYS_163,11.15,0,0.07,2.08 2E3I,GLU_94,4.69,0.15,0,0.04 3R2E,GLU_21,4.21,0.6,-0.52,-0.37 2EHG,TYR 88,9.48,-0.51,-0.29,0.28 2IN0,GLU_424,4.67,0.32,0,-0.15 1PZC,LYS_59,10.69,-0.14,0,0.34 3PP8,ARG_29,13.3,-1,1.07,0.73 3UAH,LYS_343,10.33,-0.17,0,0 4GA2,LYS 28,10,43,-0,27,0,0,2 1AD6,ASP_527,2.21,-1.56,-0.78,0.75 3OKQ,ASP_571,3.99,0,0,0.19 10XZ,ARG_299,13.04,-0.25,0.27,0.53 2C2Y,ARG_143,12.84,-1.94,1.29,1 2D8N,TYR 109,12,97,0,-0.07,3.04 3HVW,ASP_312,4.58,0,-0.12,0.9 1Y2Q,HIS_83,6.22,-0.27,0,-0.01

3IDW.ARG 56.12.91.-0.26.0.32.0.36 3V46,ARG 337,12.56,-0.41,0.0.47 1I60,HIS_26,6.38,-0.88,0.85,-0.09 2CI3,LYS_229,9.89,-0.31,0,-0.31 2X5Y,LYS 770,10.97,-0.29,0.37,0.4 1WYC.ASP 368.3.22.-0.82.-0.12.0.36 4DNU,TYR_246,12.18,0.8,0.43,0.95 3TIR,ARG_27,12.51,-0.06,0,0.07 1TR9,ARG_70,12.5,-1.13,0.37,0.76 2Q12,GLU_198,4.76,0.27,0,-0.01 1KCM,LYS 186,10,47,-0.03,0,0 2Z14,ASP_12,3.27,-0.61,-0.21,0.29 2NSN,CYS_61,9.44,0,-0.2,0.63 3AU3.LYS 435,10.62,-0.17,0.29,0 3EZ7.CYS 305.10.1.0.0.05.1.06 2P65,LYS_66,11.41,-0.41,0.83,0.49 1XEU,ASP_67,3.25,-0.93,-0.15,0.53 3ELI,ASP_88,3.32,-0.76,-0.02,0.29 3E5T,CYS 114,9.68,0,-0.04,0.72 3LJI.GLU 204,4.31,0.64,-0.83,0 3LH5,HIS_767,3.7,-1.91,0,-0.89 2RJD,ARG_269,13.32,-0.59,0.65,0.77 3JZN,CYS_150,12.38,0,-0.17,3.55 3A2Z,TYR 38,13.23,-0.18,0.56,2.84 2ILR,GLU_459,3.96,0.54,-0.6,-0.48 3LQE,CYS_288,11.2,0,-0.63,2.83 1BYI,GLU_89,4.3,0.77,-0.75,-0.22 3T5B,TYR 196,9.2,-0.85,-0.49,0.54 4F3J,ASP_235,3.46,-0.27,-0.6,0.54 2DVK,ASP_175,3.76,-0.07,-0.63,0.65 3U2R,GLU_16,4.13,0.19,-0.57,0.01 2IQT,GLU_128,3.64,0.28,-0.85,-0.3 1LZL,HIS 210,5.41,-1.62,0.39,0.15 3RE9,HIS 138,4,44,-3,26,0,98,0,22 1P4X,HIS_6,5.92,-0.24,0,-0.35 3GEC,CYS_455,9.82,0,0.13,0.68 1PNE,ARG_55,12.94,-1.52,1.4,0.56 2VGM,TYR_104,9.88,-0.29,-0.3,0.46 1F2V,ARG_104,13.14,-0.25,0.51,0.38 3IDW,TYR_3,11.3,0,0.45,0.85 3M3P,CYS_188,10.7,-0.01,-0.04,1.75 2BDV,GLU 140,4.77,0.11,0,0.16 2A1V.GLU 19.4.26.0.72,-0.66,-0.31 1ZCU,GLU_117,4.44,0.17,0,-0.24 1LTU,HIS_110,5.64,-1.71,0.84,4.16E-17 3GG6,GLU_82,2.83,1.1,-2.34,-0.44 1UXO,TYR_184,13.04,0,0.17,2.87 2D0A, ARG 224, 13.05, -0.52, 0.4, 0.67 1X7F,LYS_316,10.32,-0.21,0,0.03 2NRK,LYS_166,10.1,-0.19,0,-0.2 2CIU,LYS 120,10.5,0,0,0 1W7B,LYS_246,11.5,-0.46,0.85,0.61 1EDG,ASP_278,3.28,-0.8,-0.15,0.43 2Q34,GLU_256,4.72,0.5,0,-0.28 200K,ARG_114,13.55,-0.42,1.05,0.43 20GQ,ASP 449,2.86,-1.55,0.05,0.56 2IRM,HIS_292,5.56,-1.07,0,0.14 2OJQ,CYS_691,10.98,-0.07,-0.02,2.08 2QHT,LYS_145,10.46,-0.21,0,0.17 2IXM, ASP 95, 3.9, -0.03, 0, 0.12 3N2T.GLU 122.4.54.0.08.0.-0.04 2B61,ASP_345,4.12,0,0.14,0.18 2X5Y,TYR_826,11.95,0,0.66,1.3 1QZN,LYS_122,10.68,-0.22,0,0.41 3V75,GLU_186,3.52,1.06,-1.6,-0.43 1YR6,ASP 186,4.05,0,0,0.25 3RFF,ASP_46,3.11,-1.03,-0.1,0.43 1YG2,LYS_145,10.45,-0.05,0,0 3IU5,TYR 127,11.31,0,0.55,0.77

4AM1,LYS 118,10,52,-0,22,0,0,25 3HUE,LYS 206,10,52,-0,17,0,0,18 3ULX,ARG_78,13.6,-0.19,0.73,0.56 4ACJ,HIS_672,5.7,-0.67,0.05,-0.18 4FCU.GLU 250.3.97.0.22.-0.72.-0.03 1YM5.LYS 63.11.08.-0.18.0.12.0.63 2CBE,GLU 26,4.5,0.24,0,-0.24 2VGM,LYS_348,10.21,-0.38,0,0.09 4GCO,ASP_236,4.29,0,-0.29,0.77 2JHY.HIS 189.6.09.-1.71.0.75.0.55 4AM1.GLU 252,3,58,0,34,-0,85,-0,4 3RJX,LYS_183,10.41,-0.25,0,0.16 1T95,LYS_157,10.32,-0.35,0,0.17 3ASA,ARG_136,12.15,-0.58,0,0.23 3VHJ.ARG 52.11.49.-1.09.0.0.08 3CE7.GLU 36.4.01.0.47.-0.79.-0.17 2X5Y,LYS_813,11.27,-0.24,0.39,0.62 3G9T,ARG_236,12.27,-0.4,0,0.17 1SIG,ASP_233,3.98,0,-0.22,0.4 1Z3X,LYS 131,10.45,-0.05,0,0 1CHD,GLU_306,4.64,0.15,0,0 4F85,ASP_246,3.7,0,-0.53,0.44 1TJE,GLU_176,2.93,0.94,-1.7,-0.81 1LZL,GLU 64,3.96,0.16,-0.38,-0.32 4EVF.TYR 30.11.03.0.0.38.0.64 2IXM,GLU_301,3.74,0.62,-0.85,-0.53 1YTD,ARG_329,11.96,-2.25,0.66,1.06 3ETU,GLU_353,4.57,0.23,0,-0.16 1SUU,LYS 708,10.83,-0.35,0.15,0.52 3BA1,LYS_224,10.39,-0.11,0,0 1WXF,LYS_207,11.68,-0.29,0.84,0.63 3KT9,ARG_13,13.38,-0.29,0.76,0.41 2CXC,ARG 28,13.43,-0.7,0.88,0.73 1PGV.LYS 251.9.89.-0.77.0.0.17 3BCY,CYS_142,11.5,-0.12,-0.02,2.64 1SQH,CYS_215,9.98,-0.22,-0.14,1.35 3P2F,GLU_90,4.1,0.19,-0.58,-0.01 3Q9P,LYS 123,10.73,-0.22,0,0.46 2ZQ5,HIS_192,6.6,-1.33,0.85,0.58 4D8L,TYR_21,12.2,0,0.01,2.19 3IL3,GLU_167,4.9,1.21,-0.1,-0.71 3FNI,ASP 40,2.78,-1.83,0.0.81 20HT.ARG 196.12.83.-0.48.0.01.0.8 3O48,GLU_128,4.85,0.29,0,0.06 1QZN,TYR_43,12.24,0,0.15,2.09 1ZHV,CYS_48,10.53,0,-0.31,1.84 1C44,LYS 40,10.85,-0.41,0.44,0.32 3V4G,ASP 129,3,54,-0.64,-0.24,0.61 4AF2,TYR_159,13.64,0.79,0.49,2.36 3H5T,ARG_252,12.59,-0.32,0.03,0.38 3ETV,ASP_199,3.99,0,0,0.19 3E5T,LYS 181,11.17,-0.65,0.85,0.48 1UAJ,ASP_128,3.7,-0.84,-0.26,1.01 2F4Q,ARG_239,10.49,-2.51,0.52,-0.01 1ZCU,LYS_48,10.58,-0.14,0,0.22 3RAZ,ASP_76,4.05,-0.75,-0.11,1.11 4GA2.ARG 113.13.59.-0.57.0.93.0.73 3A7L,ASP_21,2.28,-1.82,-0.12,0.42 3LJI,GLU_282,3.09,0.48,-1.23,-0.65 20PJ.TYR 154,13.64,-0.08,0.16,3.57 2HRZ,ARG 226,12.53,-0.72,0.06,0.69 2GAU,ARG_26,12.28,-0.48,0,0.26 2CL3,ARG_90,12.42,-0.24,0,0.16 2PGX,HIS_66,6.24,-0.26,0,0 2Q13,ARG_121,13.7,-0.43,1.14,0.5 1JSX,LYS_113,10.47,-0.07,0,0.04 1SUU,HIS_556,6.29,-0.21,0,0 3EZ7, ASP 340, 3.73, 0, -0.29, 0.23 1KN3,ARG_132,12.44,-0.06,0,0

2Z14,ASP 79,4,2,0,0,11,0,29 1RHS,LYS 23,10.39,-0.15,0,0.03 3LH5,ARG_579,12.56,-0.62,0.08,0.6 4H4J,LYS 78,10.32,-0.12,0,-0.06 3CIV,ARG_99,12.7,-0.31,0.18,0.32 4DBX.LYS 99.10.2.-0.1.0.-0.21 2A0J.GLU 112.4.57.0.26.0.-0.19 3ZTA, ASP_39, 3.69, -0.49, -0.73, 1.11 3E5T,GLU_91,4.66,0.48,-0.12,-0.2 4FH3,ARG 198,12.27,-0.44,0,0.21 2HXB,TYR_72,10.5,0,0.04,0.46 2F4O.LYS 264,10.42,-0.15,0.0.07 2Y2T,TYR_17,10.48,0,0.12,0.36 3LJC,ASP_161,4.18,-0.31,-0.2,0.88 4AM1,ARG 126,8.17,-2.19,0,-2.14 2ZO5,TYR 82,10,43,0,0,08,0,35 1YB2,ARG_230,13.1,-0.37,0.5,0.47 3M16,TYR_193,11.08,0,0.48,0.6 2ZTY,GLU_53,4.64,0.14,0,0 1J33,GLU 27,3.41,1.03,-1.59,-0.53 1WLY,HIS 138,5.14,-1.91,0.75,-0.2 3EZ7,GLU_63,4.36,0.39,0,-0.52 2l6l,GLU_88,4.53,0.21,0,-0.18 2AZL,TYR 151,10.24,0,-0.15,0.4 2VAN.LYS 209.10.55.-0.12.0.0.17 1XFK,TYR_289,9.83,-0.47,-0.38,0.68 1JB3,LYS_62,11.09,-0.45,0.81,0.24 2B0J,HIS_174,2.46,-3.26,0,-0.78 1Q8B,GLU 39,2.64,1.24,-2.28,-0.83 2XHC,ARG 209,12,41,-1,21,0,29,0,83 1SNT,ASP_215,3.37,-0.85,-0.56,0.98 1IAP,GLU_141,5.01,0.37,0,0.14 1AM2,LYS_92,11.24,-1.03,0.85,0.91 1QQH,GLU 171,3.84,0.94,-1.2,-0.41 1YLN,ARG_57,12.51,-0.25,0,0.25 2P0L,ARG_250,12.44,-0.53,0.02,0.45 3CNU,GLU_94,3.39,0.3,-0.74,-0.66 2R2Y,GLU 126,4.73,0.25,0,-0.02 2CBE,LYS 39,10.29,-0.14,0,-0.08 3CAX,TYR_145,10.37,0,0.1,0.27 1SQW,ARG_30,13.78,-0.39,0.76,0.92 2H2W,HIS_75,5.58,-0.66,0,-0.26 2E3C.ARG 409.12.57.-0.09.0.0.16 10IS,GLU_329,4.52,0.16,0,-0.14 3V55,ASP_638,3.93,0,-0.17,0.3 2E3S,ASP_440,4.06,0,0,0.26 3AU3,ARG_463,12.32,-0.46,0,0.28 1XTZ,LYS_258,10.38,-0.15,0,0.03 1R7J,LYS_6,10.54,-0.15,0,0.18 10YI.CYS 34,10.74,0.34,0.71,0.69 4ANN,LYS_37,11.22,-0.63,0.85,0.49 3GS9,CYS 51,8.69,-0.44,0.04,0.09 1SJY,ARG 73,12.89,-0.21,0.13,0.47 1Q8B,LYS_82,11.03,-0.17,0.32,0.38 1Y2Q,LYS_31,11.2,-0.26,0.47,0.49 3I0C,GLU_247,2.7,1.59,-2.81,-0.59 2X5Y,HIS_810,5.98,-1.69,0.84,0.32 3ANJ,LYS_329,11.07,-0.7,0.85,0.42 2B6P.TYR 178.10.26.0.0.0.26 4DBX,TYR_189,11.26,-0.51,0.33,1.44 2ZTY,GLU 94,4.39,0.99,-0.75,-0.35 3O16,GLU_227,5.07,0.49,0,0.08 2AXO,ARG_132,12.47,-0.1,0,0.07 2FXT,ASP_411,2.27,-1.49,-0.59,0.54 2QK1,GLU_555,4.47,0.18,0,-0.21 2G3A,GLU_88,3.37,0.36,-0.77,-0.73 3FHF,TYR_128,10.2,-0.64,-0.45,1.3 2H8O,GLU_148,4.75,0.3,0,-0.06 1ZCU,ASP_112,3.39,-1.01,-0.43,1.03

1RL0,ARG_180,12.69,-2.94,0.46,2.68 2JHY,LYS 199,10.42,-0.21,0,0.13 3FWU,LYS 15,11.16,-0.35,0.41,0.6 1FO9,LYS_381,10.23,-0.13,0,-0.13 2H2Z,CYS_44,11.07,-0.68,0.34,2.42 2D2S,LYS 731,11.36,-0.56,0.85,0.57 2ZCO.LYS 190.10.42.-0.06.0.-0.01 2OSA,LYS_384,10.9,-0.19,0.21,0.38 105T,TYR_402,13.14,-0.52,0,3.66 3FS3,TYR_277,9.9,-0.25,-0.21,0.36 1TR9,HIS_212,6.37,-0.31,0,0.18 3FNI,LYS 87,10.64,-0.17,0.0.3 1WRU,GLU_128,5.11,0.85,-0.08,-0.16 2Z14,LYS 103,11.92,-0.46,0.85,1.02 2VGM,ASP 363,3.84,-0.14,-0.28,0.46 2FZ4,TYR 67,11.86,0.85,0.39,0.62 1MIX,LYS_274,10.24,-0.17,0,-0.08 3DB9,ASP_182,3.7,-0.3,-0.06,0.26 2G2D,ASP_179,3.96,0,0,0.16 3CIV,TYR_302,10.45,-0.34,0.06,0.73 3LJI.ASP 227.4.04.0.0.0.24 4FH3,HIS_273,4.28,-1.61,0.12,-0.73 3ETU,ASP 150,3,95,0,0,0,15 1O3X.TYR 253.11.92.0.78.0.39.0.76 2P0Y,LYS 161,10.16,-0.34,0,0 1Z3X,GLU_108,4.53,0.84,0,-0.8 2Z0W,ARG_76,12.02,-0.35,0,-0.13 208P,ASP_165,3.3,-0.49,-0.42,0.4 2OGQ,ASP_457,2.45,-1.79,0,0.44 2ZCO,ASP_32,3.71,0,-0.3,0.21 1NAF,GLU_203,4.16,0.24,-0.12,-0.45 2RIK,LYS 194,10.26,-0.38,0,0.14 3KB5,ARG_371,12.42,-0.08,0,0 1RI5,GLU 197,4.37,0.37,0,-0.5 1EYH,LYS 128,10.61,-0.12,0.0.23 2B0J,GLU_27,5.17,0.97,0,-0.31 4AE7,ARG_189,12.15,-0.37,0,0.01 2PLQ,TYR_116,12.23,0.84,0.45,0.93 3CAX, ASP 373, 3.25, -1.34, -0.44, 1.25 3RNV,LYS_378,10.53,-0.25,0,0.29 2GZQ,TYR_91,11.03,0,-0.14,1.17 3BJV,GLU_130,4.42,0.19,0,-0.27 3ASA,ASP_223,4.02,0,-0.08,0.31 1L2F,GLU_165,4.49,1.08,-0.85,-0.24 2BT8,ARG_262,12.22,-0.52,0.06,0.19 2AZL,LYS_41,9.51,-0.47,0,-0.52 3RJZ,ARG_105,12.8,-0.44,0.36,0.38 3CAX,LYS 298,11.07,-0.33,0.51,0.4 2Q34,TYR_170,10.09,0,-0.02,0.11 1H09,HIS_14,6.65,-0.15,0.23,0.06 2F9F,ASP_144,4.02,0,-0.08,0.31 2GEN,TYR_64,13.22,0,0.1,3.12 3ETU,ASP 161,3.19,-0.65,-0.42,0.46 3JZN,GLU_249,5.01,0.39,0,0.12 4EKU,ASP_196,4.23,0,-0.04,0.47 2G9D,ASP_131,3.84,-0.28,-0.27,0.6 4GCO,GLU_145,4.49,0.27,-0.2,-0.08 2IIA.LYS 54.10.22.-0.44.0.0.16 1BN6,GLU_202,4.62,0.38,0,-0.27 3UC9,ARG_48,12.78,-0.14,0,0.42 2QRX,LYS_72,10.85,-0.32,0.26,0.41 2P1W/ARG 111.12.3.-0.32.0.0.12 1EQ6,ASP_96,3.94,0,-0.02,0.15 3IV4,GLU_75,4.67,0.29,0,-0.11 1YM5,GLU_52,5.1,3.2,-0.61,-1.98 3AU3,GLU_461,4.43,0.22,0,-0.28 2H14.GLU 58.4.81.0.28.0.0.02 3UX2,ARG_101,12.19,-0.33,0,0.02 1NJ4,ASP_156,3.97,0,0.03,0.14

20V2.ARG 271.12.29.-0.25.0.0.04 1RSS.TYR 85.10.16.0.0.0.16 1WOU,ASP_36,2.95,-1.34,-0.05,0.54 3IL3,LYS_60,11.4,-0.49,0.85,0.55 10TM,ASP 87,2.59,-0.85,-0.65,0.29 3ETU.GLU 51.4.67.0.17.0.0 1AIL,ASP_39,3.12,-0.64,-0.48,0.44 1XAW,LYS_501,10.28,-0.16,0,-0.06 3EX9,GLU_157,4.58,0.08,0,0 3UAH.CYS 332.12.08.-0.76.-0.18.4.02 3JSN.TYR 306.10.91.0.0.21.0.7 3CBN,HIS_111,6.14,-0.69,0.18,0.15 1J33,ARG_46,13.35,-0.44,0.68,0.61 2B2H,ASP 214,3,95,0,0,0,15 1SFE.ARG 81.12.88.-0.39.0.01.0.77 2GYZ,ARG_88,12.58,-0.32,0.02,0.38 2YT4,LYS_689,9.85,-0.74,0,0.09 2F4Q,HIS_218,5.82,-0.36,0,-0.31 2FL4,ARG_139,12.36,-0.44,0.01,0.29 3ELI.GLU 61.4.58.0.08.0.0 1X7F,GLU_17,3.93,0.32,-0.61,-0.28 2EDM,ASP_105,3.3,-0.88,-0.1,0.48 4DBX,CYS_213,10.45,-0.14,0.18,1.42 2X4G.ARG 272.12.44.-0.18.0.0.13 2Q13,GLU_11,5.17,0.24,0,0.42 2F4Q,LYS_194,10.14,-0.37,0,0 2F4Q,GLU_260,3.81,0.12,-0.71,-0.09 1ZBS,ARG 38,13.21,-0.22,0.46,0.47 2RIK.LYS 49,10.39,-0.11,0.0 1EW4,GLU_44,4.43,0.3,-0.79,0.43 2AD1,LYS 31,10.35,-0.13,0,-0.02 3RJZ,ARG_28,12.43,-0.07,0,0 2AH5,TYR 81,10.28,0,0.07,0.21 2WOZ,LYS 436,11.02,-0.28,0.3,0.5 3N2T,LYS_262,9.8,-0.85,0,0.14 3HVW,ARG_246,13.09,-0.89,0.72,0.76 4H4J,ASP 188,4.02,-0.04,-0.07,0.33 1R9W.CYS 290.9.02.0.-0.19.0.21 2V4U,ASP_365,4.14,-0.82,-0.08,1.24 3IO0,ARG 120,13,79,-0,36,1.13,0.51 2IXM,LYS_242,11.62,-0.18,0.79,0.51 3PP8.ARG 269,11.99,-0.71,0,0.2 1WLY,ARG_235,12.63,-0.27,0,0.4 3GEC,ASP_276,4.53,0,-0.46,1.2 1UJ8,ASP_55,2.65,-1.54,-0.22,0.61 2H2Z,LYS_236,10.65,-0.15,0,0.3 2VAN,LYS_148,10.52,-0.33,0,0.35 1S7K,HIS 25,6.15,-0.3,0,-0.04 1YLN.GLU 188.3.97.0.86.-0.98.-0.42 1I60,TYR_199,13.9,-0.85,1,3.75 1M5I,ARG 197,12.11,-0.32,0,-0.07 3IU5.GLU 104.4.59.0.12.0.-0.03 2VGM,ASP_185,3.19,-0.78,-0.2,0.36 2EJB,LYS_116,11.21,-0.38,0.82,0.27 3G6S,LYS_197,10.71,-0.41,0,0.62 1SQW,TYR 95,9.64,-0.38,-0.38,0.4 1XAW,ARG_519,12.78,-0.24,0.24,0.27 4E8B,ASP_155,4.42,-0.19,0.17,0.63 2APL,TYR_115,11.91,0.81,0.42,0.68 3EIZ,ARG 89,12.32,-1.04,0.4,0.47 3EZ7.GLU 222.4.69.0.22.0.-0.02 3QKY,GLU_254,4.48,0.26,0,-0.28 2QK1,ARG_550,13.02,-0.45,0.31,0.66 1RKA,HIS_17,5.84,-0.66,0,0 1XKR,ASP_70,3.18,-0.8,-0.26,0.43 3BQW,GLU 302,3.42,0.41,-1.01,-0.48 4AM1,ARG_294,12.81,-0.35,0.07,0.59 3FNI,LYS_109,10.31,-0.2,0,0.01 3RJX,LYS_41,10.77,-0.29,0.23,0.32

3AUF,ARG_26,13.36,-0.39,0.82,0.44 3G9G.GLU 220.5.05.0.58.0.-0.02 3E5T,GLU_215,3.82,2.82,-0.85,-2.65 3IV4,GLU_17,4.54,0.27,-0.25,0.02 1L3K.ARG 55,12.28,-0.3,0,0.09 1RAJ.GLU 364.3.88.0.23.-0.85.0 1SUU,LYS_749,10.46,-0.12,0,0.08 1C44,ASP_41,4.04,0,6.94E-18,0.24 2V4U,ASP_470,3.84,0,-0.31,0.35 3OA7,GLU_446,4.56,0.28,0,-0.22 3F7M,ARG 225,13,48,-0.54,0.78,0.75 1FKM,ARG_254,11.33,-1.19,0,0.01 2B02,ARG_409,12.27,-0.3,0,0.07 1WYC,HIS_58,7.13,-0.14,0.69,0.07 106D,ARG_115,13.27,-0.34,0.74,0.38 4ECC,ARG 116,12,12,-2,73,0,15,2,21 3ONT,GLU_69,4.86,0.48,0,-0.11 1BN6,ASP_94,3.92,-0.84,-0.27,1.23 1ANU,ASP_114,4.01,0,-0.16,0.37 4FLE,ARG 95,13.17,-0.4,0.61,0.47 2GZQ,GLU_63,4.77,0.29,0,-0.02 1ZKZ,LYS 96,10,39,-0,32,0,0,21 4HDE,ASP_142,1.78,-1.7,-0.76,0.44 3CAX,ARG 419,12.86,-0.32,0.38,0.31 3O2C.GLU 11.3.98.0.34.-0.57.-0.29 1NWA,GLU_140,3.95,0.3,-0.51,-0.36 1H4U,CYS_373,9.01,0,-0.09,0.1 1MIX,TYR_270,11.36,-0.85,0.05,2.17 3RFY,ARG 238,12.25,-2.87,0.1,2.52 20KT,GLU_73,4.23,0.33,-0.41,-0.19 2H2W,ARG_98,12.06,-0.73,0,0.29 3LJN,GLU_18,4.57,0.19,0,-0.12 1WXF,ARG_249,12.33,-0.17,0,0 4DVD.ARG 71.12.16.-0.39.0.0.04 3CIV,GLU_121,3.96,0.47,-0.82,-0.2 2Q99,LYS_312,11.14,-1.12,0.85,0.92 1MN3,GLU_405,5.11,0.45,-0.13,0.28 2D7J,LYS 87,10.42,-0.16,0,0.08 4F85,ASP_74,3.79,0,-0.27,0.26 2D8N,LYS_63,10.31,-0.29,0,0.1 2XHC,HIS_64,6.86,-0.44,0.85,-0.05 3ETV.ASP 347.4.2.0.0.05.0.35 1ZP2,GLU 124,4,34,0.82,-0.83,-0.15 1QQE,ARG_220,12.58,-0.17,0,0.25 1I60,ARG 166,13,23,-0,38,0,59,0,52 1SQH,GLU_295,3.32,0.97,-1.7,-0.46 3MIX,LYS 478,11.06,-0.55,0.22,0.88 1WP5.LYS 141,10.42,-0.16,0.0.08 3FXH,CYS_103,12.51,-0.02,0.03,3.5 1GPP,LYS_427,10.54,-0.08,0,0.12 2RIS.LYS 141.10.42.-0.08.0.0 2CIU.LYS 180,10.42,-0.13,0,0.05 2FBI,ARG_41,12,-0.87,0,0.37 1PNE,ARG_136,12.38,-0.3,0,0.18 3GS9,GLU_247,4.7,0.16,0,0.04 2XHC,ASP_323,3.45,-0.49,-0.38,0.53 1BKB.TYR 22.11.14.0.-0.16.1.3 4AF2,ASP_151,3.72,-0.13,-0.23,0.28 2IQT,TYR_288,10.38,0,-0.05,0.43 3GE9,LYS 165,10,21,-0,29,0,0.01 3V46,ARG 289,12,48,-0,4,0,03,0,36 2G9D,ASP_279,3.73,0,-0.36,0.3 1J8B,LYS_89,10.61,-0.07,0,0.19 2GZQ,GLU_9,3.25,1.02,-1.55,-0.71 3GEC,CYS_502,9.4,-0.52,0.01,0.9 3CBN,GLU_162,4.36,0.22,0,-0.35 2B0J,GLU_229,3.57,0.37,-0.84,-0.47 1WLY,HIS_192,5.15,-0.78,0,-0.56 1J74,TYR_143,10.76,-0.84,0,1.6

2XWS.ARG 89.12.52.-0.23.0.0.25 3LJI.LYS 260.10.25.-0.26.0.0.01 1P6F,ARG_139,12.47,-0.03,0,0 1BN6,ASP_89,4.21,0,0.15,0.26 3BCY,HIS_91,6,-0.33,0,-0.18 3F1X,TYR_261,10.31,0,-0.09,0.4 30IP,ASP_145,2.79,-0.99,-0.61,0.58 1WJG,ARG_57,12.58,-0.14,0,0.21 2FD5,LYS_4,10.39,-0.07,0,-0.05 2V4X,ASP_82,3.85,-0.16,-0.07,0.28 2YWX,GLU_16,4.75,0.26,0,-0.01 2NSN,ASP_73,3.55,-0.46,-0.7,0.89 1NAF,GLU_219,4.5,0.24,-0.21,-0.03 2D7U,ARG_55,12.02,-1.06,0,0.58 2OSA, ASP 373, 4, 24, 0, 0, 25, 0, 19 2B02.GLU 435.4.7.0.2.0.0 3BB7,LYS_105,10.38,-0.12,0,0 2CN1,LYS_193,10.66,-0.24,0,0.4 4FD6,LYS_213,10.68,-0.29,0,0.47 1HF8,ARG 246,12.91,-0.85,0.73,0.53 1FQI,ARG_305,13.41,-0.63,0.78,0.76 2FG1.GLU 59.4.63.0.13.0.0 3L7N,LYS_125,11.36,-0.23,0.37,0.71 1ZYL,LYS 176,11,54,-0.21,0.85,0.4 2B0J.GLU 216.4.76.0.43.0.-0.17 2IXM,ASP_250,4.05,0,-0.47,0.73 3IVF,ASP_54,4.03,0,0.14,0.09 1SJ8,CYS_709,11.35,0,0.44,1.91 3T57,ARG 149,13.38,-0.28,0.51,0.65 2BT8.HIS 223.6.89,-0.56.0.75.0.2 2A6B,GLU_76,4.69,0.13,0,0.05 1WP5,LYS_274,10.3,-0.34,0,0.15 1JKS,ARG_254,13.68,-0.26,1.05,0.39 1C3K,GLU 69,4.61,0.5,-0.08,-0.3 3RJZ,TYR_199,9.99,0,-0.16,0.16 200K,LYS_305,10.46,-0.29,0,0.25 2BCF,GLU_218,4.22,0.37,-0.35,-0.3 300P,GLU_41,5.19,0.96,-0.15,-0.12 1AKO,HIS 16,5,76,-0,7,0,11,-0,15 4EZB,GLU_242,4.94,0.45,0,-0.02 2YT4,TYR_519,12.42,0,0.22,2.21 3CXS,LYS 167,10,46,-0,04,0,0 1NAF,HIS 186,6.34,-0.16,0,0 3GS3,GLU_54,4.67,0.22,0,-0.05 1059,TYR_343,10.27,0,0.04,0.22 1NAR,LYS_210,10.22,-0.55,0,0.26 4ESS,GLU 13,3.7,0.28,-0.85,-0.23 2B0J,LYS_2,9.88,-1.26,0,0.64 300P,ASP_31,2.88,-0.69,-0.55,0.31 1W24,HIS 117,5,72,-2,31,0,85,0.68 3M9A,CYS_93,9.41,-0.18,0.06,0.53 2PGX,ARG 241,13.21,-0.84,0.87,0.68 1NJ4,LYS 84,10,43,-0,24,0,0,16 2H2Z,TYR_37,11.71,-0.03,0.11,1.63 1RWZ,ARG_37,12.03,-0.85,0,0.38 2CIU,ASP_129,3.92,0,-0.05,0.17 1WP5,ARG_74,13.35,-0.17,0.64,0.38 3RFF,ARG_65,13.07,-0.51,0.52,0.57 2WZ9,GLU 59,4.32,0.39,-0.42,-0.14 10GL,LYS_106,10.39,-0.11,0,0 1ZCE,LYS 101,10.59,-0.09,0,0.18 2IOT.ASP 180.3.41,-0.7,-0.39.0.7 1YR6,ARG_177,12.75,-0.32,0.02,0.55 3I0C,HIS_305,5.49,-2.52,0.66,0.86 3LPZ,ARG_319,12.43,-0.07,0,0 2FXT,GLU_295,4.44,0.43,0,-0.5 1YB2,ARG_221,12.62,-0.18,0,0.29 1MTZ.TYR 176,10.52,-0.15,0.05,0.61 3FTT,LYS_6,11.51,-0.32,0.85,0.48

2OB5,HIS_49,6.49,-0.6,0.13,0.46 1R9W,ASP 275,4.02,0,0,0.22 3GT0,GLU_103,4.75,0.1,0,0.14 3CAX,TYR_448,11.01,-0.85,-0.11,1.97 10LR,TYR_128,12.71,0.14,0.01,2.56 3EIZ.LYS 175,10.49,-0.02,0,0.01 2H30.CYS 71.12.3.-0.02.0.53.2.81 1SJ8,ASP_661,4.03,0,-0.03,0.25 1K95,LYS_125,9.74,-0.83,0,0.07 3B79,LYS_123,10.34,-0.26,0,0.1 1FOLASP 399.3.89.0.-0.27.0.36 1G8P.GLU 267.4.73.0.23.0.0 1EYH,HIS_67,6.38,-0.26,0,0.14 100X.LYS 54,10.44,-0.08,0,0.02 2RH3,LYS_198,10.42,-0.08,0,0 2G3A,ASP 36,3.75,0,-0.27,0.22 3HVM,ARG_33,12.1,-0.84,0,0.44 2RJD,TYR_427,13.34,0.85,0.91,1.58 3BPP,CYS_120,12.17,-0.88,0.13,3.92 10ZN,ASP 147,3.25,-1.45,-0.03,0.93 1046.TYR 141.10.11.0.-0.25.0.37 2CBE, ASP_41, 1.64, -2.12, -0.51, 0.48 200K,ASP 34,4,0,-0.03,0.23 1YM5,HIS_295,6.67,-0.4,0,0.56 1J33,GLU 135,3.32,1.23,-1.75,-0.66 3EJG,LYS_47,10.48,-0.19,0,0.16 1Z3X,HIS_39,6.39,-0.55,0,0.43 3EVZ,GLU_57,3.31,0.66,-1,-0.86 2YYO,LYS_93,10.11,-0.12,0,-0.27 1V43,ARG_150,11.82,-1.02,0,0.34 3HVM,LYS_195,10.59,-0.15,0,0.24 2P1W.ASP 112.3.75,-0.19,-0.11,0.25 3FNI,ARG_20,12.84,-0.32,0.02,0.64 3C2E,ARG 115,12.03,-0.47,0,0.01 1DZF,LYS_201,10.04,-0.62,0,0.17 2EA9,CYS_92,12.5,-0.11,0.17,3.43 1U3Y,LYS_272,10.33,-0.17,0,0 2W0G,ASP_254,4.09,0,0.02,0.27 1DVO,ARG 101,12.33,-0.29,0,0.12 3BPV,ARG_140,12.78,-0.33,0.61,0 1WP5,LYS_228,12.44,-0.5,1.58,0.86 1MIX,GLU_350,4.05,0.7,-0.55,-0.6 2BDV,ASP_179,3.16,-0.77,-0.38,0.5 1YDL.ARG 56.12.46.-0.29.0.0.25 1UCH,LYS_210,11.36,-0.41,0.71,0.56 30DJ,GLU_49,3.85,0.5,-0.71,-0.43 2OJQ,ASP_434,4.14,0,-0.36,0.69 3V55,LYS 593,10.5,-0.09,0,0.09 3HVM,HIS_46,6.69,-0.91,0.64,0.46 3GEC,TYR_377,13.24,0,0.12,3.12 2O8I,HIS_97,6.15,-0.39,0,0.05 3BJV,ARG 77,12.24,-0.42,0,0.16 2A1V.GLU 32,4.92,0.2,0,0.22 2QOP,ARG_140,12.35,-0.32,0,0.16 3M7D,GLU_15,4.2,0.47,-0.74,-0.03 2RIK,TYR_130,10.96,0,0.51,0.45 3H5T,GLU_346,4.56,0.25,0,-0.19 2IIA.GLU 41.4.65.0.13.0.0.03 2PIM,ARG_105,12.99,-0.34,0.33,0.5 3CO1,ASP_19,3.8,-0.06,-0.21,0.28 3G9G,TYR_193,10.14,0,-0.03,0.17 2CW4,ARG 8,13,3,-0,21,0,61,0,41 4DBX,GLU_86,4.54,0.04,0,0 4F8A,ARG 662,13.22,-0.27,0.63,0.36 2BAA,ARG_114,12.96,-2.63,0.92,2.18 30DJ,ASP_183,2.95,-1.76,-0.86,1.77 3BB7,ARG 43,12,22,-0,28,0,0 1AIL,LYS_20,11.32,-0.3,0.74,0.38 4EVF,ASP_129,4.13,0,-0.14,0.49

4DNU.HIS 49.4.66.-1.82.0.15.-0.18 3C38,TYR 234,10.69,0.0.23,0.46 2P4D,HIS_109,4.85,-2.4,0.82,-0.07 3EAZ,HIS_155,7.35,-0.55,0.85,0.55 1TJE,ASP 22.3.27,-1.31,0.04,0.75 1RWZ,ASP 85,3,38,-0.83,-0.04,0.45 2XHC,LYS_73,10.42,-0.08,0,0 3HUE,ASP_59,3.57,-1.66,-0.28,1.71 1Q5Z,ARG_550,11.45,-0.86,0,-0.19 3HZO,LYS 85,10,19,-0,31,0,0 1RWZ,HIS 175.6.49,-0.64,0.69,-0.06 2OJQ,ARG_456,12.74,-0.11,0,0.34 3OA7,GLU_468,3.98,0.16,-0.68,0 1P4X.LYS 72.10.35.-0.15.0.0 3JZ9,ASP_387,2.95,-0.7,-0.4,0.25 3GMS,ASP_193,2.78,-1.64,-0.02,0.65 1WNH,GLU_59,4.83,0.3,0,0.03 3EZ7,ARG_396,12.43,-0.07,0,0 2Q13,LYS 351,10.25,-0.25,0,0 3GOZ,LYS 274,10,42,-0,24,0,0,17 1L2H,LYS_74,10.42,-0.12,0,0.04 3ASA,TYR_350,11.35,0,0.13,1.22 1I60,TYR_253,12.53,0,0.15,2.39 3UPD.LYS 19.10.38.-0.12.0.0 1HF8,CYS_48,10.25,-0.06,-0.08,1.4 1GQE,LYS_314,10.35,-0.17,0,0.03 1RL0,LYS_156,9.74,-0.51,0,-0.26 1N81,ARG 36,12.59,-0.14,0,0.23 2H2Z,CYS_160,12.82,-0.04,0.08,3.78 4ETX,GLU_238,4.43,0.15,0,-0.22 4GCO,CYS_220,10.29,-0.71,0,2 2D59,ASP_14,2.83,-1.39,0.01,0.4 2D7U,ARG 335,12.32,-1.1,0.12,0.81 3F5D.LYS 129.10.43.-0.07.0.0 3RFF,HIS_107,6.36,-0.14,0,0 1TWU,GLU_62,4.83,1.06,-0.18,-0.56 3RNV.LYS 453,10.31,-0.64,0.0.44 2I88,LYS 403,10,41,-0,2,0,0,11 1W7B,TYR_238,9.18,-0.85,-0.27,0.3 1DOV.GLU 82.4.35.0.21.-0.04.-0.32 3MIX,GLU_574,4.69,0.15,0,0.04 2Q98,LYS 190,10.2,-0.6,0.14,0.17 3FHF,TYR 86,10.02,0,-0.26,0.29 2CBE,LYS_149,10.13,-0.37,0,0 3GV0,ASP_235,3.43,-0.39,-0.32,0.33 4F8A,ARG_704,12.91,-0.16,0.12,0.45 3NR5,ASP_133,2.15,-1.78,-0.42,0.54 1SJ8,GLU_748,5.11,0.61,0,0 1LTU,ASP_235,4.07,0,0,0.27 2Z61,ARG_230,11.84,-0.75,0,0.09 2Q07,ASP_362,4.11,0,0.06,0.26 2E3S.GLU 431.3.47.2.43.-2.93.-0.52 4AE7,LYS_99,10.72,-0.15,0.37,0 2EHG,LYS_13,10.38,-0.13,0,0.01 1ZBM,GLU_186,3.77,0.35,-0.32,-0.77 2B0J,CYS_250,12,0,0.29,2.7 2RH3,LYS_137,9.57,-0.99,0,0.06 4EKU,GLU_19,4.58,0.08,0,0 3T5B,GLU_242,4.76,0.21,0,0.06 2HP7,TYR 171,10.29,0,0.03,0.26 3HNX.GLU 72.4.42.0.17.0.-0.25 2EJB,ASP_28,3.87,0,-0.16,0.22 3PBH,ARG_21,12.62,-2.92,0,3.04 4FZN,ARG_69,12.48,-0.41,0,0.38 1RI6,LYS_316,10.56,-0.34,0,0.4 3C5V,ARG_288,11.71,-1.39,0,0.61 2OJQ,GLU_561,4.67,0.16,0,0.01 208I,ARG_61,12.2,-0.3,0,0 1MN3,CYS 442,9.46,0,0.01,0.45

2PLQ,HIS_232,6.42,-1.17,0.62,0.47 1DVO.GLU 106.4.74.0.16.0.0.07 2H85,LYS_181,9.33,-1.13,0,-0.04 3QKY,ARG_180,12.36,-0.14,0,0.01 3GS9.GLU 262.5.45.1.05.0.-0.1 1JB3.ARG 10.11.23.-1.38.0.0.11 2V5B,GLU_133,3.57,0.4,-1.32,-0.01 2HRZ,CYS_296,10.22,-0.32,0.05,1.5 1YOY,GLU_158,4.61,0.14,0,-0.04 2IDC,HIS_36,6.54,-0.37,0,0.4 2EFK,ASP_23,3.81,-0.35,-0.03,0.39 2QK1,TYR_446,11.3,0,-0.01,1.31 1R53,ASP 236,3.86,0,-0.23,0.3 3M7G,ASP_119,3.98,0,-0.11,0.29 3LJC.ARG 99.12.51.-0.28.0.0.29 2BV9,ASP 113,4.09,-0.2,-0.02,0.51 4FCU,ARG_158,12.11,-0.62,0,0.22 2R0S,LYS_128,9.67,-1.4,0,0.57 2GZR,TYR_208,12.43,-0.82,0.05,3.2 3IVF,GLU 63,4.43,0.27,0,-0.35 2XHC,GLU_23,4.89,0.59,0,-0.2 2l6l.TYR 137.10.19.0.0.14.0.05 3A0X,GLU_668,4.68,0.32,0,-0.15 1IDK,TYR 229,12.66,0,1.09,1.56 2H30.LYS 148.11.3.-0.19.0.39.0.59 3ELI,GLU_146,4.58,0.15,0,-0.07 2X5Y,LYS_774,10.35,-0.55,0,0.4 1V8E,ARG_29,12.39,-0.29,0,0.18 2FBQ,HIS 83,6.46,-0.14,0,0.1 3EZ7,ARG_145,12.48,-1.38,0.9,0.48 1C44,LYS_29,10.48,-0.23,0,0.21 1HUF,LYS_26,10.3,-0.51,0,0.31 2IF4,GLU 96,4.72,0.25,0,-0.02 3GV0.LYS 232,10.39,-0.15,0.0.04 1D2K,TYR_344,10.81,0,0.06,0.74 2A4D,GLU_115,4.92,0.13,0.25,0.04 3LD1,LYS_293,10.37,-0.17,0,0.03 2IXM,ARG 41,12.23,-0.29,0,0.01 1QQE,LYS_14,11.2,-0.55,0.85,0.4 1DCF,GLU_50,4.02,0.27,0,-0.74 2JEO,ARG_122,12.25,-0.97,0.38,0.34 2ILR.CYS 319,11.08.0.0.08,2 2RJD,LYS_310,10.66,-0.1,0,0.26 3LMO,ASP_85,3.52,-0.85,-0.02,0.59 3G9G,GLU_171,4.63,0.12,0,0.01 208I,TYR_107,12.69,0.08,-0.09,2.7 2RIK,ARG 143,13.24,-0.3,0.71,0.33 1UAJ.GLU 11.4.43.0.13.0.-0.19 1FKM,ASP_462,3.26,-1.49,0,0.95 1I60,LYS_2,10.92,-0.22,0.09,0.54 2FM9.LYS 157.10.5.-0.13.0.0.13 300P,LYS 52,10,55,-0,14,0,0,19 1K95,LYS_169,10.78,-0.21,0,0.49 1QYI,LYS_141,10.36,-0.14,0,0 3L7N,LYS_38,10.22,-0.17,0,-0.1 2DFL,ASP_170,3.74,-0.31,0,0.25 1IDK,ASP 309,4,13,0,-0.02,0,36 1S7K,TYR_121,12.11,-0.86,0.23,2.75 2BLL,GLU_640,3.84,0.35,-0.75,-0.26 3BPV.GLU 25.4.38.0.47,-0.06,-0.54 3VJ8.CYS 289,12.76,-0.33,0.25,3.84 2YLF,CYS_65,12.08,0,0.07,3.02 3L3P,ARG_471,12.6,-0.3,0,0.41 3V46,GLU_360,3.39,1.33,-1.77,-0.67 2RIK,TYR_166,13.15,0,0.78,2.36 3US6,CYS_97,12.19,0,-0.02,3.22 2ZCO,GLU_198,4.1,0.35,-0.84,0.09 3LE4,LYS_342,10.44,-0.06,0,0 1NIJ,GLU_39,4.66,0.12,0,0.04

3F7M,ARG 355,13.88,-0.45,1.4,0.43 2IDC.LYS 10.10.59.-0.1.0.0.19 1YLN,ASP_157,2.86,-0.85,-0.4,0.31 1X9G,LYS_170,9.42,-1.05,0,-0.03 3JV1,GLU_71,4.64,0.1,0,0.04 3O16,LYS 61,11,15,-0.67,0.85,0.48 2PGE,ASP 115,2.86,-1.12,-0.37,0.55 1MML,ARG_121,13.12,-0.48,0.82,0.28 3F5D,ASP_12,3.44,-0.76,-0.01,0.41 2O0K,GLU_357,4.94,0.28,0,0.17 3EJG,LYS 94,10.5,-0.12,0,0.12 2Q07,TYR_447,10.65,-0.25,-0.59,1.48 3BPP,ASP_168,4.01,-0.24,-0.28,0.74 3C38,ASP_121,2.1,-1.62,-0.46,0.38 4HDE,ASP 104,3,76,0,-0,36,0,32 3FHF,LYS 88,10,38,-0,17,0,0,04 1RKA,HIS_213,5.78,-1.46,0.72,0.02 3RJX,LYS_176,11.54,-0.31,0.74,0.61 4DNU,LYS_329,10.67,-0.17,0,0.34 3JZN, ASP 144, 4.2, 0, 0.25, 0.15 3V55,ARG_551,12.83,-0.55,0.38,0.5 3K9I,ASP_156,2.81,-0.68,-0.66,0.35 3BCY,HIS_130,6.1,-0.4,0,0.01 2YWX.LYS 144.10.41.-0.12.0.0.03 100L.LYS 32.9.68.-0.96.0.0.14 3OBS,ASP_40,3.6,-0.56,-0.01,0.37 2E0T,ARG_98,12.54,-0.11,0,0.15 3CRM,HIS_240,6.33,-0.56,0,0.39 2CXA,CYS_200,9.83,-0.06,0.05,0.84 1YTQ,LYS_171,10.51,-0.13,0,0.14 3V3T,ARG_306,12.5,-0.11,0,0.11 2Z84,CYS_119,10.86,0.31,0.04,1.51 4FCU,ARG 84,12,23,-0.51,0.0.24 2G2D, ASP 72, 4.35, -0.85, 0.18, 1.22 1H4U,ARG_620,12.13,-0.41,0,0.04 1RWZ,LYS_100,11.22,-0.28,0.39,0.6 3CBN,ARG_41,12.37,-0.19,0,0.05 2Q98,GLU_70,4.49,0.1,0,-0.11 2G5X.TYR 69.11.48.-0.85.0.6.1.72 1MML,ARG_116,12.63,-0.09,0,0.22 3DTE,LYS_15,10.03,-0.37,0,-0.09 1NAR.GLU 32.5.08.1.22.0.-0.63 3LD1,GLU 57,4.42,0.36,-0.36,-0.08 3M16,GLU_260,4.78,0.36,0,-0.09 3GS9.TYR 222.10.38.0.0.19.0.19 1SUU,TYR_740,10.17,0,-0.01,0.19 3IL3, ASP 289, 2.66, -1.47, -0.5, 0.83 2Q12,LYS_70,10.66,-0.17,0,0.32 1R3F,HIS_218,6.21,-0.46,0,0.17 1ZCE.HIS 72.7.59.-0.67.0.98.0.77 3RLE,GLU_119,4.77,0.19,0,0.07 2QK1,GLU 543,4.43,0.21,-0.06,-0.22 2IF4,ARG_288,12.38,-0.13,0,0.01 2JEO,GLU_53,4.61,0.2,-0.09,0 1G5Z,LYS_165,10.18,-0.36,0,0.04 2Q99,LYS_184,10.33,-0.17,0,0 2B61,ARG_352,13.62,-0.51,0.77,0.85 4FZR,ASP_110,4,0,-0.24,0.44 1RKA,ARG_288,12.89,-0.74,0.65,0.47 2CL3,ARG_63,11.22,-1.19,0,-0.08 3IPZ,CYS 151,10.32,0,0.28,1.04 1L2F,ASP_184,2.43,-1.41,-0.38,0.42 1SIG,TYR_421,10.6,-0.16,-0.04,0.79 3L3P,TYR_402,12.38,0,0.35,2.03 3CXS,LYS_55,10.26,-0.24,0,0 3M66, ASP_378, 2.13, -1.67, -0.42, 0.42 3EVZ,GLU_146,4.52,0.12,0,-0.09 20KT,LYS_137,10.87,-0.28,0.28,0.36 3BQE,ARG_311,12.34,-0.38,0,0.23

2FXT,LYS_379,10.42,-0.19,0,0.12 3IU5,LYS 96,10.02,-0.58,0,0.1 2V4U,TYR_336,11.66,0,0.05,1.61 3T5B,ARG_320,13.51,-0.3,0.39,0.93 3CJW,GLU_210,4.88,0.65,-0.03,-0.24 1TLV.HIS 269.5.47,-1.5,0.81,-0.34 1T3YLYS 93.10.2.-0.31.0.0.01 208P,CYS_112,10.71,-0.17,-0.17,2.05 4H4J,ARG_256,11.98,-2.32,0.63,1.17 1T6L,HIS_185,6.7,-0.38,0.78,-0.2 3IPZ,GLU_115,5.08,0.35,0,0.24 2WOZ,TYR_354,10.19,0,0,0.19 105T,ARG_464,11.07,-1.65,0,0.23 2RH3.GLU 124,3.92,0.9,-1.01,-0.47 1RSS,LYS_60,10.52,-0.1,0,0.12 3S0A,GLU 5,3.62,0.27,-0.93,-0.22 3MIX.GLU 323.4.16.1.31,-0.55,-1.11 2EDM,GLU_176,3.8,0.33,-1.15,0.12 3A7L,ASP_108,2.72,-1.43,0,0.35 1RWZ.ARG 241.12.26.-0.6.0.0.37 3BJV.GLU 72.3.82.0.33.-0.76.-0.25 1GXN,TYR_360,10.55,0,0,0.55 2BV9,TYR_98,12.92,0.79,0.32,1.82 1FKM,LYS_313,11.51,-0.22,0.83,0.4 3GS3,LYS 256,10.49,-0.16,0,0.15 2Q12,CYS_99,9.58,-0.06,0.05,0.6 3G9G,GLU_107,5.48,0.77,0,0.21 3EVN,GLU_41,4.47,0.22,-0.24,0 1MD6.CYS 66,11.69,0.0.04,2.65 3GMS/HIS 284,5,39,-1,0,-0,12 2WZ9,GLU_55,3.75,0.24,-0.61,-0.38 105Z.ARG 627.12.34.-0.31.0.0.15 2FZP,TYR_271,10.38,0,0.14,0.24 4DND,ASP 60,4.59,0,0.14,0.65 1BKR.GLU 92.3.72.0.39.-0.85.-0.32 2FBQ,GLU_8,4.26,0.75,-0.56,-0.42 2RFA,LYS_229,10,-0.38,0,-0.12 1GQE,ARG_212,12.4,-0.11,0,0.01 4DNU,HIS 67,6.74,-0.49,0.66,0.07 3RLN,ASP_652,2.81,-0.74,-0.65,0.41 3FHF,ARG_57,12.23,-0.33,0,0.06 3CCY,ASP_192,2.93,-0.79,-0.38,0.31 3I4T,TYR 10,10.86,0,0.55,0.3 3EJG.GLU 80.4.54.0.18.0.-0.14 1ES5,ARG_248,10.93,-1.95,0,0.38 1BKB,TYR_99,10.09,0,0.02,0.07 3ON1,LYS_28,10.42,-0.13,0,0.05 208P,LYS 190,10.5,0,0,0 3EJG,LYS_56,11.35,-0.32,0.77,0.4 4ESS,ARG_56,12.43,-0.15,0,0.08 3GW3,GLU_13,4.6,0.09,0,0.01 1YW5,LYS_141,9.93,-0.63,0,0.06 2G9D.CYS 156.13.58.-0.16.1.38.3.36 1Q2Y,HIS_77,6.02,-0.46,0,-0.02 3V55,CYS_591,9.51,0,-0.02,0.52 3MIX,ASP_327,4.42,0,0.28,0.33 3UV9,CYS_471,11.84,-0.07,0.15,2.75 20V2.TYR 246,10.22,-0.58,-0.23,1.03 2RGY,ARG_190,12.81,-0.15,0,0.46 2H2W,GLU_236,5.04,4.18,-1.64,-1.99 3K8J,LYS_192,9.64,-1,0,0.14 4E9E,ARG 442,12,44,-0,4,0,0,34 20GQ,GLU_455,4.42,0.32,-0.47,0.07 2CXC,LYS_123,10.24,-0.26,0,-3.47E-17 3FK5,CYS_114,10.97,0,0,1.97 1X04,ASP_41,3.39,-0.42,-0.41,0.42 3VJ8,CYS 43,12,36,-0.04,0.42,2.97 2RJD,GLU_425,4.66,0.16,0,0 4DBX,HIS_68,6.37,-0.34,0,0.22

3R87.TYR 30.13.65.0.84.0.57.2.25 2FZ4,LYS 109,10.08,-0.37,0,-0.05 1O59,TYR_200,12.02,0.56,0.47,0.99 2G3A,GLU_31,4.92,0.1,0.07,0.25 3T5B,TYR 107,10.7.0.0.03,0.67 3IL3.LYS 255,10.42,-0.08.0.0 3M70,HIS_59,6.28,-0.55,0,0.32 2QEV,LYS_116,9.4,-1.05,0,-0.05 3LJC,ASP_67,3.79,-0.23,-0.13,0.36 1ANU,GLU_45,3.68,0.24,-0.68,-0.38 3T5B,ARG 344,13,19,-0,3,0,56,0,44 2PGX,TYR_88,11.33,0,0,1.33 1SIG,ASP_313,3.28,-0.84,-0.4,0.72 3DSH,GLU_270,3.9,0.32,-0.45,-0.47 3GS3,ASP 32,4.04,0,-0.01,0.25 4FH3,GLU_123,4.72,0.22,0,0 2CYG,GLU_303,4.58,0.48,0,-0.4 2EJB,GLU_132,4.58,0.08,0,0 1FKM,ASP_415,3.92,0,-0.05,0.16 1TD6.HIS 280.3.95.-2.16.0.-0.39 1X91,ARG_117,12.43,-0.09,0,0.02 3H5T,HIS_266,6.36,-0.69,0.32,0.23 1MIX.GLU 386.4.68.0.18.0.0 1UAJ.TYR 136.10.41.0.-0.02.0.43 20GQ,GLU_488,4.13,0.82,-0.8,-0.39 1YB2,LYS_129,11.54,-0.22,0.83,0.42 3H13,ASP_304,3.87,0,-0.27,0.34 4FD6,LYS 61,10.24,-0.26,0,0 1U53,ARG 75,11.81,-1.33,0.0.64 4EVF,TYR_269,12.22,0,0.19,2.03 1059,GLU_80,4.49,0.31,0,-0.32 300P,GLU_81,4.68,0.18,0,0 3BJV,TYR 43,12.75,-0.76,0.22,3.29 1MHN,LYS 97,10.47,-0.09,0,0.06 1F2V,ARG_101,12.64,-0.14,0.01,0.27 2GYZ,ARG_6,12.32,-0.18,0,0 3N2T,ARG_260,13.17,-0.64,0.83,0.48 2Z61,TYR_354,9.87,-0.16,-0.47,0.5 2IQT,HIS_253,7.45,-0.22,0.85,0.32 2OSA.GLU 377,4.53,0.21,-0.3,0.11 1TUL,GLU_92,4.48,0.23,0,-0.26 2P1W.LYS 208,10.84,-0.25,0.23,0.36 3L7N,ASP 136,3,5,-0,73,0,08,0,36 2D7U,TYR_192,10.1,0,-0.05,0.15 3JSN,HIS_12,5.58,-1.47,0,0.56 1BN6,HIS_241,6.48,-0.8,0.84,-0.06 1G8PARG 18,12,44,-0.06,0,0 1YTD,GLU_386,4.87,0.18,0,0.18 2H2W,ASP_249,4.02,0,-0.46,0.69 3K8U,GLU_40,4.49,0.15,0,-0.16 1Q46,ARG 74,13.17,-0.25,0.61,0.31 1PV5.GLU 244.4.1.0.21.-0.21.-0.4 2B61,ASP_37,3.87,0,-0.04,0.11 3OBS,TYR_17,10.27,0,-0.07,0.34 3P2F,ARG_135,13.18,-0.4,0.37,0.71 2IRM,TYR 233,12.7,-0.77,1.09,2.37 2B61,ARG_212,12.59,-1.94,0,2.02 4EUG,LYS_184,10.2,-0.19,0,-0.11 1X04,GLU_81,4.66,0.16,0,0 4ESS,ARG_157,12.8,-0.13,0,0.43 3MEW,ASP 194,5,14,0,0,33,1,01 3JSN,ARG_61,9.97,-3.12,0,0.59 1N81,GLU_113,4.46,0.15,0,-0.19 20EW,ASP_292,3.96,0,0,0.16 1SJ8,ASP_564,3.62,-0.4,-0.12,0.34 3C6B,GLU 267,4.64,0.76,-0.12,-0.51 1ZCE,ASP_80,3.28,-0.67,-0.25,0.4 1WXQ,LYS_391,10.62,-0.34,0,0.44 1RKA,LYS_91,10.47,-0.03,0,0

4H89,GLU_4,3.98,0.21,-0.63,-0.1 1R6Y.ARG 98.12.37.-0.13.0.0 1QQE,TYR_174,11.39,0,0.17,1.21 3GS3,HIS_234,5.67,-0.85,0,0.02 1TJE.HIS 125.6.29,-1.24,0.45,0.56 20HT.TYR 127.10.25.0.-0.02.0.27 1J33,ASP_270,4,0,-0.38,0.58 2G2D,ASP_38,4.02,-0.7,-0.11,1.03 1LPL,ASP_204,3.98,0,-0.02,0.2 1SJY,GLU_101,4.62,0.51,0,-0.39 2APL,GLU_40,4.55,0.33,0,-0.27 1K95,TYR_153,11.75,-0.26,0.26,1.75 3IVF.HIS 283.4.12,-2.38.0.78,-0.78 2R0S.TYR 251,13.37,-0.29,0.21,3.46 1WPA.TYR 481.11.08.0.34.0.38.0.36 1IDK.TYR 231,11.09.0.0.56.0.53 1ES5,LYS_166,10.34,-0.15,0,-0.01 1WRU,ASP_78,3.89,0,0,0.09 300P,ARG_99,13.71,-0.33,0.95,0.59 2WB3,ARG 242,12.45,-0.05,0,0 1TP6,ARG_35,12.9,-1.37,1.06,0.71 3I4T,LYS 148,10,29,-0,21,0,0 2IDC,GLU_116,4.36,0.34,-0.38,-0.1 1JT9,TYR 184,10.14,0,0,0.14 2JHY.GLU 154,4.38,0.12,0,-0.24 3HZQ,ASP_51,4.81,0,0.39,0.62 3JV1,ASP_98,3.89,-0.05,0.04,0.1 3PU6,LYS_2,10.31,-0.44,0,0.24 3H5T,GLU 261,5.15,0.52,0,0.12 3BQE,ASP_240,3.06,-0.98,-0.17,0.41 4F85,TYR_77,10.38,-0.16,0.08,0.45 2RIK,GLU_169,4.86,0.38,0,-0.01 2E3C,ARG_239,12.37,-0.22,0,0.09 1HF8,LYS 40,10,18,-0,18,0,-0,14 3FHF,HIS_-3,6.24,-0.18,0,-0.07 2G9D,ASP_118,3.23,-0.5,-0.45,0.39 2NRK,ASP_154,3.03,-0.64,-0.42,0.28 1GXN,TYR 648,11.54,0,-0.03,1.56 2VGM,LYS_221,10.35,-0.2,0,0.05 2RFA,LYS_63,10.36,-0.24,0,0.1 3C6B,ASP_103,3.33,-1.16,-0.31,1.01 2EEY,GLU 9,4,48,0.06,0,-0.08 1M5I.GLU 192.3.94.0.39.-0.74.-0.21 1ZCE,LYS_111,10.45,-0.06,0,0.01 1WXF,GLU_252,4.66,0.78,-0.61,-0.01 1RHS,GLU_169,4.6,0.23,0,-0.13 2R51,GLU 69,4.36,1.07,-0.51,-0.71 1TD6.TYR 256.9.73.-0.81.0.23.0.3 1X7F,ARG_262,12.98,-0.35,0.25,0.56 2Q12,GLU_239,4.67,0.17,0,0 3M9A, ARG 17, 12, 67, -0, 14, 0, 0, 31 1Y0K, ASP_49, 3.14, -0.79, -0.43, 0.56 3PU6,ASP_130,3.41,-0.73,0,0.34 3M7G,GLU_240,4.65,0.35,0,-0.2 20EW,LYS_101,10.51,-0.26,0,0.26 1DTO,LYS_177,10.77,-0.1,0,0.37 1N81.TYR 108,12.92,-0.6,0,3.51 2RJD,CYS_363,11.47,-0.42,0.35,2.54 3BA1,LYS_306,10.43,-0.12,0,0.05 2IOT.ASP 286.4.26.0.-0.09.0.56 1ZCE.GLU 132.2.32.0.44,-1.92,-0.7 1T95,ARG_183,12.22,-0.28,0,0 1AD6,GLU_554,5.71,1.09,0,0.12 3ERF,LYS_40,11.5,-1.14,1.24,0.89 2ZTY,GLU_21,4.29,0.25,-0.46,0 3ADO,TYR_35,10.84,0,0.16,0.68 4AM1,CYS_271,12.07,-1.67,1.5,3.24 3UAH,TYR_220,11.12,-0.01,0.06,1.07 2Q13,TYR_68,10.44,0,0.16,0.28

1K95,TYR 55,10,17,0,-0,12,0,29 2IXM,HIS 127,6.18,-0.3,0,-0.02 3PZ9,ASP_64,3.81,-0.28,-0.11,0.4 2ZO5,LYS 80,11,45,-0.36,0.85,0.46 1JSX,ARG_52,12.28,-0.36,0,0.14 20V0.GLU 61.4 68.0 21.0 -0.04 3EX9,ARG 65,12,32,-0,23,0,0,05 3B79,CYS_79,12.15,0,0.16,2.99 3CIV,GLU_118,5.03,0.31,0,0.22 2B0J,GLU_221,4.53,0.11,0,-0.09 3G9G,GLU_165,4.42,0.1,0,-0.18 3V46.LYS 263.10.5.-0.27.0.0.27 2X5Y,HIS_737,6.08,-0.38,0,-0.04 1JKS,HIS_166,3.6,-1.92,0,-0.98 1DZF.GLU 21.3.98.2.08.-1.62.-0.98 1ZCE.GLU 66.4.12.0.94.-0.63.-0.69 3EX9,ARG_14,12.36,-0.14,0,0 1BKR.HIS 60.6.39.-0.34.0.0.23 1MML,ASP_124,3.04,-0.32,-0.75,0.31 2XWS,TYR 115,10.11,0,0,0.11 2GS5.GLU 124.5.07.0.44.0.0.13 2QK1,HIS_378,5.83,-0.51,0,-0.17 1ZP2,GLU_91,4.6,0.1,0,0 2X4L,LYS 157,11.5,-0.3,0.85,0.45 3K9I,TYR 124,10.38,0,0.2,0.18 3VJ8,TYR_46,12.58,0.85,0.64,1.09 3ERF,HIS_164,6.44,-0.39,0,0.34 3V3T,GLU_170,5.06,0.83,-0.24,-0.02 2RJD,LYS 235,10.26,-0.24,0,0 3GMS.TYR 276,10.37,0.0.21,0.16 3KB5,GLU_344,4.78,0.24,0,0.05 2QK1,GLU_464,4.72,0.21,0,-1.39E-17 2WB8,LYS 768,10,47,-0,33,0,0,3 2R0S,ASP 37,3.48,-0.4,-0.22,0.31 1KN3,LYS_148,10.33,-0.17,0,0 1l60,HIS_200,11.91,-3.24,1.78,6.86 1RZ2,ASP_103,4.38,0,0.28,0.3 2R4Q,GLU_263,4.21,0.32,-0.6,-0.02 1MML/HIS 126.6.44,-0.23.0.0.17 3IU5,ARG_79,12.31,-0.2,0,0 2B78,HIS_254,4.1,-3.04,0.84,-0.2 1MIX.ARG 303.12.43.-0.88.0.3.0.51 1X04, ASP 31, 3.77, -0.08, -0.11, 0.15 208I,GLU_96,3.64,0.47,-0.83,-0.5 2P1W.ARG 91,12.09,-1.58,0.53,0.64 3ADO,LYS_130,10.45,-0.15,0,0.1 3RJX,TYR 64,10.65,-0.06,0.12,0.6 1DZF,ASP_41,4.09,0,0,0.29 1LPL,ASP_192,1.49,-2.28,-0.46,0.44 3CX2,LYS 190,10.63,-0.18,0,0.31 2R57,GLU_299,4.66,0.13,0,0.02 3DTE,TYR 246,10.57,0,0.28,0.29 20GO.TYR 562,11.76,-0.72,0.56,1.93 3HUE,LYS_76,10.44,-0.07,0,0.02 2CWY,ARG_16,12.58,-0.28,0,0.36 1T07,ARG_54,12.32,-0.18,0,0 1J74,LYS_8,10.39,-0.13,0,0.01 1RHS,GLU_227,3.65,0.33,-1.03,-0.16 2RJD,TYR 386,10,56,0,0,33,0,23 1BYI,HIS_154,6.3,-0.33,0,0.14 3U0V,TYR 66,11.63,-0.02,-0.46,2.11 2RIS,ARG 66,10,72,-1,8,0,0.02 1GXN,TYR_412,12.22,0.83,0.41,0.98 3M7G,GLU_256,4.4,0.33,0,-0.43 3BA1,LYS_178,10.33,-0.27,0,0.11 2NSN,ASP_99,3.96,0,0,0.16 1RL0,TYR_89,11.37,0,-0.09,1.47 1YW5.ASP 90.3.95.0.0.0.15 2CXA,CYS_174,11.74,0,0.03,2.71

3BPP,ASP_188,3.48,-0.67,-0.07,0.42 3T5B,GLU 152,4.67,0.26,0,-0.09 3PZ9,ASP_341,4.34,0,0.18,0.36 1EDG,LYS_127,10.53,-0.32,0,0.35 1NJ4,LYS_273,10.41,-0.12,0,0.03 4EF5.TYR 274.10.22.0.0.0.22 3EJG.ARG 93.12.19.-0.33.0.0.02 4E9E,LYS_526,10.72,-0.25,0.03,0.45 3V46,ARG_292,13.38,-0.15,0.55,0.48 2AHE,TYR_154,10.7,-0.85,0.07,1.48 1PVT,GLU_203,4.08,1.34,-1.12,-0.66 3U4K,TYR_152,11.52,0,0,1.52 2W0G,ARG_264,13.22,-0.48,0.32,0.88 3H13.HIS 283.6.73.-0.24.0.48.0 1WP5,GLU_266,3.4,0.49,-1.11,-0.48 2IXM, ASP 229, 3.87, 0, -0.14, 0.21 20VT.ARG 43.11.41.-1.27.0.0.18 2D0A,LYS_230,10.41,-0.12,0,0.03 1J33,LYS_41,10.02,-0.33,0,-0.16 1T3Y.ARG 117.13.2.-0.5.0.62.0.57 2X4L,GLU_136,2.74,0.58,-1.85,-0.49 3B4D,TYR_181,10.44,0,0.03,0.4 3DHN,GLU_46,4.47,0.14,0,-0.17 20KT,LYS 314,10,47,-0,16,0,0,13 1J7G,ASP 127,3.28,-0.68,-0.07,0.23 2EDM,GLU_112,3.76,0.42,-0.87,-0.3 3K8J,ARG_222,12.23,-0.12,0,-0.16 1BKB,GLU_16,3.95,0.26,-0.81,0 2VC8,ASP_58,3.14,-0.66,-0.38,0.38 2D7U,ARG_227,10.42,-1.89,0,-0.18 2E3C,ARG_298,12.27,-2.26,0.54,1.48 1T3J.LYS 707.10.42.-0.08.0.0 1MJS,GLU_238,4.71,2.51,-1.38,-0.91 1W7B,LYS 233,10.7,-0.23,0,0.43 2R0S,LYS 72,10.34,-0.21,0.0.06 1DZF,CYS_47,10.09,0,-0.02,1.11 1160,LYS_266,11.49,-0.22,0.83,0.38 2FM9,HIS_226,6.21,-0.59,0.21,0.1 3B79,TYR 118,10.61,0,0,0.61 2WB8,HIS_477,6.06,-0.43,0,-0.02 3HUE,LYS 172,11,42,-0,31,0,85,0,38 3M3P,ARG_155,12.15,-0.39,0,0.04 3ZSL,CYS 173,12.57,0,0.17,3.39 1X04.ASP 128.4.-0.41.0.0.61 3RJX,ARG_303,12.33,-1.22,0.46,0.59 4H4J,LYS_247,10.63,-0.22,0.08,0.27 2E3S,GLU_498,4.46,0.35,-0.11,-0.27 3ASA,ASP_183,2.31,-1.06,-0.71,0.28 3N0K,TYR_8,11.41,0,0.06,1.35 3U0V,ARG_64,12.14,-0.69,0,0.33 4EZB,GLU_146,3.32,1.03,-1.57,-0.63 1QZN,LYS_86,11.52,-0.26,0.85,0.43 1RZ2.LYS 44,10.46,-0.08,0.0.04 3IBT,ARG_198,12.11,-2.02,0.64,0.99 3GE9,GLU_180,4.85,1.12,-0.53,-0.24 3CN5,HIS_62,5.91,-0.61,0,0.02 3R2E,ARG_74,13.12,-0.48,0.7,0.39 1L2F.GLU 7.4.7.0.14.0.0.06 20BI,LYS 48,10.35,-0.43,0.0.28 3OKQ, ASP_590, 3.42, -0.45, -0.31, 0.38 4E9E,ARG_492,12.59,-0.33,0,0.42 3BOW,LYS 265,10,74,-0,24,0,0,47 2D7J,TYR_68,12.39,-0.01,0.05,2.35 2FL7,LYS 99,10.66,-0.27,0,0.43 3T8R,GLU_34,4.78,0.27,0,0.01 4FD6,LYS_107,10.42,-0.39,0,0.3 2X4L.ARG 320,13.27,-3.31,1.64,2.43 3CJW,GLU_251,6.64,3.09,-0.41,-0.53 1L3K,GLU_126,4.96,0.33,0,0.14

2ZTY.HIS 177.5.8.-0.61.0.-0.09 3U2A,ARG 69,12,-0.36,0,-0.14 3T57.LYS 70.10.69.-0.2.0.0.39 2IN0,ARG_82,12.76,-0.33,0.07,0.52 1UXO,TYR 57,10,43,0,0,08,0,35 4FZR.CYS 175,11,19,0,0,43,1,77 1Z3X,GLU_-1,4.77,0.67,-0.53,0.13 1X7F,GLU_51,4.67,0.24,0,-0.08 3KB5,ARG_401,12.22,-0.28,0,0 1XTZ,LYS 243,10.12,-0.83,0,0.44 1PV5,GLU_177,4.55,0.05,0,0 2X4G,HIS_67,6.34,-0.27,0,0.11 2IRM,GLU_42,4.58,0.29,0,-0.2 2FBQ,ASP_107,1.99,-2.8,-0.46,1.45 3L3P,LYS_266,10.65,-0.18,0,0.32 2NRR,HIS_472,6.22,-0.22,0,-0.06 3GE9,ARG_172,12.06,-0.25,0,-0.2 2HNG,ARG_109,12.54,-0.19,0,0.24 4DND,ASP_44,3.99,0,-0.01,0.2 3PBH,HIS 28,6,1,-1,01,0,71,-0.09 2R57,CYS_223,11.92,0,0.49,2.43 3H9W,GLU_58,4.75,0.12,0,0.13 1BKB.LYS 42,10.45,-0.05,0,0 2RIS.LYS 187.10.54.-0.16.0.0.2 2IDC,GLU_120,3.44,0.23,-1,-0.29 3BWT,LYS_591,10.54,-0.06,0,0.11 2X4J,GLU_112,4.42,0.41,-0.47,-0.02 1DVO,ASP_145,3.12,-1.35,0,0.68 1ZBM.ARG 222.12.95.-0.16.0.21.0.4 1U53,LYS_101,10.83,-0.22,0.21,0.33 2ILR.LYS 499,10.63,-0.27,0.08,0.31 3B7X,ASP_41,4.08,0,-0.22,0.5 1ZBP,CYS 242,10.04,0,0.13,0.92 3GEC.GLU 506.4.73.0.23.0.0 3KEY,LYS_417,10.38,-0.16,0,0.04 1NAR,ARG_271,12.35,-0.11,0,-0.04 1WLY,ARG_48,11.58,-1.04,0,0.11 1ZKZ,GLU_36,4.4,0.39,-0.13,-0.36 3GW3,HIS_360,5.33,-0.86,0,-0.31 1SFE,ASP 43,3,18,-1,12,0,07,0,43 4H4J.GLU 138.6.37.1.85.0.0.02 3GOZ.ASP 250,3.03,-0.53,-0.59,0.35 1YW5,HIS 130,6.88,-0.76,0.8,0.36 2RJD,LYS_330,10.05,-0.18,0,-0.27 3CCY,ARG_136,12.64,-0.45,0.34,0.25 2DFL,LYS_87,9.99,-0.39,0,-0.12 2CIU,TYR_204,10.43,-0.15,-0.34,0.92 3O16, ARG_19, 12.6, -0.65, 0.32, 0.43 2FD5,ASP_3,2.32,-1.94,-0.01,0.46 1YTQ,ASP_172,2.78,-1.39,0,0.37 3H13,CYS 345,10.71,-0.26,-0.2,2.16 3FWU,ASP 44,3.18,-0.92,-0.11,0.41 3GS3,HIS_76,6.23,-0.26,0,0 3EVP,LYS_75,10.28,-0.21,0,0 2V1L,TYR_50,10.62,-0.78,0.38,1.02 2PLQ,ARG 2,13.04,-0.36,0.27,0.62 2FC3,LYS_24,11.38,-0.34,0.85,0.37 3ADO,CYS_78,9.91,-0.42,-0.06,1.38 1NIJ,ASP_46,3.69,-0.57,0.06,0.4 1T95, ASP 30, 3.36, -1.19, -0.06, 0.82 1YM5,LYS 124,10,73,-0.26,0,0,5 1ZP2,TYR_63,12.91,0.83,0.59,1.49 4EVF,LYS_142,10.26,-0.67,0,0.43 1GPP,GLU_16,4.45,0.36,-0.49,0.09 3PP8,HIS_230,4.9,-2.05,0.61,-0.17 3P28,HIS 100,5.02,-1.58,0.1,0 10I7,GLU_281,4.53,0.25,0,-0.21 1VJG,ARG_137,13.42,-0.32,0.85,0.4 3LMO,GLU_21,4.06,0.29,-0.7,-0.03

3H6Q,GLU_139,4.48,0.37,0,-0.38 20HT.GLU 191.4.61.0.1.0.0.01 2R51,TYR_41,10.75,0,0.04,0.7 1W24,GLU 125,4,34,0,19,0,-0.36 3N0K,GLU_106,4.56,0.12,0,-0.06 3LJN.ARG 47.12.26.-0.24.0.0 3JZN,TYR 280,10,44,0,-0,15,0,58 2PGX,GLU_76,4.23,1.69,-1.53,-0.43 1UJ8,ARG_20,13.86,-0.53,1.13,0.77 2P52, ASP_183, 2.34, -1.93, -0.6, 1.07 3LH5,ASP_780,2,-2.23,-0.52,0.95 1TXJ,HIS_123,5.72,-0.78,0,-0.01 20JO.HIS 516.5.72.-0.78.0.0 2Q07,ASP_375,3.31,-0.8,-0.03,0.33 20KT.HIS 338.5.94.-0.32.0.-0.24 3FWU,HIS 104.6.3,-0.2,0.0 1WXQ,TYR_368,10.01,0,-0.27,0.29 1T95,ARG_19,12.87,-0.22,0.3,0.29 3LMO,CYS_16,10.85,0,0.63,1.22 3C38,TYR 185,9.49,-0.57,-0.46,0.51 3LQE,GLU_447,4.86,0.68,-0.27,-0.05 1XWM,ASP_61,4.16,0,0.04,0.32 3GS3,LYS_95,10.48,-0.41,0.01,0.39 2ATR,GLU 137,4.54,0.04,0,0 1EV8.ASP 193.3.66.0.-0.29.0.15 2APL,HIS_23,7.26,-0.82,0.85,0.73 2CL3,GLU_127,4.42,0.79,-0.44,-0.43 30NH,ASP_514,2.99,-2.01,-0.05,1.26 1DVO,ASP 167,1.98,-1.29,-0.9,0.36 3L3P,GLU_486,4.57,0.3,0,-0.23 3IRA,HIS_54,6.25,-0.59,0.37,-0.02 1PNE,GLU_46,2.84,1.49,-3.15,0 1DZF,HIS 153,5.55,-1.57,0.55,0.07 3R2E,ARG 86,12.26,-0.27,0,0.02 3IV4,GLU_46,4.67,0.15,0,0.02 3CXS,LYS_2,10.46,-0.04,0,0 1V6T,HIS_223,6.62,-1.79,0.03,1.89 2AD1,TYR 281,12.08,0,0.04,2.04 1XFK,HIS_28,5.69,-0.56,0.09,-0.33 3U0V,ARG_80,12.09,-2.68,0.14,2.15 10GL,HIS_38,6.96,-0.29,0.37,0.38 2IRM,LYS 125,11.3,-0.85,0.67,0.99 3VJ8,ASP 159,3.88,-0.11,-0.05,0.25 2P4D,ASP_91,4.07,0,0.09,0.19 3RRQ,GLU_84,4.49,0.12,0,-0.13 2V5B,GLU_168,6.66,3.19,-0.74,-0.3 3GT0,TYR_49,9.74,-0.62,-0.39,0.74 105T.HIS 445.5.12,-2.02.0.71,-0.07 1MD6,GLU_40,4.6,0.22,0,-0.12 1T95,ASP_47,4.1,0,0.04,0.25 3C38,TYR 262,11,76,-0,1,-0.06,1.92 3I47.HIS 25.6.03.-0.37.0.-0.1 1X9G,LYS_75,10.46,-0.07,0,0.04 2EJX,HIS 99,5.86,-1.58,0.73,0.2 3QAV,ASP_136,3.28,-0.43,-0.57,0.48 2F8H,ARG_25,12.85,-0.98,0.53,0.8 1RL0.LYS 211.10.25,-0.28,0.0.03 1TXJ,GLU_35,4.77,2.73,-2.19,-0.27 3UC9,GLU_99,4.58,0.3,0,-0.22 1RKA.GLU 200.4.7.0.16.0.0.04 1SIG.TYR 430.11.29.-0.52.0.08.1.71 4E8B,HIS_8,6.65,-1.29,1.22,0.21 2EJB,HIS_108,4.59,-1.84,0,-0.07 2IDC,ARG_174,12.53,-0.11,0,0.14 3RE9,ASP_150,3.33,-0.89,0,0.43 3OA7, ARG_505, 12.49, -0.13, 0, 0.12 1P4X,CYS_61,10.83,0,-0.05,1.87 4DIU,ARG_135,13.63,-0.38,1.1,0.41 2ZCX,LYS_80,10.38,-0.43,0,0.31

3BWT.ASP 834.3.43.-1.52.-0.02.1.17 1BYI,GLU 211,4.61,0.11,0,0 3VHJ,HIS_114,5.95,-0.56,0,0.01 2E3C,ASP_334,3.3,-0.65,-0.12,0.27 1ZCU,HIS_28,5.45,-1.05,0,0 3IO01YS 210.10.14-0.32.0-0.04 4DVD.HIS 92.6.15.-0.35.0.0 4EUG,GLU_52,3.78,0.87,-1.54,-0.04 1Q8B,GLU_94,4.56,0.25,0,-0.19 3RLN,LYS_594,10.58,-0.05,0,0.13 1NIJ,ASP 290,3.5,-0.45,0.04,0.12 1MD6,ARG 9,12.69,-0.2,0.0.39 2Q13,LYS_160,10.47,-0.19,0,0.16 3N0K,LYS_71,10.19,-0.32,0,0.01 2161,ARG 25,12,24,-0,26,0,0 2XWS.GLU 97.3.03.0.51,-1.45,-0.52 1AT0,GLU_268,3.72,0.43,-0.82,-0.38 1059,LYS_261,10.76,-0.42,0.25,0.44 1XWM,GLU_202,4.17,1.07,-0.84,-0.56 2R51,GLU 254,3.6,0.44,-0.64,-0.69 2RJD,CYS_264,10.33,0,-0.02,1.35 2B3M,ARG_77,12.46,-0.04,0,0 1PDB,ARG_77,12.38,-0.17,0,0.05 2APL/HIS 71,6.52,-0.48,0,0.5 1FHL.TYR 319.10.36.0.0.21.0.14 2EJB,GLU_66,5.01,0.98,-0.25,-0.23 1XDZ,ARG_147,12,-2.56,0.65,1.4 3QYB,LYS_958,10.59,-0.16,0.26,0 1R3F,ARG 34,12.42,-0.08,0,0 3G6S.TYR 196.11.44.0.0.41.1.03 1X9G,HIS_59,5.55,-1.03,0.11,-0.04 2AXO,LYS_66,11.14,-0.3,0.72,0.23 3BWT.TYR 839,9.83,-0.05,-0.36,0.23 3JRT.ASP 5,3.95,-0.06,0,0.21 1UW7,ASP_50,4.06,0,-0.13,0.4 1SFE,TYR 115,11,37,0,0,3,1,07 3FFM,GLU_110,4.89,0.39,0,0 2W0G,LYS_154,11.27,-0.46,0.85,0.38 1EYH,ARG_91,12.14,-0.4,0,0.03 3LJN,GLU_178,4.1,0.92,-0.39,-0.93 2FG1,HIS_119,4.16,-2.13,0,-0.21 2JEO,ASP_93,3.54,-0.93,-0.29,0.96 4H4J,ASP 104,3.68,0,-0.3,0.18 3PBH,ARG_41,13.86,-3.62,1.43,3.55 1Y0K,LYS_124,10.41,-0.09,0,0 3VJ8,ARG_279,12.87,-0.58,0.83,0.12 1G8P,TYR_234,11.02,0,-0.12,1.14 2QOP,ARG_105,12.9,-0.46,0.4,0.46 3M16,HIS_54,7.54,-0.43,0.85,0.61 3GFP,ASP 310,3.63,-0.72,-0.25,0.8 2E3C,GLU_238,4.32,0.47,-0.52,-0.13 2ZQ5,HIS 363,6.49,-0.1,0,0.09 3M7D,ARG_304,12.77,-0.24,0.08,0.43 1NIJ,GLU_239,5.11,0.29,0,0.32 2Q34,TYR_125,13.6,0,0.67,2.93 4ECC, ARG_121, 12.35, -0.24, 0, 0.09 1MUF,TYR_337,11.43,0,0.61,0.82 2XHC,LYS_62,10.48,-0.12,0,0.09 1ILW.GLU 35,3.44,0.39,-0.81,-0.64 1G8P,GLU_136,4.88,0.46,0,-0.09 2EDM,LYS 75,10.24,-0.34,0,0.08 1ZKZ,ARG 110,12,12,-0,52,0,0,14 1PBV,ASP_75,3.47,-0.51,-0.19,0.37 3RFF,ARG_121,12.8,-0.29,0.09,0.5 2AH5,GLU_155,4.03,0.32,-0.79,0 3H04,CYS_96,10.62,0,0.19,1.44 3MIX,ARG_616,12.52,-0.15,0,0.17 2WZ9,TYR 80,10.66,-0.33,-0.44,1.43 1UOH,HIS_78,4.49,-2.7,0.8,-0.11

1SUU,ASP_631,4.57,0,-0.03,0.8 10TM,TYR 96,10.38,0,0.07,0.31 2X4L,GLU_323,5.99,3.55,-1.27,-0.79 3M3P,LYS_97,10.13,-0.4,0,0.03 3ERF,GLU_62,4.66,0.12,0,0.04 1RKA.HIS 157.6.32.-0.33.0.0.15 3F6F.HIS 51.6.18.-0.5.0.25.-0.07 3FHF,ARG_121,12.46,-0.09,0,0.05 1XDZ,ASP_136,3.92,0,-0.02,0.14 3AU3,GLU_425,4.9,0.36,0,0.05 3OKO,LYS 561,10,28,-0,22,0,0 2YWJ,LYS 113,11.36,-0.31,0.77,0.41 3CNU,ASP_48,2.33,-1.74,-0.18,0.45 2AHE,LYS_103,11.22,-0.32,0.37,0.67 2G9D,LYS_134,10.17,-0.85,0,0.51 1JT9,LYS 124,9.71,-0.82,0,0.03 4FH3,GLU_92,5.26,0.86,0,-0.11 1MD6,ASP_142,3.52,-0.46,0,0.17 3PZ9,TYR_318,13.48,-0.82,0.7,3.6 2RFA.GLU 100.3.75.0.22.-0.6.-0.37 3RRO.ARG 114,11,99,-0.27,0,-0.24 1DZF,ASP_159,3.92,0,-0.06,0.18 2RJD.ASP 415.4.05.0.0.25 2B0A, ASP_114, 4.15, 0, 0.04, 0.31 20EW,LYS 327,10.45,-0.05,0,0 1U7U,ASP_203,3.59,-0.56,-0.38,0.73 1UCH,LYS_72,10.27,-0.3,0,0.08 1A8Q,ASP_178,3.19,-0.83,-0.17,0.38 2X4L,LYS_218,10.3,-0.14,0,-0.06 1LTU,HIS_41,5.71,-0.89,0,0.11 3NR5,HIS_69,7.45,-0.35,0.85,0.45 2WB8,CYS 487,11.28,-0.28,-0.02,2.6 1YB2,GLU_137,4.69,0.19,0,0 1QQE,ASP 139,4.28,0,-0.08,0.55 2Z0M.LYS 179.10.76.-0.43.0.23.0.46 1NJ4,LYS_219,10.6,-1.22,0.71,0.61 3F1X,ARG_50,11.68,-2.26,0.7,0.74 3G9T,CYS_64,9.64,-1.09,-0.13,1.86 1A8Q,TYR 47,10.6,-0.02,-0.28,0.91 2GS5,ASP_172,2.99,-1.69,-0.22,1.1 3I4T,TYR_239,9.88,-0.38,-0.38,0.64 3U2R,GLU_96,4.57,0.07,0,0 1DTO,HIS 0,5.93,-0.16,0,-0.41 2AZP.ARG 152,12,98,-0.24,0.34,0.38 2G9D,ASP_18,3.53,-0.56,0.14,0.15 2RIS,ARG_106,11.26,-1.43,0,0.19 2RGY,CYS_124,9.3,0,0.02,0.28 2XHC,LYS 111,10.9,-0.77,0.67,0.5 2OJQ,ASP_572,3.95,0,-0.14,0.28 2RGY,HIS_234,7.1,-0.4,0.85,0.16 4DND,LYS_79,10.44,-0.06,0,0 3GMS,TYR_200,10.48,0,0.16,0.31 2B0J.GLU 288,3.94,0.22,-0.78,0 2EFK,GLU_119,3.44,0.42,-0.81,-0.67 3B21,GLU_141,3.99,0.24,-0.75,0 2BDV,ARG_165,12.06,-1.18,0.25,0.49 4FZR,CYS_216,12.44,-0.39,0.89,2.93 3RAZ,ARG 136,12.32,-0.42,0.0.25 4ETX,ARG_252,12.59,-0.15,0,0.24 3GS3,CYS_46,10.32,-0.01,0.23,1.11 1CBY,GLU_192,3.66,1.31,-1.01,-1.13 2CYG.ASP 230.3.12.-1.58.-0.16.1.06 3BPV,ARG_87,12.39,-0.11,0,0 3DHN,ASP_59,3.95,0,-0.03,0.18 1SNT,HIS_239,6.67,-0.92,0.85,0.23 3BCH,CYS_163,12.8,-0.06,0.03,3.84 2NRR.GLU 486.3.61.0.98.-1.36.-0.51 3JZ9,LYS_461,10.39,-0.16,0,0.04 3UX2,ASP_42,3.47,-0.46,-0.27,0.4

4EKU.GLU 220.4.61.0.1.0.0.01 3K8U,HIS 87,5.67,-1.48,0.76,-0.11 1V43,LYS_113,10.41,-0.1,0,0.01 3GA2,CYS_192,11.52,-0.75,0.13,3.15 2BOO.ASP 75.3.79.0.-0.14.0.13 1N81,ARG 185,13,73,-2,79,0,76,3,24 2F8H,CYS_102,13.74,-0.14,1.74,3.14 3CXS,ARG_181,12.45,-0.05,0,0 1QZN,ASP_99,3.31,-0.36,-0.33,0.2 3HUE,HIS_242,7.17,-0.3,0.76,0.21 1N81,ARG 70,11.86,-0.6,0,-0.03 1GXN,LYS_440,10.24,-0.37,0,0.12 2XMZ,LYS_81,10.23,-0.48,0,0.21 2IDC,LYS_168,10.23,-0.19,0,-0.08 3IPZ.GLU 162.4.97.0.26.0.0.21 3IRA,GLU_59,4.18,0.82,-0.85,-0.29 3GEC,LYS_514,9.94,-0.53,0,-0.02 1WXQ,TYR_244,13.32,0.72,0.14,2.45 2IRM,TYR_62,11.63,-0.85,-0.07,2.56 2ILR.GLU 300.3.54.0.27.-0.85.-0.38 2QHT,LYS_182,10.53,-0.21,0,0.23 3BQE,LYS_315,10.78,-0.35,0.21,0.42 1NAR,LYS_233,10.44,-0.06,0,0 4H86,LYS 81,10,67,-0,21,0,0,38 2Z0M,GLU_266,4.74,0.15,0,0.09 2Z84,LYS_198,11.47,-0.37,0.67,0.66 3ASA,ARG_69,12.33,-0.42,0,0.24 2AD1,LYS 70,9.65,-1.81,0.45,0.51 3DSH,GLU_392,4.67,0.27,0,-0.1 2CWY,GLU_34,4.88,0.25,0,0.14 1WXQ,ARG_373,12.09,-0.97,0,0.56 3UAH,GLU_467,4.95,0.35,0,0.08 2OJQ,ARG 469,12.34,-0.35,0,0.19 3F1X,ARG_293,12.41,-0.2,0,0.11 3I47,HIS_182,5.5,-1,0,0 3GFP,TYR_308,10.93,0,0.06,0.88 3IVF.ARG 277.12.43.-0.08.0.0.01 2P4D, ASP_80, 2.45, -1.84, 0, 0.48 3H5T,ASP_337,3.95,0,-0.03,0.18 2HRZ,TYR_103,10.66,0,0.06,0.6 3LD1,ARG_100,13.74,-0.36,1.13,0.47 1TJE,ASP_26,3.13,-0.85,-0.25,0.43 1G5Z.HIS 162.6.78.-0.67.0.85.0.1 1TJE,ASP_64,3.86,-0.86,0.21,0.72 1DOV,HIS_231,6.25,-0.3,0.03,0.02 1HF8,GLU_162,4.59,0.14,0,-0.04 1ZYL,LYS_292,10.44,-0.08,0,0.01 3ODJ,TYR_93,12.28,-1.12,0.45,2.95 1PBV,ARG_218,12.8,-0.29,0,0.59 3ON1,LYS_78,10.15,-0.13,0,-0.22 2XHC,LYS 230,11.08,-0.72,0.26,1.04 3CGW,ARG 208,12,4,-0,78,0,12,0,56 3EIZ,LYS_149,10.33,-0.22,0,0.06 1PSW,LYS_263,10.35,-0.34,0,0.18 3JZ9, ASP_395, 2.32, -1.18, -0.7, 0.4 4F3J,TYR_151,12.83,0.17,0.59,2.07 1RI6,GLU_189,4.74,0.25,0,-0.01 1QQE,GLU_254,4.71,0.12,0,0.1 2IRM,CYS_41,9.16,0,-0.12,0.28 1XIP,LYS 24,10.94,-0.63,0.69,0.38 2B78.TYR 124.9.1.-0.97.-2.44.2.51 2PWQ,ASP_118,3.39,-0.24,-0.36,0.19 2CXA,GLU_137,4.61,0.14,0,-0.02 2QZQ,TYR_53,11.25,0,0.41,0.84 3CBN, ASP_49, 4.14, -0.24, 0.2, 0.38 3B21,LYS 175,10.72,-0.32,0,0.54 2ZCO,GLU_264,4.66,0.2,0,-0.03 3GS3,LYS_97,10.61,-0.33,0,0.45 1R53,LYS_19,10.47,-0.04,0,0

2RFA,GLU_55,4.83,0.35,0,-0.01 2D7U,ASP 148,3,23,-0.67,-0.38,0.49 2EDM,ASP_132,3.49,-0.68,-0.07,0.43 3US6.ASP 110.3.67.0.-0.33.0.2 2ZCO.GLU 193.4.39.0.17.0.-0.28 3F7M.ARG 320,12.43,-0.07,0,0 4ESS,LYS_91,10.49,-0.46,0,0.45 2RJD,GLU_204,4.56,0.06,0,0 4FCU,HIS_220,6.25,-0.88,0.25,0.38 1X04, ASP_158, 3.82, -0.13, -0.02, 0.17 3V55,ARG_576,12.31,-0.59,0,0.4 3MIX,ARG_650,12.62,-0.08,0,0.2 3LQE,TYR_399,10.25,0,0.13,0.12 2B2H,TYR_57,10.28,-0.85,0,1.13 3RFY.TYR 333.10.66.0.1.0.38.0.17 2G70,GLU_72,4.64,0.14,0,0 1SNT,ARG_123,13.75,-0.9,0.9,1.24 1X1E,ARG_34,12.5,-0.2,0,0.2 1TD6,ASP_202,3.89,0,-0.09,0.18 3I4T,LYS 166,10.49,-0.01,0,0 3E0H,ASP_121,4.18,0,0.15,0.23 3H6O,ARG 160,11.92,-1.18,0.02,0.57 1UAJ,HIS_244,6.31,-0.32,0.08,0.05 3GYW,TYR 71,9.87,-0.31,0,0.19 3M70,TYR 218,10.39,-0.08,-0.22,0.69 4HDE,GLU_184,4.01,0.24,-0.72,0 10LR,GLU_194,4.59,0.26,0,-0.17 3PZ9,LYS_304,10.47,-0.18,0,0.16 2JHY,ASP 183,2.26,-2.27,-0.42,1.15 2OB5,GLU_98,4.87,0.58,0,-0.21 3H13,LYS_249,10.42,-0.08,0,0 2GZQ,HIS_43,6.61,-1.11,1.03,0.19 3LPZ,ASP 86,2.49,-1.69,-0.18,0.58 3EAZ,HIS 134,6,38,-0,37,0,0,25 3BQW,HIS_187,5.65,-1.02,0,0.17 3A2Z,ASP_34,3.49,-0.74,0,0.43 2Y2T,LYS_52,10.36,-0.14,0,0 3IO0,HIS 104,6.28,-0.22,0,0 3B79,GLU_58,4.17,0.32,-0.42,-0.23 3VJ8,ARG_119,12.55,-0.22,0,0.27 2ZCX,HIS_187,6.25,-0.25,0,0 1UW7, ARG 39, 12, 84, -0.51, 0.46, 0.4 1XEU.LYS 173,10.19,-0.27,0,-0.04 3GE9,HIS_75,6.13,-0.44,0,0.07 1Z9L.GLU 5.4.59.0.1.0.-0.01 3PM2,LYS_79,10.47,-0.09,0,0.06 1DVO,GLU_157,3.84,0.21,-0.91,0.05 2GS5,GLU_14,4.73,0.26,0,-0.04 2HXB,ASP_45,2.68,-1.67,0,0.55 1WXQ,GLU_184,4.93,0.31,0,0.12 1MIX.GLU 335.4.69.0.49.-0.08.-0.22 3JSN,LYS 157,10.81,-0.82,0.69,0.44 1PVT,GLU_46,4.25,0.15,0,-0.39 1X9G.GLU 81.4.69.0.29.0.-0.1 1JKS,LYS_121,10.47,-0.35,0,0.33 3CBN,HIS_104,6.32,-0.52,0,0.35 1TR9,ARG 323,12,49,-0.09,0,0.08 2W2S,HIS_74,5.65,-0.44,0,-0.41 3DTE,ASP_33,3.26,-0.85,-0.2,0.51 3LMO.GLU 26.4.0.33.-0.74.-0.09 3BJV.GLU 35,3.87,0.37,-0.65,-0.35 3AU3,CYS_520,10.57,-0.73,0.07,2.23 1Q46,GLU_98,4.85,0.3,0,0.05 307K,ARG_124,12.04,-0.58,0,0.13 3FTT,TYR_20,9.95,-0.78,-0.01,0.75 1O3X,ASP_204,3.23,-0.47,-0.36,0.25 3M7G,ARG_187,12.28,-0.3,0,0.09 3CAX,ARG 173,12.15,-0.35,0,0 1LFP,ARG_30,11.73,-1.48,0.02,0.69

3JSN,ASP 237,3.62,-0.64,-0.21,0.66 3M7G,ASP 75,3.35,-0.72,-0.14,0.41 1RI6,CYS_194,13.21,-0.12,0.79,3.54 2IQT,LYS_28,10.22,-0.11,0,-0.16 4AF2,GLU_98,3.68,0.5,-0.94,-0.38 2G70,ARG 119,12,35,-0,15,0,0 2CI3,ARG 148,13,78,-0,35,0,91,0,74 1WP5,TYR_62,12.31,0,0.09,2.22 2Z61,LYS_156,11.72,-0.78,1.11,0.89 3F1X,ASP_104,3.51,-0.33,0,0.05 1X6J,GLU 70,3.6,0.42,-0.7,-0.62 1N81,HIS 44,5,7,-1,1,0,0,3 10TM,ASP_134,2.55,-1.54,0,0.3 1IAP,ARG_158,12.13,-0.49,0,0.11 4D8L,ASP_203,3.41,-0.72,-0.21,0.54 2YLF,ASP 38,3.1,-0.51,-0.46,0.27 2I88,ASP_429,3.04,-0.85,-0.42,0.5 4EKU,GLU_101,3.68,0.83,-0.85,-0.79 4E8B,CYS_142,9.87,-0.83,-0.32,2 1R3D, ARG_14, 12.44, -0.21, 0, 0.16 2WB3,GLU_292,4.63,0.13,0,0 2X4L,ASP_100,3.94,0,0,0.14 2CYG,TYR_168,10.22,0,0.04,0.18 4ETX.TYR 195,10.3,-0.85,0,1.15 1MML,GLU 176,4.5,0.33,-0.03,-0.31 1X8F,ASP_281,4.07,-0.17,0,0.44 3VJ8,LYS_248,11.46,-0.29,0.71,0.54 3RRQ,GLU_46,3.66,0.46,-0.85,-0.45 4FH3,GLU 131,4.77,0.25,0,0.02 1NIJ,LYS_58,10.18,-0.57,0,0.25 3M66,HIS_231,6.57,-0.62,0.79,-0.1 1X8F,ARG_226,12.34,-0.27,0,0.11 4H89,ASP_112,3.5,-0.77,-0.16,0.63 2XMZ,ARG 93,9.56,-3.04,0,0.09 1BKB,CYS_30,10.81,-0.15,0.12,1.85 1C44,LYS_67,10.83,-0.49,0.55,0.27 1HUF,LYS_75,10.58,-0.37,0,0.46 300P,LYS_97,10.59,-0.24,0,0.35 2E0T.ASP 202.3.31,-0.85.0.0.36 2AD1,ARG_145,12.52,-0.21,0,0.22 2BCF,ARG_222,12.88,-0.34,0.35,0.37 3H04,ARG 117,14,-0,73,1,34,0,89 1CBY.TYR 53,10.4,0,0,0.4 2IF4,LYS_262,10.69,-0.17,0,0.35 3EVN,LYS_321,10.14,-0.36,0,0 1P2F,ARG_201,12.46,-0.09,0,0.05 4EVF,ARG 249,13.41,-1.58,1.28,1.21 3GEC,LYS 378,11.16,-0.61,0.85,0.41 1KW4,GLU_76,4.66,0.25,0,-0.08 3GW3,ARG 122,12,56,-0,35,0,0,41 1XTZ,GLU_55,4.17,0.66,-0.85,-0.14 1X1E,ASP 55,3.42,-0.82,0.04,0.41 2OSA,GLU_300,4.6,0.17,0,-0.07 2B3M,LYS_141,10.9,-0.19,0,0.6 4F85,GLU_142,4.47,0.17,0,-0.2 3CS1,LYS_59,11.05,-0.29,0.45,0.39 2FG1,GLU_136,3.66,0.46,-0.85,-0.45 3BA1,ARG_154,13.03,-0.2,0.35,0.38 3N2T,HIS 201,5,45,-0.6,0,-0.46 1H09,TYR_220,10.07,0,-0.05,0.11 1X1E,GLU 38,4.48,0.1,0,-0.13 3QAV,ASP_221,2.52,-1.44,-0.86,1.02 2R51,ARG_22,12.49,-1.45,0.86,0.58 1TLV,ASP_151,3.14,-1.08,-0.31,0.73 1RI5,ARG_158,12.62,-0.31,0.02,0.41 1Q46,LYS_105,11.03,-0.5,0.54,0.48 4H89,GLU_31,4.44,0.26,0,-0.33 1RL0,ARG_69,12.09,-0.9,0,0.49 1JYH,CYS_130,11.76,-0.22,0.24,2.75

2RJD,GLU_475,4.58,0.71,-0.41,-0.22 3O16,GLU 117,4.68,0.2,0,-0.01 2YWJ,GLU_14,4.92,0.37,0,0.04 3V3T,TYR_160,13.01,-0.2,0,3.21 3IO0,TYR_189,10.72,-0.18,-0.42,1.32 1AIL.LYS 67.10.25.-0.26.0.0.01 100X.LYS 55.10.35.-0.42.0.0.28 3B4D,ASP_170,3.04,-0.52,-0.57,0.33 2B0J,HIS_294,6.02,-0.24,0,-0.23 3ULX,LYS_129,10.6,-0.3,0.02,0.37 2P0L,ASP_22,3.24,-0.83,0,0.27 2IF4,ASP 286,3.54,-1.11,-0.96,1.82 1G8P,GLU_305,4.94,0.74,0,-0.29 2H2Z,HIS_172,5.55,-1.98,0.69,0.33 1LN4,ARG_68,12.45,-0.24,0,0.19 1P4X,GLU 125,4.48,0.13,0,-0.15 2QVO,ARG_67,12.48,-0.02,0,0 3H04,GLU_229,3.87,0.46,-0.7,-0.39 1YTD,ARG_243,11.29,-1.59,0,0.37 4H89.HIS 158.6.23.-0.35.0.0.08 3V75,GLU_111,4.58,0.24,0,-0.16 10I7,ARG_18,12.31,-0.29,0,0.09 2I88,LYS 377,10.23,-0.27,0,-1.91E-17 1ZBP.GLU 18.5.01.0.31.0.0.2 3GEC,HIS 247,6.61,-0.09,0,0.2 30KQ,ASP_568,4.15,0,0.09,0.26 3GT0,GLU_137,4,0.28,-0.77,-0.02 3F5D,HIS_117,5.27,-2.01,0.8,-0.02 2H01,GLU_146,4.53,0.26,0,-0.23 1Z9L,LYS_85,10.42,-0.07,0,-0.01 4ETX,ARG_323,12.26,-0.9,0.23,0.44 3EZ7,GLU 186,4.02,0.36,-0.83,-0.01 3CS1,ARG_88,12.59,-0.27,0,0.37 2YX0,TYR 309,12.52,-0.07,-0.72,3.31 2FD4.GLU 482.4.79.0.3.0.-0.01 3LE4,HIS_312,6.12,-0.38,0,0 2P4D,TYR_88,10.15,0,-0.15,0.3 3I47,GLU_167,3.93,0.36,-0.85,-0.08 1JYH,LYS 28,10.23,-0.32,0,0.04 30DJ,ASP_47,4.11,0,0,0.32 2FB6,ASP_5,3.75,0,-0.41,0.37 3PU6,GLU_28,4.73,0.26,0,-0.03 2WOZ,GLU 577,4.5,0.32,-0.1,-0.22 1U7U.ARG 321.12.49.-1.48.0.72.0.75 3M7G,CYS_68,12.24,-0.06,-0.59,3.89 2YWK,LYS_38,11.59,-0.27,0.82,0.55 3BPP,TYR_38,10.76,0,0.21,0.55 1ZBM,ASP_221,2.79,-1.21,-0.21,0.41 1YW5,HIS_72,3.61,-2.89,0,0.01 1NIJ,TYR_233,11.05,0,-0.26,1.32 3IV4,LYS_68,10.55,-0.11,0,0.16 1EDG,LYS_280,10.6,-0.07,0,0.17 3RFY.GLU 144,4.27,0.31,-0.37,-0.17 3GE9,ASP_125,3.49,-0.63,-0.03,0.35 3G9G,TYR_19,10.61,0,0.33,0.28 1P6F,LYS_20,10.4,-0.48,0,0.39 1ZBM,LYS_215,11.74,-0.39,0.84,0.78 1ZCE,LYS 144,10.56,-0.27,0.0.33 2XJ4,TYR_159,13,-0.85,0,3.85 3L3P,ARG_340,12.5,-0.21,0,0.21 2RIK,GLU_187,5.04,0.48,0,0.06 1BGF,ARG 110,12,41,-0,11,0,0.02 3M70,LYS_285,9.84,-0.82,0,0.15 4GCO,ARG_164,12.41,-0.21,0,0.12 1SJ8,GLU_632,5.91,1.81,-0.3,-0.1 3RJZ,LYS_141,10.34,-0.34,0,0.19 2XWS.GLU 30,3.59,0.29,-0.85,-0.35 4FD6,ARG_44,12.36,-0.14,0,0 3VJ8,GLU_261,3.2,1.84,-2.29,-0.84

2R57.CYS 332.11.41.0.0.28.2.14 3I47,LYS 195,10,43,-0.09,0,0.02 3IBT, ASP_88, 3.85, 0, -0.17, 0.22 20GQ,GLU_398,4.08,0.37,-0.73,-0.06 4FH3.GLU 329.4.58.2.69,-1.66,-0.95 2H2W,GLU 245,5.34,2.09,-0.32,-0.94 20PJ,TYR_55,10.37,0,0.13,0.24 2VGM,LYS_64,9.59,-0.59,0,-0.32 2OSA, ASP_327, 2.71, -1.53, -0.02, 0.46 20EW,GLU_273,5.3,2.07,-0.75,-0.51 2P0L.GLU 145.4.63.0.13.0.0 1J85,GLU_143,2.68,1.2,-2.4,-0.62 1ES5,LYS_124,9.85,-0.65,0,0 200K,GLU_105,4.8,0.24,0,0.06 2YX0.LYS 190.10.64.-0.14.0.0.28 2FPN,GLU_101,4.49,0.34,0,-0.35 3M66,ARG_261,11.22,-1.08,0,-0.2 2H30,LYS_104,10.56,-0.34,0,0.4 1L2F,ASP_70,3.46,-0.74,0,0.39 2RIS,LYS 46,9.87,-0.71,0,0.09 1L3K,GLU_35,4.65,0.43,0,-0.28 2Q13,ASP_122,2.59,-1.91,-0.88,1.57 3CXS,TYR_151,9.89,0,-0.66,0.55 1T6L,ARG 32,13.31,-0.39,0.82,0.38 3ETU,ASP_56,3.85,0,-0.16,0.22 3BWT,GLU_803,5.07,1.47,-0.51,-0.39 4D8L,ASP_160,3.19,-0.5,-0.33,0.22 300P,LYS 133,10.44,-0.06,0,0 3BPP,TYR_87,13.32,0,0.75,2.58 2Q5X,GLU_739,3.94,0.19,-0.75,0 2DVK,ARG_43,11.94,-0.76,0,0.19 2AZL,GLU_157,4.52,0.2,0,-0.18 1SUU,LYS 607,10.5,-0.09,0,0.08 2H85.CYS 102.10.03.-1.25.0.52.1.77 2B0J,TYR_213,11.33,0,0.42,0.91 2G9D,CYS_60,12.01,0,0.33,2.67 1WRU,ASP_95,2.83,-1.15,-0.48,0.66 3JV1,GLU_179,4.54,0.11,-0.08,0 3EUR,LYS_96,10.62,-0.13,0,0.25 3ADO,LYS_51,11.3,-0.23,0.76,0.26 4AM1,LYS_175,10.37,-0.13,0,0 2YLF,GLU 210,4.55,0.26,0,-0.2 30AV.GLU 212.4.59.0.09.0.0 1ZBM,ASP_65,3.09,-0.77,-0.33,0.39 1KCM,ASP_234,2.12,-2.42,-0.26,1.01 1L3K,LYS_52,10.4,-0.09,0,-0.01 1Q46,TYR_38,12.63,-0.51,0.99,2.16 2X4G,TYR_144,10.5,-0.12,-0.5,1.12 1FHL,TYR_295,13.22,-0.85,0.2,3.88 2OGQ,CYS_405,9.99,-0.36,0.16,1.18 1X1E,ARG 16,12.24,-0.5,0,0.23 1MML.GLU 171.4.78.0.65.0.-0.37 1FKM,TYR_466,9.59,-0.57,-0.25,0.41 1R3D,HIS_240,5.55,-3.07,0.85,1.27 2RIK,TYR_259,13.13,0,0.93,2.21 2J8A,GLU_334,5.04,0.8,0,-0.26 1TD6,TYR_75,10.24,0,0.08,0.16 1S7K,CYS_155,9.75,0,0.27,0.47 1Q8B,LYS_26,10.53,-0.22,0,0.24 3UPD,ARG 320,10.27,-2.85,0,0.61 1ZP2.LYS 154.10.53.-0.09.0.0.12 3AUF,GLU_-8,4.25,0.77,-0.57,-0.44 2APL,HIS_55,6.59,-0.38,0,0.47 1EDG,ARG_208,11.26,-2.34,0.38,0.72 1YIB,LYS_220,10.23,-0.27,0,0 3JZN,GLU 325,4.86,1.13,-0.54,-0.23 3TMO,GLU_204,4.69,0.5,-0.06,-0.24 1WYC,GLU_41,3.66,2.04,-1.24,-1.64 1DZF,ARG_155,12.38,-1.81,0.75,0.94 3M7G,ARG 151,13.04,-2.16,1.53,1.16 3PAC,LYS 161,10.28,-0.72,0.0.5 4AF2,GLU_140,4.39,0.31,-0.38,-0.04 3M3P,HIS_248,6.15,-0.35,0,0 208P.ARG 11.13.78.-1.08.1.51.0.86 1GPP.GLU 415.3.95.0.29.-0.54.-0.31 1XTZ.LYS 155,10.63,-0.15,0.0.29 2QRX,ASP_164,3.03,-0.93,-0.32,0.49 2RJD,CYS_205,8.89,-0.22,0,0.11 1ZBM,ASP_64,3.9,-0.5,0.03,0.58 3EJG,LYS_158,10.69,-0.23,0,0.42 3CS1,LYS_22,10.68,-0.34,0,0.52 3F7M,HIS 119,5.87,-0.99,0.35,0.01 1RI6.TYR 103.10.96.0.0.21.0.73 2ZTY.ARG 33.12.36.-0.28.0.0.14 3EIZ,LYS 147,10,49,-0.02,0,0.01 1ZBM,LYS_249,10.9,-0.12,0.19,0.34 2R51,ARG_95,12.44,-0.06,0,0 3IL3,ARG_151,12.54,-0.23,0,0.27 2WB8,GLU 541,5.68,1.42,0,-0.24 2Q12,TYR_190,10.03,0,-0.08,0.11 200K,ARG_321,10.47,-2.14,0,0.11 3M70,GLU_200,4.54,0.29,0,-0.25 1DTO,ARG 7,12.38,-0.23,0,0.11 30KY,ARG 114,12,42,-1,22,0.09,1.06 3CN5,ASP_191,2.9,-0.85,-0.45,0.4 2P0Y,LYS_12,10.54,-0.21,0,0.25 2P52,LYS_136,10.33,-0.17,0,0 4E9E,TYR_530,11.51,0.85,0.24,0.42 2EEY,HIS 20,6.38,-0.12,0,0 1SJY,ASP_114,3.66,-0.12,-0.14,0.11 1X8F,ASP_16,3.84,-0.32,-0.3,0.65 3KEY,ASP 469,3.83,0,-0.34,0.37 3IV4,ASP 92,3.21,-0.85,-0.32,0.59 3ELI,LYS_26,9.77,-1.05,0,0.32 1WRU,GLU_266,3.86,1.18,-0.5,-1.33 1BKB,GLU_34,4.47,0.27,0,-0.3 2P65,ARG 27,12.2,-0.75,0,0.45 3N0K,LYS_13,10.14,-0.33,0,-0.02 2RIK,CYS_74,8.8,-3.6,0.47,2.92 3CIV,ARG_237,12.24,-0.4,0,0.14 2FC3.GLU 21.4.24.0.43.-0.22.-0.49 1RZ2,ARG 68,12,21,-2,1,0,71,1,1 1IAP,ARG_161,13.16,-1.13,1.11,0.68 1UXO,GLU_169,3.98,1.16,-1.46,-0.21 1WXF,LYS_193,9.5,-0.97,0,-0.02 3VJ8,LYS 45,10.3,-0.21,0,0.01 3BCH.CYS 148,13,46,-0,1,0,69,3,87 3IO0,GLU_175,4.83,0.49,0,-0.15 2NRK,TYR_88,11.52,0,-0.32,1.84 2EFK.GLU 37.4.65.0.28.0.-0.14 2WB3,TYR 340,10,4,0,0.08,0.32 1X04,GLU_220,4.52,0.19,0,-0.17 2XMZ,LYS_205,10.14,-0.36,0,0 1UJ8,ARG_39,13.29,-0.18,0.59,0.38 1SUU,ARG_771,12.56,-0.2,0,0.28 3KB5,ASP 459,3.61,-0.42,-0.72,0.94 3IVF,LYS_58,11.08,-0.17,0.24,0.52 1QQL,GLU_60,4.89,0.31,0,0.07 1TR9,ARG_18,12.22,-0.34,0,0.06 1WXF,GLU_20,4.69,0.21,0,-0.02 3EUR,TYR_30,10.49,0,0.11,0.39 2JHY,GLU_106,2.22,0.63,-2.26,-0.64 4F85,GLU_266,4.14,0.79,-0.82,-0.32 2GS5,TYR_45,10.29,0,0.19,0.1 1GXN,ARG_481,12.97,-0.61,0.73,0.35 3ETU,TYR_97,11.88,-0.03,-0.11,2.02 3CAX,ARG 158,12.36,-0.59,0,0.45 2H2Z,TYR_118,10.28,-0.86,0.11,1.04

3ASA.GLU 194.4.38.0.14.0.-0.26 1GQE,TYR 24,10.12,0,-0.24,0.36 1J7G,LYS_116,10.53,-0.18,0,0.21 1PSW.GLU 346.4.48.1.72.-0.71.-1.04 1Y2Q,ARG_32,13.18,-0.28,0.49,0.47 2APL, ARG 84, 13.33, -0.22, 0.39, 0.65 2YT4,TYR_597,10.49,0,0.02,0.47 2OB5,ASP_6,1.83,-2.33,-0.66,1 4DEZ,ARG_129,12.37,-0.69,0.01,0.54 3BWT,GLU_818,3.7,0.65,-1.09,-0.36 1ZBP,GLU 267,4.96,0.18,0,0.29 2YWK.GLU 6.3.64.0.46.-0.99.-0.32 2ILR,LYS_478,11.34,-0.24,0.67,0.41 1PV5,HIS_204,6.52,-0.5,0,0.53 208P.GLU 44.4.73.0.23.0.0 1CHD,HIS 224,6,4,-0.86,0,74,0.02 1QQE,GLU_35,3.57,0.31,-0.85,-0.4 1Q2Y,LYS_116,10.39,-0.11,0,0 2CN1,ARG_45,12.29,-0.92,0,0.72 4EKU,GLU 182,4.84,4.64,-1.49,-2.81 4EVF,LYS 18,10,27,-0,22,0,-0,01 1H09,ASP_205,3.27,-0.96,-0.25,0.69 3LJC,ASP_61,3.83,-0.05,-0.12,0.2 1X1E.LYS 62,10.63,-0.09,0.0.22 20G0.GLU 401.5.03.0.57.0.-0.04 3H13,GLU_461,3.7,0.33,-1.12,0 20RX.ARG 117.12.22,-0.71.0.0.43 3KV0,ARG_112,11.43,-1.1,0,0.03 2NYC,ASP_312,4.26,0,-0.2,0.65 2RIK,GLU_133,4.77,0.18,0,0.09 2H2W,GLU_117,4.75,0.22,0,0.03 4DEZ,ASP_117,3.39,-0.32,-0.26,0.16 4DND.GLU 66.4.75.0.14.0.0.11 3L3P.ASP 505,3.95,0,0,0.15 1F2V,ARG_191,12.28,-0.26,0,0.05 3NBI,GLU_36,4.68,0.18,0,0 3V1Q,ARG_560,12.56,-0.39,0,0.45 3M7G,GLU_161,3.49,0.68,-1.07,-0.61 1LPL/ARG 212/12/01/-0.67/0/0.18 3I4T,TYR_3,10.63,0,0.23,0.39 3R2E,GLU_33,4.51,0.69,-0.42,-0.25 1PBV,TYR_235,10.71,0,-0.02,0.73 1PBV,TYR 186,11.98,0.84,0.5,0.63 10XZ,ARG_265,12.35,-0.16,0,0.01 1UW7,ARG_111,12.43,-0.07,0,0 2GYZ,ASP_24,3.92,0,-0.08,0.2 3I4T,ARG 220,12.27,-0.8,0.06,0.51 3K8U,TYR_37,10.43,0,0.14,0.29 1AD6,GLU_533,4.46,0.19,0,-0.23 3HUE,ASP_194,2.96,-1.17,-0.23,0.57 1SI7,ASP_221,2.9,-1.12,-0.38,0.6 2FB6,ASP 76,4.27,0,0.13,0.34 3ERF,LYS 223,10.33,-0.18,0,0.02 2WB3,ARG_268,12.45,-0.05,0,0 3V75,HIS_182,5.52,-0.88,0,-0.11 2AD1,ASP_185,3.71,-0.03,-0.35,0.29 20K1.ARG 497.13.26.-0.37.0.73.0.4 1XTD,ASP_131,3.18,-0.85,-0.29,0.52 1WXF.ARG 140.12.06.-0.59.0.0.16 1TWU,TYR_84,10.69,0,0.21,0.47 2FC3,GLU 113,3.58,0.31,-0.85,-0.38 20ZO,LYS 115,10,4,-0,1,0,0 4EZB,CYS_64,9.3,-0.03,0.1,0.24 1FQI,HIS_391,6.46,-0.63,0.19,0.4 2IXM,LYS_249,10.47,-0.1,0,0.06 1YTD, ASP_19, 3.44, -0.78, 0, 0.42 3N2T,GLU 74,3.75,0.37,-0.61,-0.5 4GCO,GLU_152,4.23,0.23,-0.16,-0.34 1L2H,CYS_71,11.35,-0.85,0,3.2

2W0G,GLU_184,5.19,0.84,-0.02,-0.13 1SNT,CYS 272,12.14,-0.11,-0.52,3.77 2H2W,HIS_182,4.89,-2.37,0.65,0.11 208P,TYR_180,9.99,0,-0.2,0.19 4DNU,ASP_192,4.26,0,-0.02,0.49 2XMZ,LYS 225,10.08,-0.25,0,-0.18 1K95.ARG 75.12.57.-0.3.0.0.37 2FPN,ASP_69,2.48,-1.8,-0.1,0.58 3GS3,HIS_210,6.18,-0.44,0.08,0.04 3B7X,GLU_23,2.24,0.36,-2.13,-0.48 3CRM,ARG 80,12,11,-0,39,0,0 1M5I,ASP_147,4.04,0,-0.31,0.55 1WXF,TYR_185,11.44,0,0.37,1.07 3ZXY,GLU 191,4.62,0.22,0,-0.1 1SI7,ARG_335,11.78,-2.19,0,1.47 1UAJ,ARG 114,13,-0.93,0.71,0.73 3NR5,HIS 0,5.61,-0.25,0,-0.65 3RLN,ARG_751,13.3,-0.53,0.72,0.61 1KN3,GLU_36,4.57,0.17,0,-0.1 2EHG,LYS 93,10.3,-0.2,0,0 3VJ8.TYR 339.10.44.0.-0.22.0.66 1R7J,TYR_40,10.22,0,-0.25,0.47 3GE9,LYS 218,10.93,-0.27,0.3,0.41 100X.GLU 79.4.56.2.87.-1.65.-1.17 2D7U,ASP 168,3.47,-0.31,-0.39,0.38 4E8B,ARG 74,13.63,-0.29,0.98,0.44 2XMZ,HIS_33,5.84,-2.86,1.37,0.83 1I60,HIS_59,6.69,-0.3,0.26,0.23 3M7D,ARG_231,13.47,-1.56,1.57,0.96 2ZCX,ASP_195,2.54,-1.73,0,0.47 3M16,HIS_159,7.45,-0.81,0.95,0.8 2CL3,ASP_72,4,0,-0.08,0.28 1BYI,HIS_164,6.34,-0.16,0,0 3M7D,ASP_160,4.05,0,0.05,0.2 3E5T,ARG 10.12.64,-0.11.0.0.24 3GS9,GLU_195,4.5,0,0,0 2RGY,ASP_225,3.91,-0.48,-0.24,0.82 1TLV,HIS_237,6.49,-0.15,0,0.13 2EJB,ARG 118,12.4,-0.11,0,0.01 1OXZ,LYS_250,10.1,-0.23,0,-0.17 3LOD, ASP_141, 3.99, 0, 0, 0.19 3I4T,TYR_187,11.5,0,0.15,1.35 1XEU,GLU 284,4.66,0.16,0,0 2BV9,ASP 78,3,77,-0.66,-0.19,0.81 2YT4, ARG_670, 13.31, -0.15, 0.62, 0.34 2IQT,GLU_129,3.12,0.71,-1.62,-0.48 2Q98,HIS_97,6.16,-0.75,0,0.4 1SQW,GLU_123,4.6,0.17,-0.03,-0.04 2YYO,GLU_26,3.67,0.46,-0.83,-0.47 2A0J,LYS 53,10.32,-0.29,0,0,11 1XWM,TYR_159,10.97,0,0.24,0.74 3GOZ,LYS_249,11.2,-0.21,0.53,0.38 3IV4.TYR 65.11.14.0.61.0.04.0.48 2V5B,LYS_157,10.51,-0.07,0,0.08 2HXB,LYS_6,11.17,-0.16,0.35,0.49 3GA2,TYR_233,10.85,0,0.12,0.73 1DVO,TYR_133,11.35,-1.02,-0.39,2.75 3EAZ,HIS 84,5.82,-1.57,0.85,0.04 20EW,CYS_127,13.1,-0.1,0.33,3.87 3Q6L,LYS_101,10.33,-0.27,0,0.1 3V3T,TYR_68,9.98,0,-0.17,0.15 106D.GLU 107.4.52.0.1.0.-0.08 3V75,GLU_69,3.16,0.71,-1.55,-0.5 3M3PARG 227,13.33,-0.37,0.81,0.39 2ZCO,TYR_214,10.43,-0.09,-0.08,0.6 1DOV,LYS_120,11.16,-0.44,0.85,0.26 1EYH.ARG 124.12.99.-0.48.0.53.0.43 3HUE,TYR_319,10.3,0,0.21,0.09 1RI6,CYS_131,12.29,-0.56,0.26,3.6

3RLE.GLU 24.4.47.0.12.0.-0.15 1AD6.ARG 445.10.84.-1.7.0.0.04 2BDD,CYS_33,8.55,-0.82,-0.1,0.49 4FZR,HIS_84,5.19,-0.93,0,-0.37 3H13.GLU 434.3.99.0.47,-0.67,-0.32 1X04,GLU 170,4,59,0,23,0,-0,14 4FD6,LYS_145,9.68,-0.71,0,-0.11 1X04,LYS_150,10.21,-0.31,0,0.02 3COU,GLU_91,3.34,0.44,-1.21,-0.39 2IDC,ARG_148,12.24,-0.26,0,0 20DJ.GLU 54,4.13,0.48,-0.59,-0.27 1ANU,LYS_98,11.49,-0.31,0.74,0.57 1GQE,HIS_281,6.34,-0.32,0,0.17 4F85.GLU 279.4.82.0.24.0.0.08 30N1.LYS 51.11.18.-0.4.0.52.0.55 2FM9,ARG_100,12.4,-0.39,0.09,0.2 3ADO,GLU_97,3.81,1.92,-1.72,-0.89 3QKY,TYR_214,12.46,0.45,0.44,1.56 3EX9,GLU_137,4.72,0.91,0,-0.7 1ZCE,LYS 49,10.03,-1.0.12,0.41 1Y2Q,ASP_96,4.07,-0.08,-0.41,0.75 1R3F,ASP_186,4.94,0,0.13,1.02 3N2T,ARG_7,12.35,-0.17,0,0.02 1QYI,TYR 276,10.69,0,0.33,0.37 4F3J,ARG_110,11.16,-1.63,0,0.29 1X9G,GLU_58,5.13,1.3,-0.74,0.07 1QQL,HIS_124,6.24,-0.23,0,-0.03 2BQQ,TYR 58,10.91,-0.08,-0.31,1.3 3A2Z,GLU_61,4.19,4.25,-2.95,-1.6 2AD1,HIS_109,2.61,-3.37,0,-0.52 1XIP.GLU 320.4.84.0.36.0.-0.02 3GYW,TYR_259,10.35,0,-0.04,0.39 2YWJ,ASP 149,3.53,-0.23,-0.23,0.2 3GMS,TYR 22,9.67,-0.3,-0.3,0.27 4H4J,LYS_182,9.86,-0.68,0,0.03 4E8B,GLU_53,3.69,0.33,-0.72,-0.41 1GXN.TYR 575,11.6,-0.83,-0.14,2.57 4AM1,LYS 189,10.38,-0.12,0,0 1SUU,ARG_520,11.93,-0.57,0,0 1T6L.GLU 138.4.5.0.0.0 2WB3,LYS_306,10.48,-0.02,0,0 1U7U,LYS 318,10.33,-0.12,0,-0.05 1WOU,LYS_78,10.33,-0.16,0,0 1LTU,ASP_79,3.36,-0.91,-0.29,0.75 2FZ4,GLU_66,4.37,0.51,-0.39,-0.26 3ADO,ASP_114,2.65,-1.44,-0.41,0.69 1X1E,LYS_160,10.55,-0.12,0,0.17 3BQW,LYS_251,9.54,-0.78,0,-0.18 4H86,GLU_80,4.54,0.15,0,-0.12 3HQX,LYS_13,10.46,-0.04,0,0 3TOW, ASP 83, 3.51, -0.75, -0.13, 0.59 2VGM,GLU 234,3.5,0.89,-1.35,-0.54 3GG6,TYR_72,11.76,0.04,-0.34,2.07 3GT0,LYS_48,11.26,-0.24,0.62,0.39 3F5D,LYS_50,10.4,-0.1,0,0.01 4DEZ.HIS 7,4.66,-2.93,0.85,0.23 2Q13,TYR_161,10.77,0.01,0.5,0.27 1U3Y,ARG_281,12.86,-0.96,0.8,0.52 3TIR,ARG_89,12.51,-0.07,0,0.08 2H14,HIS 310,4.67,-1.91,0,0.07 2FXT.ASP 336.3.8.0.-0.26.0.26 1SI7,TYR_9,10.76,0,-0.33,1.09 4ESS,ARG_159,12.74,-0.79,0.77,0.27 3LE4,GLU_301,4.79,0.33,0,-0.04 4FCU,GLU_81,3.74,1.15,-1.43,-0.47 2AXO,TYR 114,11.25,-0.27,-0.18,1.71 3RFY,LYS_378,10.15,-0.34,0,0 1Y0K,GLU_75,4.29,0.5,-0.28,-0.43 2OSA,LYS_275,10.33,-0.19,0,0.02

4EVF.ASP 53.2.34,-1.72,-0.81,1.07 1PGV.ARG 255,12,47,-0.26,0,0.23 2Q34,LYS_226,10.47,-0.16,0,0.13 2E3H,ARG_298,12.24,-0.41,0,0.15 3S0A,TYR_46,12.61,0,0.17,2.43 3ANJ.HIS 113.5.27.-0.86.0.-0.36 3CE7.GLU 45.5.02.0.5.-0.03.0.05 1FQI,GLU_419,4.53,0.09,0,-0.06 1TUL,ASP_31,3.73,-0.16,-0.27,0.35 1TWU,LYS_134,10.42,-0.08,0,0 2FD5,ARG_115,12.38,-0.25,0,0.12 2DG7,GLU_9,4.83,0.64,0,-0.31 3PM2,TYR_67,10.76,-0.79,0.51,1.04 1M5I,ASP_209,3.08,-1.01,-0.3,0.58 2ZTY.GLU 71,5.88,1.68,0,-0.31 1YB2,ARG 145,12,45,-0.11,0,0.06 4AM1,TYR_203,10.14,0,-0.16,0.3 200K,HIS_24,6.13,-0.98,0.21,0.41 3D9H,ASP_224,3.41,-0.81,-0.05,0.47 2NMU,GLU 117,3.96,2.27,-2.14,-0.68 204D,ARG_112,13.44,-0.25,0.65,0.54 2P4D,LYS 130,10,43,-0.07,0,0 3R2E,ASP_31,3.59,-0.75,-0.25,0.79 1RSS,TYR 18,12.15,0.4,0.82,0.94 4EUG,ARG 179,13.6,-0.49,1,0.59 2H85,HIS_95,4.33,-2.26,0,0.09 3PM2,LYS_119,10.5,-0.07,0,0.06 1Z3X,ASP_204,2.57,-1.6,-0.04,0.42 30DJ.HIS 65,5.02,-1.43,0,-0.05 1Y0K,ARG_31,12.67,-0.83,0.57,0.42 2P0L,GLU_76,4.97,0.38,0,0.09 3JSN,ASP_186,3.96,0,0,0.16 3T57,GLU_245,4.18,0.24,-0.48,-0.08 10XZ.GLU 220.4.26.0.4.-0.34.-0.3 3JSN,LYS_155,10.99,-0.36,0.06,0.79 3L3P,HIS_355,6.51,-0.22,0,0.23 2D2S,ASP_651,3.99,0,0,0.19 1TXD,GLU 866,3.51,0.28,-0.85,-0.41 3A0X,TYR_680,10.07,0,0.02,0.05 2WB8,ASP_707,3.92,-0.62,-0.18,0.91 3T8R,ASP_113,4.12,0,0.07,0.26 3EJC,LYS 38,10,45,-0.05,0,0 3ETV.GLU 63.4.5.0.33.0.-0.32 200K,GLU_208,5.56,1.44,0,-0.38 1TLV,GLU_255,4.59,0.09,0,0 3GMS,ASP_106,3.99,-0.18,-0.04,0.41 3GS9,ASP_101,3.36,-0.42,-0.31,0.29 2AZL.GLU 266.3.78.0.49.-0.8.-0.41 1K95,GLU_67,4.84,0.32,0,0.02 1PGV,GLU_350,4.64,0.23,0,-0.09 2EYI, LYS 79, 10.3, -0.1, 0, -0.1 2A1V,LYS 118,10,34,-0,11,0,-0,04 2I88,TYR_396,13.08,0,0.3,2.78 300P.LYS 115.10.41.-0.09.0.0 20BI,LYS_20,10.38,-0.12,0,0 20KT,LYS_2,10.48,-0.16,0,0.14 2YWJ.GLU 17.4.35.0.27.0.-0.42 3C5V,ARG_222,12.63,-0.24,0,0.37 2RH3,LYS_148,10.42,-0.08,0,0 1XEU,CYS_141,9.45,0,0.07,0.38 2W0G,HIS_211,4.32,-2.27,0.78,-0.69 2Q98,ARG_129,11.74,-0.66,0,-0.09 1Q8B,LYS_21,10.57,-0.16,0,0.23 1IAP,HIS_80,4.78,-2.55,0.83,0 3E0H,ASP_122,3.91,0,-0.15,0.26 1X91,ASP_61,1.93,-2.34,-0.06,0.52 2HXB,LYS_15,10.31,-0.14,0,-0.05 3H5T,GLU_77,5.86,4.02,-1.46,-1.21 2XMZ,GLU_60,4.68,0.25,0,-0.07

2PGE,ASP_95,3.87,0,-0.12,0.19 2P65,ASP 85,2.37,-2,0,0.57 3GW3.LYS 15.10.34.-0.11.0.-0.06 2G9D,GLU_306,4.65,0.15,0,0 3UV9,TYR_401,11.42,0,0.32,1.1 105J.LYS 42.10.41.-0.09.0.0 3ZSL,ARG 162,12,44,-0.83,0.42,0.36 3DSH,ASP_309,4.19,0,0.18,0.2 3LD1,CYS_60,9.72,-0.08,0.01,0.79 2BDD,GLU_152,4.71,0.12,0,0.09 3Q6L,LYS_108,11,-0.37,0.25,0.62 3M16.GLU 275.4.55.0.24.0.-0.19 1R53,ARG_337,12.45,-0.05,0,0 1MJS,GLU_305,3.87,0.38,-0.85,-0.16 2ILR.CYS 345,12,32,-0.01,-0.06,3,39 2YX0, ARG 283, 12, 44, -0, 13, 0, 0, 07 1ANU,LYS_128,10.42,-0.08,0,0 3I82, ASP_170, 3.93, 0, 0, 0.13 2RIS,LYS_16,10.38,-0.47,0,0.35 2GKG,ASP_55,3.26,-0.75,-0.38,0.59 3NR5,ASP 124,3.03,-0.85,-0.48,0.56 1MTZ,GLU_97,4.2,1.07,-0.85,-0.51 3LQE,ARG_431,11.44,-2.51,0.42,1.01 3RE9.TYR 239.11.53.0.36.0.59.0.58 2DG7.GLU 18.4.74.0.34.0.-0.1 3RFY,LYS_189,10.66,-0.14,0,0.3 4DVD,LYS_139,10.47,-0.03,0,0 3BPV,ARG_44,12.2,-0.2,0,-0.1 1DOV,ARG_129,12.33,-0.17,0,0 2E3C,GLU_218,4.61,0.19,0,-0.08 2V4U,ARG_453,11.74,-0.98,0.1,0.12 3IL3,GLU_170,4.52,0.09,0,-0.08 1UXO.GLU 111.3.1.0.64,-1.66,-0.38 2PLQ,ASP 68,3.22,-0.9,-0.06,0.39 2GZQ,TYR_153,11.6,0.81,0.17,0.63 3PAC, ASP_66, 3.85, -0.05, -0.06, 0.17 2R51,LYS_143,10.64,-0.25,0,0.4 2WOZ,HIS_337,4.76,-2.34,0.56,0.04 2P5D,TYR 65,12,58,0,0,3,2,28 2BLL,GLU_397,4.35,0.44,-0.32,-0.28 2BV9,GLU_238,4.18,0.46,-0.44,-0.34 2D8N.TYR 32,10.74,0.0.03,0.71 2BOO.TYR 64,10.02,0,-0.12,0.13 2BT8,ASP_283,3.8,0,-0.28,0.28 3FFM,GLU_159,5.24,0.43,0,0.3 2IRM,GLU_345,4.71,0.17,0,0.04 1QQH,ASP 126,3.97,0,0,0.17 4ACJ,ARG_657,13.6,-0.93,1.38,0.66 4FLE,TYR_116,11.96,-0.05,0.07,1.94 1X1E,HIS 101,1.88,-2.85,0.81,-2.57 2BQQ,ASP_93,2.09,-1.85,-0.4,0.54 3M66,LYS 415,10.49,-0.1,0,0.09 3MTT,ASP_566,3.68,-0.11,-0.3,0.3 4EVF,TYR_214,11.45,0,0.31,1.14 3RJZ,TYR_22,10.22,0,-0.32,0.54 3HKX,ASP_44,4.41,0,0.1,0.52 3KB5,HIS 337.6.28,-0.59,0.02,0.34 4FH3,ASP_254,3.87,-0.28,-0.1,0.44 1KCM,LYS_105,10.54,-0.13,0,0.17 3DSH,ARG_247,12.26,-0.36,0,0.11 1SUU,ASP 763,3.08,-1.49,-0.55,1.32 1V43.HIS 343.6.11.-0.39.0.0 2H14,GLU_151,5.27,0.45,0,0.32 3AU3,GLU_477,4.87,1.22,-0.81,-0.05 3ZTA, ASP_113, 3.22, -0.53, -0.53, 0.49 2C2Y,HIS_215,5.82,-0.53,0,-0.15 2WB8,CYS_467,12.29,0,0.39,2.9 2B2H,LYS 292,10.35,-0.15,0.0 2QVT,GLU_79,3.56,0.43,-1.05,-0.33

3F1X,HIS_30,5.73,-0.45,0,-0.32 3IBT,TYR 212,11.8,0,-0.08,1.88 2JEO,LYS_58,10.53,-0.14,0,0.17 1JKS,ARG_54,12.36,-0.14,0,0 1YR6,LYS_80,10.48,-0.39,0,0.38 1MTZ,ASP_187,3.91,0,-0.01,0.13 4AM1.LYS 38.11.35.-0.38.0.85.0.38 1N81,TYR_125,11.27,0,0.11,1.17 1KCM,ARG_147,13.07,-0.49,0.28,0.78 2A6B,LYS_83,10.12,-0.17,0,-0.21 3FS3,ARG_268,13.06,-0.32,0.19,0.68 1YTD, ASP_216, 3.77, -0.52, -0.13, 0.62 1QQL,ARG_47,12.69,-0.4,0.04,0.55 2013.LYS 212.10.43.-0.08.0.0.01 105T,ARG_318,12.55,-0.23,0,0.28 1AD6,ARG 556,12.48,-0.29,0,0.27 1S7K.TYR 166.10.26.0.0.02.0.25 2EJX,CYS_40,10.83,0,0.28,1.55 3CAN,CYS_77,9.66,-0.42,-0.37,1.45 1AM2,GLU 155,5,52,1.63,-0.12,-0.5 1FKM.LYS 407.10.26.-0.52.0.0.28 3BCH,ARG_120,13.49,-0.28,0.8,0.48 2Q99,TYR_169,12.41,0.85,0.03,1.53 4AF2,ARG_66,13.4,-0.44,0.94,0.4 2IF4.HIS 73.5.72.-0.93.0.0.15 3IO0,TYR_249,10.36,0,0,0.36 3UX2,GLU_64,4.97,0.32,0,0.14 1X7F,ASP_61,3.78,0,-0.33,0.32 3RLE,ARG 30,12.22,-0.28,0,0 4E9E,ARG_512,11.01,-1.42,0,-0.07 3AUF,ARG_104,12.15,-0.52,0,0.17 2IRM,HIS 175,6.37,-0.49,0.09,0.26 2E0T,ASP_135,3.22,-0.85,-0.19,0.46 3CGW,GLU 24,4.08,0.37,-0.53,-0.27 3CE7.GLU 96.3.71.0.41.-0.85.-0.35 1Q5Z,GLU_573,4.02,0.59,-0.85,-0.22 3BCY,LYS_112,10.1,-0.47,0,0.07 1DCF,HIS_49,6.28,-0.39,0.03,0.15 1J33,LYS 18,10.76,-1.08,0.79,0.55 2IF4,ASP_281,3.76,-0.31,0.03,0.25 30KO.GLU 654,4.84,0.21,0.0.12 3NZL,CYS_66,10.03,-0.03,0,1.06 2OSA, ARG 403, 12.52, -0.32, 0, 0.34 3B21.GLU 29.4.68.0.21.0.-0.03 1UOH,GLU_225,3.9,0.39,-0.79,-0.19 1RAJ,LYS_200,10.39,-0.11,0,0 2P0Y,TYR_78,10.12,0,0,0.12 2GZR,HIS_66,7.3,-0.35,0.85,0.3 2FL7,CYS_177,12.21,0,0.16,3.05 3QKY,TYR_50,10.1,-0.33,0,0.43 3B7X,CYS_123,9.61,0,0,0.61 3BB7,CYS_227,13.36,-0.01,0.43,3.94 3IU5,TYR 126,9.81,-0.78,0.24,0.34 2FBQ,ASP_185,4.06,0,0,0.26 1PDB,ARG_91,11.97,-0.53,0,0 2OSA,TYR_357,9.39,-0.72,-0.44,0.55 4F3J,LYS_170,10.31,-0.63,0,0.43 1N81,HIS 28.6.26.-0.56.0.0.32 3CBN,CYS_124,6.66,-3.02,-0.63,1.3 2E3C,TYR_235,10.06,0,0,0.06 3DZ1,ARG_299,12.85,-0.18,0.15,0.37 1IDK.ASP 324.3.75,-0.27.0.0.22 1DVO,HIS_117,5.64,-0.42,0,-0.43 1T3Y,ARG_73,12.34,-0.19,0,0.03 3AU3,ARG_653,12.11,-0.42,0,0.04 2QK1,LYS_428,10.2,-0.3,0,0 1SFE,ARG 105,11.83,-0.67,0.0 208P,LYS_151,10.5,0,0,0 2GZQ,GLU_103,4.51,0.23,-0.01,-0.21

1S7K.ARG 52.12.63.-0.27.0.06.0.33 3IVF,ASP 369,3.05,-0.92,-0.46,0.62 3BPP,ASP_61,4.46,-0.46,-0.2,1.32 3HZQ,GLU_7,4.67,0.17,0,0 1X7F.GLU 258.4.4.0.21.0.-0.31 3L3P.GLU 359.4.35.0.16.0.-0.31 1GQE,ARG_337,13.2,-1.99,1.42,1.26 3P2F,GLU_18,3.47,0.77,-1.24,-0.57 1TR9,ARG_77,11.03,-1.04,0,-0.43 20BI,GLU_16,4.04,0.43,-0.88,-0.01 1T07,HIS 11.6.8,-0.23,0.45,0.07 3F1X,GLU_183,3.89,0.68,-0.58,-0.71 3CAN,GLU_165,4.45,0.13,-0.18,0 3O48,GLU_71,3.8,0.31,-0.68,-0.33 2B2H,LYS 294,10.57,-0.21,0,0.28 2D59,GLU_47,4.49,0.34,0,-0.36 3F5D,TYR_193,11.39,0.3,0.49,0.61 2V4X,GLU_72,3.96,0.63,-0.81,-0.36 2VGM,GLU_310,3.61,0.34,-0.85,-0.38 3T5B,LYS 293,9.99,-0.63,0.0.12 3H04,ASP_196,3.41,-0.83,0.09,0.35 1PSW,LYS_195,9.8,-1.07,0,0.37 3LMF.GLU 95,4.16,0.27,-0.64,0.04 2RGY,CYS 272,12.52,0,0.13,3.39 2NYC, ASP_299, 1.79, -2.37, -0.38, 0.72 1HUF,ARG_14,12.21,-0.29,0,0 3LPZ,ARG_290,12.62,-0.27,0,0.39 1ZP2,ARG 97,12.05,-0.22,0,-0.23 3ETU.GLU 322.4.56.0.29.0.-0.23 2WB8,ARG_552,12.6,-0.55,0.29,0.36 1XKR,GLU_156,5.25,1.73,-0.46,-0.51 2Z84,HIS_120,6.1,-0.41,0,0 3IV4,ARG 60,12.22,-0.37,0,0.09 3EVN,LYS 281,10.66,-0.49,0.13,0.52 3TIR,GLU_39,4.3,0.75,-0.79,-0.15 3G9G,GLU_96,4.37,0.57,-0.85,0.15 3B79.LYS 61,10.7,-0.13.0.0.34 2HP7.ARG 53.12.42.-0.12.0.0.03 4GA2,LYS_78,11.74,-0.28,0.68,0.83 2WB8,ASP 589,3,42,-0,8,0,0,42 1GPP,GLU_428,3.98,0.24,-0.81,0.05 1A80.ASP 222,2.26,-2.02,-0.38,0.87 2E3S.GLU 450.3.65.0.37.-1.1.-0.12 3PU6,GLU_72,4.61,0.3,-0.16,-0.03 3M70,TYR_248,11.22,0,0.25,0.98 3BQE,GLU_325,3.6,0.92,-1.14,-0.67 2BT8, ASP_252, 3.81, -0.78, -0.14, 0.94 2FC3,GLU 55,5.66,1.11,0,0.05 3VJ8,CYS_147,12.64,0,0.03,3.61 1V43,ARG_68,13.9,-0.23,0.8,0.83 1LFP,GLU 149,4.4,0.33,-0.11,-0.31 2YLF.ARG 89,11.99,-0.5,0,0 200K,GLU_50,4.55,0.5,0,-0.44 3I0C, ARG_337, 12.08, -0.37, 0, -0.05 3CO1,LYS_95,10.71,-0.15,0,0.36 3DB9,ARG 94,12.18,-0.95,0.26,0.36 2OB5,LYS_105,10.49,-0.15,0,0.14 3BA1,ARG_232,11.75,-1.92,0.2,0.97 3M66,GLU_400,4.88,0.3,0,0.08 3B4D,HIS 191,5.4,-1.1,0,0 1DOV,ASP_205,4.07,0,0,0.26 3TMO,HIS_334,6.83,-0.2,0.47,0.07 3M66,LYS_171,10.35,-0.12,0,-0.03 2GEN,CYS_178,9.68,0,0.11,0.57 3E7P,LYS_113,10.64,-0.13,0,0.27 1YM5,LYS 108,10.35,-0.25,0,0.1 1XKR,LYS_32,11.15,-0.63,0.85,0.43 4AE7,HIS_221,7.31,-1.5,1.7,0.61 2P5D,GLU_13,2.7,0.63,-1.57,-0.86

3T5B,ARG_119,12.41,-0.46,0,0.37 1XTZ.LYS 151.11.26.-0.26.0.59.0.42 1L2F,LYS_187,10.48,-0.1,0,0.07 1NIJ,HIS_134,7.33,-0.41,0.85,0.39 3CZC,LYS 93,10,57,-0.08,0,0,14 1WP5,LYS_205,10.42,-0.12,0,0.04 2Q13,CYS_341,10.71,0,0.23,1.48 1NJ4,ASP_295,3.52,-0.54,-0.22,0.47 1JKS,HIS_73,5.28,-1.15,0,-0.07 3BJV,LYS_149,10.93,-0.49,0.55,0.38 2BLL.TYR 443.9.78.-0.48.-0.13.0.4 1XAW,ASP_465,4.29,0,0.23,0.26 1GXN,TYR_595,11.56,0,0.01,1.55 1RL0,TYR_249,10.23,0,-0.14,0.36 1R9WLYS 318.10.34.-0.3.0.0.14 4DNU/HIS 339/3.54/-3.12/0.17/-0.01 2Q12,TYR_181,13.29,0.85,0.55,1.88 2Z84,HIS_110,6.15,-0.38,0,0.03 3ETV,GLU_239,4.77,0.29,0,-0.02 3P28,ASP 125,3.97,0,0.06,0.11 3GEC,LYS_445,10.36,-0.14,0,0 1R9W,GLU_309,3.71,0.42,-0.79,-0.42 4ESS,HIS_75,3.83,-2.67,0,0 3CIV,GLU 112,4.33,0.32,0,-0.48 3GT0.LYS 114,10.76,-0.74,0.44,0.55 3HVM,LYS_250,10.41,-0.48,0,0.39 1YTD,LYS_14,10.52,-0.21,0,0.22 1YM5,CYS_107,10.05,-1.43,0.06,2.43 1EV8,HIS 212,6.32,-1.18,0.71,0.28 4EUG,ARG_156,11.5,-1.32,0,0.31 105J,TYR_5,10.77,0,0.08,0.69 1EW4,ARG_20,11.77,-0.86,0,0.14 1XIP,ASP 151,3.22,-0.87,-0.18,0.46 3BZT,LYS 317,10.32,-0.1,0,-0.08 2EYI,GLU_75,4.5,0.39,0,-0.38 1AKO,TYR_135,11.25,0,0.25,1 3KV0,ASP_90,2.8,-1.23,-0.3,0.52 1PZC,LYS 55,10.64,-0.25,0,0.38 2PGX,HIS_151,6.33,-0.64,0.49,-0.01 2E3S,ASP_510,3.8,0,-0.12,0.12 4DIU,GLU_146,4.58,0.08,0,0 1XFK.ARG 163,12.03,-0.67,0.0.2 3AU3,GLU 536,4,31,0,17,-0,33,-0,02 2JHY,ASP_140,3.9,-0.28,-0.16,0.55 4E9E,HIS_567,5.73,-1.61,0.77,0.06 2PGX,ARG_219,11.22,-1.68,0,0.39 3HVM,TYR_110,12.12,0.6,0.79,0.73 1X91,ASP 114,4,28,-0.85,0.09,1.24 3EVZ,GLU_189,3.95,1.3,-1.58,-0.28 3M70,GLU_48,4.68,0.49,0,-0.3 2CBE,LYS 45,10,43,-0,2,0,0,13 1PSW.ARG 42,12,39,-0,23,0,0,12 2A4D,ARG_200,13.45,-0.31,0.83,0.43 3CBN.GLU 45.6.56.2.01.-0.36.0.41 2IQT,LYS_222,11.31,-0.18,0.52,0.48 1IDK,ASP_207,3.59,-1.57,-0.08,1.43 3NZL/ARG 23,12,15,-0,35,0,0 2EEY,GLU_91,4.67,0.3,0,-0.14 2W2S,HIS_128,6.52,-0.41,0.12,0.31 3FFM.GLU 87.4.66.0.1.0.0.06 2A0J,LYS 119,10,41,-0.09,0,0 2IRM,TYR_241,10.59,0,-0.29,0.88 1XDZ,LYS_48,10.47,-0.16,0,0.13 3F1X,TYR_139,10.26,0,0.12,0.15 2Q5X,ASP_773,4.07,0,-0.03,0.31 1J74,GLU_18,6.02,3.29,-1.68,-0.1 3JZ9,ARG_390,13.3,-0.59,0.7,0.68 3BPV,ARG_41,12.99,-0.61,0.69,0.41 3V55,LYS_545,10.34,-0.17,0,0.02

1UW7,ASP_78,4.05,0,0,0.25 2V4U,LYS_535,11.09,-0.19,0.62,0.17 2B0J,GLU_78,4.62,0.37,0,-0.24 1KCM,CYS_95,11.06,0,-0.56,2.62 3GW3,HIS_349,7.25,-0.59,0.78,0.56 1QQL,ARG_38,12.69,-0.07,0,0.26 1Z3X.ASP 10.3.98.0.0.0.18 1SI7,GLU_25,4.24,0.29,-0.63,0.07 3FK5,ARG_70,12.11,-0.39,0,0 3C5V,GLU_57,3.79,0.2,-0.54,-0.37 300P,GLU_7,4.68,0.18,0,0 1XEU.LYS 207.10.32.-0.23.0.0.04 2ZQ5,HIS_17,5.26,-1.66,0.83,-0.4 3ZTA,ARG_131,12.27,-0.27,0,0.04 1X1E,ASP 103,3.81,-0.68,-0.43,1.14 4DIU.LYS 154,10,45,-0.09,0,0.04 1H4U,ASP_427,2.95,-0.61,-0.6,0.36 3CO1,HIS_69,6.37,-0.29,0,0.15 3C6B,LYS_68,10.5,-0.16,0,0.15 3T5B,LYS 288,10.45,-0.18,0,0.13 3DB9,TYR_23,11.29,0,0,1.29 3HUE,LYS_210,10.43,-0.07,0,0 3G9G,LYS_37,10.29,-0.23,0,0.03 3DSH,ASP 345,4.08,0.0,0.28 3BPV.CYS 38.11.46.-0.01.0.2.47 1L3K,ASP_115,3.66,0,-0.31,0.18 3ELI,GLU_15,4.07,0.24,-0.67,0 3C6B,GLU_214,4.69,0.19,0,0 1WPA,LYS_488,9.94,-0.39,0,-0.17 1DVO.LYS 37.10.35.-0.15.0.0 3L3P,LYS_412,10.12,-0.3,0,-0.08 10TM,ASP_140,3.65,0,-0.49,0.35 2F4Q,ARG_156,12.21,-0.43,0,0.14 20EW,GLU 66,4.87,1.16,-0.85,0.06 2P1W,ARG_231,12.21,-0.35,0,0.07 2Z84,ARG_133,12.91,-0.67,0.23,0.85 3GT0,GLU_59,4.58,0.31,-0.32,0.09 3IO0,LYS 240,11.31,-0.24,0.67,0.38 2GZR/HIS 188,4.05,-2.24,0.64,-0.85 1ZCU,ASP_177,3.28,-0.59,-0.38,0.45 1C44,LYS_68,10.31,-0.09,0,-0.09 3RLE,LYS 65,10.38,-0.12,0,0 1YOY.ARG 144.12.55.-0.35.0.0.4 4EVF,GLU_141,3.96,0.66,-0.75,-0.46 2FBI,ARG_62,12.48,-0.22,0,0.21 1YTD,LYS_206,10.71,-0.23,0.33,0.11 1YR6,GLU 72,4.21,0.46,-0.74,-0.01 1EDG,ASP_3,2.85,-1.3,-0.06,0.41 2HXB,ASP_89,2.29,-1.81,-0.36,0.65 3ON1,LYS_87,10.19,-0.3,0,-0.01 2ATR,GLU_121,1.89,0.53,-2.76,-0.38 2B61,GLU_175,3.64,0.29,-0.77,-0.38 3JV1,ASP 157,2.65,-1.42,-0.15,0.41 2CN1,LYS_217,10.37,-0.15,0,0.02 1J8B,GLU_27,4.5,0.14,0,-0.15 1XTD,ASP_135,3.59,-0.56,0,0.35 2DVK.GLU 72,2.81,0.8,-2.31,-0.17 1DVO,LYS_57,10.36,-0.25,0,0.12 2YWJ,LYS_158,10.18,-0.33,0,0.01 4EUG,GLU_97,4.3,1.36,-1.07,-0.5 3AUF,GLU 193,3.91,0.38,-0.61,-0.37 3CN5,TYR_259,10.66,0.02,0.31,0.32 2VGM,LYS_207,11.4,-0.49,0.6,0.79 3GS9,ASP_199,3.64,-0.77,0.01,0.6 3M66,GLU_332,4.72,0.32,0,-0.1 3F1X,GLU_106,3.93,0.21,-0.65,-0.12 3FTT,LYS_76,9.46,-1.12,0,0.08 1P4X,HIS 227.6.2,-0.31.0.0.01 1EYH,GLU_152,4.45,0.19,0,-0.24

2CWC,ASP_78,2.55,-1.62,-0.93,1.3 1JKS,LYS 45,11.2,-0.46,0.79,0.38 1X9G,GLU_187,4.63,0.15,0,-0.02 1R3F,ASP_118,3.21,-0.8,0,0.2 3H13,TYR_423,13.99,-0.85,0.81,4.03 20V2.TYR 116.13.37.0.0.24.3.12 1R29.TYR 111.10.5.-0.78.0.19.1.08 3EIZ,ASP_168,3,-0.85,-0.41,0.45 3GS9,HIS_90,4.34,-3.05,0.83,0.07 3RLN,ARG_612,11.2,-1.33,0,0.03 3GEC,CYS_511,9.09,0,-0.11,0.2 3DHN,LYS 179,11.14,-0.32,0.19,0.77 1AT0,GLU_388,4.78,0.29,0,-0.01 3JZ9,GLU_516,4.79,0.19,0,0.1 2V4X,TYR_93,11.14,0,0.31,0.83 2P1W,LYS 160,9.74,-1,0,0.23 100X,ARG_57,12.34,-0.25,0,0.09 2BT8,ARG_185,12.3,-0.2,0,0 1TD6,GLU_257,3.73,0.54,-0.85,-0.45 1X6J,GLU_68,4.34,0.28,-0.6,0.16 4E8B,ARG 5,11.07,-1.86,0.0.43 4EZB,GLU_121,4.41,3.31,-2.95,-0.44 3ELI,ASP_91,2.19,-1.26,-0.71,0.37 1U7U,ARG 344,12.3,-0.2,0,0 1W24,ARG 104,12.51,-0.12,0,0.13 3HNX,ASP_89,3.79,0,-0.25,0.24 2AXO,GLU_162,4.66,0.33,0,-0.18 4ECC,HIS_152,6.54,-0.18,0.25,-0.03 1LZL.TYR 269.12.83.0.-0.38.3.2 2D7J,GLU_62,4.87,1.87,-1.42,-0.08 1S7K,HIS_20,5.43,-1.34,0.21,0.06 1PVT.GLU 212.5.57.2.49.-1.66.0.23 3DB9,ASP_264,4.43,0,0.04,0.59 3H04,LYS 245,10.92,-0.5,0.05,0.87 1WXF,HIS 162,5,79,-2,76,0.83,1.22 3ASA,GLU_86,4.76,0.17,-0.13,0.22 2IF4,GLU_86,6.04,1.88,-0.5,0.16 3JZN,LYS_408,10.38,-0.1,0,-0.02 2PPN,LYS 73,10.6,-0.21,0.05,0.26 3K8J,GLU_56,3.91,0.52,-1.13,0.02 3EZ7,ARG 290,12.39,-0.47,0,0.36 1EYH,ARG_135,12.36,-0.15,0,0.01 1R5Q,ARG 82,13.16,-0.31,0.66,0.31 3C6B,LYS 2,10.35,-0.15,0.0 3JZN,GLU_195,3.75,4.06,-1.44,-3.37 1X7F,GLU_332,4.51,0.32,-0.45,0.15 3P28,ASP_149,2.59,-1,-0.99,0.79 2YWJ,TYR_173,9.85,0,-0.42,0.27 1X7F,HIS_251,6.18,-0.35,0,0.02 3RFF,GLU_22,4.32,0.86,-0.85,-0.2 1RI6,HIS_186,5.07,-1.51,0,0.08 2HP7,GLU 50,4.57,0.09,0,-0.02 4H4J,LYS 102,10.55,-0.12,0.0.17 2QZQ,ARG_24,13.59,-0.42,1,0.52 1UCH,HIS_26,6.23,-0.51,0,0.24 3V75,ARG_250,12.77,-0.31,0.31,0.26 1R6Y,CYS_46,9.18,0,0.03,0.16 3HKX,ARG 48,12,27,-0.31,0,0.08 3MEW,LYS_161,10.09,-0.7,0,0.29 2CYG,TYR_336,12.69,-0.63,0.02,3.3 4DND,ASP_63,4.08,0,0,0.28 4FZR.LYS 211.10.41.-0.09.0.0 3I0C,GLU_260,3.97,0.44,-0.71,-0.25 4EKU,ARG_184,11.67,-1,0,0.17 1VSM,HIS_103,6.19,-0.3,0,-0.01 2P65,ASP_22,3.95,0,0,0.15 4EF5.ARG 191,12.29,-0.21,0,0 1AIL,ARG_37,12.4,-0.26,0,0.16 2QV2,LYS_188,11.38,-0.3,0.68,0.5

1PSW.HIS 274.5.39.-1.69.0.0.59 1X04,CYS 86,8.8,-1.06,0.33,0.54 3HVM,LYS_121,10.09,-0.72,0,0.31 1C44,ASP_53,1.74,-3.04,-0.46,1.43 3K8J,HIS 132.6.59,-0.27,0.26,0.11 1XIP.ASP 111,3.76,-0.48,0.06,0.38 2F8H,ARG_222,12.56,-0.4,0,0.46 3RE9, ASP_69, 1.89, -1.92, -0.46, 0.47 2V4X,TYR_102,10.27,0,0.07,0.19 3H13,HIS_328,6.35,-0.15,0,0 2R4O,LYS 264,11.55,-0.31,0.85,0.52 1UJ8,LYS_36,11.46,-0.33,0.85,0.44 1QYI,GLU_219,4.43,0.3,-0.07,-0.31 2G5X,TYR_148,10.86,0,-0.09,0.95 3JSN.GLU 261.4.69.0.16.0.0.04 3MTT,ARG_574,12.38,-0.86,0.17,0.57 2J8A,ARG_319,12.62,-0.27,0,0.38 1R53,LYS_311,10.38,-0.12,0,0 20JQ,GLU_406,5.06,1.62,-0.94,-0.13 2D7U,HIS 43,1.52,-2.54,0,-2.44 1WXQ,LYS_262,10.48,-0.02,0,0 2ILR,TYR_500,12.48,-0.2,0.06,2.62 3US6.LYS 129.10.43.-0.62.0.0.56 3KV0.GLU 181.4.69.0.15.0.0.04 2CIU,ARG_137,12.45,-0.08,0,0.02 2AD1,ASP_222,3.43,-0.39,-0.44,0.47 1X04,LYS_114,11.36,-0.33,0.76,0.43 2RGY,ARG 233,13.11,-0.32,0.22,0.71 4F3J,GLU_202,4.63,0.1,0,0.02 2IF4,GLU_152,4.67,1.84,-0.8,-0.87 3C2E,ARG_151,12.58,-0.67,0.07,0.68 4ECC,LYS_126,10.44,-0.06,0,0 4ECC,GLU 29,4.33,0.25,0,-0.43 3H8Y,TYR 45,10,11,0,0,0,11 2YWJ,LYS_57,10.66,-0.16,0,0.32 4ANN,LYS_91,10.41,-0.35,0.04,0.22 3F7M,LYS_362,9.58,-0.78,0,-0.14 2JKF.GLU 42,4.64.0.14.0.0.01 2NRK,ARG_86,11.75,-1.43,0.01,0.68 2NSN,GLU_56,4.62,0.12,0,0 1PGV,GLU_372,4.47,0.21,0,-0.25 1NJ4,ASP_154,3.8,0,-0.21,0.21 2FM9,LYS 213,9.85,-0.27,0,-0.38 2CL3,GLU_81,6.19,3.23,0,-1.52 3CNU,GLU_6,3.64,0.24,-0.62,-0.47 20KT,HIS_340,6.4,-0.1,0,0 2FBQ,GLU_193,4.2,0.28,-0.44,-0.14 4D8L,ASP_238,3.16,-0.76,-0.4,0.52 1TLV,LYS_134,10.3,-0.27,0,0.08 1DTO,CYS_40,10.76,-0.08,-0.04,1.88 1X8F,GLU_157,4.81,0.21,0,0.1 3V3T.GLU 257.4.58.0.28.0.-0.2 3T8R,ASP_39,4.02,-0.09,-0.09,0.41 2OJQ,ASP_411,3.7,-0.23,-0.05,0.17 3NBI,GLU_37,4.91,0.34,0,0.07 3ADO,HIS 242,6.33,-0.26,0,0.1 2AH5,TYR_193,10.27,0,-0.13,0.41 1V8E,HIS_55,4.93,-1.1,0,-0.46 109G,ARG_46,13.09,-0.37,0.69,0.26 3LJI,ASP_268,3.32,-0.53,-0.47,0.52 3HNX.GLU 60.4.33.0.33.-0.33.-0.16 4H89,TYR_76,10.38,-1.24,0,1.62 2YWJ,ASP_109,3.76,-0.14,-0.01,0.11 2GAU,GLU_137,5.21,1.84,0,-1.12 1OXZ,TYR_294,10.86,-0.27,-0.11,1.22 2QDJ,ASP 338,4.4,0,-0.06,0.65 1Z3X,CYS_122,10.75,0,-0.04,1.78 1CHD,GLU_201,4.44,0.28,0,-0.34 3CCY,ARG_39,12.55,-0.22,0.06,0.21

1TR9.GLU 257.3.57.0.31,-1.16,-0.08 301C,LYS 271,10,15,-0,49,0,0,14 2QOP,ARG_107,12.46,-0.71,0.33,0.34 3V75.TYR 130.10.1.0.0.02.0.08 2A0J.GLU 115.4.68.0.21.0.-0.03 20EW,CYS 250,10.26,0,-0.15,1.41 3GFP,LYS_478,10.39,-0.13,0,0.01 3QAV,TYR_186,12.22,0,0.42,1.81 3TMO, ASP_322, 3.92, 0, -0.14, 0.26 10LR,ASP_222,4.02,-0.11,-0.22,0.56 3I4T,HIS 91,6.82,-1.72,1.35,0.7 3BA1,CYS_203,11.48,-0.06,0,2.53 2H14,LYS 67,10.23,-0.16,0,-0.12 1X1E,GLU_93,2.62,0.51,-1.98,-0.41 1R53.ASP 369.2.88.-0.85.-0.38.0.31 3FNI,LYS 31,11,44,-0,41,0.85,0.5 3LH5,HIS_524,4.29,-3.14,0.85,0.08 4DVD,GLU_167,4.88,0.39,0,-0.01 1J33,ARG_138,12.41,-0.35,0,0.26 3N0K,GLU 39,4.61,0.27,0,-0.16 2PGE,ASP_40,2.52,-1.29,-0.44,0.44 1SI7,ASP_143,3.15,-1.4,-0.48,1.23 3G9T,CYS_179,11.62,-0.55,0.64,2.52 20KT,TYR 83,13.17,0,0.79,2.37 3UC9.GLU 144.4.73.2.25.-1.49.-0.53 2E3S,LYS_370,10.75,-0.44,0.32,0.38 2A1V,GLU_66,4.94,0.1,0,0.34 3FWU,HIS_49,6.23,-0.22,0,-0.05 20BI,TYR 53,13.78,0,0.74,3.04 1059,HIS_94,5.69,-0.82,0.12,-0.11 4DEZ,LYS_230,10.24,-0.28,0,0.02 3AU3,CYS_451,8.92,-0.25,-0.39,0.55 1PSW,HIS_199,5.88,-1.01,0,0.39 3FHF.ARG 89,11.04,-1.71,0.0.25 1AKO,ARG_200,12.36,-1.34,0.84,0.37 4E8B,ARG_88,12.42,-0.08,0,0 1VSM,LYS_164,10.17,-0.66,0,0.33 3EZ7,HIS_136,5.94,-0.38,0,-0.18 2FL7,ASP_113,3.82,0,-0.12,0.14 2F9F,CYS_11,9.23,0,-0.36,0.59 3GFP,LYS_340,10.7,-0.52,0.38,0.34 1WOU.CYS 64.9.03.-0.95.-0.02.1 3P28,CYS 22,12,2,-0,7,-0,23,4,12 3K8J,ASP_77,3.83,0,-0.28,0.32 3AU3,HIS_444,6.16,-0.48,0,0.14 4FZR,GLU_78,4.23,0.63,-0.49,-0.41 1RI5,GLU_276,5.08,0.23,0,0.34 2XMZ,ASP 139,3,53,-0.46,-0.41,0.61 4GCO,ASP_201,4.15,0,-0.37,0.72 3F6M,GLU_146,4.31,0.44,-0.2,-0.44 2PGX.ASP 160.4.01.0.0.0.21 1WP5,TYR_64,11.02,0,0,1.02 105T,GLU_386,4.5,0.39,-0.26,-0.12 1L2F,TYR_181,11.02,0,0.25,0.77 3ADO,GLU_257,4.59,0.09,0,0 3K9I,ARG_123,12.8,-0.36,0.11,0.56 3GA2,LYS 105,10,31,-0,37,0,0,17 3CAX,TYR_349,10.59,0,0.23,0.36 1RZ2,ASP_225,3.28,-1.01,-0.39,0.89 1V43,ARG_124,13.44,-0.17,0.67,0.44 1017,HIS 23,4,78,-1,66,0,-0.07 3LH5,LYS_760,9.2,-0.81,0,-0.48 3RFF,ASP_19,3.35,-1.23,-0.48,1.27 3FK5,LYS_277,10.34,-0.16,0,0 2ZTY,LYS_42,10.44,-0.22,0,0.16 1YW5,LYS_54,10.57,-0.51,0,0.58 3F6F,TYR_72,10.94,-0.08,0.03,0.98 3UC9,HIS_53,7.15,-0.34,0.71,0.28 1JKS,ASP_103,4.08,-0.25,-0.09,0.6

2PPN,ASP_79,3.63,-0.22,-0.15,0.21 2H85,GLU_128,4.56,0.06,0,0 3AUF,GLU_45,3.95,0.37,-0.38,-0.53 2R51,LYS_201,10.49,-0.16,0,0.15 1R3F,GLU_227,4.62,0.12,0,0 2D7U,GLU_310,5.01,0.3,0,0.22 3BZT,LYS_290,10.49,-0.83,0.57,0.24 3FS3,ASP_275,4.18,0,0.02,0.37 2D7J,HIS_171,6.14,-0.29,0,-0.07 2Q34,HIS_114,5.05,-1.19,0,-0.27 2QEV,HIS_91,5.26,-2.38,0.85,0.3 1GPP.TYR 48,11.5.0.0.46,1.03 1ZBP,GLU_121,4.75,0.17,0,0.08 1JSX,HIS_91,5.6,-1,0,0.1 3CN5,LYS 237,11.1,-0.56,0.66,0.5 1LFP.TYR 174,12,11,0,0,19,1,92 2PWQ,ARG_102,12.02,-0.94,0,0.47 1R3D,TYR_198,10.79,0,0.03,0.76 2OJQ,GLU_567,4.66,0.14,0,0.02 3CAN,GLU 112,3.51,0.23,-0.85,-0.37 3H9W,HIS 65,5.94,-0.63,0.0.08 1TWU,CYS_34,8.39,-0.69,-0.33,0.41 3K1H,GLU_105,4.67,0.17,0,0 1WLY.TYR 148.10.34.0.0.04.0.3 2C2Y.ARG 67.13.23.-0.65.0.81.0.58 3E7P,HIS_164,5.93,-0.45,0,-0.11 2H30,GLU_108,3.92,0.33,-0.55,-0.36 3GV0,HIS_153,5.72,-2.22,0,1.45 2W1R,ARG_79,13.5,-0.3,0.84,0.46 1IDK,ARG_349,11.66,-0.95,0,0.11 3FXH,LYS_67,10.68,-0.11,0,0.28 1L3K,HIS_168,5.49,-1.7,0.68,0 3FRR,LYS_171,10.69,-0.21,0.19,0.21 4DND,GLU_13,5,0.22,0,0.28 1X6J,ARG_8,12.32,-0.2,0,0.02 3HVW,GLU_182,4.64,0.3,0,-0.16 3OBS,LYS_108,10.58,-0.49,0,0.57 1AM2,GLU_141,4.66,0.21,0,-0.04 3L7N,ASP 198,4.05,0.0.09,0.16 4AE7,CYS_63,9.58,-1.22,0.23,1.58 3V55,LYS_665,10.28,-0.25,0,0.02 1059,LYS_19,10.35,-0.15,0,0 3FK5,LYS 23,10.42,-0.08,0,0 2DFL,LYS_27,10.18,-0.33,0,0.01 3PZ9,HIS_175,6.21,-1.94,0.85,0.8 4ETX,GLU_348,2.19,1.18,-2.44,-1.05 2GYZ,ARG 30,12.43,-0.31,0.01,0.23 3FS3,GLU_84,4.53,0.19,0,-0.15 3BWT,GLU_813,4.41,0.52,-0.62,0.01 2W2S,GLU_135,4.49,0.35,-0.26,-0.1 4H86,LYS_41,10.74,-0.1,0,0.35 3M7D,HIS 56,2.95,-2.84,0.09,-0.81 30A7,LYS 14,10,51,-0,17,0,0,18 1N81,ARG_34,13.02,-1.29,0.67,1.14 1FHL,GLU_16,3.82,1.36,-1.48,-0.56 3I0C,LYS_258,10.4,-0.31,0.1,0.12 2BAA, ARG 18, 11, 95, -1, 89, 0, 8, 0, 54 2ZCX,GLU_68,3.73,1.06,-1.51,-0.31 3GV0.ARG 141.12.45.-0.18.0.0.13 3H8Y,ASP_66,3.57,-0.3,-0.1,0.17 20JQ,ARG 422,12.35,-0.21,0,0.06 4EUG,ARG 49,12,32,-0,28,0,0,1 3DHN,ASP_156,2.71,-1.8,-0.89,1.61 1UXO,TYR_178,10.71,-0.06,0.15,0.62 2PWQ,GLU_15,4.54,0.2,0,-0.16 2VC8,GLU_51,4.2,0.54,-0.83,-0.01 3HQX,HIS_105,5.14,-1.19,0.28,-0.45 2V81,ARG_181,12.33,-0.23,0,0.06 1C3K,LYS_104,11.15,-0.24,0.37,0.52

1Q8B,GLU_45,3.73,2.07,-1.7,-1.13 1NKD,GLU 49,4.49,0.15,0,-0.16 1FKM.HIS 335.6.46.-0.31.0.0.28 2G2D,ARG_64,12.46,-0.15,0,0.11 2XHC,TYR_235,10.84,0,-0.32,1.16 4AF2.LYS 24,10.41,-0.35,0.0.26 2ZO5.ARG 37.12.76.-0.54.0.02.0.79 2B78,ASP_41,4,-0.05,0,0.25 1LPL,LYS_217,11.13,-0.28,0.57,0.33 4FZR,GLU_366,3.33,0.71,-1.68,-0.2 2Q34,GLU_231,4.31,0.31,0,-0.5 3L7N,HIS_8,7.64,-3.16,1.93,2.37 2F4Q,HIS_180,5.77,-0.47,0.05,-0.32 3H6O,ARG 55,12,77,-0,48,0,13,0.63 2VGM,TYR_111,12.6,0.54,0.75,1.31 1PDB,CYS 6,12.61,0,-0.04,3.65 3EVP,ASP_260,3.63,0,-0.4,0.22 1WPA,LYS_462,10.34,-0.26,0,0.1 3Q1C,TYR_388,13.69,0,0.63,3.06 3IVF.GLU 20.4.63.0.13.0.0 1EV8.GLU 248.4.41.0.23.-0.22.-0.1 3V55,LYS_621,10.25,-0.43,0,0.18 208PLYS 189,10,5,0,0,0 3PBH,TYR_16,9.28,-0.73,-0.36,0.37 1NJ4,GLU 18,3.82,0.25,-0.42,-0.51 1MIX.GLU 342.4.74.0.57.0.-0.33 1V43,LYS_14,11.54,-0.4,0.76,0.68 2CN1,GLU_79,4.8,0.31,0,-0.02 1W7B,LYS 212,10,72,-0,21,0,0,43 3EOD,LYS_96,10.86,-0.33,0.37,0.32 3T5B,ASP_232,2.56,-1.5,-0.21,0.47 2P0Y.GLU 119.4.67.0.17.0.0 2CYG,TYR_132,10.38,0,0.02,0.35 3ON1,ARG_15,12.29,-0.21,0,0 3UC9,ASP_167,3.96,-0.03,-0.35,0.54 3S0A, ASP_40, 2.33, -1.7, -0.45, 0.68 2AHE,GLU_138,4.49,0.28,0,-0.3 1D2K,LYS_278,10.24,-0.32,0,0.05 2B61,ASP 158,3.89,0,-0.17,0.27 2Z61,ASP_16,3.27,-0.61,-0.4,0.48 1CHD,LYS 269,10,43,-0,1,0,0,03 2FD4,LYS_435,10.5,0,0,0 3GMS,ASP_271,3.73,0,-0.35,0.28 3LJI.CYS 71,11.49,-0.05,0.13,2.41 2Z61,CYS_122,12.48,0,-0.21,3.69 3US6,ASP_70,3.11,-0.83,-0.21,0.36 3BQW,GLU_225,4.17,0.37,-0.23,-0.48 2V4U,CYS 559,10.23,0,0.12,1.11 208P,LYS_89,10.77,-0.23,0.49,0 2EDM,ASP_127,4.1,0,-0.02,0.32 3BA1,LYS_67,11.3,-0.21,0.63,0.38 3K8U,LYS_90,10.91,-0.91,0.78,0.54 2FXT.GLU 300.5.54,1.38,-0.77.0.44 1SUU,TYR_614,10.26,-0.17,0.11,0.33 3I47,GLU_206,4.28,0.48,-0.34,-0.36 2NRR,TYR_406,10.29,0,0.06,0.23 3EUR,LYS_126,9.71,-0.5,0,-0.29 105Z.CYS 589.10.7.0.0.03.1.68 3MTT,TYR_464,10.1,0,-0.04,0.14 3V1Q,HIS_592,6.81,-2.13,1.65,0.79 3V1Q,TYR_522,12.57,0,0.94,1.62 2D0A, HIS 295, 5.21, -1.2, 0, -0.09 1H09,ASP_324,3.92,0,0,0.12 2F8H,ARG_178,13.08,-0.34,0.42,0.51 4DEZ,HIS_58,5.97,-0.34,0,-0.2 2HNG,HIS_79,6.86,-0.64,0.76,0.25 1XAW.ARG 459.12.81.-0.28.0.0.59 3LD1,LYS_81,10.42,-0.15,0,0.07 1YLN,LYS_205,10.32,-0.28,0,0.11

2BV9.ARG 277.12.24.-0.26.0.0 2ZO5,ARG 134,12,23,-0,75,0,0,48 3HUE,LYS_12,10.29,-0.18,0,-0.03 2W2S,GLU_132,4.47,0.07,0,-0.11 2PLQ,ASP_70,4.2,0,0.24,0.16 2EFK,ASP 286,3.07,-0.97,0.0.23 3GYW,LYS_194,10.25,-0.37,0,0.13 4FCU,ARG_189,11.57,-1.12,0,0.19 4FD6,CYS_218,10.56,0,-0.4,1.96 3UX2.TYR 77.10.47.-0.16.0.25.0.39 20GO,ARG 483,11,79,-0,71,0,0 3CAX,TYR_435,9.53,-0.77,-0.08,0.38 3NR5,GLU_110,4.07,1.36,-1.42,-0.37 3U2R,ARG 86,12,-0.61,0,0.11 1PGV.ARG 296.11.93.-0.54.0.-0.03 1H4U,GLU_538,3.61,0.26,-0.85,-0.3 2C2Y,LYS_20,10.39,-0.11,0,0 3A7L,ASP_38,4.04,0,0,0.24 4F8A,ASP_632,3.99,0,0.04,0.15 3DB9.TYR 152.11.88.0.0.14.1.73 1R53,GLU_140,5.56,2.71,-0.75,-0.9 1NAF,GLU_271,4.76,0.14,0,0.11 1LZL,ARG 242,13,72,-1,28,1,51,0,99 3UC9,GLU 75,3.17,0.24,-1.56,-0.01 3BPV,ARG_66,12.25,-0.1,0,-0.15 2PWO,LYS 67,10.28,-0.12,0,-0.1 3C2E,GLU_153,5.63,2.53,-1.29,-0.11 2B02, ASP 452, 3.74, 0, -0.31, 0.26 100L,LYS 128,10.07,-0.13,0,-0.3 3FXH,LYS_4,10.52,-0.07,0,0.09 2EDM,LYS_88,10.22,-0.34,0,0.06 2Z0M,GLU_11,2.61,0.52,-2.11,-0.29 2E0T,ASP 63,3.17,-1.24,-0.68,1.29 3H5T,ASP 205,3.59,-0.76,-0.29,0.84 4ETX,HIS_258,6.36,-0.29,0,0.15 2VAN,LYS_289,10.25,-0.29,0,0.04 3BA1,LYS_85,12.2,-0.49,1.32,0.87 1H09.LYS 183.9.42.-1.14.0.0.06 3GEC,GLU_474,4.6,0.36,0,-0.26 2NMU.GLU 112.4.67.0.23.0.-0.06 1RAJ,TYR_81,13.36,0,-0.71,4.07 2QRX,HIS 135,5.51,-1.5,0.16.0.34 2F8H,TYR 331,11.69,-0.85,-0.27,2.81 4F85,ARG_242,12.72,-0.16,0,0.38 1I60,LYS_254,10.4,-0.29,0,0.2 3O48,TYR_99,11.25,-0.3,0.53,1.04 2WOZ, ASP_506, 3.96, 0, 0, 0.16 109G,ARG_78,12.38,-0.18,0,0.06 1WPA,HIS_509,5.52,-0.76,0,-0.22 4EZB,ARG_195,12.5,-0.17,0,0.17 3OBS,GLU 116,4.55,0.18,0,-0.13 4AM1.HIS 90.3.81.-3.13.0.84.-0.4 2XHC,LYS_19,10.37,-0.65,0,0.53 20KT,ASP_206,4.23,0,0.05,0.38 2H14,ASP_157,2.4,-1.51,-0.34,0.48 2FL4,LYS 7,10.46,-0.04,0,0 3RHE,LYS_23,10.54,-0.3,0,0.34 3ONT,LYS_141,10.4,-0.1,0,0 1T6L,ASP_149,4.07,0,-0.04,0.31 1GPP,ASP 31,1.18,-2.5,-1.01,0.89 3GOZ.GLU 157.3.24.0.45.-1.44.-0.26 2QVO,GLU_55,4.4,0.36,-0.04,-0.41 4GCO,CYS_186,11.23,0,-0.08,2.3 2B61,LYS_234,10.65,-0.25,0,0.4 2FPN,TYR_47,11.57,0,0.28,1.28 2NYC,CYS 202,11.07,0,0.01,2.05 1SIG,ARG_373,12.19,-0.27,0,-0.04 2VAN, ASP_263, 2.92, -2.19, -0.02, 1.34 3I82,ARG_213,12.42,-0.28,0,0.2

4D8L,ARG_230,13.14,-0.33,0.64,0.33 2D7J.ARG 15.12.41.-0.38.0.0.28 3EVP,ASP_287,4.03,0,-0.02,0.25 3EZ7,HIS_223,6.37,-0.31,0,0.18 1Y0K.GLU 15.4.71.0.32.0.-0.12 10LR,ASP_169,2.84,-1.68,-0.46,1.19 3IDW,ARG 28,13,28,-0.36,0.84,0.3 2X4L,TYR_236,9.88,-0.76,0.07,0.57 3ZXY,GLU_240,4.58,0.57,-0.01,-0.48 1RI6,GLU_59,4.57,0.28,0,-0.21 1DTO,ARG_165,13.8,-0.45,0.76,1 2EJX,GLU_44,3.53,0.35,-0.78,-0.55 3PBH, ASP_11, 3.38, -0.49, -0.26, 0.33 3G9G,GLU_85,4.08,0.36,-0.87,0.09 2JHY.GLU 121.4.45.0.14.0.-0.2 1L2F.GLU 88.4.56.0.13.-0.03.-0.04 1R3F,GLU_311,4.46,0.1,0,-0.15 1SNT,GLU_153,4.48,0.3,0,-0.33 3MEW,ARG_282,12.29,-0.71,0,0.5 3SMD,LYS 78,10.34,-0.18,0,0.02 2V4X,LYS_128,10.94,-0.53,0.85,0.13 1NAR,ASP_155,4.09,0,0.14,0.14 1AKO,ARG_189,12.12,-0.55,0,0.16 1GPP,CYS 17,9.94,-0.1,0.52,0.51 4FLE.GLU 132,4,54,0,11,0,-0.08 3O48,LYS_126,10.33,-0.14,0,-0.04 1ZYL,GLU_22,4.47,0.19,0,-0.21 2VGM,HIS_250,6.3,-0.33,0,0.13 2RH3,TYR 99,12.23,0,0.3,1.94 1SUU,GLU_565,5.08,0.43,0,0.15 3MTT,GLU_504,4.55,0.28,0,-0.23 1SIG,ARG_385,12.43,-0.08,0,0.01 2FPN,ASP_137,3.54,-0.3,-0.1,0.14 300P.GLU 47.3.27.0.95.-1.79.-0.39 1LTU,ASP_6,3.23,-0.85,0,0.28 3GS9,TYR_93,12.08,0,0.39,1.69 3F1X,CYS_146,8.23,-1.25,0.1,0.38 20PJ,ARG 17,13.31,-1.93,0.24,2.5 1YLN,ARG_211,13.3,-0.47,0.81,0.45 1O59,TYR_68,10.46,-0.13,-0.03,0.62 1WXF,TYR_255,11.01,-0.13,-0.06,1.2 2D7U.GLU 249.4.62.2.4.-0.26.-2.01 3K1H,LYS 136,10,49,-0,1,0,0,09 2CBE,TYR_194,13.7,-0.85,-0.13,4.66 3MEW,LYS_136,10.45,-0.05,0,0 2B0A,GLU_134,4.72,0.24,0,-0.02 1X91,HIS 88,7.11,-0.33,0.56,0.37 1J33,ARG 144,12.88,-0.82,0.81,0.39 2IXM,ARG_99,12.44,-0.06,0,0 3EAZ,ASP_123,3.98,0,0,0.18 2G3A,GLU_12,4.14,0.11,-0.47,0 100X.GLU 16.4.45.0.21.0.-0.26 2NMU,ARG_17,12.2,-0.36,0,0.06 2H2W,TYR_150,11.68,0.85,0.39,0.44 3PAC,GLU_101,4.08,0.6,-0.64,-0.38 1XEU,ASP_237,3.56,-1.2,-0.15,1.11 1UCH.ASP 216.3.64,-0.81,-0.19.0.85 4D8L,LYS_280,11.27,-0.33,0.75,0.35 3IU5,LYS_139,10.95,-0.28,0.08,0.65 1AK1.LYS 44,10.65,-0.28,0,0.44 1V8E,LYS 21,11.55,-0.38,0.85,0.56 3CAX,LYS_237,10.55,-0.22,0,0.27 2I88,GLU_373,4.23,0.41,0,-0.67 2ZCX,GLU_38,4.46,0.16,0,-0.2 1PVT,GLU_140,4.82,0.15,0,0.17 2VGY,ASP_54,3.98,0,0,0.18 3QAV,LYS_121,10.67,-0.26,0.16,0.26 3L3P,ARG_524,13.55,-0.45,0.68,0.82 2VC8,LYS_46,10.26,-0.19,0,-0.05

1RAJ.LYS 322.10.16.-0.74.0.0.39 3B21,ASP_103,3.99,0,0,0.19 3CJW,ARG_397,12.31,-0.15,0,-0.04 2FD4,ASP_473,3.14,-0.83,0,0.17 4EVF,LYS_120,10.21,-0.26,0,-0.03 3I47.GLU 246.3.48.0.46.-1.13.-0.35 3U0V,ASP 103,3,52,-0.62,-0.03,0,36 3QKY,TYR_101,10.97,-0.35,-0.31,1.63 4DND,GLU_97,4.98,0.22,0.02,0.23 2HRZ,LYS_306,11.11,-0.23,0.14,0.7 3CBN,TYR 122,10.14,0,-0.03,0.17 1L2F,GLU 148,4,48,0,19,0,-0,21 208P,ASP_148,3.72,-0.26,-0.06,0.24 3IVF,TYR_373,9.9,-0.3,0.03,0.17 2H2Z,ARG 76,12,48,-0,17,0,0,15 20HT,LYS 50,10.35,-0.1,0,-0.05 2D59,LYS_118,10.57,-0.12,0,0.19 2JKF,ASP 151,3.34,-0.81,-0.02,0.36 1H4U,TYR_440,9.72,-0.34,-0.35,0.41 1IDK,TYR 24,10.45,0,0.14,0.31 2A0J.HIS 113,5.62,-0.9,0,0.02 3BPV,ASP_51,2.52,-1.53,-0.51,0.77 1PDB,LYS_173,9.53,-0.78,0,-0.18 20VO.LYS 13,11.65,-0.41,0.85,0.71 1AK1.TYR 47.13.1.-0.85.0.96.2.99 4F85,ARG_146,12.59,-0.15,0,0.24 3UAH,HIS_198,6.5,-0.41,0.15,0.27 1UXO,GLU_48,4.94,0.28,0,0.16 2HXB,GLU_105,3.63,0.46,-0.85,-0.47 2A0J,ASP 43,3.28,-0.64,-0.15,0.28 2A6B,GLU_89,4.81,0.17,0,0.13 2WB8,LYS_659,10.36,-0.14,0,0 3M66.GLU 201.4.61.0.17.0.-0.07 3ONT,GLU 114,4.03,0.42,-0.85,-0.05 1DCF,HIS_1,6.13,-0.31,0,-0.06 2H8O,LYS_207,10.27,-0.23,0,0 2CXA,TYR_93,10.47,0,0.17,0.3 3P51,LYS 38,10.43,-0.08,0,0.01 2HNG,ASP 47,3,48,-0.86,0.04,0.5 20EW,ARG_306,12.49,-0.29,0,0.29 2B2H,ASP_3,3.91,0,0,0.11 20BI.GLU 163.2.31.0.54.-2.32.-0.41 1MN3,LYS 402,10.45,-0.12,0,0.07 2R0S,ASP_79,3.99,-0.17,-0.29,0.65 2D2S,ASP_696,4.57,0,0.16,0.6 3RFY,TYR_399,12.53,0,0.48,2.06 2JKF,TYR 5,10.21,0,0,0.21 1DZF,GLU_33,4.74,0.1,0,0.14 1YOY,ARG_161,12.46,-0.09,0,0.06 4D8L,ARG_205,13.46,-1.25,1.55,0.66 2R57,HIS_377,4.16,-2.35,0.78,-0.77 2O4D,HIS 55,6.51,-1.85,0.78,1.07 2G9D,TYR 334,10.35,-0.35,-0.17,0.87 1H4U,TYR_559,12.76,0,0.33,2.43 3UV9,HIS_363,6.67,-0.63,0.76,0.04 1S7K,GLU_77,4.79,0.27,0,0.02 307K,ARG_153,11.59,-0.93,0,0.02 2B61,HIS_135,7.02,-0.75,0.88,0.4 1XWM,GLU_140,4.33,1.03,-0.64,-0.58 1L2H,LYS_93,10.4,-0.08,0,-0.03 3BQW,LYS 75,10.37,-0.13,0,0 3CSR.TYR 3,10,46,0,0,2,0,26 3CE7,LYS_99,11.52,-0.25,0.85,0.43 2PWQ,LYS_12,10.55,-0.16,0,0.21 3F1X,GLU_168,5.59,1.31,0,-0.21 2DVK,GLU_146,4.69,0.12,0,0.07 1XTZ,ARG 23,12.74,-0.19,0,0.43 1YTQ,LYS_120,10.65,-0.25,0.02,0.39 1YLN,TYR_218,9.57,-1.65,-0.43,1.65

2CBE,ASP_110,2.49,-1.66,-0.27,0.62 1ZKZ,GLU 31,3.54,0.29,-0.99,-0.26 3C2E,LYS_48,9.95,-0.3,0,-0.27 3G9G,TYR_247,9.84,-0.74,0,0.58 3QKY,TYR_63,10.85,0,0.12,0.74 10TM.TYR 170.11.18.0.0.37.0.8 3CAX.LYS 413.10.49.-0.14.0.0.13 3RLN,HIS_694,6.5,-0.31,0.3,0.02 1RI5,ARG_275,12.45,-0.08,0,0.02 2QZQ,ASP_129,4.01,0,0,0.21 2V1L,TYR_107,10.16,0,0.07,0.09 2E0T,ARG_139,12.41,-0.24,0,0.16 3BJV,ARG_131,13.77,-0.4,1.14,0.52 1TP6.ASP 23.4.11.0.0.07.0.24 3GS3,ARG_215,12.38,-0.24,0,0.12 1V43,GLU 252,2.96,0.33,-1.24,-0.62 1LZL.GLU 224,4,45,0,18,0,-0,23 4EVF,LYS_12,10.48,-0.48,0.09,0.37 1J85,LYS_90,10.43,-0.06,0,-0.01 2BV9.TYR 208,10.63,-0.83,0,1.46 3PM2.LYS 42.10.35.-0.21.0.0.06 1R29,ASP_17,3.99,0,-0.11,0.3 106D,ARG 2,12.61,-0.2,0.02,0.29 1GPP.GLU 108.4.29.0.68.-0.78.-0.11 20EW,GLU_282,4.47,0.19,0,-0.22 2R0S.TYR 136.11.67.0.0.64.1.04 2YWJ,LYS_30,9.8,-0.35,0,-0.34 3BCH,GLU_69,2.82,0.23,-1.59,-0.33 1GPP,HIS_453,6.85,-1.67,0.46,1.57 3MEW.GLU 201,4.34,0.26,-0.18,-0.23 3RKV,ARG_287,13.49,-1.42,0.88,1.54 3F7M,ARG 156,11.51,-1.94,0.45,0.51 3SMD,TYR_126,11.39,0,0.06,1.34 3CJW,ARG 218,12.71,-0.59,0.03,0.77 3PU6,ASP 40,3.55,-0.51,-0.04,0.3 3LJI,GLU_28,3.51,0.18,-1.18,0 1MUF,ASP_256,4.04,0,-0.14,0.39 1AKO,HIS_38,6.95,-0.32,0.45,0.33 2FXT,LYS 333,9.88,-0.68,0,0.05 2VGM,ASP_61,3.46,-0.52,0,0.18 4HDE,LYS 117,10.39,-0.11,0,0 3JV1,ARG_51,12.42,-0.08,0,0 2AZP,LYS 252,10.45,-0.11,0,0.06 1KCM.GLU 54,2.81,1.33,-2.24,-0.79 2GEN,HIS_131,6.79,-0.3,0.49,0.11 1RI5,TYR_184,10.22,0,0,0.22 2AD1,GLU_121,4.59,0.25,0,-0.16 2G9D,HIS_121,6.79,-0.74,0.85,0.18 1Q42,GLU_10,3,0.32,-1.44,-0.38 1EYH,TYR_75,10.27,0,-0.39,0.66 1059,LYS_209,10.37,-0.13,0,0 3UC9,GLU_69,4.63,0.13,0,0 1SFE.ARG 160.11.57,-1.38.0.0.46 3V1Q,CYS_635,11.64,-0.14,0.67,2.1 1IAP,LYS_93,9.77,-0.87,0,0.14 1M5I,GLU_190,4.5,0.32,0,-0.31 1AD6,CYS_489,13.62,0,0.77,3.86 2CBE.GLU 14.3.75.0.38.-0.63.-0.5 2WB3,LYS_362,10.46,-0.04,0,0 3TIR,GLU_217,3.71,0.38,-1.17,0 3DTE,TYR_172,12.14,-0.85,0.01,2.98 4AF2,ARG 47,12,46,-0.5,0.09,0.38 1K95,CYS_76,11.05,0,0,2.06 2EYI,GLU_257,4.72,0.14,0,0.08 4E9E,GLU_575,4.29,0.12,0,-0.34 1DTO,TYR_102,11.59,-0.85,0.8,1.64 102Y,HIS 44,5.33,-1.68,0.68,-0.16 4D8L,HIS_152,2.89,-3.27,0,-0.33 2V4U,HIS_323,5.52,-1.02,0,0.04

3GG6.LYS 130,10.61,-1.3,0.73,0.69 3FWU.GLU 72,3.92,0.46,-0.84,-0.19 2HRZ,ARG_63,12.57,-1.05,0.43,0.69 3IRA,GLU_136,4.11,0.44,-0.68,-0.15 4AE7, HIS 158, 6, 26, -0, 24, 0, 0 3JZ9,LYS 466,11,27,-0.36,0,75,0.38 4DBX,ASP_145,3.44,-0.67,-0.07,0.39 3C2E,CYS_47,10.99,-0.81,0.14,2.66 3EYE,ARG_14,12.41,-0.21,0,0.12 3RNV,ARG 456,12.17,-0.36,0,0.04 2FBI,ARG_79,12.38,-0.17,0,0.05 1DVO,ARG_61,12.3,-0.23,0,0.03 2CWY,GLU_25,4.62,0.23,0,-0.11 1MJS,GLU_396,3.57,1.35,-1.3,-0.98 3IL3.ARG 248,11.64,-0.54,0,-0.33 2A1V,HIS_89,5.71,-0.37,0,-0.42 3Q6L,ASP_19,3.9,0,-0.14,0.25 2CBE,LYS_127,11.77,-0.31,0.74,0.84 3KEY,ASP_390,2.9,-1.24,-0.05,0.39 20VT.LYS 145,10.09,-0.41,0.0 1MN3,LYS_410,10.42,-0.14,0,0.06 4H89,TYR_160,10.19,0,0.05,0.14 1W7B,TYR 235,9.82,-0.48,-0.29,0.59 1RAJ.TYR 326,10.56,0,0.1,0.47 3F5D,ASP_54,3.35,-1.07,-0.26,0.86 3GG6,ASP_55,3.18,-1.07,-0.46,0.9 1VJG,ARG_136,11.98,-2.19,0.72,0.95 1SIG,LYS 371,11.12,-0.53,0.85,0.3 1PDB.LYS 46.9.83.-0.73.0.0.05 3GFP,HIS_355,5.77,-0.83,0,0.1 2WB8,HIS_630,3.98,-2.45,0,-0.07 1U7U,ASP_279,3.94,0,-0.16,0.29 3R87, ARG 35, 10.64, -2.21, 0, 0.34 2G9D,ARG 177,10.58,-2.2,0.02,0.26 2B61,ARG_231,12.38,-0.16,0,0.04 3N2T,GLU_258,4.66,0.24,0,-0.08 3GOZ,HIS_254,5.71,-0.59,0,-0.21 3BB7.GLU 98.4.49.1.72.-1.78.0.05 3RVC,CYS_116,9.91,-0.07,-0.32,1.3 1RWZ.ARG 16.12.12.-0.58.0.0.2 20HT,HIS 82,2.55,-2.9,0.75,-1.8 3RE9,HIS 244,6.64,-0.48,0,0.63 20G0.GLU 569.4.72.0.28.0.-0.05 2H8O, ARG_328, 12.58, -0.33, 0, 0.41 1O3X,CYS_256,11.07,0,0.01,2.06 3H13,TYR_451,10.13,0,0,0.13 2GYZ, ASP_82, 2.79, -1.23, -0.44, 0.66 2H85,CYS_333,10.36,0,0.11,1.25 3IPZ.LYS 89,10.29,-0.38,0,0.16 3T5B,LYS_103,10.84,-0.37,0.32,0.39 1YDL,LYS 17,11.32,-0.65,0.85,0.62 2HNG,LYS 67,10.34,-0.18,0.0.01 3DHN,LYS_49,10.11,-0.19,0,-0.19 1DZF,CYS_214,11.12,0.51,0.39,1.23 2XWS,GLU_22,3.42,0.48,-1.19,-0.36 1NIJ,ASP 191,3.49,-0.52,-0.07,0.27 3BQE,ASP_264,3.89,-0.47,-0.16,0.71 3QKY,LYS_58,11.01,-0.46,0.26,0.72 3RFY,LYS_123,11.51,-0.41,0.7,0.72 4F85,ARG 80,12.4,-0.48,0,0.38 20GO.TYR 445.11.76.0.0.52.1.23 1D2K,LYS_261,10.17,-0.41,0,0.08 1ANU,ASP_65,4.04,0,-0.06,0.3 4AE7,LYS_138,10.03,-0.47,0,0 3ADO,ARG_177,12.36,-0.14,0,0 1PSW,ARG 121,12.44,-1.96,0.9,0.99 1YLN,CYS_207,9.82,-0.25,0.17,0.89 1TUL,LYS 37,9.93,-0.54,0,-0.02 1H4U,GLU_448,3.58,0.35,-0.97,-0.31

3U2A,GLU_106,4.44,0.07,0,-0.14 1MIX.TYR 241,10.94,-0.45,0.29,1.11 2Q34,ARG_157,12.37,-0.21,0,0.08 1DTO.TYR 158,10.62,-0.06,0.03,0.65 2CWC,LYS 5,10.52,-0.1,0.0.11 2R51.LYS 286.10.28.-0.26.0.0.04 1WP5,LYS 59,11.84,-0.67,1.1,0.91 1ES9,ASP_192,2,-2.55,-0.56,1.31 3GW3,CYS_294,9.73,-0.06,0.21,0.58 2YWX,GLU_154,4.69,0.19,0,0 10IS,LYS 248,10.16,-0.4,0,0.07 1S7K,TYR_66,10.06,0,-0.08,0.14 3H04,TYR 60,11,59,-0.85,0.06,2.39 1TR9,LYS_275,10.15,-0.3,0,-0.05 3RFF.GLU 132.4.39.0.21.-0.27.-0.05 1X6J.ASP 66.2.65.-1.31.-0.38.0.55 2H2W,TYR_193,10.35,0,-0.16,0.51 1Z9L,ASP_37,3.94,0,0,0.14 2QVO,ASP_30,3.99,0,-0.05,0.24 3RJZ,TYR 120,10.94,0,0.25,0.68 1WJG,LYS_23,10.32,-0.2,0,0.02 109G,ARG_118,12.34,-0.2,0,0.04 1BN6,GLU_219,5.89,2.4,-0.84,-0.17 2B61.LYS 286,10.38,-0.12,0,0 3GS3.GLU 62.4.38.0.21,-0.28,-0.05 4DEZ,GLU_126,4.82,0.26,0,0.06 1WPA,TYR_420,9.83,-0.81,-0.16,0.8 30NH,CYS_452,10.32,-0.24,0.09,1.47 3UX2,LYS 111,10.47,-0.03,0,0 4H4J,TYR_152,11.51,0,0.33,1.19 3BQW,TYR_266,11.08,-0.13,0.19,1.02 2V4U,LYS_306,10.92,-0.29,0.47,0.25 3DB9,ARG_221,12.51,-0.06,0,0.07 10GL/HIS 72.6.34,-0.36.0.0.21 3F1X,GLU_149,4.49,0.29,-0.34,0.04 1ES9,ASP_20,3.28,-0.89,0,0.37 2IN0,GLU_78,3.63,0.61,-1.24,-0.24 1AK1,TYR 83,12.67,0.68,0.64,1.35 2GEN,GLU_50,3.01,0.85,-1.47,-0.86 105T,LYS_102,10.57,-0.07,0,0.14 1LTU,ARG_4,12.47,-0.03,0,0 3H04,LYS 207,10,4,-0,1,0,0 2G9D,ARG 138,12,33,-0,24,0,0.07 2CWC,ARG_40,13.24,-0.37,0.55,0.56 1RKA,GLU_107,3.99,0.21,-0.72,0 3RJZ,LYS_102,10.35,-0.16,0,0.01 2GQV,LYS 33,10.33,-0.3,0,0.13 1SOW,TYR 92,9.29,-0.76,-0.38,0.43 1YLN,ASP_66,3.21,-0.48,-0.33,0.22 3HUE,LYS_262,10.45,-0.05,0,0 3BOW.CYS 63.11.54.0.0.2.2.34 3E5T,ARG 92,12,58,-3,35,0,72,2,71 1WXF,LYS_31,12.08,-0.83,1.62,0.79 2ZTY,LYS 92,10,38,-0,15,0,0.02 2X4G,ARG_170,12.73,-0.36,0.18,0.41 3EVN,GLU_280,4.56,0.59,-0.13,-0.39 20HT.TYR 19.11.55.0.48.0.17.0.89 3LOD,TYR_79,10.86,0,0.06,0.8 4EF5,ARG_253,12.85,-0.8,0.18,0.97 1TXJ.ASP 129.3.9.0.-0.11.0.22 2IF4,GLU 120,4,9,2,25,-1,02,-0.84 1IAP,ASP_123,3.87,0,-0.26,0.33 2D2S,ASP_561,4.02,0,-0.04,0.27 3C6B,ASP_264,3.93,-0.09,-0.04,0.27 3EVZ,LYS_61,9.85,-0.28,0,-0.37 3EJC,LYS_82,10.15,-0.23,0,-0.11 1SIG,ASP_173,3.72,0,-0.22,0.14 1L2H,GLU 83,4.17,1.27,-1.2,-0.39 3GYW,HIS_227,6.06,-0.61,0,0.17

2YLF,CYS 62,13.83,-0.05,1.54,3.34 2F4Q,ASP 305,4.05,-0.31,0.27,0.3 3FS3,TYR_79,11.62,0,0.06,1.55 1TXJ,GLU_137,4.91,0.22,0,0.18 3C2E,HIS_281,4.05,-2.08,0,-0.36 3AU3.CYS 681.9.48,-0.07,-0.01.0.56 1SI7.LYS 13.10.03.-0.48.0.0 2PLQ,CYS_178,11.75,-0.66,0.33,3.09 1NAF,TYR_253,11.86,0.48,0.51,0.87 2B3M,ARG_81,12.5,-0.48,0,0.48 1NRI,LYS_137,10.39,-0.11,0,0 3OAV.GLU 114.3.68.0.34.-0.49.-0.67 3CXS,LYS_131,10.33,-0.52,0,0.34 1SNT,TYR_181,11.35,0,0.15,1.2 1TXJ.GLU 153.4.54.0.04.0.0 4DNU.GLU 88,3.94,0.67,-0.84,-0.39 3IRA,LYS_158,11.54,-0.22,0.81,0.45 2GS5,ARG_108,12.33,-0.2,0,0.03 1WJG,ARG_70,12.46,-0.35,0.07,0.24 2ILR,CYS 477,10.52,-0.02,-0.02,1.56 1BN6.HIS 70.5.36.-1.05.0.-0.09 2PP6,ARG_11,12.33,-0.17,0,0 1NWA,LYS_6,10.26,-0.46,0,0.22 1WP5,LYS 233,10.03,-0.36,0,-0.11 3G6S.GLU 89.3.86.0.29.-0.38.-0.55 3FTT,GLU_153,4.49,0.19,0,-0.2 2VC8.ARG 39.12.37.-0.14.0.0.01 10GL,ARG_268,13.36,-0.33,0.6,0.6 1J33,GLU 134,4.04,0.27,-0.73,0 20EV,ARG 126,12,31,-0,19,0,0 3BCY,HIS_144,5.82,-0.51,0,-0.18 3ZXY,ARG_93,12.32,-0.18,0,0 3IVF,HIS 228,4.23,-2.27,0.0 3CN5,ARG 39,12.05,-0.29,0,-0.16 1LFP,HIS_12,6.51,-0.31,0.56,-0.24 2QV2,GLU_170,4.52,0.06,0,-0.05 4FZN,HIS_136,2.38,-3.54,0,-0.58 3L7N, ARG 24, 13.77, -0.57, 1.31, 0.52 1MIX.ARG 297,13.8,-0.31,0.87,0.73 2F9F,ARG_57,12.4,-0.1,0,0 3LQE,ARG_228,12.29,-0.21,0,0 2YWJ,GLU_25,4.64,0.28,0,-0.14 1ZCE.GLU 24,4.53,0.15,0,-0.12 3ANJ,ASP_326,3.03,-1.55,-0.59,1.36 1YTQ,ARG_144,13.17,-0.43,0.46,0.65 1RSS,ARG_102,11.77,-0.48,0,-0.25 2A0J,GLU 131,4.05,0.27,-0.33,-0.4 3K1H,ASP_104,3.94,0,0,0.14 1V43,ASP_275,4.47,0,-0.1,0.77 3IVF.ARG 195,12.87,-0.31,0,0.67 2QVO,GLU_12,3.36,0.35,-0.85,-0.64 1V43,LYS 121,10.49,-0.2,0,0.19 1EO6.TYR 67.12.1.0.0.76.1.34 1F2V,HIS_83,6.37,-0.26,0,0.13 1NAF,ASP_204,3.45,-0.31,-0.28,0.23 1RL0,GLU_139,4.28,0.38,-0.59,-0.01 4GA2,LYS_47,10.74,-0.25,0.03,0.46 2DVK,LYS_104,11.37,-0.22,0.72,0.37 3P28.GLU 76.4.68.0.18.0.-0.01 4DVD,ASP_158,3.5,-0.53,0,0.23 2NRK,LYS 28,10.54,-0.12,0,0.16 1R5O.GLU 63.2.76.0.63.-1.59.-0.78 3DSH,ARG_263,10.16,-2.38,0,0.03 1SI7,CYS_90,11.97,-0.17,0.01,3.13 3EZ7,ARG_345,12.16,-0.74,0,0.41 2RIK,LYS_141,11.25,-0.82,0.85,0.72 2V4U,ASP_505,4.16,0,0.14,0.22 1J7G.LYS 61.10.39.-0.11.0.0 1TLV,TYR_188,9.84,0,-0.23,0.07

3FHF,GLU_185,3.87,0.46,-0.7,-0.39 1X7F,GLU 303,4.92,0.25,0,0.17 3ANJ,GLU_324,3.47,0.23,-0.85,-0.41 2Q13,ARG_46,12.4,-0.1,0,0 2GZR,ASP_126,3.21,-1.58,-0.08,1.09 2BDD,LYS 124,10.23,-0.32,0.0.06 3H6O.TYR 120.11.05.0.0.22.0.82 3B7X,ARG_104,12.45,-0.39,0,0.34 2OSA,TYR_333,12.68,0.82,0.55,1.32 3QAV,LYS_6,11.69,-0.28,0.72,0.75 1WOU,HIS_16,6.58,-0.32,0,0.4 3ETU,LYS_149,10.45,-0.05,0,0 2RIS,LYS_125,10.28,-0.53,0,0.3 3ETU,ASP 335,3.62,-0.25,-0.38,0.45 1PGV,ASP_237,3.98,-0.03,-0.02,0.23 3EYE,GLU 67,4.59,0.13,-0.08,0.05 3Q1C,ARG_231,12.34,-0.47,0,0.31 3HUE, ARG_16, 12.26, -1.61, 0.56, 0.81 4H4J,ARG_99,12.62,-1.31,0.73,0.69 3CAX,LYS 334,11.21,-0.4,0.7,0.41 3LH5,ARG 571,12,41,-0,16,0,0.07 2OB5,LYS_122,10.77,-0.31,0.17,0.41 3F6F.TYR 5,10.77.0,-0.2.0.97 3BB7,GLU_240,4.57,0.35,-0.08,-0.2 2EYI,CYS 41,12.6,-0.04,0,3.65 3K9I.GLU 125.5.31.0.26.0.0.55 1NAR,ASP_154,2.27,-1.62,-0.52,0.61 3FWU,ASP_93,3.45,-0.61,-0.08,0.34 3LJC,ARG 125,12,44,-0.06,0.0 3T5B,ARG_9,12.17,-0.6,0,0.27 20EW,LYS_215,10.31,-0.19,0,0 2RGY.GLU 222.5.57.0.85.0.0.21 3DZ1,ASP_34,2.64,-1.39,-0.43,0.67 1PDB,HIS 87,5.86,-0.94,0.44,-0.15 2B3M.GLU 45.4.54.0.32.0.-0.28 1SQH,ARG_11,12.69,-0.63,0.48,0.34 3T57,ARG_275,12.17,-0.33,0,0 3G6S,LYS_130,10.76,-0.5,0.38,0.37 1EV8,LYS 120,10.01,-0.49,0,0 3DB9,ASP_215,4.48,-0.79,0,1.47 4EVF,ASP_176,3.96,0,-0.59,0.75 1VJG,ASP_44,3.74,0,-0.35,0.29 1L2F,ARG_227,10.88,-3.01,0.53,0.86 2EYI, HIS 28, 6.37, -0.16, 0.0.03 2W1R,ASP_116,2.88,-0.78,-0.38,0.24 1ES5,LYS_254,10.34,-0.44,0,0.28 1IAP,GLU_105,3.73,0.39,-0.79,-0.37 3LH5,GLU_665,4.68,0.31,0,-0.13 1YTD,HIS_182,6.21,-1.11,0,0.82 3C6B,LYS_36,10.5,-0.22,0,0.22 1XTD,ARG_79,12.67,-0.24,0,0.41 3L3P,GLU_375,4.48,1.58,-0.97,-0.63 3H5T,ARG 226,11.92,-0.61,0,0.02 1J8B,HIS_50,6.59,-0.4,0.33,0.16 2QRX,ARG_32,12.48,-0.23,0,0.22 1RI6,CYS_248,12.57,-0.88,0.49,3.97 1ZYL,ARG_127,12.73,-0.7,0.31,0.62 3KT9.LYS 59,10.61,-0.27,0,0.37 3DSH,GLU_418,4.64,0.29,0,-0.15 3LPZ,TYR_182,12.14,0.85,0.45,0.85 1H09,ASP_67,3.07,-0.96,-0.18,0.4 1ZBP.GLU 117.4.15.0.19.-0.38.-0.17 208P,CYS_144,10.24,0,-0.06,1.3 2QEV,LYS_108,9.7,-0.63,0,-0.17 1U7U,LYS_403,10.57,-0.94,0.85,0.16 4DBX,ARG_41,13.45,-0.28,0.49,0.75 2ZCO.LYS 186.11.4.-0.25.0.73.0.42 4F85,ARG_215,13.17,-0.24,0.53,0.38 3TRE, ASP_26, 3.59, -0.42, -0.15, 0.36

2BAA.LYS 220.10.23.-0.47.0.0.2 20VT.TYR 141,10.65,-0.05,0.07,0.63 3FTT,ARG_27,11.58,-1.3,0,0.4 3HNX,ASP_5,4.07,0,-0.04,0.3 1PSW/TYR 85,11,58,-0.69,-0.03,2,31 20K1,ARG 335,13,21,-0,45,0,2,0,95 2BLL,ARG_472,12.09,-0.44,0,0.03 3CSR,TYR_155,10.36,0,0.04,0.32 2R4Q,LYS_242,10.78,-0.12,0,0.4 1VJG,ARG 71,12.53,-0.44,0,0.47 4EZB,ASP_217,4.61,0,0.5,0.31 4ETX,ARG_246,12.73,-0.21,0,0.44 3T57,HIS_199,5.11,-1.35,0,-0.03 3ASA,ARG_309,11.64,-1.34,0.1,0.38 3LJI.TYR 38.10.77.0.0.0.76 2CXA,ARG_114,12.62,-0.07,0,0.19 1MTZ,ASP_268,4.15,0,0.11,0.23 3P51,ASP_26,2.67,-1.64,-0.24,0.75 1X8F,GLU_279,4.46,0.11,0,-0.16 3M16,ARG 307,12,46,-0,27,0,0,23 4EZB,GLU_159,4.72,0.22,0,0 1V43,ARG_148,11.66,-0.84,0,0 2XMZ,ASP_251,3.75,0,-0.27,0.22 1SI7,LYS 118,11.08,-0.31,0.39,0.5 1AKO,TYR_248,11.41,-1.11,-0.25,2.78 1X6J,ASP_2,3.34,-0.52,-0.3,0.35 4DNU,ARG_323,12.63,-0.21,0,0.34 3CSR,TYR_87,10.46,0,-0.26,0.72 3CRM,ASP_262,3.63,-0.49,-0.71,1.03 1LPL,ASP_227,3.91,0,0,0.11 3T8R,LYS_62,10.46,-0.04,0,0 3C38,GLU_98,4.62,0.12,0,0 4EVF,ASP 281,2.99,-1.25,-0.11,0.55 1XEU.GLU 123.4.78.0.91,-0.51,-0.12 1P6F,ARG_164,12.21,-0.4,0,0.11 3F5D,ARG_144,12.37,-0.39,0,0.25 1SQH,ASP_161,3.54,-0.49,-0.06,0.29 3F7M,ARG_116,12.58,-1.91,1.37,0.63 3V55,ARG_719,10.99,-1.81,0,0.31 2XHC,LYS 69,10,19,-0,39,0,0,08 1CBY,ASP_196,3.52,-0.91,-0.06,0.7 2P1W,TYR 236,11.82,0,-0.07,1.88 1046,ARG 53,12,33,-0,16,0,-0,01 4H86,TYR_153,11.91,0,0.12,1.79 1YG2,GLU_24,5.47,0.86,0,0.11 2EDM,ASP_93,3.52,-0.56,-0.04,0.31 2RFA,GLU_46,4.68,0.22,0,-0.05 2R51,ARG_131,13.17,-0.89,0.75,0.81 2Z0M.ARG 298.12.6.-0.8.0.02.0.87 1UCH,ARG_66,12.68,-0.86,0.29,0.76 1TR9,ARG 67,11.88,-0.51,0,-0.1 2EYI,LYS 195,10,91,-0,1,0,2,0,32 1059,HIS_149,5.57,-1.85,0.79,0.14 3ONT,GLU_109,4.84,0.26,0,0.09 1NAF,ARG_180,12.43,-0.07,0,0 2ATR,LYS 96,10.36,-0.14,0,0 3G9T,ARG_60,12.7,-0.78,0.55,0.43 2H30,LYS_180,10.42,-0.08,0,0 3ZXY,CYS_32,11.87,-0.05,0.07,2.86 1G5Z,LYS 184,10.51,-0.16,0,0.16 208I.TYR 26.10.53.0.0.02.0.51 2D7J,GLU_168,5.39,4.62,-1.65,-2.07 4ACJ,GLU_637,2.64,0.5,-1.53,-0.83 1FQI,LYS_344,10.99,-0.2,0,0.69 2JKF,CYS_122,12.08,0,-0.03,3.11 1DUN, ARG_13, 12.58, -0.08, 0, 0.16 3ZSL, ASP_239, 2.76, -1.5, -0.24, 0.69 3E7P,LYS_256,11.69,-0.46,0.85,0.8 1JKS,LYS_29,11.18,-0.35,0.65,0.38

2WZ9,GLU_69,5.14,0.35,0,0.29 1X9G.GLU 157.5.64.1.47.0.-0.35 20KT,HIS_112,6.13,-1.23,0.82,0.04 1PBV,ASP_161,3.24,-0.84,-0.06,0.34 1KCM.LYS 128,10.34,-0.16,0.0 2W1R.ASP 154.3.24.-0.76.-0.06.0.27 1YIB,ASP_190,3.88,0,0,0.08 2AXO,TYR_82,12.5,-0.16,0.23,2.44 4F85,ASP_155,3.09,-0.58,-0.54,0.41 200K,ASP_79,4.43,-0.18,-0.05,0.86 1T6L,LYS_192,10.59,-0.31,0,0.41 2Q07,LYS_339,9.54,-0.99,0,0.02 1BKB,LYS 107,10.62,-0.2,0.0.32 2D8N,HIS_68,5.2,-1.65,0.55,-0.2 2EFK.ASP 200.3.91.-0.02.-0.26.0.41 1KCM.GLU 211,3.31,1.57,-2.22,-0.55 1ZHV,LYS_8,10.33,-0.19,0,0.02 3BB7,GLU_282,4.6,1.73,-0.85,-0.79 1J85,ARG_46,12.44,-0.12,0,0.06 1SNT,HIS 18,6.51,-0.38,0.14,0.24 3ONT,CYS_67,10.31,0.07,0.39,0.85 1DTO,TYR_155,10.56,0,0.23,0.32 1P4X,HIS_185,3.44,-2.05,0,-1.01 2V81,GLU 187,3.94,0.2,-0.72,-0.04 1TXJ.LYS 106.11.11.-0.88.0.81.0.67 1DCF,LYS_112,12.44,-0.95,1.52,1.37 1FO9,ARG_393,12.51,-0.37,0,0.38 4GA2,ASP_77,3.17,-0.68,-0.23,0.27 4EKU,LYS 57,9.92,-0.32,0,-0.26 2BDD,ARG 36,12.37,-0.42,0,0.28 1RI6,ARG_152,12.63,-0.91,0.07,0.97 2CIU,LYS_217,10.56,-0.17,0,0.23 1R3D,HIS 53,5.18,-2.23,0.8,0.11 30IP.GLU 176.4.49.0.27.-0.34.0.06 3M16,CYS_246,12.51,-0.11,0.42,3.21 3E7P,LYS_257,10.12,-1.25,0.85,0.02 1ZBP,GLU_128,4.7,0.13,0,0.07 2GZR,ASP 100,3.47,-0.79,-0.13,0.59 3O48,TYR_82,12.56,0,0.63,1.94 2Q13,TYR_378,10.22,0,0.17,0.04 2F4Q,TYR_55,10.66,0,0.18,0.49 2FC3.GLU 88.4.53.0.17.0.-0.15 2Z0M,LYS_161,11.06,-0.18,0.36,0.38 1WNH,HIS_211,6.01,-0.28,0,-0.21 2VGY,CYS_113,11.44,-0.07,0.21,2.3 2XHC,LYS_227,9.86,-0.35,0,-0.29 2DFL,ARG 157,11.41,-1.21,0,0.12 3BPP.GLU 191.3.31.0.57.-0.82.-0.94 1JB3,ARG_40,13.17,-0.3,0.7,0.27 2PP6,ARG_78,12.35,-0.2,0,0.04 105J,LYS 56,10.3,-0.59,0.0.39 20KT,LYS 131,10.4,-0.13,0.0.02 2FPN,GLU_116,5.37,1.98,-1.08,-0.04 3C6B,ARG_294,13.45,-0.31,0.67,0.59 1R53,CYS_221,12.69,-0.54,0.43,3.81 2Z0M,LYS_176,10.06,-0.4,0,-0.02 1TLV.HIS 159.3.46.-2.11.0.-0.92 2CXA,HIS_73,6.19,-0.24,0,-0.07 1GXN,LYS_405,11.33,-0.4,0.85,0.37 3CO1.HIS 57.6.32.-0.18.0.0 3SMD,LYS 77,10,76,-0,14,0,0,4 2YWK,CYS_56,9.01,-0.94,-0.13,1.07 4FD6,LYS_188,10.5,-0.34,0,0.33 2NRK,GLU_69,4.46,0.24,0,-0.28 2YX0,ARG_29,12.92,-0.49,0.55,0.36 1UOH,LYS_135,10.18,-0.71,0,0.39 1X9G,CYS_34,12.4,-0.06,0.07,3.38 3M3P,GLU 45,3.77,0.39,-0.84,-0.28 1SQW,GLU_49,4.38,0.31,0,-0.43

4DEZ.GLU 135.4.67.0.17.0.0 1X9G,ASP_119,3.63,-0.84,-0.2,0.86 1BGF,LYS_84,10.17,-0.17,0,-0.15 1ANU,LYS 28,10.62,-0.17,0,0.28 3KB5,ARG_368,11.08,-1.73,0,0.31 1T6L.HIS 56.6.57,-0.26.0.0.33 3GW3.GLU 114.4.8.0.19.0.0.11 1PDB,GLU_171,4.47,0.24,0,-0.27 3C2E,ASP_25,4.18,0,0.01,0.37 2A1V,LYS_37,10.07,-0.39,0,-0.05 2WB3,ARG 330,13.49,-0.34,0.93,0.39 3N2T.GLU 66.5.14.1.17.0.-0.52 3HUE, ASP_269, 4, -0.81, -0.13, 1.14 1H09,ASP_136,2.99,-1.27,0,0.47 2IOT,ASP 109,3.84,0,-0.08,0.11 2A0J.HIS 70.6.34,-0.34.0.0.18 2HNG,GLU_97,3.92,0.21,-0.69,-0.1 3MTT,GLU_465,4.79,0.22,0,0.08 1O59,CYS_282,9.62,0,-0.39,1 200K,LYS 60,10.38,-0.12,0,0 3CXS.CYS 150.10.6.-0.05.-0.25.1.89 3BQE,ASP_219,2.87,-0.85,-0.38,0.3 2B02,ARG_440,12.42,-0.23,0,0.15 2OSA.GLU 313.4.74.0.23.0.1.73E-17 1FOLARG 295.12.51.-0.28.0.0.29 1EV8,TYR_153,10.26,0,0.1,0.16 1XKR,LYS_54,10.47,-0.11,0,0.08 2BV9,ARG_265,13.88,-0.62,1.51,0.49 2l88,LYS_379,10.18,-0.54,0,0.21 1SJY,LYS 78,11.39,-0.27,0.78,0.38 2V4U,ASP_435,3.69,-0.47,-0.38,0.74 1DTO,TYR_178,10.27,0,0.01,0.26 2Q99,LYS_254,10.4,-0.1,0,0 1CBY,TYR 213,13.24,0,0.15,3.09 1RWZ,LYS_79,10.41,-0.26,0,0.17 3HKX,TYR_166,10.65,0,0.2,0.44 20EW,GLU_35,4.81,0.31,0,0 1A8Q,LYS 234,10.32,-0.3,0,0.13 2FL4,ASP 78,1.91,-2.08,-0.38,0.56 2Z14,LYS_29,10.42,-0.08,0,0 2QV2,ARG_130,12.89,-0.34,0.11,0.62 3CAN,GLU 82,3,45,0,36,-1,32,-0.09 1SNT.ARG 204.12.54.-0.06.0.0.11 2l88,ASP_456,3.89,0,-0.12,0.22 2WOZ,ARG_464,13.62,-0.7,1.35,0.46 2RGY,CYS_145,10.47,-0.07,0.03,1.5 1WYC,ARG_190,12.15,-0.22,0,-0.12 2E3S,TYR_381,10.1,0,0,0.1 1TD6,ASP_151,2.89,-1.45,-0.19,0.73 4EF5.ARG 281,12.39,-0.11,0,0 3BB7,GLU_273,4.42,0.41,-0.74,0.24 4ETX,ARG 330,13.57,-2.19,1.49,1.78 20BLARG 33,12,47,-0,25,0,0,22 3GMS,TYR_303,10.27,-0.18,0.1,0.36 1TWU,GLU_109,4.75,0.23,0,0.03 1PSW,GLU_164,3.64,0.28,-0.68,-0.45 10TM,ARG_184,12.32,-0.18,0,0 2FBI,ASP_75,3.53,0,-0.7,0.43 20RX.CYS 59,10.8,-0.13,0.2,1.74 3GS3,ASP_209,3.67,0,-0.28,0.15 1A8Q,ASP 74,1.69,-2.24,-1.11,1.24 3BPP.HIS 107.3.64,-2.96.0.27,-0.18 1EDG,ASP_126,2.95,-1.28,-0.46,0.88 1J33,GLU_239,3.17,1.17,-1.66,-0.85 20KT,GLU_94,4.01,0.56,-0.5,-0.56 4E6S,HIS_64,6.17,-0.26,0,-0.06 3FXH,TYR_56,9.86,0,-0.32,0.18 2CWY,ARG_56,12.35,-0.15,0,0 3EVP,LYS_119,10.26,-0.22,0,-0.01

1UOH,GLU_120,3.66,0.26,-0.81,-0.29 1YG2,HIS_128,6.1,-0.51,0,0.11 2P52,LYS_117,10.25,-0.11,0,-0.13 1R53,ASP_339,4.78,0,-0.16,1.13 2BAA,TYR_230,11.81,0.8,0.53,0.47 1WP5,HIS 125,6.08,-0.5,0.11,-0.03 3S0A.LYS 102.11.42.-0.43.0.81.0.53 1RI5,GLU_246,4.46,0.83,-0.65,-0.21 1J85,CYS_83,9.08,0,-0.17,0.26 1RI6,HIS_314,6.63,-0.23,0.31,0.06 2D7J,LYS 40,10.35,-0.26,0,0.11 2Q99,ASP_281,3.88,-0.57,-0.09,0.75 3H04,HIS_237,6.21,-0.29,0,0 301C,ARG 364,10.24,-3.36,0,1.1 3JSN,HIS_49,6.47,-0.4,0,0.37 2W0G,TYR 174,11.24,0,0.02,1.22 1H09.TYR 293.10.22.0.0.0.22 3VJ8,GLU_250,3.92,0.31,-0.78,-0.11 1SBX,GLU_183,3.9,0.42,-0.58,-0.45 1NAF,LYS 195,10.6,-0.1,0,0.2 4E8B,GLU_162,2.41,1.3,-2.07,-1.32 2PLQ,LYS_197,11.53,-0.39,0.85,0.57 1WRU,CYS_118,12.01,0,-0.09,3.11 30AV.ASP 63.2.8.-1.83.-0.45.1.27 2EHG,TYR 132,10.92,0,0.27,0.65 1FKM,ARG 370,12,-1.03,0.21,0.31 2A0J,ARG_82,11.78,-0.84,0,0.12 2P1W,GLU_184,4.95,3.03,-2.44,-0.15 1YDL,GLU_11,4.42,0.12,0,-0.19 2CN1,HIS_145,6.67,-0.4,0.57,0 3FS3,TYR_54,10.21,0,0.03,0.19 2WB8.GLU 554.4.43.0.63.-0.29.-0.42 3GS9,TYR_308,10.29,0,0.15,0.15 2QDJ,LYS 329,10.39,-0.2,0,0.08 4F85,GLU_78,4.23,0.56,-0.83,0 3HVM,GLU_145,6.57,4.66,-1.16,-1.44 2BLL,ARG_505,13.34,-1.68,1.33,1.19 1DTO,ASP_122,3.99,0,-0.01,0.2 2V1L,ASP 54,3.37,-0.61,0,0.18 3MEW,TYR_260,12.75,-0.77,0.04,3.47 2VGM,ASP 202,3.32,-0.76,-0.55,0.84 2DVK,ARG_27,12.17,-0.64,0.06,0.25 3V4G,GLU 150,4.67,0.2,0,-0.03 3AU3,ASP 539,3,58,-0.03,-0.44,0.25 106D,ARG_39,12.54,-0.65,0,0.69 3CAX,LYS_410,10.47,-0.14,0,0.11 4ECC,ARG_86,12.25,-0.89,0,0.64 2I88, ASP 473, 2.88, -0.96, -0.3, 0.35 1MIX,LYS_364,10.45,-0.05,0,0 1Z9L,ARG_38,12.02,-0.5,0,0.01 2B0J,HIS_52,5.66,-1.43,0.83,-0.23 2V4U,ARG_508,12.41,-1.3,0,1.2 3H8Y,ARG 15,12,43,-0.27,0,0.21 2YLF,TYR_117,10.07,0,0,0.07 1IAP,GLU_203,4.56,0.24,0,-0.18 1NJ4,GLU_251,3.74,1.03,-1.5,-0.31 3N0K,GLU_122,4.12,0.85,-0.65,-0.59 2HP7.GLU 60.3.9.0.38.-0.85.-0.13 4E8B,GLU_122,4.61,0.11,0,0 3RHE,ASP_80,3.43,-0.77,-0.1,0.5 1ES9,GLU_38,4.74,0.29,0,-0.05 1TWU.HIS 56.6.32,-0.26.0.0.08 2CN1,TYR_96,10.83,0,0.23,0.61 3RE9,LYS 116,11.39,-0.38,0.85,0.43 1R3F,LYS_31,10.22,-0.21,0,-0.08 3ETU,TYR_226,11.78,0,0.33,1.44 3NZL,LYS 65,11,36,-0,44,0,85,0,45 3JV1,ASP_177,4.3,0,0.27,0.22 1VSM,ARG_95,12.41,-0.09,0,0

20KT.ASP 39.3.14.-0.92.-0.21.0.46 1UOH, HIS 177, 5, 37, -2, 05, 0, 78, 0, 16 1RKA, ASP_67, 2.06, -2.74, -0.05, 1.07 1WLY,GLU_257,4.25,0.35,-0.71,0.11 2O34,GLU 158,4.62,0.37,0,-0.25 3IV4.GLU 106.4.84.0.16.0.0.18 2XHC,LYS_4,10.41,-0.15,0,0.06 2A6B,GLU_212,9.16,4.13,0,0.54 3BQW,TYR_191,10.28,0,0.12,0.16 300P,ASP_107,4.01,0,-0.07,0.29 2D0A,TYR_210,13.63,0,0.27,3.37 1UAJ,ASP_135,2.86,-0.85,-0.38,0.29 1MTZ,ASP_222,2.99,-0.74,-0.38,0.32 20EW,LYS_298,10.81,-0.13,0,0.44 3FRR.LYS 38.10.77.-0.22.0.01.0.48 3CRM,ARG_213,11.86,-0.64,0,0 2AHE,ARG_142,12.54,-0.22,0,0.27 3I4T,GLU_183,4.51,0.01,0,0 1ZP2,GLU_225,5.41,0.72,0,0.19 3EZ7.LYS 286.10.38.-0.12.0.0 2YT4,ARG_696,10.65,-1.99,0,0.14 4EVF,LYS_295,10.1,-0.49,0,0.08 3IVF.TYR 199.11.78.0.85.0.37.0.56 1RAJ,LYS 311,10.66,-0.72,0.11,0.76 2ZCO,ASP_109,4.07,0,-0.47,0.74 1NAR,LYS_197,10.51,-0.12,0,0.13 2FL7,ASP_205,3.49,-0.85,-0.73,1.27 3RHE,LYS_89,10.31,-0.21,0,0.01 1XWM.TYR 206.9.88.-0.04.-0.35.0.27 1P4X,LYS_178,10.35,-0.16,0,1.39E-17 3MTT,LYS_541,10.44,-0.12,0,0.06 1XFK,ASP_234,3.78,0,-0.25,0.24 1UOH,LYS 30,10.47,-0.05,0,0.02 1R53,ARG 132,11.01,-1.43,0,-0.06 2B0J,LYS_182,10.19,-0.31,0,0 3C2E,ARG_143,11.86,-0.51,0,-0.13 3T5B,ASP_396,4.23,0,0.21,0.21 20RX.TYR 108,11,41,0,-0,12,1.52 200K,ARG_95,12.21,-0.22,0,-0.07 3DTE,ARG 107,12,49,-0,12,0,0,11 2B0A,GLU_186,4.74,0.11,0,0.13 1V43,GLU 261,4.8,0.31,0,-0.01 1L2F.GLU 171.4.44.0.2.0.-0.25 4EVF,GLU_33,3.29,0.53,-0.84,-0.89 1PSW,TYR_135,13.2,0,1.06,2.15 1XKR,GLU_42,5.32,0.76,0,0.07 3R2E,LYS_95,10.56,-0.22,0,0.28 2P1W,HIS_106,5.42,-2.18,0.85,0.25 106D,ARG_28,13.61,-0.59,1.25,0.45 1FO9,ARG_427,12.25,-0.25,0,-0.01 2RGY,GLU 323,4.52,0.93,-0.68,-0.24 4FD6.GLU 156.4.36.1.14.-0.85.-0.42 2P65,ASP_51,3.93,0,-0.08,0.21 2A1V,CYS_17,11.79,-0.94,0.29,3.44 1ZP2,HIS_176,6.05,-0.26,0,-0.19 1T07,ASP 40,4.14,0,-0.1,0.45 2ZCX,GLU_145,4.51,1.33,-0.9,-0.41 2EYI,GLU_57,4.74,0.34,0,-0.09 3R87, ASP_83, 3.99, 0, -0.1, 0.28 1X9G,CYS 156,11.46,0,0.07,2.39 1GXN.TYR 518.10.58.0.-0.03.0.61 3BCH,HIS_193,6.97,-0.26,0.66,0.07 1MUF,ASP_161,4.03,0,0.01,0.22 1X7F,LYS_170,10.15,-0.53,0,0.18 4H86,ASP_27,3.25,-0.29,-0.41,0.16 1WYC, ASP 384, 2.7, -1.3, -0.73, 0.93 2RJD,LYS_480,10.65,-0.31,0,0.45 1C44,LYS_100,10.27,-0.13,0,-0.11 1SIG,ASP_191,3.97,0,-0.19,0.36

3C38,LYS_142,10.96,-0.2,0.32,0.34 2FC3,ASP 58,3,86,0,-0,14,0,2 1DTO,ASP_153,3.62,-1.02,-0.26,1.11 2ZTY,TYR_22,10.06,0,-0.07,0.13 1DZF,LYS 91,10,46,-0.04,0,0 3NR5,ASP_22,3.73,0,-0.21,0.14 1RL0,ASP_29,2.12,-1.86,-0.28,0.47 1ZBM,TYR_149,11,0,0.49,0.51 2AD1,ASP_27,4.26,0,0.15,0.31 2H2W,ARG_180,13.37,-0.31,0.78,0.39 4H89,ARG_144,12.22,-0.28,0,0 1VSM,GLU_157,4.97,0.43,0,0.05 3MEW, ARG_165, 12.54, -0.38, 0.03, 0.39 1X1E,GLU_92,4.65,0.11,0,0.04 2EFK.GLU 92.4.7.0.22.0.-0.01 3CBN,HIS 164,6.38,-0.09,0,-0.03 3CRM,ARG_95,12.82,-0.35,0.33,0.34 4FH3,LYS_240,11.06,-0.61,0.85,0.32 3GMS,GLU_319,4.57,0.13,0,-0.06 1XDZ,TYR 225,9.91,-0.41,-0.35,0.68 2P52,ASP_181,2.05,-1.62,-1.06,0.94 2X4J,LYS_20,10.4,-0.32,0,0.21 1EV8,GLU_223,4.61,0.16,0,-0.05 1YTQ,GLU_138,3.14,0.5,-1.39,-0.47 3LD1.CYS 356.8.68.-0.92.-0.2.0.8 1FKM,HIS_327,6.4,-0.14,0,0.04 2Z61,TYR_261,10.41,0,-0.09,0.49 1LPL,GLU_153,3.78,0.43,-0.57,-0.57 4HDE,GLU 38,4.43,0.91,-0.85,-0.13 2AZP,CYS_73,10.16,0,-0.01,1.17 1LZL,TYR_220,11.15,0,0.13,1.02 1X8F,LYS_2,10.44,-0.12,0,0.07 1JB3,GLU 12,4.75,0.5,-0.03.-0.22 1AK1.TYR 165.12.65.0.0.02.2.63 1MIX,LYS_196,10.43,-0.06,0,0 3T5B,GLU_296,5.16,0.61,0,0.06 1KCM,LYS_55,10.43,-0.07,0,0 2ZQ5,CYS 266,11.8,-0.02,0.03,2.79 3G9G,ARG_98,13.22,-0.27,0.5,0.49 1ZHV,ASP_56,3.71,-0.37,0,0.27 3GOZ,LYS_153,9.94,-0.87,0,0.3 1NRI.ARG 149.12.55.-0.36.0.0.41 2X5Y,GLU 739,2.96,0.99,-1.7,-0.84 3MM4,ARG_987,11.92,-1.15,0,0.58 3ZXY,ASP_175,2.15,-1.73,-0.58,0.64 2PLQ,ASP_294,3.57,-0.28,-0.11,0.16 1NAF,LYS 183,10.45,-0.05,0,0 2R0S.GLU 302,4.39,0.27,-0.49,0.11 4AM1,LYS_180,10.52,-0.68,0.34,0.37 1YR6,TYR_64,10.27,-0.46,0.39,0.34 2ZCO,ASP 5,2.37,-1.35,-0.46,0.38 2AXO.GLU 160.4.93.0.23.0.06.0.15 1SQH,ASP_8,2.85,-2.26,-0.19,1.49 1KCM,GLU_46,4.72,0.22,0,0 1X1E,ASP_220,2.86,-0.68,-0.71,0.45 1XKR,ASP_103,2.61,-1.63,-0.01,0.45 1ZKZ.CYS 73.9.47.0.0.19.0.28 1IAP,ASP_182,3.58,-0.5,-0.02,0.3 1TJE,ARG_123,12.48,-0.43,0.13,0.28 2APL/GLU 64/4.55/0.15/0/-0.1 301C.GLU 392.3.61.2.25.-2.35.-0.79 3V55,ASP_522,3.03,-0.79,-0.26,0.28 2Q98,ASP_41,3.55,-0.57,-0.43,0.75 1ZYL,GLU_300,4.78,0.17,0,0.11 1DOV,GLU_88,4.63,0.13,0,0 1ILW,GLU_107,4.79,1.11,-0.78,-0.04 2R51,ARG_247,12.23,-0.28,0,0.01 30IP,LYS_205,10.18,-0.38,0,0.06 1S7K,HIS_149,6,-0.28,0,-0.22

2WOZ,LYS_303,10.23,-1.01,0,0.75 2GZQ,ARG_161,12.76,-1.89,1.12,1.03 1SJ8,CYS_575,9.38,0,0.06,0.31 2VAN.TYR 173.11.81.0.-0.13.1.93 2A6B,GLU_112,4.67,0.15,0,0.02 2B0A,LYS 105,10.62,-0.35,0,0.47 2P65,ARG_79,11.86,-0.68,0,0.04 2Z0M,ASP_249,2.26,-1.3,-0.79,0.56 2IF4,ASP_48,3.84,-0.57,-0.04,0.66 1I60,LYS_17,10.44,-0.29,0,0.23 1CHD,GLU 317,4.08,0.31,-0.49,-0.25 1XKR.GLU 5.3.62.0.28.-0.76.-0.4 2E0T,ARG_81,12.47,-0.06,0,0.03 3G9G,TYR_40,9.1,-0.5,-0.84,0.45 2H2W,ARG 248,12.05,-0.24,0,-0.21 1MTZ,ASP 154,3.15,-0.5,-0.51,0.36 2H2Z,CYS_145,11.65,-0.06,0.01,2.7 3I4T,LYS_227,10.85,-0.42,0.38,0.39 3L3P,GLU_468,4.77,0.34,0,-0.07 2CXC,LYS 103,10.53,-0.26,0,0.29 1NJ4,TYR 297,10,76,0,0,3,0,45 1YTQ,HIS_180,6.89,-0.35,0.74,0 1U7U,ARG_248,12.57,-0.68,0.34,0.41 3V3T,ARG 149,13.27,-0.22,0.67,0.33 3K8JLYS 151.10.43.-0.07.0.0 2H14,ARG_154,12.78,-0.99,0.55,0.71 2H14,LYS_81,10.03,-0.73,0,0.26 2B78,GLU_302,4.51,0.01,0,0 1T95,ARG_196,12.34,-0.19,0,0.03 2WB3,LYS 368,10,46,-0,04,0,0 3QKY,HIS_67,5.99,-1,0.5,-0.01 2l6l,ASP_49,2.81,-0.85,-0.42,0.28 3V75,ARG 263,12,41,-0.5,0,15,0,25 1MML,ASP 83,3.57,-0.48,0,0.26 3I4T,GLU_47,4.61,0.11,0,0 3DHN,LYS_5,10.62,-0.09,0,0.22 1059,TYR_170,10.39,-0.85,-0.01,1.26 4DNU,TYR_201,10.34,0,-0.1,0.43 109G,ARG 42,12,82,-1,18,1,16,0,34 2FXT,ARG_294,12.28,-0.26,0,0.05 1MD6,LYS_92,10.46,-0.11,0,0.07 3UV9.ASP 368.2.23,-1.81,-0.34,0.57 2AHE,GLU 93,4.56,0.27,0,-0.21 3ANJ,LYS_333,9.97,-0.58,0,0.05 1UAJ,HIS_0,5.97,-0.35,0,-0.18 3RE9,GLU_76,4.77,0.79,0,-0.52 3CN5,HIS 210,2.56,-3.44,0,-0.5 3IO0,ASP_108,2.63,-1.36,-0.2,0.39 2DVK,ARG_78,12.24,-0.26,0,0 3V55,ARG 465,13.69,-0.84,1.1,0.92 1MD6.TYR 100.10.56.0.-0.12.0.68 3NBI,CYS 30,11.33,0,0,2.33 1FKM,ASP_259,1.94,-1.66,-0.81,0.61 3HYQ,ARG_105,12.31,-0.19,0,0 3EGN,ASP_445,2.87,-1.2,-0.02,0.3 2CN1,LYS_284,10.5,-0.22,0,0.22 4ESS,ARG_51,12.57,-0.27,0,0.35 3EVZ,ARG_70,11.57,-2.1,0.11,1.05 2FG1.GLU 106.5.61.1.02.0.0.09 1A8O.LYS 171.10.42.-0.08.0.0 1WYC,ARG 234,12.66,-1.99,0.84,1.32 2RIS.LYS 119,10.5,-0.11,0.0.11 2GZQ,LYS_140,10.91,-0.14,0,0.56 1TLV,LYS_127,9.51,-0.79,0,-0.21 3OKQ,GLU_638,3.78,0.46,-0.79,-0.38 4ACJ,TYR_717,12.53,-0.85,0.22,3.16 1KN3,ARG_49,12.83,-0.92,0.8,0.44 10TM,ASP 189,4.01,-0.85,0,1.06 2PIM,ARG_109,12.24,-0.38,0,0.12

2V81,GLU_119,4.62,0.12,0,0 2FM9,CYS 69,11.37,-0.2,0,2.56 3DHN,ASP_126,3.83,-0.05,-0.16,0.23 3ZXY,ARG_50,13.8,-0.17,0.99,0.48 1TD6,LYS_138,10.36,-0.14,0,0 105T,LYS_204,10.33,-0.19,0,0.02 3GS9.GLU 232.5.14.0.5.0.0.15 2B0J,LYS_30,10.44,-0.12,0,0.06 1X04,ASP_32,4.11,0,0.17,0.14 3U2R,ARG_23,12.51,-0.17,0,0.18 4FZN,ASP 167,4,0,0,0,2 3UAH,LYS_229,11.34,-0.44,0.85,0.44 2IQT,ARG_270,12.44,-0.06,0,0 3CO1,LYS_84,10.34,-0.33,0,0.16 1WNH,GLU 2,4.28,0.45,-0.6,-0.07 3BQW,ARG 305,13.72,-0.24,1.01,0.44 3FK5,HIS_13,4.78,-1.73,0,0.01 1JT9,HIS_56,6.28,-0.83,0.37,0.24 1DVO,LYS_119,10.32,-0.21,0,0.03 1JYH.GLU 9.4.55.0.1.0.-0.06 1R3F.GLU 217,3.92,0.37,-0.74,-0.21 2DVK,GLU_50,4.61,0.11,0,0 2ZQ5,TYR_127,10.76,0,0,0.76 3TIR.ARG 58,12,38,-0.26,0.0.14 2HRZ.GLU 2.3.92.0.27.-0.85.0 3T8R.LYS 6.10.32.-0.2.0.0.02 3EJG,HIS_64,5.93,-0.57,0,0 3TIR,ASP_200,3.8,-0.39,0,0.39 3O48,GLU_92,4.82,0.84,-0.3,-0.23 3EVN.HIS 298.6.15,-0.48.0.07.0.06 1XDZ,GLU_37,4.84,0.23,0,0.1 3B21,LYS 41,10.38,-0.42,0.0.29 1PNE,TYR_128,9.76,-0.63,0.14,0.25 2XJ4,TYR 269,9.15,-0.72,-0.39,0.26 30NT.TYR 20.11.69.0.0.31.1.38 3ZXY,ARG_237,13.15,-0.15,0.52,0.28 30NH,GLU_492,4.9,0.28,0,0.12 2IXM,LYS_183,10.16,-0.39,0,0.06 2G9D, ASP 337, 4.07, 0, -0.1, 0.36 1AK1,TYR_125,12.64,0,-0.13,2.77 3LMF,LYS 86,10.6,-0.11,0.0.23 3ETV,GLU_287,4.78,0.4,0,-0.12 4DNU,ASP 294,2.58,-1.22,-0.37,0.37 1TR9,HIS 165,5,75,-1,9,0,54,0,6 3QAV,ASP_214,3.85,0,-0.06,0.11 3KT9,LYS_75,10.55,-0.14,0,0.2 3Q2C,ASP_89,2.88,-0.85,-0.38,0.32 2D7U,TYR 288,11.32,0,0.31,1.01 1FKM,ASP_594,3.3,-0.88,-0.04,0.42 4EZB,ARG_288,12.18,-0.29,0,-0.03 3JRT,GLU_92,4.68,0.41,0,-0.23 1LTU,LYS 165,10.43,-0.1,0,0.04 302C,ARG 25,12,25,-0.58,0.0.32 3RNV,TYR_455,10.78,-0.06,0.21,0.64 2E3C,HIS_338,6.05,-0.59,0,0.15 204D,GLU_31,3.21,1.04,-2.07,-0.27 1G8P,HIS_314,5.78,-1.1,0,0.38 1J8B.LYS 12.10.41.-0.09.0.0 3BA1,GLU_300,4.27,0.59,-0.47,-0.35 3BQE,ASP_259,3.33,-0.76,0,0.29 4ETX,ARG_374,12.92,-0.2,0,0.62 1RAJ,TYR 334,10.35,-0.81,0.22,0.95 1X8F,LYS_189,10.33,-0.17,0,0 2W0G,LYS 227,10,41,-0.09,0,0 2WOZ,GLU_505,4.62,0.22,0,-0.09 1AK1,LYS_34,11,-0.71,0.85,0.36 3UV9.GLU 366.3.98.0.67,-1.04,-0.14 1Q5Z,ASP_591,4.07,0,-0.01,0.28 2YWX,GLU_24,4.78,0.37,0,-0.09

20RX.GLU 67.4.65.0.19.0.-0.04 3GV0,ARG 204,13.25,-1.11,1.25,0.61 2PPN,ASP_11,1.81,-2.53,-0.07,0.61 1PGV,GLU_281,2.88,1.03,-2.21,-0.44 3IBT.CYS 105,11.55,-0.52,-0.06,3.12 1WLY.GLU 180.4.02.0.25,-0.75.0.02 2CIU,LYS_161,10.4,-0.13,0,0.04 3E0H,LYS_12,10.67,-0.19,0.06,0.3 3EVP,LYS_203,12.15,-0.59,1.65,0.59 3ILC,LYS 157,9.99,-0.65,0,0.14 1PBV.ASP 183.4.0.0.0.2 2JKF,GLU_147,3.9,0.23,-0.5,-0.33 1WNH,TYR_158,11.5,0,0.19,1.31 1UOH,TYR_112,11.62,-0.49,0.55,1.56 1FOILLYS 378.10.39.-0.11.0.0 2APL,ASP_120,3.16,-1.04,0.09,0.31 1X9G,ARG_27,12.37,-0.22,0,0.09 3ERF,ASP_179,3.95,0,-0.02,0.18 3B4D,LYS_207,10.09,-0.38,0,-0.03 4ECC.HIS 163,4,78,-2,86,0,85,0,29 2P4D,ARG_20,12.35,-0.15,0,0 2IXM,LYS_38,11.12,-0.58,0.57,0.64 1UCH,LYS_120,11.38,-0.36,0.85,0.4 1NIJ,ARG 310,12.74,-1.09,0.76,0.57 2RIS,GLU_32,4.7,0.46,0,-0.26 1NAF,ARG_214,12.11,-0.59,0,0.21 1W24,LYS_50,10.57,-0.31,0,0.38 3A4C,LYS 509,10.27,-0.15,0,-0.08 1YR6,ARG_22,12.9,-0.2,0.3,0.3 1C3K,ASP_139,5.15,-0.16,0.05,1.45 1JT9,LYS_50,11.1,-0.2,0.33,0.48 2QK1,ARG_474,12.84,-0.69,0.68,0.35 3V75.GLU 44,3.58,0.27,-0.64,-0.56 1XEU.LYS 132,10,48,-0,11,0,0,09 2QHT,GLU_60,4.37,0.41,-0.32,-0.22 3EX9,ARG_41,12.61,-2.46,0.07,2.49 1GXN,LYS_497,11.55,-0.32,0.63,0.74 3K9I.GLU 94,4.59,0.53,-0.13,-0.31 1ZP2,ARG_217,12.3,-1.1,0.21,0.69 3U2R,ARG 9,12,45,-0.05,0,0 3K9I,HIS_107,6.16,-0.7,0.26,0.1 1A8O.GLU 270,4.04,0.21,-0.33,-0.34 3HVM,GLU 140,3.23,3.69,-2.09,-2.85 2Z14,ARG_112,13.74,-0.39,0.85,0.78 2H8O,ARG_78,12.06,-0.51,0,0.06 3PM2,GLU_75,4.2,0.25,-0.66,0.12 1AKO,TYR 63,10,41,-0,11,-0,03,0,55 3KV0,TYR_169,11.03,-0.84,-0.43,2.29 4EZB,ARG_175,12.33,-0.3,0,0.12 3ANJ,ARG_17,11.08,-1.51,0,0.09 2H85,LYS 149,10.4,-0.04,0,-0.05 3EGN,ARG 452,12,21,-0,31,0,0.02 3GYW,HIS_232,6.07,-0.44,0,0.01 3H9W,HIS_131,6.3,-0.28,0.01,0.06 3UC9,CYS_32,10.07,0,0,1.07 4AM1,LYS 255,11.46,-0.27,0.85,0.38 3BQW,TYR_188,10.07,0,-0.2,0.28 100X,HIS_236,3.41,-3.09,0.2,-0.21 1T95,GLU_42,4.52,0.13,0,-0.12 3P28,LYS 118,10.9,-0.2,0.21,0.4 20GO.ARG 441.11.29.-1.57.0.0.35 2FC3,TYR_6,11.28,-0.71,0.3,1.69 3AUF,ASP_53,3.25,-0.85,0,0.3 1XDZ,GLU_114,4.54,0.14,0,-0.1 3ULX,ARG_85,12.29,-0.32,0,0.11 3CSR,ARG 138,11.78,-0.81,0,0.09 2WB8,CYS_478,11.6,0,-0.04,2.64 3IBT,GLU_135,4.91,0.41,0,0 4D8L,HIS_79,4.99,-1.99,0.29,0.19

3C38.GLU 200.3.15.0.53,-1.34,-0.53 2HXB.TYR 48,11.06,0.0.34,0.73 3G6S,LYS_85,10.44,-0.23,0,0.16 109G.GLU 185.4.18.0.29.-0.39.-0.22 3HZO,LYS 93,10.46,-0.04,0,0 3ULX.CYS 162.13.42.-0.27.0.97.3.72 3EZ7.GLU 36.4.78.0.34.0.-0.05 2BV9,ASP_47,2.85,-1.09,-0.36,0.5 1RI6,GLU_276,2.95,2.03,-2.83,-0.74 1X7F,HIS_136,6.14,-0.46,0,0.1 4FD6,GLU_24,4.08,0.35,-0.59,-0.19 2F8H,HIS_194,6.2,-0.25,0,-0.04 2H2W,CYS_142,8.68,-2,-1.31,3 3M3P,GLU_178,3.02,3.68,-1.63,-3.53 2IN0.HIS 429.6.72.-0.41.0.33.0.29 3LH5,LYS 567,10.38,-0.12,0,0 1XEU,GLU_165,4.65,0.27,0,-0.13 3CCY,ASP_156,4.12,0,-0.03,0.35 3C38,HIS_237,7.64,-0.35,1.13,0.36 3RFY,ASP 249,3.71,0,-0.28,0.18 3EJC,ASP_21,3.57,-0.84,-0.05,0.68 1XKR,GLU_58,4.26,0.97,-1.3,0.09 1SUU,GLU_697,4.47,0.05,0,-0.07 1AK1,LYS 102,10.57,-0.06,0,0.12 3OAV.GLU 51.4.69.0.13.0.0.05 3C38,ARG_115,12.51,-2.42,1.43,1.01 4ACJ,ASP_747,2.18,-1.95,-0.41,0.74 3F6F,ARG_6,12.85,-0.69,0.43,0.6 3CAN, ARG 30, 13.5, -0.16, 0.76, 0.4 1TXJ,TYR_150,10.81,0,0.27,0.54 2G9D,ARG_106,12.61,-2.13,0.2,2.05 3M7G,GLU_171,5.48,1.32,-0.36,0.01 3NJM,LYS 56,10.38,-0.18,0,0.06 3ULX,ASP 25,4,25,0,0.05,0,4 3A2Z,ASP_41,3.06,-1.13,-0.03,0.43 2GKG,GLU_9,4.88,2.32,-1.81,-0.14 2VGM,GLU_381,5.4,0.2,0.05,0.65 1VJG,CYS 27,9.36,0,0.14,0.23 3B21,LYS_209,10.97,-1.19,0.84,0.82 2G7O,LYS_123,10.39,-0.11,0,0 1SIG,LYS_299,10.46,-0.09,0,0.06 3H04,TYR 52,12,49,-0,12,0,36,2,25 2CN1.CYS 63.10.27.-0.93.0.03.2.17 1RI5,ARG_177,12.22,-1.03,0.21,0.54 2B02.CYS 400.11.44.0.0.14.2.3 3GG6,GLU_91,6.81,2.45,-0.37,0.24 2B02,HIS 367,3.96,-3.31,0.77,0 3KEY,LYS 456,10,17,-0.35,0,0.01 1QYI,GLU_152,5.01,0.44,0,0.07 3BA1,GLU_286,4.08,0.19,-0.74,0.13 2XHC,LYS_225,10.87,-0.15,0.21,0.3 2GKG,GLU_40,3.3,0.41,-1.29,-0.31 3HQX,ARG_57,12.47,-0.48,0,0.44 2WZ9,HIS_37,4.13,-2.95,0.68,-0.09 2EEY,ARG_38,13.35,-0.14,0.59,0.4 1WXQ,ASP_201,3.99,-0.07,0.11,0.16 3BWT.GLU 769.3.7.2.52.-3.08.-0.24 2QOP,ARG_22,12.39,-0.25,0,0.14 2IN0,LYS_27,10.42,-0.25,0,0.17 3R87,LYS 117,10,45,-0.05,0,0 3VJ8,ASP 351,3,42,-0.25,-0.28,0.16 4HDE,GLU_134,4.71,0.1,0,0.11 3G9T,LYS_31,11.5,-0.23,0.85,0.37 3IVF,LYS_295,10.47,-1.08,0.64,0.4 307K,ARG_112,12.14,-0.33,0,-0.03 3T5B,ASP_156,3.94,-0.13,-0.36,0.62 2G7O,LYS_68,10.93,-0.17,0.6,0 2EJB,ARG_143,12.32,-0.21,0,0.02 1WLY,HIS_122,7.03,-0.75,0.85,0.43

3PP8,ARG 27,13,13,-0,16,0,54,0,26 2Q98,TYR 28,11.84,0.85,0.47,0.52 2G5X,TYR_233,10.37,0,0.02,0.35 2PLQ,ARG_306,12.77,-0.25,0,0.52 1LFP,GLU_146,4.58,0.15,0,-0.07 2H2Z,HIS 246,5,37,-1,22,0,0,09 1H09,LYS 195,10,47,-0.03,0,0 2JKF,GLU_168,3.65,0.39,-0.85,-0.38 2AHE,ASP_237,3.77,0,-0.68,0.65 2FXT,LYS_260,10.39,-0.11,0,0 3NZL,ARG_71,12.31,-0.28,0,0.08 1GPP.TYR 130.9.42,-0.85,-0.41,0.69 1P4X,ARG_90,13.04,-0.11,0.65,0 4ANN,TYR_97,10.62,-0.03,-0.04,0.69 3G9B,TYR 128,10,29,0,0,01,0,28 4ANN.GLU 190.4.8.0.26.0.0.04 4HDE,GLU_90,3.78,0.31,-0.65,-0.38 2IDC.LYS 165.9.63.-1.11.0.0.24 3B7X,ARG_109,12.79,-0.43,0.22,0.49 2WB3,TYR 317,10.15,0,0,0.15 2V5B,TYR_103,10.27,0,0.13,0.15 1Q42,LYS_47,11.25,-0.52,0.85,0.42 2D2S,ASP_742,3,-0.8,-0.42,0.44 3V10.GLU 607.4.46.0.11.0.-0.15 4AE7.TYR 229.11.07.-0.15.0.08.1.15 3LJI,ARG_95,13.12,-1.17,0.84,0.95 3ADO, ASP_303, 3.71, -0.79, -0.47, 1.18 1FO9,ARG_307,11.65,-3.42,0,2.56 100X,LYS 87,10.49,-0.15,0,0.13 2|88,CYS 505,11,47,-0,29,-0,21,2,98 3V3T,GLU_136,4.05,0.92,-1.05,-0.32 2PWQ,ASP_13,3.12,-0.68,-0.4,0.39 2OJQ,GLU_603,3.59,0.6,-0.76,-0.74 3HUE,GLU 57,4.52,0.15,0,-0.13 3S0A,LYS_59,10.51,-0.05,0,0.06 2B6P,GLU_254,4.61,0.11,0,0 3P28,TYR_231,10.29,0,0.14,0.15 2RIK,LYS 234,11.47,-0.92,0.85,1.04 20V2.LYS 81.10.77.-0.32.0.0.58 3CIV,ARG_37,12.3,-0.23,0,0.03 1P2F,HIS_145,6.3,-0.24,0,0.04 3GEC,CYS 241,9.82,-0.55,0.25,1.11 3KV0,ASP 191,4.26,-0.05,-0.02,0.52 1P6F,TYR_75,12.71,0,0.05,2.66 4E8B,TYR_7,11.17,0,0.29,0.89 1TR9,ARG_72,12,-0.46,0,-0.03 3PU6,GLU 79,4.15,0.32,-0.35,-0.31 2FZP.HIS 295.6.9.-0.45.0.84.0.01 1TD6,GLU_208,4.68,0.19,0,-0.01 1UAJ,GLU_222,4.11,0.47,-0.7,-0.16 1X8F,LYS_268,10.42,-0.29,0,0.21 10TM,LYS 62,10.37,-0.13,0,-0.01 4DIU.LYS 121.10.31.-0.21.0.0.03 2DG7,ARG_135,12.29,-0.38,0,0.17 3P28,ASP_213,3.34,-0.49,-0.46,0.49 1T95,LYS_41,10.78,-0.21,0,0.5 2CVB,LYS_166,10.38,-0.07,0,-0.04 1AKO,GLU_185,4.77,0.22,0,0.06 1Q42,GLU_119,4.11,0.32,-0.71,0 3IV4,LYS_42,11.23,-0.28,0.63,0.38 4GA2,TYR 52,12.27,0.85,0.51,0.92 3IRA,LYS 125,11.15,-0.3,0.39,0.57 1KW4,LYS_74,10.18,-0.2,0,-0.12 3FHF,TYR_196,11.93,0,0.26,1.66 1AKO,GLU_137,3.99,0.36,-0.79,-0.08 2QV2,LYS_25,10.73,-0.25,0.18,0.31 3BCH,ARG_155,12.62,-0.12,0,0.24 1EDG.ARG 319.10.15.-2.96.0.0.61 2JEO,HIS_226,6.1,-0.56,0,0.16

3DSH,GLU_363,4.64,0.17,0,-0.03 3O7K,ASP_58,4.11,0,0.17,0.15 1EYH,GLU_19,4.36,0.27,-0.18,-0.23 2IQT,ASP_273,3.49,-0.25,-0.28,0.21 1DUN,GLU_73,4.17,0.37,-0.62,-0.09 2EFK.GLU 184,4.54,0.26,0,-0.22 1TP6,HIS_46,6.27,-0.18,0,-0.04 2FPN,LYS_85,10.43,-0.07,0,0 1Y2Q,TYR_79,12.53,0,0.06,2.47 3ELI,ARG_127,11.99,-0.69,0,0.19 3O48, ARG_76, 12.74, -0.4, 0.06, 0.57 2AZL,GLU_164,5.29,0.84,0,-0.06 1SJ8,GLU_734,4.74,0.24,0,0 2D2S,ARG 532,12.35,-0.19,0.0.04 2H01,CYS_44,9.07,-0.31,0.09,0.29 3D9H.GLU 131,4.65,0.13,0,0.02 4ETX,GLU_251,4.93,0.37,0,0.06 3RJX,LYS_154,11.41,-0.28,0.8,0.38 1QZN,ASP_73,3.69,-0.26,0,0.15 1NFN,LYS 143,10,39,-0,11,0,0 3DHN.GLU 206.4.36.0.37.-0.05.-0.44 1NIJ,LYS_86,10.61,-0.27,0,0.38 2CXY,ARG_30,12.11,-0.48,0,0.09 1J7G,GLU_115,4.53,0.26,0,-0.23 2GZR,LYS 104,10.74,-0.17,0,0.41 205X.GLU 832.4.98.0.39.0.0.1 2EHG,ARG_65,12.52,-0.16,0,0.18 2FBI,GLU_96,4.53,0.07,0,-0.04 3LPZ,ARG_32,12.4,-0.22,0,0.11 2EJX,GLU_125,4.2,0.28,-0.66,0.07 1PDB,ASP_145,2.84,-1.31,-0.1,0.45 1X9G,CYS_112,12.78,0.63,0.91,2.24 2X5Y,CYS_867,11.11,0,0.03,2.08 1AT0, ARG_377, 12.27, -0.23, 0, 0 3BWT.GLU 622,3.99.0.83,-0.67,-0.67 3IV4,TYR_81,11.79,0,0.52,1.26 2Q99,ARG_233,12.74,-0.42,0.21,0.46 3V46,GLU_363,4.5,0.3,0,-0.31 1TJE, TYR 219, 9.6, -0.6, -0.21, 0.41 3HNX,ARG_103,12.3,-0.2,0,0 3LJC,GLU_240,4.59,0.09,0,0 1EV8,TYR_164,10.27,0,0,0.27 2GAU,GLU 47,4.67,0.33,0,-0.17 4F85,ASP 298,3.57,-0.58,-0.47,0.82 1LPL,ASP_202,3.74,0,-0.34,0.27 2D0A,HIS_235,4.92,-2.32,0.73,0.01 2IQT,LYS_188,10.7,-0.21,0,0.41 3G9T,LYS_134,10.38,-0.12,0,0 3EUR,LYS_80,11.33,-0.63,0.85,0.62 3KEY,LYS_464,10.68,-0.16,0,0.34 1XDZ,LYS_164,11.37,-0.41,0.85,0.44 3F6F,HIS_59,7.23,-0.18,0.85,0.07 3RKV,LYS 301,11.39,-0.27,0.85,0.31 1QQE,LYS_199,11.44,-0.35,0.85,0.44 20JQ,GLU_679,4.57,0.3,0,-0.23 2AZL,TYR_11,10.74,0,0.23,0.52 1NAR,ASP_59,3.16,-1.03,-0.05,0.44 3CIV.ARG 312,12,55,-0.29,0,0.34 2VGM,TYR_300,10.31,0,0.08,0.23 4ESS,CYS_49,11.19,-0.05,0.1,2.13 2H01,LYS_7,10.75,-0.12,0,0.37 3P2F,CYS 147,9,56,0,-0,16,0,71 2P0L,TYR_19,12.34,0.85,0.49,0.99 3LH5,GLU_528,4.67,0.2,0,-0.04 2Q98,CYS_199,9.67,0.62,0,0.05 1X1E,ARG_96,13.85,-0.5,1.29,0.57 1R7J.GLU 75.4.46.0.27.-0.01.-0.31 2CXA,GLU_201,4.83,0.32,0,0.01 1MN3,GLU_406,4.32,0.24,0,-0.42

1YG2,ASP_144,4,0,-0.05,0.25 2R0S,ASP 205,2.01,-1.7,-0.58,0.48 3V55,GLU_556,3.75,0.49,-0.77,-0.47 1DUP,ASP_39,3.94,0,-0.03,0.17 2BV9.TYR 179.11.8.0.0.52.1.28 105T.LYS 154,10.42,-0.21,0.0.13 2QHT,TYR_13,12.53,-0.08,-0.46,3.07 3IVF,LYS_15,10.12,-0.28,0,-0.1 3CCY,TYR_51,10.06,-0.29,-0.28,0.62 3V3T,HIS 191,6.17,-0.45,0,0.13 3F6M,ARG 85,13,-0.44,0.66,0.28 3CNU,GLU_19,3.97,0.32,-0.85,0 3C6B,HIS_37,6.12,-1.09,0.75,-0.05 3B7X,GLU_96,5.15,0.51,0,0.14 3G6S.ARG 69.11.42.-2.11.0.02.1.02 3G9G,GLU_3,4.61,0.11,0,0 1ES9,GLU_88,7.85,5.13,-0.13,-1.65 3TOW, ASP_135, 2.49, -2.46, -0.2, 1.35 2GZR,HIS 52,6.67,-0.56,0.73,0 3FHF,ARG 22,12.27,-0.86,0.17,0.45 1TLV,LYS_60,10.3,-0.2,0,0 2CXY,TYR_8,12.07,0.85,0.39,0.83 3JSN,ASP_288,4.18,0,0.17,0.21 2AH5,TYR 74,11.62,0.48,0.39,0.76 3IU5,GLU_105,4.52,0.27,0,-0.26 3ANJ,ASP_133,3.63,-0.66,-0.62,1.11 3A4C,ARG_465,12.1,-0.53,0,0.12 2IRM,GLU 266,5.15,0.79,0,-0.15 3H04,HIS_230,4.48,-1.19,0,-0.84 4EKU,ARG_148,12.97,-0.6,0.18,0.89 3ZXY,ARG_141,12.26,-0.24,0,0 2FZP,GLU_316,4.67,0.34,0,-0.17 2l6l,ARG 145,13.96,-0.47,1.53,0.4 2FM9.ASP 108.3.95.0.0.0.16 1AK1,GLU_170,4.47,0.1,0,-0.13 1YM5,LYS_270,9.44,-1.01,0,-0.06 3H04,ASP_118,3.96,0,-0.02,0.18 1YLN,LYS 231,10.1,-0.31,0,-0.1 1PBV,ARG_162,12.05,-0.52,0,0.08 3T5B,TYR_391,10.64,-0.04,-5.55E-17.0.69 2CIU,TYR_214,9.8,-0.49,-0.2,0.5 2AZL,LYS 276,10,46,-0,15,0,0,11 3KEY,LYS_338,10.57,-0.13,0,0.2 3OA7,GLU_9,4.7,0.22,0,-0.02 2B3M,ASP_146,3.82,0,-0.1,0.12 3DHN,ASP_185,2.04,-1.93,-0.57,0.74 1RI6.ASP 229.3.17,-0.92.0.0.29 2Q13,TYR_48,10.39,-0.08,0.16,0.31 2V5B,TYR_211,12.24,0,-0.02,2.27 2E0T,GLU_104,4.3,0.38,-0.46,-0.12 1YTD.GLU 376.4.3.0.29.-0.46.-0.03 3GEC,HIS_403,5.99,-0.26,0,-0.25 2QV2,LYS_154,11.09,-0.26,0.85,0 3Q1C,GLU_77,4.02,0.29,-0.78,0 1RI6,LYS 49,10.24,-0.52,0,0.27 2XHC,ARG_275,12.64,-0.46,0.29,0.32 1AM2,ARG_49,12.41,-0.25,0.03,0.13 204D,ARG 4,12.44,-0.06,0,0 2CXC,GLU_63,4.53,0.14,0,-0.11 2Q13,ARG 238,12.28,-0.23,0,0 1Y2Q,GLU_74,4.61,0.11,0,0 1AKO, ARG_14, 12.04, -1.28, 0.05, 0.77 1V43,GLU_319,3.63,0.54,-0.85,-0.55 2HNG,ASP_20,3.94,0,-0.2,0.34 1WP5,GLU_293,4.28,0.86,-0.71,-0.36 1LN4,CYS_73,10.36,-0.23,-0.34,1.93 3LD1,ARG_201,11.97,-0.72,0,0.18 2BAA, ASP_12, 3.33, -0.8, -0.58, 0.92

2G9D.ARG 322.10.47.-1.58.0.-0.45 3S0A, ARG 9, 13, 11, -0, 55, 0, 82, 0, 34 3V4G,ASP_8,3.91,0,-0.02,0.13 3V55,TYR_389,10.57,0.11,0.21,0.24 3R87.TYR 12.10.38.0.0.11.0.28 1NWA.GLU 52,7.6,3.33,-0.41,0.19 4FCU,ASP_50,3.85,-0.38,-0.59,1.03 2DVK,LYS_23,10.47,-0.09,0,0.07 3P28,LYS_59,10.43,-0.14,0,0.07 1MTZ,GLU_7,3.41,0.33,-0.85,-0.57 3LOE,ARG 537,12,45,-0.05,0,0 1W24,LYS_173,10.44,-0.15,0,0.08 2X4L,ARG_214,12.4,-0.27,0,0.18 3C5V,LYS 119,9,74,-0.63,0,-0.13 3RJZ.GLU 174,4,42,0,24,0,-0,32 2CN1,TYR_98,10.23,0,0.07,0.16 1VSM,ARG_158,12.22,-0.19,0,-0.09 2Q07,LYS_525,10.06,-0.44,0,0 2RFA,ARG 146,13.47,-0.56,0.9,0.62 1NRI,LYS 102,10.92,-0.69,0.85,0.26 1MHN,GLU_121,4.82,0.35,0,-0.04 2P4D,TYR_7,10.14,0,0,0.14 1DUN,LYS_35,10.23,-0.37,0,0.1 105J.ARG 19,12.6,-0.29,0,0.39 1SUU,LYS_514,11.36,-0.38,0.65,0.59 1QYI,TYR_257,10.33,0,-0.13,0.46 1RI6,ASP_168,3.98,0,0,0.18 2A6B,GLU_200,4.5,0,0,0 1SFE,ARG_33,12.36,-0.13,0,-0.01 3B21,HIS_96,6.6,-0.32,0.65,-0.23 4FZR,ARG_76,12.4,-0.1,0,0 3HUE,ARG_114,12.26,-0.55,0,0.3 2CVB,GLU 10,4.78,0.41,0,-0.13 2QRX,HIS_36,6.4,-0.18,0,0.1 1V8E,ASP_48,2.37,-2.15,-0.2,0.91 2PWQ,LYS_27,10.62,-0.16,0,0.28 3DHN,LYS 66,11.61,-0.27,0.76,0.61 1RHS,ARG_7,12.9,-0.82,0.72,0.5 1LTU,ARG_115,11.95,-0.84,0,0.3 1N81,LYS_170,10.35,-0.35,0,0.2 3P2F,ARG_151,12.34,-0.28,0,0.12 2BDV,ARG 137,12.42,-0.08,0,0 3TMO.HIS 279.6.46,-0.09.0.0.05 3EVN,ARG_263,12.6,-0.32,0.02,0.4 2QOP,LYS_55,10.36,-0.53,0,0.38 1WYC,ARG_301,12.68,-0.29,0.18,0.29 4ANN,GLU_93,2.98,0.42,-1.55,-0.38 1FKM,GLU_472,4.64,0.32,0,-0.19 1TD6.LYS 56.10.-0.43.0.-0.07 3F5D,GLU_60,4.44,1.65,-1.54,-0.18 1J7G,ARG_53,12.26,-0.24,0,0 20KT.TYR 56.11.05.-0.3.-1.46.2.8 1HF8,GLU_187,4.56,0.81,-0.67,-0.08 3BJV,LYS_20,10.57,-0.05,0,0.12 1SIG,ASP_167,3.82,0,-0.09,0.11 2PGX,HIS_27,7.29,-0.42,0.85,0.36 2X4G,TYR 238,12.07,-0.03,0.34,1.75 2D7U,GLU_328,4.69,0.52,-0.32,-0.01 1X04, ARG_223, 12.48, -0.28, 0, 0.27 1DTO,TYR_83,9.25,-0.77,-0.38,0.41 1SIG.GLU 146.4.83.0.35.0.-0.03 1NRI,ASP_183,3.03,-1.56,-0.26,1.05 2IQT,CYS_183,10.06,-0.71,0.21,1.55 2QZQ,HIS_84,5.97,-0.55,0.08,-0.07 3T5B,ASP 317,3.29,-0.66,-0.58,0.72 1WNH,TYR_180,13.91,0,0,3.91 1Q2Y,ARG_78,12.4,-0.37,0,0.26 2DG7,ARG_46,12.54,-0.17,0,0.21 1R6Y,CYS_37,10.36,-0.81,0.36,1.81

1H4U.TYR 431,10.16.0.-0.14.0.29 3M70.HIS 265.5.48.-0.56.0.-0.46 2BAA,ARG_215,13.92,-3.22,2.21,2.42 10IS.LYS 256.10.1.-0.4.0.0 3BWT,GLU_598,3.75,0.4,-0.85,-0.3 3UV9,CYS 451,9.47,-0.19,0.12,0.53 1C3K,ASP_50,2.12,-2.33,-0.08,0.73 2BDD,LYS_78,11.13,-0.29,0.45,0.48 2NYC,LYS_315,10.56,-0.15,0,0.21 2GAU,GLU_171,4,0.39,-0.86,-0.02 3PM2.GLU 91,2.96.0.39,-1.55,-0.38 3V3T,ASP_135,3.93,0,-0.1,0.23 1KCM.ASP 242.3.66,-0.16,-0.17,0.18 3ASA,HIS_351,5.19,-0.78,0,-0.52 3GFP,TYR 347,9.34,-0.85,-0.35,0.53 204D.GLU 64,3.36,1.3,-1.91,-0.53 4ANN,GLU_52,4.24,0.6,-0.84,-0.02 1ZBP,ARG_72,12.64,-0.32,0,0.45 1TXJ,GLU_132,5.11,0.61,0,0 3NZL,GLU_68,3.62,0.37,-0.85,-0.39 1EV8,ASP_246,2.75,-1.61,-0.56,1.11 1WLY.ARG 262.12.98.-1.18.0.81.0.85 2XHC,ARG_251,12.5,-0.39,0.16,0.23 1WPA,GLU 480,4.07,0.34,-0.53,-0.25 3M7G,GLU 221,4.85,0.2,0,0.15 2O8P,ASP_85,3.96,0,0,0.16 2QK0,ARG_36,13.79,-0.54,1.45,0.38 1YTQ,TYR_78,10.31,-0.83,0.23,0.91 3GYW, ARG 268, 12.89, -0.27, 0, 0.66 2PGX,GLU_186,3.84,0.51,-0.62,-0.55 2H14.LYS 159.10.48.-0.08.0.0.05 1TD6,HIS_35,6.45,-0.21,0,0.16 3R87,ARG 33,12.44,-0.72,0,0.66 1TD6.GLU 153.3.96.0.18.-0.85.0.13 4DNU,HIS_118,7.49,-0.21,0.84,0.36 3T8R,GLU_21,4.04,0.49,-0.78,-0.18 3V1Q,ARG_609,12.44,-0.06,0,0 2YX0,GLU_23,4.64,0.14,0,0 2OBI,LYS_105,9.91,-0.93,0,0.33 1J7G,LYS_35,10.44,-0.17,0,0.11 3HNX,CYS_83,10.2,0.43,0.48,0.29 2E3S,LYS 594,10.58,-0.24,0.01,0.32 2EYI.GLU 189.3.08.0.47,-1.53,-0.35 4AE7,ARG_223,13.03,-0.46,0.5,0.5 10IS,CYS_273,11.23,-0.01,-0.02,2.27 1V43,HIS_293,5.18,-1.81,0.14,0.35 2RIK,LYS 279,10.42,-0.08,0,0 1ES9,LYS_37,10.52,-0.16,0,0.18 2P5D,LYS_39,10.97,-0.53,0.3,0.7 1YTD, ASP_173, 3.75, 0, -0.25, 0.2 1X9G,GLU_94,4.81,0.17,0,0.14 2G5X,GLU_191,4.64,0.27,0,-0.13 3DHN,HIS_210,6.48,-1.16,0.63,0.51 1L3K.GLU 117.3.86.0.63.-0.85.-0.42 1SIG,CYS_291,12.04,-0.03,0.37,2.71 2RIS,ARG_133,11.88,-0.88,0,0.26 10ZN.TYR 157,11.38,-0.85,0.07,2.15 3HUE, ASP_72, 2.82, -2.29, -0.34, 1.65 1ZCU,GLU_78,4.07,0.45,-0.73,-0.14 3LJN,LYS_308,10.9,-0.31,0.38,0.33 3L3P,ASP 493,4.08,-0.05,-0.15,0.48 1GPP,ARG_42,12.33,-0.4,0,0.24 3P28,HIS 169.6.53,-0.73,0.83,-0.07 2ZQ5,ASP_45,4.19,0,0.01,0.38 2Q13,LYS_158,10.44,-0.06,0,0 2X4G,HIS 26,3,49,-2,02,0,-1 3D9H,ASP_116,4.11,0,-0.01,0.33 2NRK,LYS_62,10.56,-0.27,0,0.33 3A4C,ARG_493,13.24,-0.4,0.85,0.28

1ZHV.LYS 67.9.57.-0.76.0.-0.18 2VGY,HIS 91,7.11,-0.28,0.54,0.34 1NKD,GLU_24,4.79,0.25,0,0.04 3F5D,HIS_84,5.96,-0.27,0,-0.28 4DBX,HIS_202,7.25,-1.95,0.38,2.32 3U2R,GLU 118,3.63,0.2,-0.7,-0.37 3M9A.TYR 7,10.06.0.0.01.0.05 3GFP,LYS_477,10.46,-0.09,0,0.05 2BDD,LYS_43,10.44,-0.09,0,0.03 3AUF,GLU_187,3.98,0.72,-0.56,-0.69 3T8R,ARG 59,12.47,-0.03,0,0 2B3M.GLU 30.4.57.0.13.0.-0.06 3HQX,GLU_64,3.01,0.37,-1.21,-0.65 1PNE,HIS_119,6.26,-0.19,0,-0.04 3FK5,ARG 269,12.27,-0.32,0,0.1 3U2R/HIS 130.6.08,-0.28,0,-0.15 2AZL,GLU_117,5.65,1.14,0,0.01 1NFN,GLU_96,4.11,0.37,-0.23,-0.54 1BKB,TYR_11,10.06,-0.44,0.19,0.31 3C2E,GLU_212,5.19,0.48,0,0.22 2YWJ.ARG 101.11.94.-0.77.0.07.0.14 1MUF,GLU_163,4.88,0.37,0,0.01 2FD4,GLU_531,3.17,0.57,-1.13,-0.77 2VC8,HIS 42.6.74,-0.55,0.79,0 1SIG.TYR 148.11.57.0.0.23.1.34 2B78,LYS_351,10.47,-0.03,0,0 1PV5,LYS_148,11.32,-0.23,0.61,0.45 2CVB,GLU_60,3.62,0.4,-0.9,-0.38 2Cl3,LYS_105,11.74,-0.57,1.12,0.7 3CAN.GLU 93.4.55.0.3.0.-0.25 1TR9,LYS_151,10.42,-0.12,0,0.04 2V81,ASP_178,4.48,0,0.01,0.68 2FD4,ASP 439,2.75,-1.56,-0.25,0.75 3EJG,CYS 157,9.48,-0.02,0.22,0.3 2AZP,HIS_10,5.65,-0.63,0,-0.22 3HVM,GLU_21,4.57,0.24,0,-0.17 1DUP,ARG_71,11.84,-0.76,0,0.1 3Q1C,TYR_313,10.34,0,0.05,0.29 1AT0,ARG 283,13,47,-0.35,0.82,0.5 2B3M,GLU_33,4.63,0.09,0,0.04 2CWC,LYS_43,10.42,-0.13,0,0.04 1FO9,LYS_232,9.84,-0.68,0,0.02 2QRX,ASP 51,3.02,-1.19,-0.05,0.46 2FC3,GLU_116,3.57,0.31,-0.85,-0.39 200K,HIS_59,5.56,-0.99,0,0.04 3OA7, ARG_441, 12.37, -0.13, 0, 0 2F9F,GLU_78,3.53,0.27,-0.85,-0.39 1MIX.TYR 373.10.25.0.0.01.0.24 2P1W,LYS_99,10.41,-0.09,0,0 2G9D,ARG_268,12.26,-0.53,0,0.29 2O8P,LYS_185,10.49,-0.21,0,0.19 2EJX,LYS 9,10.6,-0.36,0,0.45 4EUG,GLU_30,2.02,0.68,-2.4,-0.77 2B6P,TYR_105,9.83,-0.02,-0.37,0.22 3FXH,ASP_60,3.96,-0.05,0,0.21 3EJG,TYR_151,10.35,0,0.2,0.14 2JEO, ARG_169, 12.08, -1.87, 0, 1.44 3Q2C,ARG_72,13.18,-0.28,0.15,0.82 2H2W,HIS_84,6.46,-1.5,0.85,0.61 4DBX,TYR_37,11.61,0,0.08,1.53 1PDB,ASP 168,3.08,-1.22,-0.04,0.53 2A6B,LYS 98,10,38,-0,2,0,0.08 2IXM,GLU_156,7.25,4.93,-2.47,0.29 2PIM,ARG_12,12.16,-0.26,0,-0.09 1RI6,LYS_269,9.78,-1.05,0,0.35 3N2T,HIS_88,5.96,-0.94,0.85,-0.45 3RNV,HIS_430,6.1,-0.32,0,-0.09 20EV.GLU 75.4.99.0.3.0.0.18 4GA2,ARG_10,13.31,-0.23,0.79,0.25

3IBT,LYS_61,10.49,-0.07,0,0.05

10IS.ASP 321.3.81.0.-0.12.0.13 3H04,LYS_145,10.45,-0.05,0,0 3B7X,GLU_88,4.79,0.1,0,0.18 4DNU,ARG_338,11.23,-1.05,0,-0.22 3EVP.ASP 177.3.43.-0.77.0.0.39 1042.TYR 168.13.96.0.0.18.3.78 3NZL,GLU_41,4.76,0.27,0,-0.01 4DNU,TYR_90,11.26,0,0.25,1.02 10TM,LYS_114,10.46,-0.15,0,0.1 4ACJ.GLU 643.4.69.0.17.0.0.01 1UAJ,GLU_239,3.51,0.34,-0.7,-0.63 3EUR,ASP_127,4.69,-0.02,-0.04,0.94 1FO9,ARG_429,11.56,-0.99,0,0.06 4FZN.ARG 208,13.38,-0.34,0.82,0.4 2E0T,LYS 181,10.28,-0.27,0.0.04 2NSN,GLU_80,2.56,0.89,-2.24,-0.6 2FXT,GLU_413,4.17,0.53,-0.61,-0.25 1Y0K,ARG_8,12.66,-0.23,0.39,0 3CXS.CYS 128.10.17.0.0.03.1.14 2P52,ARG_155,13.17,-1.31,1.31,0.67 2R57,HIS_262,5.73,-0.67,0,-0.09 3I0C,GLU_190,5.04,0.72,0,-0.18 3V4G,ASP 113,3.92,-0.2,-0.07,0.39 1X7F,LYS 249,10.82,-0.31,0.0.62 3LD1,TYR_341,10.38,-0.04,-0.14,0.56 2CI3,HIS_172,8.37,-2.97,0.85,3.99 3M3P,GLU_133,2.97,0.51,-1.66,-0.38 1K95,GLU 92,4.89,0.34,0,0.06 2H2W,LYS_203,10.69,-0.14,0,0.33 2ZQ5,TYR_365,9.35,-0.78,-0.17,0.31 3LJC,GLU_222,4.36,0.2,0,-0.34 2FPN.ARG 73,12,72,-0.32,0.0.55 1UXO,LYS 135,10.52,-0.17,0,0.19 1YW5,LYS_82,10.38,-0.12,0,0 1XEU,GLU_282,4.7,0.23,0,-0.03 1IDK,ASP_160,3.46,-0.69,0.02,0.33 3LJI,TYR 53,12.93,-0.55,0.23,3.24 3BWT,ASP 663,3,3,-0,38,-0,36,0,24 1RI6,GLU_334,4.52,0.2,0,-0.18 3IL3,ASP_101,4.01,0,0.03,0.18 1FO9.TYR 356.13.09.-0.72.-0.33.4.14 1O3X.LYS 210.11.08.-0.39.0.32.0.65 3V75,LYS_116,10.27,-0.35,0,0.12 1J33,LYS_263,9.73,-0.68,0,-0.09 1QYI,LYS_228,10.17,-0.74,0,0.41 1WLY,ARG 167,12.19,-0.36,0,0.05 1R7J.GLU 68,4,45,0,23,0,-0,27 2IRM,HIS_335,3.42,-2.6,0,-0.47 3KT2,GLU_21,5.75,1.25,0,0 3GOZ,LYS_102,11.06,-0.23,0.34,0.46 2GZO,ARG 83,11,49,-1,03,0,0,01 3M7G,ARG_148,11.49,-2.92,0.01,1.9 3HVM,LYS_123,10.14,-0.4,0,0.03 3NR5,GLU_19,4.67,0.23,0,-0.07 1X7F,ASP 349,3.72,-0.53,-0.48,0.91 2l6l.GLU 23.4.89.0.28.0.0.11 2QDJ,GLU_275,4.53,0.35,0,-0.32 3ERF,LYS 199,10.21,-0.29,0,0 3EVP,TYR_264,13.33,-0.85,0.07,4.11 4FH3,LYS_150,11.19,-0.32,0.54,0.46 1G8P,ARG 177,12.67,-0.7,0.16,0.72 1059,HIS_109,6.2,-0.95,0.61,0.04 2PP6,ARG_62,12.41,-0.22,0,0.13 3FHF,GLU 61,4.6,0.18,0,-0.08 1W7B.ARG 304.12.78.-1.26.0.44.1.1 2D7U,GLU_84,6.91,4.41,-1.47,-0.55 2CL3,TYR 45,12.43,0,0.23,2.2 3GMS,LYS_4,11.05,-0.4,0.3,0.65 3KEY,CYS_451,12.33,-0.02,0.34,3.01

3V75.ARG 260.12.55.-0.05.0.0.1 3U2R,ARG 50,13,23,-0,34,0,65,0,43 4EKU,LYS_60,10.4,-0.12,0,0.01 1SJ8,HIS_541,6.51,-0.3,0,0.31 3V3T.GLU 153.3.88.0.33.-0.49.-0.46 1NAR,GLU_280,5.39,3.96,-3.05,-0.02 1TWU,ARG_4,12.45,-0.05,0,0 1SIG,ARG_397,12.42,-0.1,0,0.02 2Z61,ARG_363,11.85,-1.03,0,0.38 1SJ8,HIS_663,6.64,-0.21,0,0.35 3ASA,ARG 90,12.32,-0.72,0.08,0.47 3RVC,GLU_186,4.81,0.31,0,0 3PBH,TYR_140,13.34,0.77,0.51,2.06 2BDV.LYS 75.11.33.-0.49.0.85.0.48 1PSW,TYR 28,10.04,-0.72,-0.37,1.12 2B3M,LYS_37,10.19,-0.35,0,0.04 2YWK,ARG_10,13.9,-0.53,1.01,0.91 2NRK,ASP_144,2.88,-1.08,-0.13,0.28 3V75,ASP 117,2.89,-0.91,-0.41,0.41 1TR9,GLU_95,4.55,1.2,-0.65,-0.5 3AU3,GLU_403,4.41,0.3,0,-0.39 1ANU,GLU_17,3.58,0.31,-0.74,-0.49 3PAC, ARG_167, 12.28, -0.34, 0, 0.11 2NSN.ARG 27,12.77,-0.64,0.46,0.45 3CZC,LYS_19,10.3,-0.28,0,0.08 1Y0K,ASP_204,3.96,0,0,0.16 3RJZ,LYS_32,10.51,-0.25,0,0.26 1TLV,TYR 80,10.64,0,0.23,0.41 2FM9.LYS 113.10.14.-0.34.0.-0.02 2AZP,TYR_137,12.68,0.8,0.63,1.25 4EUG,LYS_57,9.77,-1.02,0,0.28 2B3M,GLU_132,4.46,0.15,0,-0.18 1C3K.LYS 124,10.48,-0.05,0,0.03 3IU5,TYR_54,11.26,-0.02,1.39E-17,1.27 3CCY,ARG_103,13.11,-0.6,0.75,0.46 2AZL,GLU_184,3.98,0.32,-0.47,-0.38 1SQW,LYS 18,10.4,-0.26,0,0.16 4EUG,LYS_170,10.39,-0.21,0,0.1 1PNE,LYS_90,10.2,-0.34,0,0.04 2WB8,ARG 486,12.38,-0.31,0,0.18 3IPZ,TYR_142,12.14,-0.85,0.34,2.65 1ILW,GLU 169,3.2,0.51,-1.2,-0.61 1AK1.GLU 272.6.75.1.5.0.0.74 1MTZ,TYR_16,10.09,0,-0.12,0.21 1QYI,GLU_158,3.72,0.59,-0.85,-0.52 2EYI,GLU_114,4.51,0.41,-0.64,0.24 2RIK.HIS 196.6.35,-0.13,0,-0.02 4ACJ,ASP_640,4.04,0,0.02,0.23 2YT4.GLU 536.4.55.0.05.0.0 1JKS,LYS_46,10.34,-1.18,0.85,0.18 2VGY,TYR 40,10.76,0,-0.12,0.87 3ASA,HIS 33,6,12,-0,35,0,-0,03 3BA1,ASP_63,2.76,-0.85,-0.59,0.4 3CXS,ARG_129,12.39,-0.4,0,0.28 4ETX,ASP_229,3.95,0,-0.12,0.27 1P2F,GLU_20,4.48,0.3,0,-0.31 3RNV,ASP_398,3.9,0,-0.12,0.22 2H2W,HIS_281,5.63,-1.55,0.76,-0.08 1TR9,ARG_130,13.76,-1.73,1.37,1.61 4ECC,ASP_203,3.25,-0.53,-0.38,0.37 1EO6.GLU 85.3.49.2.62.-2.96.-0.65 4E8B,GLU_113,4.53,0.41,-0.74,0.37 1Z3X,HIS_82,6.07,-0.33,0,-0.1 1V6T,TYR_170,12.81,-0.81,0.09,3.53 1U53,ASP_51,2.38,-1.93,-0.43,0.93 2Z61,ASP_316,3.2,-0.89,-0.3,0.59 1BYI,TYR_31,10.14,0,-0.18,0.31 3GG6,GLU_164,3.88,0.29,-0.72,-0.19 1RWZ,LYS_12,9.73,-0.76,0,-0.01

1YTO.ASP 127.2.78.-1.49.-0.61.1.07 2B78,ARG 246,12,71,-0,48,0,0.69 1L2H,LYS_88,10.44,-0.06,0,0 2Z84,HIS 177,7.84,-1.54,1.6,1.28 1H4U,HIS_545,6.14,-0.36,0,0 2QHT,ASP_7,2.77,-1.51,-0.5,0.98 2YT4.LYS 629.11.37.-0.35.0.85.0.37 3CBN,ASP_66,3.72,-1.66,0,1.58 1QZN,GLU_123,4.9,0.26,0,0.13 3M7G,ASP 6,4.31,-0.09,-0.02,0.62 3L3P,ASP 256,3.65,-0.09,-0.31,0.25 3CCY,GLU_72,4.58,0.34,0,-0.27 1KN3,LYS_179,10.38,-0.12,0,0 2QK1,ASP_326,2.02,-1.9,-0.39,0.51 4AE7.ARG 96,12.46,-0.04,0,0 3FNI.CYS 136.11.29.-0.16.0.01.2.44 1WPA,GLU_469,4,0.24,-0.74,0 3QAV,TYR_99,10.37,-0.03,-0.17,0.56 3IRA,GLU_62,4.98,0.66,0,-0.19 3UPD,ARG 167,13.3,-0.42,0.58,0.65 1RHS,GLU_17,3.49,0.23,-0.63,-0.6 3G9T,ASP_254,2.32,-1.59,-0.52,0.64 2D7U,GLU_313,4.84,1.59,-0.86,-0.39 3E7P.HIS 221,6.13,-0.68,0.38,-0.06 3BCY.GLU 64.4.62.0.53.0.-0.41 3LMF,ARG_109,13.23,-0.37,0.51,0.61 3DB9,ASP_107,3.01,-1.59,-0.09,0.88 3JRT,ASP_151,2.86,-1.34,0,0.4 2D8N, ASP 112, 3.93, -0.1, -0.05, 0.27 3C6B,GLU_290,3.71,0.28,-0.67,-0.4 2X4G,LYS_14,10.92,-0.35,0.6,0.17 4AM1,GLU_176,4.03,0.19,-0.66,0 3PZ9,TYR 247,10.35,-0.02,0.05,0.33 1R53,ARG 209,12.51,-0.27,0.0.28 1J74,TYR_113,10.42,0,0.02,0.4 2OJQ,ARG_373,13.82,-0.44,1.13,0.63 1R3D,ARG_112,12.14,-0.35,0,-0.01 1MTZ,ARG 143,12.83,-0.71,0.18,0.86 1ZKZ,TYR_32,11.41,0,0.04,1.37 3EUR,GLU_48,5.16,0.25,0.35,0.06 3H13,CYS_406,12.93,-0.24,0,4.17 1X7F,ASP 103,2.2,-1.74,-0.32,0.46 1SNT.ASP 144.3.94.0.-0.06.0.21 1YG2,ARG_155,12.89,-0.33,0.34,0.38 3JRT,ARG_103,12.33,-0.83,0.33,0.32 2ZCO,LYS_270,10.17,-0.14,0,-0.19 3BPP,TYR_221,10.89,0,0.24,0.65 2IF4,LYS 194,9.09,-1.11,0,-0.31 2AHE,TYR_104,10.87,0.19,0.03,0.65 2RIK,CYS_261,11.36,-0.85,0,3.21 2JHY,GLU_193,4.54,0.67,0,-0.64 3L3P.ARG 349,12.42,-0.76,0.14,0.54 4DIU,TYR_76,11.78,0,0.17,1.61 2RIS.HIS 145.8.4.-1.91.1.7.2.1 3O16,GLU_96,4.33,0.24,-0.62,0.21 2NRR,LYS_419,10.24,-0.18,0,-0.07 2WOZ,LYS 399,10.84,-0.24,0,0.59 1SIG,TYR_425,10.02,0,-0.06,0.08 1P2F,ARG_182,12.42,-0.08,0,0 4H4J,TYR_106,12.6,0,0.48,2.12 1SJY.GLU 103.4.61.0.29.0.-0.18 2G9D,LYS_162,9.43,-0.67,0,-0.4 3TOW,CYS 147,10.25,0,-0.27,1.53 2NSN,LYS_46,10.44,-0.07,0,0 1JSX,HIS_153,5.58,-1.09,0.01,0.17 1HF8,ASP 235,3.03,-0.77,-0.49,0.48 3BPP,TYR_233,10.04,0,0,0.04 1MD6,LYS_78,10.32,-0.32,0,0.14 2WOZ,GLU_429,4.57,1.13,-0.85,-0.2

2EFK.ASP 264.2.09.-2.48.-0.01.0.78 3D9H,HIS_74,4.2,-2.94,0.9,-0.26 1LTU,LYS_53,10.41,-0.09,0,0 3U0V,LYS_110,10.46,-0.05,0,0.01 1059,TYR_210,10.25,0,-0.36,0.61 4ANN, ASP 84, 3.93, -0.28, -0.36, 0.78 2WOZ,TYR 438,10,3,0,-0,22,0,53 1WXQ,ARG_100,12.32,-0.36,0,0.18 1DVO,GLU_164,2.99,0.4,-1.27,-0.64 2CXA,ARG_205,12.53,-0.07,0,0.11 2CBE,GLU 106,8.75,5.23,-1.61,0.62 1SUU.GLU 655.3.52.3.63.-2.01.-2.6 4EF5,ARG_220,12.36,-0.3,0,0.16 2Z61,ARG_284,13.13,-0.52,0.5,0.66 1KW4,ASP_20,4.07,0,0.09,0.18 3R2E.CYS 50.9.5.0.0.13.0.37 2QHT,ARG_25,12.15,-0.26,0,-0.08 4DVD,ASP_49,3.85,-0.01,-0.19,0.26 3A4C,ASP_536,3.37,-0.74,-0.01,0.32 2B61,CYS 91,11.11,-1.17,0.25,3.03 1X7F.TYR 292,10,-0.02,-0.14,0.18 3RJZ,LYS_207,10.57,-0.09,0,0.16 3DHN,LYS_151,10.28,-0.22,0,0 3UC9.GLU 162.4.4.0.24.-0.37.0.02 1SUU,LYS 773,10.24,-0.32,0.0.07 1MUF,LYS_158,10.82,-0.24,0.2,0.36 4E6S.ARG 24.12.45.-0.05.0.0 3ONT,HIS_130,6.09,-0.3,0,-0.11 1U7U,LYS_345,10.66,-0.52,0,0.68 2CBE,ASP 175,3.92,0,-0.03,0.15 1J33,CYS_94,12.1,0,-0.27,3.38 2EHG,ARG_136,12.77,-0.18,0,0.45 2APL/ASP 119/2.61/-1.56/-0.42/0.8 4EKULYS 216.10.5.-0.08.0.0.07 4F3J,TYR_233,10.52,0,0.22,0.3 1T3Y,ASP_20,2.76,-0.92,-0.38,0.27 1UJ8,HIS_8,6.25,-0.15,0,-0.11 1WJG,TYR_9,11.43,0,0.25,1.17 2E3C,GLU_249,4.65,0.84,0,-0.69 2FGG,HIS_6,6.37,-0.13,0,0 1DVO,TYR_161,10,-0.02,-0.64,0.66 2FD5,ASP_143,3.96,0,0,0.16 2X5Y,LYS 755,10.81,-0.39,0.03,0.67 1VJG,LYS_167,10.5,0,0,0 2VAN,ARG_126,13.71,-0.66,1.42,0.46 3K1H,GLU_78,4.66,0.31,0,-0.16 1BYI,ARG_3,12.73,-0.42,0.35,0.31 1DCF.GLU 128,4.57,0.39,0,-0.31 3I4T,LYS_106,10.23,-0.17,0,-0.1 3QKY,ARG_96,12.82,-0.39,0.14,0.57 2YWX,ARG_138,12.55,-0.16,0,0.2 1T07,GLU 69,2.79,0.56,-1.7,-0.56 3AUF,ARG_196,12.39,-0.1,0,-0.01 3CX2,ASP_163,2.96,-1.18,0,0.34 3CZC,ASP_80,3.51,-0.8,0.15,0.36 3TOW, ARG_145, 12.36, -0.43, 0, 0.28 2F4Q,ARG_114,12.33,-0.17,0,0 3BJV,HIS_111,5.48,-1.02,0,0 4EVF,HIS_228,5.37,-0.87,0,-0.28 3M7D,TYR_268,11.74,0.85,0.31,0.57 4EKU,GLU 36,4.41,0.27,-0.57,0.2 3GMS.ASP 113.3.78.0.-0.17.0.15 2WB3,LYS_379,10.98,-0.4,0,0.87 3GA2,HIS_122,4.55,-1.91,0,-0.04 1J85,ASP_41,2.78,-1.17,-0.42,0.57 2F4Q,ARG_261,12.39,-0.11,0,0 2Y2T,ASP_75,3.35,-0.8,-0.11,0.46 3CO1,GLU_94,4.35,0.12,0,-0.26 3L3P,ARG_494,12.18,-0.31,0,-0.01

2NYC,LYS 185,10,41,-0.09,0,0 3A7L,GLU_76,4.67,0.24,0,-0.07 3FNI,ASP_46,3.1,-0.98,-0.03,0.3 2VAN,LYS_234,9.71,-0.73,0,-0.06 2FBLGLU 73.3.35.0.44.-1.16.-0.42 2XWS.TYR 111,10.07.0.0.02.0.05 4AF2,HIS_6,6.9,-0.39,0.43,0.36 1SBX,HIS_89,6.42,-0.08,0,0 1BYI,GLU_137,3.64,1.33,-1.8,-0.4 3KT9.CYS 5.11.87.0.0.31.2.56 3B7H,ASP_69,3.05,-0.84,-0.12,0.22 2R0S.TYR 318,11,59,0.0.26,1.33 2EFK,ARG_27,12.42,-0.17,0,0.09 1EDG.ASP 281.3.99.-0.83.0.29.0.73 208P.GLU 188,3.8,0.37,-0.69,-0.38 3LPZ,ARG_257,12.33,-0.3,0,0.13 1TJE,LYS_122,10.56,-0.1,0,0.16 2QOP,GLU_61,5.12,0.51,0,0.12 3ASA.ARG 340.12.46.-0.08.0.0.04 2E3C,GLU_360,4.09,0.45,-0.57,-0.3 2R0S,ASP_109,2.58,-1.64,0,0.43 3E0H,TYR_102,11.04,0,0.16,0.88 3D9H.ARG 144.13.02.-0.56.0.81.0.26 3RJX.TYR 39.11.77.0.81.0.41.0.55 3KB5,ARG_444,12.37,-0.09,0,-0.03 1EV8,ARG_166,12.23,-0.77,0,0.49 1TWU,GLU_30,4.2,0.72,-0.66,-0.36 4DNU,TYR 248,13.99,0,0.56,3.43 2GZR,ASP_272,3.94,0,-0.02,0.16 1GXN.ARG 468.12.55.-1.51.0.82.0.74 3GW3,TYR_311,12.26,0.85,0.8,0.61 3U0V/CYS 12,9.78,-0.31,-0.26,1.36 2AXO,TYR 85,9.85,-0.74,0.0.58 3IPZ,GLU_146,4.71,0.19,0,0.02 2H01,ASP_125,3.76,-1.56,-0.08,1.6 2WB8,LYS_618,10.31,-0.17,0,-0.02 1R3F,ARG 271,12.25,-0.26,0,0.02 2P1W,ASP 139,3.66,-1.21,-0.46,1.53 1ANU,ASP_40,2.95,-1.05,-0.22,0.43 1Z3X,ASP_47,3.57,-0.85,-0.15,0.77 30DJ.HIS 134.6.51.-0.13.0.0.15 3ZSL,LYS 210,11.31,-0.37,0.8,0.37 3CZC,CYS_8,8.13,-2.02,0,1.15 2D2S,HIS_611,6.49,-0.27,0,0.26 3CCY,LYS_85,11.33,-0.35,0.79,0.38 2XWS,GLU 105,3.92,0.31,-0.85,-0.03 20ZO.GLU 139.3.64.0.78.-1.64.0 1EV8,GLU_195,4.64,0.17,0,-0.03 1JT9,CYS_219,9.05,-0.13,0,0.18 1V43.ASP 279.3.93.0.-0.02.0.15 1UJ8,ASP 54,3,48,-0,25,-0,29,0,21 3M66,LYS_274,11.19,-0.31,0.73,0.27 1WXQ,LYS_152,10.47,-0.05,0,0.02 3C2E,LYS_144,10.28,-0.24,0,0.02 10IS,ASP 141,3.09,-0.85,-0.01,0.15 2CN1,GLU_259,4.65,0.09,0,0.06 3BWT,ASP_562,3.93,0,-0.1,0.23 2HRZ,ASP 61,3.13,-0.43,-0.92,0.69 2B2H,TYR_284,10.73,-0.11,0,0.83 3HNX,ASP 36,3.92,-0.56,0.14,0.54 105J,GLU_76,4.51,0.11,0,-0.11 2B61,LYS_314,10.47,-0.24,0,0.2 1V43,LYS_82,10.49,-0.27,0,0.26 3RJZ,LYS_129,10.55,-0.2,0,0.24 2D7U.TYR 52,10.09,-0.38,-0.28,0.75 4DNU,LYS_165,11.62,-0.41,0.78,0.75 3BA1,ARG_288,11.32,-1.26,0,0.08 1V43,GLU_334,4.84,0.57,0,-0.23 3F5D,HIS_188,6.3,-0.2,0,0

2CYG.ARG 232.12.45.-0.05.0.0 1NIJ.ARG 22.12.49.-0.2.0.0.19 2H85,GLU_91,4.13,0.41,-0.41,-0.37 3GYW,ASP_223,3.81,0,-0.15,0.17 3E7P,ASP 165,4.01,0,-0,12,0.32 2PWO.GLU 94.4.66.0.16.0.0 2V4X,TYR_116,11.52,-0.85,-0.33,2.7 2H01,ARG 61,13,28,-0,42,0,62,0,57 2E0T,TYR_113,11.67,-0.72,0.01,2.38 2B61,ARG_61,13.77,-0.41,1.05,0.62 2R0S,ASP 311,3,43,-0.57,-0.17,0.37 1PVT.GLU 72.4.8.0.22.0.0.09 1XIP,HIS_70,6.13,-0.93,0.76,-0.21 2X5Y,LYS 849,10.11,-0.47,0.0.07 2WOZ,TYR 317,12.67,0,0.41,2.26 3ANJ,LYS_3,10.45,-0.05,0,0 4DBX,TYR_288,11.23,0,0.43,0.81 3DTE,ARG_72,12.02,-0.23,0,-0.25 1PVT,ARG 6,12.26,-0.18,0,-0.06 20VO.LYS 7,10.41,-0.47,0.0.37 1RKA,GLU_214,4.67,0.26,0,-0.08 1FQI,GLU_345,4.2,0.29,-0.16,-0.43 1XDZ,LYS_219,10.32,-0.19,0,0 2G9D,GLU 146,4.01,0.42,-0.74,-0.18 4H86,ASP_108,2.59,-1.61,-0.15,0.54 3B21,GLU_44,3.71,0.37,-0.77,-0.38 2D0A,ARG_258,12.41,-0.22,0,0.13 3IBT,GLU_226,4.75,0.24,0,0.02 1AKO.CYS 241,10.62,-0.27,0.07,1.83 2CXC,LYS_90,10.58,-0.08,0,0.17 1RL0,GLU_99,2.84,0.71,-1.73,-0.64 2EEY,LYS 137,10,-0,34,0,-0,17 2G2D,ASP_148,4.03,0,0,0.23 3UAH,ARG_204,10.85,-2.09,0,0.43 2CXY,TYR_23,12.79,0,0.07,2.72 3M70,ASP_54,3.89,-0.2,-0.02,0.31 3LJC,ARG 17,11.09,-1.15,0,-0.27 2YWK,LYS_43,10.5,-0.13,0,0.13 3CAX,ARG_428,12.44,-0.09,0,0.03 1V43,GLU_128,4.65,0.31,0,-0.16 2PGX,ARG_101,11.77,-1.27,0,0.55 4DBX,LYS 113,10.39,-0.24,0,0.13 208P.TYR 137.11.21.0.0.05.1.16 1LZL,ARG_263,12.88,-1.07,0.71,0.74 4ETX,GLU_357,3.59,0.32,-0.73,-0.49 3IRA, ARG 81, 12, 67, -0.81, 0, 19, 0, 78 3V1Q,GLU_545,3.64,0.31,-1.17,-0.01 1YG2,ARG_148,12.27,-0.29,0,0.05 3VJ8.ASP 145.2.98.-0.78.-1.17.1.14 2AZP,TYR_185,11.42,0,0,1.42 3B21,LYS 132,10.52,-0.13,0,0.15 2R4O,LYS 193,10.2,-0.4,0,0.1 3DB9,ARG_173,11.64,-1.18,0,0.31 1UOH,TYR_161,11.26,0.22,0.53,0.5 1V8E,ARG_10,13.89,-0.56,1.48,0.47 2B6P,GLU_250,4.08,0.27,-0.68,0 1WNH,GLU_18,5.98,3.28,-0.84,-0.97 3ADO,ASP_226,4.02,0,0,0.22 2D2S,HIS_701,3.28,-2.81,0,-0.41 3CS1,GLU_29,4.75,0.21,0,0.04 3B7H,LYS 55,10.15,-0.21,0,-0.15 3UV9,CYS_380,11.92,-1.29,0.33,3.88 2XHC,LYS_24,10.57,-0.11,0,0.18 4DVD,ASP_163,3.03,-0.82,-0.29,0.34 3ZXY,HIS 30,6.21,-1.24,0.78,0.17 2EHG,LYS_82,11.28,-0.32,0.51,0.59 1L3K,LYS_130,10.61,-0.18,0,0.29 3O48,GLU_23,2.87,0.44,-1.69,-0.38 2AXO,HIS_125,5.48,-0.83,0,-0.19

2CXY,ARG_49,13.01,-0.31,0,0.82 2ZO5,ARG 214,11.15,-1.38,0,0.03 3UAH,LYS_246,10.48,-0.14,0,0.12 1X04,LYS_167,10.07,-0.24,0,-0.19 1KN3,LYS_182,10.41,-0.09,0,0 2DFL,LYS 235,10.15,-0.19,0,-0.17 2A0J,GLU_52,4.07,2.73,-2.33,-0.85 1NIJ,LYS_168,11.6,-0.23,0.84,0.49 10I7,HIS_63,5.62,-0.75,0,-0.13 3VJ8.TYR 341.10.76.-0.65.0.25.1.17 3ELI.GLU 96.4.15.0.41.-0.41.-0.35 1WNH,LYS_167,10.59,-0.27,0,0.37 3F6F.GLU 25,4,56,0,1,0,-0,04 2H85,GLU_113,3.21,0.43,-1.56,-0.16 1RZ2,TYR 124,10.38,0,0.13,0.25 3LH5,ARG_740,12.73,-1.48,0.47,1.24 3MTT,TYR_467,10.52,0,0.26,0.26 3ETU,ASP_37,3.94,0,0,0.14 1X6J,HIS_10,6.92,-0.41,0.73,0.1 1Q42,GLU_154,4.77,0.24,0,0.03 2H8O,LYS_145,10.35,-0.2,0,0.05 2D8N,LYS 22,10.35,-0.15,0.0 2QZQ,LYS_97,11.31,-0.44,0.85,0.39 1RI5,GLU 225,4.22,3.23,-2.37,-1.13 3NZL/HIS 75,6.39,-0.21,0.0.09 2OJQ,GLU_645,3.49,0.31,-1.32,0 2P5D,GLU_110,4.66,0.16,0,0 3H5T,ASP_297,3.39,-0.73,-0.14,0.46 2OGQ,CYS 372,9.25,-0.25,0.31,0.2 1PDB,ARG_36,12.15,-0.49,0,0.14 1QQE,ASP_98,3.99,-0.48,-0.09,0.75 1WPA,ARG_434,12.24,-0.27,0,0.01 1SUU,TYR 558,10.67,0,0.39,0.29 1UAJ.LYS 14,10.81,-0.15,0.0.46 4FLE,TYR_7,11.37,-1.53,0,2.89 3F7M,HIS_171,5.85,-0.82,0.01,0.16 2GAU,LYS_227,10.4,-0.09,0,-0.01 3CNU,GLU 20,4.62,0.12,0,0 3DHN,TYR_175,11.7,0,0.48,1.2 1IDK,ASP_77,4.58,-0.23,0.44,0.56 2VGM,LYS_165,10.26,-0.63,0,0.38 30N1,GLU 101,4.64,0.15,0.03,-0.04 3LD1.LYS 271.10.29.-0.38.0.0.16 2OPJ,CYS_266,12.81,0,1.11,2.7 2ZTY,ASP_32,3,-0.68,-0.65,0.53 1N81,ARG_144,12.45,-0.05,0,0 3ETV,TYR_94,10.18,-0.47,0.23,0.41 10TM.GLU 150.6.01,1.54,-0.63,0.61 1PGV,ARG_376,11.91,-0.77,0,0.18 1F2V,CYS_45,9.83,-0.97,0,1.8 1MTZ,LYS_28,11.18,-0.27,0.57,0.38 3PBH,HIS 49,6,26,-0,26,0,0.02 2F8H,TYR_148,13.62,0.85,0.68,2.09 3FTT.GLU 126.5.72.1.7.0.-0.48 2Z0W,CYS_64,10.46,0,0.33,1.14 1J7G,LYS_87,10.47,-0.03,0,0 3CAN.GLU 120,3.91,0.33,-0.85,-0.07 2QHT,LYS_173,10.39,-0.39,0,0.28 1YR6,GLU_113,3.78,0.35,-0.69,-0.38 2BV9,TYR_247,13.79,0.85,0.6,2.33 1046.GLU 99.4.59.0.23.0.-0.14 3C5V,ARG_371,12.54,-0.06,0,0.1 102Y,GLU 33,4,77,0,19,0,0.09 1C44,GLU_15,4.68,0.23,0,-0.05 3CAX,ARG_376,13.48,-0.22,0.8,0.4 1J74.LYS 24.11.-0.18.0.23.0.45 3ETU,ARG_44,12.39,-0.15,0.03,0 3CCY,LYS_172,10.25,-0.3,0,0.05 2W2S,ARG_167,12.33,-0.17,0,0

3LH5,LYS_702,10.41,-0.44,0,0.34 3VJ8.TYR 105.11.11.0.0.03.1.08 2QDJ,GLU_280,4.71,0.48,-0.16,-0.11 20JO.ARG 478,12.23,-0.84,0.0.58 3CAX,GLU_417,3.84,0.35,-0.38,-0.63 2D59,GLU 79,4.33,1.16,-1.16,-0.19 1IAP,HIS_228,5.75,-0.88,0,0.13 3DZ1,ASP_237,3.83,0,-0.12,0.16 1BN6,ARG_97,12.91,-0.32,0.17,0.57 1P2F,ARG_63,13.25,-0.14,0.39,0.5 1MTZ,HIS_264,5.83,-0.85,0,0.17 2B3M,HIS 84,5,78,-1,54,0,46,0,36 3A0X,LYS_699,10.43,-0.5,0,0.43 1059, ARG_179, 12.6, -2.17, 0, 2.27 3L7N, HIS 143, 3, 42, -2, 77, 0, -0, 31 1WPA,LYS 494,10.37,-0.13,0,0 3T5B,TYR_301,13.84,-0.05,0.92,2.97 2CBE,TYR_128,10.92,0.28,0.02,0.63 1LPL,GLU_186,4.83,0.25,0,0.08 1NJ4,GLU_342,5.08,0.98,0,-0.39 3DZ1,ASP 21,2,77,-1.06,-0.57,0.6 3C6B,ASP_230,3.61,-0.07,-0.38,0.26 1LZL,GLU_190,7.88,4.1,-0.84,0.12 1T07.TYR 10.11.24.0.0.37.0.86 2OSA, ASP 371, 3.32, -0.82, 0.0.34 3UAH,HIS_420,5.67,-1.14,0.03,0.29 3LJN,LYS 26,9,93,-0,21,0,-0,36 3IBT,CYS_31,11.69,0,-0.31,2.99 3ZSL,ARG_151,13.47,-0.35,0.79,0.52 3HYO.GLU 42.4.57.0.16.0.-0.09 1ZP2.GLU 90.3.6.1.19.-1.38.-0.71 2Z0M,ASP_296,2.83,-1.53,-0.29,0.84 4DND.GLU 49.4.83.0.33.0.0 3I47.TYR 93.10.21.0.0.0.21 3016,GLU_141,4.47,0.79,-0.32,-0.49 1J74,GLU_130,3.34,0.5,-1.58,-0.07 1MTZ,ASP_287,2.98,-0.75,-0.5,0.43 3C6B,ARG_90,12.59,-1.18,0.22,1.05 1NJ4.ARG 344,12.03.-0.91.0.0.43 3IRA,LYS_9,10.45,-0.05,0,0.01 4EZB,ARG_127,12.31,-0.19,0,-0.01 1YW5,TYR_49,12.2,-0.75,-0.31,3.26 1WJG.LYS 3,10.56,-0.07,0,0.13 3C38,TYR_266,11.99,0.39,0.66,0.94 3D9H,GLU_251,4.7,0.27,-0.01,-0.06 1WPA,ASP_466,4.05,0,-0.02,0.27 3KV0,GLU_205,3.79,0.4,-0.77,-0.33 2O99.LYS 65.10.53.-0.33.0.0.36 2D59,TYR_112,10.16,-0.85,0.02,0.99 2IXM,ARG_173,12.45,-0.16,0,0.11 3GS3,LYS_45,11.32,-0.46,0.85,0.42 2H2W,LYS 13,10.49,-0.01,0,0 3ETU,ASP_187,3.94,0,0,0.14 1FO9,ARG_192,12.26,-0.35,0,0.11 2CXC,ARG_37,13.65,-1.53,1.53,1.14 3L7N,ASP_195,4.03,0,0.09,0.15 2WB8,ARG_732,13.28,-0.26,0.69,0.34 2V1L,GLU_61,4.05,0.94,-1.26,-0.12 3E7P,LYS 37,10.32,-0.18,0,0 3BCH,LYS_89,10.01,-0.34,0,-0.15 3BQE,ASP_275,3.03,-1.59,-0.01,0.83 1T3Y,LYS 4,10.2,-0.3,0.0 2IN0,GLU_20,4.37,1.38,-1.51,-2.78E-17 3CE7,ASP_14,3.62,-0.18,-0.45,0.45 3C0C,GLU_345,4.53,0.44,-0.41,0 1WXO,ARG 299,12.97,-0.71,0.74,0.43 1YM5,HIS_185,6.31,-0.23,0,0.04 1AIL,LYS_70,10.46,-0.04,0,0 1BKR,LYS_15,10.14,-0.3,0,-0.05

4E6S.GLU 84.4.86.0.53.0.-0.17 3FTT,HIS_170,6.37,-0.37,0,0.24 2OKT,LYS_238,10.42,-0.15,0,0.09 3R87,ASP_40,3.26,-0.78,-0.16,0.4 2GKG.LYS 96.10.44.-0.06.0.0 3E7P.LYS 245,10.69,-0.62,0.42,0.38 2AHE,ASP_246,3.85,0,-0.09,0.15 1R3D,GLU_69,5.03,0.25,0,0.29 2VGM,LYS_322,10.66,-0.2,0,0.37 3EGN.LYS 396.10.48.-0.09.0.0.08 1SJ8,GLU_621,4.61,0.51,0,-0.4 3LJC,HIS 172,5,59,-0.86,0,-0.05 1QQE,GLU_12,4.59,0.14,0,-0.06 1XAW.TYR 467,10.66,0,0.43,0.23 2EJB,LYS 56,10.09,-0.35,0,-0.07 4EVF,ARG_293,12.22,-0.47,0,0.19 1U7U,ARG_206,12.62,-0.28,0.02,0.38 2PGX,ARG_164,12.09,-0.53,0,0.12 3DZ1.LYS 229.10.48.-0.2.0.0.18 3UX2,TYR_117,11.51,0.85,0.38,0.28 3BZT,HIS_265,7.09,-0.35,0.85,0.08 2FBQ,ARG_9,12.38,-0.23,0,0.12 3B79.GLU 92.4.17.0.49.-0.81.0 2G5X,ASP 7,3.59,-0.65,0.05,0.39 1RZ2,GLU_48,3.84,0.4,-0.6,-0.46 1WNH,HIS_138,4.12,-1.97,0.09,-0.51 4ECC,ASP_127,4.09,0,0,0.29 20BI,ARG 152,10.69,-1.81,0,0 3K8J,TYR_190,10.88,0,0.11,0.77 2A6B,LYS_45,10.5,0,0,0 2YT4,HIS_685,4.13,-3.16,0.8,0 1TWU,ARG 127,12.61,-0.75,0.34,0.52 1WLY,LYS 10.10.28,-0.22,0.0 3EGN,ARG_502,12.38,-0.12,0,0 1XTD.LYS 38,10,59,-0,18,0,0,27 3M3P,ASP_64,3.91,0,0,0.11 1YR6,ARG 90,12.4,-0.22,0,0.13 1FHL.ASP 127.4.18.0.0.04.0.34 1RHS,LYS_45,10.88,-0.12,0,0.5 1U7U,ARG_384,12.55,-0.27,0,0.32 20EV.LYS 15,10,14,-0,36,0,0 3IVF.GLU 350.4.57.0.44.-0.24.-0.13 3LOD,HIS_84,6.78,-0.55,0.41,0.42 3V3T,GLU_232,3.41,0.34,-0.85,-0.57 3P51,LYS_39,10.24,-0.26,0,0 2CWY,GLU 35,4.16,0.35,-0.67,-0.01 2FGG.ASP 57.4.17.-0.19.0.02.0.54 3GT0,LYS_202,10.43,-0.07,0,0 2D7U,TYR_101,9.8,-0.51,0,0.31 1NFN.GLU 45.4.57.0.19.0.-0.11 1DVO,ARG 129,12.26,-0.76,0.02,0.5 2EJX,GLU_98,4.5,0.39,0,-0.39 3K8J,ASP_265,3.84,0,-0.24,0.29 1JT9,LYS_160,10.82,-0.6,0.77,0.15 1SJ8,ASP 760,2.25,-1.52,-0.44,0.41 2Q5X,CYS_818,8.92,-0.4,0.08,0.24 1RAJ,LYS_228,11.08,-0.23,0.32,0.48 4ECC,LYS 207,11.24,-0.18,0.53,0.38 3CAX,LYS_338,10.77,-0.32,0,0.58 3GS9,ARG 239,12.16,-0.34,0,0 3CN5,LYS 161,10.37,-0.4,0.2,0.07 1D2K,ARG_120,12.56,-0.75,0.16,0.65 1YR6,GLU_58,4.17,0.45,-0.76,-0.01 1RSS,GLU 113,2.93,0.62,-1.54,-0.65 3HUE.CYS 117,10.61,-0.55,0.04,2.12 1WLY,TYR_197,10.87,0,0.09,0.77 3HVM,LYS_133,10.9,-1.03,0.77,0.66 2RIS,CYS_91,12.44,0,0.12,3.32 3HUE,GLU_227,4.54,0.21,0,-0.17

1RHS.ASP 92.3.94.0.-0.05.0.19 2012.GLU 67.4.45.0.24.0.-0.29 1KCM,GLU_181,4.79,0.29,0,0 3V55,GLU_680,4.83,0.26,0,0.06 1W7B,CYS 262,12,-0.03,-1.21,4.22 2FBO,ASP 12,3.62,-0.53,-0.67,1.02 2PGE,ARG_18,12.42,-0.08,0,0 1SQH,LYS_26,10.41,-0.32,0,0.24 3LMF,ARG_102,12.51,-0.28,0,0.29 1R3F,GLU_167,3.32,0.33,-1.06,-0.44 1YTD,LYS 170,10,42,-0.08,0,0 4FH3,GLU_43,4.4,0.24,0,-0.34 3P28,LYS_166,10.47,-0.05,0,0.02 2H01,ASP 14,3.83,-0.12,-0.07,0.21 3SMD,HIS 16,7.21,-0.28,0.85,0.13 3ZXY,GLU_106,4.99,0.51,0,-0.02 2161,ARG_6,12.48,-0.2,0,0.18 3D9H,GLU_253,4.33,0.36,-0.43,-0.09 1P4X,TYR_188,10.19,0,-0.05,0.23 3LH5.LYS 695.10.46.-0.17.0.0.13 1YM5,LYS_207,10.42,-0.08,0,0 3CAX,ARG_194,12.6,-2.19,1.34,0.94 1A8Q,ARG_54,12.37,-3.33,0.51,2.69 3LQE,ASP 366,4.09,0,-0.02,0.31 3NR5,LYS_146,10.93,-0.54,0.19,0.8 3OA7,ASP_569,4.05,0,-0.11,0.36 3V46,LYS_366,11.3,-0.31,0.74,0.38 1YIB,ASP_244,3.8,-0.32,-0.04,0.37 3ELI,ARG 92,12,35,-0,15,0,0 3V4G,LYS_146,11.02,-0.44,0.42,0.53 3GS3,CYS_60,8.97,-0.85,0.26,0.56 1ZBS.CYS 123.11.09.-0.39.0.02.2.46 2FBO.LYS 78.10.02.-0.19.0.-0.29 3IBT,LYS_115,10.33,-0.55,0,0.38 2YT4,GLU_518,3.51,0.68,-0.99,-0.69 1RKA,GLU_273,4.07,0.32,-0.42,-0.33 3RKV,GLU_234,4.11,0.28,-0.67,0 30DJ,HIS_56,4.22,-3.02,0.74,-0.01 3CCY,HIS_106,4.03,-1.96,0,-0.51 1H09.TYR 120.10.71.0.0.0.71 2BDV,ARG_33,12.29,-0.21,0,0 1SQH,ARG 142,12.05,-0.5,0,0.06 3G9T,ASP 265,4.02,0,-0.16,0.37 2H30,HIS_181,6.34,-0.16,0,0 3CBN,ARG_77,12.55,-0.28,0,0.34 2WOZ,LYS_431,10.37,-0.17,0,0.04 1R3F,ARG_75,13.13,-0.82,0.76,0.68 1EQ6,LYS_147,10.4,-0.11,0,0 1AM2.TYR 102.10.01.-0.14.-0.33.0.48 3NR5,TYR_61,10.57,0,0.19,0.38 2W1R,TYR_133,11.85,0,0.36,1.49 3CCY.GLU 56.4.78.0.34.0.-0.06 3P28,GLU_209,4.12,0.32,-0.55,-0.15 3C38,GLU_209,4.32,0.92,-1.16,0.06 3LJI,GLU_107,4.7,0.31,0,-0.11 2H85,LYS_110,10.47,-0.08,0,0.06 3AU3,ARG_414,12.13,-0.57,0,0.19 3CRM,ARG_223,10.15,-2.05,0,-0.3 1H4U,ARG_383,12.45,-0.09,0,0.04 3N2T,ARG_315,13.23,-0.34,0.55,0.52 3EIZ.CYS 115.8.61.-1.38.0.01.0.97 3F6F,ASP_58,1.2,-2.66,-0.83,0.89 2BAA,ASP_95,3.36,-0.75,-0.08,0.4 1P6F,LYS_61,11.22,-0.72,0.72,0.72 2W1R,LYS_96,10.3,-0.4,0,0.19 1NRI,ARG_113,12.45,-0.05,0,0 1A8Q,TYR_182,10.26,0,0.13,0.12 1JSX,HIS_53,5.35,-0.85,0,-0.3 3EJC,LYS_12,10.47,-0.03,0,0

3F6F,LYS_76,12.15,-0.39,0.96,1.08 1R6Y,ARG_17,12.13,-0.55,0,0.17 3BJV,ARG_70,12.63,-0.15,0,0.28 1BKB,ASP_95,1.65,-2.4,-0.77,1.01 1RI5,ARG_106,12.29,-0.21,0,0 1ZBP,TYR 235,10.4,-0.02,0.13,0.29 1UAJ,TYR_181,10.34,0,-0.05,0.39 2CYG,ASP_99,3.61,-0.13,-0.36,0.3 1XAW,ASP_451,4.14,0,-0.02,0.36 3CAX.GLU 140.4.79.0.3.0.-0.01 2V5B,HIS 188,3.61,-3.53,0.81,-0.16 2EYI,HIS_184,5.78,-0.72,0,-0.01 3JRT.GLU 74.5.9.1.82.0.-0.42 1NAF,GLU_246,3.78,0.15,-0.45,-0.42 3K8J,ARG 78,12.18,-0.39,0,0.07 2FL4,TYR 112,9,98,-0.56,0,1,0,44 1SIG,TYR_137,13.21,0.04,0.62,2.56 1L3K,LYS_105,10.68,-0.28,0,0.46 3CIV,ARG_168,13.52,-0.55,0.81,0.76 2A0J,ASP_93,2.48,-1.5,-0.36,0.53 1OXZ,LYS_295,10.38,-0.29,0,0.16 1XFK,LYS_147,10.46,-0.04,0,0 30KO.GLU 653.4.76.0.26.0.0 3A2Z,GLU 193,4.09,0.3,-0.81,0.1 1XFK.TYR 248.10.82.0.0.17.0.65 1R53,ASP_26,3.7,-0.14,-0.34,0.37 3ULX,ASP_157,4.01,0,-0.11,0.32 2H2W,LYS_76,10.62,-0.14,0,0.25 3ONH, ASP 533, 3.95, 0, 0.03, 0.12 1NJ4,HIS_216,5.99,-0.68,0.01,0.16 1SNT,ARG 182,11.67,-0.9,0,0.08 1X7F,CYS_37,12.36,0,0.79,2.57 3RAZ,GLU 129,4.19,1.31,-0.76,-0.87 3B7H.GLU 42.4.64.0.14.0.0 2P0L,ASP_195,3.58,-0.44,-0.34,0.56 3CCY,GLU_83,4.62,0.13,0,-0.01 1WPA,GLU_456,4.89,0.36,0,0.03 1XEU,LYS 72,10.44,-0.06,0,0 3GS9,ARG_176,13.03,-1.38,0.55,1.37 1G5Z,GLU_71,3.72,0.28,-0.68,-0.38 2A4D,GLU_96,4.74,0.15,0,0.09 3Q6L,ASP_18,2.87,-0.46,-1,0.53 3GFP.TYR 455,10,15,0,0,0,15 1TR9,ARG_258,12.08,-0.81,0,0.39 1R9W,ARG_294,12.92,-0.73,0.79,0.36 2FI9,ARG_27,12.51,-0.14,0,0.14 1CBY,LYS 199,9.86,-0.74,0,0.1 3DSH.CYS 388,11.87,-0.28,0.1,3.04 2I88,LYS_362,9.68,-0.85,0,0.03 1JYH,GLU_4,4.46,0.17,0,-0.22 1A8Q,LYS_263,10.38,-0.5,0,0.38 3M16.GLU 242.5.01.0.76.0.-0.26 1ES9,ARG_160,12.38,-0.34,0,0.23 3BWT,ASP_671,3.69,-0.22,-0.3,0.4 3VJ8,GLU_199,4.79,0.26,0,0.02 1RI6,LYS_4,11.42,-0.33,0.57,0.68 3RJZ,ARG 133,12,47,-0.33,0,0,3 2AHE,LYS_124,10.31,-0.23,0,0.03 2X4G,GLU_313,3.46,0.68,-1.07,-0.64 200K,ARG_162,12.35,-0.41,0,0.26 2VGM,LYS 264,10.11,-0.4,0.0.01 3CGW,LYS_87,10.06,-0.36,0,-0.06 2PGE.GLU 274,3.88,0.18,-0.74,-0.06 1ZHV,TYR_14,11.34,-0.85,0.4,1.78 1U53,LYS_140,11.45,-0.32,0.84,0.43 2BCF.TYR 258,9.88,-0.03,-0.38,0.3 2A6B,ASP_93,3.57,-1.22,0,0.99 1WYC,GLU_336,4.5,0.14,0,-0.14 3E7P,LYS_72,10.16,-0.28,0,-0.06

4DIU.HIS 53,4.06,-3,14,0,71,0 3K1H.LYS 38.10.62.-0.11.0.0.23 2P0L,GLU_46,3.92,1.38,-1.52,-0.45 1YB2,HIS 238,5.96,-0.35,0,-0.19 4FLE,LYS_24,10.33,-0.17,0,0 1A8Q,GLU 160,3.84,0.54,-0.82,-0.38 2GAU,ASP_223,4.05,0,0.09,0.15 3ELI,HIS_87,5.91,-0.8,0.43,-0.22 3K9I,LYS_148,10.36,-0.25,0,0.11 2YX0,ARG_224,13.92,-0.82,1.26,0.98 3V55,LYS 447,11.38,-0.2,0.7,0.38 1WXQ,LYS_188,10.46,-0.49,0.41,0.04 3D9H,GLU_140,3.82,1.66,-1.27,-1.07 1P6F,LYS_59,10.21,-0.41,0,0.11 20HT,LYS 175,10.46,-0.11,0.02,0.05 1KCM,LYS 179,10.19,-0.65,0.0.34 3F1X,HIS_201,5.85,-0.55,0,-0.09 10XZ,ASP_274,3.91,-0.06,0.02,0.16 2VGM,GLU_186,4.82,0.29,0,0.02 4DNU,ARG 286,11.84,-1.29,0.1,0.53 2YLF,ARG 92,12,94,-0.31,0.51,0.24 2IXM,TYR_45,11.33,0,-0.11,1.43 2AD1,ASP_196,4.65,0,-0.22,1.08 1M5I.GLU 140.3.47.0.51.-1.21.-0.34 3BWT.CYS 738,10.93,-0.1,-0.16,2.19 1ILW,ASP_110,3.96,0,-0.03,0.2 2OJO.LYS 525,10.33,-0.33,0.0.16 3TMO,ARG_187,12.47,-0.03,0,0 1D2K,HIS_251,4.09,-2.44,0.09,-0.04 1RI5,ARG 260,12.55,-0.27,0.0.32 3ETU, ARG_193, 12.16, -0.36, 0, 0.02 2IF4,GLU_173,2.63,1.01,-2.48,-0.4 3ON1,LYS_5,10.42,-0.08,0,0 1BYI,LYS 2,10.75,-0.21,0,0.47 2QVO,ARG_5,12.43,-0.07,0,0 1MIX,ARG_277,12.43,-0.07,0,0 3C5V,ASP_299,3.28,-0.58,-0.38,0.44 1GXN,TYR_616,10.13,0,-0.29,0.43 3MIX.HIS 482,4.71,-1.44,0,-0.34 4F8A,LYS_577,10.02,-0.37,0,-0.12 2RJD,GLU_522,4.73,0.23,0,0 3EAZ,ARG_89,12.61,-0.32,0,0.43 1NIJ,LYS 318,11.12,-0.31,0.46,0.47 2WB3,ASP_337,2,-1.47,-0.88,0.55 3M9A,GLU_92,4.57,0.34,0,-0.27 3CXS,GLU_120,5.86,0.96,-0.06,0.46 2IF4,GLU_197,4.91,0.25,0,0.16 3I82,ASP 206,4,11,0,-0.07,0.39 3LH5,GLU_664,3.2,0.48,-0.99,-0.78 1UXO,LYS_146,10.42,-0.17,0,0.1 3V75,ASP_206,3.65,-0.38,-0.19,0.42 3ADO.LYS 178,10.33,-0.17,0,0 1AM2,GLU_96,4.71,0.19,0,0.02 3JSN,ASP_36,3.83,0,-0.25,0.28 3LQE,ARG_268,9.97,-2.65,0,0.12 3B21,LYS_51,10.29,-0.21,0,0 1X1E,GLU_209,2.35,0.48,-1.99,-0.63 3B21,GLU_113,2.64,1.42,-2.44,-0.84 3T57,LYS 76,10,47,-0,34,0,0,31 2CW4,ASP_82,4.57,-0.2,0.01,0.97 20JQ,LYS_473,10.45,-0.05,0,0 1L2F.GLU 294,4.57.0.15.0.-0.08 3C5V,GLU_361,4.48,0.22,0,-0.23 1W7B,LYS_279,10.66,-0.2,0,0.36 1U3Y,GLU_264,4.29,0.69,-0.72,-0.17 3MEW,LYS_140,10.45,-0.05,0,0 1PDB,HIS_127,5.84,-0.92,0.02,0.23 2CW4,LYS_57,10.84,-0.29,0,0.64 2E3S,GLU_446,4.27,2.41,-1.75,-0.89

3C6B,ASP 63,2,7,-1,63,-0,46,0.99 3I4T,TYR_34,10.81,0,0.28,0.54 3V55,LYS_543,10.41,-0.09,0,0 1ZP2,ASP_130,3.87,0,-0.13,0.2 1T07.LYS 9.9.66.-1.15.0.0.31 2O99,LYS 357,10,58,-0,24,0,0,31 3C5V,LYS_293,10.48,-0.13,0,0.11 1T07,GLU_61,4.72,0.18,0,0.05 1N81,TYR_166,11.25,-0.11,0.09,1.27 2X4G.ARG 231.12.34.-0.36.0.0.19 2BV9, ASP_85, 3.68, -0.85, -0.48, 1.21 2CYG.GLU 122.5.81.1.2.-0.81.0.92 2JKF,GLU_111,4.68,0.12,0,0.06 3EUR.LYS 66.9.94.-0.48.0.-0.09 3ADO,ARG 197,12.33,-0.28,0,0.11 1L3K,GLU_24,4.71,0.17,0,0.04 1X91,LYS_24,10.21,-0.3,0,0.02 1RHS,ARG_29,12.22,-1.3,0.71,0.3 1TUL.TYR 69.12.28.-0.12.0.41.1.99 1A8Q,ASP_82,4.04,-0.1,0.04,0.3 3BQE,ARG_272,12.25,-1,0.07,0.68 105T,ARG_106,12.3,-0.22,0,0.02 1NJ4,LYS_254,10.95,-0.74,0.66,0.53 1H4U,HIS 370,6.08,-0.42,0,0 20EW,HIS_249,5.4,-1.62,0.68,-0.15 2ILR,GLU_448,5.04,0.33,0,0.2 3EIZ,LYS_95,10.62,-0.33,0,0.44 1X91, ASP 113, 3.41, -0.42, -0.29, 0.32 3PZ9,HIS_90,2.48,-3.96,0,-0.06 1UW7,LYS_52,11.34,-0.39,0.85,0.38 3DHN,ASP_165,3.8,0,-0.51,0.51 1FKM,LYS 302,10.1,-0.31,0,-0.1 1NJ4,ASP 286,3.53,-0.35,-0.13,0.21 1AK1,TYR_216,10.55,0,-0.11,0.66 1GVP,TYR_26,10,-0.07,-0.19,0.26 1BKR,CYS_12,12.16,-0.05,0,3.21 1SQH,ARG 73,12.48,-0.27,0,0.24 20ZO.GLU 127.4.18.1.05.-0.98.-0.38 3BB7,TYR_312,11.04,-0.85,0.02,1.87 3V1Q,GLU_501,4.54,1.31,-0.85,-0.41 3B79.GLU 60.4.76.0.26.0.-0.01 2IXM,CYS_164,12.44,0,0.35,3.08 2QEV,ASP_44,2.53,-0.85,-0.89,0.48 1PGV,ARG_384,12.22,-0.14,0,-0.13 2A1V,ASP_12,3.04,-1.86,0.13,0.97 3F1X,LYS 298,10.44,-0.06,0,0 2W2S,ASP 145,4,16,0,0,06,0,3 2FD5,LYS_176,9.76,-0.6,0,-0.14 3AU3,GLU_443,4.59,0.24,-0.01,-0.14 1AK1.LYS 130.10.03.-0.51.0.0.04 4DIU.TYR 133,12,21,0,0,35,1,86 4FH3,GLU_303,2.81,0.47,-1.75,-0.4 1TXD,GLU_877,4.13,1.1,-0.72,-0.77 3EGN,GLU_387,4.32,0.1,0,-0.27 3CS1,ASP 112,3.88,-0.01,-0.12,0.21 4AM1,ARG_124,10.07,-2.01,0,-0.43 3IU5,TYR_85,10.96,0,-0.14,1.09 1L2F,ASP 84,4.36,-0.11,-0.15,0.83 2G3A,ASP_105,3.18,-0.52,-0.34,0.23 3C38,ASP 97,3.72,-0.73,0,0.65 3IL3,GLU_172,4.09,0.46,-0.57,-0.31 2HP7,GLU_90,3.92,0.32,-0.62,-0.28 1GQE,LYS_282,11.36,-0.23,0.71,0.38 2E0T,ARG 192,12.34,-0.16,0,0 2YLF,TYR_49,12,-0.15,0.55,1.6 3BA1,GLU_238,5.84,1.88,-0.82,0.27 3HUE,GLU_67,3.77,0.42,-0.81,-0.36 3D9H,GLU_75,5.93,1.43,0,-0.01 3T57,LYS_131,10.89,-0.25,0.17,0.47

3EYE,TYR 124,10,34,0,0,0,34 3ADO,ARG_50,12.39,-0.3,0,0.18 2G5X,LYS_12,10.61,-0.13,0,0.24 2JKF,LYS_124,10.2,-0.52,0,0.22 2QK1,ASP_331,3.56,-0.39,-0.27,0.43 20DJ.GLU 184,4.62,0.22,-0.1,0 3GW3,ARG_332,11.89,-0.67,0,0.06 1T6L.LYS 113.11.46.-0.33.0.82.0.47 2AZL,ARG_129,12.37,-0.37,0,0.24 3LD1.LYS 284.10.52.-0.28.0.0.31 1L2F,LYS_125,10.08,-0.21,0,-0.21 2YWX,LYS_23,10.39,-0.12,0,0.01 2CN1,GLU_69,4.41,0.23,0,-0.32 3BB7.TYR 235.13.56.0.0.19.3.37 2H2W,LYS 224,10.49,-0.2,0,0.19 30DJ,ARG_82,12.25,-0.26,0,0.02 3CIV,GLU_56,4.35,0.34,-0.18,-0.31 3Q9P,ARG_136,12.09,-0.42,0,0.01 2IIA,ARG 6,12.22,-0.37,0,0.08 2H8O,ARG_227,11.22,-1.23,0,-0.05 2IRM,ASP_154,4.21,0,0,0.41 3JZN,LYS_400,10.54,-0.14,0,0.19 1ZP2,ARG_51,13.44,-0.45,0.75,0.64 4ECC,ASP 73,4.33,-0.2,-0.13,0.85 1U3Y,ARG_305,12.41,-0.09,0,0 4EZB,ASP_204,3.35,-0.56,-0.25,0.35 2E3S,ARG_544,13.55,-1.06,1.56,0.55 1SFE,ARG_151,13.05,-0.22,0.3,0.47 3CIV.GLU 291.4.87.0.26.0.0.11 3L7N,ASP_45,4.21,0,0.17,0.25 4D8L,ARG_199,13.2,-1.09,0.83,0.96 2ZQ5,LYS_306,11.17,-0.57,0.85,0.38 2G9D.ARG 233,13.24,-0.29,0.6,0.44 3BQE,ARG_244,12.53,-0.1,0,0.13 1RI5,GLU_211,4.58,0.44,0,-0.36 2AHE,LYS_204,10.48,-0.19,0,0.18 1GPP,LYS 113,10.37,-0.19,0,0.06 1X1E,ARG_95,13.47,-0.4,0.68,0.69 2XHC,GLU_27,4.61,0.11,0,0 2HXB,CYS_30,9.37,0,0.06,0.31 2G2D,CYS_39,12.07,0,0.21,2.86 1AKO,HIS 25,4.54,-1.71,0,-0.23 3I0C.TYR 237,10.87,0.0.0.87 2P65,ARG_96,12.69,-0.17,0,0.37 3P28,LYS_110,11.25,-0.54,0.85,0.43 2FXT.TYR 305,11.66,0,-0.04,1.7 3HYQ,GLU_143,4.64,0.31,-0.17,0.01 3HNX,LYS_67,10.56,-0.16,0,0.23 1WRU.TYR 100.10.96.0.22.0.3.0.45 1ES5,LYS_221,10.49,-0.21,0,0.19 1RSS,ARG 94,12.12,-0.28,0,-0.1 1SIG.LYS 392.10.35.-0.15.0.0 20BI,TYR_169,10.74,0,0.14,0.6 1X7F,LYS_287,11.17,-0.47,0.85,0.28 3GS9,ASP_24,3.92,-0.06,0,0.18 1TR9,GLU_16,4.27,0.27,-0.35,-0.15 2XWS,GLU 29,3.21,0.37,-1.12,-0.54 2Q5X,GLU_781,3.69,0.68,-0.68,-0.81 1T07,HIS_0,6.58,-0.08,0.16,0 3Q6L,GLU_15,4.65,0.16,0,0 3F6F.TYR 112,10.98,-0.17,0.32,0.84 1PGV,GLU_349,2.8,0.46,-1.65,-0.52 10XZ,GLU_219,4.75,0.31,0,-0.06 2FZ4,HIS_44,5.94,-0.39,0,-0.18 1CHD,ARG 348,12.43,-0.07,0,0 1PBV,GLU_134,4.51,0.22,0,-0.21 2DG7,ARG_136,12.09,-0.36,0,-0.06 2D7J,LYS_133,11.45,-0.51,0.85,0.61 3PAC,CYS_108,10.77,-2.19,0.46,3.5

20V2.GLU 16.4.64.0.14.0.0 3K9I.TYR 59,10.31,0.0.16,0.15 3EUR,GLU_29,3.63,0.41,-0.85,-0.43 2FG1.TYR 54,10.2,0,0,0.2 1U3Y,LYS_315,10.35,-0.17,0,0.02 2E3S,GLU 407,4.44,0.33,0,-0.38 1TLV.LYS 141.10.16.-0.34.0.0 1ANU,ARG_23,13.28,-0.35,0.68,0.45 1XDZ,ASP_209,2.81,-0.85,-0.42,0.28 1XEU.CYS 218,10,55,0,-0,11,1,66 3LOE,CYS 240,12,47,0,25,0,7,2,52 3C5V,TYR_70,12.75,-0.59,0.86,2.48 2ZCO,ARG_188,13.82,-0.72,0.74,1.29 1U7U,ASP_394,3.76,-0.3,-0.36,0.61 3R87,ASP 66,2.89,-0.81,-0.45,0.35 3CXS,LYS_15,10.41,-0.21,0,0.12 2D2S,LYS_703,10.49,-0.17,0,0.16 2ZCX,ARG_42,12.37,-0.8,0,0.66 2FPN,ARG_115,12.5,-0.31,0,0.3 2D7J.TYR 22.10.32.0.0.23.0.09 2RIK,LYS_118,10.32,-0.2,0,0.03 1MTZ.LYS 233,10.25,-0.25,0.0 3DSH,TYR_303,9.79,-0.05,-0.36,0.21 2EHG,ARG 137,12.36,-0.12,0,-0.02 1XFK,GLU_99,4.91,0.17,0,0.24 1WYC,GLU_372,4.65,0.14,0,0.02 3CJW,ARG_293,13.09,-0.38,0.58,0.4 1EV8,GLU_137,3.82,0.7,-0.88,-0.5 3CAN,ASP_176,3.37,-0.79,-0.03,0.4 2Q5X,TYR_785,10.93,-0.84,0.02,1.75 2Q12,ASP_243,3.95,0,0,0.15 2CI3,GLU_249,4.72,0.36,0,-0.14 3BCY,ASP 45,2.13,-1.97,-0.68,0.97 2NYC,LYS_246,10.46,-0.04,0,0 1X8F,TYR_174,10.06,0,0.03,0.02 1AM2,ARG_138,12.53,-0.14,0,0.17 3M66,TYR_149,10.13,0,0,0.13 2PWQ,ARG 6,13.17,-1.05,0.7,1.02 2EJX,LYS_102,10.45,-0.05,0,0 3Q6L,ASP_48,3.93,0,0,0.13 3ASA,TYR_300,9.67,-0.77,-0.27,0.7 2ZCO,LYS 272,12.31,-0.96,1.7,1.06 3HVM,HIS 302,5.85,-0.68,0.24,-0.22 3S0A,GLU_94,4.62,0.13,0,-0.02 3C2E,TYR_34,10.04,0,0,0.04 3JZN,GLU_125,4.15,0.72,-0.77,-0.29 2XJ4,GLU 272,4.21,0.59,-0.59,-0.29 2CWC.TYR 91.10.11.0.0.03.0.09 2HNG,GLU_113,4.87,0.31,0,0.06 1JT9,TYR_254,10.28,0,0.07,0.21 2FC3,GLU_28,3.34,0.43,-0.85,-0.74 2JEO.TYR 84.11.3.0.0.06.1.24 1SJY,ARG_137,13.87,-0.47,1.42,0.42 20V2.ARG 311.12.07.-1.68.0.58.0.67 3GYW,ASP_192,3.96,-0.01,0,0.17 1XTD,ASP_82,4.53,0,-0.09,0.81 3RJX.LYS 71.10.59,-0.11.0.0.2 1UXO,TYR_11,10.11,0,-0.2,0.32 20JQ,GLU_623,4.32,0.29,0,-0.47 1NIJ,GLU_37,6.48,2.22,-0.53,0.28 3V75,ARG 9,11.78,-1.98,0.63,0.63 3V55,GLU_700,4.43,0.17,0,-0.23 1DZF.HIS 99.5.85,-0.81.0.0.16 1P2F,TYR_59,11.39,0,0.18,1.22 3L7N,GLU_234,4.8,0.14,0,0.15 2FZ4,TYR 28,10,38,0,-5,55E-17,0,39 1SFE,ASP_64,3.13,-0.85,-0.31,0.49 3H13,TYR_244,12.55,0.01,0.27,2.27 1PSW,ARG_109,13.43,-0.25,0.8,0.38

3016.CYS 82,12,4,-0.01,0,16,3,25 1ES9,GLU_85,5.32,0.78,0,0.04 3KV0,GLU_95,3.49,1.81,-2.54,-0.28 3CSR,LYS_15,10.4,-0.2,0,0.1 2BDV,ASP_109,3.75,-0.43,-0.03,0.42 2H2W,TYR 246,10.6,0,0.04,0.56 20JO.LYS 438,10.6,-0.12,0.0.22 3LD1,ARG_303,13.71,-0.8,1.59,0.43 3EVN,HIS_80,4.61,-3.22,1.24,0.09 2V81,ASP_74,2.9,-1.03,-0.35,0.49 3U2R,ARG 82,12.1,-0.34,0,-0.05 1NAR, ASP_183, 3.74, 0, -0.29, 0.23 2QDJ,GLU_166,4.23,1.19,-0.85,-0.61 1AT0,TYR_295,10.58,0,-0.19,0.76 3COU.ASP 177.3.79.0.-0.24.0.22 1ES5.LYS 182.10.32.-0.18.0.0 3GA2,GLU_14,4.68,0.18,0,0 1IAP,GLU_213,4.96,0.22,0,0.24 3G9T,GLU_261,3.42,1.64,-1.41,-1.32 1IDK,LYS 12,10.39,-0.14,0,0.03 3TMO,ASP_238,2.7,-0.63,-0.74,0.27 2Q13,HIS_175,5.78,-0.64,0,-0.07 2QZQ,GLU_96,3.22,0.47,-1.6,-0.16 1ILW.ARG 122,13.89,-0.37,0.71,1.06 1ZBM.CYS 156.11.-0.42.0.6.1.82 3OKQ,CYS_676,9.17,-0.05,0,0.22 1C44,GLU_22,4.7,0.29,-0.12,0.02 3I4T,CYS_40,10.79,0,0.49,1.31 2FPN,GLU_164,4.66,0.23,0,-0.08 2V81.TYR 56.10.8.0.0.12.0.68 2IQT,CYS_127,11.18,-0.03,0.13,2.08 1MD6,ASP_154,3.8,0,-0.12,0.13 1R29,ARG 13,12,4,-0,1,0,0 1Z3X,LYS 46,11.41,-0.28,0.59,0.61 3FRR,LYS_27,10.64,-0.1,0,0.24 3CXS,HIS_77,6.28,-0.21,0,-0.01 3E7P,GLU_228,4.48,0.28,0,-0.3 2QZQ,GLU_28,3.24,0.37,-0.85,-0.78 100H,HIS 70.6.24,-0.21,0,-0.04 3T57,GLU_290,4.63,0.23,-0.09,-0.02 1SUU,CYS_691,8.89,-0.04,-0.38,0.31 3T8R,TYR_126,10.31,0,0.22,0.1 1UJ8,ASP 52,4.15,0,0.01,0.34 2Q99,ARG_204,12.13,-0.49,0,0.12 2YX0,LYS_263,11.09,-0.61,0.85,0.35 1RKA,GLU_268,4.65,0.24,0,-0.08 3C5V,LYS_133,10.38,-0.31,0,0.19 1X7F,LYS 318,10.13,-0.52,0,0.15 2WB8,GLU_613,5.1,0.84,0,-0.24 2ZCO,TYR_215,13.08,-0.8,0.71,3.17 3DB9,LYS_165,10.41,-0.09,0,0 2GAU,CYS_38,10.21,-0.48,0,1.7 3ERF,ASP_97,2.66,-1.45,-0.25,0.55 3P2F,HIS_6,5.36,-1,0,-0.13 1AM2,ASP_171,3.7,-0.48,0,0.38 2AXO,LYS_220,10.81,-0.17,0,0.48 1UCH,ARG_186,13.76,-1.23,1.13,1.37 1Z9L,ARG_50,12.41,-0.08,0,-0.01 3OIP,LYS_135,10.36,-0.14,0,0 2NMU,ASP_51,2.91,-1.27,0,0.38 2G5X,LYS 215,10.48,-0.05,0,0.02 2013.CYS 328.10.55.-0.51.0.16.1.9 100X,TYR_70,10.74,0,0.18,0.55 2JKF,ASP_8,3.24,-0.86,-0.45,0.74 1YTD,ASP_190,4.76,-0.85,-0.01,1.81 3EJC,LYS 5,10.65,-0,1,0,0.23 3EVP,GLU_282,4.71,0.17,0,0.03 3EVN,ARG_295,12.41,-0.21,0,0.12 1MTZ,ARG_202,12.06,-1.18,0,0.75

1U3Y,CYS 270,11.12,-0.05,0.09,2.08 2QVT,ASP_134,3.01,-0.72,-0.41,0.34 3UC9,ASP_126,4.18,0,0.21,0.17 3T5B,ARG_370,12.66,-0.13,0,0.28 3JZ9.GLU 381,4.1,0.26,-0.27,-0.39 1ZBM,ASP_78,3.72,-0.69,0,0.61 3BA1,LYS_141,10.42,-0.11,0,0.03 3BB7,ASP_97,3.79,-0.73,-0.06,0.78 3HUE,LYS_188,9.92,-0.65,0,0.07 2E3S.ARG 442.12.37.-2.41.0.38.1.9 1P4X,GLU_229,5.41,0.82,0,0.1 1YR6,ASP_26,3.86,0,-0.2,0.25 1SQH,LYS_28,10.17,-0.33,0,0 3HNX,ASP_27,3.94,0,0,0.14 3P28,HIS 29,6.66,-0.58,0.73,0.01 3M3P,ARG_235,12.96,-1.12,0.89,0.68 1JKS,ASP_250,1.77,-1.9,-0.81,0.67 2l88,ASP_347,3.8,-0.03,-0.17,0.19 3VJ8.ARG 77.12.83.-1.24.0.51.1.06 2R0S,TYR_93,10.67,0,-0.26,0.93 2DFL,LYS_143,11.34,-0.72,0.85,0.71 2AXO,LYS_142,10.44,-0.14,0,0.08 1LFP.ARG 136.12.29.-0.43.0.0.22 1DTO.TYR 131,13.89,0.85,0.65,2.39 3U2R,LYS_111,11.47,-0.26,0.85,0.38 3GA2,TYR_120,11.71,0,0.52,1.19 3JRT,ASP_30,3.89,-0.01,-0.23,0.34 4DNU,HIS 287,3.01,-3.06,0.09,-0.52 3V55,TYR_690,11.61,0.06,0.97,0.57 3EJG,GLU_145,4.78,0.43,0,-0.15 3V1Q,LYS_628,10.2,-0.17,0,-0.14 204D.ARG 86,12,12,-0,49,0,0,11 2VAN, ARG 254, 12, 47, -1, 97, 0, 59, 1, 34 1PSW,ASP_82,2.65,-0.85,-0.6,0.31 2AH5,ASP_189,3.93,0,-0.15,0.28 1QYI,LYS_348,10.44,-0.17,0,0.1 3FRR,LYS 130,10.44,-0.09,0,0.03 3D9H,HIS 91,5.85,-0.43,0,-0.22 3LMO,LYS_68,10.5,-0.09,0,0.09 2FZ4,ARG_192,12.17,-0.73,0,0.41 4HDE.GLU 152.4.54.0.04.0.0 2BT8.HIS 287.6.01.-0.44.0.-0.05 3H6Q,HIS_121,5.01,-2,0.82,-0.31 3M7D,GLU 171,5.22,1.32,-0.41,-0.2 1SQH,TYR_69,11.27,0,0.06,1.22 2Q98,ASP_160,3.57,-0.47,-0.01,0.24 3V75.GLU 56.4.37.0.15.0.-0.28 3UC9,GLU_46,4.53,0.21,0,-0.18 2FBQ,GLU_210,4.57,0.09,0,-0.02 1G8P,ARG_142,11.96,-0.58,0,0.03 3LOE, ASP 348, 2, 46, -1, 87, 0, 0, 53 1N81,HIS_142,7.13,-0.5,0.74,0.4 3M3P,GLU_194,3.18,1.22,-2.54,0 1T95,TYR_216,10.11,0,-0.08,0.19 1LTU,LYS 248,10.63,-0.08,0,0.21 3F5D,ASP_170,3.3,-0.84,-0.16,0.5 3CAN,HIS_138,6.24,-0.3,0,0.04 2HRZ,ASP 31,3.23,-0.66,-0.55,0.63 3LJI,ASP_91,4.18,0,0.11,0.27 1ZP2,LYS 67,10.59,-0.56,0.29,0.36 3HVM,LYS_162,10.36,-0.16,0,0.02 2IDC,LYS_35,10.59,-0.13,0,0.22 1NFN,GLU_132,3.75,0.31,-0.88,-0.18 2H2W,ARG_132,12.96,-0.35,0.16,0.65 2IQT,HIS_169,7.15,-0.54,0.85,0.35 3RJZ,ARG_159,13.07,-0.6,0.59,0.59 1CHD,LYS_212,12.01,-1.28,1.64,1.16 3IVF,GLU_317,3.24,1.96,-2.19,-1.02 1A8Q,ASP_70,3.17,-0.68,-0.66,0.71

3M7G.ARG 102.11.95.-2.92.0.3.2.08 3DSH,TYR_246,13.44,0,0.15,3.29 1H09,LYS_121,10.56,-0.38,0,0.44 1AK1,LYS_152,11.36,-0.59,0.85,0.6 20RX.GLU 151.4.43.1.75.-0.99.-0.83 2RGY,ARG 284,13.06,-0.44,0.21,0.78 2H01,LYS_28,10.41,-0.13,0,0.04 1J74,ARG_101,12.69,-0.2,0.01,0.38 2BLL,GLU_434,4.43,2.84,-1.05,-1.84 1PVT.LYS 180.10.96.-0.78.0.82.0.43 2R0S,LYS_219,10.93,-0.23,0.63,0.02 2Q98,ARG_103,12.37,-0.28,0,0.14 1R3D,HIS_243,0.83,-3.44,0,-2.23 2WOZ.LYS 583.10.49.-0.06.0.0.05 2WZ9,HIS 104,6.37,-0.27,0,0.14 3CAX,GLU_304,3.35,0.82,-1.31,-0.67 3JV1,GLU_61,4.78,0.23,0,0.04 1WYC,ASP_250,3.05,-0.71,-0.69,0.64 10GL,ARG_34,12.43,-0.36,0,0.28 3PP8,GLU_2,3.97,0.57,-0.59,-0.5 1V43,ARG_266,12.81,-0.45,0.17,0.58 3EAZ,HIS_128,5.05,-1.24,0,-0.21 3DSH,GLU_400,3.98,0.25,-0.66,-0.11 2WB3,ASP 346,3.5,-0.6,-0.05,0.36 3A0X,GLU_608,4.52,0.21,0,-0.18 1TWU,LYS_99,11.34,-0.32,0.77,0.4 3T5B,ARG_195,13.06,-0.4,0.48,0.48 2CVB,GLU 184,4.6,0.13,0,-0.02 3B7X,ASP_31,2.7,-1.75,-0.03,0.68 3F7M,ARG_268,12.56,-0.08,0,0.14 2CI3,GLU_191,4.48,0.11,0,-0.12 1P1L,HIS_74,5.93,-1.71,0.7,0.44 3K8J,CYS 178,12.48,0,0.48,3.01 3C6B,LYS_16,11.43,-0.43,0.8,0.55 3I0C, ARG_249, 13.8, -0.44, 1.16, 0.58 1WXQ,HIS_125,6.31,-0.8,0.06,0.55 1ZBM,TYR 80,10.82,-0.18,0.16,0.85 1Z9L,LYS_118,10.47,-0.16,0,0.13 2WZ9,LYS_58,11.77,-0.38,1.03,0.61 1QQH,CYS_176,10.15,-0.11,0.28,0.99 1P6F,ARG_124,12.39,-0.19,0,0.08 2HRZ,ASP_115,2.79,-1.61,-0.68,1.29 2ZO5.GLU 379.4.61.0.11.0.0 1RSS,GLU_74,3.76,1.36,-1.22,-0.88 1SNT,ASP_201,1.45,-2.88,-0.33,0.86 1LPL,ARG_199,13.67,-0.38,0.83,0.72 4D8L,ARG_187,14,-0.24,1.24,0.5 3BQW,ASP_228,3.73,-0.38,0,0.3 306L,ASP 112,3.67.0.-0.29.0.16 2IXM,GLU_134,3.82,2.15,-2.62,-0.21 3B7X,TYR 22,12.23,0,0.22,2.01 1J7G.GLU 40.4.61.0.13.0.-0.03 1RHS,HIS_94,3.63,-2.3,0,-0.57 2JKF,HIS_174,7.22,-0.13,0.85,0 1Q46,HIS_108,4.58,-1.62,0,-0.32 3UAH,TYR_426,13.09,-0.82,0.14,3.78 1XDZ,LYS_135,10.45,-0.05,0,0 3K1H,ASP_95,3.59,-0.8,-0.09,0.68 1WXF,ARG_142,11.41,-1.15,0,0.06 2NSN,LYS 78,11.12,-0.66,0.85,0.43 3UAH,TYR_259,9.95,0,-0.3,0.25 1N81,LYS_180,10.62,-0.11,0,0.23 3P28,ARG_48,9.82,-3.07,0,0.39 1BKB,HIS_43,6.34,-0.16,0,0 3M70,LYS_16,10.73,-0.19,0,0.43 3ZTA,GLU_77,3.91,0.33,-0.62,-0.31 4FH3,TYR_281,10.23,-0.17,-0.21,0.62 3EVZ,GLU_208,4.31,0.12,-0.19,-0.11 3EZ7,GLU_66,4.58,0.08,0,0

1SOH, ARG 65, 11.4, -1.29, 0, 0, 19 3E7P.LYS 92,10.27,-0.13,0,-0.11 4FCU,GLU_136,4.57,0.31,0,-0.23 2Z84,TYR_170,9.99,-0.67,0.24,0.42 1L2F,ASP_10,3.92,0,-0.27,0.39 4GA2,TYR 37,10.53,0,0.15,0.39 1MJS,ASP_309,3.66,-0.26,-0.12,0.24 1PV5,GLU_133,4.65,0.11,0,0.04 4DEZ,ASP_96,3.98,0,-0.04,0.22 2BCF,HIS_65,5.4,-1.08,0,-0.01 1K95,GLU 72,4.61,0.45,-0.49,0.14 3B7X,ARG_44,13.12,-0.36,0.62,0.36 3NZL,LYS_31,10.58,-0.1,0,0.18 3A4C,GLU_555,3.02,0.6,-1.62,-0.45 1J85,LYS 151,10.37,-0.13,0,0 3CZC,GLU_23,3.45,0.36,-1.04,-0.37 3DB9,LYS_63,10.21,-0.21,0,-0.08 2HXB,GLU_77,4.55,0.09,0,-0.05 3ASA.GLU 220,4,56,2,18,-1,46,-0,64 3GS9,TYR 291,10,34,0,0,0,34 3BCY,GLU_67,4.59,0.09,0,0 3VJ8.ASP 327.4.1.0.0.0.3 2A1V,GLU_102,4.2,0.3,-0.39,-0.21 1NAR,TYR 184,9.84,0,-0.41,0.24 1UAJ.CYS 178.9.47,-0.26,-0.14,0.87 3GS9,ASP_56,3.24,-0.72,-0.47,0.64 1WPA,ASP_461,3.77,-0.34,-0.13,0.45 2W1R,HIS_162,6.29,-0.62,0,0.42 2ZCO,ASP 195,3.24,-0.92,0,0.37 1SI7,ASP_150,3.28,-0.7,-0.36,0.55 2EFK,ARG_157,12.31,-0.19,0,0.01 2QVO,LYS_76,10.11,-0.31,0,-0.08 30IP,LYS 202,9.77,-0.85,0,0.12 2EJX,LYS 39,10,73,-0,31,0,13,0,4 4FZR,GLU_156,3.36,1.01,-1.4,-0.75 1XAW,ASP_492,3.8,0,-0.22,0.22 4ECC,ASP_179,4.35,-0.03,-0.02,0.59 2E0T,GLU 210,4.53,0.03,0,0 2NRK,GLU_163,3.77,0.42,-0.83,-0.32 1YTQ,TYR_170,10.31,-0.84,0.24,0.92 3HKX,ASP_34,3.41,-0.52,-0.33,0.45 1Y2Q,LYS 124,10.67,-0.13,0,0.3 2P0Y,ASP 190,4.51,-0.18,-0.19,1.08 3A2Z,CYS_173,9.4,0,0.02,0.38 2IXM,ARG_86,13.05,-0.31,0.5,0.37 3JZN,CYS_311,12.24,-0.7,-0.19,4.13 3F6F,LYS 129,10.61,-0.1,0,0.2 3CRM,HIS 246.6.12,-0.34,0,-0.04 3H5T,HIS_189,6.13,-1.11,0.48,0.27 3LMF,GLU_96,3.97,0.26,-0.37,-0.44 3DB9,ARG_48,12.42,-0.19,0,0.11 1R3F.TYR 251,11.09.0.0.46.0.63 3IVF,GLU_276,4.08,1.26,-1.64,-0.03 3LD1,ARG_223,12.1,-0.75,0,0.36 3KV0,CYS_162,11.46,0,0.01,2.46 1PVT,TYR_47,13.57,-0.15,0.42,3.29 3LJN.GLU 258.4.15.0.27,-0.29,-0.33 1W24,LYS_73,9.86,-0.75,0,0.1 3KT9,ARG_29,11.95,-0.44,0,-0.12 2QDJ,LYS_63,10.29,-0.25,0,0.04 2V4U.GLU 349.4.71.0.19.0.0.02 3BA1,HIS_235,4.9,-2.32,0.79,-0.07 1059.GLU 315.4.21.0.26.-0.16.-0.39 3F6F,TYR_4,11.74,0.4,0.5,0.84 2RGY,ARG_206,12.21,-0.29,0,0 1V43.GLU 369.4.97.0.5.0.-0.04 1ZHV,GLU_23,4.51,0.4,-0.4,0.02 2HXB,LYS_85,12.11,-0.33,1.15,0.79 2HRZ,GLU_304,4.58,0.35,-0.14,-0.13

1SOH,ARG 180,12.32,-0.34,0,0.16 2O34.TYR 73.10.25.0.-0.2.0.46 3GS9,GLU_39,4.27,0.58,-0.52,-0.29 1W7B,ARG 78,12,58,-0,14,0,0,21 3JRT,TYR_64,12.35,-0.83,-0.02,3.19 20KT,ASP 258,3.27,-0.82,-0.1,0.38 2GZQ,TYR_32,10.79,0.02,0.33,0.45 1XTZ,LYS_35,10.53,-0.15,0,0.18 3CCY,TYR_168,9.66,-0.66,-0.02,0.34 2XHC,TYR_224,11.98,0.61,0.07,1.29 3F1X,HIS 207,6.6,-0.5,0,0.6 1G5Z,HIS 141,6.54,-0.22,0.23,0.03 2AZP,HIS_110,6.21,-0.98,0.69,0 3BQW,GLU_278,5.11,0.62,0,-0.01 2IRM.CYS 250.10.95.0.0.03.1.92 3CNU,LYS_35,10.58,-0.35,0.05,0.37 3DSH,HIS_260,6.21,-0.3,0,0.01 2ZCO,LYS_97,10.24,-0.52,0,0.26 2DFL,ASP_46,3.99,-0.12,0,0.31 1Q8B,GLU 30,4.78,0.23,0,0.05 3L7N,ASP_132,3.24,-0.57,-0.37,0.38 1ZBM,GLU_30,4.31,0.21,0,-0.4 1LZL,ARG_107,12.4,-0.43,0,0.33 1SOW.TYR 19.12.48.-0.09.0.2.58 2GZR.TYR 83,11.08,0.0,1.08 3CS1,LYS_174,10.48,-0.15,0,0.13 3QAV,GLU_80,4.67,0.19,0,-0.02 1VJG,GLU_92,4.24,0.34,-0.08,-0.51 3QKY,ARG 65,11.78,-1.33,0.35,0.26 4H86.ASP 25.4.02.0.-0.02.0.24 4DBX.LYS 49.11.13.-0.8.0.69.0.74 3GG6,GLU_101,4.66,0.31,-0.04,-0.11 2FL4,TYR 108,11,54,0,33,0,23,0.97 3E5T.ASP 98.4.05.-0.93.0.11.1.08 1QQE,ASP_252,2.98,-1.22,-0.05,0.46 1H4U,TYR_577,12.31,-0.16,-0.74,3.21 2HRZ,HIS_241,5.58,-0.92,0,0 1PSW,LYS_223,10.53,-0.18,0,0.2 1XDZ,GLU_34,4.65,0.25,0,-0.1 1PSW,TYR_21,12.46,-0.85,0.05,3.25 3UX2,GLU_76,4.71,0.21,0,0 2G5X,LYS_159,9.83,-0.46,0,-0.22 3F5D,GLU 139,4.61,0.13,0,-0.02 3M7D,GLU_18,3.77,0.48,-0.59,-0.61 3K9I.LYS 163.10.5.0.0.0 1KCM,GLU_124,3.43,0.58,-1.18,-0.47 3Q1C,GLU_132,3.94,0.17,-0.73,0 1UAJ.LYS 32,10.53,-0.62,0.14,0.52 2EFK,ARG_146,12.58,-0.24,0,0.32 3RKV,ASP_206,4.06,0,0,0.26 3F5D,GLU_173,3.87,0.37,-1.05,0.05 1V43,LYS 30,10.54,-0.11,0,0.16 3EX9,ARG_38,10.64,-1.66,0,-0.2 3BB7,TYR_208,12.26,-0.78,0.3,2.72 1UOH,LYS_69,10.03,-0.49,0,0.02 3FXH,ASP_88,3.62,-0.59,0.06,0.34 2X4G,ASP_324,3.98,-0.13,0.03,0.28 200K,ASP_32,2.94,-0.85,-0.29,0.28 3T8R.GLU 73.4.88.0.25.0.0.12 2P1W,ARG_217,13.82,-0.95,1.06,1.23 2FL4,ASP 11,3.92,0,-0.01,0.13 3IVF,LYS 343,10,54,-0,11,0,0,15 3UX2,LYS_136,11.13,-0.22,0.85,0 4ACJ,ASP_687,3.89,0,-0.09,0.18 3CAX,CYS_399,9.91,-0.04,-0.35,1.3 1R5Q,GLU_55,5.16,0.21,0.09,0.36 3DZ1,ASP_20,3.43,-0.5,-0.13,0.26 3C6B,GLU_132,3.21,1.97,-2.88,-0.36 2X4G,ASP_38,3.67,0,-0.53,0.41

1MML/ARG 205/12/28/-0.56/0.0.34 3G9T,ASP_43,1.99,-1.89,-0.39,0.48 1Q46,ASP_150,3.75,-0.59,0,0.54 3ANJ,LYS_91,10.69,-0.21,0,0.4 3ETU.TYR 274.10.26.0.0.12.0.14 1J74,ARG 81,12,19,-0.61,0,0,3 2P5D,LYS_131,9.86,-0.35,0,-0.29 1NWA,TYR_144,10.53,0,0.12,0.41 1ZBM,HIS_143,6.06,-2.68,0,2.25 2FGG.LYS 9.10.47.-0.08.0.0.05 3US6,ARG_113,12.46,-0.43,0,0.39 3I0C,HIS 140,5.38,-1.13,0,0.03 300P,GLU_44,4.29,0.45,-0.35,-0.32 2X4L.ASP 111,3.28,-0.78,-0.12,0.38 1SBX.GLU 106.4.96.0.42.0.0.04 2RGY,ARG_143,12.5,-0.17,0,0.16 1WYC,ARG_205,12.12,-0.38,0,0 2C2Y,ASP_83,3.37,-0.57,-0.38,0.52 1WOULYS 35.10.44.-0.22.0.0.16 4F3J,GLU_132,4.62,0.12,0,0 2Q99,LYS_35,10.5,-0.21,0.05,0.17 2B78,HIS_259,6.44,-0.2,0,0.14 1PVT.TYR 51.12.04.0.0.12.1.92 1H4U.HIS 513.6.54.-0.18.0.0.22 3I4T,LYS_202,10.55,-0.08,0,0.13 3IRA,TYR_47,10.12,-0.19,-0.27,0.57 2X4G,ARG_51,11.64,-0.97,0,0.12 10I7.GLU 7,4.6,0.12,0,-0.03 109G,ARG_198,12.51,-0.3,0,0.31 3GYW,TYR_56,10.42,0,0.3,0.11 1FHL,GLU_329,5.14,0.27,0,0.37 2XHC,LYS 159,9.93,-0.45,0,-0.12 3CGW,TYR 251,11.18,-0.12,-0.07,1.38 2BDV,LYS_8,9.66,-1.42,0,0.58 1W24,LYS_181,10.93,-0.41,0.31,0.53 2RIS,ASP_122,3.41,-0.81,-0.11,0.53 3BQE,CYS_207,12.55,-0.95,1.44,3.06 1XTD.LYS 50.10.6.-0.28.0.0.38 1WLY,TYR_104,13.12,-0.03,-0.04,3.19 1U7U,ASP_377,2.83,-0.85,-0.57,0.45 2B61.GLU 54,4.21,0.92,-0.58,-0.64 3M66,LYS 267,10.5,-0.08,0,0.08 2BLL,LYS_381,10.34,-0.15,0,-0.01 3GOZ,TYR 262,10,38,0,0,1,0,28 3CAX,LYS_445,10.64,-0.22,0.37,0 3UX2,ARG 82,12.53,-0.19,0,0.22 3G6S.LYS 193.10.31.-0.19.0.0 3CCY,ASP_174,3.68,-0.26,-0.02,0.16 2E3H,ASP_216,3.13,-0.74,-0.48,0.54 3C6B,LYS 269,11.71,-0.62,0.97,0.86 2FC3,ASP 71,3.93,-0.91,-0.44,1.49 1R3F,ASP_113,3.6,-0.21,-0.22,0.23 1ZBM,ARG_43,12.88,-0.35,0,0.73 3ASA,ASP_306,3.66,-0.41,-0.91,1.19 1YG2,TYR 41,9.99,-0.46,0.02,0.43 3ASA,TYR_256,12.35,0,0.37,1.97 2P65,ARG_102,12.67,-0.3,0,0.47 2G5X,CYS 115,11.65,0,0.21,2.43 1ZBS,GLU_272,4.59,0.25,0,-0.17 2ZQ5,ASP_319,3.23,-0.64,-0.37,0.44 1LTU,ASP 11,2.66,-1.54,-0.04,0.43 1WLY,ARG_321,12.12,-1.26,0.53,0.35 2P0L,ASP_7,2.93,-0.85,-0.38,0.36 3F7M,LYS 161,10.26,-0.26,0,0.03 2W0G.CYS 203,10.07.0.2.0.46.0.4 3RVC,GLU_153,4.58,0.11,0,-0.03 1Q46,LYS_127,10.82,-0.23,0.19,0.36 2XMZ,ASP_80,3.88,0,-0.16,0.24 2EJB,GLU_180,4.55,0.11,0,-0.05

2C2Y.GLU 279.3.35.0.99.-1.57.-0.57 1R53,ARG 127,12,41,-0,12,0,0.03 2P5D,GLU_48,4.02,2.19,-1.68,-1 1XTD,ASP_104,3.65,-0.5,-0.01,0.37 3H04, ARG 242, 13, 16, -0, 46, 0, 7, 0, 42 1MD6.ARG 101.11.95.-0.94.0.0.39 3JZ9,ASP_459,4.25,0,0.27,0.18 3V75,GLU_145,4.78,0.22,0,0.06 3EGN,LYS_434,10.59,-0.17,0,0.26 2RIS,ASP_179,3.3,-0.42,-0.4,0.32 1AKO.HIS 201.6.29.-0.23.0.0.02 3DSH,ASP_298,2.87,-0.77,-0.38,0.22 1X8F,LYS_156,10.74,-0.11,0,0.34 2RIS,HIS 188,5.68,-0.88,0.33,-0.26 3ASA,ARG 376,12.2,-0.78,0,0.48 1L3K,HIS_33,4.78,-1.45,0.01,-0.28 2CI3,GLU_117,3.51,0.49,-0.77,-0.7 3UPD,TYR_193,10.12,-0.1,-0.18,0.4 2P0Y,ASP 80,4.14,0,0.11,0.22 2RFA,LYS 66,10.36,-0.14,0,0 1HF8,GLU_213,4.88,1.44,-0.79,-0.27 2AZL,TYR_200,10.6,0,-0.43,1.03 3T8R,TYR 65,10.48,-0.43,-0.03,0.93 1DTO.LYS 180.10.37.-0.14.0.0.01 2GZR,ARG_217,12.65,-0.19,0.01,0.33 3M16,HIS_299,6.34,-0.27,0,0.12 3LD1,ASP_305,1.85,-2.14,-0.52,0.71 3BPP,GLU_153,5.26,0.76,0,0 3CAX,TYR 406,9.97,0,-0.17,0.14 1J74,GLU_21,3.69,0.53,-0.84,-0.5 4HDE,ASP_93,3.67,0,-0.36,0.23 1LTU,ASP_73,4.38,-0.32,-0.28,1.17 2188.LYS 346,10.3,-0.2,0,0 4FCU,GLU_61,3.8,0.3,-0.71,-0.3 3CCY,ASP_53,3.91,0,-0.06,0.17 4AF2,ARG_110,12.96,-0.4,0.54,0.32 3U4K,ASP 68,2.27,-2.08,0,0.55 1UXO, ARG_79, 12.36, -1.31, 0.68, 0.49 1SNT,TYR_354,13.54,0,1.08,2.47 2JHY,LYS 178,10.63,-0.27,0.0.39 4GCO,CYS_254,10.18,0,-0.04,1.22 2H2W,ARG_252,12.42,-0.17,0,0.09 2B78.GLU 134.5.66.1.11.0.0.04 1DTO,LYS_34,10.56,-0.27,0,0.34 2BLL,ARG_591,12.95,-0.84,0.88,0.41 2B0J.LYS 99,11.02,-0.33,0.36,0.5 20V2,ARG 251,12,27,-0,34,0,0,11 3JSN,LYS_44,10.65,-0.11,0,0.26 3CS1,ARG 99,12,73,-0,78,0,54,0,47 4DVD,ASP_87,2.96,-0.81,-0.36,0.33 3UC9,TYR 50,11.25,-0.99,0.34,1.9 3TOW,LYS 149,10,21,-0.34,0,0.05 2AXO,TYR_102,10.4,0,-2.78E-17,0.41 3N2T,ARG_104,13.53,-0.35,0.89,0.48 4ANN,ARG_109,12.56,-0.36,0,0.41 2D0A, ASP_77, 3.15, -0.66, -0.3, 0.32 3JZ9,LYS_377,11.27,-0.33,0.7,0.41 2P52,GLU_255,4.23,2.56,-1.99,-0.83 1MIX,GLU_276,4.49,1.13,-1.09,-0.05 2W0G,LYS 273,10.42,-0.07,0,-0.02 3HVM,CYS_220,11.49,0.38,0.58,1.53 2YYO,HIS_81,3.57,-3.35,0,0.42 3O48,LYS_123,10.67,-0.22,0,0.39 10IS,ARG_308,12.59,-1.03,0.61,0.52 3RLN,GLU_622,4.43,0.12,0,-0.18 1N81,TYR_197,10.61,0,0.04,0.57 4FD6,HIS_49,6.47,-1.31,0.85,0.43 3F7M,ASP_216,3.58,-0.76,-0.43,0.97 2W0G,GLU_250,4.82,0.12,0,0.2

2FM9,LYS 217,10,42,-0,16,0,0.08 1X8FLYS 265,11.02,-0.37,0.74,0.15 3Q1C,GLU_116,4.8,0.29,0,0.01 2P1W.HIS 51.6.41,-0.23.0.0.14 1H4U,GLU_471,4.58,1.95,-1.56,-0.33 3H5T,LYS 338,10.39,-0.12,0,0 4EVF,LYS_263,9.75,-0.59,0,-0.16 4DNU.TYR 298,10.44,0,-0.19,0.62 1SJY,TYR_131,10.12,0,-0.22,0.34 1GXN,GLU_535,6.87,3.5,-1.34,0.21 1NKD.TYR 51.9.2.-0.7.-0.55.0.45 1PZC,GLU_54,4.26,0.14,0,-0.38 4ETX,ASP_320,3.88,-0.23,-0.12,0.42 2012,HIS 140,5.73,-0.67,0,-0.1 2XHC,LYS 306,10.62,-0.17,0,0.29 1WRU,TYR_305,10.19,0,0,0.19 3GW3,GLU_67,2.86,0.97,-2.16,-0.45 4ESS,ASP_50,2.29,-1.57,-0.41,0.47 3B79, ASP_33, 3.78, 0, -0.12, 0.1 2007,LYS 334,11.56,-0.4,0.85,0.6 4ETX,ARG_415,12.61,-0.24,0.01,0.34 2PGE.GLU 171.5.36.0.36.0.12.0.38 1DZF,GLU_66,4.57,0.07,0,0 3ULX,ARG 40,12.19,-0.32,0,0.01 1IAP.GLU 190,4.83,2.75,-1.58,-0.85 2QV2,GLU_147,4.63,0.13,0,0 2OSA,ARG_442,12.24,-0.33,0,0.07 3MEW, ARG_246, 13.75, -0.3, 0.65, 0.9 2PGE,ARG 230,12.53,-0.18,0,0.2 3PM2,GLU_125,4.58,0.09,0,-0.01 1TP6,ARG_7,12.39,-0.12,0,0.02 2IRM,GLU_259,5.5,1.1,0,-0.1 2GQV,ASP 28,3.21,-0.83,-0.22,0.46 3EZ7.GLU 142.4.95.1.35.-0.48.-0.42 3G9T,GLU_289,4.66,0.3,0,-0.14 2G7O,GLU_107,3.32,0.38,-1.18,-0.38 1DCF,LYS_98,10.54,-0.06,0,0.1 3EZ7,LYS 324,10.43,-0.07,0,0 2IF4,GLU_248,4.22,0.37,-0.25,-0.4 2YLF,HIS_216,7,-0.77,0.85,0.43 1R3F,GLU_98,4.51,0.2,-0.2,0 2FPN,ARG 195,12.31,-0.27,0,0.08 2H8O.CYS 116.12.44.0.0.22.3.22 1A8Q,HIS_107,6.32,-1.23,0.85,0.21 2J8A,HIS_321,5.97,-0.46,0,-0.08 3OA7,ASP_558,3.03,-0.95,0,0.18 1XKR,CYS_118,12.36,-0.04,0,3.4 2IDC.LYS 143,10.25,-0.21,0,-0.03 1X6J,ASP_50,4,0,0.02,0.18 1ZP2,LYS_30,10.51,-0.1,0,0.11 1SUU,ASP_608,3.34,-0.68,-0.12,0.34 3D9H,HIS 46,7.07,-0.37,0.59,0.36 2H2Z,CYS_85,11.6,0.27,0.13,2.19 4DEZ.CYS 70.10.04,-0.04.0.11.0.97 10LR,ASP_118,2.95,-1.64,-0.31,1.11 1P1L,LYS_37,10.35,-0.15,0,0 2GZO,LYS 180,11.34,-0.32,0.78,0.38 3CE7,ASP_81,4.37,0,0.26,0.3 4ANN,ASP_202,4.12,0,-0.09,0.42 3CX2,LYS_185,10.44,-0.06,0,0 1U7U,ARG 199,12.32,-0.45,0,0.28 3U2R,ASP_84,4.07,0,-0.19,0.46 3H13,ARG 456,13,72,-0,19,1,03,0,38 4E8B,ASP_164,2.58,-0.9,-1.47,1.15 2WOZ, ASP_311, 3.33, -0.52, -0.31, 0.36 20V2.ASP 48.3.12.-0.65.-0.37.0.34 1Y0K, ASP_74, 3.09, -1.73, -0.43, 1.44 2IF4,GLU_193,4.65,0.34,-0.19,0 1A8Q,TYR_13,11.43,0,0.54,0.9

2CVB,ARG_134,12.24,-0.88,0,0.63 2Z0M.LYS 221.10.68.-0.13.0.0.3 2ZQ5,ASP_149,4.35,-0.15,0.03,0.68 2X4L,GLU_343,3.31,0.92,-1.65,-0.45 3CN5,TYR_262,9.94,0,-0.21,0.14 3KT9,HIS 14,6.27,-0.12,0,-0.1 1ZCU,GLU_143,4.6,0.1,0,0 4FZN,LYS_193,10.17,-0.6,0,0.27 1X8F,HIS_241,6.68,-1.04,0.69,0.53 3JRT,ASP_145,2.89,-0.85,-0.41,0.35 2CWC,ARG 278,12.08,-0.26,0,-0.16 3C6B,LYS_181,10.3,-1,0.44,0.35 3V3T,GLU_297,4.83,0.14,0,0.19 3BZT,GLU_331,4.52,0.17,-0.09,-0.06 2AHE,LYS 254,10.53,-0.11,0,0.14 3GEC,ARG 422,12.35,-0.79,0,0.64 3H5T,GLU_264,4.7,0.36,0,-0.16 2BLL,CYS_439,10.29,-0.8,0.45,1.64 2X4G,ARG_75,12.22,-0.35,0,0.07 2GZQ,GLU_156,2.89,0.83,-1.93,-0.51 2DVK,HIS 65,5,76,-0,71,0,56,-0.6 2RH3,TYR_106,10.08,0,-0.12,0.19 2HXB,TYR_114,12.71,-0.85,0.09,3.48 3RJX.HIS 109.7.08.-0.55.0.85.0.28 2GZO,LYS 100,10,55,-0.6,0,0.67 1MML,LYS_62,10.44,-0.07,0,0.01 2013.TYR 283.9.21,-0.74,-0.42,0.37 1MN3,LYS_435,10.31,-0.19,0,0 2V81,TYR 100,11.44,0.79,0.25,0.39 2XMZ,ARG 200,12.69,-0.19,0,0.37 2CL3,GLU_34,4.39,0.27,0,-0.38 2IRM,ASP_16,3.81,0,-0.37,0.37 1LZL.GLU 302.4.87.0.25.0.0.12 2HXB,GLU 102,5.41,3.26,-2.33,-0.01 1U7U,LYS_303,10.46,-0.04,0,0 1P6F,ARG 168,12,56,-0.62,0.21,0.48 3U2A,GLU_18,4.65,0.15,0,0 1R29,ASP_63,3.22,-0.78,-0.18,0.39 3L7N,TYR 218,12,43,-0.02,0.01,2,45 3FHF,TYR_92,10.17,0,-0.27,0.44 1BKR,ASP_84,4.32,0,0.26,0.27 2FL7,HIS_72,5.27,-2.04,0.46,0.36 1UJ8,GLU 51,4.8,0.09,0,0.21 3L7N,TYR_206,10.43,0,0.07,0.36 1AD6,LYS_429,10,-0.22,0,-0.27 2QDJ,ASP_109,3.7,-0.85,-0.11,0.86 1RZ2,TYR_39,10.57,0,0.11,0.46 4ESS.GLU 59.4.57.0.33.0.-0.25 2DFL,HIS_304,5.62,-0.86,0,-0.02 1RL0,ARG_28,12.06,-0.51,0,0.07 1Q42,HIS_102,7.21,-0.55,0.65,0.61 2FD5,HIS 95,3.95,-2.23,0.75,-1.07 1MN3,ASP_422,3.92,0,0,0.12 3FRR,LYS_151,11.24,-0.62,0.85,0.51 1WXQ,LYS_163,10.79,-0.15,0,0.44 3HNX,GLU_22,3.06,0.43,-1.53,-0.34 4DIU,TYR_84,11.07,-0.23,0.38,0.91 2CI3,ASP_205,3.91,0,0,0.11 1GVP,LYS_3,10.6,-0.15,0,0.25 2AHE,GLU_141,5.05,0.98,-0.59,0.17 1Q42,LYS 14,11.47,-0.3,0.81,0.46 3G9T.HIS 86.6.4,-3.02.0.85,2.07 1SNT,HIS_202,8.01,-0.64,1.61,0.55 2Q07,HIS_348,4.92,-2.43,0.82,0.03 2EHG,GLU_11,5.07,0.59,0,-0.03 1BKB,GLU_28,4.07,1.4,-1.55,-0.28 2GYZ,ARG_92,12.52,-0.16,0,0.19 2FXT,ARG_255,12.1,-0.5,0,0.11 1MML,HIS_214,5.71,-0.79,0,0

3B7H.GLU 6.3.8.0.34,-1.03.0 3E5T,GLU_97,3.7,0.3,-1.09,0 2IF4,TYR 218,10.3,0.0.09,0.21 3G6S,ARG_156,12.06,-0.46,0,0.02 1Z3X.GLU 184.4.69.0.28.0.-0.09 1TR9.GLU 290.4.73.0.2.0.0.04 1SI7,HIS_69,5.9,-0.28,0,-0.31 1I60,LYS_119,10.58,-0.22,0,0.29 10GL,TYR_193,11.71,0,0.27,1.44 2R0S.ASP 137.3.92.0.-0.12.0.24 3V1Q,ARG_550,12.19,-0.31,0,0 301C,ARG 98,13,68,-1,03,1,52,0,7 2P52,TYR_226,10.38,0,0.08,0.3 3KV0.GLU 130.3.89.0.57.-1.14.-0.04 1ZYL.TYR 152,12,77,0,0,1,2,67 3M70,LYS_266,10.27,-0.23,0,0 3PZ9,TYR_46,12.71,-1.15,0.26,3.59 2ZTY,HIS_161,3.9,-2.48,0,-0.12 3UC9.ASP 174.3.75.-1.42.-0.17.1.54 3QKY,TYR_190,12.77,0.44,0.07,2.26 3P2F,ARG_154,12.51,-0.31,0,0.33 3BA1,ARG_36,13.56,-0.24,0.72,0.58 20BI,LYS 99,10.34,-0.16,0,0 2YT4,LYS 510,11.11,-0.58,0.85,0.34 2Z14,HIS_71,6.26,-0.81,0.79,-0.22 2YLF,ARG_47,12.4,-0.2,0,0.1 2X4G,ASP_331,3.98,0,-0.18,0.36 3GV0,ARG 209,13.28,-0.44,0.47,0.75 2B0A,LYS_155,10.39,-0.11,0,0 2FXT,ARG_370,12.41,-0.14,0,0.05 1YTD,LYS_280,10.52,-0.18,0,0.2 2R57.GLU 305.3.62.0.31,-0.81,-0.38 2Z14,ASP 106,2.47,-1.51,-0.3,0.48 1QQE,TYR_148,11.93,0,0.35,1.57 1JB3,HIS_127,6.63,-0.4,0.03,0.51 4FZR,GLU_209,4.6,0.1,0,0 1R3F,ASP_10,3.48,-0.47,-0.08,0.23 2Z0M.GLU 323.4.11.1.55.-1.58.-0.34 2CWC, ARG_82, 13.4, -0.75, 0.78, 0.87 20GQ,CYS_428,10.3,-0.8,0.03,2.05 2B3M,ASP 62,2,4,-1,26,-0.66,0.52 1Z9L,ASP 11,3,9,0,-0,15,0,25 2PGX,ASP_30,4.08,0,0.1,0.17 1R3F.GLU 278.4.6.0.09.0.0.01 1HF8,ARG_92,12,-0.54,0,0.03 1VJG,CYS 35,12.3,0,0,3.3 1T6L.LYS 73.10.17.-0.33.0.0 3FFM,GLU_45,4.09,0.32,-0.35,-0.38 3PBH,TYR_183,13.35,-0.48,0.61,3.22 2OSA.ASP 310.3.95.0.0.0.15 3IVF.GLU 335.4.62.0.18.0.-0.06 2Q07,ARG_359,12.75,-0.33,0.14,0.43 200K,HIS_12,3.92,-2.53,0,-0.04 3RLN,GLU_643,4.34,1.66,-1.1,-0.73 3EVZ, ASP 206, 3.22, -0.28, -0.71, 0.41 1046.TYR 101.10.33.-0.54.-0.33.1.21 307K,ARG_108,12.35,-0.27,0,0.12 2X4J,TYR 95,12.42,0.85,0.13,1.44 1SUU,GLU_546,4.74,0.72,0,-0.47 4D8L,HIS 251,7.49,-3.39,0.85,3.54 2EJB,LYS_40,10.52,-0.2,0,0.22 1X6J,CYS_49,10.33,-0.01,0.14,1.21 3IDW,ARG_50,12.56,-0.1,0,0.16 3QAV,LYS 81,10.48,-0.17,0,0.15 1JB3.GLU 23.2.52.0.63.-1.67.-0.94 2R51,GLU_26,4.4,0.28,0,-0.38 2FBQ,TYR_134,11.29,-0.85,0.64,1.5 3ETV,GLU_241,4.61,0.12,0,0 2ZQ5,ARG_109,12.31,-0.47,0,0.28

1ZP2.HIS 136.6.21.-0.25.0.-0.04 1NAR.GLU 66.4.45.0.33.0.-0.39 1U3Y,CYS_310,9.83,0,0.31,0.51 4F3J,LYS_142,10.05,-0.46,0,0.02 1R53.GLU 256.3.99.1.73.-1.61.-0.63 1VJG.TYR 76,9.89,-0.1,-0.18,0.17 2VGM,LYS_167,10.59,-0.32,0,0.41 1TR9.TYR 11.10.39.0.0.08.0.31 3G9G,LYS_7,10.65,-0.1,0,0.24 2XMZ,HIS_31,5.54,-1.18,0.49,-0.27 3EVN.TYR 284,10.11.0.-0.06.0.18 1TD6,GLU_24,3.93,0.44,-0.83,-0.19 3MTT,TYR_577,11.12,0.15,0.33,0.64 2Z14,GLU 23,3,71,0,44,-0,85,-0,38 2B78,ARG 315,12.02,-0.53,0,0.05 3RJX,LYS_190,11.46,-0.31,0.85,0.42 2EYI,ASP_117,3,-0.75,-0.54,0.49 2Q07,ARG_433,12.78,-0.42,0.11,0.58 3EX9,GLU 140,6.92,2.89,0,-0.46 2YYO,GLU_155,5.09,3.48,-2.67,-0.23 1LFP,LYS_14,9.79,-0.56,0,-0.15 3DHN,ASP_196,2.24,-3.31,-0.15,1.91 1RHS,HIS_280,6.56,-0.79,0.82,0.03 2OSA.GLU 374,5.56,0.2,0.3,0.57 3JSN,ASP_3,3.03,-0.98,0,0.2 1DUP,GLU_129,4.55,0.05,0,0 3MIX,ASP_495,3.65,0,-0.5,0.35 1WP5,GLU_5,4.82,0.29,0,0.03 2B78.GLU 169.3.74.0.48.-0.85.-0.4 3RLE,ASP_53,3.89,0,-0.13,0.23 3FHF,GLU_174,3.59,0.29,-0.61,-0.58 3CBN,ASP_73,3.33,-0.23,-0.45,0.21 3RJX.LYS 273,10.39,-0.22,0,0.11 3LD1,ARG_339,13.06,-0.26,0.18,0.63 4FZN,GLU_226,4.08,0.3,-0.41,-0.32 3G9G,LYS_219,10.34,-0.19,0,0.03 2X5Y,CYS_831,10.23,-0.84,0.02,2.06 2OBI,HIS_60,5.17,-1.29,0,-0.04 4DBX,TYR_284,10.23,0,0.06,0.17 3LD1,ARG_359,12.27,-0.27,0,0.03 3PZ9,ASP_379,3.92,0,-0.04,0.16 1X7F,TYR 115,9.97,-0.62,0.25,0.34 3EJC,HIS 124,6.88,-0.39,0.77,0 2Q13,HIS_363,5.89,-1.18,0.39,0.19 1QQL,TYR_94,10.29,-0.02,-0.24,0.55 1WPA,ASP_518,3.4,-0.27,-0.59,0.46 1CHD,ARG_238,12.78,-0.41,0.19,0.49 2GKG,ARG_46,12.29,-0.34,0,0.13 10YI.HIS 358.6.47,-0.19.0.15.0.01 1F2V,GLU_33,4.46,0.23,0,-0.27 3K1H.GLU 144,4.66,0.15,0,0.01 4EKU,LYS 54,10.37,-0.11,0,-0.01 3IU5,TYR_134,10.27,0,-0.01,0.29 2OKT,HIS_336,6.42,-0.08,0,0 2OSA,HIS_400,4.61,-3.3,0.85,0.57 1T3Y,LYS_7,11.1,-0.23,0.6,0.23 2E3C,GLU_237,4.7,0.35,-0.38,0.24 1CBY,ASP_179,2.63,-1.72,0,0.54 3GYW,HIS_182,6.09,-0.32,0,-0.1 2Q12,GLU_252,4.37,0.18,-0.31,0 3T5B.CYS 307.12.75.0.0.3.75 3L7N,GLU_112,6.2,3.16,-1.45,0 3I47,HIS_237,6.33,-0.15,0,-0.02 1WOU,GLU_5,3.05,0.36,-1.07,-0.74 3M7D,GLU 263,4.49,0.17,-0.06,-0.12 3GS9,ASP_9,2.42,-2.07,0,0.68 1MD6,CYS_121,10.77,-0.45,-0.35,2.56 3H5T,GLU_34,4.23,0.42,-0.68,-0.01 3CAX,TYR_129,11.2,0,0,1.2

1YOY,GLU_134,4.61,2.16,-1.58,-0.47 3CX2,GLU 240,4.02,0.79,-0.81,-0.46 4FCU,ASP_118,3.04,-0.79,-0.38,0.41 3B4D,TYR 217,10.34,0,-0,1,0,44 2CWY,ASP_80,3.09,-1.05,-0.02,0.37 2161.LYS 89.10.4.-0.24.0.0.13 1TR9.GLU 326.4.17.0.28.-0.53.-0.08 3LJI,GLU_136,4.63,0.15,0,-0.02 3GW3,GLU_130,4.33,0.29,0,-0.46 20YZ,GLU 59,3.24,0.56,-1.38,-0.45 1GPP.GLU 425,4.65,0.27,0,-0.12 2BDD,GLU_76,4.46,0.18,0,-0.22 2QV2,ARG_10,12.22,-0.49,0,0.2 3MIX.HIS 340.7.2.-1.1.34.0.35 301C.GLU 312.4.58.0.22.0.-0.13 3KT9,LYS_57,10.78,-0.24,0,0.51 2CN1,TYR_261,12.93,0,0.65,2.27 1XKR,ARG_6,12.39,-0.42,0,0.31 10GL,TYR_198,12.81,0,0,2.81 3EVP,GLU_190,4.62,0.18,0,-0.06 2X5Y,TYR_814,10.4,-0.39,-0.08,0.87 2Z0M.TYR 96.10.08.0.-0.32.0.4 3ONT, ASP_55, 1.91, -2.33, -0.16, 0.61 2QV2,LYS 93,10.43,-0.27,0,0.2 3M7G,ASP_121,3.37,-0.65,0,0.23 3HUE,ARG_27,12.13,-0.37,0,0 3RJX,GLU_54,7.34,4.65,-1.77,-0.04 4DIU,ASP_172,3.25,-0.52,-0.62,0.6 3HVM,TYR 217,10.85,-0.81,-0.19,1.84 1ZBM,ARG_4,12.88,-0.43,0,0.82 3KB5,ARG 326,13.2,-0.24,0.25,0.69 3A7L,TYR_70,11.03,0,0.74,0.29 2FL7,LYS 122,11.2,-0.41,0.85.0.27 2WOZ,LYS_406,10.94,-0.35,0,0.79 3ERF,ARG_210,12.39,-0.39,0,0.28 2CI3,LYS_198,10.41,-0.08,0,-0.01 2IXM,LYS_302,10.65,-0.25,0,0.4 3GFP,HIS_422,5.54,-0.85,0.17,-0.28 2PGE,ARG_151,13.03,-0.38,0.5,0.42 1R7J,LYS_86,10.41,-0.09,0,0 3KB5,GLU_392,4.3,1.35,-0.72,-0.83 3T5B,ARG 140,12.23,-0.51,0,0.24 1PVT,LYS 112,9,72,-0.6,0,-0.19 2F4Q,TYR_307,9.15,-1.31,-0.38,0.85 2l6l,GLU_115,3.53,0.89,-1.57,-0.3 1L3K,ASP_154,4.14,-0.03,-0.16,0.54 1RZ2,TYR_105,12.84,0,0.81,2.03 3I4T.CYS 193,12.66.0.0.1.3.56 3BQE,LYS_281,10.14,-0.37,0,0.01 1ZBM,GLU_211,4.2,0.26,-0.21,-0.34 1ZBP,GLU_63,4.2,0.37,-0.66,0 2E3H,ASP 254,1.82,-2.1,-0.38,0.5 3ULX,LYS_53,11.03,-0.17,0.36,0.34 1FHL.LYS 175.10.96.-0.53.0.0.99 2FL4,ARG_74,12.19,-0.85,0,0.54 3BCY,LYS_50,11.23,-0.68,0.85,0.56 1JB3.CYS 123.10.13.-0.03.0.32.0.84 2YWJ,LYS_63,10.39,-0.17,0,0.06 1QQE,TYR_80,10.65,-0.85,-0.15,1.64 1XEU,LYS_62,11.45,-0.41,0.85,0.51 3M7D,ASP 303,4.02,0,-0.07,0.28 1YR6,HIS_112,6.4,-1.46,0.85,0.51 3BPP.ASP 228.3.15.-1.38.-0.49.1.22 2R57,LYS_265,10.29,-0.32,0,0.11 3A0X,LYS_628,10.38,-0.31,0,0.19 1RWZ,LYS 118,10.31,-0.08,0,-0.11 2GZR,GLU_101,4.72,0.21,0,-8.67E-18 3RJX,GLU_179,4.49,0.3,0,-0.31 105J,HIS_0,7.15,-0.42,0.85,0.22

20PJ,ARG 67,11.92,-0.72,0.0.14 2E3I,ARG 126,13.31,-0.47,0.76,0.53 3HVM,TYR_193,11.92,0.46,0.48,0.98 3K9I,GLU_160,4.67,0.14,0,0.03 3BA1,HIS_211,7.49,-0.64,0.85,0.77 2B6P.TYR 23,12.72,-0.28,-0.43,3.43 30IP.CYS 177.9.35.0.0.13.0.22 3HVW,ARG_315,12.54,-1.41,0.7,0.75 2V5B,LYS_113,10.38,-1.23,0.83,0.28 3COU,GLU_124,3.94,1.5,-1.57,-0.49 3PP8,ASP 68,3.55,-0.36,-0.5,0.6 1P2F,LYS_148,10.7,-0.12,0,0.33 2EHG,ARG_118,12.85,-0.13,0,0.48 1BYI,TYR_4,12.07,0,0.5,1.57 1CBY,ASP_39,2.94,-1.4,0,0.55 3EZ7.GLU 293.4.56.0.21.0.-0.14 3CBN,LYS_76,10.58,-0.5,0.23,0.34 3GS3,ARG_216,12.32,-0.41,0,0.24 1R3D,GLU_72,5.18,1.14,-0.1,-0.36 3B7X,ARG 28,12.46,-0.04,0,0 2FPN.GLU 9,4.57,0.3,0,-0.23 2EFK,ARG_121,13.3,-0.45,0.66,0.59 1TLV,ARG_214,12.44,-0.97,0.48,0.43 20VO.HIS 44.6.28,-0.22.0.0 3BCH.ARG 41.12.54,-0.39.0.02.0.41 1ES9,ARG_127,13.77,-0.51,1.36,0.42 1FO9.TYR 350.12.14.-0.69.0.11.2.72 3RLN,TYR_635,10.79,-0.4,0.07,1.11 200K,LYS 40,10.23,-0.41,0,0.14 3P2F.CYS 196.9.51.0.0.3.0.21 1MTZ,TYR_165,10.57,0,0.03,0.54 1JKS,TYR_191,9.73,-0.85,0,0.58 3ERF,LYS 66,11.89,-0.39,0.94,0.84 4ESS.GLU 132.3.55.0.95.-0.93.-0.98 1MML,TYR_271,10.42,0,0.2,0.23 2D8N,LYS_196,11.07,-0.36,0.38,0.55 3GW3,ARG_113,11.99,-0.75,0,0.24 2IN0,GLU_4,4.93,0.35,0,0.09 3PM2,ARG 43,12,18,-0.39,0.0.07 1J7G,GLU_47,4.32,0.19,0,-0.37 2OSA,ARG_321,12.85,-0.17,0.06,0.45 2CVB,TYR_4,12.79,0,0.18,2.61 3F6F.LYS 82,10.74,-0.11,0,0.34 4EVF,ARG_161,12.8,-0.29,0,0.59 10GL,LYS_66,10.38,-0.13,0,0.01 1X1E,GLU_190,4.62,0.12,0,0 2BDV,HIS_65,6.39,-0.09,0,-0.02 3FTT.ARG 46.11.74.-0.76.0.0 3FTT,ASP_14,3.88,-0.69,0.19,0.58 2YT4, ASP_605, 1.81, -2.31, -0.43, 0.75 3PBH,LYS_130,10.18,-0.25,0,-0.07 2H85, ASP 310, 3.72, -0.37, -0.09, 0.39 1Y2Q,LYS_21,10.47,-0.03,0,0 2AD1,ARG_10,11.93,-0.56,0,-0.01 1UCH,TYR_85,11.91,-0.86,-0.54,3.31 3MIX,CYS_583,12.01,0,0.42,2.59 3RKV,ARG_227,12.35,-0.18,0,0.03 2B61,LYS_256,10.82,-0.18,0,0.49 2YT4,LYS 640,10.63,-0.15,0.0.27 2ZCO,GLU_76,4.6,0.18,0,-0.08 3PBH,ARG_252,11.52,-1.17,0,0.19 109G,ARG 112,11.1,-1.12,0,-0.27 2E3H,GLU_233,4.62,0.11,0,0.01 3BWT,LYS_682,11.09,-0.47,0.66,0.4 2B2H,LYS_144,10.27,-0.35,0,0.13 3FS3,HIS_227,5.75,-0.87,0.04,0.08 2Q99,ARG_71,11.91,-1.13,0.01,0.54 2Z0M,GLU_143,5.07,0.32,0,0.25 2D7J,HIS_166,9.31,-2.94,2.45,3.29

1W24, ARG 14, 12, 25, -1, 11, 0, 02, 0, 84 2D7J,GLU_173,4.01,0.41,-0.79,-0.12 1P4X,HIS_77,5.92,-0.3,0,-0.29 4FCU,LYS_2,10.01,-0.58,0,0.09 2GS5.LYS 73.10.43.-0.07.0.0 3DZ1.ASP 159.4.15.0.-0.19.0.54 2QVO,LYS_11,10.43,-0.08,0,0.01 2EFK,ASP_214,4.09,0,0.03,0.26 3DHN,ARG_214,12.36,-2.13,0.85,1.15 2EHG.GLU 52.7.82.3.34.-0.89.0.87 3DZ1,ARG_113,12.41,-0.09,0,0 3A4C,GLU_508,4.81,0.35,0,-0.04 3LQE,GLU_303,3.45,0.63,-1.67,-0.01 1SUU.ARG 790,13.53,-0.45,0.8,0.68 10GL/ARG 204/13/16/-0.81/0.82/0.66 3EGN,GLU_395,4.02,0.22,-0.09,-0.61 1YB2,TYR_62,12.23,-0.41,0.32,2.32 1R7J,GLU_65,4.63,0.21,0,-0.08 1X9G.ASP 171.3.45.-0.63.0.07.0.22 3EX9,GLU_68,3.62,0.14,-0.73,-0.29 2P1W.TYR 83,10.05.0.0.05 3IVF,LYS_98,10.46,-0.15,0,0.11 3AUF,HIS_175,5.16,-1.28,0,-0.06 1DTO.HIS 113.6.-0.43.0.-0.07 3H8Y,ARG_83,12.43,-0.09,0,0.02 4AM1,GLU_59,4.61,0.41,0,-0.3 2W1R,GLU_61,4.52,0.24,0,-0.23 2Q34,GLU 81,4.68,0.26,0,-0.06 10GL,HIS_20,5.59,-1.4,0.25,0.24 3EVN,ARG_19,12.28,-0.42,0,0.18 30IP,GLU_82,4.86,0.32,0,0.04 3V3T,LYS 4,10,43,-0,41,0,0,33 2007,ARG 384,13.69,-0.32,0.84,0.68 1R5Q,ASP_80,3.97,0,-0.02,0.19 2XMZ.GLU 214,4.05,0.29,-0.74,0 1NWA,HIS_76,3.27,-3.5,0.82,-0.54 2PWQ,LYS 39,11.16,-0.32,0.22,0.76 2F8H,HIS 87,5.77,-1.25,0.47,0.05 3MTT,ARG_458,12.45,-0.23,0,0.19 1WJG,GLU_27,4.63,0.13,0,0 1R29,ARG_94,12.42,-0.08,0,0 1J33,ARG_148,13.5,-0.33,0.85,0.49 1P1L,LYS_20,10.61,-0.14,0,0.25 3M70,GLU_263,4.12,0.29,-0.04,-0.63 4DNU,GLU_216,4.88,0.55,0,-0.18 3EAZ,ASP_159,3.51,-0.53,-0.1,0.35 2E3C,LYS 229,10,19,-0,42,0,0,1 3HQX,CYS_65,11.51,0,0.02,2.48 2AHE,CYS_189,13.36,-0.12,0.8,3.67 1NIJ.ARG 93,12.03,-0.98,0.0.5 3CRM.TYR 315.10.88.0.0.0.88 1MIX,LYS_263,11.15,-0.16,0.12,0.69 3JZN,LYS_385,10.92,-0.32,0.26,0.47 2P65,ARG_176,12.19,-0.25,0,-0.06 4EUG,LYS 94,9.98,-0.44,0,-0.08 10I7,GLU_58,4.25,0.35,-0.79,0.18 2E3C,CYS_328,12.09,0,-0.79,3.88 1T6L,ASP 109,3.95,0,0,0.15 2BLL,GLU_617,4.48,0.13,0,-0.16 1RKA,LYS 193,10.6,-0.17,0,0.26 2YWX,LYS_140,10.47,-0.25,0,0.22 3LQE,TYR_525,10.59,0,0.27,0.31 1PVT,LYS_76,10.58,-0.27,0,0.35 2IQT,ARG 10,12.18,-0.32,0,0 1WOU,GLU_122,4.72,0.08,0,0.14 3O16,GLU_215,4.75,0.11,0,0.13 1YM5,GLU_136,4.19,0.16,-0.5,0.03 20EW,ASP_325,3.76,0,-0.24,0.2 3GMS,LYS_298,10.45,-0.16,0,0.11

1RAJ.ASP 89.4.0.0.0.2 1EDG,ASP 68,2,54,-1,46,-0,4,0,61 1EDG,LYS_61,10.46,-0.24,0,0.2 2QK0,LYS_71,10.39,-0.11,0,0 2YWK.GLU 46.4.21.0.3.-0.59.0 2RIK.GLU 240.4.7.0.2.0.0 3IPZ,ARG_92,13.03,-0.68,0.56,0.65 3ANJ,CYS_176,11.91,-0.78,1.01,2.67 2NSN,ASP_54,2.13,-2.05,-0.41,0.78 2IOT.GLU 4.4.56.0.2.0.-0.14 3HUE,GLU_287,4.5,0,0,0 3V3T,LYS_155,10.37,-0.23,0,0.1 2Q13,ARG_338,12.26,-0.57,0,0.33 1JSX.GLU 48.4.37.0.16.0.-0.29 1N81,GLU 91,4.78,0.11,0,0.17 2P0Y,ASP_76,3.74,0,-0.34,0.28 1YM5,ASP_140,3.9,0,-0.23,0.33 3VJ8,ARG_218,13.76,-1.46,1.4,1.31 2FBQ,GLU_80,4.58,0.08,0,0 2H01.CYS 68.13.67.0.0.87.3.8 2B61,GLU_348,4.22,0.37,-0.45,-0.2 2V5B,GLU_248,4.74,0.63,-0.01,-0.38 3V55,CYS_596,9.6,-1.07,0.23,1.44 2D8N,GLU_25,4.68,0.22,0,-0.05 109G,ARG_108,11.74,-1.77,0.59,0.42 2PGX,ARG_118,13.86,-0.62,1.05,0.94 1WXQ,ASP_97,3.92,-0.01,-0.18,0.31 2ZQ5,GLU 342,3.81,0.29,-1.08,0.1 1JT9,HIS 132,4,88,-1,7,0,2,-0,12 3JZ9,TYR_368,13.22,-0.85,0.04,4.02 1U7U,GLU_256,2.94,0.44,-2,-0.01 3GS9.CYS 113.11.05.-0.85.0.14.2.75 3I47,HIS 60,5.13,-0.79,0,-0.58 1HF8,TYR_88,9.95,0,-0.57,0.53 3RKV,GLU_268,3.12,0.99,-1.62,-0.75 3CS1,ARG_49,12.08,-0.74,0,0.31 1TD6,GLU 27,4.73,0.24,0,-0.02 3B7H,HIS_65,6.65,-0.15,0,0.29 3GMS,ARG_232,13.3,-0.52,0.81,0.51 2X4L,GLU_261,3.71,0.4,-0.85,-0.33 3DTE,ARG_19,12.23,-0.66,0,0.39 3BB7,GLU 348,6.32,1.51,0,0.31 2H85,LYS 46,11,38,-0,24,0,41,0,71 1Q2Y,TYR_65,10.55,0,0.28,0.27 1XEU,ASP_156,4.63,0,0.42,0.41 2G9D,LYS_35,10.42,-0.4,0,0.31 2Q12,GLU_216,4.79,0.29,0,0 1D2K,LYS_149,10.5,-0.41,0.09,0.33 1BN6.HIS 283.6.89.-3.25.0.86.2.77 1UXO,HIS_9,5.16,-2.1,0.76,0 3VJ8,ARG 203,13.62,-0.39,0.56,0.95 1C44.LYS 8.10.42.-0.27.0.0.19 1Q2Y,HIS_117,6.35,-0.63,0.59,-0.11 1YTD,ASP_229,3.21,-0.68,-0.12,0.21 2NRK,GLU_161,4.95,1.71,-0.66,-0.61 2V4U,HIS_517,4.65,-2.45,0.84,-0.24 4ANN,LYS_165,10.43,-0.19,0,0.13 3G9G,TYR_183,11.93,0.85,0.48,0.6 2QEV,GLU_88,4.85,0.32,0,0.03 2RIS,GLU 95,4.65,0.09,0,0.06 3M7D,ARG_287,12.49,-0.1,0,0.09 2CVB,ASP_15,2.85,-1.86,-0.2,1.1 2WZ9,LYS_110,10.57,-0.14,0.08,0.14 3ZXY,ASP_157,4.08,0,-0.06,0.33 3JZN,GLU_90,4.41,3.23,-2.54,-0.78 4H86,LYS_107,10.34,-0.16,0,0 4FD6,LYS_219,10.99,-0.86,0.85,0.5 2EFK,TYR_231,10.43,0,-0.11,0.54 3TOW, ASP_154, 3.59, 0, -0.58, 0.38

1FHL,GLU_279,4.95,0.34,0,0.1 2G3A,ASP_33,3.91,-0.07,-0.04,0.23 3IL3, ARG_127, 12.47, -0.65, 0, 0.62 3EVP,ASP_123,2.28,-1.56,-0.4,0.44 1SFE,GLU_22,4.75,0.44,0,-0.2 2CW4,LYS 5,10.42,-0.09,0,0.01 3QAV,ASP_91,3.3,-0.84,0,0.34 4DND,GLU_41,4.61,0.11,0,0 4HDE,ASP_166,3.1,-1.85,-0.08,1.24 2AD1,GLU_275,4.7,0.15,0,0.05 2BLL/ARG 415,13,47,-0.57,0.71,0.82 2PLQ,ASP_109,3.79,0,-0.3,0.29 3C38,ARG_203,13.8,-0.43,1.34,0.38 1WYC, ARG 89, 12, 2, -0, 41, 0, 0, 1 2EJB,GLU 117,3.65,0.39,-0.82,-0.42 3I0C,HIS_145,5.24,-1.62,0.59,-0.24 2CWC,ARG_162,13.99,-0.46,1.13,0.8 3KV0,GLU_40,3.47,0.44,-1.48,0 2G5X,ASP_121,2.37,-1.66,-0.38,0.6 3G6S,ARG_147,11.83,-1.2,0,0.54 3EX9,GLU_72,3.98,0.2,-0.34,-0.37 1X8F,ASP 180,3.86,-0.25,-0.04,0.35 1H09,CYS_108,13.21,-0.06,0,4.27 1L2H,LYS 55,11.64,-0.42,0.85,0.72 2013,LYS 350,10,38,-0,27,0,0,15 2AD1,ASP_264,3.57,0,-0.6,0.37 2A1V,ASP_51,3.98,-0.61,0.24,0.55 3Q1C,HIS_250,6.28,-0.27,0,0.05 1G8P,TYR 149,13.07,-0.15,0.77,2.44 1DVO,ASP_107,2.71,-1.35,-0.32,0.58 1JKS.TYR 208,12.3.0.0.48,1.83 3V1Q,LYS_622,10.38,-0.12,0,0 1XTD.LYS 96,10.38,-0.12,0,0 4AM1.LYS 9.10.44,-0.18.0.0.12 105T,LYS_114,9.88,-0.52,0,-0.1 10TM,LYS_175,10.36,-0.14,0,0 3TMO,TYR_299,12.45,0.57,0.31,1.57 3FHF.GLU 25,3.24,0.63,-1.02,-0.88 4AM1,LYS_164,11.43,-0.33,0.85,0.41 2W1R,LYS_90,10.15,-0.34,0,0 3H8Y,GLU_53,4.71,0.21,0,0.01 307K,GLU_154,3.71,0.49,-0.75,-0.53 2IOT.GLU 265.4.12.0.76.-0.72.-0.41 2DG7,ARG_180,12.4,-0.09,0,-0.01 1YG2,ASP_94,2.83,-1.52,0,0.55 1BKR,LYS_78,10.42,-0.36,0,0.28 3TMO,HIS_240,6.36,-0.43,0.28,8.33E-17 2AZL/GLU 30.4.78.0.33.0.-0.05 3CS1,GLU_175,4.64,0.17,0,-0.03 2BDD,ASP_114,4.29,0,-0.06,0.54 3RLN,GLU_609,4.69,0.38,0,-0.18 1WLY,ARG 254,12,46,-0,27,0,0,23 3M9A,CYS_23,9.44,-0.85,0.23,1.06 3LD1.LYS 214,11.4,-0.44,0.82,0.53 2QHT,ARG_43,13.99,-0.91,1.49,0.91 1R7J,LYS_3,10.46,-0.05,0,0.01 10IS.ARG 307.13.04,-0.72.0.66.0.6 2Z61,TYR_176,13.39,-0.65,0.96,3.09 105J,ARG_97,12.36,-0.28,0,0.14 3DHN,GLU_154,4.63,0.13,0,0 2FC3.LYS 83.10.34.-0.41.0.0.25 2NYC,ASP_190,3.97,0,-0.1,0.27 2AZL.LYS 138,10.82,-0.45,0.12,0.65 3ETU,TYR_81,11.68,-0.09,0.2,1.58 2Q13,GLU_255,4.35,0.22,-0.38,0 2Z14.TYR 34.10.22.0.0.1.0.12 1UOH,HIS_137,6.31,-0.32,0,0.13 1MIX,GLU_291,4.05,0.41,-0.47,-0.39 3GG6,HIS_157,6.32,-0.22,0,0.04

3MTT,LYS 572,10.1,-0.23,0,-0.16 3N2T,LYS 147,11.07,-0.18,0.32,0.42 2P1W,ARG_90,12.35,-0.2,0,0.05 2F4Q,GLU_10,4.69,0.21,0,-0.02 2R4Q,GLU_260,4.02,0.37,-0.33,-0.52 1CBY,LYS 201,10.58,-0.13,0,0.21 3M3P.CYS 49,10.78,-0.16,0.09,1.85 1J8B,LYS_43,10.57,-0.32,0,0.39 2GZQ,TYR_118,12.8,0,0.09,2.71 3BA1,GLU_208,3.95,0.29,-0.75,-0.09 1K95,LYS 115,10.45,-0.18,0,0.12 103X.LYS 213.10.64.-0.22.0.0.37 2YX0,GLU_312,4.07,1.21,-1.15,-0.49 2EYI,ARG_133,12.82,-0.52,0.44,0.41 2013.GLU 95.4.99.0.48.0.0.01 1AK1.TYR 17.11.95.0.0.46.1.48 3BB7,ASP_193,3,-1.15,-0.11,0.45 2Z61,TYR_292,11.44,0.17,0.54,0.73 1R53,ARG_46,11.63,-1.42,0.14,0.41 3C0C,ASP 322,3.9,0,0,0.1 2VGM,TYR_230,13.43,0.71,0.78,1.95 2ZCO,TYR_284,12.42,0.6,0.56,1.25 1NAR,ARG_6,12.94,-3.24,0.51,3.17 10IS.LYS 167.11.28.-0.68.0.85.0.61 3MEW.TYR 269,10.27,-0.22,0.28,0.2 2FBQ,HIS_197,6.27,-0.33,0,0.1 1MIX,TYR_216,12.39,-0.36,-0.25,2.99 3CCY,TYR_99,9.97,-0.75,-0.57,1.3 3K1H,ARG_35,11.8,-0.82,0,0.11 1WP5.TYR 284.10.11.0.-0.13.0.24 3M66,LYS_363,10.38,-0.23,0,0.11 3RE9,TYR_180,11.01,0,0.28,0.72 2IF4,ASP 223,3.95,-0.1,-0.11,0.35 2WB8.HIS 563.5.06.-1.16.0.-0.27 1AIL,GLU_55,4.4,0.22,0,-0.31 3BWT,GLU_700,4.4,0.31,-0.33,-0.08 2HRZ,HIS_10,4.61,-1.9,0.19,-0.18 3EVN,GLU_144,4.06,0.45,-0.25,-0.64 2F4O,ASP 300.3,-0.59,-0.43,0.22 2ZCX,ARG_136,12.95,-0.14,0.59,0 1IDK,ARG_188,13.67,-0.69,1.26,0.6 3TOW, ARG_164, 12.8, -0.69, 0.26, 0.72 2GS5.GLU 123,4.85,0.1,0,0.24 2IRM,ARG_354,11.33,-2.17,0.52,0.48 1DOV, ARG_194, 13.14, -1, 0.67, 0.96 1H4U,GLU_372,4.58,0.12,0,-0.04 2P52,TYR_123,11.87,0,0.16,1.72 1X7F,ASP_194,3.13,-0.82,-0.3,0.46 1ZCE,GLU_17,4.43,0.23,-0.02,-0.27 3D9H,LYS_228,10.41,-0.11,0,0.03 3ZTA,CYS_41,11.93,-0.09,0.06,2.97 1FO9,GLU 222,4.26,1.32,-1.65,0.08 3H04,HIS_216,4.91,-3.08,1.02,0.47 1WXQ,TYR_382,12.13,0.69,0.52,0.93 2WZ9,GLU_107,4.09,0.35,-0.3,-0.46 1H09,LYS_311,10.71,-0.19,0,0.4 3GMS,LYS_309,10.25,-0.33,0,0.08 2PGE,ARG_122,12.86,-2.23,0.82,1.77 1NJ4,ASP 293,3.83,-0.25,-0.06,0.33 3CIV,ARG_210,12.28,-0.22,0,0.01 4GCO,ARG 172,13.39,-0.35,0.82,0.42 2XWS.GLU 93,3.81,0.2,-0.55,-0.34 3V3T,ASP_27,3.2,-0.62,-0.27,0.29 1O5T,HIS_170,4.04,-2.37,0,-0.09 1MIX,GLU_346,4.82,0.2,0,0.12 2Z61,ASP_283,3.33,-0.84,-0.86,1.22 3AUF,TYR_42,9.54,-0.28,-0.48,0.31 1NIJ,GLU_204,3.53,2.94,-1.58,-2.33 3IBT,CYS_182,12.61,0,0.52,3.09

20ZO.GLU 39.4.8.0.5.0.-0.21 3EAZ, ASP_161, 3.23, -0.85, -0.1, 0.37 3IU5,ARG_74,12.42,-0.16,0,0.08 3K1H,ASP_36,3.24,-0.81,0,0.25 2AZL,CYS_267,11.36,-0.49,0.01,2.84 3RJZ,GLU 80,4,52,0,27,0,-0,24 3DZ1,TYR_265,11.14,0.26,-0.08,0.95 3RFY,ARG_119,11.96,-1.62,0,1.07 2FBI,ARG_16,12.69,-0.67,0.51,0.35 3TOW, ARG_168, 13.27, -0.17, 0.57, 0.37 1GPP,GLU_125,3.76,0.66,-0.85,-0.54 2AD1.LYS 72,10.42,-0.08.0.0 3LOD,LYS_100,10.69,-0.28,0.13,0.34 2ZTYLYS 76.10.35.-0.27.0.0.12 3HVM.GLU 91,4.06,0.46,-0.69,-0.21 3NR5,GLU_10,4.78,0.21,0,0.07 2XHC,ASP_148,3.31,-0.79,-0.16,0.47 1H4U,ARG_525,12.04,-0.46,0,0 1NJ4.GLU 274.3.12.0.37.-1.7.-0.06 3JSN,TYR_169,11.94,-0.54,0.25,2.23 1QYI,HIS_39,6.65,-0.51,0.73,-0.07 1SJY,HIS_96,5.06,-1.24,0,-0.2 2EFK.GLU 270.4.51.0.3.0.-0.29 3I0C.GLU 138.3.51.1.97.-2.28.-0.68 2H2W,LYS_197,10.89,-0.34,0.12,0.61 2F4Q,CYS_291,11.02,-0.79,-0.03,2.84 4AE7,ASP_65,3.49,-0.5,-0.19,0.37 2FPN,LYS 145,10.22,-0.24,0,-0.04 1XTZ,TYR_52,11.95,0.85,0.51,0.58 1ZKZ,GLU_100,4.58,0.37,0,-0.3 2QDJ,TYR_325,11.64,-0.89,0.67,1.86 2ZTY,GLU 61,3.64,0.48,-0.76,-0.57 1TD6.TYR 119.12.56.0.6.0.3.1.67 1YOY,GLU_59,4.39,0.4,-0.43,-0.08 20RX.TYR 85,12,96,-0.85,1,15,2,67 1T95,GLU_68,3.97,0.53,-0.85,-0.22 4GCO,ASP_158,4.09,0,-0.09,0.38 2099,ARG 327,13,91,-1.05,1.53,0.92 3ONT,TYR_59,11.82,0.85,0.47,0.51 1WNH,GLU_94,4.6,0.1,0,0 3CE7.CYS 28.11.81.0.0.04.2.76 1ZBS.LYS 257.10.34.-0.16.0.0 1MUF,GLU_214,4.53,0.27,0,-0.24 3DTE,ASP_224,3.82,0,-0.29,0.31 3UV9,LYS_467,10.34,-0.23,0,0.07 1TJE,CYS 35,11.41,-0.01,-0.03,2.44 3ETU,LYS 230,10.45,-0.07,0.0.02 3BCH,ARG_191,12.39,-0.25,0,0.14 208I,GLU_151,4.26,1.65,-1.1,-0.79 4EKU.GLU 146.4.53.0.19.0.-0.16 4H86,TYR_70,13.76,-0.65,0.42,3.98 1ANU,ASP_82,4.27,0,0.15,0.33 3F6M,ASP_127,3.41,-0.15,-0.49,0.25 1SI7,LYS_190,10.6,-0.2,0.01,0.28 2QEV,GLU 80,3.78,0.42,-0.69,-0.45 2EDM,ASP_170,4.1,-0.07,-0.24,0.6 2I88,TYR_421,10.92,0,0.17,0.75 2HRZ,ASP_98,3.27,-0.7,-0.21,0.38 3RLE,TYR_135,11.5,0,0,1.49 1MTZ,ARG 153,13.12,-0.31,0.5,0.42 3PM2,ASP_112,3.95,0,-3.47E-18,0.15 2H8O,HIS_109,6.19,-1.43,0.59,0.52 2XJ4,ARG_120,13.47,-0.24,0.74,0.47 2APL,TYR 45,11.3,0,0.64,0.66 2YWJ,LYS_83,11.42,-0.45,0.85,0.52 3ETV,GLU_79,4.35,0.63,-0.74,-0.05 3RLE,LYS_68,11.2,-0.22,0.54,0.38 3Q6L,ASP_78,3.36,-0.18,-0.52,0.26 1H4U,TYR_612,12.14,0,0.43,1.71

2IOT.ARG 242.12.05.-1.09.0.0.64 3T5B,GLU_350,3.95,1.47,-1.43,-0.58 3CZC,CYS_39,10.44,0,0.28,1.17 2GKG,GLU_31,3.49,0.65,-1.42,-0.25 4DNU,LYS 304,10.35,-0.15,0,0.01 1GOE,TYR 326,12.29,-0.72,-0.78,3.79 3RRQ,LYS_131,10.48,-0.02,0,0 2E3S,CYS 503,12,25,0,-0.06,3,31 4F3J,ARG_198,13.33,-0.27,0.46,0.64 2V81.TYR 200.10.89.0.-0.17.1.06 1RI5,ARG 247,13.25,-1.34,1.16,0.94 2B3M,LYS_21,10.44,-0.06,0,0 4FCU,GLU_211,4.23,2.13,-2.28,-0.14 1AKO,ARG 209,13,-0.52,0.28,0.73 3HUE,ASP_74,4,0,0.08,0.12 1ZBM,GLU_190,3.18,0.79,-1.64,-0.47 1J85,ARG_129,12.43,-0.07,0,0 3V75,ARG_274,12.54,-0.3,0,0.33 2IN0, ARG_417, 13.19, -0.27, 0.59, 0.37 3RE9,ASP 177,2.38,-1.64,-0.6,0.83 3BCY,HIS_87,4.34,-1.86,0,-0.3 1F2V,GLU_34,4.94,1.37,-0.9,-0.02 2WOZ.HIS 298.6.43.-0.07.0.0 1KCM,LYS 156,10.76,-0.24,0,0.5 1G8P,GLU_244,4.56,0.19,0,-0.12 1YM5,ASP_32,3.4,-0.63,-0.13,0.37 2VAN,HIS_212,5.63,-0.77,0,-0.1 3T5B,ARG_29,13.19,-0.38,0.49,0.58 20DJ.GLU 287,3.4,0.26,-1.36,0 3FRR,ASP_180,3.3,-0.63,-0.29,0.42 30IP,ARG_200,13.34,-0.28,0.54,0.59 3GMS.TYR 66.11.48.0.0.12.1.36 3VHJ.LYS 37.11.2.-0.22.0.54.0.38 2Q34,GLU_238,4.63,0.27,0,-0.14 1SUU,ASP_798,3.71,0,-0.28,0.19 2V5B,GLU_158,3.49,0.33,-0.94,-0.39 2ZCX,LYS 21,10.82,-0.33,0.2,0.45 1TLV.LYS 187,10.1,-0.59,0.0.19 1G5Z,GLU_117,4.54,0.13,0,-0.08 3B21.TYR 170.10.48.0.0.2.0.28 2XHC,ARG_181,12.41,-0.09,0,0 3C2E,HIS 124,5.71,-0.65,0,-0.14 2B78.TYR 50.13.59.-0.78.0.4.37 2DVK,ARG_96,12.41,-0.28,0,0.19 1PV5,GLU_213,4.66,0.19,0,-0.04 4H4J,LYS 27,10,48,-0.09,0,0.06 1T95,HIS_126,5.94,-1.11,0.41,0.15 2YWJ,LYS_65,10.36,-0.45,0,0.31 2Z14.TYR 21.10.53.0.0.19.0.35 3BB7,HIS_226,4,-2.59,0,0.08 1LPL,CYS 152,11.35,-0.11,0.03.2.45 1BKB,LYS 114,11.39,-0.37,0.85,0.42 2QEV,ARG_69,13.86,-0.24,1.21,0.39 2QK1,LYS_363,10.54,-0.22,0,0.25 1F2V.ARG 189,12.52,-0.85,0.4,0.46 3OBS,TYR_68,10.32,0,0.06,0.26 1R9W,TYR_268,12.32,0,3.47E-18,2.32 1PZC.GLU 43.3.92.0.89.-0.72.-0.74 4FLE,HIS_9,4.28,-2.29,0.07,0 3V4G,ASP 90,3.77,-0.7,-0.16,0.83 2EJX.GLU 7,3.38,0.34,-0.85,-0.6 1AKO,GLU_23,4.65,0.15,0,0 4FZN,ARG_68,12.48,-0.25,0,0.24 1RZ2,GLU_178,3.87,0.79,-0.85,-0.58 1PBV,GLU_222,4.71,0.21,0,0 3TRE,ARG_10,12.35,-0.25,0,0.09 1WYC,ARG_76,12.59,-0.93,0.56,0.45 2ZQ5,LYS_8,10.39,-0.13,0,0.02 3EJG,ASP_82,2.87,-0.77,-0.44,0.29

3RF91YS 172.11.19-0.4.0.85.0.24 2AH5,TYR 100,10,77,0,0,05,0,72 2AHE,GLU_113,4.64,0.16,0,-0.01 1YTD,LYS_346,10.55,-0.21,0,0.25 3ZXY,ASP_130,4.22,0,0.09,0.33 1SFE,ASP_90,3.44,-0.92,-0.7,1.25 3GA2,LYS_2,10.43,-0.07,0,-0.01 2P1W,HIS_203,6.45,-0.88,0.79,0.03 1ZHV,ASP_51,3.99,0,-0.04,0.23 1LTU,GLU_133,5.4,0.71,0,0.19 3SMD.GLU 87,4.62,0.15,0,-0.04 1X9G,LYS_178,10.45,-0.05,0,0 1DZF,ARG 177,12.31,-0.22,0.0.02 2V81,CYS_108,11.46,0,0.17,2.28 1WXQ,LYS_318,10.35,-0.19,0,0.05 2NSN.GLU 53.4.69.0.1.0.0.1 3EZ7,GLU_304,4.67,0.12,0,0.05 3ZRI,GLU_110,4.98,0.43,0,0.04 2BAA.ARG 211.13.11.-0.35.0.41.0.55 3F5D,TYR_21,10.23,0,-0.02,0.25 2EFK,TYR_28,12.14,0,0.21,1.94 3D9H,ASP 36,3,76,-0.28,-0.03,0,26 3D9H,HIS_146,6.02,-1.05,0.67,-0.1 1YG2,ARG 14,12.59,-0.14,0,0.23 2E3C,ASP 373,3.82,0,-0,19,0,21 2PGE,HIS_299,4.56,-1.72,0,-0.22 3LD1,LYS_70,10.46,-0.04,0,0 3JZN,ARG_414,13.21,-1.87,1.6,0.99 2P1W,GLU 54,3.51,1.19,-1.65,-0.53 1IAP,TYR_186,11.35,0,0.17,1.18 2EJB,CYS_7,12.38,0,0,3.38 1PSW,HIS_201,5.64,-1.68,0.78,0.03 2EHG,GLU 104,4.36,0.25,0,-0.39 3F6M,TYR 83,10.93,-0.84,0.24,1.54 1RHS,ASP_82,4.04,0,0,0.24 2BLL,GLU_342,3.37,0.72,-0.85,-1 3EUR,GLU_139,4.8,0.28,0,0.02 1XKR,GLU 169,4.96,0.5,0,-0.04 2GZQ,CYS_70,11.32,0.33,-0.06,2.03 3CAX,ARG_387,13.12,-1.38,0.73,1.26 2FZP,ARG_253,12.17,-0.36,0,0.03 3IVF,ARG 33,12.55,-0.63,0.15,0.52 2Z0M,GLU_327,2.98,0.61,-1.37,-0.76 2WB8,TYR_717,12.3,0,0.38,1.92 1YLN,ARG_108,12.1,-0.4,0,0 3K9I,LYS_71,10.79,-0.09,0,0.37 3TRE,LYS_34,10.48,-0.02,0,0 1JB3,ASP 82,3.12,-0.74,-0.53,0.59 3EJC,HIS_37,7.89,-0.6,1.63,0.35 1J8B,ASP_58,3.06,-1.06,-0.09,0.41 1IAP,ARG_124,12.26,-0.38,0,0.14 4FLE,ASP 152,3.35,-0.66,-0.28,0.5 2QZQ,ASP_51,4.02,-0.01,-0.08,0.31 3IL3.TYR 117.11.26.0.0.1.26 2RIK,GLU_199,4.8,0.28,0,0.02 3CZC,TYR_51,10.61,0,0.18,0.43 3ASA,LYS 141,10,48,-0,29,0,0,27 1WLY,TYR_317,8.74,-1.38,-0.58,0.7 3CE7,GLU_69,4.97,0.23,0,0.24 1QQL,LYS_69,9.97,-0.34,0,-0.19 4ANN,LYS 87,10,75,-0.88,0,28,0.85 4F85,TYR_240,13.27,-1.7,0.97,4 3V4G,LYS 62,10.52,-0.1,0,0.13 2FB6,GLU_103,4.67,0.19,0,-0.03 2PLQ,TYR_145,10.13,0,-0.06,0.19 2B61.TYR 108.11.56.0.0.1.56 3C38,GLU_255,4.86,0.28,0,0.08 2D7J,ARG_180,12.5,-0.2,0,0.2 3JV1,LYS_128,10.21,-0.32,0,0.03

2Z84,CYS 62,11.63,-0.05,0,2.68 1YLN,GLU 41,4.64,0.34,0,-0.2 1TXJ,TYR_167,10.12,-0.63,0.06,0.68 2X4L,GLU_185,4.2,0.69,-0.77,-0.21 1T3Y,CYS_52,12.31,0,-0.19,3.5 3T5B,TYR 393,10.42,-0.41,-0.04,0.86 3GS9,TYR 286,11.05,-0.05,0.07,1.02 2V5B,ASP_35,3.43,-0.11,-0.52,0.26 4GCO,GLU_249,4.6,0.2,0,-0.1 2R2Y,LYS_34,10.43,-0.07,0,0 1LTU,ARG 50,10.8,-1.78,0,0.09 4F3J.GLU 173.4.65.0.15.0.0 2GKG,ASP_45,3.49,-0.25,-0.39,0.34 20EW,CYS_76,11.39,-0.72,0.2,2.91 1G8P.GLU 198.4.66.0.16.0.0 1X7F,ARG_164,13.34,-0.33,0.62,0.56 3GE9,GLU_231,4.63,0.13,0,0 4EVF,LYS_211,10.48,-0.07,0,0.05 3IO0,HIS_102,6.6,-0.6,0.68,0.02 1ZYL, ARG 210, 12.01, -0.33, 0, -0.15 1N81,TYR_23,9.76,-0.85,0.33,0.27 1XEU,TYR_247,10.24,0,-0.02,0.25 1MUF,TYR_287,13.48,-0.85,0.21,4.12 1SFE,CYS 135,12,17,-0.05,0.35,2.87 1046.LYS 34,10.28,-0.27,0.0.04 3M66,LYS_404,10.25,-0.24,0,-0.01 100E.CYS 160.11.38.0.-0.27.2.65 2X4L,GLU_258,3.29,2.08,-2.46,-0.83 2H85,GLU 21,4.76,0.18,0,0.08 2FZ4,GLU 187,4.63,0.29,0,-0.16 3IO0, ASP_166, 2.79, -1.3, 0, 0.28 3AU3,CYS_525,11.96,0,0.39,2.57 1NAR.GLU 97.4.72.0.22.0.0 109G,ASP 156,3.6,-0.51,-0.04,0.36 2GZQ,HIS_18,4.72,-0.86,0,-0.92 2ZQ5,ASP_369,3.24,-0.87,-0.08,0.38 1WP5,GLU_271,4.64,0.65,-0.52,0 3OA7,LYS 541,11.11,-0.18,0.41,0.38 1QQL,ARG_28,12.59,-0.2,0,0.28 2JKF,LYS_126,11.27,-0.21,0.5,0.47 3PU6,GLU_70,4.5,0,0,0 3GT0,GLU_128,4.47,0.25,0,-0.28 3U2R.ASP 81.3.1.-0.68.-0.45.0.42 2EJX,TYR_57,13.05,0,0.02,3.02 20EW,LYS_265,11.22,-0.81,0.75,0.78 1RWZ,ARG_121,12.45,-0.05,0,0 2P0L,GLU_83,5.12,0.63,0,-0.01 3ASA,ARG 110,11.84,-1.29,0,0.63 2P65,LYS_7,10.79,-0.19,0.21,0.26 1LPL,LYS_173,10.55,-0.08,0,0.14 3A2Z,ARG_45,13.57,-0.2,0.75,0.52 2VAN,GLU 216,4.43,0.28,0,-0.36 1XEU,GLU_122,4.5,0.3,0,-0.3 1V43,GLU_268,4.41,0.46,-0.17,-0.37 3M3P,ASP_37,2.38,-1.6,-0.47,0.64 1AK1,ARG_30,11.99,-0.52,0,0 3LPZ,GLU_22,4.61,0.09,0,0.02 2R4Q,HIS_215,5.91,-0.23,0,-0.36 2B78,LYS 245,10,38,-0.05,0,-0.06 3TOW,TYR_66,11.03,0,0.22,0.81 1Q46,GLU 155,4.51,0.14,0,-0.13 1T95,HIS_180,6.35,-0.5,0,0.35 20KT,LYS_16,10.36,-0.49,0,0.35 2H14,ASP_172,4.39,0,0.19,0.4 1WP5,ARG_279,12.43,-0.07,0,0 30IP,TYR_132,10.09,-0.85,0,0.94 1S7K,ASP_177,2.66,-0.98,-0.5,0.35 4DBX,GLU_262,4.25,0.33,-0.46,-0.12 1FQI,HIS_379,6.3,-0.19,0,-0.02

3F1X.LYS 24.10.24.-0.26.0.0 1XTD,GLU_163,3.94,0.44,-0.77,-0.23 1AIL,CYS_13,10.61,-0.09,-0.03,1.73 2R57,GLU_308,2.91,0.37,-1.29,-0.66 30IP.HIS 136.6.31.-0.19.0.0 2NSN,LYS_24,10.33,-0.18,0,0.01 1Q46,LYS_96,10.96,-0.18,0.47,0.18 2EJB,LYS_59,10.78,-0.14,0,0.42 2VAN, ARG_222, 12.43, -0.07, 0, 0 2FXT.GLU 373.5.1.2.52.-1.35.-0.56 1L3K,LYS_15,10.4,-0.33,0,0.23 3NBI,LYS 78,10.22,-0.12,0,-0.16 3M70,LYS_162,9.69,-0.85,0,0.04 3V55.ASP 530.4.1.0.0.07.0.24 1TD6,ASP 118,3.72,-0.16,-0.13,0.2 4E8B,GLU_140,6.01,2.47,-0.7,-0.26 1ZBM,TYR_103,10.13,0,-0.31,0.42 3CAX,ASP_457,2.95,-1.38,-0.14,0.67 2Z84.ASP 47.1.83.-2.1.-0.45.0.57 3DB9,GLU_104,4.26,0.51,-0.26,-0.48 2QEV,CYS_81,10.49,-0.8,-0.18,2.48 1YDL,ARG_5,12.34,-0.24,0,0.07 1XFK,ARG_150,13.84,-0.36,0.94,0.76 3K8U,TYR 97,12.83,0,0,19,2.64 2QV2,ASP_145,3.88,0,0,0.08 4EKU,ARG_242,12.64,-0.09,0,0.23 1SQW,HIS_40,5.98,-0.46,0,-0.07 3GG6,HIS 161,6.36,-0.3,0,0.15 4GCO,TYR_137,10.04,0,-0.02,0.06 3F6F,TYR_153,12.8,-0.85,0.55,3.1 3I4T,TYR_125,10.06,0,0,0.06 1FOLASP 371,3.94,-0.09,-0.01,0.24 1J33,ARG 334,12,36,-0.21,0,0.07 3LJN,ARG_199,13.1,-0.27,0.15,0.72 3B21.LYS 117.11.41.-0.21.0.71.0.42 2CYG,GLU_310,11.96,5.14,1.49,0.82 2NYC,LYS 289,10.54,-0.14,0,0.18 3P2F,CYS 65,9.97,-0.1,1.91E-17,1.08 3V55,GLU_534,4.75,0.16,0,0.09 3LJC,LYS_35,10.78,-0.21,0,0.48 1UW7,ARG 55,12,76,-0.25,0.01,0.5 20KT,ARG 246,12.62,-2.19,0.3,2.02 2GZR,ASP_45,3.73,-0.18,-0.22,0.33 2OB5.GLU 103.4.35.0.81.-0.85.-0.1 1XAW,TYR_474,10.59,0,0.3,0.29 2B0J,ASP 269,3.14,-0.56,-0.58,0.48 10TM,ASP 200,3.62,-0.79,0.11,0.49 2OYZ,TYR_65,9.76,-0.65,-0.14,0.55 2PPN,GLU_31,4.41,0.31,-0.42,0.03 200PARG 209,12,44,-0,4,0,0,35 2|88,TYR 367,12,51,-0.85,0,49,2,87 30NH,ASP_474,4.59,0,0.37,0.41 3P28, ASP_85, 3.21, -0.47, -0.34, 0.22 3CN5,CYS_91,9.38,-0.05,0,0.42 2X4G,GLU_297,4.53,0.18,0,-0.15 3G6S, ASP_140, 2.67, -1.85, -0.85, 1.57 3F6F,CYS_201,10.07,-0.94,-1.51,3.51 3H5T,GLU 164,4.46,0.09,0,-0.13 3LJC,ASP_105,3.98,0,-0.23,0.41 3DTE,ARG 255,12.2,-1.2,0.45,0.45 2NRR,ARG_466,12.44,-0.09,0,0.03 3CAX,LYS_432,10.64,-0.29,0,0.43 3K9I,TYR_154,10.38,0,0,0.38 2FD4,LYS 520,10.47,-0.36,0,0.34 3GFP,HIS_361,5.64,-0.77,0,-0.08 2Z0M, ASP_84, 3.95, 0, 0.03, 0.13 4GA2,ASP_59,3.25,-1.55,-0.21,1.21 1M5I,ARG_187,12.67,-0.29,0.09,0.36 2Z0M,TYR_300,12.89,-0.13,0,3.02

1TP6.ARG 17.13.25.-0.48.0.74.0.49 2G9D,ARG_179,12.98,-0.28,0.35,0.41 3EVZ,GLU_125,4.4,0.2,0,-0.29 1TLV,HIS_207,4.85,-0.89,0,-0.76 3L3P.GLU 338.4.73.0.2.0.0.03 2FPN.TYR 180,10.0,-0.07,0.07 3BQW,ASP_323,3.86,0,0,0.06 3P28,ASP_162,2,-1.66,-0.58,0.44 3H13,CYS_259,11.02,-0.73,0.21,2.54 3IVEASP 372.3.85.0.-0.05.0.1 3UAH,CYS_470,10.62,0,0.16,1.46 1V43,LYS_36,10.33,-0.17,0,1.39E-17 2I6I,TYR_110,11.58,0,0.1,1.49 1RI6.TYR 193,12,98,0,0,18,2,8 30N1.CYS 56.11.01.-0.02.0.2.03 4EZB,ARG_280,13,-0.34,0.12,0.71 20EW,CYS_90,9.06,0,-0.13,0.18 2E3S,LYS_550,10.1,-0.39,0,0 3MEW.TYR 238.10.72.0.0.4.0.33 2EFK.HIS 203.6.27,-0.29,0.0.06 4FH3,LYS_288,11.23,-0.45,0.32,0.86 3FK5,ASP_41,3.3,-1.3,-0.13,0.93 1TXD,GLU_794,4.95,0.54,0,-0.09 2IXM,ARG 193,12.94,-2.61,0.5,2.55 100X,TYR_171,11.46,0,0.15,1.31 3D9H,GLU_188,4.29,0.37,-0.11,-0.46 3I47,ARG_39,12.35,-0.35,0,0.2 1WXQ,GLU_179,4.72,0.33,0,-0.11 1SOH, LYS 136, 11.33, -0.8, 0.85, 0.78 3F5D,TYR_123,10.11,0,0.04,0.07 1P4X,HIS_244,5.59,-1.71,0.85,-0.05 2IDC.CYS 99,13.64,-0.09,0.1,4.63 2B6P,GLU_244,4.84,0.22,0,0.12 1L2F,TYR_130,9.14,-1.42,-0.38,0.94 3L7N,GLU_122,4.45,0.18,0,-0.23 2B2H,ASP_364,3.61,-0.82,-0.06,0.7 2Q13,LYS 66,10.28,-0.16,0,-0.06 1X8F.TYR 69.11.09.0.0.09.1 2ZQ5,GLU_170,4.42,0.97,-0.78,-0.26 2QEV,LYS_95,11.03,-1.08,0.6,1.01 3BCH,LYS_40,10.46,-0.2,0,0.15 3ZTA, ARG 95, 12.38, -0.12, 0, 0 2XJ4,LYS 63,10.32,-0.15,0,-0.03 2P65,ARG_177,11.92,-0.46,0,-0.12 1LFP,LYS_247,10.58,-0.22,0,0.3 3RE9,ARG_229,11.98,-0.73,0,0.21 4AM1,LYS_354,10.13,-0.26,0,-0.12 1L2H,ARG_11,11.81,-0.7,0,0.01 3AUF.TYR -5.10.1.0.0.0.1 2AXO,LYS_155,10.61,-0.14,0,0.24 3BQE,HIS 248,4.87,-1.92,0.35,-0.06 1Z3X.GLU 141.4.86.0.37.0.-0.02 1GXN,ARG_588,12.44,-0.21,0,0.15 3DHN,GLU_23,3.54,1.22,-1.46,-0.72 3O16, ARG_71, 12.63, -0.86, 0.52, 0.47 4E6S,GLU_50,4.21,0.35,-0.72,0.07 2D0A,ARG_212,12.5,-0.2,0,0.2 2RFA,GLU_116,3.89,0.24,-0.8,-0.05 3QKY,GLU_95,4.49,0.33,0,-0.34 3JSN,TYR 23,10.66,0,-0.03,0.69 3LH5,CYS_744,9.96,-0.06,-0.3,1.33 1X8F,GLU_239,5.59,3.34,-0.6,-1.65 2RFA,ARG_75,12.14,-0.88,0.15,0.36 3RKV,TYR_253,10.95,-0.47,0.16,1.26 3DZ1,LYS 232,10.09,-0.7,0,0.29 2HP7,GLU_81,4.97,0.19,0,0.28 3JV1,GLU_140,5.11,0.18,0,0.43 4ECC,ASP_134,3.73,-0.32,-0.05,0.31 1TXJ,LYS_84,10.3,-0.31,0,0.11

2G5X,LYS_150,10.21,-0.29,0,0 1MTZ.LYS 194,10.99,-0.49,0.36,0.63 2VGM,TYR_80,9.29,-1.14,-0.16,0.59 3O48,LYS 63,10,5,-0,09,0,0,1 2E3H,TYR 269,10,41,0,0,09,0,3 3M7D,ARG 112,11.73,-0.96,0.08,0.11 1X6J,GLU_19,4.03,0.3,-0.68,-0.09 2WOZ,CYS_461,9.79,-0.4,-0.15,1.33 3OA7,LYS_48,10.22,-0.33,0,0.05 30AV.CYS 18,11.36,-1.66,0,4.02 2PGE,CYS_180,12.31,0.56,-0.35,3.1 4FCU,GLU_56,4.63,0.24,0,-0.11 2E3H,GLU_248,4.82,0.2,0,0.12 2PWO,ASP 89,3.21,-0.63,-0.17,0.22 3G6S,ARG 84,13.32,-0.79,0.1,1.51 1RI5,ARG_210,12.83,-0.22,0,0.55 10XZ,GLU_246,4.71,0.59,0,-0.37 2Z0M,HIS_75,5.52,-1.14,0,0.16 3NJM,ASP_116,3.89,-0.02,-0.22,0.33 100E.GLU 258,4,86,0,2,0,0,15 2GAU,GLU_23,4.54,0.22,0,-0.18 100L.GLU 82,3.85.0.6,-0.85,-0.41 4EVF,ASP 6,4,0,-0.07,0.28 3DZ1,ASP 131,4.12,0,0.04,0.28 3B79,ARG 89,12,49,-0,16,0,0,16 2W0G,GLU_156,3.55,0.35,-0.85,-0.45 2H2W,HIS_234,10.04,-3.14,2.45,4.21 3OA7,GLU_476,4.79,0.19,0,0.11 1UW7,ARG 10,12.44,-0.26,0.06,0.14 1NIJ,LYS_159,11.29,-0.52,0.81,0.5 1LPL.GLU 140.4.51.0.23.0.-0.22 3RFY,ARG_145,12.51,-0.19,0,0.19 3V46.HIS 353,6.88,-0.44,0.82,0 3P51,GLU_78,4.09,0.25,-0.7,0.03 3EUR,ARG_3,12.37,-0.13,0,0 2YLF,HIS_232,6.17,-0.36,0,0.03 3EVN,GLU_282,9,3.71,-0.31,1.12 3GOZ,LYS 270,10.71,-0.11,0,0.32 1MHN,ASP_105,2.43,-2.06,0,0.68 1ES9,GLU_111,3.92,0.32,-0.69,-0.2 2WOZ, ASP_574, 3.88, 0, -0.06, 0.14 1RAJ,GLU 227,4,0.18,-0.32,-0.36 3HVM,ARG 83,11.69,-3.76,0,2.95 1RI6,ASP_129,3.57,-0.32,-0.22,0.32 3DSH,ARG_313,12.35,-0.74,0.18,0.41 1UAJ,GLU_225,4.81,0.19,0,0.12 3MIX,CYS 636,12.96,0,0.95,3 1V6T.TYR 95,10.04,0,-0.22,0.25 1T6L,TYR_253,12.78,0.58,0.14,2.08 1YIB,TYR_247,11.83,0.83,0.55,0.44 2JKF,ASP_60,3.26,-0.85,0,0.31 1SOW.GLU 6.4.63.0.11.0.0.01 1DOV,GLU_183,3.69,0.41,-0.84,-0.39 2AD1,ASP_217,4.11,-0.1,0.12,0.29 1KN3,GLU_172,4.76,0.27,0,-0.01 2X4G,ARG_60,11.66,-1.18,0.31,0.03 1G8P,ARG 145,11.8,-1.19,0.18,0.3 3NBI,LYS_188,10.21,-0.29,0,0 1JKS,LYS_258,10.53,-0.3,0,0.33 1JSX,TYR_180,10.96,0,0.1,0.86 3JSN,ASP 76,3.47,-0.5,-0.54,0.71 4DBX,TYR_264,11.58,0,0.89,0.69 2P5D.GLU 138.4.46.0.26.0.-0.3 3Q9P,GLU_108,4.57,0.21,0,-0.14 3EZ7,CYS_303,9.48,-0.37,-0.04,0.9 4ACJ.TYR 734,11.43,0.15,0.4,0.87 1DVO, ARG_121, 12, -0.31, 0, -0.19 1PV5,GLU_117,4.58,0.08,0,0 2HRZ,ARG_175,13.17,-0.25,0.59,0.33

3LJC,TYR_195,11.1,0.27,0.4,0.43 2AD1,GLU_57,5.31,0.76,0,0.05 3O48,LYS_97,11.45,-0.27,0.72,0.5 3M66,ASP_151,3.98,0,0.05,0.14 3G6S,ARG_165,12.13,-0.38,0,0.02 3B21,ARG 121,13.59,-0.96,1.62,0.44 1WRU.ARG 242.12.29.-0.21.0.0 3EVN,LYS_58,10.97,-0.11,0,0.59 2YT4,GLU_642,4.84,0.29,0.12,-0.08 30DJ,GLU_81,2.6,1.37,-3.18,-0.1 1VJG,TYR 48,10.22,0,-0.15,0.37 4ESS.ASP 10.2.25,-1.66,-0.42,0.54 20KT,GLU_274,5.43,3.44,-1.7,-0.8 3OKQ,LYS_608,10.42,-0.2,0,0.12 3P28,LYS 237,12,18,-0,58,1,65,0,61 1S7K,ASP_179,3.86,0,0,0.06 2FZ4,ASP_63,3.8,0,-0.74,0.74 2Z61,TYR_350,13.45,-0.36,-0.26,4.07 3UAH,TYR_423,12.88,0.85,0.59,1.44 2C2Y,ASP_18,3.54,-0.58,-0.3,0.62 1D2K,TYR 276,13,38,-0.85,0.23,4 1ILW,HIS_58,5.54,-1.84,0.8,0.08 3RRQ,ARG_147,12.59,-0.21,0,0.3 1WYC,ASP_24,3.99,0,0,0.19 3CNU,HIS 58.6.23,-0.48,0.0.21 2OSA,ARG_290,12.42,-0.49,0,0.41 2BV9,TYR_121,10.26,0,0,0.26 2QHT,LYS_187,11.39,-0.4,0.76,0.53 1TD6,HIS_11,5.66,-1.11,0.05,0.21 3DB9,ARG 156,12,14,-0,44,0,0.08 1SUU,LYS_694,10.4,-0.11,0,0.01 3ZTA,ARG_112,12.26,-0.24,0,0 204D,ARG 60,13.88,-0.34,1.35,0.38 2OSALYS 409.10.54.-0.06.0.0.09 2G9D,ARG_7,12.38,-0.27,0,0.14 2F9F,ASP_83,1.37,-2.28,-0.92,0.77 1CHD,ASP_329,2.38,-1.8,-0.04,0.42 1P2F,ARG_203,13.93,-0.34,0.75,1.02 2FI9,ARG_34,12.19,-0.31,0,0 3N0K,GLU_69,4.59,0.11,0,-0.02 4GA2,ASP_95,2.63,-1.5,-0.51,0.84 2GAU,TYR_58,10.37,0,0.12,0.26 1S7K,ASP 126,3.11,-1.29,-0.79,1.38 3EAZ,LYS_125,10.67,-0.14,0,0.31 10IS,GLU_183,5.2,1.8,-0.61,-0.49 10TM,GLU_36,4.35,0.13,0,-0.28 1WRU,ARG_176,12.98,-0.85,0.81,0.52 2099.HIS 214.6.92,-0.59.0.85.0.15 3FK5,ASP_45,4.17,0,0.11,0.25 2C2Y,ARG_129,12.22,-0.34,0,0.05 3KT9,ARG_9,13.66,-1.1,1.18,1.09 3DHNLYS 52,10,49,-0,14,0,0,13 1BKR,HIS_73,6.16,-0.35,0.07,-0.06 3H9W,LYS_23,10.13,-0.4,0,0.02 2HXB,LYS_83,10.05,-0.6,0,0.14 2Z61,ARG_286,13.56,-1.47,1.21,1.32 1DVO,GLU_75,4.19,0.3,-0.63,0.02 4ECC,GLU_197,3.54,1.44,-1.59,-0.82 1UOH, ARG 85, 11, 97, -0.62, 0, 0.09 2P0L,LYS_17,11.03,-0.5,0.47,0.56 1LFP,HIS 6,7.02,-1.22,1.45,0.29 1YLN,TYR 83,10,26,-0,1,0,22,0,14 2FXT,LYS_381,10.42,-0.08,0,0 2AZP,ARG_140,12.19,-0.46,0,0.15 2RFA,ASP_223,3.63,-0.87,-0.24,0.94 3LH5,HIS_703,5.06,-2.17,0.78,-0.05 1YW5,LYS_43,10.59,-0.19,0,0.28 3ERF,ARG_173,12.11,-0.63,0,0.24 1D2K,ARG_190,12.69,-1.8,0.57,1.42

20ZO,ASP 65,3,59,-0.85,-0.48,1,11 1EV8,GLU_82,4.74,0.27,0,-0.03 1CHD.HIS 265.6.21.-0.96.0.23.0.44 20YZ,HIS_21,6.37,-0.13,0,0 3OBS.TYR 113.10.93.-0.77.0.53.1.17 2V1L/ARG 117/12.62,-0.09/0.0.21 4DNU,GLU_53,4.98,0.2,0,0.29 1W7B,GLU_82,4.8,0.3,0,0 2CBE,HIS_64,4,-2.1,0,-0.4 3ASA.HIS 195.6.97.-0.5.0.81.0.17 3U4K,ASP_59,2.93,-0.93,-0.24,0.3 1ANU,ASP_71,3.9,-0.01,-0.02,0.14 2YYO,ASP_117,3.98,0,-0.08,0.26 2W0G.TYR 155,9.13,-0.85,-0.4,0.38 2FPN,ASP 175,3.7,-0.23,-0.08,0.21 1Q5Z,GLU_554,3.58,0.59,-0.85,-0.66 4E9E,LYS_539,11.64,-0.71,1.07,0.78 4H89,ARG_120,12.43,-0.11,0,0.03 1RSS.LYS 136.11.23.-0.29.0.82.0.2 2WB8,GLU_640,6.6,5.01,-3.11,0.2 2Q5X,LYS_791,10.03,-0.47,0,0 2RIK,GLU_209,3.76,0.42,-0.85,-0.31 2|88.LYS 433.11.39.-0.34.0.85.0.38 3EVP,ASP_234,3.4,-0.22,-0.45,0.26 1JB3,CYS_74,8.72,-0.45,-0.02,0.18 2F4Q,GLU_16,4.59,0.31,0,-0.22 3H04,LYS_44,10.41,-0.27,0,0.17 2J8A,LYS 312,10.54,-0.07,0,0.12 1PGV,GLU_325,3.35,0.73,-1.18,-0.7 2l6l,HIS_64,6.04,-1.84,1.25,0.14 2IRM,HIS_121,6.21,-0.29,0,0 3E5T,ARG 179,12.56,-0.37,0.12,0.31 1XKR.LYS 85,10.26,-0.36,0.0.12 1GPP,LYS_39,10.29,-0.26,0,0.05 3LPZ,ASP_123,3.36,-0.39,-0.24,0.2 1XDZ,GLU_206,3.56,0.5,-0.74,-0.7 10I7,GLU_130,3.57,0.43,-0.89,-0.47 1RL0.ASP 230.2.92,-1.22,-0.08.0.42 3F6M,LYS_11,10.5,-0.12,0,0.13 1T07,HIS_45,5.96,-0.66,0,0.12 3H5T.GLU 234.4.6.0.1.0.0 4DBX.GLU 152.4.72.0.31.0.-0.09 3GMS,HIS_2,6.83,-0.34,0.66,0.01 3C38.TYR 133.12.17.0.0.83.1.34 1I60,HIS_179,5.57,-1.23,0,0.31 3N0K,LYS_83,10.27,-0.58,0,0.35 4ETX.HIS 302.6.62,-2.84.0.85.2.11 20EW, ARG_290, 12.59, -0.26, 0, 0.34 3T8R,GLU_84,4.53,0.31,0,-0.27 2R51,LYS 34,11,47,-0,25,0,64,0,58 2JEO,ASP 207,3.58,-0.75,-0.28,0.81 2B0J,HIS_340,7.17,-0.25,0.8,0.14 2GEN,CYS_150,9.41,-0.02,0.11,0.32 1SJ8,ASP_525,3.54,-0.46,-0.06,0.26 1KCM,CYS 192,13.12,-0.05,0.42,3.75 3VHJ,TYR_137,10.6,-0.07,-0.31,0.98 2BLL,TYR_344,10.42,-0.34,-0.17,0.92 2IQT,LYS 293,10.13,-0.53,0,0.17 3LJC,GLU_139,4.59,0.3,0,-0.21 3F5D.ASP 40,4.48,0,0.14,0.55 2Q12,GLU_131,4.72,0.33,0,-0.11 3H13,ARG_472,13.73,-0.37,0.72,0.88 3EVZ,LYS_209,10.7,-0.11,0,0.31 20EW,TYR 258,11.3,0,0.08,1.22 2P5D,GLU_135,4.79,0.43,0,-0.13 1X04,GLU_37,5.39,0.81,0,0.07 3L3P,LYS_315,10.36,-0.21,0,0.08 3BA1,TYR_125,10.63,0,0.08,0.56 3MTT,ASP_461,4.08,0,-0.04,0.32

1FO9.LYS 186.10.12.-0.36.0.-0.03 3DSH,ASP_439,2.87,-1.36,0,0.43 1JB3,GLU_119,4.56,0.28,0,-0.22 20PJ,ARG_281,12.46,-0.13,0,0.09 1SNT,ASP 358,3.84,0,-0.22,0.26 2OK1,LYS 552,10.2,-0.22,0,-0.08 1TXJ,ASP_11,3.07,-2.01,-0.01,1.29 2FI9,GLU_86,3.86,0.24,-0.81,-0.07 1TR9,ARG_310,12.44,-0.2,0,0.14 2NRR,LYS_414,10.95,-0.47,0.85,0.07 2GS5,ARG 112,12,2,-0,3,0,0 1R7J,GLU_64,4.37,0.27,0,-0.4 2IN0,ARG_18,13.11,-0.19,0.13,0.67 1EDG,HIS 254,7.09,-3.29,0.85,3.03 3RE9.LYS 89.10.63.-0.1.0.0.24 10XZ,ARG_207,12.5,-0.23,0,0.22 3UAH,LYS_242,10.25,-0.23,0,-0.02 1TR9,ARG_55,11.28,-1.22,0,0 1U7U,ARG_399,13.27,-1.1,0.9,0.95 3ETV,ASP 173,3.32,-0.84,-0.36,0.73 3VJ8,HIS_173,5.77,-1.34,0.84,-0.22 3VJ8,ARG_66,12.33,-0.48,0,0.3 2DVK,TYR_62,11.48,0.71,0.21,0.56 103X,GLU_219,4.7,0.2,0,0 2DFL,GLU_309,4.23,0.79,-0.6,-0.45 1RL0,TYR_4,9.91,-0.75,-0.02,0.69 1Y2Q,HIS_130,6.19,-0.27,0,-0.03 3ZTA,GLU 132,4.59,0.22,0,-0.13 3M70,LYS 101,9.42,-1.26,0,0.19 2AHE,LYS_60,10.48,-0.22,0,0.19 2P1W,ASP_57,3.94,0,0,0.14 3FWU,TYR 68,12,23,-0.06,0.25,2.04 1AK1.LYS 127,10.65,-0.15,0,0.29 1PSW,LYS_125,10.24,-0.12,0,-0.14 2ATR,ASP_51,3.89,0,-0.01,0.1 1Q46,GLU_158,4.6,0.1,0,0 3ZTA, ASP 88, 4.33, 0, -0.28, 0.82 2D7U,ARG_258,12.51,-1.38,0.35,1.04 1YDL,GLU_59,4.48,0.25,0,-0.27 3EVN.TYR 242,10.39.0,-0.08.0.48 1RL0,LYS_162,10.39,-0.24,0,0.12 2QK1,HIS 544,6.38,-0.14,0,0.03 3S0A,LYS 27,11.81,-0.3,0.85,0.77 3V55,TYR_417,10.66,0,0.16,0.5 1SNT,HIS_210,7.13,-0.29,0.67,0.24 1Z3X,LYS_185,10.49,-0.16,0,0.15 1SI7,ASP_187,2.74,-1.18,-0.32,0.45 2EFK,ARG_143,12.26,-0.3,0,0.06 1NAFLYS 176,10,41,-0.09,0,0 105T,LYS_111,10.27,-0.72,0.05,0.45 2NMU,GLU 79,4.73,2.13,-1.25,-0.64 3U0V.CYS 128,11.81,-0.12,-0.54,3.45 1O3X,TYR_294,11.03,0,0.13,0.9 3P51,ARG_20,13.61,-0.71,1.13,0.69 3IU5,GLU_150,4.67,0.24,0,-0.07 1R7J,LYS_62,10.32,-0.33,0,0.16 2C2Y,HIS_147,5.03,-1.38,0,-0.09 3HUE.GLU 303,4.75,0.24,0.0.01 4FH3,LYS_42,10.55,-0.06,0,0.1 2A4D,LYS 192,10.98,-0.45,0.46,0.48 2B61.GLU 320.3.72.0.45,-0.85,-0.38 1A8Q,GLU_206,3.61,0.34,-0.85,-0.37 3EYE,LYS_153,10.21,-0.44,0,0.15 4GA2,LYS_61,10.49,-0.11,0,0.1 2ZQ5,ASP 316,4.49,0.25,-0.17,0.62 1WXQ,ASP_123,3.73,0,-0.23,0.16 3EIZ,HIS_111,5.85,-0.87,0.04,0.18 1BKB,LYS_39,10.36,-0.14,0,0 2BQQ,ARG_78,12.45,-0.05,0,0

2P52.HIS 175.6.31.-0.18.0.08.-0.09 1WXO,LYS 155,10.85,-0.16,0.24,0.28 1RL0,LYS_195,10.28,-0.25,0,0.03 2DG7.ARG 52,13.05,-0.49.0,1.05 1XFK.ARG 62.11.9.-0.6.0.0 3GV0,GLU 134,5.43,0.95,0,-0.02 2P0Y,GLU_218,4.61,0.17,0,-0.06 301C,ARG 138,12.03,-1.05,0.32,0.25 3Q1C,GLU_357,4.42,0.45,-0.02,-0.51 3ELI,LYS 75,10.17,-0.33,0,0 2IXM,LYS 27,10.61,-0.15,0,0.26 1H4U,GLU_563,4.53,0.19,0,-0.17 3V4G,ARG 57,10.64,-2.57,0.0.7 2F8H,HIS_206,5.77,-0.73,0,0 3CS1,ARG 50,12.03,-2.09,0.62,0.99 1TJE,ASP_116,2.01,-2.05,-0.38,0.64 3K8U,TYR_33,10.03,-0.3,0,0.33 100X,TYR_109,10.69,0,0.02,0.67 2P0Y,HIS 129,5,98,-0,59,0,0,07 3GEC.GLU 382,3.07.0.81,-1.86,-0.38 2P0L,ARG_80,13.02,-0.4,0.44,0.49 3G9G.GLU 189.4.58.1.06.-0.76.-0.23 20EW.TYR 233.10.1.0.0.0.1 4GA2,TYR 42,10.18,0,-0.24,0.41 1R6Y,TYR 84,12,56,0,0,06,2,5 2YLF,LYS_201,10.27,-0.18,0,-0.05 1BN6,ASP_198,3.33,-0.49,-0.33,0.35 1J33,ARG_211,12.14,-1.43,0.7,0.37 3L3P,LYS 350,9.72,-0.83,0,0.04 2P4D,HIS_143,5.4,-1.03,0,-0.07 1Y0K,LYS 63,10.51,-0.33,0.0.34 2R2Y,ARG_84,12.6,-0.3,0,0.39 1FKM.LYS 431,10.46,-0.42,0,0.38 3EZ7.TYR 38,10.88,0,-0.05,0.92 1NAR,HIS_34,1.67,-2.88,0,-1.95 3K8U,ARG_93,12.61,-0.63,0,0.73 2NRK,GLU_61,4.73,0.12,0,0.11 1BKB,LYS 47,10.14,-0.38,0,0.02 1RHS,LYS_66,10.62,-0.24,0,0.36 3ETV,LYS_316,10.25,-0.49,0,0.24 2B02, ASP_377, 1.68, -2.98, -0.6, 1.45 2ZCX,ASP 222,4.05,0,-0.02,0.27 3HVM.ARG 267,13.05,-1.25,0.77,1.03 1WRU,ARG_126,12.88,-0.2,0.08,0.5 30IP,TYR_27,11.84,0,0.27,1.57 4E8B,GLU_63,4.24,0.28,-0.37,-0.16 1U7U,HIS 370,6.71,-1.13,0.85,0.49 3OKO,LYS 660,10.38,-0.12,0.0 1RHS,GLU_61,3.82,0.63,-0.78,-0.53 1P2F,ARG_190,12.48,-0.24,0,0.21 3Q6L,ASP_88,3.81,0,-0.16,0.17 2RH3,CYS 192,10.26,-0.16,-0.26,1.68 1MIX,ARG_358,13.88,-0.25,0.93,0.69 2OJQ,LYS_690,11.32,-0.56,0.85,0.53 2R2Y,ASP_54,2.15,-1.97,-0.17,0.5 3CX2,GLU_165,3.61,0.2,-0.85,-0.25 1AIL.ASP 34,2.88,-0.66,-0.63,0.38 2DG7,GLU_99,4.44,0.25,-0.01,-0.3 3EUR,ASP_77,3.92,0,-0.05,0.16 3HKX,TYR_270,10.17,0,0.03,0.14 2Z0M,ARG 102,12,7,-0,48,0,2,0,47 3O16,GLU_226,4.61,0.22,0,-0.11 3V4G,LYS 15,10.21,-0.27,0,-0.03 4ECC,ASP_36,3.52,-0.47,-0.02,0.21 3LH5,ARG_748,12.45,-0.32,0,0.26 2CWY,ARG 52,12,19,-0,31,0,0 1DZF,ARG_192,12.52,-0.1,0,0.12 1KCM,LYS_202,10.64,-0.13,0,0.28 1DCF,ARG_71,12.24,-0.26,0,0.01

2H8O,ARG 89,10.86,-2.53,0.0.88 2DVK.ARG 128.12.83.-0.32.0.08.0.58 1LTU,GLU_184,8.93,3.85,0,0.58 1WNH, ARG 48, 12, 75, -0.24, 0, 16, 0, 32 2OSA,GLU_408,4.22,0.38,-0.51,-0.15 3MTT,LYS 500,10.46,-0.05,0,0.02 2FI9,ASP_48,3.95,0,0,0.15 1TLV,HIS_220,6.56,-0.3,0.02,0.34 2XHC,GLU_20,4.6,0.34,0,-0.23 20GQ,ARG_456,12.5,-0.08,0,0.08 1D2K,TYR 230,10.58,0,-0.05,0.63 2VGM,TYR_138,10.27,0,0.07,0.21 3LJC,TYR_116,10.5,0,0.24,0.26 3FK5,LYS_316,11.68,-0.47,0.85,0.8 301C.TYR 367.13.49.-0.85.0.08.4.27 1IDK.ASP 331.4.31.0.-0.12.0.63 1JT9,TYR_86,10.64,0,0.24,0.4 3LPZ,GLU_26,4.86,0.21,0,0.15 3ZXY,CYS_81,11,-1.17,0.15,3.02 2PLQ,CYS 246,11.87,0,0.44,2.43 2ZCX.ARG 193,12.28,-0.3,0.0.08 3VJ8,GLU_123,4.6,0.42,0,-0.32 3JZ9,ARG_453,12.43,-0.07,0,0 1T6L,ASP 72,2,4,-1.63,-0,1,0,33 1PBV.TYR 114.12.09.0.0.07.2.03 1N81,HIS_22,6.43,-0.27,0.15,0.05 4F85,ARG 116,12.08,-0.49,0.0.08 3L3P,ARG_306,12.25,-0.35,0,0.09 1Q46,ASP_163,4.05,0,0,0.25 3N2T,LYS_200,10.39,-0.17,0,0.06 1XTZ,HIS_260,6.62,-0.31,0.19,0.23 2H85,LYS_204,10.47,-0.11,0,0.08 3EVN/HIS 93,5.14,-1.7,0.2,0.14 2P1W,HIS 88,5.72,-1.1,0.85,-0.53 4DIU,GLU_151,2.15,0.62,-2.14,-0.83 2RFA,GLU_113,4.6,0.11,0,-0.01 4EKU,HIS_358,6.21,-0.37,0,0.09 1W7B,ARG_284,12.23,-0.39,0,0.13 1EQ6,GLU_190,4.35,0.25,-0.4,0 3NR5,TYR_121,12.5,0,0.61,1.89 3UPD,ARG_248,12.63,-1.01,0.25,0.88 1N81,LYS 37,10.33,-0.29,0,0.12 2CL3,TYR 208,12.26,0.85,0.42,0.99 2F8H,HIS_0,6.14,-0.21,0.01,-0.16 3BCH,ARG_205,12.41,-0.18,0,0.09 3ETV,GLU_57,4.73,0.43,0,-0.19 2YX0, ARG_184, 11.79, -1.81, 0.32, 0.77 3CAX,LYS 285,11,16,-0,96,0,85,0,76 3F6F,ASP_27,2.72,-0.85,-0.46,0.24 2QK1,LYS_549,10.5,-0.68,0.48,0.2 3U2R,ARG_78,12.5,-0.08,0,0.07 3H6Q,ASP_72,1.37,-2.44,-0.52,0.52 1SQW,TYR_45,11.14,0,0.23,0.91 2RJD,GLU_209,4.62,0.12,0,0 2H14,LYS_162,10.38,-0.12,0,0 10LR,ARG_217,12.53,-0.19,0,0.21 3U0V.HIS 90.6.15,-0.79.0.1.0.34 3IL3,GLU_195,4.69,0.19,0,0 2DVK,ARG_30,12.57,-0.1,0,0.18 3R87,HIS_37,6.13,-0.49,0,0.11 3G6S,TYR_78,11.52,0,0.07,1.45 105Z,GLU 616,4.65,0,1,0,0,05 3ULX,ARG_76,12.37,-0.7,0,0.56 2QVT,HIS_129,3.84,-2.14,0,-0.52 1EDG,ASP_188,3.91,0,-0.18,0.29 3ILC,TYR_195,11.18,0,0.02,1.16 1J7G,ASP_57,2.64,-1.77,0,0.62 1NIJ.GLU 27.4.44.0.32.0.-0.38 2P5D,LYS_22,10.71,-0.17,0.08,0.3

1SNT.ASP 60.3.16,-1.06,-0.02,0.45 4HDE,LYS_58,10.55,-0.24,0,0.29 2l6l,HIS_95,3.85,-3.31,0.85,-0.19 3HUE,LYS_94,11.04,-0.24,0.27,0.51 1SI7.ARG 299.8.54.-3.53.0.-0.43 2HRZ.ARG 294.12.54.-0.08.0.0.12 3CIV,LYS_276,9.53,-1.12,0,0.16 3RKV,ASP_294,3.83,0,-0.16,0.19 1QQE,LYS_13,10.43,-0.1,0,0.03 30AV.LYS 135.10.51.-0.57.0.08.0.49 3BB7,ARG_149,12.07,-0.43,0,0 3IV4,ASP_9,3.95,0,0.01,0.15 3ULX,ASP_158,4.3,0,0.17,0.33 3GYW.TYR 276.10.5.-0.42.-0.1.1.03 1YTD.GLU 275.3.99.1.43.-1.51.-0.45 3VJ8,TYR_73,12.69,0,0.17,2.52 1YM5,ASP_65,4.12,-0.72,0,1.04 3O16,TYR_154,10.82,0,0,0.82 3LJC.ARG 192.10.77.-1.72.0.-1.11E-16 2H85,ARG_61,11.59,-1.75,0.36,0.48 1R7J,ASP_81,3.91,0,-0.19,0.3 1MD6,GLU_80,4.78,0.43,0,-0.14 2E3C.HIS 432.4.27.-1.76.0.-0.48 2J8A.CYS 326.10.43.-0.86.-0.02.2.32 1MUF,TYR_110,10.7,-0.48,0.14,1.03 2GZR,ARG_296,11.95,-0.9,0.01,0.34 2P52,TYR_202,11.8,-0.8,0.27,2.32 3H6Q,ARG 95,12.46,-0.45,0,0.41 3DZ1,ASP_132,2.37,-1.28,-0.57,0.42 208P,GLU_22,3.79,0.57,-0.85,-0.43 3GS3,ASP_164,4.19,0,0.04,0.35 3RJX,LYS 33,10,43,-0,2,0,0,14 2R2Y.GLU 111.3.53.0.98.-1.15.-0.8 2X4G,CYS_112,12.68,-0.02,0,3.7 3GFP.GLU 314,4,42,0,22,0,-0,3 1WYC,GLU_228,7.85,4.86,-1.61,0.1 3ASA,LYS_375,10.84,-0.22,0,0.56 2GAU,ARG 143,12,41,-0,28,0,0,2 1MTZ,LYS_11,10.62,-0.11,0,0.24 2H85,GLU_56,4.68,2.05,-1.19,-0.67 2O99,LYS 229,10.61,-0.11,0.0.22 2H30,ARG 170,12,29,-0,21,0,0 1YM5,LYS_243,10.44,-0.39,0.07,0.26 1PSW,GLU_347,4.75,0.23,0,0.02 2P1W,TYR_158,9.54,-0.64,-1.28,1.45 2AH5,LYS 177,9.94,-0.78,0,0.22 20EW,LYS 334,11.12,-0.43,0.56,0.49 1KCM,LYS_31,10.42,-0.14,0,0.06 1UCH,LYS_61,10.6,-0.21,0,0.31 4ETX.GLU 173.4.76.0.26.0.0 3FHF.GLU 35.3.12.0.4.-1.57.-0.19 3JZ9,LYS_476,10.31,-0.37,0,0.19 3U2R,GLU_125,4.53,0.25,0,-0.23 1EV8,TYR_252,11.64,0,-0.14,1.78 1LN4,LYS_92,10.66,-0.31,0,0.46 1N81,ARG_74,12.69,-0.65,0.46,0.37 1PVT,GLU 22,4.63,0.15,0,-0.01 3ADO,GLU 69,2.98,0.34,-1.59,-0.28 1RI5,LYS_42,10.43,-0.07,0,0 3AU3,ARG 399,12.73,-0.17,0,0.4 4ANN,GLU_173,4.96,0.23,0,0.22 1YB2,ASP_234,3.78,0,-0.46,0.44 1RZ2,LYS_69,10.58,-0.19,0,0.27 1DZF,ARG_162,12.53,-0.09,0,0.12 2R2Y,ASP_78,3.83,0,-0.15,0.18 2CE6,ARG_67,12.83,-0.57,0.07,0.82 1RAJ,ARG_456,12.28,-0.28,0,0.08 2P52,LYS_232,10.91,-0.93,0.85,0.48 1ZBP,LYS_25,10.44,-0.11,0,0.06

20V2.LYS 142.10.45.-0.05.0.0 2RJD,GLU_213,4.64,0.14,0,0 1J33,ARG_202,12.47,-0.37,0,0.34 1BYI,LYS_148,11.4,-0.54,0.79,0.65 4GCO.TYR 159.10.1,-0.03,-0.27,0.41 3DSH.GLU 391,4.83,1.62,-0.83,-0.46 1MUF,ASP_259,4.24,-0.17,0,0.61 2CBE.HIS 122.3.6.-3.48.0.58.0 2FPN,LYS_70,10.45,-0.05,0,0 4E6S.HIS 36.5.38.-0.49.0.-0.62 1059,ARG 270,13.07,-0.26,0.47,0.36 1EQ6,HIS_107,5.98,-1.92,0.85,0.55 3AU3,CYS_417,12.1,0,0.6,2.5 3UPD.LYS 271,9.8,-0.74,0.0.05 2B61,ASP_353,3.28,-0.85,-0.46,0.8 2FPN,GLU_96,4.78,1.08,0,-0.8 3ADO,TYR_151,12.1,-0.77,0.02,2.85 1CBY,HIS_163,6.41,-0.14,0.01,0.05 2JEO,ASP 90,3.59,0,-0.52,0.31 1NJ4,LYS_339,10.45,-0.09,0,0.04 1MD6,LYS_37,10.46,-0.05,0,0.01 2P4D,TYR_39,10.51,0,0.09,0.42 3UPD,CYS_203,11.62,-0.01,-0.07,2.7 1XDZ,ARG 151,12.34,-0.33,0,0.17 1YTD,LYS_383,10.35,-0.15,0,0.01 3I0C,HIS_233,4.28,-2.22,0,0 2OBI,TYR_153,13.84,0.85,0.72,2.27 10IS,LYS 149,9.88,-0.8,0,0.19 3C2E,TYR_4,10.54,0,0.06,0.48 3LOD, ASP_6, 3.73, -0.13, -0.4, 0.45 3F6F,TYR_99,10.16,0,0.01,0.15 1MD6,TYR_19,11.94,0.82,0.39,0.74 2V81,ARG 96,13.56,-0.38,0.52,0.91 1TWU,GLU_105,3.93,0.59,-0.77,-0.39 200K,LYS_83,10.32,-0.21,0,0.02 3H04,HIS_36,5.19,-3.03,0.63,1.09 1TUL, ASP 26, 3.3, -1.65, 0.01, 1.13 1G5Z,CYS_129,10.22,-0.08,0.04,1.27 2IXM,LYS_296,9.99,-0.45,0,-0.06 3LJC,GLU_232,4.72,0.22,0,0 3PU6,GLU_32,3.36,0.18,-0.69,-0.63 3KB5,HIS 458,6.37,-0.54,0,0.43 1PZC.LYS 77.10.08.-0.79.0.0.36 1P4X,ARG_214,12.43,-0.07,0,0 1ZBP,GLU_52,4.59,0.18,0,-0.08 3O48,TYR 93,10.38,0,-0.34,0.73 3O48,GLU_58,5.51,1.88,-0.35,-0.5 1GXN,GLU_553,2.67,0.39,-1.61,-0.62 2CXY,LYS 68,10,31,-0,34,0,0,15 2FPN,LYS_26,10.41,-0.27,0,0.18 1FKM,ASP_402,3.76,0,-0.31,0.27 1RHS.LYS 292.10.48.-0.06.0.0.04 3M70,GLU_4,4.22,0.16,0,-0.44 2ZCO,LYS_221,11.51,-0.27,0.85,0.42 2BAA,LYS_87,9.64,-0.86,0,0 2CI3,TYR_160,12.05,0.37,1.03,0.65 2EEY,ASP_130,3.84,0,-0.22,0.26 2IN0,HIS_73,3.96,-2.51,0.53,-0.57 2FD5,GLU_137,4.2,0.26,-0.37,-0.2 1XFK,CYS 31,9.68,0,0.04,0.64 1XIP.LYS 33,10,44,-0.08,0,0.03 2GS5,LYS_126,10.47,-0.18,0,0.15 1W7B,LYS_308,11.34,-0.22,0.46,0.6 1BYI,GLU_115,4.43,3.83,-1.78,-2.1 1DVO,LYS 46,11.01,-0.19,0.7,0 1AIL,HIS_59,5.94,-0.25,0,-0.31 2Z14,GLU_25,4.75,0.25,0,0.01 2F4Q,LYS_265,10.44,-0.16,0,0.09 1GQE,HIS_265,5.91,-0.78,0,0.18

300P,LYS_18,10.37,-0.13,0,0 2Z14,GLU_24,3.59,0.36,-0.7,-0.57 2ILR,GLU_443,4.36,0.17,0,-0.3 3CO1.GLU 16.4.9.0.35.0.0.04 20EW,ARG_51,12.55,-0.29,0,0.34 1Q5Z,LYS 599,11.31,-0.23,0.5,0.55 1KCM,LYS_219,9.97,-0.61,0,0.07 3H04,TYR_178,9.77,-0.75,-0.06,0.58 3CBN,TYR_96,10.39,0.03,-3.47E-17,0.37 3JZN,TYR_154,10.61,0,0.08,0.53 3FHF,LYS 100,10.32,-0.17,0,-0.01 100H,TYR 169,12,32,-1,31,0,17,3,47 3HYQ,ASP_43,3.98,0,0,0.18 1SFE/HIS 70,7.3,-0.6,0.85,0.56 2CWC,ARG_11,11.44,-2.01,0,0.94 3L3P.GLU 439.3.56.0.45.-0.78.-0.61 1RAJ,ASP_455,4.21,0,0.12,0.29 1CHD,HIS_233,5.37,-1.61,0.74,-0.27 3CS1,LYS_25,10.52,-0.09,0,0.11 2YT4,HIS_625,5.59,-0.77,0,-0.14 3GMS,LYS_277,11.32,-0.48,0.85,0.45 2FZ4,ARG_60,11.94,-0.74,0,0.18 1YB2,GLU_96,6.67,2.98,-0.91,0.1 3ON1,LYS_94,10.36,-0.13,0,-0.01 3RJX,GLU 98,4.72,0.22,0,0 3MEW,LYS_200,10.53,-0.12,0,0.15 3R87,HIS_18,6.57,-0.12,0,0.18 3IVF,LYS_272,10.47,-0.13,0,0.09 2D7U,ARG_213,12.78,-0.46,0.31,0.44 1X6J,GLU 39,4.15,0.57,-0.82,-0.09 2JHY,TYR_149,11.01,0,0.04,0.97 1K95,ASP_208,4.04,0,0.07,0.17 3D9H,HIS_139,4.13,-2.84,0.8,-0.32 3LJC,LYS 211,9.86,-0.26,0,-0.38 4ETX.CYS 343.11.08.-0.82.0.27.2.63 2Q07,ARG_439,12.69,-0.17,0,0.35 4FZN,GLU_92,4.51,2.6,-1.87,-0.72 1RZ2,LYS_100,10.42,-0.12,0,0.04 3UPD,CYS_62,9.4,-0.18,-0.08,0.67 3VJ8,ARG_367,12.46,-0.36,0,0.31 1J74,LYS_133,10.02,-0.3,0,-0.18 208I,ARG_24,13.81,-0.41,1.33,0.39 1ZKZ,TYR 97,10.09,0,0,0.09 1SI7.ARG 71.12.31.-0.24.0.0.05 1J33,ARG_119,12.79,-0.79,0.61,0.47 1RZ2,GLU_201,3.54,0.39,-1.32,-0.03 2WOZ,TYR_450,11.5,0,0,1.5 2NMU,TYR 56,10.42,0,0,0.42 20VT.GLU 78.4.6.0.09.0.0.01 1Y2Q,ARG_34,13.35,-0.4,0.6,0.65 2ILR,GLU_449,4.52,0.85,-0.68,-0.15 1Y2Q,LYS_90,10.39,-0.12,0,0.01 1TWU.GLU 90.4.73.0.23.0.0 3Q1C,ASP_165,3.06,-1.08,-0.01,0.35 2ILR.GLU 427.4.53.0.07.0.-0.05 3FS3,HIS_115,6.29,-0.25,0,0.04 1Y2Q,ARG_137,12.16,-0.49,0,0.15 20JO.ARG 475.12.44.-0.06.0.0 3O48, ARG_42, 12.79, -0.81, 0.68, 0.41 2I88,LYS_381,10.89,-0.89,0.85,0.43 2Q13,LYS_153,10.43,-0.07,0,0 1UXO.ASP 179.4.08.0.-0.09.0.37 3M16,TYR_202,9.9,-0.85,0.08,0.67 2W2S.GLU 134,4.57,0.83,-0.34,-0.43 1Q5Z,LYS_601,12.32,-0.45,1.48,0.79 2FGG,ARG_44,12.35,-0.19,0,0.05 4AE7.TYR 55.10.11.0.-0.49.0.6 3IVF,CYS_336,10.55,-0.42,0.56,1.42 3IL3,GLU_258,4.35,0.23,0,-0.38 3I0C,ARG_217,12.07,-0.69,0,0.26

200P.LYS 39,10.45,-0.05.0.0 3BPVLYS 49.10.74.-0.34.0.0.58 2WOZ,ARG_597,12.23,-0.37,0,0.1 1KW4,LYS 79,10,73,-0,14,0,0.36 1QQL,GLU_45,4.72,0.54,0,-0.32 2D59,HIS 48,6.85,-0.56,0.76,0.16 1RI6,ARG 112,12,59,-0,24,0,0.33 2ZQ5,ARG_344,12.32,-0.29,0,0.11 2H2Z,ARG_105,12.85,-1.09,0.62,0.81 3P28,LYS 53,11.36,-0.22,0.68,0.39 1WPA,ARG_483,13.24,-0.26,0.53,0.48 1AKO,ARG 12,12,21,-0.32,0,0.03 1DUP,CYS_36,10.42,0.01,0.17,1.24 3CBN.GLU 93,4.57,0.31,-0.1,-0.13 3UPD.HIS -20.5.69,-0.25,0,-0.55 3JZN,ASP_431,3.21,-1.57,-0.31,1.28 3UC9,ASP_63,3.84,0,-0.3,0.34 2VAN,ASP_124,1.91,-2.23,-0.17,0.5 2GKG,HIS 98,7.08,-0.3,0.84,0.04 3ZXY,LYS 246,10.64,-0.37,0.01,0.49 2Q13,GLU_165,4.93,0.39,-0.01,0.05 2PPN,ASP_41,2.95,-0.8,-0.44,0.38 2A6B.GLU 92.9.17.3.24.0.1.43 1V8E,ASP 68,2,7,-1,5,-0,09,0,49 3ZSL,TYR_221,12.04,-0.99,0.16,2.87 3MTT.ARG 469.12.71.-0.28.0.0.49 2B78, ASP_287, 2.74, -1.58, -0.21, 0.73 3GE9,HIS_134,6.66,-0.23,0,0.38 3LJI,HIS 272,5.97,-0.25,0,-0.28 1MTZ,LYS_228,10.67,-0.15,0,0.32 4EKU,GLU_124,4.79,0.35,0,-0.06 2HNG.GLU 12.3.97.0.35.-0.81.-0.08 4ANN, ASP 68, 3.87, 0, -0.11, 0.19 3MIX,ARG_487,12.2,-0.31,0,0 1N81,GLU_167,4.96,1.83,-0.97,-0.41 3CRM,GLU_235,4.58,3.13,-3.21,0.16 1XIP,LYS_155,10.16,-0.2,0,-0.14 4FLE,TYR 103,10.66,0.0.05,0.62 3M70,GLU_165,3.11,1.67,-2.55,-0.52 2D2S,GLU_589,4.69,0.42,0,-0.22 1SQH,CYS_132,11.6,0.11,0.37,2.13 3CO1,HIS 73,6.26,-0.47,0.58,-0.36 3M3P,HIS_249,6.58,-0.12,0.22,-0.02 3UPD,TYR_36,12.44,0.85,0.78,0.82 3ZXY,ASP_14,3.45,-0.83,-0.24,0.72 2Z84,GLU_187,4.54,0.21,0,-0.16 2CYG,GLU_264,4.77,3.45,-1.7,-1.48 2B61,ASP_242,3.28,-0.85,-0.23,0.56 2P0Y,HIS_275,6.14,-0.36,0,0 1LTU,ARG_114,13.04,-0.24,0.26,0.53 3EOD,CYS 57,11.91,0,0.15,2.76 2Q99,ASP_162,2.89,-0.85,-0.74,0.67 2CBE,ASP_19,3.68,0,-0.42,0.29 1VJG,TYR_118,11.01,-0.32,0.14,1.19 3F7M,ASP_130,2.5,-1.5,-0.27,0.47 2FGG,GLU_18,4.1,0.29,-0.06,-0.62 2FB6,LYS_16,11.34,-0.41,0.85,0.41 1EDG,ASP_191,3.19,-1.57,0,0.96 2IXM,GLU_114,4.73,0.14,0,0.09 3T5B,CYS_153,10.79,-0.28,0.23,1.84 1NKD,GLU_28,4.55,0.23,0,-0.18 3LQE,GLU_356,5.16,0.58,0,0.08 1P6F,TYR_79,11.62,0,0.04,1.58 2IXM,TYR_232,10.49,0,0.12,0.37 1YR6,ARG_191,12.81,-0.21,0,0.52 2V5B,ARG_196,12.25,-0.37,0,0.11 2CYG.ASP 86.4.28.-0.39.-0.07.0.94 2Q99,ARG_69,12.22,-0.31,0,0.03

4AE7.LYS 89,10.55,-0.14,0.0.19 2AD1,LYS_38,10.1,-0.3,0,-0.1 1SQH,GLU_117,3.96,0.93,-1.01,-0.47 2BQQ,CYS_127,12.93,0,0,3.93 2F8H.ASP 256.2.94.-0.79.-0.32.0.25 3PM2,ARG 52,12,72,-0,54,0,38,0,38 1ZBS,ASP_208,3.31,-0.65,-0.18,0.34 2ZQ5,ARG_380,12.05,-0.65,0,0.2 2HRZ,CYS_166,11.11,-0.74,-0.69,3.54 1P4X.LYS 152.10.36.-0.14.0.0 3EIZ,ASP_126,2.91,-1.12,-0.15,0.38 2B0J,ARG_101,12.49,-0.99,0.35,0.63 3PAC,LYS_93,10.81,-0.24,0,0.54 2012.LYS 212.10.4.-0.1.0.0 1EV8,ARG 243,12.26,-0.24,0.0.01 1XTZ,LYS_22,11.01,-0.54,0.57,0.48 1TLV,CYS_242,11.4,0,-0.14,2.54 1SQH,HIS_188,6.43,-0.59,0.57,-0.05 200K.ARG 144.13.32.-1.02.0.86.0.97 2E3S,CYS_518,10.04,0,0.2,0.84 1L3K,HIS_156,6.67,-1.32,0.85,0.63 3ASA,HIS_324,5.19,-1.57,0,0.25 4F8A,HIS 670,5.47,-1.61,0.55,0.02 4DEZ,LYS 193,10,1,-0,4,0,0 2E3C,ARG_442,12.72,-0.44,0,0.66 1NWA,HIS_0,6.24,-0.29,0,0.03 2VAN, ASP_160, 4.08, 0, 0, 0.28 4ANN,GLU 34,4.15,0.27,-0.63,0.01 1MIX,GLU_237,4.68,1.06,-0.41,-0.47 1TJE.TYR 14.11.99.0.62.0.17.1.22 1WP5,ASP_206,3,-1.12,0,0.32 2AHE,ASP 87,3.15,-0.86,-0.2,0.4 3CO1,ASP 120,2.03,-1.95,-0.38,0.56 1EV8,HIS_186,4.54,-1.88,0,-0.08 1GPP.TYR 432.10.37.0.0.03.0.33 2W0G,ARG_166,11.8,-0.76,0,0.05 3CAN,LYS 158,10.56,-0.2,0,0.26 3GW3,GLU_218,7.31,4.17,-1.36,0 2RH3,ARG_89,12.25,-0.3,0,0.04 4FZR,ASP_98,3.79,0,-0.24,0.24 2O34,TYR 70,11.09,0.0.29,0.8 1FO9,LYS 374,10.32,-0.16,0,-0.02 3FRR,LYS_48,10.15,-0.21,0,-0.13 3G9T,ASP_264,3.85,0,-0.17,0.22 3ASA,HIS_299,6.43,-0.2,0,0.13 1N81,LYS_120,10.68,-0.15,0,0.33 2X5Y.GLU 780.3.81.1.01.-1.43.-0.27 1TR9,ASP_214,3.68,-1.39,0,1.27 10I7,GLU_267,4.38,0.22,-0.08,-0.26 2P1W,HIS 32,5.62,-0.87,0,-0.01 3DHN.GLU 195,3,78,0,73,-1,52,0.07 3M70,LYS_123,11.48,-0.66,0.85,0.78 2B0A,GLU_135,3.84,0.38,-0.89,-0.16 4E8B,LYS_126,10.24,-0.18,0,-0.08 3E0H, ASP 41, 3.72, -0.64, -0.11, 0.67 1ZBS,CYS_168,9.93,0,0.22,0.7 3BWT,HIS_719,5.27,-0.85,0,-0.37 2Q07,LYS 484,10.79,-0.17,0,0.45 2V4U,ARG_311,12.43,-0.42,0,0.36 3G9T,HIS_274,4.45,-2.13,0,0.08 4FLE,HIS 122,5.56,-0.99,0,0.04 3B21,HIS_98,5.91,-1.11,0.16,0.36 1ZYL,LYS_171,9.94,-0.7,0,0.14 2QHT,HIS 41,4.11,-3.23,0.83,0 1ZBS,CYS_114,13.36,0,0.59,3.78 3H04, ASP_76, 2.82, -1.43, -0.47, 0.93 2RFA,ARG_262,12.14,-0.36,0,0.01 2E3S,ARG_517,12.74,-0.22,0,0.46 2YWX,GLU_9,4.6,0.1,0,0

3KT9.HIS 21.6.27.-0.53.0.0.31 1W24.GLU 65.4.81.0.28.0.0.03 2R4Q,CYS_178,7.17,-2.49,-0.01,0.68 1SUU,LYS_748,10.46,-0.04,0,0 205X.TYR 755,9.7.0.-0.52.0.22 1WYC,ASP_285,3.4,-1.16,-0.54,1.29 3DB9,ASP_49,3.57,-0.47,-0.32,0.58 200K,LYS_46,11.63,-0.52,0.85,0.8 2WB3,ASP_344,4.13,0,0.17,0.16 1XKR.HIS 0.6.76.-0.13.0.39.0 2VGM.GLU 286.3.8.0.6.-0.83.-0.48 2IF4,ARG_182,12.98,-0.89,0.25,1.12 1RHS,HIS_255,3.55,-3.34,0.4,0 3U2A,ASP_68,1.67,-2.3,-0.45,0.63 2ZQ5,ARG_213,12.13,-0.81,0,0.44 2EFK,LYS_215,11.32,-0.34,0.81,0.35 200K,GLU_227,4.94,0.36,0,0.08 3A2Z,ASP_181,4.04,0,0.1,0.13 3O48, ASP_67, 4.09, 0, -0.1, 0.39 1MTZ,HIS 42,5,29,-3,16,0,85,1.09 3F7M,ASP_269,3.71,-0.68,-0.03,0.62 3N2T,HIS_63,7.72,-1.25,1.66,0.8 1QQE,CYS_86,10.37,-0.16,-0.2,1.73 1D2K.TYR 196,12.34,0,0.6,1.74 3RNV,ARG_369,12.62,-0.3,0.07,0.35 2RIS,GLU_13,4.49,0.32,0,-0.33 2Q07,ARG_354,12.7,-0.54,0.17,0.57 3HZQ,GLU 55,4.69,0.26,-0.07,0 3IVF,ASP 208,3.57,-0.71,0.1,0.38 2EA9,ASP_18,3.81,0,-0.19,0.2 3KEY,ARG_312,12.25,-0.3,0,0.05 2VGM,TYR_192,11.71,0,0.17,1.55 3OA7, ARG 439, 12.26, -0.24, 0, 0 1PBV,GLU_54,4.55,0.05,0,0 4GA2,ARG_64,13.56,-0.79,1.18,0.66 3GV0,LYS_271,10.56,-0.1,0,0.17 1059,ARG 183,11.53,-0.97,0,0 1PDB,LYS_80,10.28,-0.1,0,-0.13 3FHF,GLU_72,3.9,0.29,-0.83,-0.05 2B6P,ARG_152,13.99,-0.74,1.31,0.93 2JKF,ASP_58,4.26,-0.04,0.05,0.46 1PSW,ASP 141,3.83,0,-0.2,0.23 2Z84,CYS 43,11.05,-0.91,-0.05,3.01 2CBE, ASP_139, 2.6, -1.46, -0.42, 0.68 2VAN,ARG_183,11.53,-1.02,0,0.05 2B0J.TYR 11.13.87.-0.8.1.02.3.66 2CI3,LYS_110,10.62,-0.15,0,0.26 3JSN,HIS_75,5.89,-1.53,0.84,0.08 2ILR,ASP 286,4.05,0.0,0.25 4ESS,GLU_123,4.79,0.29,0,-0.01 3F5D,TYR 14,10.47,-0.85,0.22,1.11 3UAH, ARG 374, 11.03, -2.52, 0.03, 1.04 1J74,GLU_36,4.42,0.5,-0.01,-0.56 1HF8,TYR_237,11.44,0,0.15,1.29 2EFK,GLU_185,4.55,0.14,-0.03,-0.05 2B61, ASP_59, 1.92, -1.86, -0.48, 0.46 2ZCO,ASP 253,3.8,-0.42,-0.2,0.62 2ILR.ARG 381,12.3,-0.21,0.0.02 200K,TYR_295,10.39,0,0.19,0.21 1AK1,ASP_241,3.34,-0.78,0,0.32 3HUE,TYR 180,12,08,0,0,24,1.84 1T95,LYS_59,10.53,-0.2,0,0.23 1NWA,ARG_166,13.71,-0.69,1.32,0.58 2NSN,CYS_39,9.4,-0.08,0.13,0.35 2H85,CYS 116,10.61,0,0.18,1.43 1YTD,ARG_94,12.04,-2.38,0.72,1.21 200K,ARG_245,12.5,-0.1,0,0.1 3IO0,GLU_140,4.51,0.22,0,-0.21 3L7N,GLU_185,4.09,0.22,-0.63,0

3GE9,ASP_137,3.92,0,-0.23,0.34 2CN1.HIS 198,4.42,-2.09,0.0.01 2YX0,ARG_319,12.18,-0.4,0,0.08 2B0A,LYS_80,10.45,-0.05,0,0 1T95.LYS 234.10.42.-0.08.0.0 2AD1,HIS_203,7.07,-0.28,0.75,0.11 2YWJ,TYR_178,12.13,0,0.41,1.72 1VSM,ARG_132,12.26,-0.24,0,0 1AIL,ARG_46,13.06,-0.62,0.65,0.54 100E,HIS 132,6.38,-0.33,0.12,0.09 1RI6.GLU 270.3.42.0.54.-1.58.-0.03 3MIX,ARG_387,12.5,-0.66,0.01,0.67 2B3M,LYS 75,10.46,-0.1,0,0.06 3C5V,CYS_347,12.54,0.18,1,2.36 1YG2,GLU_49,4.57,0.09,0,-0.02 1M5I,LYS 150,10.65,-0.12,0.0.26 2NYC,CYS_274,11.72,0,0.29,2.43 2AD1,LYS_178,10.11,-0.68,0,0.29 3O16,LYS_138,10.37,-0.16,0,0.03 3DHN,HIS_224,6.36,-0.14,0,0 1DUN,LYS_10,10.28,-0.15,0,-0.07 3HVW.TYR 240,13,11,0,85,0,48,1,77 2GZQ,LYS_125,10.27,-0.14,0,-0.08 3QKY,TYR 119,12.06,0.73,0.54,0.79 3M7D,CYS 68,12,19,-0.08,-0.6,3.88 3CCY,ARG_150,12.29,-0.13,0,-0.07 2V4U,LYS_466,10.42,-0.37,0,0.3 2FG1,GLU_142,2.42,0.74,-1.86,-0.96 1059,LYS 21,9.46,-0.86,0,-0.18 4FH3,ASP_258,4.38,0,0.31,0.26 2FL7,LYS 97,10,38,-0,39,0,0,27 1NAR,LYS_236,10.15,-0.37,0,0.02 10I7,TYR 158,12.33,0,0.13,2.2 3ZTA.LYS 124,10,27,-0,24,0,0,01 2H85,ASP_202,3.81,-0.21,-0.1,0.32 1WXQ,TYR_124,10.64,-0.2,0.12,0.72 2ILR,LYS_296,11.53,-0.27,0.85,0.44 2B0J,LYS 58,10.37,-0.26,0,0.12 1ES5,LYS_186,10.38,-0.15,0,0.03 3M7G,GLU_122,3.95,1.05,-0.8,-0.8 4DEZ,ASP_177,3.98,0,0.01,0.17 1L2F,LYS 223,11.52,-0.31,0.85,0.48 3FWU,ARG 28,13,99,-0.32,1.09,0.72 1D2K,LYS_138,10.42,-0.19,0,0.11 1SJY,TYR_145,12.96,0,0.1,2.86 10GL,ARG_93,12.38,-0.7,0,0.58 2VGM,LYS_237,10.64,-0.09,0,0.23 30IP.GLU 48.4.6.0.1.0.0 3CAN,CYS_13,9.43,-0.06,0.09,0.39 2P5D,GLU_21,4.3,0.18,-0.08,-0.3 20YZ,TYR_8,9.93,-0.39,-0.17,0.48 3EJG,ARG 59,13.11,-0.3,0.48,0.43 2WOZ, ASP_407, 2.9, -1.5, -0.13, 0.74 105T.HIS 140.5.32.-2.02.0.7.0.15 3RLE,HIS_29,6.24,-0.33,0.01,0.05 2B78,ARG_24,12.45,-0.09,0,0.05 3LPZ.TYR 203.11.66,-1.55.0.33.2.88 1WLY,GLU_284,4.71,0.2,0,0.02 1FO9,ARG_131,11.24,-1.26,0,0 4EVF,LYS_59,10.4,-0.11,0,0.01 2O8P,TYR_94,10.27,0,0.05,0.22 2AXO,LYS_70,10.49,-0.14,0,0.13 4E9E,GLU 522,3.53,0.51,-0.67,-0.82 3UPD,HIS_274,2.87,-3.51,0,-0.12 2EJB,ARG_83,11.92,-0.74,0,0.15 2P1W.GLU 164.4.63.0.13.0.0 2CE6,LYS_87,12.42,-0.71,1.7,0.93 1H4U,ARG_617,12.87,-0.21,0.22,0.37 2HRZ,GLU_223,4.5,0.32,0,-0.32

2Z0M,ASP_148,3.17,-0.47,-0.41,0.25 1W7B,LYS 115,11.05,-0.56,0.58,0.53 3A0X,GLU_640,4.62,0.1,0,0.02 3VHJ.ASP 141.2.91.-0.75.-0.56.0.42 2F4Q,LYS_122,9.42,-0.8,0,-0.28 1YTQ,HIS 29,6.61,-0.33,0.27,0.17 3KB5.ASP 421.3.35.-0.69.0.0.24 2H2Z,CYS_38,12.67,0,0.14,3.53 3EGN,TYR_489,12.01,0.35,0.55,1.11 3IL3,ASP_102,3.46,-0.55,0,0.21 1ZCU,ASP 61,4.15,-0.37,0.22,0.49 2Q12,ASP_109,4.11,0,0,0.31 1WYC,TYR_140,10.69,-0.8,0.37,1.12 1XFK,HIS_195,5.55,-1.95,0.82,0.18 3M70,ASP_228,3.9,0,0,0.1 4DBX.ARG 265,12.38,-0.29,0,0.17 1YR6,GLU_57,4.12,0.55,-0.77,-0.17 20EW,TYR_294,10.7,0,0.35,0.35 1W24,LYS_127,10.44,-0.42,0,0.36 2YWK,ARG_78,12.32,-0.28,0,0.1 3V3T.CYS 143.12.33.0.-0.16.3.5 4ECC,ARG_102,12.4,-0.32,0,0.23 4DNU,GLU_224,2.89,0.59,-2.05,-0.15 1C44,LYS 38,10.29,-0.18,0,-0.02 3LD1.CYS 362.9.13.0.0.0.13 3L7N,GLU_211,4.62,0.1,0,0.02 3BWT,HIS_779,6.39,-0.49,0.21,0.17 1V43,ARG_233,12.33,-0.28,0,0.1 4FH3,TYR 221,11.99,0,-0.28,2.27 3U2A,ARG 100,12.64,-0.27,0.0.41 4DBX,TYR_282,10.81,0,-0.09,0.9 1SJ8,GLU_542,4.64,0.28,0,-0.13 2P4D,ARG 102,13.5,-0.2,0.65,0.55 2DVK.LYS 33,10.74,-0.23,0,0.47 2XHC,TYR_114,11.7,0,0.18,1.51 1RZ2,LYS_165,10.22,-0.26,0,-0.02 1JYH,TYR_143,10.48,0,0.25,0.24 1TD6,CYS_67,12.95,-0.05,0.37,3.63 2F9F,ASP_14,2.31,-1.27,-0.53,0.31 1GQE,ARG_52,13.8,-0.33,1.27,0.36 20JQ,GLU_651,4.28,0.25,-0.23,-0.23 2XHC,LYS_205,10.54,-0.25,0,0.29 1P4X,GLU 160,4.27,1.12,-1.35,0 1Z9L,ASP_112,3,-0.62,-0.72,0.54 3CZC,ASP_52,3.14,-0.86,-0.2,0.4 2H2Z,ARG_298,11.53,-1.27,0,0.3 3Q6L,CYS_118,10.99,0,-0.94,2.93 3UPD,TYR 102,9.83,-0.85,0,0.68 3ONT,GLU_110,3.94,0.29,-0.85,0 1ILW, ASP_84, 3.98, 0, -0.07, 0.24 3LJN,GLU_239,4.89,0.19,0,0.2 1WXQ,CYS 50,10.58,0,0.11,1.48 1PGV,ARG_332,12.28,-0.22,0,0 1VJG,ASP_133,2.35,-1.58,-0.68,0.81 3HVW,GLU_258,4.96,0.34,0,0.12 2AD1,LYS_283,10.67,-0.16,0,0.33 3HNX,GLU_57,4.85,0.23,0,0.12 3PP8,ASP_241,2.85,-0.85,-0.48,0.37 1JKS,GLU_64,5.3,2.79,-0.85,-1.14 1V8E,ARG_185,12.2,-0.34,0,0.04 3CAN,CYS 170,11.12,-0.03,0.14,2.01 3TOW,LYS 143,9.6,-0.25,0,-0.65 3IRA,LYS_7,10.41,-0.09,0,0 4FH3,LYS_46,10.83,-0.11,0,0.44 2P65,GLU_101,4.5,0,0,0 3DHN,HIS_207,6.44,-0.26,0,0.19 2CYG,GLU_314,3.27,2.61,-3.06,-0.79 2BDV.ARG 57,11.75,-0.68,0,-0.07 2IF4,ASP_41,3.91,-0.05,-0.01,0.16

3BWT,LYS 772,10,45,-0,43,0,0,38 2PLQ,CYS_332,9.18,0,-0.01,0.19 3DB9,GLU_114,3.26,0.74,-1.5,-0.47 3U4K,LYS_163,11.11,-0.26,0.4,0.46 1X7F.ARG 272.13.46.-0.35.1.01.0.3 3MEW,CYS_287,10.56,0.27,0.22,1.06 2Q98,ARG_10,12.29,-0.21,0,0 3V55,GLU_418,2.88,1,-1.79,-0.84 2H01,ASP_24,3.36,-0.79,-0.08,0.43 3IL3.LYS 213.10.55.-0.22.0.0.27 3ETU,LYS_170,10.64,-0.11,0,0.25 1NFN,LYS_75,11.72,-0.53,0.98,0.76 4EVF,GLU_64,5.04,0.79,0,-0.24 2I88.LYS 402,10.49,-0.22,0,0.21 3RLN,LYS 674,10.39,-0.21,0,0.11 3QAV,LYS_45,9.94,-0.38,0,-0.17 1V6T,LYS_99,10.69,-0.11,0,0.31 2X4L,LYS_208,10.46,-0.07,0,0.04 3U0V.GLU 92.4.0.21.-0.48.-0.23 1U3Y,HIS_304,6.17,-0.23,0,-0.09 3V55,LYS_358,10.29,-0.25,0,0.04 4FCU,LYS_144,8.9,-1.66,0,0.05 1XFK.GLU 96.4.6.0.1.0.0 3ANJ,ARG 196,12.25,-0.53,0,0.29 1X91,LYS_35,11.37,-0.39,0.85,0.4 2B78,LYS_82,9.76,-0.81,0,0.07 1SBX,ASP_144,4.01,0,-0.04,0.25 2CXC,ARG 13,12.46,-0.32,0.01,0.27 2G5X,ASP_18,3.85,-0.41,-0.47,0.93 2I88, ASP_398, 3.35, -0.17, -0.58, 0.3 3PZ9,GLU_300,5.29,0.73,0,0.06 2CYG,ARG 103,12,42,-0,28,0,0,2 105Z.ARG 564.12.22.-0.38.0.0.1 1RSS,ASP_45,3.97,0,-0.38,0.54 1R29,ARG_98,12.52,-0.21,0,0.23 1LFP,LYS_13,10.39,-0.16,0,0.05 1WXQ,ARG_212,12.24,-0.62,0,0.36 2CWY.HIS 21.5.48,-1.1.0.0.08 3IVF,ASP_397,4.08,-0.04,0.06,0.26 2D0A,LYS_37,10.19,-0.21,0,-0.09 1EDG,ARG 299,12.3,-0.29,0.0.09 2Z14.GLU 46.4.56.0.19.0.-0.13 1ZYL,GLU_250,4.82,0.16,0,0.16 3ETV.HIS 165.8.45,-0.37,1.68,0.64 1WYC,ASP_106,3.73,-0.82,-0.05,0.8 3RJX,GLU 229,5.67,1.58,-0.41,0 301C,ASP 191,3.51,-0.84,-0.37,0.93 2Z0M,ASP_180,3.83,0,-0.29,0.32 2D7U,ARG_141,12.33,-0.17,0,0 3COU.GLU 83.4.52.0.1.0.-0.08 1WNH.TYR 205,10,13,0,-0.08,0,21 3Q1C,HIS_304,6.68,-0.28,0.25,0.21 3IL3,LYS 130,10.4,-0.09,0,-0.01 1M5I,GLU_151,3.91,1.1,-0.81,-0.87 1NWA, HIS 47, 6.17, -1.29, 0.9, 0.05 3P2F,HIS_161,5.85,-0.89,0,0.24 2DVK,ARG_59,12.34,-0.16,0,0 1EQ6,ARG_58,12.38,-0.12,0,0 3PP8,HIS_77,6.92,-0.31,0.66,0.06 1X7F,GLU 327,4.74,0.24,0,0 2R51,HIS_84,5.62,-0.67,0,-0.22 3GW3,ASP_123,3.36,-0.83,0,0.39 1DTO,LYS_172,10.47,-0.31,0,0.27 1MTZ,GLU_276,5.97,3.85,-2.49,0.12 3D9H,ARG 252,12,51,-0.32,0,0.33 3N2T,ASP_102,1.98,-2.34,-1.01,1.52 2V81,GLU_202,3.56,0.29,-0.85,-0.38 1LZL,GLU_230,4.62,0.13,-0.01,0 2E3I,ARG_107,13.25,-0.46,0.76,0.45

1YTD.ARG 83.11.61.-0.92.0.0.03 3O48, ARG_75, 12.32, -0.34, 0, 0.17 2H2W,ARG_227,11.97,-0.79,0,0.25 2ZCO,GLU_279,4.51,0.35,0,-0.35 1JYH, ASP 120, 1.95, -2.32, -0.11, 0.57 3GMS/HIS 260.6.18,-0.29,0.02,-0.05 1L2F,GLU_21,3.16,0.39,-1.22,-0.52 2FD4.GLU 542.4.11.0.28.-0.66.0 3OA7,LYS_516,10.37,-0.23,0,0.09 2YT4,LYS_565,9.9,-0.57,0,-0.03 1TLV.GLU 168.4.63.0.13.0.0 1V43,LYS 283,10.51,-0.08,0.0.09 3U0V,LYS_215,10.56,-0.14,0,0.2 3HUE,LYS 312,11,33,-0.2,0.57,0.47 4DBX.ARG 52.12.37.-0.63.0.0.49 1KCM,HIS_116,3.07,-3.22,0.8,-1 3ASA,LYS_182,10.74,-0.3,0.49,0.05 2GAU,TYR_56,11.61,0,0.16,1.46 1RHS,LYS 174,10.37,-0.1,0,-0.03 3CRM,ARG_293,12.41,-0.09,0,0 2FG1,ARG_96,12.32,-0.5,0,0.31 1NJ4,GLU_179,6.76,3.81,-1.6,0.06 1LZL,GLU_196,4.87,0.42,0,-0.05 3EX9,HIS 22,6.27,-0.47,0.38,-0.14 3ULX,HIS_30,6.41,-0.52,0.17,0.28 1SQH,HIS_159,7.04,-0.73,0.93,0.34 1ZYL,TYR_302,12.58,0,0.36,2.22 3RRQ,LYS_135,10.03,-0.47,0,0 2V1L.TYR 133.10.65.0.0.11.0.54 3CCY,ASP_114,3.37,-0.54,-0.15,0.26 2IN0,HIS_30,6.28,-0.51,0,0.29 2EDM,ARG_64,11.89,-1,0,0.39 2FBI,GLU 110,4.75,0.27,-0.01,-0.02 2CL3,GLU_69,3.81,0.31,-0.82,-0.18 3ETU,ASP_40,3.91,-0.11,0,0.21 2D7J,TYR_101,12.12,0,0.98,1.14 3O7K,GLU_30,4.67,0.17,0,0 2XJ4,HIS_250,5.66,-0.64,0.05,-0.25 2D7U,LYS_147,10.56,-0.3,0,0.35 3GEC,ARG_283,12.31,-0.41,0,0.22 200K,ASP_265,3.89,0,-0.12,0.21 2G70,LYS 112,10.45,-0.1,0,0.06 30KY,ARG 133,12,46,-0,39,0,0.35 2GKG,ASP_74,3.99,0,-0.01,0.19 2WB8,ARG_692,11.48,-2.15,0.6,0.51 2IQT,GLU_275,3.84,0.19,-0.85,0 1X8F,ARG_218,12.34,-0.21,0,0.05 2IRM,GLU_228,4.64,0.14,0,0 3M7D,ARG 135,10,75,-1,56,0,-0,2 2CN1,LYS_119,10.45,-0.2,0,0.14 1R6Y,ASP 45,3.38,-0.79,-0.09,0.46 2YWJ.GLU 62.4.38.0.13.0.-0.25 2D7U,ARG_259,11.9,-1,0,0.4 2E0T,TYR_106,12.66,0,0.32,2.34 3G9G,LYS 242,10,58,-0,25,0,0,33 1Y0K,ARG_25,12.5,-0.06,0,0.06 2CL3,LYS_122,11.17,-0.34,0.49,0.51 3E7P,GLU_237,6.03,1.79,-0.22,-0.05 2QZQ,LYS_157,10.42,-0.08,0,0 2P52,GLU 218,5.06,0.45,0,0.11 1UAJ.LYS 83,11.5,-0.51,0.85,0.65 1P6F,ARG_145,12.72,-0.35,0.18,0.39 1ZP2,ASP_207,2.1,-1.77,-0.51,0.58 2OJQ,GLU_635,4.59,0.27,0,-0.18 2ATR,HIS_17,6.62,-0.76,0.84,0.03 3ASA,ASP_344,4.15,-0.1,-0.37,0.82 3AUF,ARG_49,13.58,-0.27,0.66,0.68 2CE6,GLU_57,2.61,0.34,-2.2,-0.02 3RLE,TYR_166,13.61,0.85,0.99,1.78

2PGE,ARG_309,12.6,-0.74,0.41,0.43 3LJI,HIS 83,6,48,-1,27,0,84,0,41 2Q99,ASP_178,3.23,-0.85,-0.58,0.85 3NR5,ASP_126,3.58,-0.55,0.07,0.26 3RFY,ASP 310,3,95,0,0,0,15 3MTT.GLU 492.4.66.0.27.0.-0.12 2D7U,GLU_241,4.5,0.5,-0.32,-0.17 30IP,ASP_150,2.99,-1.3,0,0.49 1UOH,LYS_95,10.22,-0.28,0,0 1N81,ASP 95,3.3,-0.46,-0.46,0.42 3M66.TYR 301.13.94.0.0.3.94 2HP7,LYS_226,10.54,-0.06,0,0.1 3KB5,ASP_329,2.57,-1.2,-0.63,0.6 2R2Y,GLU_81,4.27,0.31,0,-0.54 1MUF,HIS 116,6.15,-0.35,0,-0.01 208P,LYS_124,10.31,-0.22,0,0.03 3ONT,ASP_112,4.06,0,0,0.26 1XKR,ASP_143,3.49,-0.67,0,0.36 1L3K,ARG_31,12.79,-0.41,0,0.71 3RJX,TYR_156,12.54,0.71,0.51,1.31 3BQW,TYR_77,10.41,0,0.17,0.24 1Y2Q,GLU_62,4.01,0.28,-0.32,-0.45 2A4D,ARG_87,11.73,-1.1,0,0.33 2A0J,CYS 47,10.76,0,0.02,1.75 2IOT.GLU 45,4,36,0,37,-0,57,0,06 3H5T,GLU_339,4.68,0.16,0,0.01 4H4J,HIS_178,7.04,-0.42,0.81,0.15 1X91,GLU_84,4.43,0.26,0,-0.32 4GCO,GLU 168,3.41,0.42,-0.82,-0.69 2A1V,ASP_96,2.41,-1.88,-0.08,0.57 1HUF.HIS 83.6.03.-0.99.0.33.0.19 3EVZ,LYS_106,10.39,-0.11,0,0 2PP6,ARG 10,12.35,-0.15,0,0 2R2Y,CYS 80,11,25,0,0,13,2,13 3IRA,ARG_4,13.11,-0.62,0.08,1.14 2CVB,ARG_126,12.73,-0.21,0,0.44 1EDG,TYR_116,11.31,0,0.3,1 1H09,ARG_212,12.26,-0.24,0,0 3KV0,GLU_105,4.59,0.31,0,-0.21 3FHF,GLU_162,4.87,0.24,0,0.13 2A0J,LYS_127,10.79,-0.18,0.33,0.14 4ECC,GLU_109,4.73,2.3,-0.85,-1.21 1UXO,LYS 121,9.56,-1.08,0,0.14 1D2K,TYR_113,12.03,0,0.06,1.96 1Q8B,HIS_52,7.03,-0.38,0.85,0.07 1SFE,LYS_124,10.09,-0.2,0,-0.21 2EEY,LYS 98,11.49,-0.41,0.66,0.75 3V46.CYS 338.11.31.0.-0.48.2.78 3B4D,GLU_234,4.87,0.13,0,0.24 1MUF,GLU_271,4.56,0.06,0,-0.01 1CHD,ARG_273,12.34,-0.16,0,0 4H89,ASP 66,4,23,0,0,28,0,15 3E7P,ARG_98,11.72,-0.78,0,0 4FZN,ARG_25,12.39,-0.91,0.34,0.46 3E7P,GLU_25,5.24,1.54,-0.01,-0.78 1EV8,TYR_71,11.11,-0.03,0.11,1.03 106D,ARG 59,12,1,-0,55,0,0,15 2A4D,TYR_134,12.69,-0.15,0.23,2.61 3EZ7,LYS_81,10.23,-0.21,0,-0.05 2BAA, ARG_183, 12.3, -0.24, 0, 0.04 1AK1.ARG 46.13.35.-0.73.0.31.1.26 3P51,TYR_5,11.52,0.5,0.41,0.6 2ILR.GLU 312.4.09.0.39.-0.61.-0.19 1V6T,TYR_65,12.37,0,0.39,1.98 3VJ8,LYS_41,9.98,-0.46,0,-0.04 1J85,HIS 86,5,41,-1,29,0,0,19 1LZL,CYS_133,13.43,0,0.57,3.85 1NWA, ASP_113, 2.96, -0.95, -0.38, 0.49 1WJG,ARG_16,13.74,-0.21,0.79,0.65

2RJD,GLU_312,4.54,0.07,0,-0.02 4AF2,GLU_113,3.45,0.44,-1.45,-0.04 3ETU,HIS_116,2.04,-3.5,0.45,-1.4 4FZR,LYS 189,12.09,-1.27,1.46,1.41 109G,GLU_114,4.8,0.25,0,0.06 1RKA,ASP 302,4.26,-0.29,-0.36,1.12 3CXS.TYR 85,11,45,0,0,22,1,24 3ZSL,ASP_178,4.18,0,0.22,0.16 1V6T,LYS_120,10.35,-0.19,0,0.03 3U0V,ASP_106,3.95,0,-0.21,0.38 1YB2,LYS 130,10.43,-0.23,0,0.16 1YM5,LYS_293,10.38,-0.12,0,0 2CIU,HIS_175,5.59,-1.58,0.52,0.14 1GQE,ARG_278,12.5,-0.1,0,0.1 2RIK.GLU 102.3.64.0.32.-0.77.-0.4 3CZC,LYS 87,11.55,-0.43,0.68,0.8 2BDV,GLU_197,4.2,0.23,-0.25,-0.27 1QYI,GLU_109,4.68,0.2,0,-0.02 1TD6,GLU_97,3.72,0.76,-0.85,-0.7 1X04,ARG_217,12.64,-0.26,0.05,0.36 3HOX,HIS 8.6.35,-0.15,0.0 1SJY,ASP_147,4.19,-0.31,-0.25,0.95 1RWZ,ARG_231,12.45,-0.35,0,0.3 306L/ARG 109/12/23/-0.45/0/0.18 3LJN.GLU 220,4,96,0.62,-0.25,0.08 3BPV,ASP_113,3.95,0,-0.21,0.36 1U53,GLU_171,3.59,0.47,-0.85,-0.52 1F2V,ARG_8,12.3,-0.28,0.08,0 1XWM,GLU_18,3.88,0.54,-0.77,-0.38 3CIV.ARG 190.12.53,-0.12.0.0.15 3GA2,ARG_81,12.51,-0.21,0,0.21 2B78,GLU_373,4.51,0.47,-0.51,0.05 2G9D.HIS 63.0.03.-3.03.0.-3.45 3I4T,GLU 211,4.78,0.21,0,0.07 4EUG,TYR_66,13.71,0,0.11,3.6 30IP,CYS_93,11.04,-0.03,-0.08,2.15 2P65,ASP_98,3.59,-0.36,-0.3,0.44 2A4D,LYS_142,11.02,-0.24,0.27,0.5 1UXO,LYS 187,10.37,-0.31,0.0.18 3LJN,GLU_15,4.39,0.09,0,-0.2 3HVW,ARG_187,12.74,-0.63,0.4,0.48 4EVF,ARG_35,10.39,-2.65,0,0.53 2WOZ.HIS 445.5.61.-0.88.0.-0.01 2E3C,ARG_197,12.98,-0.67,0.68,0.47 4ACJ,ASP_794,4.63,-0.07,-0.06,0.96 3CJW,ARG_228,12.74,-1.1,0.81,0.51 2QVO,TYR_23,10.52,0,0,0.52 3TRE,ARG 40,12,65,-0,26,0,0,41 1AKO,LYS_49,10.45,-0.05,0,0 2DVK,CYS_40,9.45,-0.79,-0.5,1.74 3CJW,ARG_366,11.75,-0.9,0,0.15 1Z9L,HIS 0,6.44,-0.06,0,0 1SI7,GLU_319,3.91,0.61,-0.84,-0.35 3CAX,TYR_461,10.4,0,0.05,0.35 1EQ6,LYS_97,10.63,-0.18,0,0.32 2FGG,ARG_35,12.39,-0.27,0,0.16 1KN3,LYS_150,10.09,-0.37,0,-0.04 2PIM,ASP_41,2.63,-1.14,-0.76,0.73 10LR,LYS_26,10.84,-0.34,0.42,0.26 1MUF,HIS_310,2.1,-3.91,0,-0.49 1N81,CYS 109,12.3,0,0.44,2.86 3RLE,ASP 57,2.89,-0.85,-0.42,0.36 1TLV,LYS_115,10.79,-0.16,0,0.45 1RWZ,GLU_178,4.7,0.2,0,0 1V6T,LYS_189,10.58,-0.33,0,0.41 3OBS,GLU_138,4.67,0.25,0,-0.09 1KN3,HIS_15,6.22,-0.36,0,0.08 2EEY,ARG 26,11.77,-0.89,0,0.16 3U4K,ARG_37,12.32,-0.18,0,0

1RAJ,LYS 431,10.75,-0.11,0.0.37 1SQH,LYS_290,10.21,-0.42,0,0.13 2P0L,ARG_38,12.43,-1.05,0.46,0.52 3BB7,TYR_165,10.8,0,0.04,0.76 4FD6.LYS 123.10.42.-0.08.0.0 1046.ASP 16.4.03.0.-0.02.0.26 4F3J,HIS_244,5.75,-0.41,0,-0.33 2AXO,GLU_144,4.63,0.13,0,0 1ES9,GLU_157,2.91,0.44,-1.28,-0.75 2R51.TYR 116.10.72.-0.02.0.09.0.65 1ZYL, TYR_37, 10.41, 0, -0.01, 0.43 1YR6,GLU_45,4.64,0.11,0,0.03 4DBX,LYS_97,10.87,-0.68,0.85,0.2 4ESS.ARG 3.12.33.-0.31.0.0.15 3TRE.CYS 22.10.86.0.0.12.1.74 1T95,GLU_26,4.96,1.14,-0.79,0.12 2CXY,LYS_6,10.71,-0.29,0,0.49 1MUF,LYS_107,10.33,-0.17,0,0 1MUF,ASP_306,3.94,-0.09,-0.54,0.77 2DG7,ARG_3,12.4,-0.1,0,0 1HUF,ASP_106,3.71,-0.7,-0.3,0.92 3F5D,ASP_191,4.05,0,0,0.25 20EW.ASP 299.3.92.0.-0.07.0.18 105T,CYS 394,10.27,-1.11,0.22,2.16 1KW4,ASP_37,3.98,0,0,0.18 2FBI,HIS_30,6.87,-0.53,0.68,0.22 2FGG,HIS_20,6.16,-0.31,0,-0.02 1AM2,GLU 55,4.65,0.23,0,-0.08 2D59,GLU_138,4.78,0.46,0,-0.17 2CWC,ARG_180,13.12,-0.74,0.74,0.61 1NWA,TYR_148,10.22,0.04,-0.09,0.28 2E3C,ASP 313,3.25,-0.67,-0.31,0.44 3DTE,ASP 215,4,23,0,0,1,0,33 1TD6,LYS_220,10.59,-0.09,0,0.19 4DVD,ASP_164,3.19,-1.55,-0.37,1.31 3I0C,LYS_314,10.75,-1.01,0.85,0.42 1DZF,GLU 148,4.36,0.14,0,-0.28 3BPV.CYS 131,9.35,0,-0.04,0.39 2FXT,LYS_355,9.63,-0.9,0,0.03 3HVM,TYR_249,12.17,-0.62,0.58,2.21 1G8P.GLU 222,3.95,0.17,-0.71,0 2D2S,ASP 525,3.69,-0.16,0.0.05 2XHC,LYS_270,10.62,-0.15,0,0.27 3BJV.LYS 136,10.53,-0.15,0,0.18 1DUP,ASP_47,3.36,-0.79,0,0.35 3AU3,GLU 578,4.73,0.22,0,0.01 2PGX.GLU 145.4.66.0.21.0.-0.04 1GQE,ARG_116,11.02,-2.41,0.02,0.91 1ANU,ASP_50,3.94,0,-0.23,0.37 2F9F,LYS 165,10,34,-0,14,0,-0.02 3U2A,ARG 61,13,72,-0.52,1,19,0.54 3G9G,GLU_232,4.72,0.2,0,0.02 1JT9,ARG_158,12.24,-1.23,0.49,0.48 3LH5,ARG_677,12.32,-0.24,0,0.06 3A2Z,GLU 166,4.32,0.3,-0.1,-0.38 4FCU.CYS 58.11.23.0.0.03.2.19 3BQW,ARG_116,12.09,-0.4,0,-0.01 4AM1,LYS_98,10.3,-0.27,0,0.07 1JKS,GLU_182,5.34,1.59,-0.7,-0.06 1YTQ,ASP 102,3.14,-0.82,0,0.16 4DND,ASP_5,3.77,0,-0.32,0.29 1GPP,ARG_35,13.56,-1.18,1.27,0.97 2IQT,LYS_118,10.43,-0.15,0,0.08 3FTT,LYS 179,10.34,-0.17,0,0.01 2FD5.LYS 80.10.58.-0.23.0.0.3 2FD5,ARG_9,13.93,-0.48,1.49,0.42 1WXQ,ASP_381,4.12,0,0.14,0.18 3M3P,HIS_231,6.23,-0.84,0.64,-0.06 1L2F,TYR_59,10.91,0,0.49,0.42

3H5T,TYR 30,11.03,0,0.2,0.83 4EVF,ASP_125,3.49,-0.65,-0.42,0.76 2RGY,GLU_245,4.3,0.45,-0.66,0 2CW4,CYS_119,12.05,0,0.08,2.97 2FB6,LYS 31,10.05,-0.42,0,-0.03 2B78,TYR 115,13.9,-0.85,1.38,3.36 1SNT,ARG_78,12.26,-0.29,0,0.05 1H4U,HIS_497,6.01,-0.49,0,0 2YT4,LYS_525,10.23,-0.12,0,-0.15 4ECC.LYS 210.11.03.-0.88.0.7.0.72 3Q6L,ASP_111,3.92,0,-0.02,0.14 3BQE,ASP_352,3.77,0,-0.38,0.36 3CNU,GLU_24,4.74,0.22,0,0.02 30KY,LYS 120,10.33,-0.28,0.0.1 3G6S,ASP_206,4,-0.1,0,0.31 3GEC,TYR_253,10.29,0,-0.04,0.33 3OA7,LYS_4,10.63,-0.12,0,0.24 3L3P,ASP_528,3.95,-0.31,-0.3,0.77 2WB8,ASP_596,3.76,-0.23,0.03,0.16 1F2V.LYS 122.10.2.-0.33.0.0.03 2BDV,GLU_80,5.1,1.78,-0.6,-0.58 1TP6,ARG_60,12.38,-0.27,0,0.15 2AZL,LYS_152,10.35,-0.25,0,0.1 1TLV.LYS 177,10.69,-0.47,0,0.66 3HUE,HIS_150,4.77,-1.74,0,0.02 1LFP,LYS_16,10.23,-0.35,0,0.08 1AK1,HIS_201,5.49,-0.91,0,-0.1 10IS,HIS_299,5.77,-0.5,0,-0.23 3LOE, TYR 317, 12, 74, 0, 0, 28, 2, 46 3VJ8,LYS_170,11.68,-0.37,0.8,0.75 1PBV,GLU_119,3.62,0.29,-0.75,-0.41 1YDL,GLU_25,4.7,0.18,0,0.02 3E5TLYS 227.10.45.-0.05.0.0 2P0L,GLU_143,5.23,0.39,0,0.35 3EX9,GLU_131,4.94,0.33,0,0.12 3GE9,GLU_24,4.56,0.06,0,0 3F7M,GLU_147,4.38,1.3,-1.38,-0.03 3SMD, ARG_89, 13.13, -0.36, 0.63, 0.36 3M16,CYS_160,13.64,0.2,1.05,3.39 1LZL.LYS 20.10.72.-0.19.0.0.41 1FO9,TYR_365,12.13,0,-0.27,2.39 4DBX,LYS 255,10.3,-0.2,0,0 2D0A,LYS_266,10.96,-0.6,0.53,0.52 1PSW,HIS_225,6.83,-0.35,0.56,0.12 2OBI,LYS_90,11.58,-0.3,0.85,0.52 3LJC.ARG 212,12,26,-0,26,0,0.02 1C44,LYS 46,10,29,-0,3,0,0,09 3QAV,TYR_193,11.67,0,0.01,1.66 2AHE,GLU 213,4.08,0.3,-0.72,0 2H01,LYS_159,10.75,-0.15,0.4,0 2QEV,ASP 137,3.38,-0.46,-0.32,0.37 3LJC,ASP 205,4,1,0,-0.02,0,32 4HDE,LYS_174,10.38,-0.23,0,0.12 1WRU,LYS_232,10.3,-0.12,0,-0.08 3HNX,ARG_24,12.16,-0.29,0,-0.05 1EW4,ASP_23,4.33,0,0.25,0.28 2RGY,ARG_175,12.16,-1.79,0.7,0.74 2E3H,LYS_213,10.56,-0.08,0,0.14 105T,ARG_381,12.56,-0.5,0.22,0.34 1T3J,LYS_700,10.35,-0.15,0,0 2E3I,ASP 56,3,47,-0,4,-0,02,0,1 2CXC,LYS_83,11.19,-0.28,0.57,0.4 1MTZ,TYR_198,10.39,-0.4,-0.34,1.12 3ERF,LYS_110,10.43,-0.2,0,0.12 2DVK,GLU 108,3.48,0.32,-0.72,-0.62 2B2H,TYR_390,10.82,0,0.01,0.81 2JKF,ASP_65,2.99,-1.31,-0.01,0.5 2W1R,HIS_72,6.45,-0.99,0.54,0.4 1RI6,ASP_209,2.14,-2.05,-0.32,0.7

4FH3,ARG_139,12.44,-0.06,0,0 3JRT,LYS 101,10.39,-0.25,0,0.15 3Q9P,GLU_166,3.53,0.38,-0.71,-0.63 3KB5,LYS_279,10.49,-0.09,0,0.08 4DEZ.TYR 110.12.65.0.0.55.2.1 1LZL,ASP_245,2.33,-1.52,-0.35,0.39 3JSN,GLU_106,4.87,0.49,0,-0.13 4AF2,ARG_133,10.53,-2.17,0,0.2 2W1R,LYS_118,11.48,-0.18,0.78,0.38 3B21,ASP_38,3.48,-0.06,-0.83,0.57 1TUL,ASP 21,3,12,-0.84,-0.29,0.46 1NFN,ARG_136,12.44,-0.2,0,0.14 2H01,ASP_56,3.83,0,-0.17,0.2 1BYI.LYS 45.10.45.-0.06.0.0.01 1H4U,CYS_588,9.07,0,-0.05,0.12 1XDZ,TYR_56,12.04,0,0.26,1.78 1WYC, ARG_278, 13.85, -1.24, 1.49, 1.1 2H85,TYR_237,12.97,0,0.13,2.84 3GEC,HIS_429,4.77,-1.18,0,-0.55 3IU5.CYS 69.10.58.-0.1.0.18.1.5 4FH3,ASP_249,1.75,-2.45,-0.67,1.07 105Z,LYS 581,10.52,-0.13,0,0.14 4E9E,ASP_510,2.97,-0.85,-0.41,0.43 1TR9,LYS 300,10.38,-0.21,0,0.09 1IAP.HIS 101.7.25.-0.46.0.79.0.42 1DUN,GLU_78,4.74,0.25,0,-0.02 1J33,GLU_288,4.45,0.24,0,-0.3 1CBY,LYS_216,10.47,-0.32,0,0.29 2JKF,ASP 13,3.98,0,-0.08,0.26 3IPZ,ARG_126,13.22,-0.36,0.7,0.38 4ANN,GLU_106,4.45,0.26,-0.13,-0.19 1X8F,ARG_36,12.27,-0.24,0,0.01 3CZC,GLU 90,4.65,0.26,0,-0.11 1YTO,ASP 191,3.88,0,-0.1,0.18 2OJQ,LYS_574,10.39,-0.22,0,0.12 1X9G,GLU_108,4.94,1.55,-0.71,-0.4 3Q1C,ASP_238,2.53,-1.25,-0.38,0.37 3C2E,CYS 162,11.59,-0.16,0.01,2.75 2H2Z,GLU_240,6.04,1.44,0,0.09 1X1E,GLU_208,3.66,0.47,-1.03,-0.28 2Q12,HIS_180,6.29,-0.21,0,0 2YLF,GLU_124,3.03,0.42,-1.44,-0.44 3EAZ,GLU 154,4.6.0.17,0,-0.07 1QYI,LYS_315,10.95,-1.06,0.85,0.65 3RJX,GLU_270,4.36,0.28,0,-0.42 2ILR,ARG_460,11.68,-0.92,0,0.11 1TD6,ASP_31,3.74,0,-0.28,0.23 3HNX/CYS 23/10.12/-0.85/0.03/1.94 1RI6,ARG_231,13.58,-0.82,1.31,0.59 1DCF,LYS_24,10.28,-0.24,0,0.02 4EVF,GLU_156,3.82,0.34,-1.13,0.11 2AD1.TYR 194,10.23,0,-0.98,1.21 1X8F,HIS_202,1.46,-2.46,0,-2.58 3FTT.CYS 32,11.4,-0.35,0.27,2.49 2Q07,ARG_269,12.18,-0.28,0,-0.04 1F2V,ARG_22,12.1,-0.72,0,0.32 1042,ARG 114,12,38,-0,37,0,0,25 2G3A,GLU_111,4.25,0.44,-0.26,-0.42 1XEU,HIS_160,6.12,-0.26,0,-0.11 3GFP,ARG_369,12.74,-0.35,0.16,0.44 3G6S,LYS 157,10,31,-0,77,0,0.58 3B21,ASP_171,3.18,-0.73,-0.39,0.51 3TMO.GLU 284.5.58.1.14.0.-0.06 3TOW,LYS_89,10.74,-0.21,0,0.44 1BGF,HIS_95,6.89,-0.29,0.68,0 1PBV.LYS 57.10.3.-0.12.0.-0.09 3ANJ,GLU_374,4.17,2.02,-2.44,0.07 3VJ8,ASP_245,1.95,-1.65,-0.82,0.62 2Q99,CYS_97,12.43,0,0.61,2.82

2CVB,ASP_137,2.65,-1.6,-0.19,0.64 3MTT,ASP_557,4.03,0,-0.14,0.36 4FZN,GLU_247,4.55,0.26,0,-0.2 3EZ7,HIS_95,6.57,-0.28,0,0.35 3NR5,ASP_108,3.56,-0.63,0,0.4 1QYI,GLU 271,4.3,0.28,-0.24,-0.23 4DNU,ARG 15,12,31,-0.27,0,0.08 2CWC,LYS_77,10.56,-0.17,0,0.23 2XJ4,TYR_31,13.12,0.38,0.63,2.11 2QDJ,LYS_319,11.04,-0.33,0.46,0.42 2B0J,GLU 207,8.05,5.14,-1.41,-0.17 2DG7.GLU 22.3.73.0.42,-0.66,-0.53 2CBE.CYS 206.11.54.-0.17.-0.19.2.91 3H13,ARG_268,13.49,-0.42,0.78,0.63 1MD6.TYR 149.10.18.0.-0.1.0.27 3PBH,TYR_75,10.32,0,0.03,0.3 4AM1,ARG_244,12.25,-0.43,0,0.18 3VHJ,GLU_29,3.93,0.49,-0.68,-0.38 2R0S,TYR_92,11.97,0,0.43,1.55 3BQW,TYR 227,11.07,0,-0.15,1.22 30IP.LYS 75.9.14.-0.42.0.-0.94 3PP8,ARG_181,11.89,-0.67,0,0.06 3JV1,ASP_174,3.25,-0.82,0,0.27 1PZC.GLU 116.3.9.0.3.-0.82.-0.08 3JZN, ASP 91, 2.32, -1.23, -0.61, 0.36 2CBE,ARG_246,10.47,-2.52,0,0.49 20KT.ARG 157.12.38.-0.22.0.0.1 2FXT,ASP_244,3.94,0,-0.03,0.17 3EVP,GLU_253,3.93,0.61,-0.83,-0.34 3RJX.HIS 90.5.2.-2.0.56.0.15 1RHS,ASP_238,1.44,-2.46,-0.42,0.52 1NAR,GLU_98,4.89,0.33,0,0.06 3ADO.GLU 189.3.98.1.26.-1.51.-0.27 2E3H,LYS_252,10.3,-0.17,0,-0.03 1ZHV,HIS_133,6.23,-0.21,0,-0.06 3L7N,CYS_178,13.1,-0.38,0.73,3.75 4ETX,ASP_450,3.85,-0.19,0.02,0.23 2ZCO,TYR_73,10.04,-0.19,0.05,0.18 3CX2,ARG 238,13.2,-0.68,0.81,0.57 3PBH,CYS_42,12.8,0,0.5,3.3 1DTO,LYS_66,10.68,-0.18,0,0.36 2CYG,ARG_138,12.16,-0.46,0,0.12 1N81,TYR 65,10.48,0,0.31,0.16 1RZ2,GLU_54,4.75,0.53,-0.29,0 1PV5,HIS_48,6.72,-0.32,0.21,0.32 3V46,LYS_361,9.49,-1.02,0,0 4EKU,CYS_180,12.71,0,-0.01,3.72 3V10,ARG 657,12,14,-0,36,0,0.01 1QQE,LYS_183,10.51,-0.22,0,0.24 1EDG,LYS_15,10.13,-0.27,0,-0.1 1PSW,GLU_78,4.61,0.14,0,-0.03 2GZQ,ARG 85,12.43,-0.15,0,0.08 4D8L,ARG_63,12.26,-1.27,0.54,0.5 2R57,LYS_326,10.39,-0.23,0,0.12 1NJ4,GLU_249,5.12,0.98,0,-0.35 1Q46,ARG_63,12.28,-0.22,0,0 3V1Q,ARG_650,12,-0.4,0,-0.1 3H6Q,ASP_35,4.12,0,-0.16,0.48 3ETU,LYS 133,10.22,-0.28,0.0 2R2Y,ARG_104,12.21,-0.29,0,0 3GMS,GLU 304,4.89,0.28,0,0.1 1BGF,HIS 32,5.89,-0.59,0,-0.02 1Y2Q,GLU_50,2.93,0.59,-1.67,-0.5 1JSX,LYS_33,10.42,-0.08,0,0 3ANJ,ARG_150,12.27,-0.23,0,0.01 2IF4.GLU 160.5.33.1.06.-0.09.-0.16 1NAF,ARG_255,13.16,-0.24,0.6,0.3 3ZTA,TYR_107,10.35,-0.46,-0.28,1.08 1ZBS,ARG_152,11.7,-0.97,0,0.16

20B5,LYS 3,10,47,-0.03,0,0 3V55,CYS_441,8.81,-1.5,-0.03,1.34 3GS3,ASP_171,2.56,-1.49,-0.32,0.57 2XHC,LYS_3,10.35,-0.1,0,-0.04 3KB5.ARG 409.11.7.-0.97.0.0.17 3GFP,ASP_370,3.9,0,-0.21,0.31 2AD1,HIS_226,6.3,-0.2,0,0 2VAN,GLU_203,4.71,0.12,0,0.09 2H2W,TYR_168,12.17,-0.19,0.05,2.31 2V1L.HIS 28.6.31.-0.29.0.0.11 3EIZ,LYS_113,10.49,-0.02,0,0.01 3CJW,GLU 379,5.31,1.51,-0.79,0.09 4DEZ,GLU_118,4.71,0.16,0,0.05 3PU6.TYR 39.10.72.0.0.23.0.49 1LTU,ASP_245,4.18,0,0,0.38 2E3S,ASP_389,3.33,-0.81,-0.07,0.41 4FLE,ARG_164,11.67,-0.86,0,0.03 1XFK,ARG_317,13.17,-0.42,0.58,0.52 3AUF.HIS 128.6.29.-0.21.0.0 1JB3,GLU_121,4.84,0.41,0,-0.08 4FZR,ARG_67,13.47,-0.57,0.84,0.7 2ZCO,GLU_71,4.38,0.73,-0.83,-0.03 2B2H.GLU 323.4.62.0.1.0.0.02 2DFL.ARG 295.11.22.-1.28.0.0 1ZBS,LYS_74,10.3,-0.19,0,0 2X4G,GLU_56,4.5,0.1,0,-0.11 2QEV,LYS_120,10.34,-0.16,0,0 1XEU,LYS 116,11.45,-0.36,0.85,0.46 3BCY,LYS_94,10.57,-0.25,0,0.33 1N81,ASP_155,2.21,-1.81,-0.39,0.6 2B02,GLU_453,4.58,0.13,0,-0.04 2BDV,ARG 81,13.22,-0.22,0.52,0.42 3GV0.TYR 118.9.84.-0.37.0.0.21 2QZQ,LYS_170,10.24,-0.42,0,0.16 3A2Z,ASP_194,3.71,-0.51,0.13,0.29 3GOZ,GLU_41,4.91,0.35,0,0.06 2FPN,LYS_34,10.46,-0.06,0,0.02 3EUR.TYR 71,11.8,-0.63,0.74,1.69 2RIK,LYS_63,10.43,-0.07,0,0 1L2F,LYS_100,10.34,-0.16,0,0 1JT9.TYR 128.10.93.0.0.07.0.85 2P1W.LYS 175,10,-0,72,0,0,21 3QAV,GLU_160,4.67,0.17,0,0 2V4X,ARG_85,12.5,-0.06,0,0.06 2AD1,ASP_218,3.8,-0.03,-0.12,0.16 1J7G,TYR_108,11.69,0.85,0.33,0.5 2GEN.ARG 179,13.7,-0.55,1.31,0.45 1WNH,GLU_92,3.89,0.18,-0.74,-0.05 1PVT,ASP_33,1.99,-1.85,-0.62,0.67 1GOE,LYS 109,10.08,-0.44,0.0.02 3H5T,ASP 78,4.02,0,-0.06,0.28 1R3D,ARG_108,12.65,-0.34,0.1,0.38 2FD5,HIS_47,5.85,-0.49,0,-0.16 1T95,LYS_20,10.12,-0.3,0,-0.08 2V1L,ASP 69,2.76,-1.33,-0.01,0.3 2Q98,GLU_93,4.72,0.49,0,-0.27 4DNU,ARG_368,12,-0.52,0,0.02 3M66,GLU_185,3.61,0.29,-0.77,-0.41 1KCM,CYS_231,12.19,0,0.12,3.07 1MHN,GLU 147,4.83,0.23,0,0.1 3CIV,GLU_172,4.51,0.33,0,-0.32 2RIK,TYR_156,10.8,0.09,0.29,0.41 4F8A,TYR_699,11.53,0,0.14,1.38 3RHE, ASP 101, 3.84, 0, -0.07, 0.11 3GW3,ARG 362,12,48,-0,36,0,0,34 1ZBP,GLU_39,6.25,1.76,-0.1,0.1 3QAV,LYS_150,10.48,-0.22,0,0.19 2Q99,ARG_273,11.23,-1.81,0,0.54 3S0A,LYS_111,10.13,-0.39,0,0.02

1SOW.ARG 80.12.28.-0.22.0.0 2RIS.TYR 15.13.11.-0.85.0.08.3.88 2W1R,ASP_64,2.25,-1.4,-0.59,0.44 3BA1,TYR_172,10.09,-0.8,-0.25,1.13 100E,ASP 130,3.85,-0.33,-0.16,0.54 4FZN,ASP 95,2.98,-1.06,-0.08,0.32 2YWJ,LYS_53,10.39,-0.15,0,0.04 3B79,GLU_87,4.55,0.05,0,0 4FLE,TYR_74,11.54,-0.7,-0.07,2.32 3H8Y,GLU_97,4.53,0.09,0,-0.06 4DEZ.ARG 22,12,97,-0.32,0.39,0.4 3B7X,GLU_106,4.48,2.02,-1.34,-0.71 1U3Y,CYS_259,8.49,-1.81,0.63,0.67 1X1E,ARG 206,13,11,-0.29,0.57,0.33 3IVEASP 205.2.02.-2.05.-0.38.0.64 1SQH,GLU_259,5.13,1.12,0,-0.49 3CGW,ARG_274,12.91,-0.32,0.46,0.26 1EV8,LYS_259,10.44,-0.06,0,0 1T95,ASP 221,4.15,0,0.14,0.21 1I60.TYR 275.11.21.0.23.0.46.0.51 4FH3,GLU_376,4.55,0.16,0,-0.12 3UPD,LYS_33,10.12,-0.58,0,0.19 3F1X,TYR_57,10.55,0,0.21,0.34 2ILR.LYS 425.10.48.-0.54.0.0.52 2G9D,ARG_276,12.54,-0.22,0,0.26 4H4J,LYS_164,10.78,-0.24,0,0.53 3T5B,ARG_87,12.34,-0.16,0,0 2PGE,ARG_117,12.71,-0.17,0.01,0.37 1DOV,ARG_211,11.6,-0.9,0,0 1DVO,GLU_50,4.1,0.3,-0.7,0 2JEO,HIS_88,6.23,-0.68,0,0.41 2ILR.LYS 282,10.46,-0.04,0.0 3CN5,ARG 265,12.4,-0.19,0,0.09 3M66,TYR_229,13.09,0.85,0.44,1.8 3H13,HIS_335,5.48,-0.45,0,-0.58 2H14,LYS_272,10.3,-0.2,0,0 3GA2,ARG_182,12.29,-0.27,0,0.07 3ETV,LYS_332,9.79,-0.47,0,-0.24 3C6B,LYS_223,10.42,-0.26,0,0.17 1CBY,LYS_29,10.42,-0.08,0,0 3QAV,LYS_84,10.41,-0.09,0,0 2D59,TYR 59,9.75,-0.21,-0.42,0.38 2CYG.GLU 251,3.82,0.73,-0.5,-0.9 2BLL,HIS_340,6.66,-0.32,0.28,0.2 3FTT,HIS_132,6,-0.54,0,0.04 3EZ7,LYS_261,10.82,-0.75,0.39,0.68 1RI6,HIS_24,6.44,-0.24,0,0.18 20EW,HIS_279,6.78,-1.26,0.85,0.69 4H86,TYR_137,10.12,0,-0.06,0.18 2IF4,ARG_167,12.46,-0.27,0,0.23 1PZC,GLU_13,4.07,0.32,-0.22,-0.53 3N2TARG 155,12.61,-0.55,0.1,0.56 3GFP,LYS_474,10.64,-0.08,0,0.22 2XMZ,ARG_174,10.42,-2.71,0,0.64 2EHG,TYR_53,12.96,0,0.17,2.79 3BA1,CYS_10,10.77,0,-0.04,1.81 2EJB,ARG_126,12.52,-0.31,0,0.34 1ES9,CYS_205,13.91,0.59,0.53,3.79 3CIV,LYS_286,10.56,-0.14,0,0.2 2GAU,GLU 185,3.27,1.62,-1.95,-0.9 2H85.LYS 109.10.57,-0.09.0.0.15 2Z14,GLU_54,3.12,0.8,-1.59,-0.6 3LOD,CYS_133,8.79,-0.23,-0.17,0.19 1GXN,ARG_417,12.26,-0.57,0,0.33 4FZR,TYR 356,10.39,-0.03,-0.18,0.61 1FO9,GLU_276,4.34,0.54,-0.68,-0.02 3U4K,LYS_90,10.37,-0.45,0,0.32 1SUU,ASP_596,3.39,-0.55,0,0.14 2X4J,HIS_125,6.66,-0.39,0.24,0.31

1XTZ.HIS 152.6.27.-0.48.0.0.25 3F1X,CYS_153,9.47,0,0.08,0.39 3PZ9,LYS_125,10.06,-0.47,0,0.03 2PWO,ASP 60,3.64,-0.55,-0.02,0.4 1CHD,ASP_216,3.24,-0.81,-0.09,0.34 1XIP,LYS 84,10.28,-0.26,0,0.03 2FI9,ASP_30,3.86,0,-0.06,0.13 2YLF,ARG_37,12.39,-0.25,0,0.14 1NAF,GLU_257,4.11,0.4,-0.48,-0.31 3HZO,LYS 3,10.45,-0.05,0.0 3CJW,LYS 340,10,1,-0,49,0,0,09 3EVN,HIS_285,3.84,-2.37,0,-0.28 3G9B,LYS_116,10.46,-0.23,0,0.19 3RKV,ASP 212,4,11,0,0.03,0.27 3LMF,ASP 82,3.34,-0.51,-0.54,0.58 3GS9,ARG 64,12,26,-0,42,0,0,18 1JKS,LYS 222,10,44,-0,48,0,0,42 1NFN,TYR_118,11.12,-0.36,-0.28,1.76 3JSN,ARG_133,12.14,-0.86,0,0.5 1NAR, ASP_94, 3.72, -0.13, -0.8, 0.85 1YW5,ARG_81,12.24,-0.26,0,0 1BKR.ASP 6.3.93.0.-0.22.0.35 3TOW,CYS_161,10.11,-0.12,-0.47,1.69 3CAN,GLU 59,2.3,0.74,-2.32,-0.62 2AD1,HIS_174,2.9,-2.77,0,-0.84 2IQT,ASP_48,4.05,0,-0.08,0.34 3RJX,ARG_76,13.66,-0.97,1.26,0.86 3ELI,GLU_142,5.02,0.59,0,-0.07 2CL3,GLU 181,4.66,0.22,0,-0.06 2E3C,GLU_220,3.87,0.47,-0.68,-0.41 3H13,ASP 269,4.01,0,-0,19,0,4 3HYQ,ASP_168,3.35,-0.82,-0.16,0.53 2CBE, ASP 34, 3.78, -0.53, 0.1, 0.4 2B0A, HIS 40, 7.09, -1.93, 0.92, 1.59 2ZQ5,HIS_271,6.22,-0.4,0,0.12 1R3D,ARG_95,9.78,-2.58,0,-0.15 1L3K,LYS_78,10.31,-0.17,0,-0.02 4FZN,ARG 109,12.84,-0.46,0.46,0.35 1SNT,ARG_56,11.46,-1.26,0.05,0.19 3CIV,GLU_164,4.7,0.98,-0.62,-0.16 2CYG,GLU_322,5.52,1.11,0,-0.09 2EJX,ASP 124,3.26,-1.68,0,1.14 3IV4.CYS 30.8.31,-1.23,0.01,0.54 3H5T,GLU_246,5.8,4.11,-2.17,-0.65 1XIP,GLU_261,4.33,1.55,-1.23,-0.49 2BQQ,TYR_138,11.98,-0.83,0.44,2.36 3BQW,GLU_105,4.31,0.54,-0.51,-0.21 2R4O,LYS 171,10.59,-0.3,0,0.39 3EZ7,GLU_190,4.86,0.16,0,0.2 2QK1,LYS_486,10.66,-0.32,0,0.48 4EF5,ASP_297,3.84,0,-0.25,0.3 3P28,GLU 174,6.49,2.89,-0.85,-0.05 4ETX,ARG_382,12.77,-0.47,0.33,0.42 2JKF,LYS_164,11.54,-0.64,0.85,0.83 1ZYL,ARG_58,12.09,-2.12,0.54,1.16 4AF2,LYS_33,10.47,-0.15,0,0.11 4H86.GLU 170.4.33.0.49.-0.66.0 2AZP,HIS_293,6.03,-0.32,0,-0.15 1YW5,GLU_108,4.54,0.17,0,-0.13 1QQL,ARG_24,11.88,-1.06,0,0.43 1ILW.ARG 152,12.39,-0.14,0.0.03 2CWY,ARG_36,12.03,-0.47,0,0 2YWJ.LYS 27,10.43,-0.48,0.0.42 1NIJ,ASP_82,3.68,-0.44,-0.21,0.53 3A0X,LYS_750,11.25,-0.53,0.85,0.43 1R53,LYS 287,10.5,-0.15,0.0.15 2APL,ASP_39,4.08,0,-0.04,0.32 3F6F,ASP_87,3.05,-0.94,-0.18,0.36 1YB2,TYR_110,10.16,0,0.09,0.06

2CIU,GLU_136,3.39,0.66,-1.51,-0.26 1H09,TYR_17,10.92,0.21,0.4,0.32 3G9B,LYS_96,10.24,-0.35,0,0.08 2EEY,LYS 153,10,43,-0.07,0,0 1BKR,LYS_5,11.35,-0.46,0.85,0.46 3PZ9,GLU 308,4.48,0.17,0,-0.19 2BDV.GLU 16.4.05.0.29.-0.5.-0.24 3C6B,TYR_279,10.02,0,-0.05,0.07 3EVZ,GLU_216,4.53,0.28,0,-0.25 1T95,ARG_115,12.07,-0.48,0,0.05 3E7P,GLU 199,4.18,0.45,-0.42,-0.35 3AUF,GLU_180,4.67,0.58,0,-0.4 2CWC,TYR_267,12.37,0,0.49,1.88 3LD1,ARG_281,12.34,-0.18,0,0.02 1SIG.ASP 125,2.94,-0.85,-0.4,0.39 1T95,ARG 237,13,25,-0,25,0,73,0,27 1WNH,ARG_12,12.24,-0.83,0,0.56 3K8U,TYR_82,10.84,-0.85,0.04,1.65 3UC9,GLU_182,4.59,0.15,0,-0.06 1VJG,ARG_10,12.67,-0.47,0.1,0.54 3GE9.CYS 14,9.79,-0.47,0.05,1.21 3LMO,GLU_86,2.87,0.4,-1.59,-0.44 3ASA,GLU_303,4.71,0.33,0,-0.11 3KEY,ASP 335,3.58,-0.29,-0.2,0.27 1MJS.ARG 291,12.34,-0.28,0,0.13 1XDZ,CYS_90,12.49,0,0,3.49 2BDV,LYS_106,10.54,-0.23,0,0.28 2G9D,ARG_225,12.49,-0.12,0,0.11 3VJ8,GLU 137,4.6,0.1,0,0 1V43,TYR 259,10.34,-0.22,0.28,0.28 1SQW,ARG_43,12.99,-0.38,0.24,0.63 3GS3,GLU_36,4.79,0.34,0,-0.06 3V75,ASP 174,3.15,-1.73,-0.19,1.27 2CI3,LYS 99,10.52,-0.11,0,0.13 2FZ4,LYS_188,10.17,-0.3,0,-0.03 2GZQ,GLU_64,4.53,0.21,0,-0.18 3IPZ,LYS_77,10.43,-0.07,0,0 109G,ARG_75,12.58,-0.2,0,0.28 1R6Y,LYS 82,10.28,-0.22,0.0 2IF4,ARG_75,12.37,-1.11,0.28,0.68 4FH3,HIS_194,4.17,-1.66,0,-0.66 1D2K,TYR_81,10.14,-0.12,-0.35,0.61 3V4G,GLU 20,3.87,0.43,-0.72,-0.35 3JSN,GLU_48,4.41,0.2,0,-0.29 3JSN,TYR_275,11.12,-0.79,0,1.91 2ILR,GLU_467,4.1,0.24,-0.62,-0.02 3ZRI,HIS_147,6,-0.31,0,-0.19 1WLY.CYS 233,12,39,0,-0.02,3,41 1OXZ,GLU_271,4.68,0.11,0,0.07 3GE9,TYR_60,10.86,0,0.11,0.76 2JKF,ASP_31,3.42,-0.95,0,0.57 1FHL,CYS 118,11.59,-0.37,0.01,2.95 3HZQ,TYR_63,10.2,0,0,0.2 20EW,GLU_45,4.15,0.3,-0.14,-0.5 2P5D,LYS_89,10.05,-0.33,0,-0.11 2ZQ5,ARG_92,12.01,-0.6,0,0.11 3CCY,ARG_73,12.89,-0.43,0.39,0.44 2H2Z,HIS_164,1.6,-3.43,0,-1.47 3CGW.CYS 239,10.4,0.0.01,1.39 1PDB,ARG_65,11.67,-0.97,0,0.14 3HUE,GLU 124,4.41,0.28,-0.38,0 2IF4.GLU 276.3.53.0.28,-0.53,-0.71 4FD6,GLU_157,4.02,0.38,-0.46,-0.4 3PZ9,LYS_118,11.75,-0.5,0.85,0.9 3RLN,ASP_576,3.75,0,-0.31,0.27 2ILR/LYS 528/10.18/-0.42/0.0.09 1NWA,ARG_22,12.96,-0.91,0.78,0.6 3ETU,ARG_267,13.51,-1.08,0.85,1.24 2B0A,CYS_42,10.64,-0.84,0,2.48

3B21,ARG 79,11.76,-0.84,0.0.1 2P0Y,GLU_293,4.67,0.3,0,-0.13 3M7D,ASP_365,3.76,-0.05,-0.21,0.22 3GW3,ARG_148,12.15,-0.3,0,-0.04 2Z0W.LYS 51.10.13.-0.15.0.-0.23 1NFN,CYS 112,10,79,-0.02,-0.24,2.05 20EW,LYS_202,10.69,-0.33,0,0.51 1SJY,ARG_124,12.57,-0.54,0,0.61 100X,ARG_216,13.06,-0.37,0.53,0.39 2GZO.CYS 167.9.97.0.0.0.97 2CXY,ASP_21,2.31,-1.67,-0.38,0.56 1QQE,TYR_134,10.44,0,0.04,0.4 2P1W,CYS_182,10.23,0,0.09,1.14 2DVK.HIS 94,6.7,-0.73,0.62,0.31 3V3T,LYS 302,10,59,-0,5,0,16,0,44 3N2T,ARG_40,12.24,-0.34,0,0.09 2C2Y,ASP_13,3.49,-0.35,-0.41,0.43 2B2H,LYS_361,10.26,-0.24,0,0 1UAJ.ARG 154.12.4.-0.19.0.0.09 2NRK,GLU_71,4.08,0.41,-0.85,0.02 3EGN,GLU_393,3.86,0.48,-1.13,0 2APL,LYS_15,9.76,-0.94,0,0.2 2AZL,ARG_90,12.98,-1.22,0.81,0.89 2YYO,ARG_158,12.4,-0.21,0,0.11 1AK1,ARG_31,11.99,-0.44,0,-0.07 2P4D,TYR_124,13.14,0.85,0.6,1.7 1JKS,GLU_59,3.89,0.21,-0.53,-0.29 1RWZ,LYS 65,10.04,-0.98,0,0.51 2P4D,LYS_40,10.34,-0.16,0,0 3LH5,GLU_570,4.02,0.32,-0.34,-0.47 3IU5,ASP_108,3.16,-1.05,0,0.42 2P0L,ASP 25,4,12,0,-0.03,0.34 3CGW/CYS 277,10,79,0,0,19,1.6 3RNV,LYS_340,10.39,-0.2,0,0.09 4F8A,TYR 609,12,97,-1,26,1,91,2,31 3M66,LYS_350,10.33,-0.17,0,0 3S0A, TYR 110, 11.51, 0.82, 0.09, 0.59 1AK1.GLU 20.3.96.0.26.-0.65.-0.15 2VGY,GLU_112,3.8,2.15,-1.68,-1.18 3M7G,LYS_248,10.37,-0.13,0,0.01 2R0S.LYS 95,10.43,-0.22,0.0.15 1TWU.ARG 14.12.5.-0.63.0.18.0.46 3C38,GLU_105,4.74,0.17,0,0.07 2FI9,ARG_95,12.25,-0.27,0,0.03 3G9B,CYS_55,9.1,-0.18,0,0.28 3PU6,CYS 7,12.59,-0.02,0.04,3.57 3CS1.TYR 71.10.42.0.6.94E-18.0.41 3M66,LYS_186,11.56,-0.26,0.85,0.47 3B79,ASP_109,4.16,0,0.04,0.33 2PP6.ASP 6.3.98.0.0.0.18 1AKO.GLU 183,4.04,4.22,-2.98,-1.69 1J33,ARG_279,13.52,-0.32,0.92,0.41 2CWC,TYR_141,11.1,-0.2,0.05,1.26 1Q2Y,LYS_52,10.54,-0.21,0,0.24 3RFF,GLU 98,4.41,1.36,-0.8,-0.66 3TMO,GLU_197,4.75,0.19,0,0.06 2IQT,ASP_38,3.79,-0.15,-0.08,0.22 3Q6L,LYS_82,11.66,-0.24,0.85,0.55 3FWU,ASP_55,3.84,0,-0.19,0.22 1EW4.HIS 7,6.93,-0.37,0.32,0.47 1WXQ,ARG 311,12.85,-0.69,0.4,0.64 2P0L,ASP_236,4.36,0,0.22,0.35 2H8O,ARG_293,12.83,-0.38,0.35,0.36 3BWT,ASP_594,3.4,-0.78,-0.01,0.39 2BV9,TYR_167,11.74,-0.01,0.08,1.67 3BB7,LYS_358,11.49,-0.34,0.85,0.49 2AZP,ARG_17,13.55,-1.96,1.57,1.44 3C2E,CYS_66,11.24,0,0.02,2.23 3CS1,GLU_106,5.1,0.44,0,0.17

4E9E.ARG 468.12.28.-0.22.0.0 2FZ4,GLU_147,4.27,0.29,-0.09,-0.45 2R4Q,GLU_223,4.78,0.15,0,0.12 3ONT,LYS_134,10.72,-0.21,0.43,0 4FH3.ASP 82.3.92.0.-0.05.0.17 2VAN.GLU 288,4.31,0.2,-0.16,-0.23 1WRU,ARG_270,12.89,-1.07,0.5,0.96 3I4T,HIS 205,6,52,-0,22,0,16,0,08 208P,ASP_155,4.38,0,0,0.59 2WOZLYS 494.10.72.-0.3.0.06.0.45 3A7L,LYS 11,10,25,-0,28,0,0,03 3ETV,LYS_343,10.39,-0.11,0,0 3GEC,LYS_500,10.69,-0.1,0,0.28 1CHD,LYS 205,10,44,-0,17,0,0,11 2R2YLYS 113.10.45.-0.05.0.0 2HXB,ASP_150,3.87,0,-0.23,0.3 4D8L,ARG_70,12.49,-0.97,0.45,0.51 1EYH,ARG_114,12.49,-0.05,0,0.04 1ILW,ASP_88,3.71,-0.34,-0.08,0.33 3GE9.GLU 130.4.58.0.12.0.-0.04 3U2R,ARG_121,13.51,-0.29,0.7,0.6 3C6B,GLU_93,3.87,0.39,-0.78,-0.23 2Z14,TYR_39,11.42,-0.05,-0.02,1.47 2NRK,GLU 14,4.69,0.16,0,0.04 105T,LYS_264,10.37,-0.29,0,0.16 3H5T,LYS_292,10.36,-0.29,0,0.14 2Z0M,LYS_331,11.35,-0.44,0.85,0.44 1MJS,LYS_408,10.29,-0.21,0,0 3BWT.HIS 721.5.71.-0.78.0.0 2CWY,TYR_18,10.22,0,0.06,0.15 4AM1,TYR_89,11.21,-0.05,-0.07,1.33 2FZ4,LYS_37,10.61,-0.29,0,0.4 3TRE,LYS 47,11.3,-0.35,0.73,0.42 2GYZ,ARG_63,12.24,-0.26,0,0 2R2Y,LYS_44,10.24,-0.09,0,-0.16 1YTQ,LYS_41,11.32,-0.23,0.67,0.38 2P4D,ARG 13,13.76,-0.41,0.97,0.7 3EJC,ARG_155,12.2,-0.41,0,0.11 2Z61,LYS_265,10.59,-0.64,0.15,0.58 3DTE,GLU_102,4.76,0.2,0,0.06 307K,ARG_115,12.47,-1.04,0.11,0.89 3US6, ASP 12, 3.86, 0, -0.22, 0.28 3E7P.TYR 146.11.18.0.-0.01.1.19 1P2F,LYS_129,10.77,-0.92,0.48,0.71 1IAP,ASP_211,3.4,-0.76,-0.08,0.45 2YLF,ARG_147,11.89,-0.86,0,0.25 1F2V,ARG_127,12.44,-0.32,0,0.25 3DTE,ASP_232,4.07,-0.02,0,0.3 3F5D,GLU_176,4.24,0.23,-0.3,-0.19 3RFY,ASP_391,3.72,-0.31,0,0.23 2Q99,ASP_70,3.34,-0.59,-0.21,0.33 1DZF.TYR 208.10.1.0.0.04.0.07 2Q5X,TYR_866,12.03,0,0,2.03 2YX0,LYS_116,11.26,-0.55,0.75,0.57 4EKU,GLU_119,6.22,2.18,-0.62,0.17 4FH3,GLU_333,5.08,0.99,0,-0.4 1RI5,ARG_47,12.18,-0.27,0,-0.04 1PNE,CYS_127,12.11,-0.95,0.22,3.85 3GYW,TYR_75,10.49,0,0.2,0.29 1LTU,TYR 262,12.24,0,0.09,2.15 2B3M,TYR 19,12,93,0,7,0,79,1,44 1FQI,LYS_397,10.3,-0.2,0,0 3FHF,LYS_32,10.05,-0.66,0,0.22 3M66,HIS_345,6.09,-1.05,0.84,-0.21 2VAN,ARG 152,12.01,-0.64,0,0.15 3M7G,GLU_54,5.16,0.37,0,0.28 3SMD,TYR_90,10.46,0,0.2,0.27 3JZN,LYS_268,10.46,-0.04,0,0 2IXM,GLU_141,4.11,1.97,-0.85,-1.49

1FHL,HIS_81,5.15,-3.28,0.69,1.25 3BQW,GLU_157,4.61,0.11,0,0 3BQW,TYR_253,11.71,0,0.53,1.17 20BLCYS 37.12.73.0.0.02.3.71 3LH5,HIS_566,5.66,-1.05,0.21,0 2AD1,HIS 98,6.34,-0.17,0.21,-0.2 1WRU,GLU_111,4.43,0.92,-0.58,-0.41 1R53,GLU_232,4.55,0.72,-0.39,-0.3 2J8A,LYS_320,10.38,-0.1,0,-0.01 3C6B,LYS 203,10.32,-0.19,0,0.01 2C2Y,LYS 102,10.5,-0.14,0.0.14 1DVO,LYS_42,10.42,-0.08,0,0 1N81.GLU 135.4.41.1.06.-0.59.-0.56 4F8A,HIS_579,4.9,-1.61,0,0.02 1MTZ.ASP 80.4.23.0.-0.02.0.44 2PLQ,LYS_36,10.45,-0.2,0,0.15 3BJV,ASP_21,3.11,-1.01,-0.21,0.53 1LZL,GLU_146,3.7,0.41,-0.76,-0.44 2O4D,ASP_109,3.84,0,-0.15,0.2 2IOT.HIS 96.6.01,-0.64,0.03,0.12 3QKY,TYR_112,10.87,-0.59,-0.13,1.59 1PSW,ARG 334,12.31,-0.27,0,0.07 3BCH,TYR_156,9.96,-0.16,-0.19,0.3 3U2R.GLU 34,4.55,0.22,0,-0.17 1Q8B,ASP_25,3.62,-0.2,-0.13,0.15 2ZQ5,ARG_256,12.19,-0.74,0.06,0.37 2QEV,ASP_53,3.42,-0.89,-0.46,0.97 3IU5,GLU_70,4.69,0.24,0,-0.04 2IN0,TYR 79,10.53,0,0.34,0.2 3ERF,TYR_92,10.54,0,0.09,0.45 3ASA,ARG 348,13.33,-0.37,0.73,0.47 2P52,TYR_104,10.41,0,0.01,0.4 4GA2,GLU 142,4.49,0.26,0,-0.26 1YLN,LYS_177,10.4,-0.35,0,0.24 3BQE,ASP_223,3.94,-0.45,-0.06,0.66 3KT9,GLU_50,3.31,0.65,-1.25,-0.59 1X1E,GLU_53,3.92,1.09,-1.29,-0.4 3BWT,LYS 857,10.42,-0.32,0,0.25 20PJ,ARG_142,12.39,-0.19,0,0.07 1ANU,GLU_126,4.59,0.4,-0.39,0.09 3BQW,HIS_91,5.2,-1.07,0,-0.23 1UW7,CYS_73,9.5,0,-0.1,0.61 1EV8,ASP 110,2.3,-2.64,-0.51,1.65 3MIX,HIS_480,6.37,-1.15,0.85,0.17 2G9D,TYR_206,12.01,0,0.58,1.44 1D2K,TYR_50,12.14,0.77,0.62,0.75 2PGE,LYS_150,10.36,-0.39,0,0.25 3CN5.TYR 145.12.86.0.-0.11.2.97 2QV2,ASP_149,4.15,-0.03,0,0.39 1JKS,GLU_294,4.48,0.32,-0.32,-0.02 2Z0M,HIS_302,6.1,-1.37,0.85,0.12 105Z.HIS 611.7.25.-0.29.0.85.0.19 3GYW,TYR_49,10.29,0,0.03,0.26 1O5T,ASP_322,4,0,-0.79,0.98 2Q13,GLU_216,4.74,0.25,0,-0.01 1YOY,CYS_65,9.45,-0.02,0.07,0.4 1EDG,LYS 114,10.3,-0.17,0,-0.03 3RHE,LYS_59,11.53,-0.25,0.85,0.43 3JSN,ARG_173,12.27,-0.13,0,-0.1 1AK1,ASP_278,3.5,-0.32,-0.36,0.39 20RX.LYS 64,10.44,-0.1,0.0.04 2XHC,ARG_183,12.79,-0.3,0,0.58 3OBS.GLU 5,3.37,0.32,-0.76,-0.69 1RHS,GLU_143,4.61,0.13,0,-0.02 2IDC, ASP_133, 3.66, -0.2, -0.27, 0.34 4GA2.GLU 144.4.54.0.04.0.0 3GMS,ARG_175,11.92,-0.68,0,0.11 4H4J,GLU_176,4.02,0.41,-0.68,-0.21 1QQL,CYS_17,10.31,-2.01,-0.05,3.37

3VHJ,ASP_125,3.06,-0.55,-0.56,0.38 3CS1,GLU 131,4.86,1.59,-0.77,-0.45 3MTT,GLU_493,4.55,0.2,0,-0.15 3BPP.TYR 44,11.62,0,0,01,1.61 3HKX,ASP_229,4.32,-1.38,0.18,1.71 1T07,TYR 79,12.33,0.85,0.54,0.94 3ASA.GLU 157.4.78.0.24.0.0.04 3LPZ,GLU_142,3.57,1.21,-1.6,-0.55 1WXQ,GLU_240,4.5,0.57,-0.38,-0.19 3V46,TYR_342,11.09,0,0.06,1.02 2R57,CYS 263,9.88,-0.21,0.35,0.75 3JSN.LYS 265.10.17.-0.33.0.0 2IDC,GLU_39,4.84,0.36,0,-0.02 3LJC,GLU_201,5.07,0.29,0,0.28 2B61,ASP_343,2.93,-2.02,0,1.14 2OSA,LYS 316,11,59,-0.55,0.8,0.85 3TOW,HIS_196,6.78,-0.44,0.68,0.04 3K8U,TYR_6,10.25,0,-0.07,0.33 3DHN,GLU_132,4.56,0.06,0,0 4EZB,ARG_289,12.28,-0.28,0,0.06 300P,ASP 61,2,45,-1,67,-0,06,0,39 3B21,GLU_196,3.61,1.26,-1.27,-0.89 1XKR,ASP_55,3.44,-0.74,0,0.38 1U53.LYS 76.10.36.-0.14.0.0 2FZ4.CYS 112.10.51.-0.32.0.54.1.29 1WPA, TYR_467, 10.78, 0, 0.54, 0.23 3GEC,ASP_432,4.28,-0.47,-0.53,1.48 1NWA,ASP_59,2.72,-1.52,-0.03,0.47 1R9W,GLU_338,5.18,0.88,0,-0.2 2F4O,ARG 227,12.46,-0.84,0,0.79 2O4D,CYS_73,9.13,-0.18,-0.17,0.47 3DB9,GLU_204,4.09,0.36,-0.76,-0.01 1DCF.GLU 15.4.64.0.06.0.0.07 2D7JLYS 45.10.3.-0.21.0.0.01 1RSS,GLU_57,4.5,0.14,0,-0.14 2CXA,HIS_128,5.68,-0.82,0,0 2D59,GLU_115,3.92,0.22,-0.26,-0.55 1T3Y,LYS_75,10.01,-0.37,0,-0.11 2AZL,ARG_259,12.39,-0.11,0,0 3RVC,ARG_88,12.42,-0.16,0.07,0 4DBX,GLU_184,3.04,0.52,-1.55,-0.43 3NJM,ASP_91,4.74,0,0.03,0.91 1RWZ,ASP_72,4.43,0,0.2,0.42 1TXJ,ASP_140,3.47,-0.86,-0.06,0.59 1VSM,ASP_82,4.18,-0.72,0,1.1 1BN6,ASP_291,2.94,-0.85,-0.42,0.41 208P,GLU_32,3.92,0.64,-0.85,-0.37 3TMO,ASP_256,3.9,0,0,0.1 1L2F,ARG_104,12.39,-0.11,0,0 2Q13,LYS_172,10.97,-0.16,0.24,0.39 2FBQ,LYS_128,11,-0.17,0.4,0.27 4EVF,LYS 242,10.46,-0.04,0,0 3V4G,CYS_68,10.95,0,0.39,1.57 1RI5,LYS_267,10.34,-0.19,0,0.03 3MTT,GLU_482,4.65,0.15,0,0 1RHS,ARG_229,12.56,-0.37,0,0.43 1X9G,LYS_182,10.21,-0.38,0,0.09 2GZQ,HIS_130,6.58,-2.06,0.97,1.17 1ZBS.CYS 89.10.1.-0.35.-0.02.1.47 1M5I,ARG_213,13.2,-0.48,0.47,0.7 1Q2Y,ASP 140,4.25,0,0.2,0.26 3T8R/LYS 121,11.03,-0.39,0.35,0.58 1WXF,LYS_9,10.43,-0.07,0,0 1H09,HIS_132,6.49,-0.18,0,0.17 1FQI,LYS_398,10.65,-0.09,0,0.25 3LH5,ARG_663,12.64,-0.3,0.01,0.43 2X5Y,HIS_807,4.86,-1.75,0,0.11 3BZT,LYS_287,10.73,-0.25,0,0.49 1SFE,ARG_129,12.34,-0.17,0,0.01

10ZN,LYS 119,10,25,-0,25,0,0 1SJ8,GLU_567,5.29,0.29,0.26,0.24 1YW5,ASP_36,3.98,0,0,0.18 4F8A,ASP_566,3.87,-0.08,-0.22,0.37 2CE6.LYS 77.10.37.-0.29.0.0.15 2JKF,TYR 55,10,54,0,0,28,0,26 1JT9,ARG_33,12.08,-0.43,0,0.01 2BAA, ASP_32, 1.88, -1.92, -0.39, 0.39 1JSX,ASP_194,3.89,0,0.03,0.06 2D7U.ARG 96.10.67.-1.85.0.0.03 3ETV,ASP_68,2.84,-1.06,-0.48,0.58 3NR5.TYR 48.11.39.0.0.41.0.98 3CBN,CYS_58,11.61,0.04,0.83,1.73 2A4D.ASP 114.4.04.0.0.07.0.17 1NAR,LYS 182,10.61,-0.13,0.0.24 1LFP,LYS_72,10.2,-0.36,0,0.06 2IXM,HIS_237,5.64,-0.82,0,-0.03 2DVK,HIS_66,6.13,-0.24,0,-0.14 3M70,ASP 229,3.88,0,-0.04,0.12 1EYH,GLU_42,3.95,0.3,-0.52,-0.34 2CN1,HIS_243,6.04,-0.5,0,0.04 1MTZ,GLU_71,4.17,0.77,-0.84,-0.27 2PLO.ARG 241.13.53.-0.23.0.84.0.43 1WNH.GLU 154,3.92,1.91,-1.63,-0.86 1XKR,ARG_200,12.33,-0.42,0,0.25 4GA2,HIS_63,5.86,-1.36,0.77,-0.06 2YX0,ASP_106,3.82,-0.91,0.19,0.75 3GW3,ASP 197,4.72,0,-0.25,1.17 3ANJ,LYS_194,10.56,-0.07,0,0.14 3F6F,TYR_44,12.16,-0.85,0.35,2.66 1WRU,GLU_184,4.64,0.27,0,-0.13 309PASP 100.3.67,-0.35,-0.06,0.28 1SOH, ARG 245, 12.32, -0.44, 0, 0, 25 2H01,GLU_64,5.59,1.42,0,-0.33 2P5D.LYS 20.10.36,-0.25.0.0.1 3GMS,HIS_9,7.24,-0.42,0.85,0.3 3LJC,GLU 126,4.86,0.16,0,0.19 2XWS,HIS 24,5.53,-0.75,0,-0.22 2DFL,ARG_83,12.12,-0.38,0,0 3HKX,ASP_120,2.66,-1.68,-0.31,0.86 3ANJ,HIS 219,3.14,-3.05,0,-0.31 2C2Y,ASP 72,3.94,-0.01,-0.06,0.22 2IN0,HIS_41,6.14,-0.38,0,0.02 3H04,HIS_59,5.89,-0.4,0,-0.21 3LJC,GLU_194,5.02,0.24,0,0.29 1KCM,LYS 235,10.58,-0.37,0,0.44 1MJS.ASP 407.4.03.0.0.23 4F85,GLU_89,6.72,3.5,-0.84,-0.44 1MD6,GLU_33,4.49,0.31,0,-0.32 3KEY,GLU_450,4.89,1.05,0,-0.66 1NWA, ARG 105, 13, 09, -0, 18, 0, 46, 0, 3 2HRZ,ARG_1,12.46,-0.04,0,0 4ETX,ASP_310,2.77,-0.86,-0.47,0.3 2B2H,TYR_327,10.44,0,0,0.44 4DNU,HIS 26,2.67,-3.19,0.09,-0.72 3EAZ,GLU_100,3.59,0.36,-0.85,-0.43 1SI7,ARG_116,11.87,-0.64,0,0.01 1DTO,ASP 13,4.08,0,0,0.28 2AH5,GLU_186,4.64,0.19,0,-0.05 1R3F,ASP_27,3.59,-0.34,-0.13,0.26 2QDJ,LYS 164,9.93,-0.66,0,0.08 10IS,TYR_240,10.1,-0.31,-0.06,0.48 3M7D,ARG_250,10.89,-2.81,0,1.21 3IVF,GLU 386,4.65,0.15,0,0 3BOW, ASP 183, 2.68, -1.42, -0.11, 0.4 1V6T,ARG_2,12.86,-1.01,0.83,0.54 1NIJ,HIS_170,5.88,-0.69,0,0.07 3EIZ,LYS_164,11.51,-0.26,0.85,0.42 2YLF,TYR_134,11.09,0,0.74,0.34

30KO.GLU 627.4.11.0.57.-0.85.-0.1 20DJ.LYS 136.10.44.-0.64.0.0.58 2GEN, ARG_120, 12.42, -0.1, 0, 0.01 1TXJ,ASP_16,2.78,-1.21,-0.45,0.63 1ZBS.ASP 108.3.91.0.-0.09.0.21 1HF8,LYS 231,10.37,-0.13,0,0 3QAV,GLU_47,4.57,0.07,0,0 2Y2T,LYS_49,10.55,-0.17,0,0.23 1X04, ARG_80, 12.41, -0.23, 0, 0.13 3COU,GLU_70,3.04,1.61,-2.43,-0.65 3TRE,HIS 93.6.37,-0.37,0.06.0.17 2FZP,ARG_265,12.42,-1.1,0.46,0.56 3B4D,HIS_193,7.52,-0.19,0.85,0.37 4FH3.CYS 159.13.05.0.0.45.3.6 10XZ,LYS 174,11.53,-0.28,0.42,0.88 2YWJ,GLU_33,4.12,0.3,-0.7,0.02 2X5Y,LYS_758,11.32,-0.28,0.59,0.51 3ONT,ARG_133,12.51,-0.25,0.25,0 1TJE,ASP_168,4.26,0,0.15,0.3 3GW3.LYS 104.10.4.-0.1.0.0 3GS9,GLU_137,4.99,0.55,0,-0.06 1RAJ,HIS_80,5.14,-1.69,0.7,-0.38 2H2W.ASP 202.3.96.0.-0.03.0.19 3HQX,GLU 56,5.61,1.55,-0.42,-0.02 3M70,ASP_175,3.3,-0.84,-0.11,0.46 2X4J,ASP_120,4.05,0,0.03,0.22 3LOD, ARG_77, 12.91, -0.89, 0.68, 0.62 1Q42,TYR 24,9.83,-0.95,0.07,0.71 3V3T.ARG 167,12.68,-0.93,0.34,0.77 2BT8,CYS_222,10.72,-0.31,0.19,1.84 3GEC,ASP_405,4.07,-0.75,-0.19,1.2 1RI5,HIS_144,5.09,-3.3,0.76,1.13 2B6P.TYR 219.12.04.0.66.-0.03.1.39 3EJC,LYS_47,10.45,-0.05,0,0 2GZR,GLU_230,3.78,0.57,-1.25,-0.04 3P28,CYS_240,10.2,-0.15,5.55E-17,1.35 3DSH,LYS 243,10.35,-0.29,0,0.14 3DHN,ARG_106,13.08,-1.63,1.26,0.94 1AKO,GLU_165,2.78,0.41,-1.51,-0.62 4FZR,ASP_352,2.7,-1.15,-0.36,0.41 4DBX,LYS_70,10.21,-0.28,0,-0.01 1WPA,LYS 506,10.48,-0.57,0,0.55 200K.LYS 111.10.49,-0.19.0.0.19 3JSN,GLU_46,3.85,2.46,-2.39,-0.73 2161,ASP_38,3.23,-0.54,-0.47,0.44 1BKB,ASP_98,2.42,-1.84,-0.18,0.64 2HRZ,GLU_167,4.67,4.09,-2.45,-1.46 2XJ4,ARG_225,12.63,-0.27,0,0.4 3I4T.GLU 104.4.59.0.19.0.-0.1 3C6B,TYR_126,13.19,0,1.16,2.03 3ILC,TYR 173,11.98,-0.69,0.19,2.48 2R51.TYR 183.12.89,-0.8,0.45,3.23 3UPD,HIS_280,6.51,-1.59,0.9,0.69 1ES9,TYR_191,11.08,0,0.52,0.56 2R2Y,CYS_88,9.47,0,-0.06,0.53 1PGV,GLU_301,4.55,0.66,-0.46,-0.16 2Z0W,ARG_23,12.2,-0.3,0,0 1YLN,ASP_80,3.84,-0.43,0,0.46 4DNU,GLU_271,4.43,0.15,0,-0.22 3RJX,HIS 235,3.79,-2.71,0,0 4D8L,TYR 156,11.84,-0.24,-0.13,2.23 1DZF,LYS_161,10.94,-0.85,0.85,0.44 3ONT,ASP_105,3.77,-0.13,0,0.1 3RLE,GLU_187,4.59,0.09,0,0 1RWZ,ASP_134,2.89,-1.63,-0.02,0.75 2ZTY,TYR_122,10.3,0,0,0.3 10TM,GLU_241,4.54,0.11,0,-0.07 2XMZ,GLU_203,4.36,0.45,0,-0.58 3CJW,GLU_189,5.4,3.68,-1.21,-1.56

3HUE,ARG 49,12.05,-0.43,0,-0.02 3BCH.TYR 204.10.42.-0.11.0.31.0.22 2H14,CYS_134,13.75,-0.2,0.96,3.98 1FO9.GLU 354,4.08,0.31,-0.79,0.07 1PSW,ASP_329,3.34,-0.81,-0.06,0.41 3LJN,ARG 34,13.5,-0.27,0.82,0.44 10IS,LYS 320,10.35,-0.18,0,0.04 2FC3,LYS_117,11.33,-0.32,0.72,0.43 1ES9,GLU_150,4.6,0.34,0,-0.24 3LJN,ASP_63,3.99,0,-0.04,0.23 1X04.GLU 94.4.17.0.73.-0.35.-0.72 3RLN,GLU_595,4.51,0.15,0,-0.14 2X5Y,ASP 883,4.08,-0.3,-0.42,1 3MTT.GLU 593,3.48,0.35,-0.85,-0.52 1R3D,GLU 149,3.82,0.31,-0.75,-0.24 1NFN,ASP_154,2.29,-1.3,-0.88,0.67 10LR,TYR_161,11.69,-0.05,-0.05,1.79 1V43,LYS_20,10.11,-0.76,0,0.36 20YZ,ASP_72,3.49,-0.45,-0.21,0.35 2WB8,TYR_747,13.97,-0.78,0.96,3.79 3BA1,ARG_175,12.51,-0.1,0,0.11 3LD1.GLU 222.4.57.0.3.0.-0.24 3F6F,HIS_57,5.89,-0.65,0,0.03 2B78, ASP 43, 3.58, -0.18, -0.3, 0.25 1NRLARG 17,12.38,-0.13,0.0.01 1LPL,TYR_168,10.71,0,0.15,0.56 2IN0,GLU_99,4.7,0.09,0,0.11 1SUU,CYS_552,11.47,-0.69,-0.02,3.17 3HUE,GLU 83,4.48,0.1,0,-0.12 10XZ,GLU_172,4.55,0.15,-0.1,0 3JZ9.GLU 425.2.44.1.25.-2.74.-0.56 3V55,TYR_407,12.94,0.11,0.17,2.66 2R2Y,GLU 119,3.57,0.34,-0.66,-0.61 3F6F,ASP 81,2.65,-1.2,-0.35,0.41 3H5T,TYR_53,10.29,0,0,0.29 1W24,HIS_124,6.32,-0.41,0,0.23 3BPV,ARG_24,12.44,-0.08,0,0.02 2V4U,ASP 496,3.29,-0.8,-0.09,0.38 1DCF,GLU_64,4.8,0.3,0,0 2RGY,ARG_138,12.7,-0.4,0.04,0.56 2QVT,ASP_108,3.63,-0.53,-0.02,0.38 3GW3,ARG 249,12.38,-0.28,0,0.16 1046.TYR 113.10.66.0.0.32.0.33 3IVF,GLU_38,4.2,0.34,-0.64,0 2F9F,GLU_98,5.24,1.96,-0.85,-0.37 2APL,ARG_74,11.88,-0.83,0,0.22 10I7,LYS_42,10.37,-0.14,0,0.01 2PWO,LYS 69,10.22,-0.31,0.0.02 3HVM,LYS_233,10.6,-0.2,0,0.3 1059,LYS_326,10.08,-0.88,0.04,0.41 1HF8,ARG_206,12.27,-0.79,0,0.57 1WPA.LYS 485,10.35,-0.21,0.0.06 1RHS,CYS_254,12.52,-0.01,-0.85,4.39 2A6B,HIS 56,5,21,-1,42,0,0,13 1EYH,GLU_55,4.43,0.48,-0.85,0.3 3ULX,ARG_107,12.74,-0.1,0,0.34 1T3Y.GLU 84.4.94.0.21.0.0.23 3LMF,ARG_47,12.44,-0.15,0,0.09 3G9T,ARG_286,13.67,-0.93,1.09,1.02 1SIG,ASP_160,3.89,0,-0.19,0.28 1RL0.GLU 116.3.25.0.83.-1.27.-0.82 2R0S,ARG_60,12.52,-0.26,0,0.27 1YLN, HIS 106, 5, 51, -0.8, 0, -0.18 2P0L,TYR_82,12.87,0.67,0.68,1.51 3LJC,GLU_210,4.7,0.31,0,-0.1 109G,HIS 183.6.33,-0.31.0.0.15 2VC8,ARG_24,12.23,-0.3,0,0.02 3GMS,ASP_313,3.85,0,-0.18,0.23 2W1R,TYR_67,10.24,0,0.07,0.16

1P6F.HIS 176.6.94,-0.88,0.85,0.47 3EJG,ASP_100,3.24,-0.42,-0.42,0.28 2CXC,GLU_11,3.1,1.35,-1.88,-0.88 1SOW.TYR 46.12.3.0.0.26.2.02 1LTU,LYS_205,10.08,-0.31,0,-0.12 3QYB,LYS 945,10.45,-0.05,0,0 3TRE, ASP_78, 2.82, -1.34, -0.23, 0.59 200K,ASP_116,3.36,-0.73,-0.35,0.63 1ZP2,ASP_105,3.92,0,-0.18,0.3 2QOP,GLU_136,4.81,0.17,0,0.14 1BYI,TYR 68,10.98,-1.3,-0.19,2.46 10IS,LYS_204,10.23,-0.26,0,-0.02 3BOW,LYS 242,10.42,-0.13,0,0.05 2PP6,ARG_66,12.63,-0.11,0,0.23 1MIX.TYR 395,10,47,0,-0.01,0,47 1AKO.GLU 45,4,77,0.09,0,0.18 3PZ9,TYR_340,10.26,0,0.06,0.2 3ILC,TYR_22,11.71,0.85,0.38,0.47 1Z3X,ARG_115,12.68,-0.3,0.01,0.47 1U53,LYS_117,10.32,-0.24,0,0.06 1P6F,ARG 50,12.56,-0.28,0.07,0.27 2PGE,ARG_227,12.09,-0.7,0,0.29 1R53,ARG_285,12.44,-0.06,0,0 1JT9,ASP 98,2.31,-2.22,-0.65,1.37 3I47.CYS 133.10.34.0.-0.22.1.56 3FFM,GLU_136,4.73,0.24,0,-0.01 10LR,ASP_179,4.96,0,0.24,0.92 1160,LYS_194,10.32,-0.52,0,0.35 2NRR,CYS_449,11.85,-0.02,0.19,2.68 2CXA.HIS 9.6.31,-0.18.0,-0.02 1R53,CYS_234,9.17,-0.13,-0.05,0.35 4E8B,GLU_149,4.84,0.51,0,-0.16 3EUR/CYS 43,11,4,-0,22,0,44,2,18 2QV2,ASP 92,3.91,-1,-0.25,1.37 3PBH,HIS_145,4.87,-1.7,0.27,-0.19 1P4X,ASP_59,3.65,-1.04,-0.47,1.36 4D8L,ASP_227,3.3,-0.64,-0.28,0.42 1AK1,ARG_310,12.59,-0.27,0,0.37 3N2T,GLU_252,2.69,0.5,-1.4,-0.91 1NJ4,LYS_64,11.4,-0.24,0.75,0.38 3UV9,TYR_364,12.65,0.85,0.47,1.33 1DVO,LYS_40,10.4,-0.1,0,0 2XJ4,GLU 65,4.27,0.16,-0.4,0 3LH5,TYR_520,9.66,-0.75,-0.22,0.63 3F6F,ARG_35,12.46,-0.07,0,0.03 2H85,HIS_14,6.62,-0.87,0.81,0.18 2WB8,ARG_772,12.23,-0.27,0,0 2FZP,LYS 278,10.85,-1.12,0.85,0.62 1NWA,GLU_55,3.64,1.53,-1.53,-0.86 1KCM,LYS_168,10.55,-0.35,0,0.4 3M16,LYS_269,10.8,-0.53,0,0.84 3LOD,GLU 69,4.57,0.07,0,0 1SNT,TYR_20,9.36,-1.53,-0.02,0.91 3N2T,ASP_235,3.32,-1.15,-0.56,1.23 3JZN,LYS_398,12.15,-0.44,1.7,0.38 2EJX,ASP_77,2.94,-1.22,-0.34,0.71 3CN5,ARG_190,12.29,-0.35,0,0.14 1UOH,ARG_41,12.63,-1.66,0.76,1.03 2VGM.GLU 361.4.89.0.38.0.0.01 1LTU,CYS_52,10.59,-0.48,0,2.07 1ZYL,GLU_151,5.2,2.75,-0.07,-1.98 1YTQ,GLU_24,4.75,0.3,0,-0.05 2X5Y,LYS_727,10.28,-0.44,0.04,0.17 109G,HIS_73,4.17,-2.26,0,-0.08 1SBX,LYS_119,10.56,-0.3,0,0.36 3TOW,LYS_170,11.45,-0.28,0.85,0.38 1X9G,ARG_179,12.28,-0.29,0,0.07 3GEC,HIS_430,5.86,-0.59,0,-0.04 20JQ,GLU_491,3.98,0.74,-0.85,-0.41

2FC3.GLU 13.4.76.0.11.0.0.14 2X4G,ARG_195,12.36,-0.19,0,0.06 3E7P,GLU_151,6.34,4.78,-1.87,-1.07 1S7K,ARG_124,13.97,-1.04,0.78,1.73 2APL.ARG 37.11.91.-0.94.0.0.34 1UOH,HIS 119,5,95,-0,91,0,41,-0.06 1SI7,ARG_147,12.68,-1.25,0.58,0.84 3HYQ,GLU_169,3.77,0.38,-0.91,-0.21 3LE4,TYR_333,10.6,0,0.05,0.56 2BAA.ARG 13.12.24.-0.26.0.0 1R3F,LYS_207,10.16,-0.26,0,-0.08 3IL3, ASP_150, 4.22, -0.93, 0.19, 1.15 3LJC,LYS_146,10.25,-0.19,0,-0.06 2G5X.TYR 99.10.13.0.-0.17.0.31 3S0A, ASP_37, 4.16, -0.1, 0.13, 0.32 2P65,ASP_71,2.49,-1.17,-0.44,0.3 1SQW,ARG_38,12.28,-0.93,0.02,0.69 3KEY,LYS_329,10.41,-0.07,0,-0.02 3UAH.ASP 177.2.97.-0.81.-0.36.0.35 2IF4,GLU_259,4.64,0.25,0,-0.11 2E0T,ARG_206,13.08,-0.26,0.85,0 1TR9,ARG_192,12.49,-0.3,0,0.29 2Z61.LYS 56.10.42.-0.1.0.0.02 2BLL.TYR 423,11.01,0.49,0.0.52 10IS,LYS_227,11.61,-0.24,0.82,0.53 3P2F,GLU_131,5.04,1.31,-0.37,-0.4 1U53,TYR_153,11.87,-0.87,0.32,2.42 3CSR,LYS 156,10.42,-0.14,0,0.07 3CE7,ARG_50,12.29,-0.21,0,0 2RFA,TYR_162,11.31,0,0.36,0.95 3T8R,ARG_108,13,-0.3,0.48,0.33 1FKM,LYS 283,10,44,-0.31,0,0.25 1J33,ASP 297,3,78,-0.21,-0.15,0.33 2Z0M,ARG_104,12.38,-0.12,0,0 10GL,ARG_116,12.36,-0.23,0,0.09 2QHT,ARG_64,12.43,-0.37,0,0.29 1BYI,ARG_32,12.37,-0.25,0,0.12 1NIJ.ARG 120.13.91.-0.48.1.35.0.54 3FS3,TYR_62,10.14,0,0,0.14 1NJ4,ARG_248,12.49,-0.52,0,0.5 3I4T.ASP 66.3.81.0.0.0.01 105Z.LYS 615.10.22.-0.33.0.0.06 1UOH,GLU_201,4.9,0.29,0,0.1 3M16.TYR 126,12.89,-0.85,0.31,3.43 3BPV,ARG_133,12.37,-0.13,0,0 1F2V,TYR_181,10.45,0,-0.06,0.51 2BLL/ARG 404/12.3/-0.67/0.0.49 4DIU,GLU_124,4.61,0.11,0,0 1XAW,LYS_497,10.67,-0.29,0.05,0.4 1YB2,ASP 153,4,11,0,0,08,0,23 2G5X,LYS 39,10,73,-0,13,0,0,36 1EDG,ASP_160,2.31,-1.62,-0.62,0.75 3FTT,ASP_30,4.01,0,0,0.21 2E3C,ARG_257,12.12,-0.65,0,0.27 2WB3,ARG 332,12.63,-0.39,0.54,-0.02 20K1,LYS 444,10.9,-0.32,0.19,0.52 1P2F,TYR_123,11.95,-0.82,0.52,2.24 2CYG,ARG 72,12.2,-0.48,0,0.19 1AKO,LYS_70,10.35,-0.37,0,0.23 2IQT,GLU 285,3.12,0.4,-1.33,-0.45 2PP6,ARG_63,12.41,-0.09,0,0 2AXO,GLU_264,4.6,0.1,0,0 2FPN,GLU_153,4.62,0.15,0,-0.02 1EDG,HIS 85,6.8,-2.11,1.15,1.27 1G8P,ARG 117,12,42,-0,1,0,0,03 3O48,GLU_78,5.71,1.17,0,0.04 2RIK,ASP_252,4.05,-0.07,-0.04,0.37 3EGN,TYR_438,11.83,0.78,0.62,0.43 1NAR,TYR_190,12.34,-0.63,0.5,2.48

1TLV.LYS 110.10.4.-0.1.0.0 4F85,TYR_59,13.88,0,1.2,2.68 1YM5,ASP_273,4.11,0,0.11,0.2 1M5I,GLU_152,5.11,0.64,0,-0.02 1HF8.GLU 255,4.46,0.22,0,-0.27 20BLLYS 164,10.35,-0.31,0,0.16 3K8J,ARG_272,12.4,-0.12,0,0.02 1R5Q,ASP_29,3.72,-0.21,-0.1,0.23 2XMZ,ARG_171,12.59,-0.49,0,0.58 3EYE,ASP_38,3.75,-0.78,0.02,0.72 2A6B,LYS_193,10.5,0,0,0 3EIZ,ASP_160,3.72,-0.35,0.06,0.2 3BCH,HIS_24,5.59,-0.87,0,-0.04 1SUU,LYS 527,10.5,0.0.0 4DIU.ARG 140.12.67.-0.22.0.06.0.33 3K8U,GLU_56,4.36,0.3,0,-0.44 1P4X,ASP_66,3.54,0,-0.56,0.3 3GEC,LYS_532,10.43,-0.12,0,0.05 3B7X,TYR 64,10.3,-0.24,0.13,0.41 1Z3X.TYR 136.10.06.0.-0.17.0.22 1YIB,ARG_241,12.46,-0.08,0,0.04 1VSM,HIS_198,6.28,-0.28,0,0.05 3BCH,TYR_37,11.21,0,0.13,1.08 3M3P,GLU 213,3.49,0.37,-0.93,-0.45 20EW,LYS_48,10.79,-0.15,0.14,0.3 1X04,LYS_127,10.41,-0.33,0,0.23 3H5T,LYS_18,10.47,-0.31,0,0.28 1RZ2,ARG 116,12.27,-0.36,0,0.12 1BN6.HIS 65.6.82.-0.8.0.85.0.27 1PBV,ASP_137,4,0,0,0.2 1ZP2,ASP_44,4.77,0,0,0.98 1V6TLYS 201,10.82,-0.17,0.0.5 1WXF,TYR 85,10.08,0,-0.38,0.46 3MTT,LYS_447,10.34,-0.15,0,-0.01 3C6B,LYS_178,9.8,-0.72,0,0.03 1PGV,ASP_343,3.7,-0.82,-0.46,1.18 3GG6,ARG 39,13.03,-0.23,0.38,0.39 2HP7,GLU_117,6.47,3.13,-0.91,-0.26 2P52,HIS_107,6.56,-0.8,0.7,0.15 4H89,HIS_154,6.18,-0.32,0,0 3CE7,LYS_43,10.51,-0.31,0,0.31 1LFP,TYR_181,11.91,0,-1.73E-18,1.91 1EDG,TYR 293,10.53,-0.03,-0.02,0.59 1RL0,ARG_53,13.08,-1.26,1.3,0.55 3EVN,HIS_258,5.97,-0.47,0,-0.06 1EO6.LYS 180.10.51,-0.04,0.0.05 1W24,GLU_123,4.96,0.46,0,0.01 2E0T,GLU_107,4.58,0.08,0,0 2BQQ,ASP_108,2.56,-1.55,-0.02,0.33 3F1X,ASP_141,3.87,-0.39,-0.3,0.76 2CL3,TYR 226,10.87,0,-0.11,0.98 2F4O,ARG 41,11.95,-0.65,0.0.09 3GS3,ASP_199,3.25,-0.51,-0.22,0.18 2X4G,ASP_306,3.71,-0.59,-0.44,0.94 1KCM,LYS_153,10.13,-0.19,0,-0.17 1RKA,GLU_267,2.94,1.12,-1.69,-0.99 3LJN,CYS_271,11.04,-0.84,-0.03,2.91 3GS3,CYS_127,12.64,-0.06,0.17,3.53 1XKR,LYS_132,10.55,-0.07,0,0.12 1RSS,ARG_76,11.86,-0.46,0,-0.18 2FG1.LYS 19.9.78.-0.63.0.-0.1 3BB7,HIS_49,6.44,-0.11,0,0.05 3H13,TYR_305,11.19,0,0.64,0.56 2CVB,LYS_65,10.35,-0.17,0,0.02 1GQE,ASP_231,3.74,-0.23,-0.01,0.19 2IDC,GLU_142,3.96,0.4,-0.82,-0.13 1MTZ,ASP_146,2.85,-0.85,-0.5,0.4 2Q99,LYS_27,10.4,-0.1,0,0 3G9G,ASP_243,3.06,-0.81,-0.36,0.43

1TWU,HIS_76,6.5,-0.27,0,0.26 2EJB.GLU 136.4.65.0.17.0.-0.02 208P,LYS_201,10.63,-0.14,0,0.27 3RRQ,ARG_139,12.17,-0.38,0,0.05 2HXB,ARG 16,13.2,-0.42,0.41,0.71 1MML,LYS 264,10.23,-0.35,0,0.08 1WYC,ARG_229,12.98,-0.71,0.78,0.41 3CGW,TYR_137,10.09,-0.12,-0.11,0.32 3RAZ,CYS_133,9.55,-0.12,0.31,0.37 2EFK,CYS_145,9.53,0,-0.01,0.55 2R51.GLU 62.4.27.0.34.-0.25.-0.33 3U4K,ASP_76,3.67,-0.04,-0.5,0.41 4EZB,ARG 232,12,42,-0,1,0,0,03 2ATR.LYS 11,11.07,-0.15,0.11,0.61 3I47,CYS 121,12.58,-0.2,0.27,3.5 1JKS,ASP_11,3.99,0,-0.1,0.28 3A0X,GLU_605,4.59,0.15,-0.01,-0.04 1I60,LYS_61,9.82,-0.8,0,0.12 30A7,ASP 45,4.01,0,-0.05,0.26 1ZBM.GLU 208,3,79,0,46,-0,85,-0,32 3VJ8,ARG_133,11.65,-0.94,0,0.09 2OJQ,ASP_560,4.14,0,-0.48,0.82 4D8L,ASP_133,3.88,0,-0.1,0.18 2GS5,GLU 11,4.56,0.08,0,-0.02 3GT0.LYS 72,10.46,-0.11,0.0.07 1TR9,HIS_173,7.55,-0.34,0.85,0.54 1M5I,GLU_202,4.71,0.21,0,0 1HF8,ARG_243,13.52,-0.89,0.95,0.96 3CAN,CYS 31,9.44,-0.01,-0.08,0.53 1PNE,TYR_24,11.16,0,-0.06,1.21 3CIV.GLU 186.4.33.4.29.-3.56.-0.9 3JZN,LYS_344,10.4,-0.16,0,0.06 1AT0,ASP 347,3.99,-0.08,-0.2,0.47 3GT0,GLU_217,4.28,0.22,-0.13,-0.31 100X,LYS_200,10.8,-0.21,0.14,0.36 3CCY,ARG_121,12.67,-0.36,0,0.53 3DTE,ASP_55,3.96,0,-0.16,0.33 3I4T,HIS 139,6.4,-0.1,0,0 1NWA, ARG_162, 12.3, -0.22, 0, 0.02 1JSX,ARG_101,12.97,-0.51,0.53,0.46 4ETX,ARG_360,12.84,-0.15,0,0.48 2QVT,LYS 143,9.93,-0.46,0,-0.12 3I47.LYS 238.11.04.-0.85.0.85.0.55 1NAR,GLU_207,4.79,0.22,0,0.07 2QEV,ASP_49,2.91,-0.92,-0.64,0.67 2BCF,TYR_111,10.24,-1.11,-0.3,1.65 2ZCX,ASP_166,4.24,0,0.08,0.35 3LJI.ARG 199,12.34,-0.26,0.0.1 1TP6,HIS_121,5.68,-0.68,0,-0.14 1I60,HIS_230,3.76,-2.81,0,0.06 3IDW,GLU_29,3.61,0.26,-0.84,-0.3 3F5D,LYS 108,10,49,-0,22,0,0,21 3RE9,GLU_107,2.46,0.75,-1.93,-0.87 3M66,ASP_239,3.29,-1.15,-0.13,0.76 2BLL,ARG_535,8.9,-2.13,0,-1.47 1AIL,ARG_44,12.39,-0.24,0,0.13 1V8E,ARG 122,12.01,-0.64,0.0.14 2XMZ,TYR_215,10.5,0,0.23,0.27 4EKU,HIS_103,5.83,-1.86,0.85,0.35 3MIX,GLU_623,4.67,0.17,0,0 20EW.GLU 34.5.24.0.41.0.0.34 3PBH,ASP_254,3.99,0,-0.01,0.19 3L3P.GLU 484.4.6.0.1.0.0 2V81,ASP_167,4.26,0,0.16,0.3 4EZB,TYR_221,9.79,-0.03,-0.53,0.34 3E7P.CYS 255.12.76.0.0.3.76 1U7U,TYR_323,13.57,0,0.29,3.27 1T95,LYS_84,10.64,-0.24,0,0.38 2Q13,TYR_262,10.53,-0.05,0.29,0.29

20KT,TYR_121,11.05,-0.56,0.14,1.48 3HUE.CYS 66.11.53.0.-0.09.2.62 1JT9,ASP_95,3.88,0,-0.47,0.55 2DG7,ARG_14,12.75,-0.22,0.01,0.46 2Z84,CYS_23,9.76,-0.16,0.2,0.71 1059,ARG 75,12.47,-0.11,0,0.08 1UOH,LYS 149,10.16,-0.19,0,-0.15 2D2S,ASP_568,3.99,0,0,0.19 3PU6,GLU_11,3.94,0.73,-0.86,-0.43 1QZN,ASP_100,4.08,0,0.09,0.2 3P28,LYS 108,10.42,-0.08,0,0 3H9W,HIS_107,6.5,-0.36,0,0.37 1PSW,TYR_214,11.41,0,0.53,0.88 3U0V,LYS_153,11.47,-0.39,0.85,0.51 2PGX.LYS 238,10,49,-0.05,0,0.03 1ZBM.GLU 51,4.26,1.58,-1.24,-0.58 3BQE,GLU_358,4.03,0.24,-0.41,-0.31 2HXB,LYS_62,11.36,-0.43,0.65,0.64 1WYC, ASP_323, 3.89, 0, -0.15, 0.23 1RI6,ARG 280,8.45,-1.89,0,-2.16 3GE9.HIS 96.4.76.-1.47.0.3.-0.56 1G8P,GLU_71,4.7,0.35,0,-0.15 2CXC,ARG_97,12.4,-0.1,0,0 1T95,ASP 202,2.54,-1.37,-0.25,0.35 1LZL,ASP 73,3.88,-0.38,0.02,0.43 2YX0,GLU_336,4.65,0.15,0,0 2X5Y,LYS 836,10.63,-0.17,0,0.31 3JZN,CYS_84,10.68,-0.29,0.19,1.78 3M66,LYS 327,11.23,-0.32,0.62,0.43 20DJ.LYS 94,11,43,-0.38,0.85,0.46 2AD1,HIS_113,5.7,-0.87,0,0.07 3RVC,ARG_118,12.79,-0.54,0.07,0.76 4FCU.GLU 152.3.06.0.46,-1.41,-0.49 10GL.GLU 237.4.86.0.16.-0.06.0.26 3EIZ,LYS_136,11.45,-0.36,0.85,0.47 10ZN,TYR 95,11,57,-0.89,0.56,1.9 1T3Y,GLU_121,4.89,0.33,0,0.07 3H6Q,ASP_62,4.02,0,-0.05,0.27 2WB3.GLU 289.4.6.0.1.0.0 3EVN,LYS_138,10.21,-0.36,0,0.07 3GMS,HIS_300,5.59,-0.56,0,-0.35 1GPP,CYS_1,10.93,-0.06,-0.16,2.14 3VJ8,LYS 92,10.56,-0.37,0.11,0.32 3OBS,TYR_63,9.4,-0.75,-0.16,0.32 4F85,ASP_190,4.45,0.1,0.21,0.35 2WB3,LYS_327,10.3,-0.3,0,0.09 3UV9,HIS_312,6.35,-0.1,0,-0.05 1WRU,ARG 24,13.07,-2.67,0.4,2.84 3Q1C,TYR_151,10.07,0,0,0.07 2P52,ARG_172,12.79,-1.6,0.96,0.93 3RNV,ASP_420,3.74,-0.48,-0.07,0.49 3GS9,TYR 62,11.36,-0.3,0.7,0.95 3H9W,ASP_96,1.86,-1.68,-0.89,0.64 2B0J,ARG_192,13.74,-1.01,1.67,0.57 1NRI,CYS_225,9.47,-0.12,0.06,0.53 3EVP,LYS_199,10.41,-0.23,0,0.14 2G2D,GLU_41,3.1,0.32,-1.34,-0.38 2R51,TYR_128,13.26,-0.81,0.36,3.7 10XZ,ASP 269,3,15,-0,32,-0,59,0,26 2GEN,GLU_80,3.79,0.33,-0.83,-0.21 2PLQ,LYS 37,10.41,-0.26,0,0.16 3Q2C,GLU_31,4.59,0.09,0,0 2FD5,LYS_65,10.7,-0.19,0,0.39 1ES5,LYS_177,10.3,-0.2,0,0 3FNI,ASP_37,2.18,-1.99,-0.41,0.78 3TMO.GLU 297,3.99,1.19,-1.31,-0.39 1MTZ,LYS_92,10.39,-0.4,0,0.3 3H6Q,TYR_27,10.87,0,-0.03,0.9 4FZR,CYS_54,10.34,0,-0.09,1.44

4GA2.LYS 25.10.24.-0.26.0.0 2VAN,ARG_283,11.77,-1.13,0,0.4 1SJ8,ASP_514,3.08,-0.47,-0.46,0.22 1EV8,ASP_20,3.34,-0.88,-0.11,0.53 1UCH.LYS 108.9.91.-0.71.0.0.13 1XKR.TYR 121.12.69.0.0.2.69 1DOV,ASP_242,2.79,-0.92,-0.91,0.82 3DHN,GLU_213,3.68,0.66,-0.95,-0.52 3KEY,LYS_391,11.35,-0.24,0.71,0.38 1XAW.ASP 461.3.91.-0.22.-0.15.0.49 1UJ8,ASP_32,3.96,0,0,0.16 3K8J,ARG_89,12.47,-0.05,0,0.02 1X04,LYS_77,10.25,-0.23,0,-0.02 1Q8B,GLU_70,4.68,0.23,0,-0.05 2O34,TYR 175,11,47,-0.05,0.44,1.08 1QQE,TYR_201,10.96,-0.61,0.18,1.4 3BQE,LYS_253,10.18,-0.68,0,0.36 3IVF,ASP_222,4.84,0,0.09,0.94 1TR9.TYR 178.12.19.0.85.0.59.0.75 3PM2,LYS_71,10.09,-0.2,0,-0.2 1TR9,ARG_148,12.12,-0.47,0,0.09 3P28,GLU_67,3.78,0.39,-0.47,-0.65 1HUF.ARG 104.12.54.-0.39.0.05.0.38 3ETU.GLU 190.4.78.0.14.0.0.14 2B02,CYS_459,12.08,-0.45,0,3.53 2YWX,LYS_48,11.3,-0.43,0.85,0.38 3HVW,ARG_305,12.5,-0.19,0,0.18 3BWT,GLU 825,4.78,0.28,0,0 3AU3,ASP_556,2.69,-1.54,-0.03,0.47 2YWJ,LYS_100,10.52,-0.16,0,0.17 2B3M,LYS_25,10.22,-0.22,0,-0.06 2IDC.GLU 32.4.73.0.24.0.-0.01 1XKR,ARG 111,12,23,-0.32,0,0.05 2E3I,GLU_112,3.54,0.2,-0.78,-0.38 1HUF,ASP_72,2.07,-2.93,-0.68,1.87 4EVF,GLU_20,4.37,1.55,-1.25,-0.43 3L7N,LYS 152,9.97,-0.57,0,0.04 2H14.TYR 243.11.21.0.0.05.1.16 1YW5,ASP_97,3.83,-0.01,-0.17,0.22 1R5Q,TYR_25,11.98,0.85,0.42,0.71 30KO,ASP 640,4.05,0.0,0.25 20ZO,LYS 150,10,36,-0,13,0,-0,01 1DOV,ARG_126,12.23,-0.23,0,-0.04 3I4T.ARG 141.12.73.-0.2.0.0.43 2BV9,HIS_170,3.5,-3.09,0.09,0 2V81,GLU 113,3.91,0.39,-0.98,0 3M16.GLU 241.4.77.1.18.-0.62.-0.29 3M70,CYS_93,11.66,0,0.17,2.48 2YYO,HIS_160,5.76,-0.69,0,-0.05 3RLN.GLU 692.4.59.0.27.0.-0.19 3GOZ.GLU 70,3.86,0.37,-0.76,-0.24 2G9D,HIS_210,5.72,-1.03,0,0.25 3M7G,GLU_165,3.72,0.63,-0.95,-0.46 2F9F,GLU_3,4.5,0.12,0,-0.13 4E6S,ARG 29,12.39,-0.37,0.05,0.21 10LR,ARG_213,12.33,-0.69,0,0.52 4DBX,LYS_269,10.22,-0.27,0,-0.02 1GQE,ARG 213,13.1,-0.35,0.49,0.45 2HRZ,ASP_246,3.25,-0.71,-0.19,0.35 1DOV,LYS 216,10.35,-0.15,0,0 4DNU,ARG_173,12.52,-0.18,0,0.21 2X4G,TYR_122,13.11,0,0.43,2.68 1YW5,LYS_116,10.2,-0.3,0,0 2W0G,ASP 177,3.06,-0.65,-0.4,0.31 3CGW,ARG 264,13,78,-0.42,0.8,0.9 1IAP,ARG_181,12.48,-0.02,0,0 2NSN,HIS_33,6.64,-0.26,0.46,-0.07 3FHF,LYS_204,11.32,-0.41,0.85,0.38 10I7,HIS_224,6.25,-0.37,0,0.12

2J8A.GLU 352.4.61.0.25.0.-0.13 3GMS,TYR_54,10.51,0,-0.28,0.8 2J8A,LYS_332,10.43,-0.4,0,0.33 3KB5,ARG_309,12.47,-0.17,0,0.14 1XTD,LYS 61,10.47,-0.03,0,0 3ASA,ARG 27,11.82,-0.72,0.0.03 1G5Z,LYS_60,10.54,-0.14,0,0.18 2H2Z,LYS 61,10,72,-0.52,0.09,0.65 1KCM,ASP_146,2.57,-1.71,-0.09,0.57 1RI5.LYS 248.11.36.-0.46.0.69.0.62 3US6.ARG 135.12.45.-0.29.0.0.23 2BV9,HIS_286,6.13,-0.4,0,0.03 3CN5,ASP_240,4.06,0,0.01,0.25 4AM1.TYR 304.10.54.0.0.09.0.44 1YTD.LYS 366.10.43.-0.08.0.0.01 3CAN,ASP_52,3.25,-0.52,-0.63,0.6 2IDC,LYS_41,10.65,-0.4,0,0.56 2PLQ,LYS_113,10.7,-0.14,0,0.34 1SQH,GLU_111,4.39,0.72,-0.44,-0.39 1QZN,ASP_12,3.2,-1.13,-0.32,0.86 1ZCE,GLU_78,4.92,0.22,0,0.2 3DHN,LYS_90,10.5,0,0,0 1QQH,TYR_165,10.05,0,0,0.05 1SUU.LYS 659,10.5,0,0,0 3RRQ,TYR_68,9.85,-0.83,-0.2,0.88 1SIG,ASP_332,3.9,0,-0.13,0.22 1HUF,HIS_9,6.38,-1.04,0.85,0.06 1X8F,GLU 76,4.11,0.34,-0.34,-0.38 1SOH, LYS 194, 10, 43, -0, 34, 0, 0, 27 2I88,LYS_366,10.36,-0.21,0,0.07 3MIX,LYS_491,10.28,-0.21,0,0 4FZN,LYS 77,10,19,-0.84,0.08,0.44 1U53,ASP 87,3.89,0,-0.2,0.29 1TXD,CYS_967,13.01,0,0.02,3.98 3HVW,ASP_313,3.19,-0.74,-0.34,0.46 3LD1,CYS_234,10.42,-0.14,-0.01,1.57 1VJG,LYS 40,10.37,-0.2,0,0.06 1059,ARG_161,12.95,-0.28,0.23,0.5 2B78,HIS_265,5.01,-1.54,0,0.06 1ZP2,ARG_62,11.43,-1.31,0,0.25 2QDJ,TYR_225,10.63,0,0,0.63 2H01,ARG 142,12.44,-0.06,0,0 2HNG.GLU 10.3.77.0.29,-0.76,-0.26 3HUE,CYS_291,9.83,0,0,0.83 2X4L,ASP_233,3.97,0,0,0.17 3CE7,GLU_46,4.74,0.26,0,-0.01 3CIV,GLU_106,4.75,0.26,0,-0.02 3B79,TYR_114,12.23,0,0.14,2.09 2V4U.CYS 313.9.47.-0.26.-0.09.0.83 3CXS,LYS_147,10.38,-0.36,0,0.24 1GVP,GLU 5,3.67,0.42,-0.77,-0.48 2D7J.LYS 92,10.65,-0.12,0.0.28 3IV4,GLU_16,4.69,0.13,0,0.05 2P65,ARG_41,12.43,-0.07,0,0 2BCF,ARG_59,12.54,-0.37,0,0.41 1X6J,ARG_18,12.45,-0.16,0,0.1 2JEO,ARG_165,11.43,-1.9,0,0.84 1TXJ,ARG_41,13.51,-0.45,0.66,0.8 4FZR,ARG_191,12.24,-0.34,0,0.08 3ERF,ARG_50,12.25,-0.31,0,0.07 2Z14.TYR 38.10.38.0.0.07.0.3 1R29,ASP_75,3.39,-0.85,0,0.44 3PP8,ARG_167,12.12,-0.38,0,0 2P52,ARG_287,12.56,-0.19,0,0.24 108B,TYR 15,10.28,0,0.05,0.23 3DB9,CYS_158,10.14,-0.86,-0.09,2.1 2EDM,CYS_172,10.34,0,0.19,1.15 2XHC,LYS_351,10.24,-0.4,0,0.14 1H09,LYS_308,10.15,-0.62,0.06,0.22

2H85,LYS_12,10.52,-0.12,0,0.15 1YR6.LYS 225,10.59,-0.19,0.0.28 300P,GLU_114,4.69,0.18,0,0.01 2YLF.HIS 159.6.42.-0.9.0.8.0.02 2D7U.GLU 153.4.72.0.22.0.0 3DZ1,ARG_209,13.61,-0.43,1.11,0.42 2O4D,GLU_145,4.55,0.05,0,0 2Y2T,ASP_85,2.58,-1.74,-0.02,0.54 1MD6,LYS_73,10.47,-0.03,0,0 3G9G,LYS 69,10.66,-0.11,0.0.27 1TD6.ARG 26.12.34.-0.28.0.0.12 2C2Y,TYR_49,10.23,0,0,0.23 3U0V,HIS 132,4,26,-3,13,0,33,0,58 3ETU,HIS 328,5,58,-1,82,0,89,0,02 1GQE,LYS 162,10.46,-0.15,0,0.11 1BYI,HIS_83,6.18,-0.52,0,0.2 1SIG,LYS_343,9.87,-0.3,0,-0.32 2BLL,GLU_411,5.15,0.37,0,0.28 3MEW,ASP 266,3,33,-0,93,0,01,0,45 2PIM.GLU 77,4.01.0.22,-0.8.0.09 4GA2,CYS_141,9.43,-0.17,0.15,0.45 3F6M,ASP_128,4.11,0,-0.05,0.37 2VAN,LYS_331,11.65,-0.36,0.85,0.67 2RGY,LYS 340,10.41,-0.09,0,0 2X5Y,TYR 889,12,77,0.85,0.35,1.59 1GPP,GLU_144,4.83,0.23,0,0.1 1R7J,LYS_42,10.75,-0.14,0,0.38 1ZBP,GLU_201,4.84,0.13,0,0.21 2B02,LYS 417,10.4,-0.18,0,0.07 1V43,LYS_9,10.68,-0.21,0,0.4 4EVF,ASP_19,3.79,-0.56,-0.01,0.56 3S0A, ASP_87, 2.14, -1.67, -0.38, 0.4 2X4J,HIS 31,6.7,-0.52,0.8,-0.09 1WXF,TYR 237,13.32,0.61,0.54,2.17 3HVW,ARG_323,13.11,-0.66,0.78,0.48 2PWQ,LYS_145,10.41,-0.21,0,0.12 2EJB,GLU_65,4.61,0.2,0,-0.09 2RH3,LYS 110,10.28,-0.24,0,0.01 3F1X,LYS_234,10.47,-0.03,0,0 3P51,GLU_87,2.96,0.56,-2.1,0 1AM2,ARG_17,13.65,-0.32,0.92,0.55 3NBI,HIS 158,6.19,-0.41,0,0.1 2098,LYS 42,10,47,-0,23,0,0,2 1NAR,TYR_216,13.12,-0.85,0.47,3.51 3CXS,ASP_4,2.6,-1.59,-0.06,0.44 1X7F,GLU_267,4.53,1.09,-0.53,-0.52 2OB5,ARG 18,12.41,-0.09,0,0 1PGV,ARG_380,12.4,-0.39,0,0.29 2A6B,ASP_217,3.3,-0.85,-0.51,0.86 3DHN,HIS_211,7.36,-0.37,0.85,0.38 109G,GLU_136,4.08,0.37,-0.25,-0.55 1RI6.TYR 304,11.93,-1.15,0.56,2.51 2NRR,ARG_489,13.2,-0.3,0.51,0.48 3UX2,CYS_155,9.52,0,-0.13,0.66 3A7L,GLU_46,4.62,0.1,0,0.03 3JZ9,GLU 528,4.61,0.11,0,0 3JV1.GLU 63.3.89.0.53.-1.07.-0.06 1AD6,GLU_559,4.33,0.33,0,-0.5 1JKS,GLU_94,4.28,1.72,-1.37,-0.58 208I,GLU_5,4.66,0.11,0,0.05 1XAW.TYR 493,9.75,-0.05,-0.84,0.65 2IRM,TYR_177,11.98,0.15,0.55,1.27 2JKF,CYS 37,11.33,0,-0,16,2,48 1ANU,TYR_110,10.37,0,0.16,0.21 2H2Z,GLU_290,5.84,2.35,-0.53,-0.49 3M70,TYR 137,12,27,0,0,59,1.68 1PDB,GLU_154,4.7,0.1,0,0.1 1JT9,HIS_19,5.11,-2.14,0.85,-0.1 3B21,ASP_178,2.91,-1.1,0,0.21

4E8B,GLU_225,3.22,0.38,-1.15,-0.52 3016,GLU_111,4.9,0.16,0,0.24 2Z0M,GLU_89,4.22,1.39,-0.75,-0.92 3FTT.GLU 5.3.56.0.18.-0.69.-0.42 1Q46,ARG_87,12.18,-0.35,0,0.02 3AUF,ASP 82,2.26,-2.17,-0.66,1.29 2H14.GLU 279.2.94.2.1.-3.24.-0.42 2P1W,LYS_46,10,-0.41,0,-0.1 2H30,GLU_162,4.54,0.44,-0.03,-0.38 1NAF,ASP_274,3.63,-0.33,0,0.16 3AUF,ARG 65,11.96,-0.15,0,-0.39 1JYH,TYR_111,10.47,0,0.23,0.24 2EFK,ARG_223,12.56,-1.3,0.7,0.67 1RWZ,LYS_107,10.39,-0.18,0,0.06 1XTZ.LYS 195,10.03,-0.47,0.0 3ON1,ASP 88,3.21,-0.94,-0.04,0.39 1ZBP,GLU_157,1.37,3.97,-2.68,-4.41 3EVN,LYS_310,10.19,-0.63,0,0.32 1SUU,GLU_575,4.6,0.91,-0.8,0 1U3Y,ARG 255,12.74,-0.32,0.01,0.55 1EV8,ASP 122,4,15,0,0.08,0,27 1L2F,GLU_211,5.27,1.3,-0.37,-0.16 3ON1,GLU_23,3.97,0.51,-0.78,-0.25 2WOZ,LYS 472,10,19,-0,3,0,0 3CRM,HIS 299,5,16,-0,96,0,-0.38 3UPD,LYS_208,10.44,-0.06,0,0 1EV8,GLU_74,4.71,0.24,0,-0.03 2NSN,GLU_110,4.53,0.03,0,0 1CBY,GLU_152,4.89,0.34,0,0.05 2AZP.ARG 314,13.17,-0.22,0.45,0.45 3JZN,ASP_338,3.17,-0.79,-0.26,0.43 3UC9,LYS_62,10.67,-0.1,0,0.26 1MHN.GLU 104.5.5.0.67.0.0.33 4EZB,ASP_37,3.29,-0.8,-0.01,0.3 1OXZ,ASP_204,3.79,-0.05,-0.29,0.33 1ZBP,GLU_98,4.59,0.09,0,0 1FQI,TYR_410,11.58,0,0.11,1.47 3PZ9,HIS_48,3.35,-3.44,0.35,-0.06 3M9A.GLU 34.4.56.0.06.0.0 3LOD,LYS_92,10.18,-0.32,0,0 1T07,ASP_62,3.45,-0.8,-0.08,0.53 2OBI,ASP_7,3.94,0,-0.02,0.16 2B61,ASP_76,3.01,-1.6,-0.31,1.11 1SFE,ARG_148,13.57,-1.68,1.53,1.23 2BQQ,ARG_59,13.03,-1.05,0.82,0.77 2BDV,GLU_143,3.15,0.29,-1.4,-0.23 1WPA,LYS_512,11.33,-0.29,0.85,0.28 3HKX,HIS 122,6.85,-0.25,0,0.59 2AH5,HIS_23,5.78,-0.68,0,-0.03 1ZYL,GLU_253,4.12,0.44,-0.84,0.02 2HXB,ASP_44,3.52,-0.35,-0.23,0.3 3LJC,GLU 41,4.54,0.18,0,-0.14 2V4U,GLU_423,5.65,1.11,0,0.04 2B3M,ARG_98,11.97,-1.09,0.02,0.54 2EA9,TYR_86,10.3,0,0.06,0.24 1YB2,GLU_198,4.9,0.25,0,0.14 1L2F,ARG_153,12.76,-0.34,0.16,0.44 3LPZ,TYR_139,11.16,0,-0.12,1.28 2PGE,ASP 13,2.97,-1.87,-0.51,1.54 200K,LYS_63,10.21,-0.39,0,0.09 3GW3,ARG 238,12.34,-0.25,0,0.08 2D0A.LYS 300,10,44,-0.06,0,0 20KT,HIS_263,7.02,-0.42,0.66,0.28 3CS1,LYS_56,10.27,-0.31,0,0.07 2CWC,HIS_159,3.28,-2.49,0,-0.73 3CIV,GLU_295,3.96,0.35,-0.9,0.02 3M66,LYS_295,10.56,-0.23,0,0.29 2J8A,LYS_269,9.95,-0.29,0,-0.25 2WB8,GLU_728,4.6,1.05,-0.7,-0.26

1SOH.GLU 196.4.45.1.61.-0.76.-0.9 2NMU,ASP_91,3.19,-1.22,0,0.61 3G9G,TYR_118,12.16,0,0.03,2.13 3ERF,ARG_215,12.11,-0.74,0.03,0.32 3EUR.LYS 81.10.54.-0.11.0.0.16 4DIU.GLU 193,4.12,0.93,-1.44,0.13 10I7,TYR_30,11.24,-0.82,0.14,1.93 2BAA, ARG_130, 12.19, -0.31, 0, 0 2DG7,ASP_50,3.17,-1.34,-0.51,1.22 2013.ARG 339.12.76.-0.28.0.1.0.44 3UPD,TYR_107,13.49,0.16,0.75,2.58 3V55.GLU 653.3.81.0.32.-0.86.-0.16 2G5X,ASP_105,3.2,-0.46,-0.45,0.31 3GW3.CYS 59.13.49.-0.09.1.31.3.28 10IS.GLU 312.2.42.0.74,-2.23,-0.6 2PWQ,GLU_33,5.15,0.93,0,-0.27 1X7F,CYS_197,11.68,-0.08,-0.33,3.09 3TIR,ASP_179,3.74,-0.06,-0.27,0.28 3JRT,ASP_112,2.49,-1.46,-0.29,0.44 3ANJ,HIS_114,6.67,-1.27,0.83,0.6 1XWM,LYS_15,10.75,-0.54,0.44,0.34 2YX0,LYS_341,10.36,-0.16,0,0.03 1JT9.GLU 197.4.22.0.66.-0.11.-0.83 1X91,LYS 130,10,29,-0,19,0,-0,03 2PWQ,CYS_87,9.65,-0.21,0.39,0.46 1WNH,GLU_73,3.54,0.71,-0.85,-0.82 2C2Y,ASP_27,3.21,-0.85,0,0.26 3RE9,LYS 134,10.35,-0.45,0,0.29 2P5D,TYR_6,11.16,0,0.46,0.7 1FQI,ARG_318,12.26,-0.3,0,0.06 3RJZ,LYS_205,10.72,-0.16,0,0.38 1XFK.HIS 27.5.29,-0.96.0.5,-0.75 10IS.GLU 216.3.96.0.6.-0.66.-0.48 1WPA, ASP_451, 3.3, -0.73, -0.2, 0.43 1DTO,HIS_130,6.56,-0.3,0.07,0.3 1EV8,ASP_253,3.34,-0.29,-0.5,0.32 20EW,ARG_322,12.66,-0.18,0,0.33 3DHN,HIS 222,5.84,-0.47,0,-0.2 2CWC,LYS_33,10.07,-0.7,0,0.27 3RLN,ARG_638,13.99,-0.32,1.07,0.74 1W24,ASP 107,3.67,0,-0.35,0.21 2DFL/HIS 215.6.49,-1.23.0.97.0.25 2QOP,LYS_53,10.69,-0.08,0,0.27 2YYO,HIS 21,6.63,-0.25,0.34,0.04 2BLL,ARG_424,12.35,-0.18,0,0.03 1C44,GLU 23,3.99,0.66,-0.85,-0.32 2WB8.GLU 466.4.21.1.33.-0.7.-0.92 2QHT,GLU_15,4.8,0.3,0,0 1PGV,LYS_265,10.61,-0.38,0.14,0.35 3C0C,GLU 329,4,77,0,17,0,0,1 1SJY,ASP 26,3.27,-0.94,-0.45,0.86 1W24,GLU_44,4.75,0.27,0,-0.02 2H30,GLU_74,4.01,1.91,-1.67,-0.73 2D2S,ARG_636,10.8,-1.98,0,0.28 3EZ7,LYS 67,10.52,-0.13,0,0.15 2P5D,LYS 122,10,43,-0.07,0.0 2V4X,TYR_66,10.97,-0.19,-0.35,1.51 4FD6,TYR_85,10.58,0,0.24,0.35 4E8B,GLU_75,4.75,2.35,-1.29,-0.81 3EZ7,ARG 134,11.11,-2.05,0,0.66 1AKO,LYS_121,11.18,-0.28,0.55,0.41 3OKQ,LYS_628,10.26,-0.13,0,-0.11 1Q46,LYS_169,10.44,-0.39,0,0.33 3EVP,LYS_184,10.6,-0.09,0,0.19 2G3A,TYR_110,11.71,0,0.09,1.62 2VGY,CYS_63,11.6,-0.05,0.15,2.49 1SQW,TYR_109,10.1,0,-0.01,0.11 2GQV,ARG_76,12.6,-0.15,0,0.24 3V55,ASP_595,4.09,0,0.14,0.16

2V81.GLU 46.4.17.0.54.-0.86.0 30AV,LYS 41,10,58,-0.09,0,0,17 2QOP,GLU_150,4.55,0.27,0,-0.21 1SBX,GLU_108,4.77,0.27,0,0 1V43,HIS 328,6.54,-0.95,0.85,0.14 3PM2,ASP 158,3.88,0,-0.04,0.12 3CRM,HIS_62,5,-2.13,0.7,-0.05 1IDK,LYS_122,10.81,-0.22,0,0.53 4DBX,HIS_50,6.16,-0.99,0.88,-0.23 4EUG,HIS_181,5.23,-1.22,0,-0.05 4EZB.TYR 31.11.02.0.0.29.0.73 1XEU,LYS_236,10.22,-0.3,0,0.02 3LPZ,TYR_168,12.53,-0.09,0.83,1.8 3K9I.TYR 60.10.64.0.0.28.0.36 3CCY.ASP 145.1.89.-1.88.-0.38.0.35 3V46,GLU_281,3.96,0.35,-0.55,-0.34 2IF4,HIS 125,5,1,-1,43,0,12,-0.09 1Q42,GLU_65,3.68,0.38,-0.85,-0.35 2EYI,GLU_81,3.32,0.28,-0.98,-0.48 3BWT.ARG 629.13.07.-1.41.1.19.0.79 3IBT,TYR_13,10.36,-0.56,-0.04,0.96 1TJE,LYS_169,10.34,-0.26,0,0.09 1MJS,ARG_287,12.41,-0.15,0,0.07 2JHY,ARG 134,12.52,-0.44,0.08,0.39 3M7G,GLU_263,4.47,0.32,0,-0.35 3HQX,HIS_53,6.44,-0.14,0,0.08 3F6M,ARG_84,12.78,-0.33,0.37,0.25 100X,HIS 82,4.54,-1.91,0,-0.05 2AH5.CYS 58.9.85,-0.43.0.1.29 3LQE,ASP_321,3.9,0,-0.05,0.15 3UAH,HIS_414,5.12,-2.64,0.85,0.4 300P.ARG 80,12,42,-0,48,0,13,0,26 2AD1,GLU 65,4.84,0.48,0,-0.14 3V55,CYS_464,10.07,0,-0.19,1.25 3A4C,GLU_457,4.58,0.33,0,-0.25 20BI,TYR_63,11.31,0.55,0.28,0.48 3BPP,TYR 146,12.29,0,0.41,1.88 3H13,GLU_242,4.36,0.18,0,-0.32 1RZ2,ARG_108,12.68,-0.41,0,0.59 1U53,ARG_125,12.24,-0.37,0,0.11 4DNU,LYS_296,10.78,-0.18,0,0.47 2EFK.LYS 114,10.3,-0.2,0,0 3V46,ASP_309,3.96,0,-0.23,0.38 2H2Z,TYR_209,12.71,-0.53,0.35,2.89 3UAH,ARG_210,12.6,-0.24,0,0.34 1J33,GLU_242,4.61,0.15,0,-0.05 2EHG,LYS_31,12.06,-0.36,1.13,0.79 2QV2,TYR_78,10.45,0,-0.68,1.14 3ETV.TYR 286.10.24.0.0.09.0.15 3M70,LYS_210,10.44,-1.09,0.62,0.42 1WRU.TYR 243,10.51,0,0.24,0.27 1JYH,TYR_74,10.12,0,-0.08,0.2 1X8F,ARG_70,12.31,-0.3,0,0.11 3IVF,TYR_70,10,0,-0.19,0.19 1WLY,ARG_32,14,-0.56,1.24,0.82 3JZN,GLU_107,4.55,0.05,0,0 3ETU,GLU 223,4.57,0.28,-0.21,0 1FO9,GLU_149,4.22,0.36,-0.29,-0.35 1JKS,LYS_249,10.18,-0.43,0,0.11 3M16,ARG_248,12.61,-1.24,0.53,0.82 200K.GLU 72.4.48.0.29.-0.32.0 3CGW,ARG_104,12.11,-0.47,0,0.08 3COU, ARG_42, 12.51, -0.28, 0.06, 0.23 3C38,ASP_245,4,0,0,0.2 4DBX,ASP_256,2.93,-1.2,-0.12,0.44 3EZ7,ASP_208,3.57,-0.46,0,0.24 2FL4,GLU_30,4.66,0.16,0,0 4E8B,HIS_79,4.89,-1.33,0,-0.28 3BQW,ARG_158,13.08,-0.36,0.59,0.35

3RNV,LYS_371,11.41,-0.33,0.85,0.38 4FH3,TYR 265,10,23,0,-0.01,0,25 1XDZ,LYS_223,10.42,-0.05,0,-0.03 3L3P,HIS 282.6.78,-0.44,0.28,0.43 2V81.ASP 30.3.94.0.-0.13.0.27 3MM4,ARG_984,13.85,-0.3,1.2,0.45 1AM2.GLU 12.4.61.0.11.0.0 20HT.ARG 112,12,58,-0,29,0,0,37 2YLF,LYS_135,10.33,-0.2,0,0.04 1RI6.TYR 246.13.41.0.0.09.3.32 3I4T,ASP 256,3.87,-0.23,-0.09,0.4 3RRQ,ARG_96,12.34,-0.16,0,0 2BDV,ARG_206,12.42,-0.09,0,0.01 3G9T,GLU_111,2.25,0.69,-2.34,-0.61 1XDZ,HIS 95,6.18,-0.37,0.19,-0.14 1YR6,GLU_231,4.87,0.75,-0.67,0.29 3BA1,LYS 124,10.84,-0.28,0,0.62 3EJG,LYS_160,10.39,-0.27,0,0.15 2B2H,TYR 351,11.55,0,0,1.55 2AZL,ASP 222,4.08,0.0.0.29 3KB5,GLU_323,4.48,0.11,0,-0.14 1RSS,ARG 72,13,12,-0,57,0,67,0,52 1XWM,ARG_79,12.91,-0.77,0.64,0.54 10TM,LYS 142,10.04,-0.53,0,0.06 1TLV.LYS 245,10.27,-0.43,0,0.19 2YWJ,ASP_134,3.17,-0.37,-0.61,0.36 1FO9,ARG_376,12.35,-0.18,0,0.03 4ETX,GLU_213,4.59,0.42,0,-0.33 1NAR,LYS 152,9.72,-0.78,0,0 3A4C,ARG_471,12.26,-0.29,0,0.05 1Z3X,GLU_20,4.91,0.42,0,-0.01 2G70,CYS_73,9.31,-0.01,0,0.32 2RGY,GLU 194,4.19,0.56,-0.43,-0.43 3US6,LYS 82,9.91,-0.31,0,-0.27 1XAW,LYS_488,9.94,-0.34,0,-0.22 3H5T,ASP_313,3.34,-0.56,-0.33,0.42 1ZKZ,LYS_38,10.81,-0.19,0.13,0.37 2QHT,TYR 122,10.41,0,0.12,0.29 1QYI,GLU_259,4.57,0.23,0,-0.17 3N2T,LYS_294,10.77,-0.15,0,0.41 1PVT,GLU_7,5.42,1.29,-0.48,0.13 1YLN,ASP_183,3.53,-0.69,-0.17,0.6 3M70.LYS 275,10.6,-0.13,0.0.23 1R9W,GLU_256,4.56,0.12,0,-0.06 3CQ1,ARG_65,12.46,-0.36,0,0.33 2HNG,GLU_25,4.58,0.13,-0.04,0 2AD1,LYS_122,10.5,-0.27,0,0.28 20KT,GLU_59,6.02,2.72,-1.26,0.05 2NRR,TYR_375,10,0,0,0 1D2K,ASP_324,3.54,-0.85,-0.19,0.79 3CBN,LYS_149,10.13,-0.18,0,-0.2 2R57.GLU 183.4.77.0.24.0.0.03 10I7,LYS_227,9.36,-1.42,0,0.27 1YW5,LYS 104,10.5,-0.15,0,0.15 2H14,ASP_333,3.08,-0.85,-0.09,0.21 2XJ4,TYR_224,12.67,0,0.2,2.47 2AHE,GLU 30,4.8.0.16.0.0.13 3C38,ARG_91,11.99,-0.51,0,0 1ZHV,ASP_111,3.4,-0.47,-0.41,0.49 3SMD,LYS_115,10.28,-0.32,0,0.1 3F6M,ARG 2,12.64,-0.29,0.11,0.32 1WPA,ASP_479,3.89,0,-0.21,0.3 20PJ.ARG 22.10.84,-3.33.0.1.67 1P4X,GLU_106,4.55,0.24,0,-0.19 2F9F,LYS_148,10.4,-0.36,0,0.26 3EZ7,HIS 282,6,11,-0,35,0,-0.04 1KCM,LYS_163,11.87,-0.61,1.65,0.33 1PVT,LYS_144,10.24,-0.16,0,-0.1 2DFL,ASP_67,3.87,-0.08,-0.15,0.3

1X1E.TYR 239,10.25,0.0.08,0.16 3LJI,ASP 224,4.46,-0.77,-0.14,1.57 1P2F,LYS_100,11.58,-1.03,0.85,1.27 2V1L,ARG_92,12.77,-0.41,0,0.67 1Q42,ARG_108,12.01,-0.49,0,0 2A4D,ARG 121,12.98,-0.31,0,0.8 1YOY,LYS 152,10,41,-0,31,0,0,21 1YW5,ARG_96,13.74,-0.28,0.93,0.58 1YTQ,LYS_119,11.14,-0.53,0.7,0.46 1XAW,ARG_483,13.62,-0.18,0.92,0.38 3DZ1,TYR 140,11.74,-0.26,0.47,1.53 3M7D,ARG_20,13.78,-0.75,1.17,0.87 1AKO,HIS_62,6.15,-0.27,0,-0.08 1W7B,ARG_168,12.1,-0.4,0,0 3EVN, HIS 177, 3.25, -3.25, 0.0 1UXO.TYR 157,10.32,0,-0.14,0.47 3EX9,HIS_126,3.74,-3.21,0.73,-0.29 2QHT,ARG_100,12.42,-0.08,0,0 1X8F,LYS_259,10.37,-0.13,0,0 2QK0,TYR_81,9.93,-0.89,0,0.83 2CIU,HIS_170,5.79,-0.69,0,-0.02 3V46,TYR_264,11.9,0,-0.1,2 3RFY,TYR_343,10.49,0,0.23,0.26 2BLL.GLU 481.4.71.0.23.0.-0.03 3PM2.GLU 17.4.45.0.22.0.-0.27 4EKU,TYR_238,11.51,0,0.26,1.25 4DVD.LYS 168.10.4.-0.08.0.-0.02 3F5D,ASP_78,3.75,-0.01,-0.21,0.17 20EW,HIS_162,5.21,-1.12,0,-0.18 1UXO,HIS 164,6,-2,65,0,85,1,3 3NZL,HIS_10,6.28,-0.17,0,-0.06 3OKQ,LYS_600,10.18,-0.32,0,0 1ZP2.ASP 19.3.99.0.0.0.19 1R3F,GLU 189,3.72,0.81,-1.02,-0.56 2E0T,TYR_170,11.69,0.85,0.32,0.52 2ZTY,ARG_79,12.01,-0.87,0.05,0.32 2XHC,LYS_191,11.23,-0.31,0.7,0.35 2H8O,LYS_319,10.25,-0.28,0,0.03 1N81,GLU_129,2.94,4.5,-1.68,-4.38 1L2F,GLU_253,3.29,0.32,-1.16,-0.38 3UPD,ARG_8,13.29,-1.02,1.2,0.61 3M70,GLU_25,3.85,0.23,-0.85,-0.03 3F7M,TYR 129,11.18,0,0.03,1.15 1DUN,LYS_119,10.43,-0.07,0,0 1SBX,GLU_145,4.64,0.11,0,0.03 1SUU,LYS_781,10.31,-0.2,0,0.01 2V1L,LYS_15,10.41,-0.09,0,0 1GXN.TYR 404,11,27,0.6,0.09,0.58 4FCU,HIS_72,6.7,-0.31,0,0.52 3KB5,LYS_462,10.43,-0.1,0,0.02 1WLY,LYS_144,11.5,-0.55,0.85,0.71 2D0A, ARG 17, 12.02, -0.54, 0, 0.05 1LN4,ARG_86,13.57,-1.01,1.31,0.79 1SFE,LYS_126,10.36,-0.14,0,0 3ASA, ARG_81, 10.7, -2.02, 0, 0.22 1RWZ,TYR_219,10.21,0,0.05,0.16 3ZRI,ARG_54,11.97,-0.64,0,0.11 2H2Z,ASP_56,3.11,-0.61,-0.38,0.31 3K1H.GLU 119.4.57.0.1.0.-0.03 1PVT,ARG_66,13.14,-0.24,0.52,0.36 4GA2,TYR 132,10.21,0,0,0.21 1PDB.GLU 150.4.74.0.17.0.0.07 3C6B,ASP_42,3.52,-0.42,-0.02,0.16 2P52,GLU_195,3.21,0.36,-1.27,-0.38 2Q13,GLU_162,4.9,0.35,0,0.05 2B0J.LYS 34,10.52,-0.4,0.05,0.36 2GEN,ASP_177,3.98,0,0,0.18 2JEO,GLU_197,4.72,0.33,0,-0.11 3GS9,ASP_194,3.89,0,0,0.09

1JKS.TYR 12.11.41.0.73.0.3.0.38 3QKY,TYR_76,10.29,-0.01,-0.28,0.57 1HF8,GLU_91,4.04,0.46,-0.85,-0.07 1QQH,LYS_125,10.97,-0.37,0.23,0.6 103X.LYS 195.10.45.-0.05.0.0 2AHE,ASP 120,3.8,-0.51,-0.29,0.8 3RRQ,ARG_148,12.57,-0.12,0.19,0 109G,GLU_38,1.74,1.56,-3.39,-0.93 2XHC,GLU_80,5.74,2.41,-0.53,-0.64 3CBN.ARG 31.12.43.-0.19.0.0.12 1AK1,ARG_33,12.31,-0.19,0,0 2X4L,ASP_280,3.72,-0.4,0.01,0.31 3M7D,GLU_17,4.77,0.26,0,0 2WOZ.ASP 516.3.93.0.-0.42.0.54 2H2W.GLU 215,4,46,0,43,-0,46,0 20PJ,ARG_126,12.05,-1.04,0,0.58 3Q1C,TYR_86,10.74,0,0.41,0.32 1SQW,ASP_29,4.07,0,0,0.27 2D0A.TYR 162.12.83.0.0.2.83 1RAJ,HIS_423,2.17,-3.54,0,-0.79 2IF4,GLU_45,4.09,0.55,-0.14,-0.83 3LD1,GLU_157,5.53,1.34,0,-0.31 2P52,ARG_280,12.27,-0.4,0,0.17 3M70,HIS 76,4.54,-2,1,0.83,-0.69 3M70,TYR_143,12.04,0,0.3,1.74 3OA7,LYS_491,10.28,-0.22,0,0 3LPZ,ASP_49,4.31,-0.15,-0.21,0.86 3K9I,TYR 90,10.22,0,-0.07,0.28 3EUR,TYR_24,10.92,-0.04,0,0.96 1RI5,ARG_84,11.73,-0.8,0,0.02 3DSH,HIS_452,6.24,-0.26,0,0 2D0A, HIS 19.6.01, -0.43, 0, -0.06 3S0A,LYS 114,11.01,-0.26,0.41,0.37 3OBS,ARG_50,13.36,-0.35,0.73,0.47 2CI3,LYS_56,10.32,-0.18,0,0 3V55,TYR_569,10.11,-0.85,-0.06,1.02 2YT4,HIS 600,6.06,-0.37,0,-0.08 3M3P.GLU 102.4.66.0.17.0.-0.01 1C3K,LYS_19,10.45,-0.05,0,0 10XZ,GLU_173,4.81,0.14,0,0.18 1FQI,ASP_366,1.99,-1.84,-0.46,0.5 3DZ1,ARG 123,12,41,-0,31,0,0,22 1TLV,GLU_253,4.63,0.21,0,-0.08 2GZR/TYR 190/10.36/-0.01/-0.29/0.65 3FFM,LYS_48,11.36,-0.33,0.8,0.38 2WB8,GLU 531,3.69,0.84,-1.2,-0.46 2DG7.ASP 85.4.3.0.0.0.5 1YB2,LYS_219,10.25,-0.26,0,0.01 3GE9,GLU_207,5.18,2.18,-1.61,0.11 2JEO,LYS 42,11,24,-0.36,0.72,0.38 4DNU,GLU_345,3.75,0.41,-0.85,-0.31 2H30,GLU_103,4.83,2.74,-2.33,-0.08 1WLY,GLU_86,4.05,1.61,-1.59,-0.47 4F85,ASP_107,2.95,-1.21,-0.36,0.71 2RGY,GLU_202,4.63,0.3,0,-0.17 1WP5,LYS_186,9.98,-0.28,0,-0.24 1RZ2,ARG_43,13.37,-0.43,0.72,0.58 3M70,GLU 244,4.51,1,-0.8,-0.18 10TM,ASP_195,3.99,0,-0.34,0.53 1IDK,TYR 97,10.62,0,0.41,0.21 3IL3, ASP_30, 4.02, 0, -0.21, 0.43 1ZBM,GLU_223,3.73,0.26,-0.85,-0.17 3CZC,GLU_35,4.36,0.27,0,-0.4 2NYC,GLU_228,4.45,0.29,-0.62,0.29 2Q99,ARG_355,12.85,-0.73,0.64,0.44 1T6L,LYS_18,10.4,-0.1,0,0 3V75,ARG 17,11.72,-0.94,0,0.17 1ES5,ASP_194,3.86,-0.01,-0.11,0.18 3EVN,GLU_66,4.44,0.17,0,-0.23

2D2S.LYS 598.10.3.-0.23.0.0.03 1PSW,ARG 196,12.31,-0.85,0,0.66 2W0G,GLU_221,4.97,0.42,0,0.05 1TR9,GLU_312,3.95,0.16,-0.7,0 2B61.GLU 129.3.78.0.57,-0.85,-0.44 1IDK.ASP 201,3.97,-0.01,-0.04,0.22 3M7G,ARG_245,12.36,-0.24,0,0.1 3EZ7,LYS 117,9,78,-1.07,0.0.35 3DZ1,ARG_290,12.78,-0.34,0.13,0.49 3LJN,LYS_257,10.48,-0.02,0,0 3E0H,ASP 145,3.73,-0.25,0.0.17 1UOH,GLU_87,4.24,0.18,-0.44,0 1P6F,TYR_122,10.54,-0.11,0.27,0.38 1P6F.GLU 183,4.59,0.18,0,-0.09 1JT9,ARG 126,12.52,-0.32,0,0.35 2GZQ,LYS_163,10.41,-0.16,0,0.07 1C44,LYS_30,11.44,-0.31,0.85,0.4 3EUR,GLU_78,4.47,0.29,0,-0.32 3D9H,LYS 90,10.31,-0.14,0,-0.05 1LN4,LYS_59,9.87,-0.44,0,-0.2 1C3K,TYR_89,11.07,0,0.61,0.47 3JRT,CYS_61,12.32,0,-0.08,3.4 3M70,GLU_96,4.52,0.97,-0.74,-0.21 3ZSL,GLU 205,2.6,0.49,-1.65,-0.74 2J8A,HIS_280,6.42,-0.3,0,0.23 3GE9,GLU_37,4.19,1.47,-1.6,-0.18 3GE9,ASP_28,2.71,-1.53,-0.02,0.46 2E3C,ASP_318,2.43,-1.66,-0.24,0.54 1HUF,LYS 82,10,51,-0,17,0,0,17 1WXQ,TYR_143,9.65,-0.85,0.03,0.47 1X8F,ASP_153,4.1,0,-0.08,0.39 1EV8,LYS_158,10.55,-0.18,0,0.22 1G5Z.LYS 177,11.49,-0.35,0.79,0.56 2YX0,LYS_130,10.43,-0.07,0,0 3PZ9,ARG_111,13.93,-1.63,1.98,1.1 3H04,ASP_256,3.94,0,0,0.14 3EZ7,GLU_332,4.72,0.29,-0.01,-0.06 1Z3X,HIS_69,5.73,-0.76,0,0 1WJG,CYS_131,10.13,-0.29,-0.03,1.45 2YT4,GLU_540,4.39,0.28,-0.04,-0.35 2HP7,LYS_49,10.44,-0.06,0,0 2A0J,LYS 123,10.48,-0.34,0,0.32 20JO,ARG 606,13,44,-0.2,0,76,0.38 3BB7,TYR_56,10.86,0,0.01,0.84 1M5I,GLU_135,4.51,0.22,0,-0.22 2GS5,ARG_133,11.04,-2.14,0.08,0.6 1XAW,ARG_468,12.71,-0.19,0.4,0 3CX2,CYS_239,12.48,0,0.19,3.29 2ZO5.HIS 85.4.65.-1.61.0.-0.24 2VAN,ARG_326,12.48,-0.08,0,0.07 2DFL,ASP 248,4.01,-0.27,-0.74,1.21 3G9G,HIS 159,6,26,-0,31,0,0.07 2X4L,LYS_159,10.56,-0.13,0,0.19 1J33,GLU_61,4.05,0.45,-0.77,-0.13 2D59,TYR_44,11.59,0,0.33,1.25 3A4C,GLU_455,4.56,0.09,0,-0.03 2OSA,CYS 268,9.73,-0.11,0.03,0.81 1V8E,ASP_154,2.95,-1.59,-0.08,0.81 1X9G,ARG_66,12.68,-0.12,0,0.29 3IBT,GLU 152,5.41,1.48,0,-0.56 1XTZ,LYS 220,11.51,-0.26,0.77,0.51 2NMU, ARG_108, 12.44, -0.54, 0.23, 0.26 2NRK,GLU_59,4.34,0.35,-0.37,-0.14 3Q9P,GLU_119,3.58,0.33,-0.58,-0.67 1SQH,TYR 36,11.88,0,0.14,1.74 2YT4,ASP_579,4.04,0,-0.08,0.31 3CGW,ARG_166,13.38,-0.46,0.77,0.57 2EYI,GLU_53,4.82,0.12,0,0.2 1R53,ARG_9,12.65,-0.35,0.08,0.42

2V1L.GLU 137.4.6.0.1.0.0 30NH,CYS 537,9.32,-0.07,0.2,0.19 2CXY,GLU_108,4.43,0.09,0,-0.16 3IL3,ASP 21,2.67,-1.19,-0.36,0.43 2R4Q,HIS_184,6.37,-0.22,0,0.09 2R0S,ASP 51,3.04,-0.85,-0.81,0.91 2Z84.CYS 212.11.66.0.0.02.2.65 1QQE,ARG_114,12.69,-0.14,0,0.32 3Q1C,ARG_170,12.29,-0.5,0.03,0.26 1WRU,ARG_155,13.68,-1.21,1.09,1.31 1DUPASP 135.3.96.0.0.0.16 3CAN,GLU_164,4.59,0.09,0,0 4E9E,TYR_485,10.73,0,-0.19,0.92 1M5I,LYS_139,10.61,-0.12,0,0.23 1U7U,HIS 211,6.46,-0.11,0,0.07 3DHN,LYS_40,10.42,-0.16,0,0.08 1P6F,GLU_55,4.12,0.35,-0.73,0 3LJN,LYS_205,10.48,-0.02,0,0 3EX9,GLU_93,4.06,0.38,-0.36,-0.45 2FB6,ASP_14,3.78,-0.21,-0.08,0.28 1V43,GLU_205,3.84,2.65,-2.51,-0.8 3OBS,LYS_10,10.4,-0.1,0,0 1BN6,CYS_72,12.38,0,0.03,3.35 2D7J,GLU 176,4.89,0.41,0,-0.02 2A6B.GLU 16.3.59.0.26.-0.79.-0.38 2Q99,LYS_99,10.81,-0.54,0.02,0.81 2HRZ,ARG_118,13.47,-0.36,0.72,0.61 3QKY,ARG_229,11.92,-1,0.16,0.25 2QV2,ASP_184,3.39,-0.68,-0.44,0.7 3HYQ,HIS_32,6.12,-0.18,0,-0.21 2CXA,GLU_139,4.77,0.23,0,0.05 4AF2,LYS_46,10.23,-0.27,0,0 3M66,LYS 196,11.52,-0.29,0.85,0.46 3FTT,ASP 59,3.9,0,-0.17,0.27 1QQE,LYS_88,10.81,-0.61,0.3,0.62 3I0C,TYR_309,11.95,0,0.34,1.62 4DNU,ARG_212,13.75,-0.74,1.33,0.67 2EFK,LYS 140,11.26,-0.4,0.85,0.32 3EZ7,GLU_94,4.34,0.37,-0.24,-0.29 2BT8, ASP_249, 2.67, -1.5, -0.29, 0.67 3V4G,GLU_119,4.77,0.27,0,0 3K8J,LYS_176,10.67,-0.37,0.42,0.11 3E5T,LYS 220,10.35,-0.89,0.0.74 2V4U,LYS_331,10.33,-0.18,0,0.01 1JT9,ARG_91,12.31,-0.38,0,0.19 1YTQ,ASP_169,3.85,0,-0.37,0.41 3FXH,TYR_49,10.5,0,-0.38,0.87 3RJX,LYS 343,10.04,-0.82,0.0.36 2G5X,TYR_187,10.15,-0.16,0.13,0.18 1X91,ARG_119,12.47,-0.03,0,0 1LTU,GLU_207,6.88,3.12,-0.85,0.11 2C2Y.ASP 90.3.98.0.-0.03.0.21 2CBE,ASP_101,3.15,-0.84,-0.37,0.56 4H86,HIS 175,6,71,-0.68,0.84,0.05 2FBQ,ASP_214,4.04,0,0.07,0.17 1F2V,TYR_14,10.1,-0.07,-0.39,0.56 2OB5.GLU 119.4.33.0.38.-0.17.-0.38 3BA1,GLU_263,4.39,0.18,0,-0.29 20EW,GLU 62,4.56,0.12,0,-0.05 3HQX,GLU_31,4.7,0.18,0,0.02 3PP8,ASP 35,2.03,-1.81,-0.68,0.72 2E3S,HIS_422,4.95,-1.73,0,0.18 2CVB.ARG 63.13.32.-0.45.0.9.0.38 3CRM,CYS_31,11.53,0,0.13,2.4 1GVP,GLU_40,4.58,0.08,0,0 1RAJ,LYS 383,10.68,-0.09,0.0.28 3DSH,ARG_353,12.1,-0.47,0,0.07 3CZC,HIS_59,6.47,-0.22,0,0.19 1QQE,GLU_122,4.05,1.21,-1.15,-0.51

3M7D,ARG 276,12,59,-0.08,0,0,18 1WXQ,ARG 352,13.3,-0.44,0.8,0.44 2BDD,GLU_139,4.73,0.23,0,0 2YWK,GLU_18,3.14,0.59,-1.42,-0.53 3U2R,ASP_26,4.06,0,-0.13,0.38 3AU3,ASP 651,3.57,-0.3,-0.11,0.18 2098/HIS 173,5.18,-0.91,0,-0.42 1UJ8,ASP_34,2.55,-1.4,-0.38,0.53 3BZT,TYR_345,10.2,0,0.14,0.06 3F6M,GLU_81,3.34,0.49,-1.03,-0.62 1XKR,GLU 57,4.8,0.12,0,0.18 3T5B,LYS_354,10.15,-0.44,0,0.09 3B7X,TYR_61,11.81,0.74,0.43,0.63 2ATR,GLU_107,4.61,0.15,0,-0.04 3PP8,ARG 192,13,-1.61,0.86,1.24 1U7U,HIS 320.6.4,-0.24.0.0.14 2IQT,ARG_56,13.55,-0.7,1.02,0.74 4FH3,CYS_75,10.73,-0.25,0.14,1.84 3HVM,HIS_54,5.67,-1.34,0,0.5 1SJY,ARG_95,12.33,-1.74,0.68,0.89 10GL.TYR 209.9.64,-0.5,-0.29,0.43 3M16,ARG_188,10.44,-1.88,0,-0.18 30IP,HIS_12,6.31,-0.19,0,-0.01 4DIU.ARG 32,11.76,-0.43,0,-0.31 2APL,HIS_146,6.33,-0.17,0,0 3FXH,GLU_12,4.52,2.74,-2.47,-0.26 1AK1,ARG 240,13,19,-0,33,0.66,0.36 3E7P,ASP_43,2.63,-1.17,-0.38,0.39 3DHN,ARG 176,12.32,-0.2,0,0.02 3IBT.ARG 183,13.62,-0.79,1.09,0.81 2RIK,ASP_225,2.88,-0.85,-0.41,0.35 3G9G,LYS_44,10.55,-0.18,0,0.22 1T95,GLU_103,4.57,0.14,0,-0.08 1YDL,GLU 55,4.66,0.18,0,-0.02 3U2R,ARG_27,13.75,-0.32,1.17,0.4 20EW,LYS_269,10.5,-0.3,0,0.31 3FTT,LYS_183,10.43,-0.07,0,0 1L2F,GLU_22,4.51,0.49,-0.32,-0.16 2NMU,HIS_137,6.21,-0.29,0,0 3RKV,GLU_327,4.95,0.38,0,0.07 3RFY,GLU_178,4.82,0.19,0,0.13 3IL3,LYS_24,10.55,-0.08,0,0.13 3RE9,TYR 111,8.95,-0.85,-0.51,0.31 3EUR,GLU_97,3.86,0.88,-1.14,-0.37 1HF8,TYR_44,10.58,0,0.31,0.27 3CNU,GLU_39,3.43,1.06,-1.66,-0.47 3DHN,LYS_153,10.4,-0.12,0,0.02 2XJ4.GLU 256.4.84.1.95.-0.93.-0.68 30DJ,HIS_39,5.65,-1.11,0.59,-0.33 2H2Z,CYS_22,10.17,-0.09,-0.52,1.77 2GAU,ARG_199,12.38,-0.12,0,0 3VJ8,HIS 347,7.38,-0.35,0.85,0.38 4AM1,GLU_8,4.47,0.12,0,-0.15 2QV2,GLU_12,3.99,0.36,-0.76,-0.1 1YOY,LYS_30,10.23,-0.34,0,0.07 1L3K,ARG_53,12.42,-0.11,0,0.03 2CN1,LYS_27,10.53,-0.09,0,0.12 2IF4,TYR_208,10.82,-0.01,-0.22,1.06 2O34.LYS 234.10.9.-0.11.0.0.52 20KT,GLU_233,3.82,0.26,-0.66,-0.28 1WLY,LYS 9,10.34,-0.16,0,0 2HRZ,ARG 209,12,76,-1.58,1.2,0.65 3V3T,GLU_237,4.49,0.33,0,-0.34 1GXN,ARG_353,12.29,-0.26,0,0.05 3JZ9,LYS_370,11.26,-0.47,0.85,0.38 1SJ8,LYS 540,10.4,-0.52,0.0.42 1WXQ,CYS_55,8.14,-1.07,0,0.22 2D8N,LYS_194,10.07,-1.35,0.85,0.07 4DBX,TYR_252,12.89,0,0.83,2.06

3GOZ.HIS 8.6.35,-0.23.0.0.08 4DVD,ASP_11,3.71,-0.48,-0.02,0.41 1QZN,LYS_60,10.54,-0.09,0,0.14 1RWZ,ASP_70,3.44,-0.89,-0.24,0.78 2IRM.ARG 40.12.05.-0.81.0.0.37 1RSS.GLU 90.4.69.0.19.0.-0.01 10LR,LYS_76,10.26,-0.33,0,0.1 3JZ9,LYS_491,10.1,-0.48,0,0.07 2YWJ,GLU_16,4.87,0.58,0,-0.2 3UC9.HIS 31.6.29.-0.27.0.0.06 3OA7,ARG_566,13.1,-0.28,0.42,0.45 2R0S.LYS 162.10.41.-0.09.0.0 3CAX,LYS_420,10.26,-0.14,0,-0.1 3FRR.TYR 64,10.51,0,0.02,0.5 3HKX,HIS 28,5,26,-1,17,0,-0.07 200K,GLU_33,4.67,0.24,0,-0.07 1W7B,ASP_200,3.48,-0.47,-0.57,0.71 1XTZ,LYS_72,10.61,-0.18,0,0.28 2B2H,ASP 268,2.88,-1.73,-0.12,0.94 4E8B,ARG_223,13.2,-0.13,0.41,0.42 4DVD,ARG_52,12.81,-0.12,0,0.44 3016,ARG_16,13.22,-0.8,0.84,0.68 3IO0.ASP 192.3.94.0.0.0.14 2AZP.ARG 54,12,27,-0.96,0.46,0.28 1ZP2,ARG_49,12.25,-0.23,0.05,-0.06 3PM2,LYS_86,10.67,-0.13,0,0.3 2BDD,GLU_61,4.67,0.31,0,-0.13 3F7M,ARG_168,12.79,-0.37,0.17,0.49 2CI3,HIS_235,4.34,-2.22,0.06,-0.01 2AXO,ASP_124,3.28,-1.01,-0.66,1.16 2XHC,TYR_215,10.12,0,-0.14,0.26 2V5B,LYS 60,10,51,-0,28,0,0,3 2EDM,ASP 177,3.2,-0.8,-0.13,0.32 3F1X,GLU_77,4.64,0.14,0,0 3CZC,LYS 71,10.32,-0.27,0.0.09 1JKS,ASP_238,3.8,0,-0.18,0.17 2FGG,ARG 63,11.82,-0.44,0,-0.24 2P1W.GLU 205,4.17,0.21,-0.23,-0.31 1WYC,ASP_248,3.92,0,-0.06,0.19 3FTT,GLU_48,4.57,0.21,0,-0.15 2E3S.HIS 509.6.21,-0.49.0.0.19 3JZN.GLU 145.5.92.2.66.-1.33.0.09 4F8A,HIS_601,7.4,-0.3,0.85,0.34 3EYE, HIS 79, 6, 16, -0, 26, 0, -0, 09 1XTD,CYS_49,10.78,-0.21,0.33,1.65 3EVP,HIS 235,6.2,-0.3,0,6.94E-18 2YX0,ASP 161,3.15,-0.85,-0.42,0.61 2EJX,ASP_117,2.93,-0.84,-0.38,0.35 1ZBM,GLU_36,3.82,0.78,-1.03,-0.43 1DOV.TYR 237.10.23.0.0.04.0.19 2CXY.GLU 107.4.56.0.16.0.-0.1 3GYW,LYS_70,10.57,-0.25,0.31,0 3GS9,ASP_131,3.15,-1.62,-0.02,0.98 1QQE,ASP_290,2.94,-1.02,0,0.16 2X4L,TYR 328,12.45,0,0.4,2.05 1PDB,ARG_28,12.23,-0.3,0,0.03 2EFK,ARG_278,12.45,-0.05,0,0 1QYI,GLU 233,4.27,0.28,0,-0.51 3DZ1,GLU_253,6.23,4.9,-1.14,-2.03 3V55,LYS_582,11.26,-0.32,0.7,0.38 2EEY,GLU 114,4.5,1.26,-0.77,-0.48 2D0A,CYS_291,11.45,-0.45,-0.01,2.92 1JKS,GLU_109,4.5,0,0,0 3GW3,TYR_202,13.98,-0.26,0.92,3.33 1W7B.GLU 142.3.03.0.46.-1.54.-0.39 3QYB,LYS_888,10.41,-0.09,0,0 2B0A, ASP_173, 3.04, -0.59, -0.38, 0.21 2P4D,GLU_164,4.59,0.38,-0.01,-0.29 1PGV,ARG_248,12.33,-0.21,0,0.04

1RZ2,ASP_127,2.5,-1.42,-0.42,0.54 1J8B,LYS 66,11.15,-0.17,0.82,0 208P,ARG_53,12.92,-1.61,1.15,0.88 3GS9,LYS_182,10.46,-0.27,0,0.22 2|6|,LYS 26,10,46,-0.06,0,0.01 3CRM,HIS 217,5,45,-0.61,0,-0.45 3U0V,LYS_195,10.36,-0.14,0,0 1P4X,GLU_29,4.63,0.14,0,-0.01 3COU, ARG_129, 12.39, -0.19, 0, 0.08 1R5O.TYR 18.13.27.0.0.09.3.19 2H2Z,LYS 102,10,79,-0,17,0,0,46 1IDK,TYR_211,11.94,0.13,0.38,1.42 2FGG,CYS_11,9.28,0,-0.05,0.33 1FO9.GLU 211.7.79.2.82.-0.85.1.32 4EUG,GLU 14,4.39,0.96,-0.85,-0.22 1ZBM,ASP_125,3.99,-0.13,-0.09,0.41 3LJN,TYR_245,12.28,0,0.66,1.62 4H89,CYS_107,12.01,0,-0.11,3.11 1IAP,ARG 111,12.22,-0.41,0,0.14 3IRA,ARG_140,12.64,-0.67,0.25,0.55 3GS3,GLU_66,4.83,0.54,0,-0.19 1YTQ,LYS_107,11.3,-0.39,0.61,0.57 3ODJ,TYR_125,12.75,0.17,0.02,2.57 2YWK, ASP 9, 3.36, -0.6, -0.17, 0.33 1QQE,ARG_50,12.59,-0.4,0,0.5 1V43,ARG_307,12.95,-0.34,0.37,0.43 1SI7,ARG_92,12.54,-0.2,0,0.24 3US6,LYS 72,10.52,-0.06,0,0.08 2YLF,ARG 222,12,25,-0.3,0,0.05 3LMF,ASP_44,4.49,0.11,0.38,0.2 1X9G,TYR_8,11.5,0.03,0.46,1.01 2IIA.ARG 73,12,73,-0,16,0,01,0,38 2FC3,GLU 38,4.13,0.3,0,-0.66 1K95,GLU_143,4.76,1.04,-0.88,0.09 3GW3,CYS_35,12.64,0,0,3.64 2CW4,ARG_46,12.8,-0.22,0,0.53 2FBQ,HIS 162,6.33,-0.88,0.8,-0.08 3CCY,ARG_13,12.88,-0.48,0.17,0.69 1PSW,ARG_105,11.35,-1.15,0,0 1AD6,ASP_511,2.8,-1.6,-0.12,0.72 1WYC,ARG_387,13.07,-0.52,0.74,0.35 1W7B,LYS 157,10.77,-0.2,0.02,0.45 1LZL,ASP 47,3.84,0,-0.11,0.14 3GV0,ASP_201,3.43,-0.76,-0.47,0.87 3PP8,ASP_307,4.12,-0.08,0.16,0.24 3M7D,ASP_336,3.96,0,0,0.16 2FZ4,GLU_207,4.67,0.17,0,0 2JEO,HIS_120,5.37,-1.08,0,-0.05 3JRT.ASP 131.3.95.0.0.0.15 2Q13,LYS_63,11.29,-0.29,0.7,0.38 1NWA, ARG 93, 12.46, -1.43, 0.68, 0.71 1RHS.LYS 13.11.27,-0.18.0.63.0.31 2C2Y,ASP_114,3.43,-0.79,-0.24,0.66 2F8H,ARG_166,11.62,-1.79,0.8,0.11 1BKB,GLU_36,4.57,0.16,0,-0.09 4AM1,LYS_289,11.38,-0.55,0.85,0.59 1PSW,CYS 243,11.88,0,0,2.88 3HNX.ARG 63,12,38,-0,28,0,0,15 1RI5,TYR_226,9.78,-0.85,0.19,0.44 3K8U,GLU_130,3.74,1.64,-1.6,-0.8 3VHJ,LYS 116,11,24,-0,41,0,69,0,46 2FC3,GLU_93,4.63,0.11,0,0.01 2HP7,CYS_214,12.94,0,0.08,3.86 3HVM,HIS_227,5.12,-1.94,0.25,0.31 1BKR,TYR_98,12.61,-0.85,0.08,3.38 3P51,ARG_130,12.2,-0.33,0,0.03 3GT0,TYR_180,10.18,0,0,0.18 3JZN,ARG_201,12.38,-0.2,0,0.08 4AF2,GLU_74,4.3,0.31,-0.42,-0.09

2F8H,ASP_305,3.82,0,-0.23,0.25 2H30,LYS 120,10,44,-0,17,0,0,11 4EKU,CYS_298,10.74,0.43,0.31,1 3GOZ.GLU 99.2.81.0.4,-1.71,-0.39 1X7F,ARG_333,13.94,-0.38,1.36,0.46 1BKR.LYS 43.10.27.-0.23.0.0 100X,GLU_249,4.33,0.65,-0.38,-0.44 3CQ1,ASP_20,3.93,-1.21,0,1.33 2VAN,LYS_262,10.21,-0.52,0,0.22 3M7D,HIS_373,6.37,-0.23,0,0.11 1R53,LYS 162,10.25,-0.17,0,-0.08 3EVN,GLU_22,4.48,0.33,-0.23,-0.13 4H86.GLU 38.4.44.0.25.-0.01.-0.29 1059.HIS 244.7.06.-0.61.0.53.0.64 1YOY,GLU 102,4.45,0.11,0,-0.16 2EFK,LYS_173,10.96,-0.26,0.21,0.52 3VJ8,LYS_115,10.42,-0.2,0,0.13 1ZHV,ASP_75,3.8,0,0,0 3UPD,GLU_303,3.37,0.71,-1.45,-0.38 2YX0,GLU_152,6.48,4.45,-2.42,-0.04 3V55,CYS_439,11.68,0,0.08,2.6 30IP.LYS 13,10.33,-0.17,0,-0.01 1JSX,LYS_21,9.59,-1.14,0,0.23 1R3D,HIS 150,6.45,-0.28,0,0.24 2EEY,GLU 148,3.46,0.4,-0.79,-0.64 3I4T,CYS_247,12.14,0,0.11,3.04 2RGY,TYR_100,13.45,0,1.05,2.4 3V3T,ASP_88,3.87,0,-0.29,0.37 1PZC,ASP 94,3.68,-0.03,-0.24,0.15 3BCH,ARG_102,12.28,-0.22,0,0 3ADO,GLU_271,4.67,0.1,0,0.07 200K,GLU_303,4.52,0.27,0,-0.25 1YTQ,TYR 111,10.09,-0.46,-0.43,0.99 1NAR.GLU 138,2.78,0.65,-1.99,-0.38 3CCY,ASP_104,3.1,-1.01,-0.67,0.98 3CIV,CYS_243,10.38,0,0.3,1.08 2GZR,ASP_179,3.83,-0.51,-0.31,0.86 4ESS,ARG 5,13.13,-0.27,0.64,0.26 2DG7,GLU_144,4.77,0.19,0,0.08 2E3C,ARG_356,13.26,-0.46,0.57,0.65 3PP8,GLU_101,4.65,0.3,0,-0.15 3V75,ARG 70,12.59,-0.99,0.68,0.4 1WYC,ARG 328,11.29,-1.71,0,0.49 1LZL,ASP_43,4,0,0,0.2 1X7F,GLU_131,3.24,0.43,-0.97,-0.73 1L2F,LYS_123,10.44,-0.32,0,0.28 3DB9,ARG 179,12.29,-0.27,0,0.06 2BDV.GLU 104,5.24,3.89,-3.33,0.19 3BPP,TYR_142,10.74,0,0,0.74 3FXH,ASP_68,3.62,0,-0.4,0.23 3MTT,GLU_436,4.57,0.07,0,0 20KT.TYR 9,12.65.0.85.0.56.1.24 3BQW,LYS_349,11.69,-0.34,0.85,0.69 3M9A,TYR 25,10,38,0,-0,05,0,43 2H8O, ARG_69, 13.5, -1.04, 1.44, 0.6 2BQQ,LYS_54,10.5,0,0,0 2XMZ.GLU 161.4.61.0.11.0.0 1JKS,LYS_33,10.68,-0.38,0,0.56 2RH3,ARG_179,12.32,-0.24,0,0.06 100X,TYR_105,9.13,-0.78,-0.41,0.31 1XTD,HIS 116,7,37,-0.33,0.85,0.35 3H9W,ARG_95,12.43,-0.2,0,0.13 1059,HIS 0.6.17,-0.15,0,-0.18 3ERF,GLU_207,4.47,0.22,-0.18,-0.06 1IDK,TYR_149,10.45,-0.61,0.1,0.96 2B78,ARG 16,12,19,-0,38,0,0,07 1EDG,TYR_296,12.25,0,-0.09,2.34 2YWK,ARG_74,12.32,-0.18,0,0 1QYI,GLU_195,5.6,1.27,0,-0.17

3N0K,TYR_132,10.05,0,0,0.05 2PLQ,ASP 311,3.57,-0.51,-0.09,0.37 1ES9,HIS_79,4.32,-1.99,0,-0.19 3JZN,HIS_295,6.19,-0.34,0.15,-0.12 300P,ASP_11,4.12,0,0,0.32 1X91,ARG 44,11.95,-0.55,0,0 4E8B,ARG_238,12.19,-0.31,0,0 2ZQ5,HIS_121,3.04,-2.62,0.46,-1.31 2FBQ,HIS_91,5.84,-0.54,0,-0.12 2R57,ARG_364,11.98,-2.4,0.79,1.09 1LFP,LYS 58,10.34,-0.49,0,0.33 4E6S.GLU 32,4,25,0,27,-0.05,-0.47 3I47, ASP_5, 3.33, -0.65, -0.39, 0.57 1Z3X,LYS_21,10.45,-0.05,0,0 1G8P,ARG_343,12.37,-0.13,0,0 3MIX.ARG 533,12.26,-0.24,0.0 2DG7,ASP_26,3.88,0,-0.16,0.25 1M5I,GLU_201,4.92,0.28,0,0.14 2APL,CYS_46,10.11,-0.01,0.41,0.71 2GZR,ASP 96,3.68,0,-0.46,0.35 2PLO.LYS 205.10.1.-0.54.0.0.14 3CIV,ASP_100,2.73,-1.44,-0.22,0.6 3ULX,GLU_9,5.06,0.7,0,-0.13 1WP5.GLU 122.4.13.0.33.-0.11.-0.58 3AU3,ARG 527,12,39,-0,12,0,0 3CS1,CYS_74,11.79,-0.74,0,3.53 3BPV.ASP 82.3.19.-0.83.-0.43.0.65 2Q12,LYS_191,10.96,-0.68,0.85,0.29 1MUF,TYR 281,10.36,0,0.12,0.25 1TWU,LYS 97,11.23,-0.38,0.69,0.43 2FZ4,ASP_89,4.04,0,0,0.24 3FXH,GLU_87,1.76,0.38,-2.32,-0.78 106D.GLU 52.5.71.1.75.0.-0.54 2QDJ,GLU 322,2.97,0.36,-1.13,-0.76 3ANJ,LYS_370,10.25,-0.36,0,0.11 2JEO,LYS_204,10.98,-0.24,0.43,0.28 3DTE,ASP_59,2.21,-1.74,-0.44,0.6 2PIM,ASP_123,4,-0.01,-0.03,0.23 4FZR,GLU_180,4.27,0.46,-0.61,-0.09 1SJY,LYS_142,10.37,-0.39,0,0.27 2A1V,ARG_58,12.26,-0.32,0,0.08 2A1V,ARG_67,13.97,-0.71,1.56,0.62 3ZRI.LYS 145,11.01,-0.26,0.4,0.37 4EUG,HIS_180,5.25,-1.68,0.52,-0.09 2B61,LYS_255,10.47,-0.09,0,0.06 3M3P,HIS_182,6.49,-0.24,0,0.23 2D2S,LYS_746,10.52,-0.1,0,0.12 3GS3,ASP 146,3,92,0,0,0,12 3M7G,TYR_177,10.19,-0.29,-0.19,0.67 1WP5,LYS_222,10.4,-0.2,0,0.09 1PDB,GLU_143,4.66,0.2,0,-0.03 1NKD.GLU 41,4.95,0.26,0,0.18 2FZ4,TYR_183,10.24,0,0.1,0.15 3LH5,HIS_759,5.97,-0.23,0.03,-0.33 1SI7,ARG_230,12.3,-0.2,0,0 1U7U,LYS_187,10.37,-0.13,0,0 2EYI,ARG_187,13.36,-0.34,0.84,0.36 3ETU,GLU_67,4.74,0.24,0,0 2RIS,CYS_59,12.49,0,0.75,2.74 3FS3,LYS_233,10.43,-0.07,0,0 3M66,ASP 335,3.43,-0.66,-0.04,0.33 1YG2.LYS 99.10.51.-0.21.0.0.22 2RIK,GLU_41,4.29,0.23,0,-0.43 3ETV,LYS_249,10.46,-0.04,0,0 2ZCO,TYR_154,11.45,0,0.45,0.99 1ES9,ARG_93,12.28,-0.23,0,0.02 2Q34,GLU_163,4.15,0.2,-0.52,-0.03 2Z0M,ARG_238,12.41,-0.09,0,0 1T3Y,ASP_116,3.34,-0.76,-0.02,0.32

1Y0K.GLU 39.3.51.1.14.-1.57.-0.56 3GMS,ASP_30,4.09,0,0,0.29 2A4D,GLU_135,3.87,0.32,-0.79,-0.16 1NRI,ASP_253,3.56,-0.34,0,0.1 1PSW.ARG 27.12.72.-0.32.0.05.0.48 2H85,CYS 290,8.76,-0.23,-0.29,0.28 1SI7,ARG_186,12.44,-0.06,0,0 1X7F,ASP_126,2.25,-1.44,-0.64,0.53 2FZP,HIS_251,5.57,-0.69,0,-0.23 100L.GLU 36.4.46.0.38.-0.15.-0.27 4E8B,LYS_91,10.32,-0.54,0,0.36 3BJV.GLU 49.4.82.0.24.0.0.08 2OJQ,ARG_496,12.55,-0.34,0,0.38 1H09.LYS 207.11.39.-0.24.0.47.0.65 3UPD.GLU 148.5.32.3.15.-1.52.-0.82 2FPN,GLU_160,4.06,0.48,-0.4,-0.52 2EEY,LYS_14,10.37,-0.26,0,0.13 4FZN,ARG_94,12.74,-0.47,0.09,0.62 1FO9.LYS 332.10.4.-0.1.0.0 1X04,GLU_160,4.36,0.43,-0.24,-0.34 2G3A, ASP_19, 3.26, -0.85, -0.05, 0.37 105T,GLU_414,3.85,0.57,-0.76,-0.45 3C6BLYS 270.10.69.-0.2.0.0.39 1X9G.CYS 17.12.78.-0.1.0.46.3.41 2P52,GLU_221,4.24,0.33,-0.56,-0.02 2FD4,LYS_453,10.6,-0.29,0,0.39 1MML,ARG_159,12.04,-0.46,0,0 1QQE,ASP 246,4.08,0,-0.1,0.38 1G5Z,GLU_61,4.41,0.31,-0.02,-0.38 2FZP.GLU 315,3.87,0.31,-0.55,-0.39 3Q1C,LYS_309,10.71,-0.15,0,0.36 1WP5.ASP 309.3.44,-0.93,-0.04,0.61 2D7U,LYS 109,11,29,-0.56,0.83,0.52 2P0Y,LYS_282,10.31,-0.25,0,0.06 1DZF,GLU_172,3.43,0.3,-0.85,-0.51 2FC3,ARG_25,13.01,-0.25,0.22,0.54 2DVK,ASP_153,2.46,-0.98,-0.62,0.27 3DSH,LYS 441,10,43,-0.07,0,0 1ZBP,ARG_146,12.2,-1.22,0.05,0.86 3LD1,HIS_352,6.05,-0.92,0.16,0.3 2C2Y,ASP 7,3.28,-0.77,-0.2,0.45 2E3S,HIS 430.6.46,-1.46,0.85,0.57 1QQE,ASP_289,4.06,0,0,0.26 1CBY,LYS 140,10.54,-0.27,0.0.3 1P2F,LYS_29,10.62,-0.18,0,0.3 2B3M,GLU 35,4.6,0.1,0,-0.01 1X1E,CYS 218,12,2,0,-0,31,3,51 2ZQ5,ASP_28,2.28,-1.58,-0.43,0.49 2AH5,LYS_61,10.46,-0.04,0,0 2012.LYS 158.10.58.-0.08.0.0.16 1WP5.GLU 92.3.65.1.73.-2.48.-0.11 3NR5,LYS_100,10.31,-0.23,0,0.03 4EVF,GLU_10,5.07,0.54,0,0.04 2EEY,TYR_157,9.69,0,-0.7,0.39 3M7G,ASP 160,4.06,0,0.06,0.2 1EV8,GLU_58,6.64,2.96,-0.82,0 1RHS,LYS_135,10.53,-0.18,0,0.2 2IQT,LYS_94,10.51,-0.11,0,0.12 3RFY,ASP_197,3.81,0,-0.18,0.19 4ECC,ARG_18,11.86,-3.35,0,2.71 3M7G,GLU 8,3.22,0.38,-1.67,0 3EJC,TYR_88,11.01,0,0.03,0.98 2JEO,TYR_115,12.21,0,0.17,2.05 1K95,GLU 71,4.39,0.35,-0.72,0.25 4EZB,GLU_200,3.02,0.61,-1.45,-0.65 3A4C,CYS_491,11.34,-0.01,0.29,2.07 3I4T,GLU_21,4.55,0.17,0,-0.11 2D8N,ASP_61,2.95,-0.83,-0.41,0.38 3CAN,LYS_180,10.49,-0.15,0,0.14

2XHC.ASP 75.3.36.-0.83.-0.08.0.47 3GEC,ARG 272,13,28,-0.37,0.53,0.62 2IN0,HIS_439,6.37,-0.98,0.73,0.13 3FRR,TYR_128,11.93,0,0.06,1.88 3OBS,LYS 90,10,29,-0,42,0,0,21 2E3C,ASP_386,4.03,0,-0.3,0.53 3ERF,GLU_123,4.63,0.61,0,-0.48 3HNX,ASP_82,1.97,-2.05,-0.38,0.6 1S7K,ARG_146,12.61,-0.29,0.1,0.3 1NRI.GLU 177.4.84.0.32.0.0.02 1WRU,ARG 262,11.8,-0.56,0,-0.14 1D2K,ARG_39,11.41,-2.16,0,1.07 3L3P,LYS_496,10.45,-0.05,0,0 2YLF.ARG 75.12.31.-0.16.0.-0.03 1ZBS.GLU 48.4.37.0.58.-0.71.0 2E3S,ARG_574,13.08,-0.35,0.6,0.33 3RLN,LYS_696,11.02,-0.53,0.54,0.52 300P,GLU_35,2.92,0.44,-1.46,-0.55 2D0A,HIS 86,6.08,-0.29,0,-0.13 3PU6.TYR 82.9.83.-0.41.-0.15.0.39 1WXQ,GLU_230,4.46,0.11,0,-0.15 2YT4,GLU_594,4.65,0.15,0,0 3K8J,LYS_200,10.38,-0.18,0,0.06 109G,GLU 141,4.9,0.86,0,-0.45 2EEY,CYS_76,10.77,0,0.42,1.35 3FHF,GLU_110,4.58,0.08,0,0 20PJ,ARG_49,12.1,-0.56,0,0.16 4AM1,LYS 24,10.59,-0.15,0,0.23 1ZCE,ASP_87,4.68,0,-0.13,1.02 3H5T,CYS_247,12.48,-0.01,0.35,3.15 2XHC,TYR_172,10.74,-0.91,0.11,1.55 1VJG,GLU_67,4.12,0.81,-0.55,-0.64 20PJ.ARG 190,13.66,-0.3,0.98,0.48 2EEY,ASP_71,3.84,0,-0.22,0.26 1WRU,ASP_131,1.31,-2.68,-0.52,0.7 307K,ARG_49,12.27,-0.39,0,0.15 3IVF,ASP 125,3.65,-0.01,-0.38,0.25 2DFL,ARG_223,12.4,-0.1,0,0 1XFK,LYS_216,10.35,-0.11,0,-0.03 2RIS.CYS 181,11.88,-0.28,0.32,2.85 3HKX,ASP_258,2.97,-0.85,-0.48,0.51 1SBX,ASP 156,3.84,-0.08,-0.35,0.47 2A0J.HIS 41.6.58.-0.31.0.0.39 1P2F,LYS_142,10.44,-0.07,0,0.02 2D59,ARG_36,12.57,-0.2,0,0.27 3N0K,GLU_81,4.76,0.15,0,0.11 1Q5Z,ASP_568,3.44,-0.74,-0.68,1.05 2CXY,GLU_28,4.7,0.14,0,0.06 3FWU,ARG 16,12,39,-0.28,0,0.18 2G9D,ARG_103,12.27,-0.25,0,0.02 3BA1,LYS 89,10.43,-0.19,0,0.12 2W2S.GLU 126.4.49.0.11.0.-0.12 3DSH,ASP_442,3.59,-0.55,-0.01,0.36 3BWT,GLU_658,3.07,0.98,-1.15,-1.26 1WP5,ARG_298,13.05,-0.2,0.26,0.49 3H13,TYR_322,10.56,0,0,0.56 3OA7,GLU_434,4.68,0.18,0,0 1ZCE, ASP_102, 3.57, -0.3, -0.18, 0.26 2WOZ,TYR_571,10.78,-0.19,-0.1,1.08 2GZR,ASP 59,3.03,-0.85,-0.27,0.36 2G5X.LYS 155,10.36,-0.14,0,0 1MTZ,LYS_257,10.41,-0.22,0,0.13 4DNU,ASP_208,2,-2.13,-0.46,0.78 1P1L,LYS_57,9.84,-1.01,0,0.36 1WLY,TYR 46,10.17,0,0,0.17 2FXT,ASP_410,3.98,0,0.01,0.18 2NRR,ARG_478,12.2,-0.46,0,0.16 2H85,GLU_233,4.69,0.97,-0.79,3.47E-18 3AUF,ARG_23,13.69,-0.33,0.91,0.61

3GOZ.GLU 16.4.83.0.31.0.0.02 1ZKZ,LYS 64,10,41,-0.09,0,0 3CXS,GLU_37,4.48,0.1,0,-0.12 1AT0.GLU 297.3.56.0.28.-0.78.-0.44 4AM1,ARG 202,12.07,-1.14,0.0.71 2PGE.ARG 71.12.47.-0.11.0.0.09 1WNH,GLU_60,4.06,2.44,-2.64,-0.24 1BN6,ASP_42,3.74,-0.16,-0.07,0.17 2V81,ARG_188,12.2,-0.31,0,0.01 3RE9.LYS 120.10.49,-0.36.0.0.34 3M7D,ARG 83,12,52,-1,58,0.67,0.94 1P4X,GLU_207,3.66,0.31,-0.85,-0.3 3UC9.GLU 133.4.64.0.13.0.0.02 1IAP.GLU 50.3.35.0.39.-0.9.-0.65 3M7G,TYR 66,13.91,0.85,0.14,2.92 2EA9,TYR_104,10.78,-0.1,-0.16,1.05 30IP,ARG_122,12.44,-0.66,0,0.61 2EJB,ARG_109,12.96,-0.46,0.52,0.39 1WLY,GLU 20.3.19.0.19.-0.85.-0.65 2B3M,TYR_112,10.62,-0.85,0.12,1.35 3F6M,ARG_80,12.96,-0.48,0.56,0.39 1Z9L,HIS_4,6,-0.36,0,-0.14 3BA1,LYS_132,10.29,-0.21,0,0 3ERF,HIS 134,5.81,-0.64,0,-0.04 1ZBS.LYS 18.10.49.-0.14.0.0.13 2B78,GLU_172,4.94,0.27,0,0.17 1U53,ASP_33,3,-2.44,-0.22,1.87 2EYI,GLU_235,3.89,0.66,-0.24,-1.04 3ASA,GLU_267,5.36,1.09,0,-0.22 1SIG,HIS_331,6.47,-0.33,0,0.31 1MML,LYS 267,10.38,-0.12,0,0 1G5Z,LYS_110,10.75,-0.26,0.02,0.49 100L.TYR 22,10.52,0,-0.11,0.63 3HKX.GLU 107.4.43.0.7.-0.74.-0.02 4EVF,ARG_78,12.14,-3.23,0.08,2.78 1XDZ,GLU_46,4.77,0.14,0,0.13 3EVP,GLU_61,5.24,2.17,-0.99,-0.43 1ZKZ,TYR 35,10.26,0,-0.02,0.28 2XJ4,ARG_50,12.07,-0.6,0,0.16 4GA2,CYS_105,10.62,0,0.01,1.61 4H4J,ASP_38,3.82,0,-0.24,0.26 3TMO,ASP 209,3.59,0,-0.56,0.35 1I60.TYR 252,11.92,-0.73,0.14,2.52 2ZCO,LYS_283,11.33,-0.47,0.85,0.46 3EJG,LYS_129,10.54,-0.15,0,0.19 3L7N,ASP_151,3.87,-0.01,-0.04,0.12 3E0H,LYS 118,10.67,-0.26,0,0.44 2Z14,TYR 84,10.96,-0.84,0.01,1.78 1WYC,GLU_139,4.74,0.22,0,0.02 2QHT,GLU_74,4.43,0.16,0,-0.22 3I0C, ASP_259, 3.33, -0.77, -0.17, 0.47 306L,LYS 53,10.8,-0.2,0,0.5 2WZ9,ASP_101,2.73,-1.33,-0.52,0.78 2RIK,LYS_99,10.4,-0.5,0,0.4 208l,HIS_41,6.04,-1.35,0.79,0.1 1GPP,ASP_12,2.43,-1.71,0,0.34 3U0V,ASP 95,3.47,-0.68,-0.7,1.05 1W7B,LYS_169,10.48,-0.2,0,0.18 1NJ4,LYS_294,9.96,-0.32,0,-0.22 2FB6,GLU_79,3.99,0.34,-0.86,0 30KY,TYR 56,9.43,-0.37,-0.72,0.52 3AU3,ARG_554,12.27,-0.23,0,0 3M16,LYS 194,10.68,-0.3,0.0.48 3LH5,TYR_722,10.19,-1.98,-0.16,2.33 1AKO, ARG_77, 12.07, -0.57, 0, 0.13 3EIZ.ASP 98.4,-1.08.0.02,1.25 3FRR,ARG_109,11.2,-1.28,0,-0.03 3LQE,ARG_437,12.32,-0.27,0,0.09 2XHC,GLU_142,4.75,0.15,0,0.1

1PDB,GLU_104,4.77,0.28,0,-0.02 1UAJ,HIS 72,6.25,-0.61,0,0.35 3GS3,LYS_84,10.52,-0.66,0.31,0.37 2CXC,GLU_111,4.53,0.05,0,-0.02 3UC9,ASP_28,4.23,0,-0.05,0.48 1R29,ARG 24,12.22,-0.25,0,-0.03 1HUF,ARG 10,13.32,-0.24,0.73,0.32 3QAV,TYR_32,11.32,-0.79,0.46,1.65 2FBQ,ARG_59,13.76,-1.94,1.57,1.62 3C2E,TYR_46,9.38,-0.64,-0.4,0.42 3H9W,HIS 98,7.3,-0.44,0.85,0.39 1YM5.GLU 131.4.49.0.35.0.-0.36 3HKX.ASP 82.3.92.0.-0.13.0.25 2P0Y,LYS_266,10.43,-0.14,0,0.07 3UAH.TYR 424.10.1.0.-0.15.0.25 3U2R,ARG 99,12,44,-0.06,0,0 3IV4,LYS_73,10.23,-0.2,0,-0.07 2GKG,GLU_101,4.11,0.84,-0.82,-0.41 2R0S,ARG_86,12.4,-0.36,0,0.26 2E0T,ARG 84,12.29,-0.21,0,0 1RZ2,ASP_89,3.83,0,-0.2,0.23 3G9G,ASP_212,4.14,0,0,0.34 1PSW,ARG_146,12.66,-0.24,0.02,0.38 2WOZ.CYS 593.11.78.-0.52.0.03.3.27 2GZR.ARG 206.12.24,-0.39.0.0.13 1P4X,LYS_200,10.33,-0.17,0,0 2EJX.LYS 51,10.33,-0.16,0,-0.01 1V43,CYS_49,10.04,-0.97,-0.71,2.71 2AZL,LYS 127,10.28,-0.17,0,-0.06 1FO9,GLU_249,4.14,0.24,-0.27,-0.33 3DTE,ARG_77,11.23,-1.57,0,0.31 3JSN,ASP_226,4.21,0,0.13,0.28 2D2S,ASP 630,4,29,0,0,0,49 3L3P.GLU 314.4.53.0.38.0.-0.34 3EVZ,HIS_193,6.04,-0.96,0.65,-0.16 3ZTA,LYS_60,11.02,-0.21,0.24,0.49 2Z0M,ARG_209,12.58,-0.12,0,0.2 2EDM,ASP_47,3.44,-0.78,0,0.42 2P52,ARG 210,11.08,-1.44,0.0.02 2IQT,ASP_89,3.52,-0.85,-0.43,1 1YTD,TYR_214,10.72,0,0.13,0.59 1SJY,ARG_6,13.47,-0.33,1.3,0 1J74,LYS 129,10.42,-0.08,0,0 10IS,LYS_144,10.19,-0.49,0,0.19 3FXH,ARG_108,12.42,-0.09,0,0.01 2E3C,ARG_226,13.57,-0.3,0.75,0.62 3A2Z,GLU_92,4.76,0.32,-0.05,0 3BB7.LYS 108.10.21.-0.35.0.0.07 3DTE,ARG_32,11.5,-1.21,0,0.21 1PDB,GLU_172,4.38,1.3,-0.95,-0.47 10I7,LYS_112,10.58,-0.14,0,0.21 2Q5X,GLU 803,5.12,0.77,0,-0.17 1ZHV,GLU_76,4.5,0,0,0 1SJY,ASP_60,4.14,0,0.05,0.29 1XDZ,GLU_196,3.87,0.8,-0.97,-0.46 1W7B,ARG_309,13.29,-0.27,0.65,0.41 1XTD.LYS 58.10.44.-0.06.0.0 2Q34,GLU_47,2.9,0.36,-1.47,-0.49 2E0T.HIS 151,3.95,-2.66,0.06,0.05 3BA1,GLU_19,2.92,0.51,-1.44,-0.64 2DFL,TYR 33,10.68,0,0.04,0.64 1T95.GLU 168.3.25.0.75.-1.37.-0.63 3Q1C,TYR_292,10.19,-1.43,0.17,1.46 1ZP2,CYS_100,10.16,-0.07,-0.15,1.38 2CWY,GLU_66,4.22,0.78,-0.73,-0.33 2B0A.TYR 96,9.55,0,-0.72,0.28 2H01,GLU_114,3.66,0.39,-0.79,-0.44 1V6T,TYR_235,11.75,0.85,0.51,0.38 1NWA,GLU_127,3.77,1.3,-1.49,-0.54

3BWT.TYR 760,10,38,0,0,06,0,33 2B78,LYS_13,10.94,-0.95,0.85,0.54 2YWJ,LYS_56,10.5,-0.14,0,0.14 1GXN,LYS_490,9.99,-0.5,0,-0.02 1SUULYS 669.10.25.-0.46.0.0.21 2WB8.GLU 604.3.96.1.72.-1.65.-0.61 3JSN,GLU_65,3.7,0.17,-0.72,-0.25 1RAJ,HIS_398,5.53,-0.65,0,-0.33 3HVM,TYR_189,13.33,-1.58,0.55,4.37 3LE4.HIS 321.6.13.-0.44.0.0.07 3ADO,GLU_278,4.67,0.17,0,0 3H8Y,LYS 29,11.32,-0.2,0.5,0.51 1XEU,ARG_204,11.98,-0.52,0,0 2G9D.CYS 328.8.66.-0.75.-0.58.0.99 2B3M,TYR 136,10,58,0,0,08,0,5 1PVT,HIS_192,5.28,-1.16,0,-0.05 1DCF,CYS_43,11.64,0,-0.04,2.67 1UOH,GLU_57,5.02,0.3,0,0.23 1ES9.ARG 29.12.26.-0.44.0.0.2 2CBE,GLU_69,3.8,1.24,-1.5,-0.44 3FFM,ASP_97,2.68,-1.55,-0.1,0.52 1AKO,GLU_139,4.65,0.21,0,-0.06 2H30,HIS 102,6.31,-0.14,0,-0.05 2X5Y,ASP 823,3.23,-0.8,-0.5,0.73 3M7G,GLU_21,4.88,0.4,0,-0.02 3K8U,HIS_28,5.63,-0.69,0,-0.18 1RKA,LYS_289,10.38,-0.18,0,0.07 3C38,GLU 257,4.52,1.11,-0.77,-0.32 2FZ4,LYS_46,10.46,-0.1,0,0.06 1WNH,GLU_86,4.28,0.28,-0.16,-0.34 1UCH,ASP_218,3.84,0,-0.07,0.11 3FFM.GLU 69.4.67.0.16.0.0.01 2AH5,ARG 44,12,34,-0,29,0,0,14 2F8H,ASP_85,3.17,-0.79,-0.23,0.39 20YZ.GLU 92.4.8.0.38.0.-0.07 2VAN,GLU_186,4.54,0.19,0,-0.15 3IBT,GLU_169,5.46,1.6,0,-0.64 3HKX.ARG 180.12.22.-0.28.0.0 1YLN,GLU_221,4.58,0.17,0,-0.09 3M16,GLU_10,3.81,0.33,-0.36,-0.66 2FM9,ASP 130,2.77,-2.4,-0.27,1.64 1DZF.LYS 197.10.05.-0.46.0.0.01 4EKU,LYS_229,10.01,-0.26,0,-0.23 1AT0, ASP_282, 3.62, -0.79, -0.18, 0.79 3IRA,GLU_150,4.62,0.22,0,-0.1 1WLY,LYS 142,10.35,-0.22,0,0.08 2CXA.ARG 204.11.44.-1.18.0.0.12 4FD6,ARG_143,12.23,-0.51,0,0.24 2CXY,GLU_9,4.5,0.32,0,-0.32 3P51.GLU 69.4.47.0.21.0.-0.23 1TD6.GLU 113.4.45.0.25.0.-0.3 3H13,LYS_460,10.71,-0.19,0,0.4 2X5Y,GLU_895,4.64,0.13,0,0.02 2X5Y,HIS_735,5.89,-0.32,0,-0.3 2ZCO,CYS 130,12.68,-0.03,0.38,3.32 2RJD,ARG_461,12.74,-0.24,0,0.48 2G3A,ARG_18,12.54,-0.14,0,0.18 2D59,ARG 135,13.8,-0.29,0.77,0.83 3DB9,ARG_20,12.41,-1.66,1.02,0.55 3BJV,TYR 58,12.44,-0.85,0.44,2.85 3I0C,GLU_107,4.66,0.16,-0.02,0.01 1WXF,LYS_41,10.35,-0.15,0,0 1PZC,TYR_74,11.87,-0.01,0,1.87 3FRR,CYS_136,10.51,-1.15,0.03,2.63 2GEN,TYR_43,10.35,0,0.04,0.32 1RL0,ASP_21,3.93,0,-0.77,0.91 1AT0, ARG_272, 12.38, -0.12, 0, 0 2NMU,GLU_70,4.35,0.34,-0.23,-0.26 2IRM,LYS_112,10.69,-0.1,0,0.29

2D59,GLU 17,4.71,0.58,-0.03,-0.34 2RIS,GLU_27,4.81,0.21,0,0.1 2GEN,ASP_122,4.27,0,-0.37,0.84 3CS1,GLU_45,4.65,0.21,0,-0.05 1TXJ,LYS 92,10,19,-0,21,0,-0,1 3ZRI.ARG 112.13.72.-1.79.1.6.1.41 2DVK,GLU_161,4.66,0.14,0,0.02 2GKG,TYR 102,11,51,-0,78,0,32,1,97 1TLV,TYR_64,10.44,0,0.24,0.2 4ECC.LYS 153.10.15.-0.24.0.-0.11 1CBY,LYS 94,10.06,-0.56,0,0.11 3RNV,GLU_438,3.49,0.59,-0.85,-0.76 3N0K,GLU_117,5,0.3,0,0.19 1MIX,TYR_377,9.96,-0.11,-0.16,0.24 1MUEARG 249.10.81.-1.75.0.0.06 3C2E,HIS_250,6.42,-0.08,0,0 1YDL,LYS 71,10.07,-0.43,0.0 3V46,ASP_237,4.27,0,-0.29,0.76 3FHF,ASP 64,3.06,-0.83,-0.27,0.36 3U0V.HIS 204,5.46,-0.89,0,-0.15 1FO9,LYS_256,11.31,-0.47,0.79,0.48 2FM9,LYS_89,9.97,-0.53,0,0 1SNT,ARG_283,13.24,-0.35,0.69,0.4 2AXO,ASP_72,3.38,-1.16,-0.41,1.15 2IIA,ARG_68,12.37,-0.16,0,0.03 2EFK,ASP_220,3.55,-0.7,-0.88,1.34 3HYQ,HIS_101,6.32,-0.17,0,0 2IF4,GLU_163,3.32,0.76,-1.02,-0.92 102Y,GLU 26,4,54,1.37,-0.83,-0.49 2AXO,ASP_136,4.21,0,0.12,0.29 3GFP,TYR_420,11.78,-0.59,-0.09,2.46 3RKV.CYS 252,11.24,-0.08,-0.07,2.39 2RGY,GLU 158,3.9,0.2,-0.63,-0.18 2EEY,HIS_6,6.04,-0.35,0,-0.12 2B78,TYR 183,13,98,-0.02,0.06,3.95 3IPZ,LYS_130,10.05,-0.25,0,-0.21 3RJZ,LYS 177,10.24,-0.32,0,0.06 3ONT,TYR_57,9.45,-0.34,-0.44,0.23 3T5B,GLU_243,3.96,1.05,-0.85,-0.74 1TD6,ASP_272,3.8,0,-0.17,0.17 2CL3,LYS_169,9.75,-0.73,0,-0.02 10XZ,GLU_302,5.12,0.45,0,0.17 3ADO,CYS 94,12.66,-0.85,0.5,4.01 1SQW,GLU_22,4.59,0.1,0,-0.01 3BQW,ARG_343,13.91,-0.21,1.16,0.46 1RI6,ASP_139,2.63,-1.79,-0.11,0.75 3F6F,GLU_143,3.81,0.21,-0.82,-0.08 3GMS,TYR_330,13.03,0.85,0.57,1.61 3L7N.ARG 35.12.62.-0.13.0.0.25 3KT2,ARG_41,12.39,-0.11,0,0 2QDJ,LYS 143,11.42,-0.42,0.85.0.49 2WZ9,ARG 99,13.39,-0.78,1.11,0.56 4H4J,ASP_195,4.03,-0.82,-0.06,1.12 1BKB,TYR_132,10.53,-0.16,-0.02,0.7 3FHF,LYS_77,10.36,-0.34,0,0.19 10IS,CYS_232,11.95,0,0.09,2.85 3LJC,TYR_228,10.54,0,0.38,0.16 3PM2,LYS_94,10.54,-0.19,0,0.23 3P51,GLU_15,3.89,0.31,-0.71,-0.21 2DFL,TYR_247,10.2,0,-0.05,0.24 300P,ARG 122,12,52,-0,11,0,13,0 3EUR,ARG_83,12.54,-0.34,0,0.38 1AKO,GLU_166,4.56,0.08,0,-0.01 2FBQ,TYR_129,10.19,-0.85,0.01,1.03 4EVF,GLU 105,4.09,0.44,-0.82,-0.05 2G3A,GLU_134,4.46,0.42,-0.14,-0.32 3AU3,LYS_581,10.76,-0.2,0.03,0.44 3EIZ,ASP_112,3.08,-0.43,-0.73,0.44 3EZ7,ARG_54,12.47,-0.13,0,0.1

3KT9,ARG_16,12.29,-0.48,0,0.27 2F9F,LYS 37,10,42,-0,21,0,0,13 1VJG,GLU_166,3.98,0.75,-0.85,-0.42 1EW4.CYS 32,11.04.0.0.45,1.6 4DBX,ARG_163,12.39,-0.11,0,0 3F5D,TYR 184,9.97,0,-0.28,0.25 4EZB,ASP_270,3.65,0,-0.31,0.16 3LH5,LYS_660,11.13,-0.45,0.85,0.23 300P,LYS_60,10.1,-0.54,0,0.14 1RL0.LYS 92.10.32.-0.5.0.0.32 2Z61,GLU_174,5.02,0.18,0,0.34 2G9D,LYS_256,10.54,-0.19,0,0.23 3RHE,ASP 110,2,57,-1,58,-0,37,0,73 2RFA,LYS 263,10.05,-0.18,0,-0.27 20JOLYS 654.10.69.-0.56.0.08.0.67 1Q46,GLU_167,4.18,0.47,-0.48,-0.31 1W24.CYS 36.12.61.-0.82.0.93.3.5 3KV0,TYR_164,10.21,0,0.15,0.06 2Z84,GLU_103,3.57,1.78,-2.22,-0.5 2CBE,ASP_52,3.53,-0.41,-0.14,0.28 3ZRI,ARG_123,13.67,-0.35,0.61,0.91 1XKR,LYS_196,10.65,-0.32,0,0.47 2BV9,LYS_80,10.17,-0.33,0,0 1MUF,ARG 152,12.49,-0.18,0,0.17 3CE7.GLU 62.5.37.0.39.0.0.47 3E0H,ARG_23,12.18,-0.54,0,0.22 10XZ,ASP_247,3.95,0,-0.09,0.24 2X4G,ARG_116,12.45,-0.05,0,0 3IBT,ARG 87,12.51,-0.07,0,0.08 3MEW,GLU_221,4.78,0.31,0,-0.03 3V55,LYS 516,11,49,-0.92,0.85,1.06 2BQQ,TYR_125,11.29,-0.61,0.53,1.37 1XTD.ASP 129,1.93,-2,-0.4,0.52 3TRE.HIS 4.6.95.-0.42.0.85.0.03 1WP5,LYS_76,10.45,-0.17,0,0.12 3AU3,CYS_483,11.63,-0.04,-0.36,3.03 2HXB,ASP_5,2.81,-1.01,-0.35,0.38 3L7N, ASP 104, 3.85, -0.5, 0, 0.54 2AHE,GLU_239,3.68,0.73,-1.68,0.14 2VAN, ASP_314, 4.16, 0, 0.09, 0.27 2B0A,HIS_136,6.34,-2.15,1.06,0.94 2Z0M,ARG 306,11.01,-1.58,0,0.09 3GS9.ARG 169.12.18.-0.65.0.0.33 4DIU,GLU_242,3.87,0.65,-1.08,-0.2 2YT4,LYS_562,10.42,-0.09,0,0.01 2PWQ,LYS_73,10.18,-0.35,0,0.03 3FWU,CYS_105,9.54,0,-0.02,0.55 1NIJ.GLU 72.4.61.0.15.0.-0.05 3LJI,ARG_140,12.1,-0.41,0,0.01 2G2D,LYS_115,10.37,-0.13,0,0 3PAC,LYS_117,11.09,-0.73,0.85,0.47 2A6B,HIS 116,5,81,-0,74,0,0,04 2CXC,GLU_34,4.1,0.3,-0.45,-0.25 3GT0,LYS_111,10.14,-0.43,0,0.07 3VHJ,ASP_134,2.2,-1.63,-0.39,0.42 3VJ8,GLU_116,5.47,0.73,0,0.24 3G6S.TYR 83,11.69.0.0.42,1.27 1RI5,ARG_239,12.52,-0.13,0,0.15 1SI7,LYS_212,11.35,-0.37,0.82,0.4 3US6,HIS_77,5.82,-0.55,0,-0.14 1PBV.LYS 70.10.28.-0.12.0.-0.09 4FH3,TYR_348,10.08,0,-0.01,0.08 105T.ASP 454.3.76.0.-0.24.0.2 1BKR,TYR_61,10.21,0,0.01,0.21 2B0J,ASP_126,3.97,0,-0.23,0.4 20DJ.GLU 237.3.31.0.46,-1.43,-0.21 3C38,GLU_228,2.66,0.79,-2.38,-0.24 3U2R,ASP_11,3.38,-0.53,0,0.11 1RL0,CYS_220,10.29,-0.18,0.02,1.45

3M9A,TYR_69,10.91,0,-0.04,0.95 3ETV.GLU 295.5.77.1.3.0.-0.02 1GPP,TYR_420,10.29,0,-0.04,0.33 2G3A,ARG_35,12.12,-0.25,0,-0.13 1059,TYR_181,13.84,0,1.53,2.3 2E3C,TYR 384,10.07,0,0,0.07 3PAC.CYS 110.9.88.0.-0.3.1.17 1Q2Y,GLU_41,4.63,0.23,0,-0.11 2YT4,LYS_501,10.47,-0.14,0,0.12 2QHT,GLU_6,3.63,1.13,-1.58,-0.42 1MJS,TYR 297,10.62,0,0,0.62 1SNT,HIS_297,5.07,-3.49,1.89,0.18 2GEN/HIS 45,5,53,-0.38,0,-0.59 4F85,CYS_162,9.98,-0.06,0.09,0.96 3AU3,ASP 434,3.77,-0.15,0.0.13 3TMO.GLU 290.3.67.0.75,-1.58.0 2AD1,LYS_219,10.51,-0.05,0,0.06 1U3Y,LYS_334,10.39,-0.23,0,0.13 2F9F,LYS_42,11.65,-0.24,0.81,0.56 3H04,ARG 253,12.39,-0.08,0,-0.03 1AT0.TYR 401,10.5.0.0.33.0.17 4EKU,GLU_340,4.98,1.23,-0.77,0.01 1W7B,ARG_179,10.53,-2.13,0,0.16 1K95,ARG 95,12,45,-0,43,0,0.38 3VHJ.HIS 126.6.26,-0.33.0.0.09 3CBN,ASP_121,3.68,-0.18,-0.13,0.19 2B2H,HIS_134,6.5,-1.8,1.5,0.29 3CIV,ARG_108,12.23,-0.28,0,0.01 2FZ4,TYR_209,11.01,0,0.35,0.65 3CAX,HIS 123,4.04,-2.17,0,-0.29 3CGW,GLU_273,4.9,0.32,0,0.08 3HVM,LYS_246,10.34,-0.19,0,0.02 4ACJ.LYS 735.9.66.-0.84.0.0 4EZB,ARG_34,13.36,-0.61,0.94,0.52 3PAC,GLU_183,4.35,0.32,-0.22,-0.24 1KN3,TYR_81,10.16,0,0,0.16 2NYC,TYR_239,10.2,0,0.02,0.18 2BLL,GLU_561,4.06,1.32,-1.31,-0.45 3UC9,LYS 41,10,44,-0,12,0,0,06 1SJ8,ARG_741,13.4,-0.35,0.84,0.42 3LD1,CYS_357,11.54,0,0.14,2.4 2R57.LYS 289.10.43.-0.07.0.0 1X91,GLU 87,4.83,0.19,0,0.13 1Q2Y,LYS_62,10.44,-0.2,0,0.13 30KQ,GLU_604,4.62,0.17,0,-0.06 3GV0,ARG_155,12.71,-1.6,0.7,1.12 3MTT,ARG_571,12.52,-0.27,0,0.28 2EHG.GLU 123.3.11.0.63.-1.29.-0.73 3AU3,HIS_462,6.81,-0.68,0.85,0.14 2R57,LYS_340,10.45,-0.09,0,0.04 3RLE,TYR_17,11.17,-0.09,0.3,0.96 1A8Q,LYS 210,10.47,-0.13,0,0.1 1T3J,GLU_727,4.85,0.23,0,0.12 3B7X,TYR_116,11.54,0.54,0.45,0.55 1FHL,TYR_77,13.86,-0.84,0.52,4.18 1SIG,ARG_423,12.83,-0.17,0.04,0.45 2XJ4,ARG_176,12.87,-0.76,0.59,0.53 1RKA,ARG_307,12.27,-0.29,0,0.06 2IF4.HIS 90.6.48.-0.16.0.0.14 2APL,ARG_13,13.09,-0.44,0.7,0.32 1BGF,CYS 108,11.44,-0.85,0.34,2.95 20PJ.ARG 86,12,48,-0,19,0,0,17 1J33,ARG_316,11.62,-1.29,0,0.41 3UAH,TYR_379,13.69,0.41,-0.17,3.46 2G3A, ASP_45, 3.2, -0.84, 0, 0.24 2A6B.GLU 179.4.5.0.0.0 3DB9,ASP_261,3.39,-1.02,-0.81,1.41 2R57,LYS_315,10.46,-0.19,0,0.15 2WZ9,LYS_126,10.46,-0.04,0,0

1UW7.GLU 68.3.53.0.45.-0.85.-0.57 2FD4,ARG_536,13.18,-0.17,0.44,0.41 2FZ4,ARG_31,12.55,-0.1,0,0.16 2D7U,LYS_290,10.45,-0.07,0,0.02 20KT.ASP 38.2.52.-2.2.-0.25.1.17 1XFK,HIS 117,5.99,-0.62,0.16,-0.05 3C6B,GLU_67,4.98,0.39,0,0.09 3A7L,GLU_6,4.6,0.11,0,-0.01 2HXB,TYR_81,8.86,-0.85,-0.63,0.34 3H5T.LYS 327.10.17.-0.39.0.0.05 2HRZ,GLU_316,3.87,2.44,-2.96,-0.11 3D9H,GLU_213,3.66,0.2,-0.73,-0.31 3ASA,ASP_258,2.23,-1.7,-0.38,0.51 2Z61.TYR 322.10.66.0.0.16.0.5 1RI6.GLU 114.4.45.0.27.0.-0.32 2H85,ARG_135,12.26,-0.35,0,0.11 2IF4,LYS_101,10.53,-0.57,0.13,0.47 20PJ,ARG_28,12.24,-0.28,0,0.02 1XTZ,ASP_239,4.07,0,-0.41,0.68 1WJG,ASP_44,4,0,0,0.2 3GW3,ASP_346,3.21,-0.74,-0.33,0.49 2XJ4,GLU_152,2.99,0.36,-1.5,-0.36 1P4X.ARG 84.12.36.-0.14.0.0 3CRM,ASP 69,2.1,-2.05,-0.36,0.71 2H01,LYS_170,10.47,-0.03,0,0 1JKS,TYR_240,10.55,0,0.32,0.23 1NJ4,GLU_354,4.73,0.14,0,0.09 3UX2,GLU 58,3.95,0.31,-0.93,0.07 1P4X,GLU_48,4.52,0.18,-0.09,-0.06 3TRE, ARG_44, 12.18, -0.3, 0, -0.03 3EVN,GLU_313,4.63,1.14,-1.06,0.05 3F1X.CYS 92.10.44.0.21.0.33.0.88 3RLE.GLU 64,3,45,0.65,-1.7,0 1BGF,HIS_81,5.89,-0.26,0,-0.35 4EF5,ARG_178,11.9,-0.93,0,0.32 2Z61,ARG_66,12.76,-0.72,0.1,0.88 2IXM,ARG_200,12.21,-0.29,0,0 20PJ.GLU 82.4.71.0.15.0.0.06 2Z61,LYS_291,11.05,-0.33,0.52,0.35 1WYC,GLU_168,6.53,2.19,0,-0.16 1WLY,LYS 229,11,49,-0,43,0,59,0.83 3A2Z,ASP 29,2,35,-1,65,-0,2,0,4 2X4L,ASP_201,4.21,0,0,0.41 1H4U,HIS_429,6.12,-0.5,0.04,0.09 3FTT,GLU_24,4.22,0.71,-0.65,-0.35 3AU3,ARG_405,12.21,-0.29,0,0 1ILW.GLU 168.4.73.0.29.0.-0.06 3GE9,GLU_151,4.49,0.32,0,-0.33 1JYH,ASP_145,2.63,-1.44,-0.38,0.64 10TM,ASP 79,3,47,-0.37,-0.3,0.34 1DZF,LYS 166,10,44,-0.06,0,0 3CIV,GLU_282,7.82,3.13,-0.02,0.21 3F5D,ASP_31,1.66,-1.91,-0.86,0.64 3VJ8,GLU_165,4.51,0.89,-0.81,-0.08 1MTZ,LYS 221,11.36,-0.27,0.74,0.38 2H85,LYS_307,9.71,-0.79,0,0.01 3CSR,ARG_111,12.21,-0.29,0,0 3ULX,ASP_131,3.78,0,-0.35,0.33 1059,HIS_324,4.9,-1.5,0.47,-0.57 1WXF,TYR_37,10.17,0,0,0.17 3US6,ARG_55,12.79,-0.31,0.12,0.48 2F4Q,ARG_214,12.12,-0.39,0,0.01 3M7G,LYS_134,9.98,-0.15,0,-0.37 100X,GLU_179,3.73,0.35,-0.81,-0.32 2OSA,ASP_322,3.54,-0.06,-0.71,0.5 3QKY,GLU_178,3.36,1.79,-1.82,-1.12 1V43,ARG_56,12.96,-0.36,0.43,0.39 2YYO,GLU_156,4.47,0.38,-0.53,0.12 2ZQ5,HIS_212,3.28,-3.22,0,0

2AD1,ASP 24,4.05,0,-0.05,0.3 1GPP.ARG 417,13,42,-0,31,0.69,0.54 2H2W,LYS_169,10.32,-0.24,0,0.07 3FWU,ASP_29,2.85,-1,-0.38,0.42 109G,ASP 86,4,14,0,0,03,0,3 2CWY,GLU 6,4,47,0.2,-0.06,-0.18 3N2T,ARG_120,12.22,-0.31,0,0.03 3JSN.HIS 40.6.41.-0.31.0.0.22 3CAX,TYR_284,13.87,0.06,0.91,2.91 3TMO.LYS 216.11.52.-0.27.0.84.0.44 2EYI,HIS 44,3,41,-2,32,0,21,-0.98 3ILC, ARG_139, 12.28, -0.38, 0, 0.16 1V6T,ASP_134,2.67,-1.45,-0.4,0.73 1JT9.CYS 239.12.19.-0.46.0.23.3.43 1ZP2.ASP 192.3.38-0.71-0.09.0.38 2G5X,TYR_92,10.3,0,-0.06,0.36 3H04, ASP_204, 3.92, 0, -0.04, 0.16 2IN0,LYS_74,10.47,-0.21,0,0.18 1SI7,ARG 210,13.53,-2.53,1.65,1.92 1WP5.GLU 93.4.25.1.33.-0.69.-0.89 3K8J,ARG_173,12.79,-1.08,0.71,0.65 3QYB,LYS_896,10.41,-0.09,0,0 1AT0.GLU 350.4.66.0.16.0.0 10GL.LYS 207.10.49.-0.1.0.0.09 1YG2,LYS_34,10.4,-0.1,0,0 3GG6,HIS_175,6.16,-0.25,0,-0.1 2G9D,TYR_164,10.21,-0.6,-0.1,0.91 1JKS,LYS 69,10.13,-0.38,0,0 3ERF,LYS 149,10.4,-0.12,0.0.02 1T95,ARG_17,13.34,-0.31,0.43,0.72 2BLL,LYS_382,11.15,-0.31,0.27,0.68 3PBH,LYS 158,10.44,-0.16,0.0.11 3I0C.ARG 81.13.61.-1.07.1.51.0.68 3I0C,LYS_75,10.23,-0.27,0,0 2J8A,ASP_309,3.87,-0.1,-0.12,0.29 1YR6,TYR_142,12.39,-0.02,0.13,2.28 2J8A,LYS 339,10.21,-0.33,0,0.04 3KV0,ASP_174,3.87,0,-0.04,0.11 2GYZ,ARG_40,12.04,-0.54,0,0.08 1H09,ASP_157,2.5,-2.03,-0.07,0.79 1IAP,ASP_156,2.42,-1.35,-0.69,0.65 2CE6,ARG 25,12.59,-0.48,0.12,0.44 2CXA,ASP 138,3.54,-0.37,-0.06,0.17 3BQE,ARG_199,13.54,-0.73,0.69,1.09 2ZCO,LYS_64,10.36,-0.46,0,0.33 1WPA,LYS_444,10.38,-0.15,0,0.03 1MTZ,TYR_81,11.92,0,0.53,1.38 1WYC,ASP_172,3.33,-0.82,-0.05,0.39 2D8N,ARG 43,12,76,-0.33,0,0.59 3G9T,HIS_112,6.11,-0.4,0,0.02 3LMF,GLU 42,3.47,0.5,-1.37,-0.17 3FS3,HIS 182,5.83,-0.45,0,-0.22 2QVO,ASP_89,3.23,-0.51,-0.38,0.32 1N81,LYS_62,11.22,-0.15,0.5,0.37 4DBX,TYR_88,10.34,-0.4,0.03,0.71 3BJV,CYS_135,10.52,0,0.14,1.39 2H2Z,LYS_269,9.97,-0.77,0,0.24 3KT9,GLU_102,4.55,0.07,0,-0.01 20PJ,ARG_211,12.68,-0.55,0.37,0.36 1ZYL,TYR_328,10.11,0,0.06,0.05 2X4J,ASP 127,3.57,-0.24,-0.32,0.33 1UJ8,ASP_56,4.12,0,0.14,0.19 3M66,GLU_154,4.63,0.12,0,0 3O16,LYS_47,10.42,-0.29,0,0.22 1LFP,ARG 37,12.62,-0.57,0.02,0.67 1SQW,LYS_72,10.07,-0.25,0,-0.17 3FHF,GLU_117,4.36,0.34,-0.06,-0.41 3LJN,LYS_262,10.88,-0.3,0.29,0.38 2ZCO,TYR_200,11.71,0.85,0.38,0.48

1D2K,LYS 204,11.1,-0.84,0.85,0.58 1UCH,LYS 121,10.54,-0.18,0,0.21 1D2K,ARG_349,12.67,-0.31,0.03,0.45 1LZL,ARG_313,12.24,-0.25,0,-0.01 3LJN.LYS 167.11.52.-0.4.0.76.0.66 2VGM.LYS 7.10.46.-0.04.0.0 4EVF,ARG_289,12.67,-0.53,0,0.7 2FXT,ASP_405,3.8,-0.55,-0.08,0.64 3EVZ,LYS_75,10.47,-0.28,0,0.25 3T5B.ASP 147.4.-0.23.0.17.0.26 2FM9.CYS 197.9.26.0.0.02.0.24 2NRK,LYS_24,10.25,-0.37,0,0.13 3IBT,GLU_260,3.87,0.28,-0.82,-0.09 10I7,GLU_109,4.63,0.41,-0.22,-0.06 2RIS.TYR 201,11.64,0.85,0.38,0.41 2OB5,HIS_22,6.97,-0.4,0.5,0.36 208I,LYS_38,10.6,-0.12,0,0.22 2FD5,GLU_22,4.99,0.63,0,-0.14 3AUF,TYR 89,12.88,-0.29,0.36,2.8 10LR,GLU_18,5.13,1.5,-0.85,-0.02 2Q5X,ASP_772,2.07,-2.28,-0.26,0.81 3F6F,ASP_2,4.18,-0.97,-0.41,1.76 2P52,ARG_171,12.08,-0.68,0,0.27 2GEN, ASP 8, 3.37, -0.26, -0.48, 0.31 1SIG.CYS 132,9.88,-0.12,-0.25,1.24 2RGY,ASP_157,3.14,-0.73,-0.4,0.47 3E0H,TYR_39,13.79,0,0.15,3.64 3EZ7,ARG_184,13.64,-0.36,0.85,0.65 1XIP,GLU 329,4.71,0.16,0,0.06 1SNT,TYR_27,11.65,0,0.07,1.57 100X.GLU 78.4.93.1.17.-0.75.0.02 2FC3,ARG_31,12.42,-0.23,0,0.15 2APL,TYR 131,12.05,0.46.0.29.1.3 1RZ2.GLU 157.4.78.0.23.0.0.05 2FGG,ARG_25,12.55,-0.31,0.06,0.29 1YTQ,LYS_67,10.49,-0.11,0,0.1 1SFE,ASP_20,3.15,-0.59,-0.37,0.31 1UOH,LYS 162,10.41,-0.11,0,0.02 4D8L,HIS_116,5.42,-0.76,0,-0.33 1X04,LYS_53,10.86,-0.15,0.52,0 2V81,ASP_148,3.44,-0.36,-0.21,0.22 20PJ,CYS 159,11.3,0,0.49,1.8 2X5Y,LYS 729,10.72,-0.16,0.06,0.32 3CN5,ARG_187,12.73,-0.15,0,0.38 3GMS,ARG_40,9.28,-3.33,0,0.11 3HYQ,ARG_50,12.32,-0.28,0,0.1 2Q98,GLU_35,4.74,0.31,0,-0.08 208P.HIS 54.6.19.-0.4.0.0.09 3O48,TYR_88,11.27,0,0.37,0.9 1V6T,LYS_228,11.23,-0.38,0.56,0.56 1KN3,LYS_157,13.23,-0.5,1.95,1.28 2CIU.LYS 149,10,43,-0.07,0,0 2Q98,ARG_89,12.52,-0.85,0.45,0.42 1X04,GLU_35,3.78,0.39,-0.6,-0.52 3P28,ARG_25,12.18,-0.4,0,0.08 1GQE,HIS_253,6.23,-0.29,0,0.01 1NJ4,TYR 222,10,48,0,-0,04,0,52 3L3P,LYS_479,12.17,-0.71,0.99,1.38 3LH5,LYS_787,10.52,-0.35,0,0.37 3ETU,GLU_136,4.49,0.09,0,-0.1 3TOW,TYR 176,11,83,0,59,0,04,1,19 3FHF,ARG_148,12.19,-0.41,0,0.11 1059.LYS 318.10.5.0.0.0 1WLY,GLU_310,4.6,0.29,0,-0.19 3UAH,TYR_230,9.62,-0.72,-0.35,0.69 1XKR.GLU 199.4.52.0.18.0.-0.16 3UV9,LYS_475,10.23,-0.3,0,0.03 1Z9L,ASP_62,3.82,0,-0.27,0.28 3QAV,TYR_82,12.66,0.85,0.78,1.03

2ATR/LYS 6,10.3,-0.31,0.0.11 1DTO,GLU_2,4.41,0.1,0,-0.2 3FNI,GLU_153,4.63,0.16,0,-0.02 1JKS.TYR 234.11.91.0.-0.23.2.14 1RWZ.LYS 53.10.57.-0.16.0.0.22 3T57,CYS 127,10.3,-0.82,0.28,1.86 2OB5.GLU 113.4.61.0.13.0.-0.02 3BWT,HIS_885,6.17,-0.24,0,-0.08 1TLV,GLU_251,4.44,0.33,0,-0.39 2G9D,ARG_247,12.78,-0.3,0,0.59 4F85,CYS 232,11.07,-0.22,0.01,2.27 2B6P,LYS_238,10.42,-0.12,0,0.04 4FZN,TYR_9,12.33,-0.67,0.34,2.66 2R4Q,ASP_224,3.17,-0.67,-0.32,0.36 3ZXY,ASP_100,2.34,-1.96,-0.33,0.83 3CN5,LYS 138,9.97,-0.34,0,-0.19 2CBE,ARG_89,13.09,-0.82,0.85,0.56 10LR,ASP_109,3.28,-0.76,-0.13,0.38 4DVD,HIS_73,5.47,-1.56,0.61,-0.08 1YTD, ARG 282, 12.17, -0.62, 0, 0.29 2GKG,ASP 108,3.24,-0.86,0.0.31 4HDE,LYS_191,11.17,-0.31,0.65,0.33 2B3M,TYR_40,11.13,0,0.05,1.09 2JEO.ARG 168,11.85,-0.69,0,0.04 1NJ4,ARG 287,12,49,-0,37,0,0,37 3V55,LYS_481,10.48,-0.02,0,0 4H86,LYS 8,10,44,-0.06,0,0 3PBH,LYS_50,10.41,-0.09,0,0 2CI3,LYS_250,10.33,-0.17,0,0 2FGG.HIS 85.6.32.-0.18.0.0 4HDE,ARG 30,12.39,-0.09,0,-0.02 2HRZ,GLU_78,3.86,0.31,-0.58,-0.37 3ADO.HIS 90.4.06.-3.13.0.8.-0.11 3IRA,GLU 29,4.41,0.37,-0.05,-0.4 30IP,HIS_45,5.75,-0.66,0,-0.08 3EYE,LYS_81,10.27,-0.23,0,0 3RLE,HIS_18,4.83,-2.17,0.8,-0.29 2Q12,ARG_238,12.33,-0.17,0,0 3HUE,LYS_171,11.08,-1.1,0.52,1.15 3RLN,ARG_721,10.8,-1.72,0,0.01 2RIK,GLU_211,4.55,0.26,0,-0.21 3ILC,ASP_133,3.58,0,-0.41,0.18 2H85,LYS 173,10.63,-0.13,0,0.26 2X4L,GLU_303,3.5,0.42,-1.39,-0.04 2V4U,GLU_510,6.62,4.15,-1.32,-0.69 1NIJ,TYR_258,13.17,0,0.13,3.04 2H85,ASP_132,3.91,-0.01,-0.12,0.25 3MEW.TYR 183,9.6,-0.79,-0.38,0.77 1Q46,ARG_6,12.14,-0.98,0,0.62 1P4X,ASP_122,3.43,-1.07,-0.59,1.29 2RIK,GLU_111,4.03,0.4,-0.62,-0.26 4EKU,GLU 24,4.56,0.06,0,0 1PBV,ARG_170,13.12,-0.75,0.34,1.03 3E7P,GLU_112,4.65,0.13,0,0.01 3JRT,GLU_124,4.62,0.17,0,-0.05 2V5B,GLU_189,3.76,0.51,-1,-0.24 3I47,GLU_156,4.41,0.12,0,-0.21 1JSX,LYS_187,10.49,-0.16,0,0.15 106D,LYS_20,10.38,-0.11,0,-0.01 2P0L,ARG_65,12.31,-0.37,0,0.18 2D7J,LYS 123,11.77,-0.27,0.85,0.69 3LH5,LYS 749,10.65,-0.82,0.85,0.12 4FZR,HIS_325,6.18,-0.46,0.09,0.04 10IS,GLU_267,3.77,0.78,-0.7,-0.81 3P28,GLU_42,4.07,0.44,-0.81,-0.06 3LD1.HIS 355.5.43.-1.68.0.68.-0.08 2D7U,GLU_236,4.8,0.73,0,-0.44 2P0Y,ASP_220,3.95,0,0,0.15 3CX2,TYR_213,10.42,0,-0.05,0.47

2CXA,LYS 167,10.18,-0.33,0,0.01 1P6F,ASP_66,4.03,0,-0.04,0.27 3ZSL,LYS_199,11.34,-0.39,0.85,0.38 1KW4,ARG_51,12.38,-0.12,0,0 1HF8.ARG 157.12.5.-0.34.0.0.34 2B61.TYR 243.10.16.0.-0.01.0.17 2QV2,TYR_279,12.71,0,0.28,2.43 3IVF,TYR_378,13.52,0.73,-0.07,2.86 1Z9L,CYS_121,10.51,-0.77,-0.07,2.36 3OKO.ASP 625.3.45.-0.67.-0.05.0.36 2CWC,ARG_204,12.34,-0.22,0,0.07 1KCM,GLU_138,4.34,0.39,-0.05,-0.51 1YW5,ASP_135,1.77,-2.38,-0.76,1.11 3NBLARG 133,13.87,-0.55,1.41,0.51 1YM5,GLU_76,4.12,1.84,-1.36,-0.86 2XHC,ARG_37,13.91,-0.36,1.35,0.42 3TIR, ARG_170, 13.88, -0.47, 1.44, 0.41 3M7D,ASP_6,2.72,-1,-0.48,0.41 1MIX.HIS 250.5.56.-0.98.0.0.05 3E7P,GLU_204,4.28,0.41,-0.57,-0.06 2H2Z,GLU_288,4.36,1.51,-1.15,-0.5 3I47,LYS_24,10.56,-0.17,0,0.23 3HUE.LYS 41.10.43.-0.04.0.-0.03 1R53.LYS 270.11.31.-0.45.0.85.0.41 1YW5,GLU_64,3.9,0.24,-0.81,-0.04 1A8Q,GLU_243,4.27,0.75,-0.57,-0.43 2A4D,GLU_97,4.03,0.44,-0.46,-0.46 3RKV,ARG 282,11.08,-1.51,0,0.1 4ECC,ARG_149,12.64,-0.94,0.71,0.37 3P2F,HIS_159,6.78,-0.39,0,0.67 1PDB,LYS_63,10.35,-0.15,0,0 20YZ.GLU 69.3.88.0.29.-0.9.0 3U2A, ASP 35, 2.85, -1.29, -0.14, 0.48 3AU3,HIS_598,4.72,-1.62,0.22,-0.38 3PZ9,TYR 220,10.51,-0.32,-0.13,0.96 3OA7,TYR_548,10.09,0,0,0.09 2XMZ,HIS 51,2.64,-3.66,0.78,-0.97 2WOZ.TYR 468,11,56,0,0,25,1,31 2FPN,LYS_124,10.52,-0.1,0,0.12 1X7F,LYS_109,10.36,-0.36,0,0.22 2X5Y,GLU 763,4,28,0,22,-0.06,-0.38 2FI9,CYS 39,12,52,0,-0.06,3,57 2D59,CYS_132,10.94,-1.44,0.75,2.63 1XIP.ASP 146.4.23.0.0.0.43 1YB2,ASP_235,3.25,-0.5,-0.42,0.38 1Q46,LYS 79,10.54,-0.1,0,0.13 2GZR/LYS 271,10.37,-0.13,0.0 3OA7,TYR_517,10.03,0,-0.05,0.08 2V1L,TYR_76,12.46,0.85,0.65,0.96 10TM,ASP 222,3,34,-0.68,-0.05,0.26 1YTD, LYS 223, 10, 88, -0, 37, 0, 3, 0, 44 1WXQ,TYR_140,10.41,0,0.12,0.29 1F2V,GLU_3,4.59,0.09,0,0 307K,GLU_110,4.79,0.29,0,0 2NYC, ARG 263, 12.35, -0.17, 0, 0.02 1UCH,ARG_134,11.32,-1.85,0.01,0.66 2ZCX,ARG_67,11.4,-1.41,0,0.31 3ETV,LYS_137,10.38,-0.18,0,0.06 3ASA,GLU_53,4.61,0.11,0,0 2B0J,TYR 228,9.98,0,-0.37,0.34 2D8N,LYS 131,10.83,-0.23,0.21,0.35 2Z14,TYR_105,11.13,0,0.46,0.67 3CO1,LYS_122,10.98,-0.95,0.85,0.59 3HZQ,LYS 29,10.6,-0.26,0,0.37 3CRM.GLU 78.3.49.0.42,-1.21,-0.22 1XAW,LYS_504,10.71,-0.13,0,0.35 10GL,GLU_110,4.73,0.23,0,0 1Q2Y,CYS_72,11.91,0,-0.65,3.55 3E0H,GLU_130,4.53,1.78,-1.38,-0.36

3LJC.HIS 109.6.3.-0.42.0.0.21 2FL7,TYR_90,12.75,-0.85,0,3.6 3LPZ,ARG_318,12.39,-0.11,0,0 2RGY,GLU_131,4.52,0.31,-0.04,-0.26 1JYH, LYS 128, 10, 46, -0, 77, 0, 21, 0, 52 2AHE,GLU 97,4.68,0.19,0,-0.01 3GA2,LYS_8,10.55,-0.09,0,0.14 3KT9,LYS_39,10.53,-0.1,0,0.13 3G9T,LYS_246,10.69,-0.36,0,0.56 2O34.GLU 104.4.02.0.37.-0.52.-0.33 1PBV.LYS 102,10.32,-0.25,0,0.07 4DND,GLU_58,3.71,0.64,-0.84,-0.59 4GCO,LYS_155,10.67,-0.18,0.16,0.19 2R51.GLU 13.4.37.0.3.-0.1.-0.33 2R0S.TYR 133,10.24,0,-0.09,0.34 3N2T,GLU_94,4.5,0.73,-0.78,0.06 2AH5,GLU_82,3.2,0.62,-1.64,-0.29 3ZRI,ASP_154,3.92,0,-0.04,0.15 1ZHV,LYS 6,10.23,-0.27,0,0 3ZXY,LYS 206,10,49,-0,19,0,0,19 2B61,TYR_335,9.64,-0.63,-0.22,0.49 2PGE,TYR_9,11.91,0.85,0.4,0.66 4FLE,ARG_154,13.32,-0.13,0.38,0.56 2FPN,GLU 33,4.18,0.31,-0.38,-0.25 2CN1,GLU_93,4.66,0.12,0,0.04 2R2Y,GLU_70,2.45,0.51,-1.99,-0.57 3F6F,LYS_86,10.65,-0.11,0,0.27 1H09,TYR_231,11.25,0,0.15,1.09 2IOT,LYS 125,10.62,-0.11,0.0.23 3C6B,LYS_148,10.17,-0.34,0,0.01 3IVF,ASP_221,3.38,-0.57,-0.44,0.59 2AD1,GLU_204,3.8,1.74,-1.6,-0.84 3H13.HIS 302,5.15,-2.12,0.77,0.01 1ES5,CYS_223,11.41,-0.83,-0.22,3.45 3EVZ,ARG_237,12.9,-1.26,0.56,1.1 1PNE,ASP_80,3.75,-0.15,-0.13,0.23 1BGF,ARG 85,12.29,-0.21,0,0 2QEV,GLU_28,3.68,0.47,-0.6,-0.68 1TP6,HIS_11,5.88,-0.34,0,-0.29 1LTU,TYR_36,13.05,-0.84,0.15,3.74 2ILR,GLU_463,4.66,0.12,0,0.04 105J,ARG 36,12.46,-0.15,0,0.11 3PZ9,ARG 387,12.68,-0.8,0.37,0.62 2GYZ,GLU_25,4.35,0.36,-0.54,0.03 3MTT,TYR_460,10.28,0,-0.14,0.41 2DFL,HIS_279,6.32,-0.21,0,0.03 2XMZ,LYS_5,11.02,-0.63,0.11,1.03 1MTZ,GLU_70,4.1,0.46,-0.78,-0.07 3TIR.ARG 194,12.03,-0.51,0.0.04 2V5B,GLU_105,3.37,1.09,-1.26,-0.96 2DG7,ARG 105,12.42,-1.46,0.63,0.76 2WOZ,LYS 576,10.83,-0.2,0.0.52 2B78,ARG_140,12.31,-0.47,0,0.28 3IO0,CYS_111,9.99,0,0.12,0.87 2WB8,HIS_647,3.91,-3.62,0.76,0.28 2IXM,GLU_72,4.39,0.15,0,-0.26 3GOZ,TYR_213,11.54,0,0,1.54 2FBI,LYS 136,10.38,-0.18,0.0.06 1TJE,TYR_103,10.94,-0.04,0.06,0.93 1R7J,ARG 77,12.45,-0.3,0,0.26 2P0Y,HIS 141,6.07,-0.42,0.02,-0.02 3GW3,ARG_50,11.39,-1.33,0,0.2 1G8P,HIS_325,4.05,-2.77,1.05,-0.73 1PZC,GLU_51,4.65,0.11,0,0.04 1X7F,GLU_298,4.62,0.12,0,0 1KN3,LYS_113,10.29,-0.21,0,0 1D2K,TYR_354,12.12,0,0.15,1.97 2YX0,ARG_238,10.06,-3.12,0,0.67 1BKB,ASP_130,3.8,0,-0.2,0.19

4ACJ.LYS 652,10.43,-0.22,0.0.15 1X7F,ASP_274,2.22,-1.44,-0.52,0.38 3JSN,LYS_184,10.64,-0.14,0,0.28 3IO0,ASP_169,4.34,0,0.17,0.37 3RHE,ARG_115,13.05,-1.02,0.69,0.88 3016,HIS 132,6.82,-0.62,0.62,0.31 1LZL,GLU_268,5.59,0.78,0,0.31 1TJE,ARG 191,11.78,-0.8,0,0.08 3BB7,TYR_291,11.81,-1.21,-1.24,4.26 3M66,ARG 374,12.23,-0.27,0.0 3CSR,LYS 88,10,74,-0,37,0,0,61 1UJ8,ASP_28,3.97,0,0,0.17 3FK5.LYS 243,10.41,-0.2,0,0.12 2EA9,LYS 54,10.31,-0.25,0.0.06 2IF4,ARG 175,11.37,-0.88,0,-0.25 1V6T,GLU_22,4.37,0.21,0,-0.34 3M9A,GLU_48,4.56,0.22,0,-0.16 3G9T,ARG_187,12.96,-0.5,0.54,0.42 1EYH,ASP_113,2.93,-1.28,-0.33,0.73 3C6B,LYS 258,10,44,-0.06,0,0 3FK5,ARG_53,12.17,-0.65,0,0.32 1L2F.GLU 132.4.72.0.21.0.0.01 2V5B,GLU_108,4.1,0.33,-0.56,-0.17 3V55,LYS 524,10.12,-0.36,0,-0.03 4AF2.ASP 139.3.39.-1.26.-0.11.0.96 3IRA,LYS_168,10.64,-0.14,0,0.27 2XJ4,CYS_104,10.41,0,-0.17,1.58 2ZCO,GLU_31,4.08,0.47,-0.43,-0.46 3G9T,GLU 279,4.85,0.84,-0.67,0.18 2GZR,ASP_220,3.95,0,-0.2,0.36 4EKU,TYR 90,13,19,-0.85,0,71,3,31 1GPP,CYS_416,9.5,-0.24,-0.55,1.29 4DNU,ASP_367,3.34,-1.51,-0.49,1.54 2CWC,ARG 153,13,14,-0,73,0,84,0,54 1X8F,CYS_166,13.5,0,0.3,4.2 1IAP,GLU_176,4.65,0.22,0,-0.08 4EVF,LYS_128,10.71,-0.11,0,0.32 3MEW, ASP_223, 3.65, -0.83, 0.01, 0.67 3CAX,GLU_159,4.97,0.37,0,0.1 2WB8,GLU_694,3.59,0.71,-0.83,-0.79 3R2E,ARG_114,13.98,-0.39,1.41,0.48 2W2S,CYS 178,9.62,-0.13,0,0.76 1SUU.GLU 761.4.28.0.27.-0.33.-0.17 1DUP,ARG_104,12.21,-0.29,0,0 3QKY,TYR_230,10.89,-0.75,-0.08,1.72 1GQE,TYR_27,11.94,0.85,0.47,0.62 2YYO,LYS 130,10.44,-0.06,0,0 2EFK.HIS 17.6.28.-0.45.0.0.22 100X,LYS_34,11.3,-0.28,0.85,0.22 3JSN,GLU_158,4.72,0.21,0,0.02 3H9W,ARG_91,13.95,-0.56,1.33,0.69 1P6F.TYR 32,9.99.0,-0.23,0.23 1Q46,CYS_97,11.57,0,0.54,2.02 1Y2Q,GLU_28,3.9,0.25,-0.47,-0.37 3F6F,ASP_209,4.13,0,0.03,0.31 1W7B,GLU_139,3.39,2.35,-0.97,-2.5 3FNI.ARG 111.12.32.-0.18.0.0 1FKM,HIS_473,6.55,-0.29,0.18,0.17 3DB9,HIS_252,3.94,-2.59,0.17,-0.14 2FM9,ASP_53,4.01,0,0,0.21 2EJB,HIS 134,6,17,-0,54,0,0,22 2O4D,GLU_122,3.09,0.66,-1.77,-0.3 1WNH,TYR 8,10.02,0,-0.18,0.2 1DUP,ASP_92,3.78,-0.18,-0.05,0.21 3GA2,GLU_107,4.79,0.1,0,0.19 1DUP.ARG 116,12.62,-0.23,0.05,0.3 2BDV,ARG_41,12.19,-0.37,0,0.06 2X4L,LYS_265,11.14,-0.21,0.85,0 4EZB,GLU_149,4.63,0.32,-0.19,0

2PGE,ARG_284,12.38,-0.13,0,0 3RKV.LYS 319.10.71.-0.13.0.0.34 1TD6,TYR_239,12.42,0,0.15,2.27 1SOH,ARG 216,12,72,-0,29,0,0,5 1PZC,LYS_106,10.45,-0.05,0,0 3KV0,ARG_77,12.43,-0.45,0,0.38 2A4D,ASP_113,3.03,-1.08,-0.08,0.39 1XTZ,ARG_223,12.41,-0.13,0,0.04 2E3C,TYR_446,10.46,-0.17,-0.44,1.06 1YB2,GLU_41,4.98,0.28,0,0.19 200K,LYS 23,10.31,-0.2,0,0.02 1PSW,ARG_47,13.8,-0.88,1.62,0.56 2JEO, ASP_150, 3.88, 0, -0.34, 0.41 3GV0,ARG_196,12.32,-0.69,0,0.52 3RHE,ASP_88,3.92,0,-0.14,0.25 1MJS.TYR 237,10,77,0,-0.01,0,77 3L7N,LYS_172,10.63,-0.59,0,0.73 1ANU,LYS_62,10.7,-0.1,0,0.29 3FS3,ARG_68,12.44,-0.22,0,0.16 3B4D,GLU_189,3.74,0.46,-0.85,-0.37 2013.LYS 6.10.57.-0.16.0.0.23 3EJC,GLU_70,4.76,0.52,-0.26,0 2IDC,TYR_111,12.36,0,0,2.36 2098,CYS 191,8.76,-0.52,-0.1,0.38 2CVB.GLU 119.4.78.3.8.-2.53.-0.99 4GCO,ASP_198,4.13,0,-3.47E-18,0.34 2R4Q,ASP_269,2.81,-0.85,-0.39,0.26 1R29,ARG_28,12.36,-0.14,0,0 4FCU,HIS_182,3.25,-3.13,0,-0.12 1SUU,ARG_678,13.14,-0.3,0.44,0.5 4DEZ,ARG_127,12.3,-0.29,0,0.08 2EHG,ARG_94,12.47,-0.36,0,0.34 3LJN,LYS 153,10.86,-0.26,0.25,0.37 4ECC,CYS 191,8.72,-0.09,-0.53,0.34 2H2W,LYS_17,10.41,-0.1,0,0.01 3B21,GLU_183,4.66,0.13,0,0.03 3HYQ,ASP_108,2.81,-1.57,0,0.57 1LZL,GLU_53,4.48,0.28,0,-0.3 2GS5,ARG_5,12.44,-0.09,0,0.02 3IL3,ARG_4,12.51,-0.69,0.1,0.6 1YTQ,LYS_75,10.23,-0.23,0,-0.04 20KT,LYS_288,9.73,-0.68,0,-0.09 4D8L,HIS 33,5.01,-3.23,1.55,0.18 3FHF,ARG_169,13.38,-0.51,0.7,0.69 1GPP,LYS_152,10.66,-0.16,0,0.33 2AD1,GLU_175,4.88,0.65,0,-0.28 2OSA,HIS_277,6.8,-0.46,0.82,-0.06 3RKV,LYS 285,10.57,-0.58,0.43,0.22 4EUG,HIS_73,3.94,-2.39,0.01,-0.18 2FG1,GLU_47,2.66,0.59,-1.81,-0.62 2A0J,ARG_51,12.13,-0.56,0,0.19 2XJ4,ARG 56,13.45,-0.37,0.73,0.59 1V6T,ASP_41,2.68,-1.86,0,0.75 2VGM,ASP_98,3.95,0,0,0.15 1GXN,ARG_604,12.39,-0.4,0,0.28 3P2F,ARG_155,12.42,-0.08,0,0 3RNV,CYS_446,8.25,-0.85,-0.26,0.36 20EW,GLU_293,4.72,0.17,0,0.05 4DVD.ASP 124.3.48.-0.51.-0.15.0.34 4DEZ,LYS_148,11.25,-0.85,0.85,0.75 2QVO,LYS 58,10.44,-0.06,0,0 2E0T.HIS 172.6.35.-0.15.0.0 1UOH,HIS_45,4.63,-2.73,0.54,0.33 3V55,HIS_503,6.45,-0.09,0,0.04 1BKB,ARG_131,13.38,-0.81,0.9,0.79 105T,LYS 412,10.39,-0.3,0.0.19 2Z0M,ARG_263,12.77,-0.39,0.17,0.48 2XWS,GLU_19,4.39,0.23,-0.17,-0.17 3PU6,ARG_138,12.63,-0.31,0.11,0.32

2FM9.LYS 135.10.61.-0.15.0.0.27 3I0C,TYR_255,10.6,0,0.18,0.42 3EVP,TYR_113,10.34,0,0.07,0.28 3IVF,ASP_233,2.78,-0.85,-0.48,0.3 2WZ9.ASP 98.1.63.-2.34.-0.88.1.04 3L3P,GLU 509,4.6.0.13.0,-0.02 2FI9,ARG_108,13.06,-0.31,0.52,0.34 1G5Z,GLU_63,5,1.09,-0.44,-0.15 3NR5,GLU_132,4.55,0.05,0,0 3JSN.GLU 167.7.82.3.63.-0.19.-0.12 2YWJ,ASP_34,2.54,-1.59,-0.29,0.61 2VAN,TYR_296,10.84,0,0.42,0.42 2HXB,LYS_157,10.33,-0.28,0,0.1 2D0A.ARG 38,12.31,-0.42,0,0.23 1R7J.GLU 53,3.8,0.26,-0.61,-0.35 2HXB,GLU_53,4.57,0.07,0,0 2JEO,ASP_161,4.26,0,0.27,0.19 3LD1,ARG_153,12.36,-0.89,0.22,0.54 30NH.ASP 488.3.55.-0.88.0.0.63 2F8H,ARG_227,12.79,-0.29,0.14,0.45 3P51,ARG_16,12.23,-0.32,0,0.07 2EJB,LYS_44,10.32,-0.12,0,-0.06 3C6B,ARG_226,12.41,-0.09,0,0 3CGW.GLU 19.4.84.0.57.0.-0.22 3LMF,ASP_92,3.52,-0.11,-0.35,0.19 2QHT,GLU_181,3.86,0.5,-0.76,-0.38 3RE9,GLU_186,4.67,0.42,0,-0.25 3CCY,GLU 10,4.53,0.13,0,-0.11 2HNG,CYS_103,11.2,0,0.06,2.14 3CS1,LYS_23,10.5,-0.1,0,0.1 4ECC,LYS_100,10.58,-0.07,0,0.15 2D0A, ASP 14, 3, 57, -0.59, -0.01, 0.37 2W1R,GLU_103,5.07,0.31,0,0.26 1IDK,HIS_247,4.81,-2.94,0.52,0.74 1LZL,GLU_96,4.95,0.46,0,-0.01 208P,GLU_140,3.28,0.85,-1.45,-0.62 1MUF,GLU_177,4.45,0.08,0,-0.13 1BYI.GLU 94.3.99.0.34.-0.85.0 2F4Q,ASP_59,3.81,-0.42,-0.13,0.57 1WOU,LYS_40,10.44,-0.06,0,0 3CXS.GLU 156.4.81.0.7.-0.01.-0.38 3KV0.ARG 93,13.82,-0.6,1.24,0.68 3JSN,GLU_47,4.74,0.2,0,0.05 3F6F.TYR 114,11.31,-0.85,0.02,2.14 3CCY,TYR_9,10.14,0,0.07,0.07 1WYC,ARG 251,12.42,-0.41,0,0.34 3IL3.ARG 291,12.8,-0.94,0.7,0.54 1SBX,ASP_133,3.85,0,-0.1,0.16 3OA7,HIS_8,6.24,-0.36,0,0.1 2012.GLU 69.4.48.0.22.0.-0.23 2ILR.GLU 276.4.56.0.06.0.0 1BN6,TYR_57,12.26,-0.01,-0.11,2.36 2J8A, ASP_286, 1.92, -2.62, 0, 0.73 2DFL,LYS_74,10.5,-0.25,0,0.24 1NKD,CYS 54,9.54,0,-0.01,0.55 3RRQ,ARG_94,13.71,-0.95,1.44,0.72 1WXQ,TYR_268,11.38,0,0.25,1.12 2V81,GLU 92,3.66,0.32,-0.61,-0.56 2RIK,LYS_186,11.12,-0.5,0.74,0.38 1J74.ASP 40,3.61,-0.34,-0.16,0.31 2Q99,ASP_211,3.5,-0.85,-0.59,1.14 3US6,GLU_40,5.02,0.43,0,0.09 3V1Q,LYS_662,10.81,-0.12,0,0.42 10I7,HIS_86,7.11,-0.34,0.8,0.14 3V4G,GLU_64,4.24,0.27,-0.36,-0.17 1T07,ARG_63,12.32,-0.2,0,0.03 3CIV,CYS_91,13.69,-0.33,1.19,3.84 1V43,TYR_231,12.68,0.85,0.14,1.7 2YT4,LYS_567,10.43,-0.46,0.04,0.35

2H01.HIS 76.6.8.-2.91.1.6.1.61 3IBT.HIS 126.5.78.-1.05.0.07.0.26 3LMO,GLU_95,4.43,0.23,-0.01,-0.29 1WLY,GLU_204,5.38,0.22,0.32,0.34 1RZ2,LYS 152,9,79,-0,3,0,-0,42 4DNU,ARG 209,12.4,-0.27,0.0.18 3C0C,ARG_328,13.28,-0.31,0.39,0.7 3IDW,ASP_38,4.09,0,0.04,0.26 2D7U,ASP_289,3.99,-0.63,-0.17,0.98 2CW4.ARG 101.12.33.-0.82.0.0.65 2B78,LYS 15,11.08,-0.23,0.44,0.37 1L2F,LYS_129,11.3,-0.53,0.85,0.48 3GOZ,TYR_218,10.21,0,0.04,0.17 2GZR.ASP 62.0.94.-2.76.-0.73.0.63 2VGM.LYS 271,10.45,-0.19,0,0.13 3A2Z,GLU_164,2.59,0.43,-1.57,-0.77 1V8E,ARG_120,12.43,-0.07,0,0 2FG1,LYS_140,10.68,-0.27,0,0.45 2A1V,GLU 70,4.7,0.24,0,-0.04 2CXY,GLU_29,4.63,0.18,0,-0.05 2XWS,HIS_74,5.75,-0.89,0,0.14 3U0V,HIS_175,5.01,-2.46,0.87,0.11 1P4X,GLU_213,4.58,0.12,0,-0.04 1YTD.HIS 364,7.35,-0.23,0.67,0.4 2DG7,HIS_23,6.41,-0.26,0.01,0.17 1ZBM,ARG_68,11.69,-0.83,0,0.02 2Q12,LYS_160,10.5,-0.27,0,0.26 3EUR,TYR 115,12.25,0,0.54,1.71 3FK5,ARG_35,12.15,-0.45,0,0.1 20PJ,ARG_215,12.36,-0.27,0,0.14 1R6Y,HIS_38,7.19,-0.34,0.85,0.18 3CRM,ASP_307,3.62,-0.35,-0.05,0.22 1R5Q,ASP 87,2.97,-1.27,-0.34,0.78 3HVM,TYR_228,10.07,0,-0.27,0.34 3GV0,ASP_126,1.69,-2.53,-0.43,0.86 1V43,GLU_247,4.98,0.6,0,-0.11 3GA2,HIS 227,5.89,-0.69,0,0.09 1ES5,ASP_81,2.38,-2.22,-0.61,1.42 3ULX,GLU_11,4.44,0.1,0,-0.16 1NIJ,ASP_265,4.11,0,0,0.31 1YTQ,CYS_66,9.28,-0.18,-0.25,0.71 2G9D,HIS 19,6.62,-0.15,0,0.27 2V4X.ARG 129,12.6,-0.29,0.0.38 2H85,GLU_3,4.34,0.39,-0.55,0 2E3C,ARG_310,11.92,-0.54,0,-0.04 1MML,LYS_274,10.42,-0.25,0,0.17 1N81,ARG_83,12.83,-0.33,0.04,0.62 3FTT,ASP_99,3.21,-0.77,-0.2,0.39 2GEN,GLU_55,2.9,1.61,-2.16,-1.05 1V43,LYS_116,10.46,-0.05,0,0 1Y0K,LYS 148,10.49,-0.34,0,0.33 3EVZ.TYR 71,10.23,0,-0.34,0.57 1VJG,ASP_153,3.52,-0.35,-0.23,0.29 3C6B,TYR_180,12.36,-0.02,-1.24,3.61 2D8N,LYS_5,10.38,-0.12,0,0 1UOH,GLU_171,4.93,0.18,0,0.24 2CN1,ARG 17,12.55,-0.17,0,0.22 3FXH,ARG_79,13.8,-0.67,1.5,0.46 1S7K,ARG_174,11.65,-0.85,0,0 1PDB,ASP_94,3.74,-0.39,-0.3,0.63 3F6F,ASP 80,3,5,-0,57,-0,14,0,41 1F2V,ARG_16,12.33,-0.17,0,0 2H2W,GLU 159,4.64,0.19,0,-0.05 1T95,GLU_24,3.68,0.49,-0.71,-0.6 2IRM,CYS_21,7.86,-2.62,-0.57,2.05 1SIG,GLU_154,4.73,0.33,0,-0.1 2X4L,LYS_102,10.43,-0.07,0,0 2PPN,GLU_107,4.09,0.27,-0.42,-0.25 3LJC,ASP_85,3.83,-0.36,0,0.39

2EHG,LYS 106,9,76,-0,71,0,-0.03 1ZYL.LYS 238.10.38.-0.12.0.0 3RAZ,ARG_110,12.24,-0.26,0,0 3R2E.GLU 78.3.05.0.79.-1.54.-0.7 4ANN.TYR 205,10,74,0,0,11,0,63 4DIU,LYS 139,10.57,-0.11,0,0.19 2DFL/ARG 320,11,45,-1,42,0,0,37 2AHE,ARG_40,11.46,-2.2,0.32,0.85 3QAV,LYS_123,10.69,-0.17,0.35,0 1NIJ,HIS_215,6.54,-0.41,0.51,-0.05 2EJX,TYR 64,10,19,0,-0,15,0,34 3MEW,ASP_258,2.69,-1.29,-0.41,0.59 1DOV.GLU 95.3.91.0.36,-0.52,-0.43 3I4T.ASP 93.3.09.-0.72.0.0.01 106D,LYS 10,11.22,-0.43,0.7,0.44 1FKM,LYS 263,11,39,-0,34,0.85,0.39 2Q34,LYS_178,10.6,-0.13,0.05,0.17 2B61,TYR_266,13.66,0.07,1.02,2.57 1X91,ARG_69,12.31,-0.23,0,0.04 2AZL,GLU_247,4.71,0.39,0,-0.18 4EF5,TYR_182,12.49,0.8,0.53,1.16 1AIL,ARG_35,12.35,-0.31,0,0.15 3EZ7,TYR_59,10,0,0,0 3VJ8,CYS 70,13.2,-0.01,0.6,3.6 3JRT,LYS 63,10.32,-0.36,0.0.18 3BQE,ASP_357,3.26,-0.48,-0.53,0.47 1Q2Y,GLU_21,4.92,0.52,0,-0.1 1V6T,LYS_246,10.24,-0.22,0,-0.04 1T95,ARG 98,12.17,-0.4,0,0.07 3M3P,ASP_105,3.2,-0.83,0,0.24 100L/HIS 102,5.26,-0.83,0,-0.4 1MJS,ARG_372,12.76,-0.9,0.52,0.65 2HXB,LYS 168,12.16,-0.59,1.7,0.56 3IPZ.GLU 76,4.65,0.19,0,-0.04 2O8P,TYR_67,9.9,-0.8,-0.37,1.08 2EEY,GLU_42,3.9,0.4,-0.59,-0.4 3IL3,LYS_256,10.82,-0.34,0.43,0.24 1SJY,GLU 12,3.35,0.43,-1.58,-0.01 3A7L,GLU_111,3.74,0.68,-1.7,0.26 1BN6,ASP_84,3.36,-0.83,-0.26,0.65 2A1V,GLU_25,4.46,0.94,-0.76,-0.21 3A2Z,TYR 47,9.4,-0.75,-0.33,0.47 2GZO,ARG 89,11.76,-1.33,0.18,0.41 1XEU,ARG_170,13.59,-0.57,0.65,1.01 4F85,ARG_286,13.51,-0.32,0.82,0.51 2V4U,ASP_418,3.42,-0.24,-0.5,0.36 2A6B,GLU_43,4.68,0.17,0,0.01 3HVM,CYS 158,11,21,-1,21,-0,19,3.6 3BB7,TYR_180,10.41,0,0.05,0.37 2O8P,LYS_100,10.44,-0.11,0,0.05 3Q1C,HIS_240,6.4,-0.18,0,0.08 3NR5,ARG 157,12.64,-1.27,0.52,0.89 2BV9,ASP_140,4.31,0,-0.33,0.84 3B79.TYR 15.10.24.0.0.04.0.2 2PGX,ARG_114,11.27,-1.27,0,0.05 2NYC, ARG_288, 13.37, -0.22, 0.82, 0.28 2007.TYR 441.10.16.0.-0.02.0.18 4DEZ,ARG_95,12.44,-0.3,0,0.24 3DHN,ASP_180,2.92,-0.85,-1.01,0.97 3FK5,ARG_220,12.25,-0.33,0,0.09 300P.TYR 4,10.14,0.0.07,0.06 3HVM,LYS_65,10.82,-0.17,0,0.49 1N81.TYR 86.10.16.-0.67.-0.32.1.15 2F4Q,ARG_313,12.51,-0.06,0,0.07 4EKU,LYS_284,10.21,-0.25,0,-0.04 1AD6,ASP 507,3.7,-0.27,-0.1,0.27 2OSA,LYS_280,10.39,-0.09,0,-0.02 3KT9,ASP_37,2.44,-1.68,-0.18,0.5 2A1V,ASP_30,3.95,0,0.05,0.1

3O6L.LYS 22,10,58,-0,19,0,0,28 1WXQ,TYR 64,10.93,-0.04,0.45,0.51 3CIV,HIS_183,4.95,-1.94,0.12,0.27 3PU6, ASP_75, 2.96, -1.65, -0.35, 1.16 3IU5,ASP_107,3.88,-0.27,0.11,0.24 3BPP,GLU 218,4.48,0.15,0,-0.17 4E9E,LYS 514,10.32,-0.28,0.0.1 3N2T,GLU_199,4.93,0.43,0,0 1Z3X,HIS_211,4.98,-2.37,0.82,0.03 1IDK,ASP_255,3.32,-1.15,-0.42,1.1 3AUF,ASP 165,3.55,-0.69,0.06,0.39 2CVB,ASP_141,2.83,-1.17,-0.24,0.44 1J7G,GLU_58,4.58,0.08,0,0 1PVT,GLU_37,4.34,0.09,0,-0.24 20JO.GLU 387.4.77.0.31.0.-0.04 4FCU,ARG 243,13,1,-0,38,0.62,0.37 3CXS,LYS_115,10.17,-0.66,0,0.34 2W2S,TYR_138,13.1,0,0.25,2.85 3CAX,HIS_400,6.29,-1.08,0.79,0.08 3O16,GLU_20,4.57,0.11,0,-0.03 3CGW.GLU 139.4.92.0.31.0.0.11 4GA2,GLU_57,4.45,0.15,0,-0.2 3CCY,ASP_36,2.53,-1.35,-0.27,0.35 3TMO.GLU 200.4.39.1.17.-0.79.-0.48 3UV9.CYS 486.6.29,-3.08,-0.43,0.8 1J74,GLU_121,4.14,1.1,-1.02,-0.44 10XZ,CYS_256,10.88,-0.02,-0.02,1.92 3T8R,GLU_72,4.71,0.14,0,0.07 2V5B,GLU_98,4.68,0.28,0,-0.09 1TR9.TYR 83.10.65.0.0.02.0.62 3CIV,GLU_41,4.7,0.23,0,-0.03 3ONH,LYS_523,9.98,-0.52,0,-0.01 2R51,LYS 59,10.38,-0.08,0,-0.04 2B6P,GLU 232,3.49,0.5,-1.22,-0.29 2AZP,TYR_139,10.41,0,0.07,0.34 1RSS,ARG_79,12.3,-0.2,0,0 3ZXY,ASP_52,2.58,-1.16,-0.38,0.32 4AF2,TYR_118,12.98,0,0.11,2.88 3L7N,ASP_47,1.36,-2.12,-0.93,0.61 2IXM,GLU_57,4.62,0.42,0,-0.3 2Q5X,LYS 841,10.42,-0.08,0,0 3M70,HIS_150,6.54,-0.33,0.01,0.36 3CS1,GLU 111,4.87,0.25,0,0.12 1MN3,GLU_429,3.78,0.36,-0.71,-0.37 1DZF,GLU_160,3.33,0.93,-1.56,-0.55 3H04,ARG_263,12.43,-0.26,0,0.19 3CAN, ASP_111, 3.41, -1.26, -0.03, 0.91 3UAH,ASP_195,3.68,-0.15,-0.56,0.59 2B78,GLU_151,4.47,2.08,-1.59,-0.52 2H2Z,ASP_248,4.27,0,0.15,0.33 2VAN, ASP_116, 3.87, 0, -0.09, 0.16 2CN1,ASP_236,2.52,-1.6,-0.85,1.19 1DZF,LYS_56,10.82,-0.2,0,0.53 3HUE,LYS_318,10.44,-0.22,0,0.16 1T95,ASP_218,4,0,-0.01,0.21 1NIJ,ASP_223,3.83,-0.24,-0.03,0.3 2H85,ASP_78,3.79,-0.85,-0.14,0.98 2NRK,LYS_95,10.37,-0.13,0,0 2E3C,GLU 332,5.32,1.26,0,-0.45 3G9T,ARG_30,13.58,-0.99,1.59,0.48 3GS9,TYR 149,11.22,0,0.16,1.06 200P,LYS 80,10,56,-0,18,0,0,23 4DIU,ASP_175,3.89,0,-0.11,0.21 1DOV,GLU_197,4.82,0.26,0,0.06 3BB7,TYR_51,11.51,0,0.13,1.39 1P1L,LYS_91,10.65,-0.08,0,0.23 2APL,GLU_22,4.61,0.28,0,-0.17 3M3P.GLU 200.4.96.0.21.0.0.25 2VAN,LYS_120,10.53,-0.15,0,0.18

3H5T.GLU 207.4.63.0.17.0.-0.04 1TR9,TYR_223,11.44,0,0.6,0.85 3GW3,GLU_293,4.58,0.17,0,-0.09 2AD1,GLU_69,4.67,0.23,0,-0.07 1CBY.ARG 212.12.52.-0.28.0.0.3 1BKR/HIS 44,5.55,-1.52,0.82,-0.24 4EF5,ARG_180,12.2,-0.32,0,0.02 1BN6,HIS_50,4.73,-3.46,0.8,0.89 1KCM,ASP_160,1.67,-2.43,-1.24,1.52 2IF4.GLU 203.5.22.0.81.0.-0.08 3UAH,LYS_288,10.64,-0.38,0,0.52 1EV8.LYS 140.10.45,-0.06.0.0.01 1ILW,CYS_126,12.58,0,0.06,3.53 2GS5.ARG 179.12.23.-0.7.0.0.43 2D7U.ASP 158.3.11.-1.03.-0.39.0.72 3EJC,LYS_65,11.4,-0.33,0.85,0.38 2YX0,LYS_247,10.7,-0.18,0,0.38 1X6J,ARG_41,12.81,-0.32,0,0.64 1R29.CYS 121.10.58.-0.02.0.01.1.6 2BV9,HIS_290,7.03,-0.33,0.77,0.09 4H4J,GLU_86,4.58,0.08,0,0 2PGX,TYR_134,11.9,0,0.15,1.75 3TIR,GLU_99,3.78,0.31,-0.8,-0.24 3SMD,ASP 141,3.61,-0.15,-0.38,0.35 3COU,LYS_113,10.39,-0.68,0,0.57 2WOZ, ASP_397, 3.84, 0, -0.29, 0.33 1ANU,ASP_121,2.95,-1.38,-0.13,0.67 2G9D,ASP 274,3.51,-0.31,-0.26,0.28 1YOY,ASP_154,3.77,0,-0.18,0.15 3JV1,ASP_62,3.96,0,-0.21,0.36 3ONT,HIS_118,6.46,-0.34,0,0.3 2ZCX.ASP 160.3.41,-0.91,-0.04,0.57 1L3K.GLU 118.3.61.0.29.-0.84.-0.34 30IP,LYS_129,10.01,-0.32,0,-0.17 3H13,LYS_473,10.32,-0.32,0,0.13 3VJ8,GLU_167,3.76,0.54,-0.82,-0.47 3GA2,LYS_186,9.92,-0.3,0,-0.27 1ZP2.GLU 120.4.75.0.25.0.0 1WYC,HIS_31,6.35,-0.61,0,0.46 1BKB,LYS_37,10.16,-0.31,0,-0.03 4FCU,LYS 38,10,72,-0,23,0,0,46 2R4O,GLU 221,2,53,0.63,-1.92,-0.68 2Y2T,LYS_78,10.34,-0.2,0,0.03 200K.LYS 153,10.67,-0.2,0.0.36 2D7U,GLU_311,5.07,0.66,0,-0.08 1HF8,HIS 41,5.26,-0.66,0,-0.58 3VJ8.ASP 108.3.83.0.-0.16.0.18 3CCY,ARG_60,12.38,-0.38,0,0.25 2Q99,ASP_160,3.65,-0.26,-0.06,0.17 2CXA,ARG 2,12.35,-0.16,0,0.01 3LOD,GLU_91,4.65,0.34,0,-0.19 1160, ARG_34, 13.61, -1.41, 1.16, 1.36 20BI,CYS_107,9.72,0,0.11,0.61 1U3Y,GLU_284,3.45,0.76,-1.44,-0.37 4FCU,GLU 101,7.67,2.68,0,0.49 2G5X,GLU_131,4.1,0.46,-0.67,-0.19 1P4X,ARG_208,12.21,-0.33,0,0.04 1XTD,GLU 91,4.01,0.39,-0.85,-0.03 3JZN,ASP_303,3.99,0,-0.05,0.23 4GCO,ARG 195,12.54,-0.36,0.13,0.28 1RSS,GLU_123,5.15,2.09,-1.12,-0.33 2EFK,LYS_56,10.46,-0.04,0,0 3VJ8,LYS_315,10.27,-0.17,0,-0.05 1EDG,ARG 217,10.1,-2.4,0,0 1IAP,TYR_100,11.1,0,0.47,0.63 1R53,GLU_302,4.95,0.59,0,-0.15 3E7P,GLU_136,4.01,0.63,-0.79,-0.32 2FZ4,TYR_97,9.28,-1.11,-0.35,0.73 3ILC,GLU_92,4.21,0.32,-0.81,0.19

30N1.ARG 81.12.1.-0.41.0.0.01 3T5B,LYS 2,10.52,-0.19,0.0.21 3DHN,LYS_139,10.41,-0.25,0,0.16 3BA1,GLU_247,3.56,0.29,-0.8,-0.43 4DEZ,LYS 43,10.39,-0.11,0,0 1KCM,ASP 52,3,31,-0.89,0,0.39 3EJC,HIS_133,6.53,-0.73,0.45,0.31 1SI7,ASP_26,2.64,-2.05,-0.4,1.3 1JSX,GLU_115,4.56,0.12,0,-0.06 3FK5.ARG 203.11.89.-0.77.0.0.16 1ZHV.ASP 117.4.04.0.0.0.24 2WOZ,LYS_471,10.6,-0.11,0,0.21 2B0A,TYR_163,10.36,0,-0.15,0.51 30AV.GLU 104.4.19.1.57.-1.13.-0.75 2Z14.LYS 40.11.56.-0.54.0.58.1.02 1T95,ARG_130,12.34,-0.22,0,0.05 1L2F,LYS_57,10.52,-0.37,0,0.39 1J74,GLU_39,4.69,0.13,0,0.06 2Z84,TYR_135,13.45,0.84,0.6,2 30YB,LYS 904,10,53,-0,34,0,0,36 2QK1,ARG_519,12.18,-0.39,0,0.07 2V4U,GLU_493,3.48,0.24,-0.85,-0.41 2R57,ARG_374,12.01,-0.57,0,0.08 2H2Z,TYR 239,12.67,0,0.21,2.45 1PGV,ASP_223,3.19,-0.83,-0.13,0.35 10TM,LYS_139,10.54,-0.16,0,0.21 2D0A,CYS_227,10.24,-0.34,-0.24,1.83 3V55,HIS 540,6.37,-0.12,0,-0.01 2FGG,ASP 67.2.77,-1.46.0.0.43 2IF4,LYS_272,9.59,-0.97,0.21,-0.15 3BQW,ASP_280,3.3,-1.23,-0.36,1.08 3NR5,CYS_41,8.63,-0.71,-0.23,0.56 2ILR,TYR 396,10.51,-0.29,0.07,0.73 3I4T,TYR_49,12.78,0,0.27,2.51 1V8E,LYS_73,10.03,-0.93,0,0.47 4AF2,ASP_76,3.79,0,-0.15,0.14 1X1E,GLU 161,4.56,0.23,0,-0.17 1RAJ,HIS_199,6.64,-0.36,0.5,0 2CXA,ARG_21,12.94,-0.23,0.38,0.28 2FGG,ASP_79,3.98,0,-0.16,0.34 1R29,LYS_66,10.43,-0.21,0,0.14 1DZF,ASP_74,3.97,0,0,0.17 3N2T,ARG 270,11.88,-2.09,0.52,0.95 4ECC,GLU_25,4.66,0.22,0,-0.05 2WOZ, ASP_474, 3.46, -0.37, -0.59, 0.62 1Q8B,HIS_14,5.77,-0.6,0,-0.12 2PLQ,ASP_11,1.94,-2.31,-0.35,0.8 3F6M,LYS_106,10.43,-0.07,0,0 1WP5.TYR 166.10.57.0.0.17.0.39 4FH3,ASP_148,2.54,-2.71,-0.06,1.51 1BYI,ARG 193,12.27,-0.23,0,0 3LMO,ARG 7,12,28,-0,27,0,0.06 3AUF,ASP_58,3.31,-0.64,-0.21,0.36 3GW3,HIS_339,3.81,-1.96,0,-0.73 1MUF,GLU_176,4.53,0.09,0,-0.06 3LPZ,ARG_165,13.16,-0.53,0.77,0.42 3GE9,CYS_43,9.4,0,0,0.4 2B3M,ASP 120,3.92,-0.81,-0.25,1.18 3BQW,GLU_185,3.92,0.27,-0.45,-0.4 3PZ9,GLU 384,4.26,0.28,-0.37,-0.14 1NIJ.ASP 136.3.58.-0.43.-0.52.0.72 1LPL,LYS_206,10.37,-0.23,0,0.1 3RJX,ARG_195,10.6,-2.01,0,0.11 2GYZ,HIS_21,6.03,-0.43,0,-0.03 3ANJ,TYR 187,10.31,0,0.07,0.24 1RZ2,TYR_167,10.77,0,0.43,0.33 3M3P,GLU_157,4.3,0.21,0,-0.4 2X4G,TYR_208,10.62,0,0.09,0.53 1BN6,GLU_296,4.61,0.44,0,-0.33

20PJ,ARG_149,12.29,-0.36,0,0.16 1PBV.GLU 228.4.7.0.19.0.0.02 3P51,ARG_145,13.29,-0.49,0.62,0.66 1NRI,LYS 224,10.4,-0.28,0.0.18 1K95,ASP_69,2.97,-1.15,-0.26,0.58 1ZBP,LYS 29,10.23,-0.18,0,-0.09 3TRE,LYS_31,10.33,-0.17,0,0 3CXS,TYR_165,11.63,0,0.29,1.33 3H5T,GLU_163,3.5,1.09,-1.3,-0.81 3JSN,ASP 124,4.02,0.0.0.22 3M16.GLU 145.3.97.1.1.-1.37.-0.25 1PV5,ARG_34,12.4,-0.61,0,0.51 3V75,GLU_85,5.2,0.87,0,-0.17 3FHF,HIS_-1,6.14,-0.31,0.03,-0.07 2IDC,GLU 105,5.04,1.89,-0.72,-0.62 3Q1C,ARG_245,13.77,-0.35,1.2,0.41 2CXA,ARG_218,12.43,-0.07,0,0 2CE6,TYR_41,9.7,-1.09,-0.16,0.95 2IXM,GLU_67,4.57,0.07,0,0 1LFP,HIS_171,5.71,-1.27,0.11,0.37 1XIP,LYS_126,10.44,-0.12,0,0.05 1SJY.GLU 118.4.75.0.26.0.-0.01 3MIX.GLU 630.4.57.0.35.0.-0.28 1GQE,LYS 334,10.41,-0.29,0,0.2 1FHL,LYS 280,10.58,-0.19,0.0.27 3RNV,LYS_357,10.44,-0.18,0,0.12 2X4G,HIS_43,6.35,-0.95,0.8,0 2JKF,HIS_130,3.71,-2.79,0.36,-0.35 3RFY,TYR 394,11.56,0,0.58,0.98 2IRM,GLU_344,4.53,0.11,0,-0.08 3C2E,GLU_81,3.97,0.31,-0.66,-0.18 3CN5,ARG_225,9.95,-2.87,0,0.32 3PP8,GLU 297,3.54,0.57,-1.06,-0.48 1AIL.ASP 29,3.14,-0.83,-0.16,0.34 1L2F,GLU_296,4.64,0.32,0,-0.18 1MTZ,TYR_243,10.83,0.28,0.27,0.28 3M16,HIS_223,6.26,-0.62,0.43,-0.04 3G6S,ASP 63,4.02,-0.07,-0.57,0.87 4FZR,HIS_292,5.37,-1.13,0,0 1WXQ,GLU_52,4.48,0.2,0,-0.21 2D0A,GLU_21,4.56,0.1,0,-0.04 3LPZ,HIS 151,3.89,-1.95,0,-0.65 4EKU.GLU 268,4,41,0,38,-0,09,-0,38 2IF4,ASP_148,3.92,-0.61,-0.18,0.92 1M5I,LYS_153,11.47,-0.2,0.77,0.4 4D8L,GLU_117,4.35,0.23,0,-0.39 2HRZ,HIS 152,6.53,-0.33,0.36,0 2AZL,LYS_272,10.24,-0.25,0,-0.01 3UAH,TYR_290,13.73,0.79,0.94,2.01 2HNG,GLU_34,4.59,0.1,0,-0.01 2P52,ARG_246,13.19,-0.8,0.72,0.76 2RIS.ASP 28.3.47,-0.78.0.15.0.29 1QYI,LYS_221,10.38,-0.33,0,0.22 2G2D,ASP_56,3.32,-0.97,0,0.49 1X7F,GLU_233,3.96,0.23,-0.65,-0.11 1J7G,LYS_48,10.21,-0.31,0,2.78E-17 2J8A.GLU 277.4.63.0.21.0.-0.08 20PJ,ASP_148,4.01,0,-0.15,0.36 1P2F,TYR_213,10.74,-0.56,-0.18,1.49 1PVT,ASP_50,4.18,0,0.06,0.32 2P5D,LYS 100,11,32,-0,41,0,85,0,38 2XHC,LYS_139,10.59,-0.11,0,0.2 1M5I.TYR 159.10.39.0.-0.06.0.45 3EX9,TYR_30,12.06,-0.07,-1,3.13 2ZTY,GLU_99,4.6,0.2,0,-0.09 2CVB.ASP 75.2.68.-1.38.-0.42.0.68 2Q99,LYS_300,10.48,-0.11,0,0.09 3Q6L,CYS_2,9.04,-0.67,-0.36,1.06 1R9W,ASP_220,3.95,0,-0.11,0.26

2XMZ,GLU_263,4.41,0.29,0,-0.39 1RAJ,GLU_382,4.3,0.51,-0.72,0.01 4EVF,ARG_116,13.13,-0.32,0.47,0.49 1XIP.GLU 114,5.05,0.17,0.0.38 3LOD,GLU_58,4.74,0.28,0,-0.04 2EYI,CYS 180,12.17,-0.11,0.08,3.2 2R0S,HIS 54,7,34,-0.58,0.81,0.61 1HUF,GLU_50,4.69,0.26,0,-0.08 2XMZ,ASP_59,3.89,0,-0.08,0.18 3H5T,TYR_340,10.47,0,0.18,0.29 2AXO,LYS 195,10.39,-0.11,0,0 1G8P,GLU_73,3.31,0.33,-0.9,-0.62 2CL3,LYS 29,10.62,-0.26,0.0.38 1MML,ASP_216,3.91,0,-0.07,0.18 3BB7.TYR 245.10.23.0.0.06.0.16 3CS1,ASP 68,3.87,-0.15,-0.03,0.25 1F2V,CYS_76,13.63,0,0.93,3.7 2BDD,LYS_96,11.4,-0.44,0.68,0.66 2CBE,GLU_234,3.43,0.16,-0.85,-0.38 2RIK, ASP 255, 2.89, -1.88, -0.58, 1.55 3M66.GLU 170.4.82.0.3.0.0.02 2GAU,GLU_117,3.94,0.25,-0.43,-0.38 3MIX,TYR_651,10.36,-0.11,0.19,0.28 3MTT,LYS 558,10,47,-0.08,0,0.04 3BWT,HIS 849,6.39,-0.43,0.0.32 3C5V,GLU_295,4.7,0.28,0,-0.08 1XIPLYS 5,10,41,-0,12,0,0.02 3ERF,GLU_142,4.35,0.2,-0.35,0 2EJX,ASP_15,3.74,-0.25,-0.14,0.34 1NAF,LYS 295,10.39,-0.19,0.0.09 2HXB,TYR_32,11.99,-0.8,0.39,2.39 4EUG,TYR_93,13.21,0,0,3.21 20VO,LYS 52,9.67,-0.77,0,-0.06 3K8J.GLU 64.4.63.0.3.0.-0.17 3DTE,ASP_94,4.06,0,0.13,0.14 2VGM,ASP_75,3.65,-0.34,-0.17,0.36 3UV9,LYS_372,9.94,-1.54,0.55,0.43 2PLQ,TYR_192,12.2,-0.83,1.06,1.97 1EV8,TYR 242,10,58,-1,42,-0.08,2.08 3LD1,ARG_152,12.25,-1.54,0.75,0.55 3IVF,TYR_71,10.84,-0.84,0.3,1.39 2R51,TYR_284,11.1,0.27,0.18,0.65 1KW4.GLU 43.4.63.0.11.0.0.02 3LJI,ARG_267,12.85,-0.61,0.53,0.44 1FHL,LYS_67,9.88,-0.61,0,-0.01 1YM5,LYS_201,10.47,-0.69,0.18,0.47 1MD6,ASP_138,4,0,0,0.2 1R3F.GLU 285,3.11,0.89,-1.64,-0.63 1WPA,ARG_459,12.38,-0.21,0,0.08 3I47,GLU_9,4.32,0.29,-0.32,-0.15 3E5T,HIS_193,5.38,-2.23,0.85,0.26 30DJ,LYS 10,10.48,-0.05,0,0.02 2JHY,ARG_152,12.56,-0.52,0,0.59 2ZCO,TYR_248,11.87,-0.29,-0.93,3.09 2E3C,GLU_207,4.58,0.08,0,0.01 2YX0,LYS_50,10.63,-0.19,0.07,0.25 1SUU,LYS_623,10.22,-0.5,0,0.22 3L7N,ARG_164,11.67,-0.92,0,0.09 3BJV.LYS 8,10.41,-0.15.0.0.06 3Q1C,LYS_237,10.55,-0.21,0,0.25 1R5Q,ASP 37,2.9,-0.74,-0.55,0.39 3CO1.CYS 55.11.49.-0.14.0.02.2.61 2CWY,LYS_30,10.42,-0.08,0,0.01 2DVK,GLU_74,4.05,0.34,-0.5,-0.3 1YG2,ARG_76,12.19,-0.33,0,0.02 2BAA,ASP_141,3.83,-0.16,-0.7,0.88 1YM5,ASP_191,3.71,0,-0.26,0.17 3RFF,ARG_78,12.27,-0.24,0,0.01 2QV2,HIS_226,6.4,-0.88,0.62,0.15

1TUL,LYS 58,10.66,-0.31,0.39,0.08 1ZCU,GLU_56,4.45,0.79,-0.8,-0.03 1DUP,GLU_17,4.74,0.37,0,-0.13 3ZSL,HIS_158,5.91,-2.1,1.1,0.41 1EW4.ARG 82.12.61.-0.14.0.0.25 2X4L.LYS 220,10.02,-0.68,0.0.2 3M70,LYS_45,12.47,-0.47,1.59,0.84 1WXQ,ASP_315,3.46,-0.4,-0.45,0.51 1WLY,LYS_224,10.67,-0.12,0,0.3 3GS3.GLU 99.4.18.0.69.-0.71.-0.32 105T,ASP_209,3.88,-0.13,0,0.21 20GO.HIS 538.6.06.-0.25.0.-0.19 3ANJ,LYS_135,10.6,-0.2,0,0.3 200K.HIS 293.5.62.-1.63.0.77.-0.01 2B6P.ARG 5,12.36,-0.14,0,0 1WP5,HIS_81,5.79,-0.89,0.11,0.06 3H5T,ARG_162,12.21,-0.39,0,0.1 2H85,GLU_145,4.55,0.52,0,-0.47 3CIV.CYS 143.11.57.-0.86.0.31.3.12 1CBY,ARG_25,12.41,-0.09,0,0 2ZCX,GLU_204,4.63,0.22,0,-0.08 3U2R,TYR_18,9.72,-0.53,0,0.26 3BA1,ARG_260,12.72,-0.12,0,0.35 3EVN,ARG 38,12,45,-0,11,0,0.06 1P1L,ASP_95,4.19,0,-0.01,0.4 3SMD,GLU_59,4.23,0.4,-0.73,0.05 3CS1,GLU_52,4.47,0.31,-0.03,-0.32 3CNU,GLU 55,3.59,0.52,-0.85,-0.57 3BWT,LYS_619,12.21,-0.62,1.22,1.1 2H2W,ASP_200,3.23,-0.85,-0.32,0.59 2F8H,ARG_38,12.28,-0.34,0,0.12 1DTO.ASP 28.3.11,-0.85,-0.43.0.58 20GO.ARG 507.12.55.-0.06.0.0.12 2CN1,TYR_249,13.42,0,0.53,2.89 1RL0.ASP 219.2.29.-1.6.-0.39.0.48 1PBV,LYS_71,10.11,-0.33,0,-0.05 3B4D,GLU_186,4.9,0.21,0,0.19 1KCM,ASP_16,4.1,0,0.05,0.25 3GMS,TYR_124,12.13,-0.79,0.03,2.88 3F5D,LYS_192,10.79,-0.29,0,0.59 3HVM,LYS 129,10.36,-0.25,0,0.11 1L2F.GLU 120.4.4.0.33.0.-0.43 1X04,TYR_57,10.21,-0.49,-0.01,0.7 2G2D.GLU 140.3.85.1.22.-1.58.-0.29 3N0K,ASP_150,4.28,0,0.29,0.19 3RLN,GLU_607,4.14,0.33,-0.64,-0.04 3GE9.GLU 138.4.51.0.22.0.-0.21 2I6I,TYR_2,12.95,0,0.15,2.8 2D0A, ASP_130, 3.77, 0, -0.3, 0.27 1YLN,ASP 152,3.87,0,-0.11,0.19 2BLL,ARG 601,12.34,-0.16,0.0 1T07,GLU_13,4.29,0.22,-0.42,-0.01 3LH5,HIS_692,6.09,-0.23,0,-0.18 1NFN,ARG_114,11.69,-1.05,0,0.25 2CXY,GLU_100,3.54,1.83,-2.4,-0.38 1R7J,LYS_78,10.64,-0.15,0,0.29 1R53,ASP_61,3.83,0,-0.5,0.53 3BZT,ARG 313,12.28,-0.23,0,0.01 1AKO,GLU_254,4.55,0.08,0,-0.03 1I60, ARG 74, 12.41, -0.57, 0.12, 0.37 2Q34,ASP_194,4.18,0,0.05,0.33 3M7G,GLU_13,4.57,0.07,0,0 1ZCU,LYS_208,10.38,-0.46,0,0.34 3GS3,LYS 22,10.47,-0.03,0,0 3IRA.GLU 82.4.96.0.29.0.0.17 2FXT,LYS_307,9.69,-1,0,0.18 1P6F,HIS_15,5.63,-0.96,0.01,0.08 4H86,ARG_-6,12.46,-0.04,0,0 4DIU,GLU_12,4.18,0.34,-0.62,-0.04

1XDZ.CYS 74.13.74.-0.08.1.04.3.78 2l6l,ASP_47,3.63,-0.82,0.24,0.41 1ILW,LYS_43,10.13,-0.6,0,0.23 2PGE,ASP_92,3.82,-0.12,-0.03,0.17 2098.LYS 115.10.26.-1.08.0.4.0.43 3GV0.LYS 65,10.49,-0.05,0.0.05 2Q5X,ASP_828,4,0,-0.03,0.23 1CBY,ASP_147,3.58,-0.71,0,0.48 3BQW,TYR_314,10.6,-0.74,0.09,1.26 3ETU.GLU 78.5.1.0.53.0.0.06 2A0J.ARG 130,12.07,-0.52,0,0.1 3CBN,GLU_82,3.94,0.34,-0.78,-0.14 1XWM,HIS_153,6.87,-0.37,0,0.73 1MIX.GLU 252,2.66,0.29,-1.47,-0.66 2EFK.LYS 150.10.59.-0.22.0.02.0.29 3BCY,ASP_41,4.35,0,0.28,0.28 2FBI,LYS_82,10.26,-0.24,0,0 4DEZ,GLU_88,4.97,0.21,0,0.25 3RFY,GLU_379,6.3,1.81,0,-0.01 3HKX.ARG 206.11.64.-1.53.0.0.67 2B3M,LYS_47,10.58,-0.18,0,0.26 2F4Q,ASP_306,3.3,-0.82,-0.13,0.46 1BYI,CYS_20,12.33,-0.07,0.67,2.72 3JSN,ARG 270,12.51,-0.29,0,0.31 1WNH,LYS_134,9.79,-0.71,0,-0.01 2V4U,TYR_554,12.11,-0.33,0.55,1.9 2XHC,ARG_326,13.3,-0.25,0.49,0.56 3DHN,GLU 152,3.19,0.95,-1.79,-0.46 2FG1.CYS 25.12.84.0.0.15.3.7 3OKQ,GLU_668,4.65,0.15,0,0 3M70,TYR_98,11.72,0,0.24,1.48 3GFP,ASP_442,2.2,-1.69,-0.5,0.59 100X,GLU 88,3.94,0.29,-0.74,-0.11 3KEY,ARG_374,12.69,-0.27,0,0.45 3O16,ASP_124,3.39,-0.15,-0.55,0.29 1NAF,GLU_172,4.7,0.2,0,0 3UPD,LYS_263,10.47,-0.13,0,0.1 3GOZ,TYR_35,10.19,0,0,0.19 1RL0,ASP_134,2.17,-1.75,-0.35,0.49 3IO0, ARG_112, 12.19, -0.34, 0, 0.03 2QVO,ASP_75,3.86,0,-0.08,0.14 1XDZ,GLU_207,4.65,0.32,-0.09,-0.08 3M7G,TYR 30,12,2,0,0,52,1,69 1EYH,GLU_125,4.45,0.23,0,-0.28 1H09,ARG_298,12.45,-0.05,0,0 1ES9,HIS_187,5.87,-0.29,0,-0.34 2B3M,ARG_41,12.39,-0.22,0,0.1 1EV8,ARG_234,13.36,-0.55,0.8,0.6 105T.GLU 408.5.05.0.68.0.-0.13 3U4K,TYR_117,10.19,-0.07,-0.02,0.28 1W7B,LYS 47,11.58,-0.33,0.85,0.55 2ATR.GLU 97.4.59.0.09.0.0 3FTT,ARG_39,12.29,-0.21,0,0 3C0C,HIS_349,6.39,-0.29,0,0.19 3CIV,GLU_263,4.85,0.52,0,-0.17 2CXA,HIS_82,5.57,-1.04,0,0.12 3QKY,ARG 278,12.24,-0.1,0,-0.16 2RH3,ARG_156,13.04,-0.94,1.01,0.47 3MIX,LYS_498,10.54,-0.24,0,0.28 10LR,GLU_205,7.21,2.77,-0.79,0.73 2B78.GLU 323.4.64.0.09.0.0.05 3M7G,TYR_149,11.33,-1.27,-0.48,3.08 3PZ9,ASP_337,3.95,-0.85,-0.09,1.08 4EKU,GLU_172,4.83,0.33,0,0 10IS,LYS 265,10.38,-0.19,0,0.07 1XAW,LYS_433,10.39,-0.24,0,0.12 3MIX,GLU_378,4.67,0.61,-0.1,-0.34 1EYH,ASP_66,2.88,-1.32,-0.49,0.9 3I0C,ARG_187,11.67,-0.95,0,0.11

3LJC,LYS_176,10.53,-0.33,0,0.35 3RLE,ASP 140,3.08,-0.85,-0.29,0.42 1ZBS,ARG_259,13.4,-0.31,0.79,0.42 1V43,ASP_37,3.82,-0.32,0.04,0.31 3FNI,GLU_49,5.05,0.24,0,0.31 2AXO,ARG_181,11.74,-0.77,0,0.02 1WRU,ARG_73,12.19,-0.32,0,0.01 2EFK,HIS_181,6.34,-0.19,0,0.04 1MIX,GLU_293,4.12,0.3,-0.42,-0.25 3EVN.GLU 31,4.24,0.26,0,-0.52 2CVB,HIS 44,6,45,-1,34,0,85,0,44 2X4L,ARG_182,13.58,-1.05,1.13,0.99 3BQW,ARG_231,12.39,-0.51,0,0.4 1KCM.ASP 256.3.97.0.0.0.17 2B78,LYS_277,10.15,-0.11,0,-0.24 2CI3,ARG_98,11.43,-0.72,0,-0.35 1DCF,TYR_66,11.76,-0.18,0.6,1.33 2GS5,ASP_4,3.07,-0.68,-0.28,0.22 2ZTY,LYS 108,10.33,-0.17,0,0 3O48,LYS_117,10.98,-0.36,0.4,0.43 3GS9,ARG_123,12.76,-0.33,0,0.58 2B2H,LYS 293,10.3,-0.2,0.0 2BV9,ARG_33,11.8,-1.15,0,0.45 1ZCU,ARG 29,12.44,-0.06,0,0 1Y2O.GLU 143.4.54.0.18.0.-0.14 2H14,LYS_70,9.72,-1.01,0,0.23 2Z0M,ARG_247,13.46,-0.36,0.79,0.53 2ZCO,LYS 72,10.52,-0.18,0.19,0.02 3HVM,GLU_221,4.3,0.54,-0.24,-0.5 3JZ9,GLU_347,4.56,0.22,0,-0.15 3A2Z,GLU_196,4.84,0.37,0,-0.02 2JKF,GLU_64,4.69,0.19,0,0 3Q6L,LYS 121,10.61,-0.13.0.0.24 2FI9.GLU 65.4.15.1.08.-1.28.-0.15 1WNH,HIS_7,5.94,-0.44,0,-0.12 1NWA,GLU_136,4.08,0.4,-0.61,-0.22 3ZSL,ARG_224,13.37,-1.04,0.93,0.98 3RJX,TYR 95,10.66,0,0.43,0.24 2D7J,ARG_121,12.62,-0.26,0,0.38 100X,LYS_17,10.46,-0.35,0,0.31 3ERF,GLU_172,4.45,0.11,0,-0.16 2FPN,LYS 187,10.27,-0.38,0,0.15 1ZCE,ARG 89,13,44,-0.35,0.51,0.77 3NR5,ASP_60,3.88,-0.2,0,0.28 3IBT,CYS_209,11.16,-0.2,-0.71,3.08 1SQH,GLU_137,4.66,0.27,-0.05,-0.06 2EHG,LYS 89,10.36,-0.14,0,0 2ZCO.GLU 139.3.66.2.17.-2.54.-0.47 3BQE,GLU_312,5.42,1.63,-0.21,-0.51 4FCU,ASP_91,4.18,0,0.18,0.2 2B61,ARG_271,12.98,-0.55,0.53,0.5 30NT,HIS 125.6.13,-0.32,0,-0.05 2GZR,LYS_46,10.43,-0.26,0,0.2 3H6Q,TYR_157,11.59,-0.02,-0.22,1.83 3M3P,ASP_48,4.09,0,-0.03,0.32 1X9G,LYS_12,10.32,-0.3,0,0.13 1YTD.ARG 318.12.47.-0.03.0.0 1LZL,CYS_102,13.24,-0.01,0.34,3.91 2F8H,GLU_93,4.66,0.06,0,0.1 1C3K,LYS_49,10.43,-0.38,0,0.31 3ASA.GLU 151.4.71.0.31.0.-0.1 2ZCO,HIS_12,6.23,-1.39,0.85,0.27 3ZSL,ASP_207,3.71,0,-0.29,0.19 3TIR,ARG_97,12.42,-0.08,0,0 2VAN,GLU_117,4.6,0.32,0,-0.21 3JZ9.LYS 362.10.39.-0.11.0.0 1RSS,ARG_95,13.26,-0.91,1.22,0.45 2JEO,HIS_98,6.11,-0.54,0,0.16 2BT8,TYR_180,10.32,-0.06,0.1,0.27

3UC9,ASP_91,2.88,-1.56,-0.29,0.94 1AM2.ARG 145.12.29.-0.3.0.0.09 307K,GLU_104,4.53,0.15,0,-0.12 3BB7,LYS_167,9.47,-1.15,0,0.11 1BKB,ASP_57,1.56,-2.34,-0.49,0.59 2OJQ,ASP 500,3.91,-0.01,-0.18,0.3 1FKM,ASP 588,4.04,0.0.08,0.17 2ZQ5,GLU_138,4.84,0.35,0,-0.01 3T5B,GLU_316,4.79,0.18,0,0.11 1YR6,HIS_240,5.96,-1.56,0.84,0.18 4FH3,GLU 61,4.2,1.38,-1.3,-0.38 1H4U,GLU_542,4.04,2.77,-1.43,-1.8 3NR5,CYS_112,9.57,-0.06,0.21,0.4 2VAN,ARG_299,12.2,-0.35,0,0.05 1DOV,LYS 181,11.31,-0.4,0.54,0.67 4H89,ASP_36,3.3,-0.84,-0.01,0.35 30NH,GLU_501,3.47,0.5,-1.15,-0.38 3IU5,CYS_138,9.28,-0.11,-0.4,0.78 1NAF,ARG_207,12.85,-0.21,0,0.56 3BQE,LYS 260,11.58,-0.31,0.85,0.54 2B0J,ASP_287,4.18,0,0.12,0.26 2B78, ASP_358, 4.29, -0.31, 0, 0.8 20BI,LYS_125,10.3,-0.17,0,-0.03 2PGX,ASP 91,3.38,-0.83,-0.63,1.05 1X7FLYS 171.10.54,-0.17.0.0.21 3C38,ASP_194,3.9,0,-0.33,0.43 3BCY,TYR_123,13.67,0.82,0.58,2.27 3IVF,ASP_264,4.38,0,0.29,0.3 2W2S,TYR 83,12.6,0,-0.01,2.62 100H.LYS 68.10.78.-0.14.0.0.41 3UX2,GLU_153,4.88,0.38,0,0 2R2Y,LYS_103,10.28,-0.32,0,0.1 1FHL.LYS 107.10.39.-0.28.0.0.17 3V10.ARG 629.12.63.-0.21.0.13.0.2 1UXO,ASP_118,3.38,-0.65,-0.15,0.39 1L3K,ARG_178,12.45,-0.41,0.09,0.27 3GS3,LYS_121,10.16,-0.29,0,-0.05 1UXO,GLU_167,3.15,0.43,-1.44,-0.34 1WXO.ARG 258,11.86,-1.51,0.06,0.82 3RFY,ASP_405,3.83,0,-0.2,0.23 3CRM,ARG_276,12.67,-0.28,0,0.45 2OSA,GLU_449,5.11,0.91,-0.14,-0.17 1FHL.LYS 228.10.36.-0.14.0.0 1JKS,LYS_175,9.71,-1.03,0,0.24 3EVN.LYS 85.11.75.-0.28.0.76.0.76 3U0V,HIS_20,5.44,-1.23,0.23,-0.05 2DVK,HIS_52,5.58,-0.77,0.29,-0.44 109G,HIS 207.6.14,-0.66.0.0.3 1WP5,TYR_195,10.7,-0.09,-0.29,1.08 1SJY,GLU_125,3.98,0.34,-0.72,-0.14 1SIG,LYS_426,10.36,-0.33,0,0.19 2ZTY,HIS 40,4.91,-1.53,0,-0.06 3RFY,ASP_114,3.74,0,-0.26,0.2 1AT0,CYS_258,9.54,-0.8,-0.23,1.57 2D8N,LYS_55,10.39,-0.15,0,0.05 1W7B,ARG_295,12.99,-3.11,1.41,2.18 1RAJ,ARG_437,12.27,-0.25,0,0.02 2JKF,GLU_146,4.78,0.34,0,-0.06 1DZF.ARG 167.12.94,-0.2.0.05.0.59 3E5T,GLU_175,4.69,0.38,0,-0.18 2QV2,ARG 57,13.38,-0.53,0.74,0.66 2CIU,LYS 193,10,5,0,0,0 2H2Z,TYR_126,12.73,-0.85,0.86,2.7 2R0S,LYS_78,11.82,-0.37,0.92,0.77 2BQQ,ASP_130,4.15,-0.83,-0.05,1.23 1Q46,LYS_136,10.25,-0.41,0,0.17 1Y2Q,CYS_127,10.08,0,0.28,0.8 2BAA,HIS_206,7.18,-0.36,0.87,0.18 3LQE,TYR_250,10.28,0,0,0.28

1GXN.LYS 501.10.39.-0.15.0.0.04 1QQL,TYR_74,11.85,0.29,0.64,0.92 3EVN.HIS 237,4.41,-1.61,0,-0.48 3RHE,TYR_11,12.53,0.05,-0.15,2.63 2ZCO.LYS 35.10.5.-0.63.0.0.62 3G6S,ARG 116,12,32,-2,04,0,31,1,55 1ES9,HIS_91,6.21,-0.3,0,0.02 2HRZ,ARG_273,13.47,-0.33,0.69,0.62 3C38,HIS_74,6.54,-0.58,0.34,0.28 2013.ARG 299.12.11.-0.68.0.0.29 3M66,LYS_246,9.75,-0.41,0,-0.35 1MTZ.TYR 19.9.94,-0.78,-0.31,1.03 1NIJ,CYS_66,12.84,0.53,0.86,2.45 3GFP.ARG 463,13.6,-0.32,0.72,0.7 105T.TYR 214.10.28.0.0.01.0.27 3BCH,ARG_80,12.07,-1.23,0.19,0.6 3CZC,GLU_43,3.7,0.25,-1.05,0 1AKO,ARG_216,12.96,-0.32,0.23,0.56 2VGM.TYR 113.10.12.0.-0.04.0.16 2FG1,LYS_87,10.38,-0.16,0,0.04 4ETX,CYS_446,11.27,0,-0.09,2.36 2E3C,ARG_290,12.21,-0.44,0,0.15 3UPD,GLU_89,4.87,0.26,0,0.12 1W24.LYS 30.10.34.-0.16.0.0 1AK1,LYS_188,10.46,-0.24,0,0.19 3EZ7,HIS_323,6.31,-0.21,0.17,-0.14 3BPV,ARG_124,13.19,-0.29,0.22,0.74 20EW,CYS 231,10.98,0,0.01,1.97 3FNI,HIS_154,5.7,-0.26,0,-0.55 4GCO,ARG_252,12.48,-0.12,0,0.1 1WRU,ARG_158,11.1,-1.15,0,-0.25 20V2.ARG 327.12.58.-0.41.0.0.49 3IBT.GLU 15.2.75.0.76.-1.67.-0.84 1TP6,ARG_70,12.41,-0.08,0,-0.02 1PNE.GLU 82.4.81.0.29.-0.01.0.04 3G9T,LYS_281,10.15,-0.46,0,0.12 3CZC,GLU 83,2.5,0.66,-2.26,-0.39 4DBX.CYS 34,11.73.0.0.09.2.65 3IL3, ASP_147, 3.89, -0.49, -0.07, 0.65 1AK1,ASP_42,3.59,-0.35,-0.3,0.43 3UC9.GLU 124.4.52.0.16.0.-0.15 1WXO.GLU 380.3.87.0.5.-0.8.-0.33 1LTU,TYR_155,12.97,-0.85,0,3.82 4F85,ARG_238,12.35,-0.1,0,-0.06 1ZBM,GLU_189,4.59,0.21,0,-0.13 3NBI,GLU_193,4.88,0.28,0,0.1 3T5B,ARG 327,13.1,-0.39,0.31,0.67 2X5Y,GLU_811,4.44,0.22,0,-0.28 1RZ2,ASP_101,2.66,-1.58,-0.05,0.49 3CZC.GLU 63.3.11.0.27.-1.01.-0.64 4E8B.TYR 210.11.14.0.45.0.34.0.36 4FH3,ARG_73,12.15,-0.74,0,0.39 3ZRI,LYS_146,10.41,-0.09,0,0 3U2A,LYS_77,11.38,-0.28,0.85,0.31 2P5D,LYS_80,11.17,-0.21,0.52,0.35 3EVP,ASP_291,3.32,-0.34,-0.35,0.2 1YOY,HIS_15,6.31,-0.17,0,-0.02 1YTD,ARG_260,12.76,-0.49,0.46,0.29 3EIZ,LYS_122,10.44,-0.21,0,0.14 2FPN,TYR 92,10.22,-0.19,-0.45,0.86 100X,GLU 158,4.12,0.32,-0.27,-0.43 2YX0,LYS_256,10.75,-0.24,0,0.48 4ESS,GLU_82,3.89,0.46,-1.12,0.05 2QK1,LYS 427,10.38,-0.13,0,0.01 300P,GLU_76,4.54,0.15,0,-0.11 4E8B,LYS_60,10.48,-0.05,0,0.03 1ZBM,GLU_118,4.62,0.22,0,-0.1 3BPP,ARG_156,12.17,-3.55,1.18,2.03 10I7,LYS_285,10.4,-0.1,0,0

3I82.ARG 15.12.39.-0.11.0.0 2YX0,GLU_113,3.75,1.31,-1.65,-0.41 2F9F,ASP_154,3.6,-0.3,-0.21,0.29 1PSW,ARG_303,12.34,-0.33,0,0.17 1T95.GLU 96.4.21.0.22.-0.52.0 3S0A,LYS 82,10.64,-0.17,0.0.3 2AXO,LYS_43,11.57,-0.33,0.7,0.7 4DIU, HIS 22, 2.36, -3, 78, 0, 75, -1, 11 3H5T,ARG_224,10.96,-3.69,0,2.15 3RJX.TYR 97.10.32.0.-0.09.0.41 20KT.GLU 13.5.3.1.03.-0.22.0 2D7U,GLU_86,3.88,0.33,-0.58,-0.37 1ILW,GLU_131,4.92,2.02,-1.98,0.39 3F5D.TYR 128.11.46.0.0.39.1.07 2EYILYS 84.10.44.-0.09.0.0.04 2P1W,GLU_189,4.62,0.13,0,-0.01 1QZN,ARG_152,12.18,-0.38,0,0.06 2CVB,CYS_42,11.55,-1.61,0.83,3.34 1ES5,HIS 76,6.22,-0.57,0,0.3 2CL3.GLU 55.4.1.1.19.-0.85.-0.75 3UC9,CYS_61,11.66,0,0.46,2.21 2IN0,GLU_426,4.71,0.27,0,-0.06 1YR6.TYR 124.10.5.0.0.41.0.09 2WB8.TYR 688.13.94.-0.69.0.25.4.39 3VJ8,LYS_311,10.12,-0.39,0,0.01 1N81,GLU_116,4.68,0.12,0,0.06 2WB8,LYS_672,10.2,-0.33,0,0.03 1SIG,ASP 278,3.49,-0.23,-0.42,0.34 3RJX.CYS 125.12.6.-0.13.-0.02.3.75 4ECC,GLU_34,4.6,0.38,-0.21,-0.07 2FXT,GLU_421,4.91,1.28,-0.13,-0.75 2ZQ5,GLU_298,3.29,0.58,-1.37,-0.41 3BOW.TYR 328.10.8.0.0.45.0.35 3ELI,ASP_115,3.76,-0.35,-0.75,1.06 3UPD,LYS_47,10.49,-0.29,0,0.28 1NJ4,TYR_25,11.23,0,-0.19,1.41 1MUF,LYS 195,9.72,-0.43,0,-0.35 1HUF,GLU_52,3.37,1.96,-2.75,-0.35 3GV0,ASP_213,2.49,-1.23,-0.54,0.46 2FI9,GLU_57,4.71,0.11,0,0.1 3NZL,LYS_74,10.16,-0.37,0,0.04 2G2D,HIS 87,6.11,-0.3,0,-0.09 1RKA, HIS 113, 6, 37, -0, 32, 0, 0, 19 3LJI,GLU_265,4.05,0.26,-0.84,0.13 1X9G,GLU_29,4.35,0.13,0,-0.28 1ZBS.CYS 70.11.63.-0.09.0.23.2.5 2AH5,HIS_200,6.86,-0.28,0.45,0.19 3B7X,ARG_103,12.42,-0.31,0,0.23 1WXO.GLU 129.4.88.0.23.0.0.15 1SI7,ASP_315,3.76,-0.09,-0.14,0.19 2ZCO,ARG_85,12.76,-0.48,0.06,0.69 2AXO.GLU 260.4.98.0.64.0.-0.15 1NAR,GLU_132,4.52,1.97,-0.8,-1.14 1R3F,TYR_312,10.44,0,-0.05,0.49 105J,GLU_50,3.64,1.27,-2.37,0.24 4F8A,CYS_602,10.96,0.02,0.58,1.36 3C2E,CYS_207,11.69,0,0.34,2.34 3BPV,ARG_117,12.33,-0.27,0,0.11 3HVM,GLU_255,5.01,0.66,0,-0.14 1Q8B,ASP_86,3.22,-0.32,-0.7,0.45 3L7N,LYS 75,10,44,-0,12,0,0,06 106D,ARG_27,12.33,-0.38,0,0.21 3DTE,ARG_195,12.21,-0.36,0,0.07 2WOZ,LYS_518,10.61,-0.15,0,0.27 2W1R,ASP_129,3.87,0,-0.09,0.15 2YLF,GLU_154,5.18,0.24,0.09,0.36 3HNX,ARG_8,13.03,-0.5,0.73,0.29 1WRU,ASP_144,3.69,0,-0.36,0.25 2C2Y,TYR_152,10.18,-0.79,0.18,0.79

1FO9,ARG 312,12,27,-3,5,1,52,1,75 1YOY.GLU 108.4.56.0.06.0.0 2J8A,LYS_357,9.96,-0.58,0,0.04 2RJD.GLU 245.6.47.4.15.-2.14.-0.04 2V4U,HIS 355,6,94,-0,33,0,6,0,16 2WOZ.GLU 523.4.76.0.51.0.-0.25 2BV9,HIS_289,6.27,-0.14,0,-0.1 3LOE,LYS 540,10,47,-0.03,0,0 2FZ4,TYR_160,10.65,0,0.36,0.29 1GPP,GLU_121,4.65,0.15,0,0 2D2S,LYS 725,10,4,-0,1,0,0 1VJG,ASP_24,1.48,-3.43,-0.48,1.59 1FHL,TYR_325,11.97,0,0.88,1.1 2ATR.TYR 99,10.08.0.0.0.08 2V1L,ASP_47,2.05,-2.39,0,0.65 3KB5,GLU_289,4.34,1.2,-0.85,-0.51 2BV9,LYS_249,9.67,-0.85,0,0.01 2AHE,GLU_153,3.94,0.31,-0.83,-0.05 3H5T,TYR_286,10.87,0,0.26,0.61 3CRM,GLU_55,3.85,0.22,-0.78,-0.1 3JV1,ARG_117,11.89,-1.37,0,0.76 3H6O.GLU 138.4.77.0.18.0.0.08 3HVW,ARG_229,11.91,-0.73,0,0.14 3Q6L,LYS 97,10.57,-0.15,0,0.21 3M16,TYR_217,12.13,0,0.72,1.41 2F4Q,ASP_185,3.2,-1.09,-0.13,0.62 2AZP,HIS_-1,6.91,-0.14,0.55,0 2R57,GLU_187,4.65,0.15,0,0 2AXO,GLU_99,4.74,0.35,0,-0.11 1F2V,ARG_89,11.76,-1.32,0.13,0.45 3O7K,GLU_57,4.74,0.24,0,0 1TUL,GLU_20,4.64,0.1,0,0.04 1Q5Z,GLU 597,3.67,0.18,-0.63,-0.38 2G3A.ASP 10.4.07.0.0.0.27 1MN3,GLU_408,4.61,0.43,-0.33,0 3C0C,GLU_341,4.07,0.14,-0.76,0.19 2FZ4,GLU_200,6.18,2.07,-0.03,-0.35 1A8Q,GLU 248,4.71,0.11,0,0.11 3M7D,ARG_148,11.57,-3.01,0.01,2.05 2AXO,ASP_81,3.32,-1.01,-0.22,0.74 2W0G,TYR_189,12.84,0.85,0.5,1.48 2QEV,LYS 107,10.07,-0.47,0,0.03 2EHG,CYS 10,10.29,-0.58,0.04,1.83 1SQH,ARG_246,12.4,-0.28,0.13,0.05 3QKY,TYR_45,11.93,0,0.25,1.68 1UXO,HIS_18,5,-1.76,0,0.26 2RJD,LYS 298,10.41,-0.26,0,0.17 20DJ,LYS 236,10.26,-0.46,0.0.22 1MD6,ASP_50,2.55,-1.55,0,0.3 3NR5,GLU_74,4.75,1.04,-0.79,0 2QVO,GLU_24,4.91,0.73,-0.27,-0.06 3BWT.ARG 872,12,22,-0,28,0,0 2FXT,LYS_380,10.22,-0.34,0,0.05 3GT0.LYS 62.10.42.-0.11.0.0.03 3H9W,GLU_70,4.83,0.2,0,0.12 2FD5,ARG_126,12.51,-0.23,0,0.25 2G3A,LYS 91,11.19,-0.25,0.39,0.55 3Q1C,HIS_255,6.51,-0.24,0,0.26 2D59,ARG_65,12.5,-0.73,0.17,0.55 2Z61,LYS_343,10.67,-0.13,0,0.3 2FXT,ASP 361,4.06,0.0.0.26 1DTO,LYS_182,9.9,-0.54,0,-0.06 1LPL.CYS 203,10.5.0.0.04,1.47 3LJN,GLU_147,4.52,0.02,0,0 2B2H,LYS_113,10.26,-0.34,0,0.11 4GA2,ASP 43,3.83,0,-0.22,0.25 3T5B,LYS_53,10.93,-0.21,0,0.64 3GYW,TYR_62,10.18,0,0.03,0.15 3NR5,LYS_35,10.17,-0.32,0,-0.01

3M7G,TYR 107,11,47,-0,74,0,28,1,94 3F6F,GLU_43,4.06,0.31,-0.74,-0.01 3N0K,HIS_93,5.07,-0.98,0,-0.45 1NAR,GLU_168,4.25,0.7,-0.81,-0.14 1RI6,GLU_215,4.92,0.26,0,0.16 1BN6,TYR 25,10.2,-0.04,-0.37,0.6 1LFP,GLU_178,3.96,0.31,-0.63,-0.22 3U2A,GLU_117,3.75,0.37,-0.79,-0.32 2CL3,GLU_200,4.02,0.37,-0.85,0 1OTM,LYS_209,10.27,-0.12,0,-0.1 2E3H,LYS 280,10.42,-0.28,0,0.21 1ZP2.GLU 24.4.61.0.14.0.-0.03 3RLN,ASP 619,3,98,0,0,0,19 3IRA,HIS_58,6.57,-0.2,0,0.27 20HT.GLU 98,3.92,0.24,-0.44,-0.38 3LD1,GLU_318,4.77,0.27,0,0 2AXO,HIS_265,6.37,-0.13,0,0 3RVC,LYS_110,10.35,-0.15,0,0 3DTE,ARG_150,13.32,-0.38,0.7,0.5 2GS5,ASP_176,4.51,0,-0.1,0.81 1YW5.GLU 159.4.96.3.78.-2.3.-1.03 3U2R,ASP_67,3.92,0,-0.05,0.16 2HRZ,CYS_190,12.11,-0.61,-0.08,3.79 3ADO.CYS 252.9.47.0.0.06.0.41 1WXF,LYS 138,10,27,-0,39,0,0,16 3PM2,LYS_169,10.15,-0.27,0,-0.07 3IO0.LYS 151,11.32,-0.27,0.85,0.23 3JRT,TYR_116,9.99,0,-0.25,0.24 3EOD,ARG_76,12.51,-0.37,0,0.38 3UV9,ASP 302,2.66,-1.45,0.0.31 3JV1,GLU_54,4.7,0.2,0,0 3LQE,GLU_494,4.97,1.06,-0.4,-0.18 1J8B.ASP 56.3.86.0.-0.18.0.24 2W0G.GLU 272.4.7.0.24.0.-0.05 1R3F,ARG_201,13.69,-1.02,1.29,0.92 1SI7,ARG_269,13.48,-0.39,0.96,0.4 2Y2T,GLU_40,4.59,0.31,0,-0.21 1NJ4,LYS_325,10.36,-0.15,0,0 1ZP2,GLU_193,4.57,0.07,0,0 2RIK,ASP_110,3.84,0,-0.28,0.33 1AKO,GLU_71,4.72,0.17,0,0.05 2ILR/HIS 533.6.37,-0.2.0.0.07 1NFN.TYR 74.10.92.-0.04.0.17.0.78 2G70,GLU_116,4.72,0.22,0,0 2QRX,ARG_98,11.96,-1.26,0.2,0.51 3PP8,ASP_235,3.3,-0.99,0,0.49 1QYI,GLU_244,6.97,2.47,0,0 20ZO.ASP 80.3.91,-0.02.0.0.13 1EV8,HIS_73,6.5,-0.17,0,0.17 1FKM,ASP_614,3.03,-1.09,-0.13,0.46 10TM,ASP_156,3.29,-0.96,0.05,0.39 3CJW,GLU 393,4.76,0.59,-0.09,-0.24 3FTT,ASP_187,3.86,0,-0.04,0.1 3RJX,GLU_144,5.36,0.93,0,-0.08 2Z84,ARG_123,12.25,-0.26,0,0.01 3M7D,ASP_121,4.42,0.05,0.31,0.25 3IU5,CYS_50,11.31,-0.02,0.17,2.17 3RLE,LYS_159,10.18,-0.41,0,0.09 3FWU,CYS_59,9.82,0,-0.37,1.19 1MTZ,TYR_106,13.83,0,0.74,3.1 2EEY,GLU 39,3.52,0.28,-0.84,-0.41 1DVO.GLU 159,4,0.35,-0.83,-0.02 3GS3,GLU_81,4.18,0.4,-0.31,-0.41 20KT,LYS_266,11.16,-0.3,0.47,0.48 1X7F,GLU_12,4.06,0.9,-1.14,-0.2 4FH3.LYS 243,10.16,-0.32,0,-0.02 1R3D,GLU_216,4.23,0.34,-0.61,0 2G9D,ASP_271,3.61,-0.01,-0.49,0.32 1QYI,LYS_346,10.48,-0.13,0,0.11

2VGY,CYS 79,11.24,-0.07,-0.03,2.34 1WPA, ASP_465, 4.24, 0, 0.19, 0.24 2A6B.GLU 196.4.5.0.0.0 1BKB,GLU_112,3.77,0.28,-0.97,-0.03 1PGV.GLU 375.4.93.0.24.0.0.19 1MML/ARG 71,12,75,-0.4,0.03,0.63 3I47,GLU_226,4.61,0.12,0,-0.01 3B21,LYS_25,10.36,-0.11,0,-0.03 3US6,GLU_131,4.53,0.52,0,-0.5 3CJW.LYS 301.10.97.-0.44.0.85.0.07 2C2Y,CYS_190,9.46,-1.1,0,1.56 2F4Q,ASP_197,4.08,0,-0.02,0.3 2GZQ,ASP_68,3.98,0,-0.07,0.24 1UJ8.LYS 63.10.42.-0.08.0.0 1BN6.CYS 187.11.91.0.0.27.2.64 2DFL,LYS_205,10.09,-0.72,0,0.31 2GZR,TYR_51,13.99,0,0.09,3.9 3KT9,GLU_23,4.63,0.15,0,-0.02 2013.ARG 149.12.41.-0.09.0.0 3ZTA,GLU_84,5.09,0.62,0,-0.02 1AKO,ARG_142,12.38,-0.23,0,0.1 3IBT,HIS_165,3.53,-2.76,0,-0.2 2FG1,LYS_105,11.12,-0.43,0.85,0.2 1NKD,ASP 48,2,41,-1,1,-0,8,0,51 1XEU,ASP_49,3.5,-2.22,0,1.92 3ASA,LYS_105,10.17,-0.27,0,-0.06 3IPZ,ASP_93,3.81,0,-0.27,0.28 3EVZ,ASP 150,3.76,-0.8,-0.02,0.79 1V43,GLU_160,3.26,1.06,-1.21,-1.1 2B2H,GLU_297,7.57,4.7,-1.75,0.11 2CN1,LYS_72,10.43,-0.09,0,0.02 3K8J.CYS 144.12.33.0.-0.06.3.38 3LPZ.TYR 285.11.55.0.0.1.55 1X04,GLU_176,4.44,0.61,-0.52,-0.15 3RLN,LYS_713,10.97,-0.23,0.29,0.4 3LJN,LYS_298,9.93,-0.67,0,0.1 1TJE,ASP_209,3.22,-0.92,0,0.34 4E8B.GLU 196.4.53.0.16.0.-0.13 2Q34,TYR_82,11.6,-0.11,-0.05,1.76 1QQH,TYR_160,13.51,0.83,1.11,1.56 3N2T,LYS 219,10,25,-0,22,0,-0,03 3FS3.TYR 49.10.34,-0.03.0.04.0.33 2VGY,ASP_66,4.15,-0.24,0.08,0.51 3P51.TYR 124.11.13.0.0.19.0.95 3F1X,GLU_19,3.92,0.24,-0.82,0 2E3H,LYS 224,9.77,-0.62,0,-0.1 2BLL.TYR 378,9.6,-0.27,-0.38,0.25 2VAN, ASP_92, 3.77, -0.04, -0.1, 0.11 1PVT,ARG_35,13.33,-0.29,0.23,0.89 3EYE, ASP_132, 3.05, -1.97, -0.2, 1.41 1TLV.TYR 265.10.97.-0.48.-0.4.1.85 3T8R,ARG_56,12.2,-0.24,0,-0.05 1GQE,ARG_200,12.01,-0.47,0,-0.02 3A7L,LYS_103,9.72,-0.98,0.01,0.2 3BCH,TYR 202,12.59,0,0,2.59 2CWC,TYR_83,12.05,-0.02,-1.22,3.3 3CAN,HIS_37,6.25,-0.38,0,0.13 2J8A,TYR 300,13.39,0,0.27,3.11 1GXN,LYS_348,10.16,-0.37,0,0.02 1LZL,TYR 33,11.91,-0.12,0.1,1.93 2B0A, ARG_99, 12.85, -0.29, 0.16, 0.49 3HYQ,TYR_99,11.04,0,0.38,0.67 2X4L,ASP_113,4.08,0,0.15,0.13 3EVN,ASP_314,3.41,-0.69,-0.64,0.93 3LJC,ARG 164,12,25,-0,42,0,0,17 2A6B,LYS_23,10.43,-0.08,0,0.01 2BAA,ARG_240,12.39,-0.11,0,0 3BQW,LYS_178,10.78,-0.19,0,0.47 3UX2,GLU_34,4.72,0.18,0,0.04

3R2E,TYR 18,10.21,0,0.08,0.12 2EFK.GLU 112.3.13.0.62,-1.29,-0.71 4ESS,LYS_150,10.44,-0.06,0,0.01 3A7L,ASP_56,3.54,-0.59,0.11,0.23 2G70.GLU 127.4.73.0.23.0.0 2XHC.ARG 86,13.25,-0.22,0.62,0.35 2PLQ,TYR_151,10.04,-0.4,-0.12,0.57 1A80.HIS 59.6.41.-0.33.0.0.24 1P4X,LYS_55,12.25,-0.75,1.45,1.05 3RVC,GLU_159,4.07,1.75,-1.39,-0.8 1TUL, ARG_108, 12.49, -0.24, 0, 0.23 3GG6,LYS_133,10.46,-0.04,0,0 1R53,TYR_13,10.15,-0.85,0.18,0.81 2VGM,ASP_225,4.13,0,-0.04,0.38 3TOW, ARG 98, 12.29, -1.1, 0.02, 0.87 4AM1,LYS_29,11.93,-0.32,0.98,0.76 2I88,TYR_445,13,0,0.86,2.14 3RFF,GLU_30,4.11,0.42,-0.5,-0.31 4FZN,TYR 54,13.21,0,0.25,2.97 3TOW, ASP_77, 3.1, -1.25, -0.26, 0.82 2BDD,LYS_153,10.27,-0.29,0,0.05 3T5B,ASP_387,3.08,-1.06,-0.5,0.83 1PV5,GLU_141,3.64,1.29,-1.55,-0.6 2CN1.CYS 23.9.45.0.0.11.0.34 3FRR,LYS_127,9.68,-0.78,0,-0.04 4EKU,ARG_93,12.54,-2.04,0.46,1.62 3FHF,LYS_60,10.25,-0.19,0,-0.06 1J8B,GLU 67,4.6,0.1,0,0 2GZR.TYR 132,10.3.0.-0.16.0.45 3ZRI,CYS_28,11.07,0,0.03,2.03 1R53,ARG_62,12.41,-0.09,0,0 2PWQ,GLU_17,3.74,0.32,-0.71,-0.37 1C3K,HIS 57,6.34,-0.38,0,0.21 3GA2,ARG_27,12.4,-0.29,0,0.2 3G9G,GLU_236,3.76,0.72,-1.15,-0.32 4H4J,ASP_49,3.29,-0.41,-0.27,0.17 1QYI,TYR 295,11.19,0,0.01,1.18 3JZ9.TYR 532.10.0.0.0 1ZCU,ASP_224,2.55,-1.33,-0.35,0.44 4FCU,GLU_195,4.54,0.73,-0.25,-0.44 2ZCX,GLU_43,4.56,0.23,0,-0.17 3MIX,ASP_357,3.05,-1.06,0,0.31 1T6L.ASP 98.3.86.0.-0.12.0.19 2V5B,TYR_87,10.16,0,-0.31,0.47 2V1L,ASP_141,3.95,0,-0.16,0.31 1YB2,ASP_57,3.47,-0.52,-0.41,0.6 2CW4,ASP_79,3.87,-0.22,-0.09,0.38 3A0X,ARG_648,13.82,-0.68,1.49,0.52 3H5T,HIS_254,6.11,-0.7,0,0.31 3IO0, ASP_182, 3.88, -0.71, 0, 0.79 3IL3,ASP 27,3.7,0,-0.24,0.14 3H5T.GLU 39.4.27.0.17.-0.39.-0.01 1WNH,TYR_146,10.5,0,-0.05,0.55 1WXF,CYS_201,10.86,0,-0.05,1.92 2P65,ASP_28,3.88,0,-0.12,0.21 1YM5,GLU_271,3.67,0.41,-0.85,-0.4 1UOH,TYR 138,10.29,0,0.14,0.15 3G6S,CYS_114,8.93,-0.31,-0.34,0.58 3HKX,ARG_280,12.58,-0.09,0,0.17 2B78, ASP_271, 3.57, -0.9, -0.02, 0.69 1ZHV.ASP 60.2.29,-1.76,-0.38,0.63 3PBH,ARG_8,13.19,-1.29,1.11,0.87 20YZ,GLU_34,3.92,0.36,-0.84,-0.1 3RFY,LYS_179,10.54,-0.26,0,0.3 4DNU,ASP_107,3.66,-0.84,-0.07,0.77 2B3M,GLU_13,4.41,0.19,0,-0.27 1GPP,GLU_80,4.71,1,-0.64,-0.15 3HKX,TYR_135,10.95,0,0.65,0.29 2P1W,ARG_65,12.92,-0.4,0,0.82

3K8J,TYR_101,11.37,-1.04,0.06,2.35 1MML.LYS 102.10.42.-0.08.0.0 2I88,ASP_509,2.64,-0.96,-0.58,0.38 1EQ6,ASP_99,3.2,-0.89,-0.11,0.4 1PBV.LYS 77.12.4.-0.45.1.38.0.98 1MTZ,GLU_172,4.23,0.34,-0.3,-0.3 1XIP,ASP_69,4.12,0,-0.13,0.44 1XTZ,HIS_264,6.57,-0.21,0,0.28 1RI6,HIS_211,7.23,-0.22,0.53,0.41 4FZN,LYS 119,10,18,-0,31,0,0 2H01,GLU_47,4.93,1.8,-0.83,-0.53 3FHF,HIS_-4,6.4,-0.1,0,0 1AD6,TYR_529,10.66,0,0.39,0.27 2B78,ASP_189,3.76,0,-0.53,0.49 1S7K,ARG 135,13.39,-0.41,0.64,0.67 3L3P.GLU 398.4.7.0.15.0.0.05 1SIG,TYR_143,11.91,0,0.18,1.73 3QYB,HIS_978,4.81,-1.91,0.1,0.12 3M7D.ARG 241,12.72,-0.12,0.0.33 208I,HIS_17,6.77,-0.25,0.3,0.22 3PP8,ARG_89,11.91,-0.67,0,0.07 2G3A,ARG_90,13.52,-0.41,0.75,0.68 10LR,ARG_75,12.49,-0.56,0.2,0.36 3HUE,GLU 189,4.04,0.44,-0.84,-0.07 1X6J.ARG 83,12,51,-0,76,0,5,0,26 3RKV,ARG_325,12.82,-0.37,0.09,0.6 3FS3,TYR_191,10.35,0,0.03,0.32 2H8O,ARG_246,12.39,-0.35,0,0.24 3CXS,GLU 175,4.45,0.11,0,-0.16 1R29,ARG_26,12.2,-1.71,0.68,0.73 2RIS,GLU_10,4.71,0.16,0,0.05 10XZ,ARG_214,12.2,-0.63,0.01,0.33 1PVT,LYS 110,10.6,-0.18,0,0.28 1ZBP.GLU 99,4.53,0.16,0,-0.13 3KT9,LYS_53,10.83,-0.12,0,0.46 1GPP,GLU_22,4.68,0.14,0,0.04 2CN1,LYS_51,10.62,-0.1,0,0.22 1XIP,GLU_85,4.77,0.24,0,0.04 1WNH,LYS_217,10.46,-0.18,0,0.13 1WPA,GLU_470,4.1,0.31,-0.71,0 1WLY,TYR_275,10.32,-0.85,0.05,1.13 1L3K,ASP 123,3.83,0,-0.29,0.32 3F6M,ARG 144,12.71,-0.32,0.2,0.33 2CXY,ARG_22,12.28,-0.32,0,0.1 3A2Z,LYS_177,10.83,-0.23,0.1,0.46 2V4U,GLU_343,5.08,1.29,-0.7,-0.01 2IXM,ARG_69,12.58,-0.13,0,0.21 1YR6.CYS 242.9.33.-0.27.0.1.0.51 3KT9,CYS_40,10.94,-0.09,-0.03,2.06 1ZBM,TYR_67,12.31,-0.1,-0.03,2.43 3ANJ,LYS_16,10.4,-0.1,0,0 4E6S,HIS 9.6.41,-1.18,0.85,0.24 1LTU,HIS_138,3.76,-2.95,0,0.21 3E7P,CYS 201,11,-0.65,0.15,2.51 3LD1,GLU_17,4.03,0.47,-0.78,-0.15 1TUL, ARG_54, 12.92, -0.24, 0.18, 0.48 1TD6.GLU 39.4.64.0.07.0.0.07 1PVT,GLU_179,4.59,0.27,0,-0.18 200K,ARG_104,12.45,-0.05,0,0 1QQE,GLU_288,4.81,0.46,-0.47,0.3 1ZBS,ASP 221,3.24,-0.79,-0.58,0.8 2V5B,TYR_224,12.11,0,0.2,1.9 3JZN.GLU 337,4.54,0.07,0,-0.02 1XWM,ASP_115,3.66,-0.44,0,0.3 4FLE,TYR_160,13.57,-0.85,0.92,3.51 2V1L.TYR 82.10.34.0.0.01.0.33 1EDG,HIS_176,6.47,-0.51,0.21,0.27 2P52,GLU_201,2.88,0.52,-1.66,-0.48 1P6F,LYS_52,10.19,-0.16,0,-0.14

1T6L.GLU 270.4.78.0.12.0.0.16 2Z84,ARG 49,13.89,-0.48,1.44,0.43 2QK1,LYS_531,10.4,-0.14,0,0.04 1LN4,HIS_43,6.06,-0.23,0,-0.21 1ES5,CYS_98,11.44,-0.57,-0.43,3.44 3M3P,GLU 230,2.91,0.8,-1.66,-0.72 4HDE,CYS 69,7,49,-3,0.01,1.49 4DIU,GLU_235,4.77,0.43,0,-0.16 1DTO.LYS 14,11.31,-0.6,0.85,0.55 1KCM,GLU_248,5.45,0.91,0,0.05 1SNT,TYR 91,10.59,0,0.02,0.57 3HNX.TYR 3,12.87,0,0.09,2.77 3LPZ,ARG_11,12.14,-0.29,0,-0.06 2DFL,ARG_72,12.58,-0.09,0,0.17 4AM1,GLU_73,3.35,0.53,-1.68,0 2E0T.TYR 70.11.16.0.0.41.0.75 1YTD,ARG_142,11.77,-0.63,0,-0.11 2B0J,GLU_125,4.55,0.29,0,-0.25 3IRA,GLU_165,4.53,0.3,0,-0.27 300P,GLU_110,4.9,0.17,0,0.22 3TOW, ASP_74, 2.01, -1.83, -0.4, 0.44 2QHT,TYR_63,10.71,-1.07,0.01,1.77 3GS3,ASP_114,3.39,-1.59,-0.47,1.65 2099,LYS 193,10.23,-0.26,0,-0.01 3RJX,LYS 116,10,46,-0,12,0,0.09 2GEN,HIS_21,6.32,-0.33,0,0.14 2IDC.TYR 101.11.76.-0.2.0.51.1.45 3M7D,GLU_375,6.34,1.65,0,0.18 3H04,HIS_234,6.01,-0.45,0,-0.04 3CJW,ARG 246,12.51,-0.35,0.09,0.27 20KT,GLU_315,4.55,0.09,0,-0.03 1J74,ASP_38,4.22,0,0.11,0.31 3RKV.GLU 277.4.28.0.31.0.-0.53 3BZT,ARG 338,12.44,-0.12,0,0.06 2B0A,ARG_138,13.2,-0.38,0.72,0.36 3ZTA, ASP_64, 2.99, -0.62, -0.56, 0.36 2Z0M,ARG_77,12.59,-1.08,0.75,0.42 2R0S,LYS_174,11.31,-0.39,0.49,0.7 1BKR,TYR_19,11.35,0,0,1.35 1SIG,ARG_157,12.46,-0.24,0,0.21 1P1L,LYS_25,10.53,-0.11,0,0.15 3R87,HIS_51,6.45,-0.27,0,0.22 3M7D,ARG 144,13.09,-2.78,0.71,2.65 3EZ7,HIS_138,6.18,-0.32,0,0 3BQW,LYS_290,10.29,-0.25,0,0.05 1SFE,GLU_30,4.16,1.63,-1.28,-0.69 2FBI,GLU_17,3.68,0.33,-0.73,-0.42 1J85,LYS 61,10.64,-0.11,0.0.24 2V4U,HIS_330,6.19,-0.73,0.8,-0.37 200K,CYS_257,12.89,0,0.07,3.82 30NH, ARG_484, 13.01, -0.62, 0.81, 0.32 1NJ4,LYS 6,10.56,-0.2,0,0.25 2GAU,GLU_27,4.9,0.18,0,0.22 3CXS,GLU_106,3.12,0.58,-0.85,-1.11 3H13,ASP_325,3.36,-0.84,-0.03,0.44 1AKO,ASP_208,3.54,-0.21,-0.38,0.33 2IF4,TYR_202,12.33,-0.62,0.52,2.42 3SMD,TYR_139,12.72,0,0.06,2.66 1NIJ,ASP_52,3.97,-0.01,-0.01,0.2 2GAU,ARG_183,11.64,-0.9,0,0.03 1X91,ASP 57,3.26,-0.82,-0.07,0.35 4ACJ.GLU 732.4.88.0.33.-0.08.0.13 2WB3,ASP_291,3.64,-0.42,-0.22,0.48 3JSN,GLU_271,4.63,0.22,0,-0.09 3H6Q,TYR_64,10.81,-0.19,-0.04,1.05 3IVF.ARG 303,12,46,-0,59,0,08,0,47 4GCO,TYR_214,11.07,0,0.23,0.83 3M16,LYS_274,10.46,-0.04,0,0 3SMD,GLU_53,4.27,0.68,-0.85,-0.05

1WXF,ARG 25,12.81,-0.38,0.0.69 106D,LYS_93,10.16,-0.32,0,-0.03 3M3P,GLU_138,11.09,4.6,-0.04,2.03 3BJV,GLU_9,4.62,0.35,-0.03,-0.21 1ZCU.CYS 130.10.1.0.0.27.0.83 2ZTY.ASP 51.4.0.0.01.0.19 1A8Q,ARG_266,12.49,-0.08,0,0.07 3HVW,TYR_175,10.14,0,-0.02,0.16 2OGQ,TYR_453,9.62,-1.7,0.13,1.18 3ERF.HIS 114.6.97.-0.71.0.83.0.35 1D2K,LYS_199,10.5,-0.09,0,0.09 3T8R,GLU_125,4.11,0.32,-0.35,-0.36 2AXO,TYR_204,11.91,0,0.19,1.72 1RI5.ARG 232.12.51.-0.22.0.0.22 2P4D.LYS 62.10.33.-0.2.0.0.03 2PPN,TYR_80,10.38,-0.04,0.05,0.38 3O16,ASP_112,3.71,-0.51,0.12,0.29 4ECC,GLU_64,4.63,0.13,0,-0.01 3GEC.CYS 312.10.38.-0.27.-0.57.2.21 4ECC,GLU_141,4.61,0.34,0,-0.23 4ETX,GLU_394,4.39,0.12,0,-0.24 1QQH,TYR_179,10.6,0.05,0.07,0.48 1NIJ,GLU_308,4.9,0.24,0,0.16 3ASA, ASP 339, 3.34, -1.57, 0, 1.12 3EVN,GLU_245,4.45,0.26,-0.02,-0.29 1UOH,CYS_48,12.66,0,-0.1,3.76 2FB6,GLU_72,4.21,1.65,-1.36,-0.59 1WPA, TYR 432, 10.68, -0.6, 0.08, 1.2 2C2Y,HIS_103,6.94,-0.43,0.81,0.06 3LQE,TYR_370,10.61,0,0.12,0.49 4H4J,HIS_148,6.14,-0.37,0,0.01 3LJC,LYS 143,10,44,-0,26,0,0,21 4AE7.CYS 218.12.25.-0.41.0.35.3.32 2RFA,GLU_71,4.6,0.14,0,-0.04 2RGY,HIS 205.6.33,-1.16.0.78.0.2 1NJ4,CYS_115,11.37,-0.01,-1.51,3.91 2Z14,ARG 35,12.8,-0.41,0.32,0.39 1PGV.ARG 232,12,23,-0.32,0.0.05 3M70,LYS_94,10.77,-0.21,0,0.49 2X4G,TYR_15,12.57,0.71,0.6,1.26 1YG2.HIS 37.6.11.-0.39.0.0 1DOV.ASP 172.3.7.-0.38.0.0.28 1CBY,LYS_26,10.22,-0.35,0,0.06 3LJC,LYS 48,10.56,-0.22,0.0.27 3ONT,CYS_122,9.67,0,0.08,0.58 2EHG,GLU 61,5.09,1.01,0,-0.42 3HKX.ARG 93,12.66,-0.25,0.03,0.38 208P,CYS_59,11.81,-0.02,0.05,2.78 3GS9,TYR_189,11.17,0,0.13,1.04 3N2T.GLU 127,10.33,4.87,-0.11,1.07 2X5Y,TYR 793,10.05,-0.2,0,0.25 3P28,LYS 114,10.16,-0.46,0,0.12 4EVF,LYS_246,10.29,-0.39,0,0.19 2FL7,LYS_120,10.45,-0.21,0,0.17 3SMD,LYS 113,10.34,-0.16,0,0 3FK5,ARG_210,12.19,-0.32,0,0.01 3F6F,LYS_189,10.41,-0.21,0,0.12 3CRM,ARG 63,12.47,-0.34,0.02,0.29 1J8B,GLU_26,4.13,0.25,-0.62,0 2YYO, ASP 39, 3.8, 0, -0.15, 0.15 2FBI,TYR_91,10.31,0,-0.05,0.35 3MIX,GLU_398,5.1,0.45,0,0.15 4DIU,TYR_119,11.57,0.85,0.24,0.47 3RJX,LYS_219,10.63,-0.11,0,0.24 2ZCX.TYR 192.10.33.0.0.0.33 1NRI,ARG_70,13.92,-0.93,1.6,0.75 2RFA,HIS_257,5.26,-0.96,0.09,-0.38 2OGQ,LYS_556,12.13,-0.37,1.2,0.79 1P4X,TYR_42,11.79,-0.48,0.04,2.23

1VJG.GLU 26.4.5.0.27.-0.23.-0.05 2R2Y,LYS 83,10.26,-0.45,0.0.21 2RFA,GLU_104,3.81,0.43,-0.87,-0.25 2QOP,GLU_118,4.71,0.43,0,-0.22 1ZBM,GLU_134,3.53,0.18,-0.79,-0.36 30KO.GLU 644.4.75.0.14.0.0.12 1WJG,ASP_79,4.36,-0.02,-0.27,0.85 3C0C,ASP 307,3.45,-0.48,0.0.13 1PBV,ARG_145,11.65,-1.26,0,0.42 1D2K.LYS 422.10.55.-0.25.0.0.29 3F7M,ASP 266,3.41,-0.8,-0.05,0.46 2XJ4,LYS 62,10.03,-0.47,0,0 3G9T,ARG_205,12.03,-0.59,0,0.11 2A6B.LYS 74,10.5.0.0.0 2WOZLYS 460.10.79.-0.12.0.0.4 1ZCE,GLU_128,4.41,0.21,0,-0.3 3HUE,LYS 80,10.33,-0.2,0,0.03 1AM2,TYR_178,10.91,0,0.01,0.9 3GV0,ARG_234,12.92,-0.35,0.39,0.37 3P2F.ARG 58,13.61,-0.62,1.24,0.49 3NBI,GLU_204,4.88,0.22,0,0.16 3U0V,ASP_140,2.85,-1.05,-0.66,0.75 3LMO,GLU_63,4.18,0.41,-0.42,-0.3 105JLYS 63.10.55.-0.09.0.0.14 3ERF,GLU_121,4.19,1.75,-1.03,-1.03 3TOW, ASP_48, 3.92, 0, -0.21, 0.32 1YTQ,ASP_82,3.19,-0.7,-0.38,0.48 2R2Y,ASP_79,3.43,-0.84,-0.01,0.47 2FL7.HIS 114.7.11.-0.56.0.85.0.31 2AZL,LYS_93,10.01,-0.63,0,0.14 1NAR,ASP_272,3.94,0,0.03,0.1 3M66,HIS_314,5.5,-0.74,0.21,-0.48 4H4J.TYR 69,11.11,-1.57,0.24,2.44 2E3I,CYS_111,10.46,-0.02,0.05,1.43 2QVO,LYS_39,10.41,-0.16,0,0.07 3T57,ARG_271,12.03,-0.31,0,-0.16 2IQT,ASP 202,3.01,-0.85,-0.29,0.35 2F4Q,ARG_24,12.43,-0.07,0,0 3BPV,ARG_79,12.05,-0.81,0,0.35 2IXM,GLU_241,4.71,0.19,0,0.01 2Z84,GLU_132,3.18,0.35,-1.29,-0.38 1YR6,GLU_234,3.88,1.06,-1.69,0.01 1ILW,HIS 54,4,45,-2,77,0,84,-0,11 1YR6,TYR_97,13.31,0,1,2.3 3ZXY,ASP_176,4.06,0,0.02,0.24 2ZO5.LYS 226.12.26.-0.7.1.7.0.76 1Z9L,ASP_15,3.11,-0.41,-0.72,0.43 2FZ4,GLU_158,4.55,0.11,0,-0.06 3K8J,LYS 73,10.55,-0.17,0.0.21 1TR9,GLU_73,4.56,0.15,0,-0.08 3RFY,HIS 172,7.48,-0.43,0.85,0.58 1H09,ASP 333,3,94,0,-0.03,0,16 1YTQ,GLU_77,4.7,0.2,0,0 3JRT,CYS_48,8.77,-0.26,-0.37,0.41 2X5Y,TYR_886,11.25,-0.75,0.2,1.8 4D8L,ARG_92,13.37,-0.21,0.56,0.52 4E9E,LYS 518,10.53,-0.18,0,0.21 2BLL.LYS 587,10.52,-0.08,0,0,1 1XDZ,LYS_234,10.24,-0.21,0,-0.05 3IVF,ARG_358,12.82,-0.23,0.16,0.39 1BKR.LYS 53.11.6.-0.2.0.72.0.59 2VGM,TYR_32,11.94,0.11,0.8,1.03 1YM5,LYS_143,10.58,-0.11,0,0.19 1JSX,TYR_63,10.4,0,0,0.4 4HDE,GLU_109,4.63,0.13,0,0 1KCM,TYR_24,11.56,0,0.46,1.09 1GQE,TYR_296,10.58,0,0.18,0.41 2EJB,LYS_19,10.36,-0.48,0,0.34 2YYO,TYR_88,12.63,0.85,0.8,0.99

2AD1,TYR_141,10.48,0,-0.08,0.56 2YX0,GLU_165,2.81,0.69,-1.62,-0.76 3ZRI,ARG_77,12.45,-0.05,0,0 3CBN.GLU 51.3.52.0.3.-0.85.-0.43 2CYG,HIS_291,6.41,-1.89,0.81,0.99 4DNU,HIS 78,6.79,-2.97,1.6,1.66 3PBH,ASP_60,3.33,-0.56,-0.02,0.11 1YB2,CYS_86,9.74,-0.45,0,1.19 1BN6,GLU_225,4.52,0.17,0,-0.15 1MIX.LYS 284,11.32,-0.29,0.73,0.38 3CJW,TYR 312,12,72,0,0,13,2,59 3ETV,HIS_128,2.12,-3.56,0.56,-1.37 3CCY,ARG_185,12.3,-0.27,0,0.08 4H4J,ASP 220,3.52,-0.11,-0.32,0.15 3GMS,ARG 57,11.78,-0.79,0,0.07 2QVO,TYR_46,10.14,0,-0.25,0.38 3BA1,ASP_237,4.46,0,0.06,0.59 3ETU,ARG_208,12.32,-0.45,0,0.28 3U4K,CYS_178,9.12,0,0,0.12 109G,LYS 225,10,41,-0.08,0,-0.01 1NAR,HIS_130,2.87,-2.96,0,-0.67 3N2T,LYS 259,10.39,-0.24,0.0.13 1RI5,HIS_127,5.96,-0.33,0,-0.22 4ESS.ARG 39,12.35,-0.2,0,0.05 2F8H,ASP 335,3.68,-0.83,0,0.71 3US6,LYS_58,10.51,-0.12,0,0.12 2P65,GLU_30,4.25,0.73,-0.73,-0.25 2Z0W,ARG_12,12.48,-0.02,0,0 3US6,ASP 59,3.75,0,-0.36,0.3 1YLN,GLU_72,4.77,0.36,0,-0.09 3IRA, ARG_84, 14, -0.42, 1.53, 0.39 1YB2,ASP_157,3.38,-0.54,-0.02,0.15 3M7G,ARG 20,12.37,-0.46,0,0.32 1SUU,ARG 681,12.2,-0.23,0,-0.07 1GXN,LYS_521,11.26,-0.54,0.85,0.45 3QAV,LYS_137,10.46,-0.15,0,0.12 3IRA,ARG_101,12.11,-0.6,0,0.21 2QRX,ASP_18,3.98,0,0,0.18 2APL,ARG_97,12.56,-0.16,0,0.22 2IQT,GLU_185,4.63,0.19,0,-0.06 1K95,HIS_105,6.4,-0.28,0.01,0.16 1KW4,LYS 53,10.21,-0.13,0,-0.15 3K9I,LYS 102,10.38,-0.12,0.0 4E9E,LYS_554,10.31,-0.28,0,0.09 1XIP,ARG_189,12.42,-0.08,0,0 2QDJ,CYS_102,11.75,-0.02,0,2.77 1PVT,CYS_78,11.42,0,-0.01,2.43 1SOW, ARG 154, 12.4, -0.14, 0.0.04 3VHJ,GLU_163,3.25,0.4,-0.85,-0.8 1Q46,TYR_32,10.43,0,0.09,0.35 3S0A,LYS_109,11.62,-0.4,0.85,0.67 2013.GLU 28,4,73,0,19,0,0,04 2D7J,LYS_120,10.37,-0.27,0,0.14 1XFK,ARG_94,12.92,-0.24,0.22,0.44 2ZCO,HIS_79,6.18,-0.22,0,-0.09 3EAZ,GLU_108,4.28,0.83,-0.83,-0.21 20KT.TYR 333,10.76.0.-0.11.0.86 3L3P,GLU_519,4.45,0.78,-0.39,-0.44 2R51,ARG_260,12.37,-0.31,0,0.18 2A1V,HIS_75,5.92,-0.58,0,0 1PVT.HIS 123.6.69,-3.11.1.28.2.02 2FPN,LYS_62,10.64,-0.22,0,0.36 3DZ1.TYR 121.11.3.0.0.1.3 3GYW,TYR_277,9.95,-0.23,-0.19,0.37 2Q99,LYS_28,10.26,-0.3,0,0.05 1160,LYS 94,10.62,-0.14,0,0.26 3UX2,GLU_35,4.22,0.37,-0.6,-0.04 3NBI,GLU_150,3.58,1.59,-2.19,-0.33 3VJ8,LYS_138,10.57,-0.4,0,0.47

3GE9,GLU_74,4.05,0.32,-0.3,-0.47 2JEO,ARG 155,12.3,-0.68,0,0.48 1P1L,GLU_92,4.01,0.28,-0.77,0 3EVP,ASP_68,3.86,0,-0.51,0.56 2CVB,ARG_186,12.31,-0.19,0,0 3GS9,TYR 57,10.58,0,0.14,0.44 1KW4,ASP 10.3.73.0.-0.29.0.22 1FHL,TYR_151,11.48,0,0.25,1.23 3R2E,ASP_45,3.89,0,0,0.09 3EZ7,GLU_189,4.63,0.13,0,0 3OBS,ARG 64,13.51,-0.12,0.75,0.37 3MYI,HIS_974,6.09,-0.38,0.08,-0.11 1AK1.GLU 94.3.81.1.2.-1.15.-0.74 3V46,ARG_300,12.35,-0.32,0,0.17 3VHJ,ARG 135,13.69,-0.4,0.79,0.79 2JHY,HIS 131,5.09,-0.65,0,-0.76 3CQ1,CYS_54,9.28,0,0.05,0.23 4DNU,ARG_99,11.32,-2.76,0,1.58 3CXS,HIS_107,6.31,-0.42,0.05,0.17 1R53,CYS_23,11.76,0,0,2.76 2P4D,HIS 74,6.69,-0.56,0.69,0.06 3HYQ,ARG_172,12.52,-0.58,0.23,0.37 1NRI,LYS_124,10.45,-0.05,0,0 1AM2,HIS 52,5.93,-0.95,0.36,0.02 3GW3,ARG 193,13,47,-0.82,0,78,1.02 3IVF,ARG_220,13.53,-0.92,0.85,1.1 2FGG.GLU 58,4.25,0.32,-0.62,0.04 1WRU,GLU_311,4.75,0.35,0,-0.1 20EW,ASP_302,3.56,0,-0.55,0.31 10ZN,ASP 151,4.32,0.0.28,0.24 1Q5Z,HIS_595,6.52,-0.47,0.42,0.07 2RIS,ASP_105,1.52,-2.76,-0.3,0.78 1XTZ.CYS 125.11.69.-0.07.1.28.1.48 1WOU.TYR 68.12.77.0.85.0.44.1.47 1SI7,HIS_117,5.76,-1.23,0.19,0.29 1JSX,GLU_67,4.74,0.16,0,0.07 4ACJ,LYS_649,10.57,-0.29,0,0.36 3OA7,HIS_570,6.44,-0.21,0,0.15 3M7G,GLU_255,3.75,0.28,-0.7,-0.33 3ADO,LYS_279,10.28,-0.22,0,0 2FC3,LYS_84,10.54,-0.18,0,0.22 3E7P,HIS_235,7.37,-0.47,0.85,0.5 2FC3,CYS 70,12.03,-0.05,0.14,2.95 1IDK,TYR_179,13.62,0,0.04,3.58 3I4T,CYS_26,11.25,0,0.04,2.21 3FS3,HIS_120,6.95,-0.65,0.78,0.31 4ESS,HIS_146,6.25,-1.49,0.85,0.39 1V8E,ARG 201,12,75,-0,18,0.09,0.34 2VGM,ASP_285,4.11,0,0,0.31 2Q07,LYS_394,10.43,-0.07,0,0 1G5Z,LYS_80,10.34,-0.16,0,0 109G,ARG 217,12.24,-0.26,0,0 1V6T,CYS_221,13.32,-0.53,1.78,3.08 1U3Y,ARG_252,12.43,-0.08,0,0.01 109G,LYS_121,10.5,-0.19,0,0.19 1GXN,LYS_467,9.97,-0.4,0,-0.13 1C3K,TYR_90,10.11,0,0.01,0.1 1MN3,GLU_440,4.81,0.21,0,0.11 3EZ7,TYR_101,11.49,0,0.41,1.08 3O16,ARG_83,12.53,-0.12,0,0.15 1V8E,LYS_184,10.41,-0.06,0,-0.04 3HKX,ASP_43,2.73,-1.46,-0.64,1.03 3UC9,LYS_9,11.25,-1.13,0.85,1.02 1P4X,ASP_88,3.19,-0.99,-0.06,0.44 1T95,GLU_137,4.64,0.2,0,-0.06 1RZ2,GLU_66,4.9,0.2,0,0.19 2IXM,ARG_187,12.97,-1.06,0.67,0.85 2GKG,TYR_63,11.52,0,0.13,1.41 3MEW, ASP_153, 3.57, -0.37, -0.06, 0.2

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1UXO,ASP 30,2,46,-1,49,-0,39,0,53 2QRX,CYS_69,11.47,0,-0.04,2.5 3GMS,ARG_267,12.22,-0.47,0,0.18 1R6Y,ASP_91,3.09,-0.85,-0.38,0.53 1V43.LYS 278.10.54.-0.12.0.0.16 20JO,ASP 693,4.08,0.0,0.28 3BPP,TYR_209,10.3,0,0,0.3 3BA1,GLU_87,4.75,0.16,0,0.1 2P0Y,ARG_165,11.85,-0.62,0,-0.02 1XDZ,ARG_227,13.95,-0.91,1.59,0.77 1UW7,LYS_92,10.55,-0.12,0,0.18 3G6S.GLU 259.4.63.0.32.0.-0.19 3BQW,GLU_246,4.61,0.11,0,0 2F8H.HIS 340.5.63.-1.6.0.0.74 1DZF.ARG 169,12,46,-0.04,0.0 1UAJ,ARG_68,13.09,-0.38,0.5,0.47 100X,LYS_20,9.86,-0.5,0,-0.14 1KCM,ARG_220,12.46,-0.44,0.02,0.38 2HP7,ASP_168,3.98,0,0,0.18 2G5X,ARG_76,12.5,-0.43,0,0.43 3U2R,GLU_32,4.4,0.82,-0.66,-0.27 4ACJ,GLU_788,4.95,0.3,0,0.15 1WXOLYS 364.10.34.-0.12.0.-0.03 3H9W.CYS 82,8.3,-0.77,-0.3,0.38 4FCU,TYR_163,10.22,0,0.03,0.18 1ZBM,GLU_49,4.38,0.28,0,-0.4 3GOZ,HIS_238,6.32,-0.18,0,0 2HXB,GLU 46,4.57,0.07,0,0 2A0J,HIS_12,5.93,-1.13,0.2,0.36 2FBQ,GLU_131,4.45,0.38,-0.2,-0.24 3KV0,HIS_101,6.5,-0.47,0,0.47 1SUU,ASP 788,3.77,0,-0.28,0.25 1L2F.GLU 66.4.65.0.15.0.0 3IDW,LYS_63,10.42,-0.08,0,0 1WOU.ASP 45,3.96,-0.1,0.0.26 3P2F,ARG_104,12.62,-1.73,1.36,0.5 2RIS,GLU 200,4.66,0.29,-0.06,-0.06 1RKA, ARG 53, 11, 78, -2, 04, 0, 52, 0, 81 1Q5Z,HIS_612,5.05,-2.26,0.82,-0.01 1YM5,ASP_61,2.95,-1.07,-0.22,0.44 3JV1.GLU 59.2.62.0.51,-1.96,-0.43 3A0X,TYR 619,10,78,0,0,27,0,51 20GQ,LYS_474,10.44,-0.06,0,0 1J74.GLU 68.4.61.0.35.0.-0.24 1KCM,GLU_33,4.66,0.27,0,-0.11 2PGE,ARG 10,12.39,-0.11,0,0 3ETV.HIS 340.5.66,-1.96,1.09.0.03 2GEN,GLU_9,4.43,0.16,0,-0.23 2HRZ,LYS_336,10.29,-0.1,0,-0.11 2IXM.LYS 197,10.07,-0.52,0.0.09 1UW7.CYS 23.10.32.0.-0.08.1.4 3PP8,ARG_185,12.37,-0.13,0,0 3L3P,ASP_503,3.33,-0.65,0,0.18 2FBI,LYS_85,10.48,-0.07,0,0.05 1WRU,ARG 72,12.31,-0.23,0,0.03 2YWK,TYR_65,10.17,0,0.06,0.11 3CGW,TYR_252,13.75,0,0.29,3.46 3VJ8,ARG 110,12.42,-0.35,0,0.28 3BCH,TYR_47,10.08,-0.02,-0.31,0.41 4FZN,ASP 65,3.84,0,-0.25,0.29 1FO9,TYR 184,10.29,0,0.11,0.19 2QVO,LYS_79,10.49,-0.09,0,0.08 4EVF,ASP_271,2.43,-1.45,-0.26,0.35 1X1E,LYS_4,9.58,-0.73,0,-0.19 2NRK.HIS 99,4.28,-1.99,0,-0.23 2BT8, ASP_170, 3.9, 0, 0, 0.1 3CGW,LYS_213,10.55,-0.2,0,0.25 3RE9.CYS 220.8.79.-1.34.-0.19.1.32 2EHG,ARG_126,13.34,-0.48,0.57,0.74

1H09,LYS 87,11,17,-0.6,0,72,0,54 1ANU,ASP_123,4.12,0,0.09,0.23 3V75,ARG_48,13.65,-0.21,0.81,0.54 1RWZ,LYS_139,9.88,-0.71,0,0.09 2W0G.LYS 268.10.55.-0.11.0.0.17 1IAP.GLU 71,4.65,0.52,0,-0.38 3H6Q,ARG_127,13.85,-0.58,1.47,0.46 3OAV.HIS 44,5,46,-0.6,0,-0.45 2NMU,ARG_38,12.07,-0.38,0,-0.06 2ZCO.TYR 208.13.49.0.0.03.3.46 204D,LYS 118,11.6,-0.27,0.83,0.54 2R4Q,GLU_237,4.59,0.15,0,-0.06 2YX0,TYR_33,11.83,0,0,1.83 3K8J,ARG 248,12.28,-0.22,0.0 3ZSL,GLU_230,3.43,0.35,-0.79,-0.63 2WB8,LYS_798,10.39,-0.28,0,0.17 30NT,ARG 140,12,31,-0,19,0,0 1IDK,LYS_148,9.52,-0.98,0,0 4FCU,ASP_44,3.86,-0.85,-0.41,1.33 2BV9.LYS 96.10.38.-0.12.0.0 4EF5,HIS_157,6.19,-0.28,0,-0.04 1Q42,ARG_137,12.06,-0.23,0,-0.21 1X6J,ARG_15,12.83,-1.29,0.75,0.87 4E9E.GLU 572.4.74.0.2.0.0.04 2R2Y,HIS_120,5.93,-1.39,0.3,0.52 2CWY,GLU_19,4.49,0.31,0,-0.32 2AHE,ARG_206,11.2,-1.54,0,0.24 1NAR,LYS_49,10.66,-0.23,0.13,0.25 2JEO.ASP 215.3.77.0.-0.19.0.16 3BWT,ASP_574,3.89,0,-0.2,0.3 2XMZ,GLU_151,4.73,1,0,-0.77 2EJX,LYS_58,10.63,-0.18,0,0.32 4AM1,LYS 40,12.45,-0.55,1.67,0.83 1P4X,TYR_3,13.22,0.31,0.7,2.21 3M66,ASP_395,3.05,-0.82,-0.58,0.64 1UOH,LYS_18,10.43,-0.14,0,0.08 1NRI,ARG 246,12.32,-0.18,0,0 2P0Y,ARG_246,12.66,-0.43,0.08,0.52 1ANU,ASP_57,2.9,-1.69,0.01,0.79 1TJE,HIS_195,7.28,-0.4,0.78,0.4 3N2T,LYS_98,10.33,-0.17,0,0 1F2V,ARG 40,11.13,-1.59,0.07.0.16 105T.LYS 349.10.44.-0.07.0.0.02 1BN6,GLU_194,4.25,0.28,-0.51,-0.01 3PZ9,LYS_68,10.45,-0.33,0,0.28 3RAZ,ASP_83,3.06,-2.15,-0.04,1.44 3L7N,LYS_41,10.5,-0.11,0,0.1 2Z0M,ASP_241,3.74,-0.23,0.01,0.16 1WOU,LYS_98,11.54,-0.39,0.8,0.62 4AE7,LYS_139,11.4,-0.51,0.85,0.57 3Q1C,ARG 120,12.17,-0.36,0,0.02 2PGE,TYR 337,11.73,-0.01,-0.52,2.26 2Q98,HIS_195,5.69,-0.35,0,-0.46 1FKM,ASP_340,3.02,-1.79,-0.29,1.29 4H4J,LYS_166,10.38,-0.17,0,0.05 3B21,ASP_182,4.03,0,0.01,0.22 2ZTY,GLU_121,5.44,0.34,0,0.6 3L7N,TYR_116,12.16,-0.03,0.34,1.85 1G8P,LYS_239,11.35,-0.28,0.51,0.61 1HF8,ARG_100,12.72,-0.6,0.36,0.46 1FHL,ASP 167,3.34,-0.85,-0.03,0.42 4FZR,GLU_316,5.39,3,-1.3,-0.82 4ECC,ASP_159,3.74,0,-0.22,0.17 2WB8,GLU_535,5.54,3.08,-1.12,-0.92 3UAH,ARG_455,12.2,-1.04,0,0.73 3M70,LYS_30,10.35,-0.15,0,0 20JQ,ARG_446,11.89,-0.63,0,0.02 1XDZ,LYS_47,11.42,-0.57,0.79,0.7 1R3F,CYS_58,11.51,-0.67,0,3.18

4GA2,TYR_11,11.15,0,0.15,1 3HKX,ASP_269,3.56,-0.6,-0.01,0.38 1QYI,GLU_45,4.94,0.26,0,0.19 1XTZ.CYS 75.12.33.0.0.3.33 2GEN, ASP 24, 2.79, -0.7, -0.54, 0.23 2A6B,ASP 109,3.32,-0.72,-0.08,0.32 3DTE,TYR_160,10.5,0,0,0.5 2PGX.CYS 111.11.58.0.-0.02.2.6 2FPN,GLU_46,4.66,0.19,0,-0.03 1NKD, ARG 16, 13, 17, -0, 43, 0, 7, 0, 41 1SI7,ASP 5,3.99,0,-0.09,0.28 2FZP,GLU_263,4.59,0.09,0,0 3ADO.GLU 246,4.62,0.13,0,-0.01 1V6T.ARG 206.12.36.-0.18.0.0.03 2WZ9.CYS 46.10.38.-0.69.0.2.08 1GXN.GLU 624,1.66,0.54,-2.62,-0.76 2J8A,ASP_265,4.46,-0.04,-0.14,0.84 3CXS,GLU_76,4.27,0.04,-0.28,0 2BOO.ASP 117.3.79.0.-0.18.0.17 4ECC,HIS 92,7,48,-0.84,1,43,0.38 2P52,HIS_190,3.59,-2.16,0,-0.74 3M7G,ARG 206,13.83,-0.41,1.06,0.68 1YR6,ARG_179,12.96,-0.3,0.08,0.69 3EVP,GLU 192,4.8,0.28,0,0.02 4FH3.GLU 128.3.61.0.35.-0.55.-0.7 105J,TYR_92,11.19,0,0.32,0.87 4HDE,LYS_82,10.39,-0.17,0,0.06 3GFP,GLU_368,4.45,0.35,-0.24,-0.17 1QQH,TYR 139,11.22,-0.74,0.83,1.14 3EJC,GLU_93,3.96,0.26,-0.68,-0.11 1UW7,LYS 36,10,47,-0.03,0,0 1VJG,ARG_53,12.4,-0.27,0,0.17 1V8E,GLU 109,4.15,0.35,-0.76,0.07 4F8A,HIS 570,5.55,-0.3,0,-0.65 3T57,HIS_180,6.52,-1.53,0.85,0.69 2V81,HIS_24,5.52,-1.29,0,0.31 3LPZ,CYS_183,12.8,0,0.08,3.72 3BCY,TYR 153,13.73,0,0.39,3.34 2FZ4,LYS_100,10.52,-0.12,0,0.14 2XJ4,LYS_13,11.19,-0.24,0.52,0.41 3Q6L,ARG_31,12.82,-0.53,0.46,0.39 1YB2,GLU 213,4.74,0.47,0,-0.23 1RI5.ARG 188.12.58.-0.41.0.0.49 2BLL,TYR_436,12.93,-1.07,-0.26,4.26 1EYH,LYS_149,10.55,-0.12,0,0.17 3GOZ,ASP_156,3.95,0,-0.03,0.18 1UAJ,ASP_119,2.6,-1.48,-0.38,0.67 3ASA,CYS 68,7.62,-1.48,-0.17,0.27 1YIB,ASP_191,3.91,0,0,0.11 2FPN,LYS_146,10.35,-0.17,0,0.02 3CJW,ASP_330,3.42,-0.63,-0.12,0.38 4DBX.LYS 65,10.2,-0.38,0.0.08 3ERF,GLU_85,5.28,0.67,0,0.11 2P0L,CYS_149,10.85,-0.02,-0.34,2.22 2QHT,ARG_49,11.99,-0.55,0,0.04 1NJ4,LYS_184,10.5,-0.17,0,0.18 3IV4.TYR 45,10.29,0.0.12,0.17 4DIU,GLU_218,3.17,0.53,-1.37,-0.49 2XMZ,LYS_181,10.06,-0.73,0,0.29 3CE7,GLU_51,4.66,0.26,0,-0.1 3C0C,LYS 312,10,37,-0,15,0,0.02 1SNT,ASP_169,2.41,-2.33,-0.49,1.43 2CI3.LYS 195,10.63,-0.15,0.0.27 1SJ8,GLU_599,4.15,0.53,-0.82,-0.06 3ULX,CYS_33,10.01,-0.15,0.02,1.12 1AD6.ARG 500,12.36,-0.23,0.0.08 1R3F,ARG_307,12.8,-0.46,0.43,0.33 1GPP,GLU_156,3.88,0.72,-0.42,-0.91 1L3K,HIS_120,5.87,-0.52,0,-0.11

2XWS,ARG_18,11.66,-0.79,0,-0.04 1DUP.ARG 13.13.98.-0.42.0.96.0.93 2QK1,HIS_465,7.96,-1.52,1.99,1 3BQW,LYS_168,9.95,-0.57,0,0.01 3GE9,TYR_44,10.32,0,0.18,0.14 1FQI,ARG 382,12.67,-0.31,0.23,0.25 3T57.GLU 294.3.83.0.23.-0.55.-0.34 3PBH,HIS_190,6.34,-1.4,0.61,0.63 3LJN,GLU_183,4.69,0.16,0,0.03 2Q34,HIS_51,6.16,-0.28,0,-0.06 2BDV,ARG 47,12.49,-0.72,0,0.71 2X4J,ASP_49,2.24,-1.67,-0.38,0.49 3U4K.ARG 102,13,18,-0,49,0,8,0,37 3JZN,LYS_335,10.56,-0.14,0,0.2 1J8B.GLU 63.4.63.0.13.0.0 2012,ARG 46,12,43,-0.07,0,0 1IDK,GLU_95,4.67,0.17,0,0 1QYI,HIS_41,6.79,-0.87,0.76,0.4 3A0X,GLU_697,4.61,0.19,0,-0.09 2CI3,GLU 263,3.1,1.45,-2.12,-0.73 3L7N.TYR 101.11.88.0.0.1.88 2Q99,LYS_264,10.65,-0.17,0,0.33 1G8P,CYS_153,11.62,0,-0.17,2.79 1NJ4.TYR 20.10.76.-0.63.0.02.1.38 1DOV,LYS 155,10,55,-0,23,0,0,27 2V81,LYS_59,10.44,-0.19,0,0.13 3HVW,TYR_216,10.19,0,0,0.19 3GS3,LYS_197,10.42,-0.11,0,0.04 3QAV,ASP_198,4.04,0,0,0.24 1PV5.TYR 111.12.01.0.0.37.1.64 3V55,ASP_701,3.76,-0.44,-0.08,0.48 1LZL,LYS_219,10.21,-0.56,0,0.27 1NRI.GLU 38,3.91,0.28,-0.45,-0.42 2B6P.ARG 241.12.34.-0.21.0.0.05 1XDZ,GLU_178,4.56,0.09,0,-0.03 2D0A,TYR_4,11.24,0.46,0.38,0.39 1ZCU,HIS_150,6.8,-0.23,0.32,0.22 4FLE,LYS_133,10.43,-0.12,0,0.04 1GQE,ARG_343,12.2,-0.34,0,0.04 1R29,ARG_67,12.3,-0.27,0,0.06 1PZC,GLU_1,4.63,0.15,0,-0.01 1XTZ,TYR_245,12.64,-0.07,0.59,2.14 1XDZ,HIS 54,3.06,-2.4,0,-1.04 20KT,ASP_201,2.73,-1.33,-0.12,0.39 4DBX,HIS_254,6.62,-1.38,0.85,0.65 2PLQ,TYR_67,13.51,-0.06,0.9,2.67 4H86,CYS_120,11.6,-0.07,0.45,2.22 3M9A.LYS 95,10.49,-0.37,0.0.36 1XWM,GLU_56,5.88,0.97,0,0.4 3NR5,ARG_43,12.31,-0.22,0,0.03 3A2Z,GLU_125,4.98,0.37,0,0.11 3EVZ,ASP 113,3.14,-1.06,-0.24,0.64 2Q5X,HIS_862,6.02,-0.37,0,-0.1 1YTD,ARG_141,12.25,-0.28,0,0.03 1EQ6,GLU_102,4.66,0.22,0,-0.06 2B78,LYS_312,10.39,-0.3,0,0.18 1DOV,CYS_228,9.64,-0.14,-0.4,1.18 2Q99,CYS_364,11.22,0,-0.01,2.23 3PAC.GLU 175.4.37.0.26.0.-0.39 3JZN,TYR_138,11.49,0.1,0.3,1.08 3R87,LYS 59,10.74,-0.17,0,0.41 3BQW,ASP_268,3.2,-1.01,-0.25,0.66 1WLY,LYS_304,10.51,-0.22,0,0.22 1SQW,HIS_165,6.55,-1.56,0.99,0.62 4H4J,GLU_68,5.02,3.75,-1.45,-1.78 3EVP.HIS 239.6.03,-0.73.0.0.27 1XTD,GLU_128,4.01,0.42,-0.98,0.08 3M66,ARG_318,11.89,-0.6,0,-0.01 1PDB,LYS_176,10.64,-0.13,0,0.27

1BKB.LYS 18.10.43.-0.07.0.0 1YB2,HIS_33,6.26,-0.26,0,0.02 1YR6,LYS_29,10.46,-0.26,0,0.22 3P2F,LYS_41,10.94,-0.26,0.4,0.31 3K8ULYS 60.10.-0.35.0.-0.15 2Z61.LYS 4.10.46.-0.04.0.0 3GE9,GLU_3,4.54,0.13,0,-0.09 2E3S,ASP_444,3.84,0,-0.29,0.33 2RIK,GLU_148,4.54,0.07,0,-0.03 3V10.LYS 576.10.77.-0.18.0.0.45 3IVF,TYR_377,10.18,0,0.02,0.16 2PIM,ARG_9,13.11,-0.33,0.53,0.4 3CE7,ARG_53,13,-0.21,0,0.71 4D8L.GLU 276.4.01.0.22.-0.67.-0.04 2BAA, ASP 51, 3.66, 0, -0, 41, 0, 28 1PDB,TYR_177,12.33,0.32,0.65,1.35 1FKM,ASP_408,2.36,-2.32,0,0.89 3RE9,GLU_191,4.57,0.29,0,-0.21 2YT4.TYR 553.13.59.0.0.32.3.27 1Y0K,ARG_29,12.21,-0.46,0,0.16 1PVT,TYR_88,12.03,0,0.19,1.84 2AD1,HIS_293,6.45,-0.32,0,0.27 2PP6.GLU 35,4.22,0.51,-0.44,-0.35 3CX2,ASP 214,2.62,-1.48,-0.02,0.31 3TRE, ASP_66, 3.59, -0.55, 0, 0.34 1DCF,LYS_75,9.55,-1.04,0,0.09 1ZKZ,ARG_14,12.72,-0.31,0.16,0.36 2H8O,LYS 286,10.36,-0.14,0,0 10GL,TYR_245,10.6,-0.85,0,1.44 3FHF,LYS_27,11.23,-0.87,0.85,0.76 1GVP,LYS_24,10.42,-0.08,0,0 1SI7.ARG 122.12.35.-0.15.0.0 3UX2,ARG 48,12,49,-0.36,0.0.34 2CIU,GLU_210,4.67,0.3,0,-0.13 3ASA,ASP 211,3.81,-0.04,-0.44,0.5 2EJX,GLU_42,4.43,0.3,-0.15,-0.22 2IRM,GLU_75,4.81,0.55,0,-0.23 2BAA.GLU 67.4.55.2.55.-0.62.-1.88 2AZL,LYS_261,10.51,-0.49,0,0.49 2V5B,LYS_198,10.14,-0.36,0,0 1NFN.GLU 131.4.22.0.23,-0.38,-0.13 3LMF.ASP 8.3.94.0.0.0.14 2CI3,HIS_254,6.89,-1.38,1.3,0.47 1YB2,TYR 15,11,34,0,-0,15,1,49 4ETX,ASP_209,2.66,-1.34,-0.18,0.37 1T95,ASP_154,3.59,0,-0.4,0.19 3HOX,ASP 97,3.99,0,-0.03,0.22 3T8R,ASP_128,3.98,0,0,0.18 3V75,GLU_163,4.61,0.11,0,0 1YDL.LYS 31.10.52,-0.14,0.0.17 2R2Y,CYS_121,11.4,0,0.3,2.1 2YYO,LYS_127,10.68,-0.59,0,0.76 1CBY,HIS_227,6.3,-0.2,0,0 3ETV,GLU_266,4.43,1.32,-0.85,-0.54 1YLN,GLU 224,4.45,0.09,0,-0.14 100X.LYS 40.10.58.-0.2.0.0.28 3BQW,ASP_198,4.1,0,-0.02,0.32 1WOU, ASP 83, 4.03, 0, -0.16, 0.39 2FPN,ASP_136,3.93,-0.34,0.1,0.36 2JHY,GLU 87,4.6,0.25,0,-0.14 3MTT,GLU_507,3.41,0.18,-0.6,-0.67 3CZC,ASP_81,3.74,-0.17,-0.3,0.41 1BN6,TYR_98,10.95,0,0.11,0.84 2AZP,HIS_124,5.54,-0.79,0,-0.18 1JT9,ASP_195,3.67,-0.79,-0.44,1.1 3ASA,LYS_21,10.52,-0.12,0,0.13 3ZTA,GLU_139,4.47,0.25,-0.27,-0.01 2FZP,GLU_303,4.21,0.31,-0.65,0.06 3CQ1,ARG_4,12.47,-0.03,0,0

1N81.ASP 69.2.81.-1.68.-0.15.0.84 1TXJ,LYS_170,10.45,-0.05,0,0 1PBV,GLU_104,4.3,0.18,0,-0.38 1SIG,LYS_257,11.56,-0.7,0.67,1.08 1TLV.GLU 271.4.99.0.43.0.0.07 3IL3.HIS 178.6.2.-1.32.0.73.0.29 2B02,HIS_401,5.99,-0.61,0,0.1 30NH,GLU_516,4.24,0.36,-0.71,0.1 2FD5,ARG_173,12.18,-0.29,0,-0.04 1XDZ,HIS_199,5.63,-0.88,0,0.01 1XFK.HIS 67.5.94.-0.45.0.-0.11 3FXH,GLU_66,4.55,0.4,0,-0.35 1SBX,ARG_152,12.44,-0.14,0,0.09 1LFP,LYS_11,9.6,-1.03,0,0.13 4EKU.ARG 68.13.37.-0.43.0.62.0.68 1P4X,ARG_10,12.12,-0.64,0,0.26 2GAU,TYR_90,11.65,0,0.42,1.24 4EKU,HIS_192,6.27,-0.21,0,-0.02 3DZ1,ASP 98,3.94,0,-0.08,0.22 1DTO,LYS 52,10.39,-0.05,0,-0.06 2CW4,GLU_88,4.28,0.35,0,-0.57 3IDW,ASP_4,3.46,-0.72,-0.02,0.4 2CN1,GLU_211,4.59,0.13,0,-0.04 2E0T.LYS 147.10.35.-0.23.0.0.09 2B02,LYS_419,10.49,-0.4,0,0.38 3GV0,GLU_231,4.7,0.13,0,0.08 3L7N,CYS_91,9.65,-2.8,0.46,2.98 3V4G,GLU_36,5.38,0.81,0,0.07 1TR9.HIS 37.7.45.-0.26.0.85.0.36 3IL3,ARG_217,12.42,-0.33,0,0.25 1UCH,HIS_102,3.25,-3.36,0.02,0.1 1FHL,ASP_239,4.06,0,0.07,0.19 3ZTA,LYS 15,10.14,-0.32,0,-0.03 10IS,ASP_269,3.74,-0.4,0,0.34 1X04,ARG_100,12.89,-0.32,0,0.72 3G9T,CYS_54,11.7,0.27,0.66,1.77 2FM9,TYR 123,13.33,0,-0.04,3.37 1JSX,ARG_123,12.37,-0.22,0,0.09 4GA2,GLU_119,3.95,0.25,-0.18,-0.6 1R9W,LYS_219,10.48,-0.2,0,0.18 3O16,ARG_119,11.64,-1.61,0.51,0.23 3LH5,LYS 577,10.32,-0.29,0,0.1 3JV1.ASP 180.3.95.0.0.0.15 1A8Q,ASP_141,4.09,0,-0.02,0.32 1SQW,GLU_104,5.1,0.59,0,0 2RJD,ASP 383,3.8,-0.29,0.02,0.26 1WYC.ARG 187,13.03,-0.34,0.48,0.38 3QAV,LYS_134,10.78,-0.43,0.33,0.37 4FH3,HIS 224,4,45,-2,0,-0,04 1BN6,GLU_262,3.12,0.89,-1.46,-0.81 2H2W,HIS 170,3.32,-3.51,0.5,-0.17 3HVW,ARG_227,12.97,-0.35,0.39,0.42 3M7G,TYR_268,9.74,-0.78,-0.03,0.56 1ES5,ARG_31,11.78,-0.73,0,0.01 3HVW,ASP_228,3.44,-0.39,-0.39,0.42 4EKU,ASP_139,3.89,-0.21,0,0.31 3AUF,ARG_176,13.45,-0.39,0.71,0.63 200K,CYS_113,12.07,0,0.32,2.75 1QYI,TYR_207,11.94,0,0.02,1.92 1J33,HIS_276,5.97,-2.26,0.35,1.39 2JKF.GLU 77,5.02,2.77,-2.13,-0.11 4E6S,ARG_31,12.35,-0.19,0,0.03 3OA7,HIS_50,6.33,-0.17,0,0 3OA7,ARG_555,12.38,-0.12,0,0 2B0J,LYS_335,11.12,-0.16,0.4,0.38 1PBV,GLU_94,4.16,0.2,-0.27,-0.27 1XWM,ARG_106,12.09,-0.52,0,0.1 4FH3,TYR_370,11.02,0,0.21,0.82 3GMS,ARG_87,12.13,-1.06,0,0.69

1XDZ,ARG_20,12.21,-0.32,0,0.03 1L3K,ARG 140,12.46,-0.04,0.0 1WNH,ASP_121,2.94,-0.85,-0.35,0.34 1WP5,CYS_65,11.89,0,0.16,2.73 3JZN.LYS 89,10.63,-0.22,0.0.36 2GOV.CYS 47.9.37.0.0.02.0.35 3C2E,LYS_94,11.33,-0.21,0.59,0.45 2CN1,TYR_82,11.17,-0.06,0.38,0.85 1DOV,LYS_193,10.28,-0.25,0,0.03 2XHC.LYS 188.10.36.-0.12.0.-0.03 1DOV,LYS_199,10.49,-0.07,0,0.06 2H85,CYS_292,11.4,0,-0.13,2.52 4D8L.GLU 142.4.16.0.22.-0.32.-0.25 3HVM,LYS 2,9.69,-0.6,0,-0.2 2P52,ARG 193,12.35,-1.29,0.42,0.74 2VAN, ASP_170, 2.23, -1.69, -0.42, 0.54 1L3K,ARG 122,13,41,-0.39,0.84,0.46 3I82,CYS_201,11.56,-0.02,-0.12,2.7 2R4O,ARG 245,12.22,-0.3,0.0.01 1EYH,LYS 69,10.52,-0.08,0,0.09 3RJX,GLU_212,4.59,0.3,0,-0.21 2GKG,LYS_71,10.3,-0.19,0,-0.01 1LPL,TYR_200,9.88,-0.82,-0.14,0.83 4EZB,ARG 143,13.75,-0.95,1.57,0.62 2CXC.TYR 74,11.04,0.26,0.34,0.45 1KN3,CYS_168,12.18,-0.31,-0.16,3.65 3V46,ARG_393,12.62,-0.08,0,0.2 3BQE,GLU_301,4.99,1.58,-0.97,-0.12 3BZT,TYR 316,10.09,0,-0.36,0.45 1PDB,LYS_178,10.35,-0.29,0,0.14 2DFL,ASP_301,4.18,0,-0.3,0.68 1SIG,ASP_213,3.95,-0.05,0,0.2 1NFN,LYS 72,9.99,-0.54,0,0.03 3GT0.ARG 117.12.89.-0.81.0.66.0.55 1T3J,ASP_703,4.01,0,0,0.21 3PP8,GLU_153,4.54,0.18,0,-0.15 4HDE,LYS_170,11.44,-0.35,0.85,0.44 1ZBS,HIS 247,5.8,-0.62,0,-0.08 2Q5X,LYS_753,10.36,-0.14,0,0 20EW,CYS_40,9.86,-0.11,0.01,0.96 1XEU,GLU_101,3.53,0.4,-0.92,-0.45 3LJC,GLU 185,5.34,0.98,0,-0.15 2PWO,LYS 130,10.88,-0.32,0.24,0.46 1QQE,LYS_242,10.38,-0.17,0,0.05 1EV8,ARG_35,12.53,-0.24,0,0.26 4E8B,HIS_172,6.11,-0.49,0,0.1 2QOP,HIS_95,6.1,-0.93,0,0.54 1KN3.ASP 59.3.25,-0.75,-0.17,0.37 3DZ1,ASP_30,2.97,-1.28,-0.6,1.05 3C0C,ASP_340,3.27,-1.04,0,0.52 2XMZ,LYS_202,10.38,-0.21,0,0.08 3H04.GLU 58.4.4.0.32.0.-0.41 1L3K,LYS_113,10.37,-0.13,0,0 2QVT,HIS_115,6.22,-0.25,0,-0.03 2DG7,ARG_36,13.35,-0.38,0.66,0.58 2FG1,LYS_33,10.65,-0.21,0,0.37 20RX.ARG 167.12.63.-0.83.0.5.0.46 3UAH, ASP_203, 4.59, 0.17, 0.3, 0.31 2QVT,HIS_110,6.28,-0.17,0,-0.06 3M3P,GLU_243,4.51,0.01,0,0 2V81,ARG 201,12,42,-0,29,0,0.22 4H86,CYS_31,8.63,-1.06,0.04,0.65 1NRI.GLU 180.4.59.0.12.0.-0.04 3BQW,ASP_53,3.68,-0.47,0,0.35 2A1V,GLU_124,2.95,0.65,-1.69,-0.5 4DIU.ASP 227.2.92.-1.29.0.0.41 3C5V,GLU_51,3.77,0.4,-1.13,0 3LE4,HIS_343,6.94,-0.49,0.85,0.07 2RIK,GLU_228,4.29,0.38,0,-0.59

3Q1C,ARG_69,12.41,-0.09,0,0 2WB3.LYS 272.10.47.-0.03.0.0 3B7X,GLU_66,3.58,0.63,-1.58,0.02 10IS,ARG 263,12.93,-0.39,0.15,0.67 3UX2,CYS_107,9.33,0,0,0.33 2WB8,LYS 455,11.92,-0.32,0.97,0.78 3U2R.HIS 124.6.92.-0.56.0.8.0.17 3EJG,ASP_10,3.8,-0.05,-0.18,0.22 1PV5,GLU_180,4.7,0.11,0,0.09 1L2F,GLU_78,4.58,0.22,0,-0.14 2B0J,GLU 102,4.02,0.21,-0.36,-0.34 2PGE,LYS_17,10.31,-0.19,0,0 3ETU,GLU_254,4.25,1.12,-0.85,-0.52 2RIK,TYR_235,11.12,0,0.08,1.03 1UW7.LYS 58.10.11.-0.39.0.0 3K8J,ARG 161,13.57,-1.75,1.56,1.26 3JSN,LYS_298,10.41,-0.09,0,0 3DHN,TYR_145,10.81,0,-0.46,1.27 1ES9,GLU_90,3.2,0.62,-1.36,-0.56 2IRM,TYR 114,12.23,-0.94,0.44,2.73 3LOD,ARG 132,12,48,-0,56,0,0,54 2FBQ,ARG_160,12.51,-0.59,0.23,0.38 3PU6,LYS_147,10.78,-0.24,0,0.52 2G3A,TYR 113,12,74,0,74,0,42,1.57 1MML/HIS 77.5.54,-0.7.0,-0.26 2Q34,ASP_224,3.78,0,-0.18,0.15 2VGM.GLU 26.4.82.1.09.-0.64.-0.12 105T,ARG_134,11.21,-1.7,0.26,0.14 3GW3,CYS_65,11.94,-0.03,0.09,2.88 2DVK,ARG_79,12.22,-0.36,0,0.07 3BB7,ASP_68,4,-0.05,0.14,0.11 2AH5,LYS_164,10.71,-0.21,0,0.41 3CAN, HIS 73, 4, 92, -1, 33, 0, -0, 25 2JKF,ASP 145,3.51,-0.72,-0.53,0.97 3NR5,ASP_117,3.13,-0.63,-0.69,0.64 3COU,ARG_38,12.21,-0.29,0,0 1UAJ,LYS_75,10.47,-0.51,0,0.48 3KEY,LYS_410,10.59,-0.19,0,0.28 3G9G,GLU_65,3.66,0.28,-0.81,-0.31 4EVF,ASP_241,4.51,0,-0.1,0.8 1U53,LYS_178,11.43,-0.3,0.85,0.38 2W2S,GLU_147,4.62,0.08,0,0.04 2V81,LYS 139,10.41,-0.1,0,0.01 1WP5,TYR_25,10.96,0,0.05,0.91 2BAA, ASP_77, 2.93, -0.85, -0.4, 0.39 2R0S,ASP_218,3.09,-1.1,0,0.39 2X5Y,HIS_828,5.29,-1.2,0,-0.02 3EVN,ARG 317,13.67,-0.32,0.69,0.8 3GV0,GLU_307,3.74,0.73,-0.72,-0.77 3JV1,ARG_58,12.62,-0.09,0,0.22 3I4T,ARG_186,12.29,-0.27,0,0.06 2A0J,GLU 85,4.71,0.21,0,0 3T5B,ASP_388,3.87,0,-0.07,0.13 20B5,GLU_80,4.99,0.41,0,0.08 1UCH, ARG_47, 13.01, -0.72, 0.73, 0.51 1UOH,LYS_153,10.46,-0.14,0,0.1 2P1W,ARG_237,13.53,-0.37,0.78,0.6 3ETU,GLU_227,4.77,0.27,0,0 10I7,ASP_103,4.08,-0.01,-0.11,0.39 1QYI,LYS_144,11.11,-0.62,0.71,0.52 1QZN,ARG 77,12.31,-0.19,0,0 2OSA.ASP 269.3.02.-1.28.-0.25.0.75 2V5B,ASP_86,3.89,0,-0.04,0.13 1ZBS,GLU_250,3.84,0.47,-0.74,-0.39 3U2R,ARG_53,12.26,-0.62,0.13,0.24 3BZT.GLU 299,4.66,0.26,0,-0,1 1G8P,ARG_326,10.84,-2.14,0.3,0.17 1PSW,ARG_77,12.1,-0.35,0,-0.05 1CHD,ARG_219,12.44,-0.31,0,0.25

1YDL.CYS 12,9.57,-0.18,0.2,0.56 2GZQ,GLU_23,3.56,0.18,-0.85,-0.27 1059,CYS_143,11.91,0,0.05,2.87 4AM1,LYS_146,11.43,-0.26,0.75,0.44 3F6F.ARG 67.12.89.-2.35.0.62.2.11 1SI7.ARG 199.10.62.-1.91.0.0.02 1W7B,GLU_247,4.85,1.17,-0.7,-0.12 2YX0,LYS_126,10.19,-0.27,0,-0.04 2WOZ, ARG_297, 12.43, -0.13, 0, 0.06 10YLASP 43.3.74.-0.37.-0.05.0.35 1WYC,HIS_180,6.02,-3.2,0.85,1.88 2R4O,ARG 240,13,25,-1,33,1,43,0.65 1ES9,CYS_55,9.47,-0.02,-0.03,0.52 2WB8.ASP 504,3.75,0,-0.2,0.15 1UXO,LYS 101,11.03,-0.48,0.63,0.37 2R51,TYR_78,10.4,0,0.15,0.24 3Q1C,ARG_354,12.29,-0.68,0,0.47 2BCF,ARG_251,12.97,-0.52,0.53,0.47 1J74.ASP 37.3.47.-0.3.-0.3.0.26 3M70,GLU_183,3.51,0.24,-0.85,-0.38 2XWS,LYS_92,9.24,-1.28,0,0.02 1SQW,TYR_128,10.12,0,-0.1,0.21 2HRZ,TYR 112,10.55,0,0.27,0.28 1TR9.LYS 125.10.46.-0.04.0.0 3UX2,LYS_113,10.44,-0.06,0,0 3D9H,HIS_41,4.93,-2.39,0.79,0.03 2Q5X,ARG_817,12.37,-0.18,0,0.05 3CAX.HIS 179,7.42,-3.49,1.67,2.74 3D9H,LYS_184,10.66,-0.16,0.11,0.21 3I0C,LYS_124,10.3,-0.2,0,-0.01 3BA1,HIS_302,6.25,-1.21,0.85,0.12 3V46.LYS 371.11.15.-0.27.0.47.0.46 3I4T.HIS 238.6.26.-0.29.0.0.05 3C6B,LYS_47,10.35,-0.15,0,0 3I0C,TYR_206,11.25,0,0.16,1.1 3A0X,GLU_696,4.31,0.16,0,-0.35 3LD1,LYS_52,10.42,-0.08,0,0 1L2F,ARG 144,12,71,-0,16,0,04,0,33 3IVF,GLU_346,4.75,0.19,0,0.07 1RZ2,ASP_199,3.57,-0.2,-0.29,0.25 3EZ7.GLU 350.4.81.0.42.-0.03.-0.09 3RLE,TYR 198,10,11,0,-0.02,0,12 1Z9L,ASP_77,3.93,0,0,0.13 4HDE,LYS 138,11,72,-0,31,0,85,0.67 1FQI,GLU_324,3.9,0.71,-0.74,-0.57 3JV1,ASP 151,3.21,-0.84,-0.17,0.39 3HUE,LYS 104,10.02,-0.23,0,-0.25 1GPP,ARG_162,13.41,-0.62,0.79,0.72 3HZQ,LYS_6,10.46,-0.04,0,0 3H04,GLU 257,4,35,0,23,-0,05,-0,32 3EVZ.LYS 101.9.98.-0.54.0.0.01 3B4D,ARG_200,12.54,-0.1,0,0.13 2FI9,GLU_116,4.59,0.26,0,-0.17 3CBN,ASP_138,3.17,-0.83,-0.36,0.55 3CJW,GLU_297,2.96,0.46,-1.37,-0.65 3Q6L,ARG_127,11.9,-2.31,0.24,1.47 3A0X,GLU_664,4.74,0.43,0,-0.19 1A8Q,ASP 133,4.07,0,0,0.26 2RIK,LYS_202,10.49,-0.21,0,0.21 2B78,ARG 280,12.34,-0.46,0,0.3 30DJ,ASP_32,4.02,0,0,0.22 1PDB,LYS_108,9.32,-1.17,0,0 3K8U,ARG_126,12.54,-0.11,0,0.15 1RI5,GLU_285,5.35,2.49,-1.16,-0.48 1RHS,LYS 236,10,45,-0.05,0,0 2CYG,TYR_329,10.39,0,0,0.39 1Y0K,ARG_181,11.35,-1.15,0,0 3RKV,GLU_295,4.61,0.31,0,-0.21 2FI9,TYR_21,9.48,-0.52,-0.3,0.31

2PLO.LYS 21.10.83.-0.52.0.54.0.31 3FWU,LYS_75,10.48,-0.23,0,0.21 3ETU,LYS_222,10.21,-0.19,0,-0.1 2B61,ARG_184,11.78,-1.52,0.7,0.1 3LJI,ASP 90,3.81,-0.32,1.39E-17,0.33 3ADO,ARG 185,12,99,-0,4,0,64,0,25 3GA2,ARG_183,12.52,-0.16,0,0.18 3A7L.LYS 8,10.39,-0.27,0,0.16 1ZBS,ASP_126,2.58,-1.5,-0.23,0.51 1PBV,GLU_156,3.99,0.28,-0.62,-0.17 2YLF.GLU 148.4.62.0.12.0.0 3F7M,CYS_177,10.23,-2.49,0.04,3.68 1D2K,LYS_177,11.22,-0.46,0.85,0.33 3OA7.HIS 562.6.1.-0.47.0.0.06 4H86.LYS 156.10.13.-0.54.0.0.17 4F85,TYR_185,11.97,0,0.62,1.35 3U2A,ARG_38,12.82,-0.29,0.2,0.4 3FNI,TYR_133,10.98,-0.02,-0.02,1.03 3BPP,TYR 36,10.18,0,0.05,0.13 2HRZ,ARG 233,13.82,-0.63,1.2,0.75 3JRT,TYR_31,9.88,0,-0.3,0.17 3EVP,GLU_290,4.58,0.09,0,-0.01 4EF5,GLU_296,4.91,0.34,0,0.07 3F6F.GLU 75.5.03.0.53.0.0 1HF8,HIS_83,4.59,-3.33,0.85,0.58 3EGN,GLU_402,4.15,0.23,-0.59,0 10GL,LYS_63,9.98,-0.18,0,-0.34 1F2V,TYR_4,10.07,0,0,0.07 1T95,ASP 76,3.25,-0.51,-0.37,0.33 1QYI,TYR_305,11.82,0,0.12,1.7 3CAX,ASP_344,3.37,-0.6,-0.18,0.36 1L2H,ARG_4,12.42,-0.23,0,0.15 2W2S,GLU 108,3.88,0.36,-0.44,-0.54 3Q9P,ARG_96,13.28,-0.27,0.71,0.34 3N0K,HIS_107,6.13,-0.43,0,0.06 1YLN,ARG_155,13.52,-0.35,0.98,0.39 3G9T,HIS 233,3.91,-3.37,0.26,0.52 3ULX,ARG_126,12.4,-0.1,0,0 1SJ8,ARG_765,12.41,-0.16,0,0.06 2P52.GLU 225.4.65.0.15.0.0 3VHJ,ARG_148,12.48,-0.31,0,0.29 100X,ARG 148,12.23,-0.31,0,0.05 3SMD.LYS 80.11.57,-0.41,0.85,0.63 1RZ2,ARG_141,12.05,-0.68,0,0.23 3BPP,LYS_194,10.46,-0.26,0,0.22 1VJG.LYS 115.10.5.0.0.0 3P28,LYS_92,10.35,-0.29,0,0.13 3B7H,TYR_73,12.38,0.85,0.4,1.13 3UX2,LYS 103,10,39,-0,11,0,0 1YG2,LYS_46,10.55,-0.1,0,0.16 3KV0,GLU 72,4.05,0.26,-0.51,-0.2 106D,GLU_74,3.82,0.43,-0.74,-0.38 1YTQ,LYS_100,10.39,-0.06,0,-0.05 1J33,ARG_116,13.19,-0.6,0.84,0.45 1UJ8,LYS_15,11.2,-0.35,0.25,0.8 2HXB,LYS_139,10.7,-0.2,0,0.39 3GFP,ASP_375,3.9,0,-0.28,0.38 3R2E,ASP_46,3.37,-0.68,0,0.25 3C38,ARG_171,12.38,-1.36,0.34,0.89 3HUE,GLU 203,4.82,0.17,0,0.15 3IV4.TYR 52.11.06.-0.08.0.3.0.85 1TJE,HIS_13,6.32,-0.27,0,0.09 1UXO,TYR_6,10.66,-0.85,0.32,1.19 2JKF,GLU_113,4.69,0.31,0,-0.12 3UC9,ARG_80,11.74,-1.12,0,0.36 3UC9,TYR_5,10.12,0,0,0.12 1JT9,CYS_118,11.28,-0.12,0.33,2.07 3GS3,CYS_34,10.83,0,0.01,1.82 1TR9,ASP_38,2.36,-1.68,-0.25,0.5

1EV8,ARG_99,12.73,-1.25,0.97,0.51 2D7U,ASP 90,3.61,-0.09,-0.35,0.25 109G,ARG_132,12.57,-0.32,0.25,0.14 3IPZ.GLU 82,4.73,0.25,0,-0.02 4FZN.ARG 242.12.34,-0.26.0.0.1 3LH5,TYR 755,10.22,0,-0.09,0.31 1Q5Z,ASP_647,2.23,-2.28,-0.73,1.45 2XWS,CYS_59,10.48,0.03,0.21,1.24 2GZR,TYR_67,13.48,-0.02,0.69,2.83 1JYH, ASP 105, 3.26, -0.66, -0.27, 0.38 3F7M,TYR 299,10.21,0,-0.16,0.37 2BV9,ARG_52,12.62,-0.35,0,0.47 3LJI,GLU_293,4.9,0.34,0,0.06 3P2F,ARG 139,12.06,-0.51,0.0.07 1TD6,ASP 38,1.75,-2.57,-0.06,0.59 2PLQ,TYR_284,10.14,0,-0.16,0.3 1SNT,ARG_243,13.75,-3.69,0.54,4.4 2OGQ,LYS_480,9.62,-0.58,0,-0.3 3CAX,ASP_296,3.4,-0.54,-0.03,0.16 3C38,HIS_154,5.47,-1.11,0.08,-3.47E-18 1YB2,LYS_17,10.31,-0.19,0,0 1YTO, ARG 89, 13, 74, -0.24, 0.91, 0.57 1DOV,LYS_246,10.4,-0.12,0,0.02 3HKX.HIS 20,7.46,-0.25,0.85,0.36 3LPZ.GLU 141.4.85.0.39.0.-0.04 3C6B,TYR_39,11.8,-0.06,0.02,1.83 1GXN,HIS_513,4.03,-3.27,0.81,-0.01 2D59,LYS 103,10,57,-0,14,0,0,21 3RNV,ASP 370,3.68,-0.07,-0.42,0.37 1WPA, ASP_437, 3.98, 0, -0.27, 0.45 3M16,LYS 48,10.32,-0.24,0,0.06 1PVT,GLU_172,4.4,0.49,0,-0.59 1LN4,GLU 64,4.61,0.25,0,-0.14 4FH3,TYR 324,10,29,0,-0,06,0,35 1Q8B,CYS_19,9.77,-0.04,0.13,0.68 3GFP,ASP_467,3.35,-0.56,-0.19,0.3 3N0K,ASP_114,3.67,-0.3,-0.03,0.2 3UPD,HIS -17,7.18,-0.78,0.87,0.58 3N0K,ASP_82,3.41,-0.85,0,0.46 1PDB,TYR_156,13.05,0,0.57,2.49 1NKD,HIS_46,6.68,-0.17,0.15,0.21 2AZP,ARG 132,12.32,-0.5,0,0.33 2CWC.ARG 243,11.83,-1.06,0.03,0.38 1GQE,GLU_16,4.61,0.22,-0.29,0.17 2R51,HIS_63,5.77,-1.09,0.32,0.03 2E0T,HIS_138,6.06,-0.47,0,0.03 1DOV,LYS 87,10.45,-0.16,0,0.11 4FH3.ARG 340.12.2.-0.38.0.0.08 3LJI,CYS_56,11.65,0,0.08,2.57 2RFA,GLU_176,3.9,0.36,-0.69,-0.27 2ZQ5,GLU_15,4.02,0.29,-0.74,-0.03 3FNI,LYS 125,10,41,-0,11,0,0.02 1YR6,TYR_181,10.46,0,-0.42,0.87 1RAJ,GLU_226,4.64,0.59,0,-0.45 3AU3,HIS_652,5.78,-0.83,0,0.11 3CJW,GLU_311,5.07,2.95,-2.47,0.08 2HNG,LYS 8,11.31,-0.42,0.85,0.38 1YM5,GLU_40,5.04,0.57,0,-0.03 2B78,LYS_84,10.2,-0.46,0,0.15 1ZBM.GLU 204.4.7.0.2.0.0 2E3H.CYS 242.11.24.0.0.1.2.14 3O48,ARG_108,12.55,-0.16,0,0.2 20BI,GLU_158,4.23,0.35,-0.56,-0.06 1WOU,GLU_20,4.49,0.28,-0.02,-0.27 1UXO, ARG_12, 12.56, -0.17, 0, 0.23 4E9E,TYR 540,12,37,-0.66,0.63,2.39 1UCH,HIS_193,4.71,-2.6,0.85,-0.04 2QVO,ARG_72,13.49,-0.26,0.7,0.54 2l6l,LYS_56,10.18,-0.32,0,0

3LOE, ASP 410, 4, 34, 0, 0, 24, 0, 29 3IO0,HIS_195,3.78,-2.36,0.01,-0.35 2QRX,ASP_8,4.01,0,0,0.21 3GV0.ARG 179.12.05.-0.79.0.0.34 3F7M,ARG_222,11.96,-0.6,0,0.07 1RWZ,CYS 202,12.05,-0.06,-0.23,3.34 3CCY,GLU 97,4.38,0.62,-0.39,-0.35 3DSH,GLU_354,4.19,0.25,-0.18,-0.38 2VGM,LYS_82,12.26,-0.49,1.33,0.92 3RFF,HIS_60,7.1,-0.55,0.85,0.31 1X04,ASP 169,4.28,0,-0.06,0.53 2IQT,GLU_247,4.14,0.25,-0.3,-0.31 1X1E,TYR_224,10.04,0,-0.01,0.05 1R3D,HIS_166,6.79,-0.24,0.32,0.21 4FZR.ARG 210.12.96.-0.77.0.46.0.77 1WOU.GLU 50.4.02.1.36.-1.43.-0.41 3JV1,TYR_189,10.95,-0.07,-0.03,1.05 1H4U,GLU_523,4.43,0.23,0,-0.3 1V43,GLU_292,3.84,2.13,-1.63,-1.16 4HDE,LYS 31,10.44,-0.06,0,0 2AHE,ASP 228,4,11,0,0,09,0,23 1X91,LYS_10,11.47,-0.45,0.85,0.57 1D2K,LYS_369,10.39,-0.13,0,0.02 2V5B,ARG 162,13,11,-0.61,0.84,0.37 2VGY,ASP 69,3.25,-1.58,-0.47,1.49 1Y0K,GLU_113,4.39,0.27,-0.37,-0.01 1GOE, ARG 22, 11, 91, -1.03, 0, 0, 44 2CXY,TYR_95,10.6,-0.05,0,0.65 1DTO,ASP_25,4.01,-0.11,0.06,0.25 2IRM.TYR 339,10.94,0.0.23,0.72 3RLN,LYS_695,10.51,-0.12,0,0.12 2YLF,ASP_212,4.04,0,-0.06,0.29 1MML.LYS 103,10.08,-0.33,0,-0.09 2CW4,ARG 114,12.91,-0.31,0.2,0.52 3T8R,ASP_109,3.03,-0.51,-0.7,0.43 4EKU,GLU_88,5.06,1.25,-0.71,0.01 2GZR,LYS_262,10.56,-0.14,0,0.2 1LTU,ARG_233,12.34,-0.33,0,0.18 4FZR,HIS_29,6.62,-0.66,0.74,0.04 3A2Z,ARG_64,10.87,-2.34,0,0.71 2FZP,GLU_292,4.7,1.6,-0.85,-0.54 4ANN,CYS_160,11,-0.01,-0.2,2.21 3GG6,CYS 100,11.37,0,0.12,2.24 2FD5,ASP_169,3,-0.67,-0.6,0.46 1DOV,CYS_116,9.12,0,0,0.12 2OJQ,CYS_524,9.84,0,-0.16,1 2H2Z,HIS_163,2.22,-3.39,0,-0.89 3PZ9,ASP 154,3.28,-1.03,-0.13,0.63 2AZL,LYS_238,11.3,-0.42,0.8,0.41 1NIJ,ARG_69,11.97,-0.95,0,0.42 1MUF,GLU_329,3.59,0.61,-1.38,-0.14 1G8P,GLU 115,3.86,0.52,-0.54,-0.62 4FCU,GLU_253,4.84,0.24,0,0.09 2JEO,LYS_76,10.21,-0.31,0,0.02 2IF4,HIS_252,5.89,-1.55,0.8,0.14 1X9G,ASP_122,4.1,-0.02,0.11,0.21 1XTZ,TYR_67,9.8,-0.53,0.18,0.15 2CWC,CYS_64,10.97,-0.01,0.04,1.94 2O4D,TYR 50,10,49,0,0,26,0,22 3ZSL,GLU_193,3.46,0.32,-0.79,-0.56 3K8U,ARG_66,12.13,-0.49,0,0.12 3IDW.TYR 22,11.88.0.0.26,1.63 2QHT,ASP_135,4.17,-0.11,-0.25,0.73 3T5B,TYR_274,13.33,-0.08,0.21,3.2 2DFL,TYR_220,10.47,-0.15,0.14,0.48 1X7F,CYS_146,12.73,0,-0.11,3.84 3TRE,LYS_97,10.33,-0.19,0,0.02 3COU,HIS 21,5,79,-1,21,0,51,0 1XWM,LYS_85,10.36,-0.33,0,0.18

100E,CYS 164,12.02,0.12,0.43,2.47 3ERF,ASP_79,2.33,-1.83,0,0.36 4EVF,HIS_92,5.42,-1.28,0,0.2 1RI6,GLU_126,4.23,0.37,-0.64,0 3C6B.GLU 117.4.31.0.46.-0.55.-0.1 3M7D,ARG 102,12,23,-2,88,0.69,1.92 1NRI,ASP_121,3.97,0,-0.15,0.32 1XTZ,LYS_90,10.47,-0.24,0,0.2 3GMS,TYR_190,10.34,0,0.1,0.25 1GVP.GLU 30.3.36.0.44.-0.95.-0.63 20GQ,GLU_575,2.85,0.34,-1.49,-0.5 1R29,ARG 40,12.5,-0.07,0,0.07 3K8J,GLU_271,4.42,0.13,0,-0.21 3E7P.GLU 214,4.34,1.95,-1.65,-0.46 20RX,LYS 44,10,29,-0,27,0,0,06 1GQE,TYR_187,10.67,-0.02,-0.43,1.12 3K8J,ASP_259,3.53,-0.44,-0.11,0.28 2R0S, ASP_277, 4.98, 0, -0.03, 1.22 4ETX.ASP 434.3.44.-0.64.0.0.28 30DJ,HIS_169,5.59,-0.91,0,0 3BPP,GLU_163,3.64,0.37,-0.85,-0.38 3RNV,ARG_445,12.52,-0.23,0,0.25 2ZCO,ASP 56,2.94,-1.35,0,0.49 3EVP.ASP 179.3.27.-0.52.-0.49.0.48 2E3C,LYS_192,11.68,-0.26,0.85,0.58 1SI7,ASP_250,3.35,-0.53,-0.25,0.34 4AF2,ASP_-3,4.02,0,0,0.22 3PU6,CYS 102,10.49,-0.37,0.07,1.8 1SUU,LYS_734,10.48,-0.05,0,0.02 20PJ,ARG_124,12.45,-0.05,0,0 1JSX,ASP_146,3.2,-0.92,-0.04,0.36 3H6O,LYS 31,10.92,-0.24,0,0.67 2F9F,GLU 141,3,76,0.5,-1,5,0.27 1WPA,ASP_516,1.98,-1.59,-0.68,0.45 3NBI.GLU 199.4.84.0.14.0.0.2 1J85,GLU_68,4.61,0.11,0,0 2HP7,ARG_152,12.13,-0.39,0,0.01 20K0.GLU 67.4.65.0.17.0.-0.02 1EDG,LYS_317,11.45,-0.3,0.83,0.43 3H04,GLU_3,4.53,0.31,0,-0.3 1KN3,ARG 82,12,36,-1,03,0,31,0,57 1RI6,ARG 243,12.66,-0.16,0.0.32 3JZN,ASP_390,3.23,-0.75,-0.25,0.42 1WXQ,HIS_341,5.75,-0.75,0,0 2CXC,LYS_108,11.52,-0.2,0.73,0.49 1QYI,ARG_17,13.13,-1.52,0.61,1.53 3EVN,LYS 82,10.66,-0.2,0,0.36 3T5B,ASP_44,3.39,-0.83,0,0.42 1LFP,LYS_145,10.13,-0.15,0,-0.22 105T,ASP 382,3.85,-0.06,-0.07,0.17 4ECC,LYS 144,10.77,-0.15,0.0.43 1DCF,GLU_99,4.67,0.17,0,0 3CS1,LYS_55,10.45,-0.19,0,0.14 1AKO,GLU_46,4.14,0.36,-0.69,-0.03 1WP5,ARG 19,12.2,-0.78,0,0.48 1PVT,TYR_13,10.32,0,0,0.32 3C6B,TYR_278,12.29,-0.89,0,3.17 2W0G,LYS 240,9.97,-0.61,0,0.08 1S7K,GLU_18,4.53,0.5,-0.23,-0.24 2H85,GLU 191,4.6,0.1,0,0 1QQE,GLU_250,4.58,0.24,-0.43,0.27 2XHC,LYS_132,10.58,-0.08,0,0.16 3UPD,LYS_213,10.47,-0.13,0,0.11 1WYC,ARG 33,12.43,-0.07,0,0 1V6T,LYS_17,10.17,-0.38,0,0.04 3KV0,ASP_29,3.52,-0.52,0,0.24 1NAR,TYR_116,12.31,-0.64,0.31,2.64 4DBX,TYR_190,10.07,0,0,0.07 2l6l,LYS_30,10.33,-0.25,0,0.08

3E5TLYS 71.10.31.-0.19.0.0 3JZ9,ASP_480,2.45,-1.59,-0.06,0.3 3BQE,GLU_335,4.79,0.23,0,0.06 1YOY,GLU_16,2.55,0.6,-2.18,-0.38 10GL,LYS 216,11,-0.99,0.85,0.63 2ILR/HIS 317.6.17,-0.74,0.35.0.06 3RFY,TYR_265,11.64,0,0.02,1.63 3JRT,LYS_29,11.39,-0.88,0.85,0.91 2Q98,HIS_30,4.9,-1.22,0,-0.38 3M7G.GLU 217.4.18.2.39.-1.54.-1.19 1MTZ.LYS 151,11.81,-0.37,0.87,0.82 3LMF,LYS_72,10.59,-0.1,0,0.19 2XWS,ASP_110,3.35,-0.84,0,0.39 3BOW,LYS 26,10.35,-0.17,0.0.02 2I88, ASP 410, 2.84, -0.79, -0.75, 0.59 3I47,GLU_255,4.57,0.23,-0.1,-0.06 3LH5,LYS_737,10.21,-0.19,0,-0.1 3HVM,LYS_178,11.38,-0.32,0.79,0.41 1ZCU,GLU_118,5.68,2.87,-1.61,-0.08 2HRZ,GLU_297,4.58,0.2,0,-0.12 20EW,LYS_207,10.32,-0.15,0,-0.04 2EDM,ARG_51,12.25,-0.18,0,-0.07 3DTE,ARG_149,12.89,-0.28,0.48,0.18 1SUU.GLU 598,2.91,1.22,-2.53,-0.27 1WRU,TYR_207,11.53,-0.75,-0.15,2.43 3EVP,TYR_197,10.32,0,0.18,0.14 2B0J,LYS_161,10.41,-0.22,0,0.13 3H04,GLU 152,4.38,0.14,0,-0.26 3EZ7.GLU 65.4.85.0.39.0.-0.04 30IP,LYS_77,10.39,-0.11,0,0 1PBV,ASP_225,3.15,-0.76,-0.25,0.35 1MUF,GLU_135,4.5,0.09,0,-0.08 3RE9.TYR 124,10.3,0,-0.48,0.77 1U7U,GLU_335,4.44,0.36,0,-0.42 1Y0K,TYR_164,11.97,-0.04,0.07,1.93 2E3C,LYS_311,10.01,-0.34,0,-0.15 4ECC,LYS 138,10.67,-0.12,0,0.28 2G5X,ASP_77,3.08,-0.78,-0.36,0.42 1P1L,GLU_61,3.6,0.26,-0.7,-0.46 1XDZ,ARG 210,12,94,-1.08,0.57,0.96 3GS9,ASP_76,3.95,0,-0.06,0.2 1L2F,ARG 160,12.44,-0.21,0,0.15 1SIG.ARG 374,12,43,-0,11,0,0,04 3BPV,LYS_106,10.07,-0.33,0,-0.1 2GEN,ASP_91,3.23,-1.31,-0.46,1.2 3RHE,LYS_13,10.47,-0.05,0,0.03 3RFF,ASP_94,3.5,-0.67,0,0.37 2BAA, ASP_209, 1.69, -2.09, -0.74, 0.71 3GV0,ARG_187,13.31,-0.4,0.72,0.48 3ELI,GLU_104,4.64,0.35,0,-0.21 1SI7,GLU 145,3.94,0.96,-1.39,-0.13 1ZHV,HIS 135,6,39,-0,11,0,0 1YW5,GLU_98,3.66,0.28,-1.05,-0.08 3NR5,HIS_24,7.05,-0.41,0.6,0.37 3QKY,ARG_145,13.35,-0.44,0.57,0.72 3FHF,GLU_192,5.18,1.56,-0.83,-0.06 1SBX,GLU 159,4.66,0.25,0,-0.09 1IDK.TYR 305,10.36,0.0,14,0.22 3PP8,LYS_121,10.41,-0.09,0,0 2ZCO,HIS_207,6.59,-0.3,0,0.39 1PZC,ASP 29,2.67,-1.25,-0.44,0.57 3LJC,GLU_243,4.71,0.21,0,0 1ZYL,ARG_197,10.6,-1.98,0,0.09 3CAX,LYS_239,10.84,-0.6,0.54,0.39 1PSW,LYS 2,10.37,-0.38,0,0.24 1SUU,GLU_732,4.2,0.34,-0.26,-0.38 2IQT,ARG_261,12.03,-0.49,0,0.03 208I,LYS_152,10.28,-0.22,0,0 2QEV,ARG_17,13.26,-0.33,0.66,0.43

1IDK,LYS_47,10.64,-0.44,0.22,0.36 1ILW,HIS 71,5.94,-2.73,0.88,1.29 3IVF,TYR_216,12.43,-0.28,-0.24,2.94 4GA2.GLU 41.4.52.0.4.-0.12.-0.27 4ESS,ASP_81,3.79,0,-0.18,0.17 3RFY,ASP_300,4.06,0,-0.1,0.36 3RFY,LYS 116,10.67,-0.12,0,0.3 1PNE,GLU_116,4.7,0.24,0,-0.04 1P6F,GLU_117,4.13,0.36,-0.71,-0.02 1DZF.GLU 81.5.07.1.8.-0.83.-0.4 3K1H.LYS 131,10.76,-0.95,0.22,0.99 4FLE,GLU_47,4.97,0.39,0,0.08 4F85.GLU 239.4.52.1.03.-0.64.-0.37 1FOI.GLU 348,4.82,0.42,0.16,-0.25 3P51.ARG 52.12.81.-3.48.0.67.3.13 1IAP,GLU_212,4.63,0.08,0,0.05 1XDZ.GLU 26,4.06,0.77,-0.79,-0.43 2FL7,ARG_169,12.32,-0.41,0,0.24 3TRE.GLU 80.4.88.0.21.0.0.17 1U3Y,LYS 343,10,11,-0,24,0,-0,15 1059,LYS_168,12.47,-1.32,1.3,1.99 2BCF,ARG 109,13.63,-0.4,0.9,0.62 3C38,ARG_95,12.31,-0.4,0,0.21 3UPD,GLU 309,4.54,0.12,0,-0.09 3F6M,LYS 71,10.28,-0.22,0.0 1P2F,TYR_204,11.4,-0.21,0.26,1.34 2FM9,LYS_118,10.58,-0.16,0,0.24 3GEC,ARG_522,12.36,-0.14,0,0 1GPP,ARG 33,13.16,-0.15,0.56,0.25 3UAH,TYR_255,11.05,-0.84,-0.43,2.31 1WP5.LYS 220.10.58.-1.18.0.83.0.43 3I0C,LYS_82,10.02,-0.43,0,-0.05 2Q13,GLU 27,4.69,1.5,-0.85,-0.46 3EOD,ARG 99,12,36,-0,14,0,0 1RI5,LYS_195,10.59,-0.24,0,0.33 2YWJ,LYS_174,11.51,-0.3,0.62,0.69 1RI6,HIS_286,5.94,-1.23,0.7,-0.03 2Q34,GLU 134,3.19,0.59,-1.72,-0.18 1PVT,GLU_55,3.77,0.44,-0.38,-0.79 1RWZ,ASP_157,3.1,-0.7,-0.64,0.64 3CAX,ASP_249,3.45,-0.58,-0.49,0.73 3P2F,ASP_190,3.05,-0.65,-0.36,0.27 3N2T,ASP 12,3.82,0,-0,13,0,15 2FC3,LYS_49,10,-0.52,0,0.03 2IXM,TYR_151,13.86,-1.65,1.16,4.36 2B6P,GLU_134,6.05,4.29,-2.54,-0.2 2VGM,ASP_296,4.87,0,0.54,0.53 2B3M,GLU 70,4.55,0.14,0,-0.09 2R57,HIS_345,6.18,-0.84,0.04,0.48 2F4Q,TYR_225,13.87,0.77,0.43,2.67 1JB3,TYR_44,11.48,0,0,1.48 3CO1.GLU 94,3.71,0.22,-0.81,-0.19 3CQ1,TYR_34,10.41,-0.3,-0.37,1.09 1TR9.HIS 260.6.26.-0.25.0.0.01 2H2Z,GLU_178,4.88,0.21,0,0.18 3ONH, ASP_496, 3.7, 0, -0.29, 0.19 2P5D,LYS 114,10,38,-0,12,0,0 3BB7,CYS_249,10.9,-1.46,0.05,3.32 3GEC,ARG_345,12.33,-0.22,0,0.05 1H4U,ARG_403,12.38,-0.27,0,0.16 1UOH,LYS 213,11.54,-0.53,0.85,0.73 2Q98,TYR_169,11.03,0,0.21,0.82 1DUPASP 107.3.95.0.-0.03.0.18 1ZBM,GLU_253,4.13,0.34,-0.19,-0.53 2BT8,TYR_289,10.44,0,-0.05,0.49 2RFA.LYS 209.10.09.-0.41.0.0 1WRU,ARG_286,13.57,-1.23,1.34,0.95 2IF4,LYS_274,10.65,-0.97,0.85,0.26 4AF2,GLU_152,3.2,0.54,-1.87,0.04

1F2V.GLU 24.4.71.0.2.0.0.01 3M7D.ARG 245.12.34.-0.16.0.1.39E-17 3I82,LYS_167,11.49,-0.24,0.77,0.46 3GG6.GLU 53.4.53.0.1.0.-0.06 2QDJ,GLU_137,4.61,0.19,0,-0.09 4F85,HIS 189,6.63,-0.33,0,0.45 2HXB,LYS 57,11.07,-0.17,0.35,0.38 3F5D,ARG_183,13.06,-0.45,0.38,0.63 3T57,LYS 55,10,46,-0.04,0,0 3FK5,LYS_159,10.5,-0.24,0,0.24 2IXM,HIS 155,4.76,-2.69,0.5,0.44 3MTT,GLU_440,4.37,0.39,-0.23,-0.29 2WB8,LYS 759,10,-0.36,0,-0.14 3E7P,GLU_84,4.17,0.26,-0.08,-0.51 2A4D,ARG 157,12,4,-0,4,0,0,31 4FZN,ASP 190,3.52,-0.59,-0.11,0.43 3HVM,LYS_184,10.32,-0.18,0,0.01 3HUE,ASP_9,3.98,0,-0.01,0.19 1RL0,ARG_237,12.73,-0.32,0.22,0.33 2V81,LYS 69,10.46,-0.15,0,0.11 1KW4,LYS 70,10.37,-0.37,0.0.24 3GV0,GLU_227,4.86,1.56,-0.63,-0.58 4F3J,GLU_200,4.37,0.17,-0.19,-0.11 2G5X.GLU 22.3.66.0.41,-0.85,-0.39 1YM5,LYS 246,10,43,-0.07,0,0 3PU6,LYS_48,10.62,-0.21,0,0.33 1YW5,LYS 87,10,13,-0,8,0,0,43 3CAX,ARG_430,12.52,-0.08,0,0.1 3FHF,LYS 103,9.86,-0.7,0,0.07 2G9D.ARG 173.12.48.-0.24.0.0.22 2JEO,HIS_153,5.57,-1.08,0.38,-0.24 1J33,ARG_32,10.99,-2.01,0,0.5 1BYI.TYR 36.13.22.0.0.12.3.11 1WPA.TYR 474.10.57.0.0.28.0.28 3G9G,GLU_77,4.59,0.09,0,0 2CXA,GLU_100,4.79,0.35,0,-0.06 3ETU,CYS_257,12.92,-0.08,0.31,3.69 1ZYL,LYS_315,10.57,-0.19,0,0.26 1VSM,HIS_93,4.52,-1.69,0,-0.3 3A7L,LYS_105,10.56,-0.15,0,0.21 2QDJ,CYS_283,10.31,0,-0.04,1.35 1P6F,CYS_27,9.8,-0.72,-0.08,1.61 1GOE.LYS 74,10.61,-0.16,0,0.27 2AZP,ARG_173,13.13,-0.29,0.61,0.31 3RJX,GLU_257,4.5,1.22,-1.24,0.02 3GYW,ARG_105,13.3,-0.31,0.51,0.6 2D0A,ARG_283,12.24,-0.29,0,0.03 1RI5.ASP 129.2.97.-0.55.-0.55.0.27 208P,HIS_153,4.98,-2.27,0.85,-0.1 3JZ9,GLU_386,4.25,0.74,-0.83,-0.15 2YWJ,GLU_36,4.48,0.18,0,-0.2 2B2H.TYR 377,10.06,0,0,0.06 1F2V,ARG_52,12.7,-0.25,0.07,0.39 2RH3,ASP_100,4.22,-0.82,0,1.24 1YOY,TYR_119,11.45,0.27,0.41,0.77 3BPP,LYS_178,10.55,-0.09,0,0.14 1RSS,ARG_115,12.42,-0.25,0,0.17 4ECC,GLU_147,4.74,1.37,-1.07,-0.06 2GEN,ASP_33,2.89,-0.9,-0.38,0.38 2P65,GLU_169,4.66,0.37,0,-0.21 4F85,ARG_197,13.73,-0.79,1.42,0.59 2098.LYS 142.10.26.-0.17.0.-0.07 4GCO,ASP_173,3.96,-0.54,0,0.7 3V46,ARG_377,12.84,-0.23,0.29,0.27 3JSN,ASP_90,2.49,-1.42,-0.36,0.48 1QQH,LYS_173,10.58,-0.09,0,0.16 3US6,ARG_7,12.16,-0.33,0,-0.01 1LTU,GLU_109,4.48,0.38,-0.17,-0.22 1NAF,ASP_269,3.78,0,-0.32,0.3

2034,ARG 88,13,4,-0,31,0,81,0,39 20YZ,LYS_14,10.39,-0.12,0,0.02 3FK5,CYS_219,9.96,-0.25,-0.09,1.3 3M7G,GLU_190,4.5,0.18,0,-0.19 1ZP2.ASP 31.4.0.-0.04.0.23 3MIX.GLU 621.4.66.0.64.-0.24.-0.24 2JHY,TYR_133,9.72,0,-0.73,0.45 2PLQ,LYS_93,10.44,-0.18,0,0.12 1PGV,ASP_234,2.87,-0.93,-0.66,0.65 3CNU.GLU 52.2.69.0.31.-1.39.-0.73 1EDG,LYS_142,11.27,-0.57,0.85,0.5 3V4G.GLU 28.4.65.1.02.-0.85.-0.01 2CW4,TYR_90,12.01,-0.85,0.38,2.47 3MTT.ASP 575,3.59,-0.14,-0.58,0.52 3MEW, ARG 209, 12, 15, -0, 39, 0, 03, 0, 01 2OSA,LYS_325,10.46,-0.33,0,0.29 3RVC,GLU_196,4.65,0.1,0,0.06 3LPZ,TYR_171,11.45,0,0.08,1.37 3ETV.GLU 20.5.15.0.54.0.0.11 3E0H,GLU_30,3.44,0.26,-1.3,-0.02 2Z14,ARG_70,12.97,-0.58,0.28,0.76 3E5T,LYS_207,10.44,-0.1,0,0.04 1MIX.ASP 397.3.89.0.-0.06.0.15 3EVZ.ARG 132.12.25.-0.28.0.0.02 2F4Q,GLU_315,4.95,0.32,0,0.14 3QAV,TYR_148,12.07,0.75,0.12,1.2 3GW3,ASP_355,4.45,0,-0.17,0.83 3JSN,GLU 41,3.18,0.62,-1.51,-0.43 2CI3,ASP_209,3.42,-0.44,-0.23,0.29 3KV0,GLU_129,4.16,0.4,-0.85,0.11 2GS5,ARG_102,12.45,-0.05,0,0 1PBV.LYS 64,10.15,-0.33,0,-0.01 4FZN.GLU 90.6.3.1.31.-0.02.0.52 3RKV,GLU_274,4.62,0.12,0,0 3JZN, ARG 436, 13, -1.47, 0.85, 1.13 3TOW, ASP_118, 2.7, -0.85, -0.57, 0.32 3FTT,GLU_10,4.61,0.17,0,-0.06 1YW5.ASP 65.4.26.0.0.21.0.25 3N2T,ASP_193,3.67,-0.7,-0.22,0.79 307K,LYS_12,10.47,-0.06,0,0.04 4EZB.HIS 229.5.95.-0.48.0.-0.06 1EDG,LYS 248,9.89,-0.77,0.0.16 1RL0,GLU_106,3.08,1.14,-2.03,-0.55 10I7.GLU 199.2.63.1.1,-1.99,-0.98 1R3D,HIS_211,5.16,-1.34,0,0 3BQE,ASP_265,2.76,-1.91,-0.43,1.3 3FHF,HIS -2,6.37,-0.13,0,0 1IAP,LYS_94,10.43,-0.12,0,0.05 1ZP2,CYS_172,10.73,-0.28,-1.19,3.2 2FZP,TYR 272,12,36,-0.03,-0.17,2,56 3S0A.GLU 78.4.39.0.14.0.-0.26 2FPN,ASP_19,3.07,-0.85,-0.38,0.5 4E6S,GLU_19,4.02,0.19,-0.66,0 20BI,HIS_15,5.2,-1.28,0,-0.01 1X04,LYS 149,11.43,-0.39,0.62,0.71 2FB6,LYS_37,10.61,-0.11,0,0.22 3FTT,ARG_182,12.32,-0.18,0,0 3H13,ARG_338,12.29,-0.18,0,-0.03 10IS,ASP_233,2.81,-1.62,-0.05,0.68 1GXN,GLU_527,3.75,2.65,-2.19,-1.21 1SNT,TYR_151,10.81,-0.53,-0.24,1.59 1BYI,ARG_51,12.3,-0.6,0,0.4 2RH3,GLU_197,4.73,1.81,-1.71,0.12 2AD1,CYS_124,11.19,-0.13,0.09,2.22 2DG7,LYS_51,9.47,-1.33,0,0.29 2Z61,LYS_45,10.79,-0.12,0,0.41 1UAJ,ASP_231,3.81,0,-0.12,0.13 3ERF.TYR 68.10.05.0.0.0.05 1FQI,LYS_352,10.6,-0.18,0,0.28

1R50.GLU 94.3.54.0.34.-1.27.-0.03 2CBE,LYS 252,10.38,-0.38,0.0.26 2H14,ARG_181,12.38,-0.14,0,0.01 2AH5,ASP_62,3.54,-0.56,0,0.29 3I4T.ASP 257.4.01.0.0.06.0.15 1R6Y,LYS 26,10.31,-0.2,0.0.01 3DSH,LYS_358,11.66,-0.37,0.46,1.09 3F6F.CYS 12.11.29.-1.57.-0.29.4.16 1RWZ,ASP_150,3.32,-0.57,-0.22,0.31 1J8B,ARG_82,12.47,-0.31,0,0.28 4EVF.GLU 147.4.65.0.17.0.-0.02 3BA1,LYS_145,9.95,-0.7,0,0.17 2R57,GLU_182,4.64,0.09,0,0.05 2FG1.TYR 86.9.79.0.-0.37.0.16 3M70,CYS 122,11.44,0,0.41,2.03 1X04,TYR_148,9.89,0,-0.34,0.23 3LOD, ASP_105, 3.98, 0, 0.02, 0.16 3O16,ASP_143,3.74,-0.77,-0.09,0.8 2A6B,TYR 163,11.46,0,0.34,1.12 3HQX,ASP_32,2.31,-1.81,-0.08,0.4 2H14,HIS_178,2.39,-2.67,0,-1.44 1DUP,HIS_78,6.08,-0.34,0,-0.08 2RJD,LYS_307,10.38,-0.12,0,0 1G5Z,GLU 171,4.93,1.35,-0.68,-0.24 3RE9,ARG_233,13.1,-1.27,0.79,1.09 2QDJ,TYR_239,12.44,0.16,0.46,1.81 1TLV,LYS_257,10.65,-0.15,0,0.3 3U0V,ARG_11,13.01,-0.79,0.77,0.53 3G9G,ARG 26,13.54,-0.31,0.84,0.52 4FH3,ARG_323,12.29,-0.21,0,0 1X04,ARG_221,12.83,-0.43,0.3,0.46 2Z0W,ARG_67,12.45,-0.09,0,0.04 1ES9,HIS 188,6.33,-0.25,0,0.08 1XTD,ASP_53,3.68,0,-0.41,0.29 1PGV,GLU_225,4.43,0.38,-0.07,-0.37 3LH5,LYS_733,9.67,-0.3,0,-0.53 3N2T,HIS_80,6.03,-1.34,0.47,0.4 4AE7,LYS_213,10.75,-0.4,0,0.66 4ETX,ARG_273,12.62,-0.24,0,0.36 2D2S,ARG_753,12.47,-0.03,0,0 1MML,LYS_152,11.2,-0.64,0.73,0.61 1MUF,ARG_258,12.39,-0.14,0,0.03 1JKS,HIS 80.6.08,-1.01.0.0.59 3B21,HIS_68,3.58,-3.5,0.83,-0.26 3DZ1,ARG_263,12.41,-2.67,0,2.57 4H86,LYS_79,10.7,-0.16,0,0.36 3C0C,TYR_359,10.45,0,0.18,0.26 1V43,ASP_333,3.93,0,-0.07,0.2 1017,ASP 277,3.99,0,-0.01,0.2 1PDB,ASP_21,3.75,-0.24,-0.1,0.29 3F1X,HIS_194,5.16,-1.11,0,-0.23 1YLN,ASP 192,1.46,-2.76,-0.32,0.75 3M66,ARG_245,12.2,-0.34,0,0.04 4FH3,LYS_98,10.35,-0.3,0,0.15 3UC9,LYS_51,10.62,-0.16,0,0.28 3GYW,GLU_118,5,0.35,0,0.14 2DFL,HIS 125,3.55,-3.18,0.86,-0.62 3GV0,GLU_145,4.61,0.26,0,-0.15 3FFM,TYR_44,9.91,-0.45,0.18,0.18 2B0J,GLU 168,4.68,0.1,0,0.08 1C44,LYS 58,10,57,-0.09,0.0.16 3U2R,TYR_25,10.09,0,-0.19,0.28 1EDG,HIS_123,6.17,-2.34,0.66,1.34 1WNH,LYS_162,11.11,-0.66,0.85,0.42 3LD1,TYR_26,12.44,0,0.41,2.03 2CIU,GLU_143,4.53,0.65,0,-0.61 3COU, ARG_54, 12.75, -0.21, 0.23, 0.23 2NRK,LYS_33,10.63,-0.18,0,0.31 3MIX,ARG_373,12.32,-0.22,0,0.04

3ANJ,ASP_328,4.64,0,-0.11,0.95 2P0Y,LYS 31,10.84,-0.24,0.23,0.34 4EKU,LYS_188,10.25,-0.76,0.11,0.4 1T95,ASP_77,3.48,-0.78,0.08,0.38 2DG7,GLU_165,4.52,0.11,0,-0.1 10IS,LYS 286,10.89,-0.41,0.62,0.18 3EYE,LYS 122,11.39,-0.42,0.85,0.47 1P4X,TYR_203,10.65,-0.08,0.05,0.68 3I4T,HIS_33,6.08,-0.69,0,0.27 2B61,ASP 58,3,93,-0.21,0,11,0.23 109G.ARG 137.13.01.-0.7.0.75.0.46 1J33,ARG_320,12.33,-0.35,0,0.18 3IVF.GLU 126.3.83.0.43.-0.83.-0.27 3CE7.CYS 57.9.5.-0.08.0.36.0.23 2YT4,GLU 652,4.23,0.38,-0.33,-0.32 2G2D,ARG_141,12.07,-0.3,0,-0.12 3E7P,LYS_88,10.73,-0.22,0,0.46 1X1E,LYS_58,10.42,-0.32,0,0.24 1ANU.TYR 69,10.2,0.0.0.2 1XWM.ARG 139.12.37.-0.36.0.0.23 3GV0,LYS_302,10.41,-0.26,0,0.18 3FHF.TYR 155,10,47,0,0,3,0,17 2H2W/TYR 136,10.83,0,0.13,0,7 2AZL,GLU 281,4.56,0.21,-0.15,0 3ADO,ARG 31,13.81,-0.2,1.1,0.42 3LJN,GLU_150,4.15,0.27,-0.25,-0.37 2WB8,LYS_658,9.89,-0.78,0,0.17 1TXJ,LYS_122,10.4,-0.1,0,0 2P52,CYS 179,9.41,-0.08,0.13,0.35 1U7U,ARG_339,12.62,-0.37,0,0.5 2XWS.TYR 17.11.14.-0.73.-0.09.1.95 3LJC,ARG_132,12.5,-0.2,0,0.2 2NYC,TYR 272,10.4,0,-0.05,0.45 3CRM,LYS_267,10.6,-0.18,0,0.28 2APL,ASP_47,4.08,0,0,0.28 3GEC,TYR_318,9.23,-0.58,-0.45,0.26 1NKD,CYS_40,9.75,0,0.05,0.7 2EEY,TYR 41,10.12,-0.22,0.02,0.32 1RAJ,GLU_449,4.69,0.21,0,-0.02 1D2K,LYS_221,10.31,-0.36,0,0.18 3C6B,TYR_175,12.43,0.07,0.54,1.82 3H6Q,GLU 167,4.68,0.18,0,0 3NBI.GLU 80,4,7,0,22,0,-0,01 1TWU,HIS_44,6.29,-0.21,0,0 3IVF,ASP_53,3.38,-0.77,-0.05,0.4 1YM5,LYS_188,10.57,-0.12,0,0.19 1AKO,GLU 249,3.66,0.21,-0.85,-0.21 1RHS.GLU 77.3.93.0.34,-0.83,-0.08 2EJX,LYS_87,11.2,-0.39,0.25,0.83 2EJX,LYS_135,10.45,-0.05,0,0 2B0A, ARG_180, 13.9, -0.27, 1.21, 0.46 2F9F,ASP 40,3,45,-0,41,-0,25,0,31 3CRM,GLU_72,3.87,0.4,-0.83,-0.19 3HOX,LYS 14,10.21,-0.29,0.0 2l6l,GLU_43,4.91,0.32,0,0.09 2ILR,LYS_393,11.13,-0.59,0.45,0.76 2EFK.ARG 16,12.4,-0.22,0,0.12 1H4U,LYS_614,10.78,-0.13,0,0.41 2R51,LYS_264,10.56,-0.13,0,0.19 3A4C,HIS_553,6.38,-0.12,0,0 2HP7.GLU 180.5.03.0.53.0.0 1Z3X,GLU_36,4.1,0.39,-0.56,-0.23 2GZR/LYS 153,10.3,-0.4,0,0.22 3EYE,LYS_48,10.42,-0.08,0,0 1MML,ARG_173,12.1,-0.76,0,0.36 2IF4.LYS 191,10.09,-0.41,0.0 3EUR,LYS_101,12.56,-0.64,1.7,0.99 3PZ9,HIS_228,6.73,-2.18,1.66,0.75 2HRZ,GLU_94,4.13,0.3,-0.4,-0.27

3HVM,GLU_263,4.01,0.23,-0.6,-0.12 30DJ,ASP 130,3.93,0,-0.15,0.28 1O3X,ARG_260,12.27,-0.38,0,0.15 3UC9.HIS 102.6.21,-0.29.0.0 3M66,LYS_389,9.78,-0.73,0,0.01 1WOU,LYS 86,10.35,-0.43,0,0.28 3OA7,LYS 507,9.9,-0.3,0,-0.3 3NBI,LYS_125,10.43,-0.07,0,0 3N2T,ARG_232,13.39,-0.81,1.34,0.37 2D2S,LYS_685,10.65,-0.11,0,0.26 1XKR,LYS 8,11.31,-0.35,0.76,0.4 2YWJ,LYS_28,10.63,-0.33,0,0.45 2GZQ,ARG_154,12.16,-0.34,0,0 2B61,ASP_277,2.63,-2.21,0,1.03 3G9G,LYS 113,10.81,-0.15,0.17,0.29 1RZ2.GLU 173.3.49.0.95.-1.46.-0.5 4EVF,LYS_56,10.5,-0.15,0,0.16 1WP5,GLU_306,4.6,0.56,0,-0.45 4EKU,ASP_32,3.98,0,0,0.18 3M16,LYS 13,10.18,-1.14,0.36,0.45 3JRT.CYS 143.9.9.-0.8.0.04.1.67 4ACJ,GLU_721,4.48,1.88,-1.38,-0.51 4FZR,TYR_195,11.01,0,0.05,0.97 1T6L,ARG 16,12,27,-0.36,0,0,13 2P5D,TYR 47,12,54,0,0.03,2,51 3GA2,TYR_147,11.67,0,0.33,1.33 2P65,LYS_94,10.85,-0.2,0.49,0.06 3VHJ,HIS_67,5.52,-2.34,0.88,0.49 2YLF,ASP_158,4.52,-0.09,-0.14,0.95 2IXM,CYS 165,13.63,-0.04,1.02,3.63 3ZXY,HIS_15,6.51,-0.23,0,0.23 3H04,LYS_5,10.47,-0.08,0,0.05 3UAH.GLU 501.4.63.0.13.0.0 1LTU.LYS 239.9.98.-0.24.0.-0.28 3LJI,ARG_275,12.27,-0.25,0,0.02 1WXF,LYS_144,11.25,-0.39,0.67,0.46 3HUE,HIS_35,7.08,-0.52,0.85,0.25 2WB8,GLU_776,4.61,0.63,0,-0.51 3CGW,LYS_115,10.3,-0.2,0,0 3ZSL,ARG_168,12.4,-0.11,0,0 1X9G,ARG_40,11.45,-1.66,0,0.61 1X7F,LYS 118,10.07,-0.53,0.0.1 4GCO,ARG_256,12.26,-0.5,0,0.25 3GE9,ARG_83,12.54,-0.3,0.05,0.29 3ANJ,LYS_26,12.31,-0.39,1.43,0.76 1N81,GLU_61,4.62,0.12,0,0 1J8B,ARG_53,12.56,-0.18,0,0.23 2D8N,LYS 150,10.37,-0.47,0.0.34 1K95,HIS_197,6.2,-0.26,0,-0.04 3CAX,ASP_292,2.57,-1.37,-0.38,0.52 2Z0M,TYR_91,9.91,-0.2,-0.44,0.55 4ETX,CYS 264,13.52,0,1.16,3.36 1FKM,ARG_499,12.2,-1.85,0.42,1.13 3V4G,ARG_83,12.21,-0.42,0,0.14 3M3P,HIS_170,4.09,-2.57,0,0.16 1P2F,LYS_17,10.34,-0.23,0,0.07 3ERF,ASP_167,3.63,-1.17,-0.24,1.24 3EVP,LYS_271,10.93,-0.29,0.36,0.36 3OA7, ARG_452, 12.67, -0.21, 0, 0.38 3BPV,LYS_125,10.44,-0.08,0,0.02 3G6S,ARG 5,13.57,-0.68,0.85,0.91 1SIG.ARG 218.12.91.-0.19.0.0.6 3BQW,GLU_181,4.58,0.24,0,-0.16 3BCH,HIS_169,6.11,-0.42,0,0.04 1QQE,ASP_3,3.52,-0.44,-0.25,0.41 1WRU.GLU 280.3.8.0.66,-0.81,-0.54 1NAR,GLU_56,3.53,1.09,-1.6,-0.47 10TM,HIS_219,6.27,-0.38,0,0.15 1L2H,GLU_113,2.83,1.15,-2.37,-0.45

3A0X,ASP 638,3,55,-0.93,0,13,0,55 20KT,ARG_287,12.39,-0.15,0,0.04 2P65,ARG_10,12.77,-0.73,0.65,0.35 1Q8B,GLU_46,4.56,0.11,0,-0.04 4EVF.ARG 89.12.46.-0.06.0.0.02 1Y2O.GLU 142.3.98.0.17.-0.62.-0.07 2EA9,CYS_82,10.63,-0.13,0.45,1.3 2VGM,ASP_78,4.28,0,0.26,0.22 3QKY,ARG_251,12.8,-0.12,0,0.42 2PWO.HIS 133.6.06.-0.44.0.0 2BAA,TYR_84,13.82,-0.85,0.38,4.29 3O48.TYR 45.11.36.0.0.13.1.23 3CCY,GLU_184,3.89,0.28,-0.69,-0.2 3V55.GLU 531,3.51,0.47,-0.85,-0.61 2IOT.HIS 134,7,47,-0.36,0.85,0.49 3IO0,CYS_191,9.29,-1.03,0.16,1.17 1RI6,ASP_115,3.12,-0.56,-0.34,0.21 1XAW,GLU_472,4.62,0.12,0,0 2H2W.GLU 18.3.38.1.13.-1.62.-0.62 2QEV,ASP_5,3.23,-0.82,-0.12,0.37 2P52,CYS_121,10.99,0,0.61,1.38 3M3P,GLU_193,3.93,0.27,-0.84,0 2H14.ASP 242.3.32.-0.82.-0.2.0.53 1ANU,ARG 72,12,41,-0.09,0,0 2Z0M,ARG_160,10.85,-1.65,0,0 1SIG,ARG_422,13.4,-0.6,0.38,1.13 3P2F,ARG_75,12.17,-0.21,0,-0.11 3B7X,TYR 118,12.19,0,0.46,1.73 2ILR,LYS_468,10.43,-0.25,0,0.18 2G9D,GLU_251,4.46,0.24,0,-0.28 3K9I,ASP_72,3.3,-0.73,-0.06,0.29 1SFE,ASP 82,3.92,0,-0.26,0.38 3LJC,ARG 38,12.69,-0.2,0,0.39 2DFL,ARG_294,12.05,-0.31,0,-0.14 3LJI.TYR 176.10.24.0.0.0.24 1DOV,LYS_105,10.52,-0.05,0,0.07 1NIJ,TYR 280,10.41,0,0.16,0.25 3V10.TYR 519,10.2.0.-0.15.0.34 2D7U,ARG_244,12.49,-0.24,0,0.22 3HNX,ASP_45,2.86,-1.32,0.06,0.31 2P0L,ASP 233,3.63,-0.49,0.0.32 2IDC/HIS 53.6.74,-0.35,0.32,0.27 1R9W,CYS_273,11.12,0,0.35,1.76 1LPL.GLU 176.3.55.0.26.-0.75.-0.45 20EW,GLU_86,5.28,0.78,0,0 2EDM,LYS_85,10.57,-0.18,0,0.25 3I4T,ASP 261,4,28,0,0,18,0,3 1X91,GLU_76,4.95,0.28,0,0.17 1WYC,ARG_51,13.61,-0.26,0.92,0.45 1PSW.CYS 41.10.86.0.0.1.86 3GMS.TYR 100.11.27.0.05.0.56.0.66 3A2Z,ARG_91,13.8,-0.55,1.21,0.63 2VGM,GLU_343,5.15,0.76,-0.12,0.02 3M66,HIS_213,5.39,-0.83,0.13,-0.42 1QQL,GLU 104,4.31,0.16,0,-0.35 1RL0,GLU_119,4.86,0.79,-0.61,0.18 1SQH,ARG_278,11.78,-0.41,0,-0.31 2FZP,CYS 238,12.27,0,0.09,3.17 1EDG,ASP_234,3.81,0,-0.15,0.16 3EVN,TYR 104,10.37,0,0.09,0.28 2VAN,GLU_249,4.57,0.07,0,0 1PSW,GLU_133,5.1,1.31,-0.66,-0.05 3IL3, ARG_42, 9.67, -2.79, 0, -0.04 4GA2,TYR_48,10.33,-0.12,-0.38,0.83 3R87, ASP_125, 3.37, -0.44, -0.36, 0.37 2Q12,GLU_155,3.55,0.36,-0.82,-0.47 2ZQ5,GLU_156,4.18,0.28,-0.51,-0.09 3RFY,LYS_344,11.09,-0.25,0.54,0.29 2X4J,ARG_79,12.44,-0.06,0,0

2FL4.GLU 132.2.59.0.5.-1.99.-0.42 2EDM,ARG_103,12.45,-0.05,0,0 3F6F,GLU_126,4.44,0.1,0,-0.16 1T3Y,ARG_18,12.67,-0.35,0.07,0.45 1N81.TYR 168.10.08.0.0.02.0.06 3FHF,ASP 161,3.87,0,-0.06,0.13 3CCY,HIS_154,6.24,-0.2,0,-0.06 20EV.LYS 9,11.51,-0.29,0.85,0.45 1YLN,ARG_165,12.26,-0.41,0,0.17 2ILR.GLU 474.3.62.0.21.-0.67.-0.42 3HKX.ASP 40.3.16,-0.72,-0.33,0.4 2D0A,ARG_278,12.83,-0.26,0.33,0.26 1TJE,ASP_109,3.81,0,-0.2,0.21 1LZL/HIS 141,5.69,-0.81,0,0 30KY.TYR 257.10.18.-0.27.-0.13.0.59 1JSX,ARG_160,13.52,-0.79,0.96,0.86 2CBE,HIS_15,6.04,-0.41,0.47,-0.52 3GV0,GLU_92,4.37,0.44,-0.19,-0.39 2Z14,TYR 98,10.3,0,-0.11,0.41 2RGY,GLU_135,4.7,0.33,-0.16,0.02 4F85,GLU_132,3.84,2.25,-1.57,-1.34 3LQE,ARG_476,12.35,-0.26,0,0.11 1DZF,ARG_52,13.34,-0.21,0.67,0.38 1ZYL, ARG 26, 12.79, -0.14, 0, 0.43 3RJZ,GLU_114,2.7,0.39,-1.4,-0.78 2EFK,LYS_132,10.57,-0.11,0,0.17 3GMS,LYS_29,10.69,-0.15,0,0.34 1J74,GLU_139,4.5,0.22,0,-0.21 1YR6.ASP 195.3.96.0.-0.12.0.27 1QQH,ASP_147,4.95,0.03,0.37,0.74 3ZRI,HIS_-6,6.26,-0.24,0,0 3FHF,HIS 133,3.21,-2.76,0.85,-1.38 3V55.LYS 513,10.63,-0.27,0,0.4 3N2T,ASP_133,2.88,-2.18,-0.01,1.29 3US6,GLU_122,4.04,1.28,-1.26,-0.48 1XWM,ARG_92,13.9,-0.56,0.83,1.14 3RNV,TYR 337,11.53,0.48,0.43,0.62 3I47.LYS 249.11.22.-0.21.0.43.0.5 3A2Z,GLU_37,5.56,0.24,0.29,0.53 3GOZ.LYS 266.10.5.0.0.0 3H04,GLU_227,5.83,3.02,-1,-0.68 3G9T,ARG 126,12.25,-0.35,0,0.09 3HVW,ARG 317,13.3,-0.31,0.74,0.37 1J85,GLU_10,3.47,0.57,-1.32,-0.29 2RIK,HIS_223,5.95,-0.65,0,0.1 4F8A,GLU_682,4.71,0.22,0,-0.01 1AT0,ARG_369,12.52,-0.24,0,0.26 1XAW,LYS_512,11.29,-0.3,0.78,0.31 3PU6.GLU 43.4.19.0.43.-0.8.0.06 3P2F,ARG_123,13.15,-0.37,0.65,0.36 3T5B,GLU 139,4.66,0.19,0,-0.02 2A0J.GLU 107.4.51.0.16.0.-0.14 1HF8,GLU_220,4.48,0.29,0,-0.31 1HF8,LYS_38,11.2,-0.27,0.59,0.38 4E8B,GLU_157,4.14,0.28,-0.45,-0.2 1ZBP,GLU_96,4.59,0.09,0,0 2Q5X,ARG 778,13.16,-0.23,0.46,0.44 200K,ARG_154,11.72,-0.56,0,-0.22 4DEZ,GLU_18,4.71,1.28,-0.85,-0.22 1ES5,ASP 140,4.06,-0.09,-0.14,0.5 2FZ4,HIS 202,7.34,-0.26,0.85,0.25 1F2V,TYR_6,10.17,-0.08,0.01,0.24 2NRK,ARG_96,12.07,-0.56,0,0.13 1C44,ASP_66,3.65,-0.28,0,0.13 2H30,ASP_149,3.38,-0.39,-0.24,0.22 1JYH,TYR_123,10.39,0,0.09,0.3 1ZP2,GLU_21,4.63,0.13,0,0 3FRR,LYS_134,10.19,-0.19,0,-0.12 109G,LYS_231,10.05,-0.19,0,-0.26

3FHF,CYS 44,13.31,0,0,25,4.07 1JSX.ASP 134.3.06.-1.55.-0.12.0.92 2CIU,GLU_165,4.57,0.13,0,-0.06 3CGW,LYS 61,10,48,-0.09,0,0.08 2FBO.GLU 156.2.92.0.69.-1.91.-0.35 3C38.GLU 139.4.2.0.48.-0.32.-0.45 3T57,ASP_129,2.57,-0.99,-0.94,0.7 1UOH,LYS_23,10.63,-0.29,0,0.42 4EZB,ARG_23,12.43,-0.26,0,0.19 2R57,ARG 250,11.64,-1.8,0.0.95 109G,ASP 15,1.94,-2.26,-0.79,1.19 3C5V,LYS_206,10.37,-0.13,0,0 20PJ,GLU_83,4.59,0.26,0,-0.17 2AD1.CYS 169,12.34,-0.04,0.09,3.29 10IS.GLU 225.3.65.0.35.-0.82.-0.38 3GEC,HIS_395,3.38,-3.12,0,0 20EW,ARG_41,12.36,-0.21,0,0.07 2OSA,TYR_443,10.17,0,-0.23,0.4 3KV0.GLU 46.3.95.0.48.-0.7.-0.34 1SUU,CYS_665,12.83,0,0,3.83 3LOD,GLU_26,4.74,0.15,0,0.1 1YM5.LYS 58.10.34.-0.41.0.0.25 3H6Q,GLU_99,4.65,0.17,0,-0.02 3CIV,GLU 218,4.74,0.33,0,-0.1 2F9F.GLU 124,3.93,0.21,-0.41,-0.38 3BQW,LYS_164,10.13,-0.48,0,0.1 2GYZ,ARG_22,12.43,-0.17,0,0.09 2YWK,GLU_61,4.02,0.37,-0.68,-0.16 3BZT,TYR 324,10.43,0,0.06,0.38 4E9E,HIS_454,6,-0.53,0.01,0.03 2CXA,ARG 76,12,46,-0.04,0,0 3FHF,LYS_39,10.04,-1.19,0,0.73 3RLE,GLU 208,3.28,0.25,-1.47,0 1G8P.ARG 224,12.34,-0.26,0.0.1 3BZT,LYS_296,10.37,-0.19,0,0.06 2P0Y,ASP_115,3.55,-0.52,0,0.28 3GG6,ARG_147,13.69,-0.45,1.07,0.57 2F4Q,LYS 174,10.14,-0.17,0,-0.19 3HUE,LYS_267,10.41,-0.09,0,0 1RI5,TYR_61,12,0,0.6,1.41 30KQ,GLU_593,4.94,0.29,0,0.16 3LJC,GLU 10,4.5,0.33,0,-0.34 30KY,TYR 81,10.88,-0.26,0,1.14 1MHN,ARG_120,12.47,-0.07,0,0.04 3B4D,LYS_243,10.34,-0.18,0,0.02 2Q07,ARG_400,12.35,-0.76,0.09,0.53 3IVF,LYS 320,10.47,-0.03,0,0 1DCF.GLU 42.3.72.0.44,-1.03,-0.19 1W24,ASP_154,3.45,-0.52,-0.42,0.59 3M7D,HIS_246,5.77,-1.62,0.84,0.05 2IRM,GLU_97,4.02,0.23,-0.68,-0.03 3G6S,LYS 27,10.85,-0.28,0.0.64 3DB9,ASP_25,3.88,-0.08,-0.01,0.18 3LD1.LYS 257.10.03.-0.57.0.0.1 1X6J,ASP_51,2.98,-1.18,-0.49,0.84 1YLN,GLU_138,4.41,0.37,0,-0.48 3I47,ASP 12,3,86,-0,24,-0,11,0,4 3HVM,CYS_98,10.95,-0.28,0.12,2.11 3JV1,LYS_224,10.36,-0.14,0,0.01 1EW4,LYS_65,10.38,-0.12,0,0 2G9D,HIS 147.6.64,-0.36.0.12.0.38 3VJ8,GLU_156,2.36,0.81,-2.15,-0.79 3HVW.CYS 263.11.94.-0.03.0.02.2.96 2IDC,TYR_112,10.59,0,-0.1,0.69 3LMF,GLU_115,4.81,0.24,0,0.06 3V46.LYS 236.10.36.-0.16.0.0.01 2A1V,ARG_45,12.25,-0.33,0,0.08 3KV0,GLU_182,4.4,0.61,-0.81,0.09 3COU,ARG_105,12.31,-0.19,0,0

1ILW.GLU 4,4.65,0.6,0,-0.45 3CO1.GLU 70.2.94.0.43.-1.5.-0.48 2BQQ,ARG_111,13.04,-0.27,0.38,0.42 1CBY,LYS_115,10.19,-0.78,0.09,0.38 1WOU,GLU_107,4.87,0.24,0,0.13 2Q98, ARG 177, 12.44, -1.45, 0.2, 1.17 109G,TYR 64,12,46,-0.01,0.37,2,1 3IL3,HIS_85,6.29,-0.28,0.06,0 1SQH,GLU_244,4.48,0.3,0,-0.32 2YWJ,ARG_129,12.35,-0.41,0,0.26 4H86,ARG 141,12.08,-2.17,0.76,0.99 3C38,GLU_107,3.54,0.36,-1.02,-0.3 4H86,TYR_73,10.62,0,0.39,0.23 2IF4,ARG_245,12.98,-0.35,0.25,0.58 3IBT.GLU 249.4.99.1.67.-1.2.0.03 100LGLU 81.4.1.0.41,-0.19,-0.63 2ZCO,HIS_151,6.36,-0.22,0,0.08 1J85,TYR_7,11.47,0.29,0.31,0.87 2CN1,ARG_52,11.43,-1.62,0,0.55 1RSS,LYS 70,9.98,-0.65,0,0.14 1IAP.GLU 121.4.81.0.37.0.-0.06 1T95,GLU_179,3.52,0.38,-1.12,-0.25 3N2T,ARG_17,10.68,-1.82,0,0.01 3PM2.LYS 13,10.32,-0.57,0,0.39 2RIS.GLU 65.4.61.0.11.0.0 1L2F,GLU_221,3.33,0.31,-1.11,-0.38 2QRX,ASP_177,3.96,0,-0.08,0.25 3RHE,LYS_17,10.43,-0.07,0,0 1SBX,LYS 162,10.09,-0.54,0,0.13 2RFA,ARG_190,12.53,-0.45,0,0.48 2A6B,ASP_24,4.39,0,-0.01,0.6 3I0C,CYS_284,12.94,0,0.42,3.52 1UJ8.GLU 62.4.64.0.14.0.0 1WXO.ASP 151.3.46.-0.24.-0.32.0.21 3P2F,CYS_177,11.58,-0.1,0.24,2.44 1XKR,LYS_48,10.3,-0.21,0,0.01 3LJI,LYS_45,10.25,-0.22,0,-0.03 2WB8,ARG_723,12.88,-0.47,0.46,0.39 1017.GLU 131.2.99.0.61.-1.6.-0.54 2RH3,ASP_122,4.15,0,-0.54,0.88 2ZCO,ASP_147,4.15,0,0.03,0.32 3S0A,GLU_13,3.54,0.82,-1.44,-0.34 3EVZ,GLU 114,3.77,0.18,-0.78,-0.13 3BCH,ARG_128,12.63,-0.42,0,0.55 1BKR,ASP_52,3.71,-0.41,0.07,0.25 1QQE,GLU_142,4.96,0.71,-0.12,-0.14 1QQH,HIS_108,6.58,-0.53,0.32,0.29 3C6B.GLU 6.3.78.0.42,-0.77,-0.37 2B0J,LYS_188,10.68,-0.12,0,0.28 2FPN,TYR_50,12.82,0,0.32,2.5 2YWK, ASP_44, 2.09, -2.18, -0.25, 0.7 2E3S,ASP 545,3.93,0,0,0.13 1HF8,LYS_252,10.74,-0.13,0,0.36 1ZCE,HIS_54,5.47,-1.31,0,0.28 2I6I,ARG_150,12.04,-0.47,0,0.01 1WOU,LYS_104,9.89,-0.63,0,0.02 2HXB,LYS_141,10.35,-0.29,0,0.14 2OSA,LYS_362,11.17,-0.33,0.53,0.47 1WXO.HIS 107.4.51.-2.86.0.62.0.25 1SQH,ASP_58,3,-0.92,-0.46,0.58 3LMF,ASP 16,4.09,0,-0.03,0.32 3RKV.LYS 189.10.46.-0.04.0.0 4GCO,ARG_216,11.72,-1.38,0,0.6 1T3Y,LYS_130,10.39,-0.1,0,-0.01 1RAJ,ASP_349,3.7,-0.12,-0.32,0.35 3BB7.TYR 343.10.13.0.0.0.13 3VJ8,ASP_253,4.01,0,-0.01,0.22 1L3K,TYR_167,10.12,0,0,0.12 2BLL,ARG_497,11.63,-0.88,0,0.01

2013.HIS 180.6.29.-0.26.0.03.0.01 1O6D,LYS_121,11.47,-0.26,0.85,0.38 1Q8B,LYS_33,10.47,-0.17,0,0.14 2P4D,TYR_54,10.33,0,0.01,0.32 2FG1.GLU 133.4.09.0.18.-0.54.-0.05 1PDB.TYR 162.9.65,-0.65,-0.43,0.73 2VAN,HIS_285,6.26,-0.65,0.39,0.02 1IDK,TYR_252,11.4,0,0.19,1.21 3IRA,ARG_35,12.39,-0.31,0,0.2 30AV.GLU 34.4.77.0.95.-0.7.0.02 2YYO,CYS_101,10.72,-0.47,-0.11,2.29 2B78,LYS_56,10.26,-0.11,0,-0.14 109G,ASP_50,3.74,-0.17,0,0.11 20V2.ASP 254.3.36.-0.81.-0.16.0.52 3GFP,ARG 429,12,15,-0,34,0,-0,01 2DFL,LYS_63,9.9,-0.52,0,-0.08 2GZQ,HIS_157,6.34,-0.16,0,0 4DIU,ASP_178,4,-0.15,-0.01,0.36 2WB8.ARG 648.12.22.-3.65.1.51.1.86 1HF8,LYS_226,10.43,-0.07,0,0 3T57,ASP_204,3.94,-0.82,0.01,0.96 3U2R,GLU_58,4.66,0.13,0,0.04 2B2H,ARG 370,12,57,-1,3,0,67,0,7 3FXH,HIS 5,6.81,-0.89,0.77,0.43 2CN1,TYR_135,10.86,0,0.4,0.46 2VAN,ARG_112,12.27,-0.25,0,0.02 4DIU,TYR_104,12.38,0,0.41,1.97 1KN3,ARG 76,11.73,-0.8,0,0.02 3CRM,ARG_253,12.28,-0.27,0,0.05 3RKV,GLU_273,3.18,0.42,-1.47,-0.27 3HVM,GLU_71,4.81,0.5,0,-0.19 1DVO.GLU 178.4.63.0.13.0.0 3ZXY,ARG 267,12.57,-0.1,0,0.17 1TD6,HIS_33,6.13,-0.43,0,0.06 1BKB.LYS 78.10.39.-0.3.0.0.19 3RLN,TYR_704,10.28,-0.03,-0.09,0.4 3JZN,ARG 236,12.6,-0.26,0,0.36 1PZC,ARG 114,11,46,-1,18,0,0,14 3BWT,GLU_771,3.92,0.4,-0.62,-0.35 4AM1,ARG_264,12.06,-1.08,0,0.64 2VGM.TYR 219.11.1.0.0.35.0.74 4DEZ.GLU 236.4.62.0.18.0.-0.07 3LPZ,TYR_190,13.33,0,-0.05,3.38 3DZ1,ARG_251,12.21,-0.39,0,0.09 2D59,GLU_122,4.81,0.24,0,0.07 3BPP,LYS_81,10.45,-0.13,0,0.08 2P0L/LYS 198/10.55/-0.14/0.0.2 1QQE,ARG_10,12.91,-0.31,0.41,0.32 1NJ4,GLU_33,4.67,0.44,-0.1,-0.17 1ZHV.ASP 30.3.88,-0.04,-0.09,0.21 1DTO,LYS 45,10.97,-0.21,0.31,0.36 2OSA,TYR_360,12.47,-0.45,0.64,2.28 1XTZ,ARG_56,13.86,-0.82,1.13,1.06 10XZ,LYS_195,10.5,-0.08,0,0.08 3ZXY,ARG 213,12.33,-0.3,0,0.14 4ESS,GLU_98,4.41,0.34,0,-0.42 4FD6,ARG_94,13.16,-0.39,0.36,0.68 1WXF,TYR_147,12.91,0.84,0.56,1.52 1YW5,TYR_24,10.3,0,-0.17,0.47 1L2F,ARG 232,12.6,-1.34,0.77,0.67 3C5V,GLU_374,4.61,0.19,0,-0.08 4AM1,ARG_280,12.36,-1.69,0.75,0.79 3C5V,LYS_236,10.11,-0.55,0,0.16 3ADO, ASP 100, 3.91, 0, -0.06, 0.17 1ILW,GLU_25,4.35,0.2,0,-0.35 3M66,ARG_282,12.29,-0.24,0,0.03 2FZ4,GLU_170,4.46,0.95,-0.6,-0.39 3V55,ASP_377,3.9,0,-0.21,0.31 3G9T,LYS_213,10.52,-0.16,0,0.18

3GEC.ASP 248.3.8.-0.16.-0.2.0.36 2QDJ,GLU_170,4.58,0.27,0,-0.19 1Z9L,LYS_45,10.21,-0.31,0,0.02 3PM2,ASP_101,2.88,-0.81,-0.35,0.23 3UAH,LYS 253,10.31,-0.19,0.0 2BLL.TYR 477,9.61,-0.76,-0.28,0.65 3C2E,LYS_136,10.43,-0.11,0,0.04 2CWC,ARG_72,12.75,-0.32,0,0.57 2H85,HIS_249,4.21,-2.76,0.8,-0.33 20KT,ASP_177,3.5,-0.65,-0.04,0.39 1FKM,LYS 354,10.31,-0.23,0.0.04 1WOU,GLU_73,4.99,0.35,0,0.14 3BQW,LYS_148,10.52,-0.56,0,0.58 1TLV,ARG_124,11.99,-1.26,0.01,0.74 3Q1C,ASP 335,3.96,0,0,0.16 2CE6,ARG_63,11.94,-0.6,0,0.03 4ETX,ASP_177,3.48,-0.6,0,0.28 1KCM,ARG_253,12.43,-0.07,0,0 3IVF.LYS 268.10.33.-0.09.0.-0.08 1JKS.ARG 63.13.5.-1.05.1.26.0.8 3RKV,LYS_329,10.38,-0.12,0,0 3BWT,LYS_634,10.56,-0.21,0,0.27 3JSN.LYS 211.10.38.-0.18.0.0.06 3M66.ARG 226.12.65.-0.94.0.66.0.42 4E8B,ARG_123,12.25,-0.32,0,0.06 1ZBP,LYS_102,10.47,-0.15,0,0.13 3PBH,ARG_202,12.28,-3.17,0.11,2.83 1LTU,ASP 23,3.17,-1.35,0.29,0.43 3CJW,TYR 177,10.08,0.0.0.08 3NR5,LYS_44,10.52,-0.44,0,0.47 2ILR,CYS_328,12.09,-0.31,0.31,3.08 2B78,TYR_39,10.19,0,-0.2,0.39 2E3C,LYS 228,10.55,-0.18,0,0.24 4FZR,ARG_322,13.42,-0.41,0.49,0.85 3GE9,HIS_98,6.22,-0.19,0,-0.08 2ZCO,HIS_263,6.88,-0.42,0.65,0.15 1QZN,LYS 29,10.42,-0.16,0,0.07 2P4D,ARG_29,12.68,-0.29,0.06,0.42 1YR6,ARG_61,12.44,-0.16,0,0.09 2XMZ,LYS_136,10.29,-0.15,0,-0.06 1DCF,ARG_80,12.45,-0.05,0,0 4ECC,GLU_37,4.13,0.36,-0.84,0.12 4E6S,LYS 45,10,46,-0,04,0,0 3QKY,TYR_171,10.66,-0.4,-0.11,1.17 3LJI,LYS_168,10.43,-0.07,0,0 3ELI,GLU_7,4.34,0.34,0,-0.48 105T,LYS 374,10.35,-0.15,0.0 2CI3,GLU_100,7.11,5.18,-1.48,-1.06 3V55.GLU 368.4.4.1.28.-0.85.-0.53 2FB6,ARG_95,13.87,-0.47,0.96,0.89 2WZ9,GLU_78,4.62,0.1,0,0.01 3US6.ASP 65.4.0.-0.21.0.41 4ESS,ARG_71,13.65,-0.33,0.86,0.62 2BQQ,ARG_63,12.58,-0.27,0,0.35 3QAV,LYS_204,10.26,-0.25,0,0 1UXO,ASP_153,3.67,-0.09,-0.25,0.21 1Q2Y,GLU 32,4.61,0.11,0,0 2AD1,TYR_15,10.3,0,-0.12,0.42 3BA1,GLU_88,4.03,0.32,-0.47,-0.32 2V81,GLU_37,7.37,3.46,0,-0.59 2P0L.TYR 179.12.82.0.0.71.2.12 3MIX,GLU_612,4.7,0.2,0,0 3EZ7,LYS_9,10.32,-0.13,0,-0.05 3BWT,LYS_744,10.54,-0.33,0,0.37 3RKV,LYS_292,11.46,-0.33,0.69,0.61 1J85,TYR_142,10.7,0,0.06,0.64 2BT8, ARG_282, 12.25, -0.57, 0, 0.32 1Q8B,LYS_81,10.47,-0.29,0,0.25 1FO9,ARG_295,12.05,-2.74,0.6,1.7

2P5D,LYS_37,10.39,-0.18,0,0.08 1X1E,TYR_144,12.2,-0.07,-0.03,2.3 2PWQ,ASP_122,2.53,-2.62,-0.02,1.37 1XIP.ASP 264,3.66,-0.78,-0.01,0.65 1046.ARG 54,12.38,-0.06,0,-0.06 30KO.GLU 560.4.52.0.23.0.-0.2 2CVB,TYR_26,10.42,0,0.11,0.31 3UAH,GLU_469,4.74,0.26,0,-0.02 1R29,CYS_53,10.78,0,0,1.78 3CAX,LYS 147,10.2,-0.22,0,-0.08 3AU3,ARG 402,12,46,-0,5,0,0,45 2B78,LYS_86,10.56,-0.13,0,0.2 2Q13,CYS_368,9.72,-0.04,-0.01,0.77 1SI7.GLU 86.4.55.1.02.-0.63.-0.35 20V2.ARG 263.12.43.-0.32.0.0.25 3QAV,GLU_43,4.04,0.39,-0.51,-0.34 2PPN,LYS_47,10.48,-0.16,0,0.13 2CYG,CYS_32,13.28,-0.89,0.86,4.31 3IVF,CYS 29,11.17,-0.03,-0.23,2.44 1W24,ASP_109,3.24,-1.18,-0.76,1.38 2Z61,ARG_285,12.6,-2.29,1.25,1.15 4FLE.GLU 119.4.06.0.31,-0.16,-0.59 2FZP,LYS_230,10.23,-0.29,0,0.02 3U2A,GLU 74,2.55,0.37,-1.64,-0.69 1TR9.TYR 84.13.34.0.0.3.34 2AH5,HIS_138,6.47,-0.25,0,0.22 1UXO,ASP_52,4.23,0,0.15,0.28 3FHF,CYS_42,12.99,0,-0.26,4.25 200K,HIS 191,5.96,-0.46,0.17,-0.26 3RJX,GLU_187,2.94,0.54,-1.33,-0.76 1R53,ASP_194,3.35,-1.36,0,0.9 4EKU,LYS_35,10.47,-0.03,0,0 200K,GLU_2,4.55,0.05,0,0 3AUF,ASP 40,3.89,0,-0.03,0.12 1X7F,HIS_183,6.53,-1.14,0.84,0.33 1PV5,GLU_6,4.41,0.1,0,-0.19 3IV4,ASP_95,3.97,0,-0.06,0.23 1AM2,LYS 150,10.5,-0.11,0,0.11 2PGX,GLU_205,4.62,0.23,0,-0.11 1UAJ,LYS_27,10.23,-0.3,0,0.03 2Z0M,LYS_122,11.05,-0.22,0.34,0.43 1TJE,HIS 16,7.39,-0.31,0.85,0.35 3P28,ARG 194,12,58,-0,24,0,0.33 1NRI,GLU_227,4.48,0.28,-0.31,0 2BLL,GLU_521,4.96,0.45,0,0 3GMS,HIS_157,5.35,-1.77,0.64,-0.01 3GG6,GLU_86,4.18,0.28,-0.69,0.09 2CIU,HIS 169,7.97,-0.59,1.7,0.38 2B0J,LYS_240,10.73,-0.35,0,0.58 1V43,GLU_168,4.85,2.25,-1.44,-0.47 3GW3,TYR_236,11.51,0,-0.19,1.71 2EYI,ASP 210,3.05,-0.85,-0.4,0.49 3FHF,LYS_16,11.97,-0.39,0.85,1.01 1059,LYS_87,11.06,-0.5,0.56,0.5 2D0A,ARG_281,11.85,-0.35,0,-0.31 3T57,ARG_246,12.4,-0.19,0,0.08 2FBO.GLU 183.4.73.0.24.0.-0.01 3R87,ASP_50,3.89,0,-0.19,0.27 2ATR,GLU_13,4.3,0.33,-0.44,-0.09 2IRM, ASP_56, 2.62, -1.53, -0.12, 0.48 3EVZ.TYR 43,10.29,0,0,0.29 3PAC, ASP_21, 2.94, -0.85, -0.38, 0.37 2R2Y,CYS_60,11.05,-0.34,0.5,1.89 3L7N,ASP_230,2.55,-1.93,-0.51,1.18 1YOY,LYS_56,10.4,-0.12,0,0.03 3CGW.GLU 179.3.89.0.26.-0.43.-0.44 3CJW,CYS_343,10.03,0,0.38,0.66 4AM1,LYS_216,11.43,-0.45,0.85,0.53 3RVC,GLU_172,4.01,0.19,-0.59,-0.09

1RI5.GLU 277.3.63.0.99.-1.85.0 3FK5,HIS 50,6.19,-0.4,0,0.09 2WB3,GLU_260,4.55,0.05,0,0 1QQE,ASP_74,3.63,-0.25,-0.46,0.55 4ETX,GLU_445,3.5,0.28,-0.72,-0.54 3GS9,GLU_280,4.5,0,0,0 2G9D,ARG_255,12.38,-0.21,0,0.09 1GPP,LYS_4,10.9,-0.13,0,0.53 3DZ1,GLU_127,4.7,0.15,0,0.05 1G8P,ARG_328,12.47,-0.03,0,0 3IO0,TYR_200,10.99,-0.01,0,1 2D2S,GLU_608,4.55,0.31,0,-0.26 1GXN,ARG_567,11.69,-0.81,0,0 2CL3,ARG_150,12.03,-2.13,0.77,0.88 3CAX.HIS 301.5.86.-0.88.0.0.24 3UX2,LYS 52,10.99,-0.52,0.4,0.6 2R51,HIS_27,4.9,-1.62,0,0.02 3CIV,ASP_256,3.84,0,-0.17,0.21 3GA2,HIS_131,3,-2.88,0,-0.62 1T6L,TYR 20,13.43,-0.85,0.17,4.11 1AK1.GLU 174.4.79.0.2.0.0.08 1X1E,TYR_27,10.34,-1.28,-0.27,1.89 1WXQ,GLU_239,6,2.07,-0.68,0.1 2BOO,ASP 86,3,49,-0.85,-0.08,0.62 1ES9.HIS 209.5.79,-0.7.0,-0.01 1TP6,TYR_5,10.56,0,-0.13,0.7 3GS3,GLU_193,4.58,0.05,0,0.03 3G9T,LYS_201,10.31,-0.19,0,0.01 1NWA,TYR_44,12.23,0,1.38,0.84 2AZP,HIS 170,5,18,-1,65,0,34,-0.02 3EGN,GLU_405,4.69,0.22,0,-0.04 3DZ1,LYS_151,10.27,-0.1,0,-0.13 3PU6,TYR 97,9.88,-0.49,-0.38,0.75 3M7G.ARG 252.12.54.-0.22.0.0.26 1WRU,LYS_106,10.07,-0.43,0,0 1Q5Z,GLU_543,3.89,1.23,-1.36,-0.49 1R9W,ARG_287,13.85,-0.92,1.54,0.74 2CI3,GLU_85,5.05,0.32,-0.14,0.38 1W24.TYR 129.11.78.0.0.1.1.68 1YTD,HIS_334,4.62,-1.48,0,-0.39 3K8J,TYR_217,13.7,0.77,0.55,2.38 1ZBP,LYS_227,10.55,-0.17,0,0.21 1I60,GLU 12,4.81,0.33,0,-0.03 1ZP2,GLU_143,4.62,0.32,0,-0.2 2GS5,ASP_99,3.33,-0.75,-0.03,0.31 3ASA,GLU_29,3.94,0.24,-0.79,0 1WXQ,GLU_137,4.81,0.33,0,-0.02 1R53,LYS 207,11,29,-0,28,0,16,0.89 2VGM,GLU_40,5.02,0.84,0,-0.32 3MEW,TYR_154,11.32,-0.3,0.46,1.15 3RJX,LYS_330,10.48,-0.11,0,0.09 1YW5,GLU 149,4.04,0.53,-0.85,-0.14 1Y0K,ARG_132,12.43,-0.37,0,0.3 1AKO, ARG_173, 12.29, -0.21, 0, 0 3TOW,HIS_198,6.52,-0.17,0,0.2 3GS3,GLU_222,4.72,2.09,-0.85,-1.02 3M3P,HIS_247,7.18,-0.16,0.84,0 3TOW,GLU_103,4.58,0.08,0,0 3FK5,LYS_217,10.24,-0.11,0,-0.15 3HYQ,ARG_174,12.37,-0.3,0,0.16 3CN5,HIS_193,6.31,-0.17,0,-0.03 3V3T,ASP 301,4,13,0,-0.01,0.35 1X91,TYR_75,12.3,-0.85,0.18,2.97 3IV4,ARG_47,13.02,-0.35,0.38,0.5 2IQT,GLU_191,4.32,0.25,0,-0.43 3CIV,HIS_223,5.56,-0.95,0,0.01 2EYI,ARG_156,13.83,-0.29,1.23,0.38 2RFA.ASP 57.3.37.-0.72.-0.1.0.39 1J33,GLU_224,4.4,1.01,-0.7,-0.4

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3016.GLU 218.3.23.0.47,-1.02,-0.71 2GEN,TYR_57,11.61,0,-0.24,1.86 2Q5X,GLU_852,3.88,0.28,-0.8,-0.09 3IBT,ASP_64,3.87,-0.02,-0.13,0.21 2FZP.GLU 252.3.55.0.56.-0.95.-0.56 1JSX.HIS 152.6.86.-0.57.0.83.0.11 1SI7,LYS_120,10.07,-0.35,0,-0.08 1XFK,CYS_319,12.32,0,-0.01,3.34 1AK1,HIS_116,3.23,-3.27,0,0 1O3X,ARG_255,12.65,-0.17,0,0.32 4GA2,ASP_111,2.75,-1.14,-0.37,0.46 2BDV.ARG 23.12.63.-0.14.0.0.26 4FCU,LYS_119,11.45,-0.8,1.01,0.73 2VGY.ASP 34,3.98,-0.1,0.1,0.19 3M7G,ARG 135,11.25,-0.91,0,-0.34 1WYC,ARG_376,12.27,-0.23,0,0 2YWX,ARG_111,12.46,-0.21,0,0.17 1DCF,ASP_125,3.9,0,-0.25,0.36 2FZP.ARG 210.13.15.-0.28.0.55.0.38 1N81,GLU_90,4.39,0.36,0,-0.47 3PAC,LYS_25,11.49,-0.24,0.85,0.38 3ZRI,HIS_40,4.08,-2.1,0,-0.32 3PZ9,ARG_374,12.75,-1.44,0.71,0.98 2IIA.ASP 42.3.18.-0.75.-0.21.0.34 1X91,LYS_100,10.41,-0.27,0,0.17 2X4G,GLU_97,4.62,0.12,0,0 1MUF,TYR_305,12.1,0,0.02,2.08 1MTZ,GLU 147,4.74,0.57,-0.02,-0.31 3JZN,GLU_238,5.96,1.68,0,-0.22 3K8U,TYR_29,10.94,0,-0.03,0.98 4FZR,ARG_71,12.29,-0.21,0,0 1K95,ARG 166,12.64,-0.19.0.0.33 30A7.GLU 19.4.56.0.06.0.0 30IP,ARG_86,12.18,-0.43,0,0.11 2VC8.CYS 14.10.3.0.0.11.1.19 2BT8, ARG_226, 13.28, -0.85, 0.89, 0.74 3F1X,HIS 28,6.72,-0.34,0.56,0 4DIU.GLU 168,4.72,0.27,0,-0.05 1IAP,ASP_98,4.3,0,-0.14,0.64 2RFA,HIS_153,6.34,-0.61,0.66,-0.2 1G5Z.LYS 47.10.96.-0.18.0.31.0.33 4DEZ.ASP 181.3.75.-0.37.-0.06.0.39 1H4U,LYS_476,10.36,-0.39,0,0.26 2G3A.LYS 34,10.23,-0.27,0.0.01 1FO9,ARG_296,12.23,-0.45,0,0.19 4E8B,LYS 65,11.31,-0.32,0.72,0.41 2OK0,LYS 88,11.31,-0.35,0.57,0.58 2H2W,CYS_291,13,0.18,0.73,3.09 1SQH,ARG_262,12.2,-0.44,0,0.14 1YG2.LYS 23.10.5.0.0.0 3EUR,ASP 118,3,15,-1,46,-0,16,0,99 307K,ASP_13,3.88,0,-0.07,0.15 2DFL,ASP_201,1.95,-2.09,-0.55,0.79 4EZB,GLU_91,4.79,0.12,0,0.18 3GA2,ARG 220,12.22,-0.41,0,0.13 2BDV,HIS_162,6.44,-0.19,0,0.14 1059,HIS_312,5.39,-1.63,0.77,-0.24 3M7G,ASP 239,2.63,-1.32,-0.33,0.49 4HDE,ASP_102,4.03,-0.85,-0.33,1.41 1SQW,LYS 50,10.4,-0.36,0,0.25 2WB3,LYS_309,10.45,-0.05,0,0 3RJZ,TYR_103,9.33,-0.59,-0.35,0.28 3RFF,LYS_55,10.21,-0.27,0,-0.02 1ES5,ARG 171,12.17,-0.33,0,0 2AZL.GLU 241,4.54,0.32,0,-0.28 3A2Z,ASP_121,3.58,-0.68,-0.12,0.58 2AXO,GLU_62,3.49,0.21,-0.72,-0.51 3BB7,TYR_199,13.89,0,0.52,3.36 2YYO, ASP_76, 4.04, 0, 0, 0.24

4FH3.GLU 64.4.6.0.35.0.-0.25 1P2F,ARG 117,12.2,-0.27,0,-0.03 3PZ9,TYR_370,11.97,0.85,0.47,0.65 3MIX,ASP_366,4.07,0,0.08,0.19 3FRR,ASP_77,3.93,0,-0.24,0.37 1X04,ASP 145,3,48,-0,38,-0,53,0,61 2C2Y,GLU_84,3.38,0.89,-1.52,-0.48 2JHY,LYS_98,11.62,-0.39,0.85,0.66 3S0A,LYS_7,12.56,-0.55,1.7,0.91 3M7G,ASP_124,4.27,-0.01,0.21,0.27 1P4X.GLU 211.4.61.0.11.0.0 4EKU,LYS 295,10,49,-0.01,0,0 1I60,LYS_114,10.45,-0.2,0,0.15 2H80, ARG 244, 12, 89, -0.86, 0.84, 0.41 1G8P.GLU 132.5.07.0.45.0.0.12 2I6I,ASP_75,2.47,-1.53,-0.4,0.59 30IP,ARG_116,12.76,-0.22,0,0.48 1ZBM,ARG_196,12.25,-0.53,0,0.28 1FO9,ARG_165,12.27,-0.37,0,0.14 2F4O,ARG 94,13,48,-1,43,1.54,0.87 3B79,LYS_2,10.41,-0.08,0,-0.02 1X8F,GLU_98,4.67,0.23,0,-0.05 1FKM,ASP_464,4.11,0,0.15,0.16 1PSWLYS 301.10.21.-0.3.0.0.01 2QK1,GLU_397,5.37,1.57,-0.85,0.16 3IL3,ARG_294,11.75,-1.27,0.46,0.06 2P52,ARG_264,11.71,-0.84,0,0.05 1S7K,ARG_64,12.32,-0.26,0,0.08 1059.GLU 142.4.65.0.19.0.-0.04 3EAZ,TYR_133,11.44,0,0.19,1.26 1YTD,LYS_279,11.33,-0.29,0.85,0.27 1EQ6,ASP_167,4.21,0,0.16,0.25 3IBT.ARG 46,13.4,-0.3,0.82,0.38 2XHC,LYS_95,10.62,-0.33,0,0.46 1S7K,ARG_14,12.95,-0.64,0.74,0.34 3FRR,ARG_12,13.66,-0.47,1.24,0.38 1PVT,GLU 113,4.51,0.22,0,-0.21 1XDZ,GLU_119,4.54,0.15,0,-0.1 3L3P,ASP_332,3.99,0,-0.02,0.21 2PGE,ARG_311,13.47,-0.48,0.88,0.57 3ZSL,LYS_233,10.25,-0.26,0,0.01 1SUU,LYS 744,10.94,-0.37,0.78,0.03 20HT.HIS 24.5.66.-1.52.0.94.-0.27 3T5B,GLU_284,4.67,0.3,0,-0.13 3DTE,ARG_17,13.12,-0.36,0.38,0.61 2BDV,GLU_176,3.76,0.49,-0.89,-0.34 3UC9,GLU_127,4.68,0.51,-0.03,-0.28 2FI9,ASP_67,3.86,0,-0.07,0.13 3SMD,LYS 86,10,17,-0,14,0,-0,19 2D2S,ASP_706,4.25,0,-0.43,0.86 20EW,HIS 61,6.75,-0.26,0,0.5 3BPP,ARG_220,13.07,-0.27,0.1,0.74 2QZQ,LYS_44,9.88,-0.33,0,-0.28 2G5X,ARG_21,12.72,-2.54,1.21,1.56 3JZ9,ARG_418,12.51,-0.07,0,0.08 1EW4,ARG_106,13.3,-0.49,0.47,0.81 2V4X,TYR_29,10.21,0,0.01,0.2 3OA7,HIS_530,6.01,-0.52,0,0.04 1AIL,HIS_17,6.05,-0.44,0,-0.02 3RVC,GLU_96,2.91,0.46,-1.63,-0.42 4DBX.ASP 19.3.94.0.0.0.14 2FPN,HIS_186,6.55,-0.41,0.08,0.38 2B6P,HIS_172,3.49,-3.23,0.73,-0.51 2ZQ5,TYR_370,11.4,-0.55,0.49,1.44 1TUL,ASP_82,3.41,-0.81,0,0.42 2NRK,LYS_136,11.3,-0.32,0.74,0.38 3F7M,LYS_184,10.69,-0.15,0,0.34 1PGV,GLU_233,4.71,0.17,0,0.03 4ANN,TYR_74,11.17,-0.74,-0.23,2.12

1MTZ.LYS 291.11.51.-0.24.0.75.0.5 1Z9L.GLU 108.4.69.0.17.0.0.02 2E3H,ARG_261,13.32,-0.51,0.88,0.44 10ZN.ASP 141.4.25.0.0.17.0.27 2WOZ,GLU_513,4.24,2.86,-2.18,-0.94 1P4X,HIS 70,6.09,-0.93,0.6,-0.07 2DVK,GLU_98,4.22,0.27,-0.08,-0.48 4H89,ASP_15,2.29,-2.1,-0.4,0.99 2YX0,TYR_210,12.88,0,0.19,2.68 2O34.GLU 248.3.83.0.27.-0.83.-0.11 1A80.HIS 219.5.08.-3.02.0.83.0.78 105J,HIS_73,4.62,-2.06,0.29,-0.11 3M16.GLU 91.4.92.0.6.0.-0.17 1PGV,ARG 315,13,35,-0.54,0.82,0.57 2188.LYS 426.10.41.-0.14.0.0.05 2V5B,ARG_139,12.4,-0.21,0,0.11 2WOZ,ASP_372,2.65,-1.5,-0.05,0.39 3JZ9,LYS_350,11.37,-0.5,0.83,0.54 2XHC,GLU_146,3.76,0.33,-0.67,-0.4 3DSH,HIS_364,6.27,-0.42,0,0.19 1SI7,ASP_142,3.98,0,0.01,0.18 1X7F,ARG 243,11,47,-1,36,0,0,33 1FKM.TYR 365,11,22,-0,76,0,44,1.54 1RI6,GLU 13,4.57,0.46,0,-0.39 3LJN.GLU 101.3.7.0.29.-0.57.-0.52 3ETV,TYR_123,11.09,0,-0.25,1.34 4D8L,GLU_158,4.64,1.11,-0.45,-0.53 1UCH,ASP_177,2.52,-1.51,-0.13,0.36 1GQE,ASP 68,4.54,0,0.15,0.59 1V43,ARG_263,13.34,-0.23,0.39,0.68 2OK0,LYS 43,10,35,-0,18,0,0,03 3CAX,ASP_342,2.09,-2.05,-0.48,0.82 1X91.LYS 133,11.35,-0.48,0.85,0.48 4GA2,ARG 84,12,49,-0,39,0,04,0,34 2D7U,TYR_270,10.24,0,-0.04,0.28 2WB3,ASP_377,4.05,0,0,0.26 1PSW,LYS_142,10.36,-0.26,0,0.11 1TJE,LYS 63,10.46,-0.21,0,0.16 1G8P,ARG_208,12.73,-0.85,0.56,0.52 2EDM,ASP_89,4.09,0,0.08,0.2 1W24,ASP_47,3.81,0,-0.39,0.4 1H4U,GLU_424,4.53,0.27,-0.17,-0.06 1|60,LYS 118,11,55,-0,46,0,85,0,65 3N2T,HIS_43,6.3,-1.03,0.78,0.04 2ZTY,ASP_64,2.42,-1.59,-0.46,0.68 1FO9,GLU_282,3.7,1.06,-1.34,-0.53 3H9W,ARG_110,12.35,-0.2,0,0.06 1KCM,ASP 51,3.91,0.0.03,0.08 3CCY,ARG_26,13.47,-0.48,1.01,0.45 1A8Q,ASP_221,3.5,-0.85,0.01,0.55 1WPA,TYR_517,11.23,0.38,0.27,0.58 2YX0,ASP 206,2,52,-1,65,-0,55,0,92 3RHE,TYR_22,10.61,0,0,0.61 3K8U,LYS 69,9.98,-0.52,0,0 1FHL,LYS_70,10.67,-0.24,0,0.41 3C5V,CYS_105,11.84,0,-0.03,2.87 3MIX.TYR 660.11.72.0.0.87.0.85 20EW,GLU_356,4.6,0.17,0,-0.06 1TJE,LYS_197,10.35,-0.2,0,0.05 20GQ,ASP_447,1.78,-2.57,0,0.54 1T3J,ARG 716,12,38,-0,12,0,0 1W24,GLU_143,4.66,0.2,0,-0.05 20VO,LYS 85,11.65,-0.26,0.51,0.9 1RAJ,GLU_93,4.58,0.08,0,0 3H5T,ARG_150,11.99,-0.54,0,0.03 3BWT,LYS 807,10.62,-0.32,0.0.44 1UW7,TYR_31,11.75,0,0,1.75 4DVD,GLU_33,2.85,0.46,-1.45,-0.66 1R3F,LYS_190,10.34,-0.24,0,0.07

1SUU,TYR_526,12.53,0,0.27,2.27 2RIS,GLU_147,4.27,2.31,-2.05,-0.49 3M3P,CYS_89,9.2,-2.03,-0.64,2.87 3IDW,ARG_67,12.44,-0.43,0,0.36 1RZ2,ASP_114,3.8,0,-0.2,0.2 1UW7,HIS 48,6.3,-0.47,0,0.28 2FG1.TYR 153,11.33,-0.77,0.02,2.07 2AHE,LYS_90,10.83,-0.12,0,0.45 2BDV,GLU_172,3.81,0.24,-0.76,-0.17 2QK1,HIS_468,5.64,-0.58,0,-0.28 3VHJ,LYS 164,10.69,-0.09,0,0.28 3HYQ,GLU_77,4.56,0.41,-0.39,0.04 10YI,LYS 114,9.3,-1.3,0.0.09 3CNU,ARG_92,13.19,-0.28,0.69,0.28 4AE7.GLU 210.4.34.0.31.0.03.-0.49 2W1R,LYS 163,11.62,-0.31,0.85,0.57 1FO9,ARG_189,12.08,-0.97,0,0.54 2QK0,ASP_73,1.39,-2.54,-0.38,0.5 3BQE,LYS_328,11.28,-0.63,0.85,0.55 1ZHV,HIS_134,6.28,-0.19,0,-0.03 2G3A,ASP 7,3.71,-0.2,0,0.11 3DZ1,ARG_181,12.26,-1.52,0.58,0.7 3A0X,LYS_652,10.95,-0.6,0.85,0.2 2D0A,LYS 64,10.95,-0.3,0.38,0.37 2BOO.GLU 123.4.84.0.35.-0.15.0.14 1RSS,TYR_154,10.14,0,0.05,0.08 20EW,ASP 210,3.64,-0.8,-0.42,1.05 1AM2,GLU_65,4.34,1.31,-1.45,-0.01 2NSN, ASP 48, 3.99, 0, 0, 0.19 1BKR,ARG_32,12.4,-0.45,0,0.35 3JZN,ASP_395,2.7,-0.85,-0.55,0.31 1V43,ASP_365,2.31,-2.01,-0.01,0.54 2VAN.TYR 250.10.55.0.0.3.0.26 3TIR.ASP 166.3.9.-0.24.0.1.0.25 3BPP,GLU_49,3.6,1.72,-2.09,-0.53 3G9T,ASP_159,2.68,-1.61,-0.41,0.9 3MIX,GLU_407,4.02,0.92,-0.51,-0.88 2P0Y,GLU_222,5.79,1.39,0,-0.11 1DTO.GLU 20.4.69.0.17.0.0.02 3IO0, ASP_270, 3.94, 0, -0.01, 0.15 2OJQ,LYS_553,10.23,-0.28,0,0.02 1T95,ARG_121,12.56,-0.06,0,0.12 2YX0,LYS 22,10.36,-0.1,0,-0.04 2YWJ,LYS_20,10.69,-0.21,0,0.41 1WXF,GLU_66,2.55,0.87,-1.98,-0.84 2GAU,GLU_104,4.63,1.13,-0.46,-0.54 3HVW,ARG_231,12.25,-0.27,0,0.02 3PAC.GLU 9.5.42.1.59.-0.38.-0.29 3PBH,ASP_69,3.95,-0.06,-0.05,0.26 3ZTA,LYS_65,12.2,-0.81,1.37,1.14 1WPA, ARG_418, 12.46, -0.04, 0, 0 2EYI,HIS 186,4.97,-1.92,0.84,-0.45 3UV9,HIS_461,6.32,-0.18,0,0 2P5D,GLU_88,4.21,0.79,-1.07,-0.03 3LQE,HIS_242,3.49,-3.66,0.63,0.01 2Z0M,ARG_216,12.18,-0.34,0,0.02 3MIX.TYR 350,10,17,0,0,0,17 1X1E,GLU_180,4.59,0.49,0,-0.4 1T3Y,LYS 110,10.52,-0.27,0.0.29 2E3S,TYR_576,12.13,0,0,2.13 1TR9,GLU 12,4.61,0.13,0,-0.02 1Z3X,ARG 60,11.81,-1.51,0.42,0.41 1ES5,HIS_138,5.97,-0.65,0,0.12 1ILW,LYS_39,11.87,-0.48,1.1,0.74 1L3K,ASP_42,3.56,-0.45,-0.07,0.28 1FKM,HIS 442,6.38,-0.12,0,0 1Y0K,ASP_153,3.35,-0.73,-0.14,0.42 2CXY,CYS_53,10.1,-0.03,-0.1,1.23 3G9G,ARG_141,12.16,-0.39,0,0.05

3TIR.ASP 87.3.28.-0.7.-0.23.0.41 1JB3,GLU_11,4.43,1.64,-0.85,-0.87 3UX2,GLU_57,3.61,0.5,-1.14,-0.25 2VAN,GLU_123,4.7,0.13,-0.04,0.11 2B0J.TYR 200.13.72.0.0.06.3.66 3G9T,GLU 5,4.21,0.44,-0.72,-0.01 2P5D,TYR_56,9.36,-0.85,-0.42,0.64 3IPZ,GLU_131,3.53,0.48,-1.24,-0.22 3RNV,TYR_345,12.2,0,0.22,1.98 3GA2.LYS 25.9.41.-1.1.0.0.01 1XWM,ASP_47,4.22,-0.01,0,0.43 3DTE,HIS 63.6.28,-0.25,0.01,0.02 2BV9,LYS_216,10.2,-0.73,0,0.42 2V5B.TYR 102,10.39,0,0.22,0.17 3TOW,LYS 87,10,1,-0,14,0,-0,27 2JKF,GLU_66,4.57,0.07,0,0 3QKY,TYR_87,9.75,-0.5,-0.56,0.82 3ANJ,ASP_145,4.24,-0.85,0.06,1.22 100X.CYS 234.12.59.-0.37.0.22.3.72 2D2S,GLU_542,4.96,0.37,0,0.09 3CS1,LYS_153,10.4,-0.4,0,0.3 3CAX,LYS_275,9.93,-1.33,0,0.76 3CGW.GLU 182.4.51.0.14.0.-0.13 2ZCO.ARG 246,12,43,-1.26,0,47,0,72 2H2W,GLU_212,4.76,0.73,-0.28,-0.19 1YW5,LYS_105,10.42,-0.1,0,0.02 3HVW,ASP_300,4.04,0,0,0.24 4AF2,ASP 124,3.27,-0.83,-0.07,0.36 2FG1,ASP_154,3.97,0,-0.29,0.46 2Z84,HIS_137,4.39,-2.52,0.82,-0.4 1TD6,HIS_243,6.23,-1.2,0.84,0.09 204D,GLU 93,2.54,1.71,-2.65,-1.03 2NMU,ARG 55,12.36,-0.35,0.0.2 3IBT,HIS_20,6.55,-0.09,0,0.14 2GEN,ARG_32,13.61,-0.35,0.9,0.55 2l6l,ARG_31,10.93,-1.82,0,0.24 2EHG,LYS_122,10.45,-0.11,0,0.06 3ADO,ARG 40,12,44,-0.06,0,0 1S7K,ASP_17,2.54,-1.36,-0.27,0.37 2ZCO,GLU_125,4.25,0.52,-0.91,0.14 3S0A,LYS 42,10,41,-0,19,0,0,1 1UOH, ARG 118, 11, 77, -0, 74, 0, 0, 01 3RJZ,LYS_229,11.06,-0.85,0.71,0.7 3ADO,LYS_139,10.4,-0.13,0,0.03 1IDK,LYS_335,10.34,-0.48,0,0.32 1DTO,GLU_118,4.23,0.43,-0.61,-0.08 1Y2O,LYS 106,10.93,-0.42,0.37,0.48 3NBI,TYR_201,11.04,0,0.19,0.85 3T57,ARG_315,12.57,-0.67,0.05,0.7 1LFP,ARG_108,13.85,-0.54,0.71,1.19 2P4D,TYR_63,12.31,0,0.18,2.12 2FPN,GLU_12,4.9,0.47,-0.13,0.05 4DIU,TYR_204,10.12,0,-0.21,0.33 3CQ1,ARG_70,12.38,-0.12,0,0 2H30,GLU 79,4.25,0.69,-0.83,-0.11 1H4U,HIS_436,6.31,-0.23,0,0.05 1SJ8,LYS_613,10.99,-0.34,0.47,0.37 1ZCE,GLU_57,4.71,0.2,0,0.01 2NRR,LYS_443,10.63,-0.14,0,0.27 3EVZ,LYS 207,10.42,-0.29,0,0.21 3HUE,ASP_259,3.58,-0.54,0,0.31 1EV8,GLU_245,3.97,0.36,-0.81,-0.08 1DOV,TYR_148,9.39,-0.85,-0.08,0.33 3HVM,LYS_30,10.4,-0.06,0,-0.04 4DND,ASP_104,3.15,-0.84,-0.16,0.35 2VAN,LYS_141,10.41,-0.27,0,0.18 1U7U,LYS_378,10.54,-0.25,0,0.29 2QDJ,TYR_173,11.73,-0.85,0.37,2.22 4DNU,CYS_37,11.52,-0.04,0,2.57

200K.ASP 69.3.45.-0.56.-0.05.0.26 2PLO,LYS 314,10.7,-0.19,0.01,0.38 3HYQ,LYS_56,10.44,-0.04,0,-0.01 3ZTA,ARG_42,13.18,-0.31,0.31,0.67 1P6F.GLU 112.4.68.0.18.0.0 3T5B,TYR 32,13.33,-0.14,-0.24,3.7 4ETX,LYS_329,10.48,-0.33,0,0.31 2P4D,ASP_84,2.17,-1.98,-0.26,0.61 1UW7,ASP_60,3.96,-0.11,0,0.27 3DB9.LYS 213.10.42.-0.08.0.0 2H30,ARG 154,12.02,-0.54,0,0.06 3IU5,LYS_61,10.43,-0.12,0,0.05 1PSW,ARG_281,12.67,-1.33,0.71,0.79 3V55.GLU 451.3.61.0.26.-0.7.-0.46 1SI7.ASP 60,4,0,-0.36,0.56 4EVF,GLU_191,4.39,0.19,0,-0.3 4DIU,LYS_215,10.56,-0.61,0.19,0.49 4HDE,ASP_149,4.09,0,0,0.29 1X04,GLU 173,4.75,0.14,0,0.12 2R51,HIS_223,6.22,-0.3,0,0.03 4GA2,ARG_2,12.48,-0.02,0,0 2OGQ,ASP_588,3.82,-0.02,-0.26,0.3 2FD4,LYS_464,11.12,-0.21,0.83,0 4H4JLYS 262.10.33.-0.48.0.0.3 2CXA,CYS_187,12.18,0,0.77,2.4 1EV8,GLU_6,4.57,0.22,0,-0.15 3M7G,ARG_112,13.36,-0.54,0.78,0.62 2BLL,GLU 571,3.94,1.11,-0.85,-0.82 3H13.HIS 396.6.36.-0.15.0.0.01 3RFF,ASP_75,4.08,0,-0.01,0.29 1P4X,GLU_102,4.95,0.21,0,0.24 3LJC,ASP_160,4,0,0,0.2 1PDB,ASP 152,3.28,-0.69,-0.29,0.46 1Q46,ASP_93,2.69,-1.39,-0.14,0.42 2R51,HIS_204,9.04,-0.51,2.21,0.82 1SNT,LYS_9,10.01,-0.65,0,0.16 2A0J,GLU 36,5.04,1.75,-0.85,-0.36 1W24,TYR_139,10.03,-0.02,-0.3,0.35 3MEW,LYS_217,10.11,-0.49,0,0.11 3CXS,CYS_113,9.3,0,0,0.3 2FZP,TYR_196,10.48,0,0.22,0.26 1HF8,LYS 28,10.06,-0.26,0,-0.18 3FHF,LYS 124,9.81,-0.39,0,-0.3 1T95,ARG_70,13.14,-0.26,0.36,0.54 2Z0W,TYR_41,10.32,0,0,0.32 2AHE,LYS_62,9.79,-0.73,0,0.01 2E3S,GLU_373,4.1,0.23,-0.32,-0.32 2IDC,ASP_37,4.12,0,-0.06,0.38 3FK5,ARG_135,12.41,-0.56,0,0.47 1XWM,GLU_161,4.71,0.22,0,-0.01 3P28,LYS 83,10.81,-0.29,0,0.6 3PP8,ASP 40,4.61,0,-0.05,0.86 3I0C,GLU_174,4.77,0.24,0,0.03 1TXJ,LYS_105,10.52,-0.16,0,0.17 1LTU,TYR_181,12.74,0,-0.26,2.99 1WOU,ARG_17,12.46,-0.1,0,0.06 2IF4,LYS_244,10.93,-0.26,0.14,0.55 2D59,TYR_93,11.66,0,0.44,1.21 1W24,CYS_15,9.63,-0.85,-0.06,1.54 1D2K,CYS_108,11.21,-1.44,0.39,3.25 10LR.ARG 220.12.73.-0.28.0.0.5 3CSR,ASP_112,3.91,0,-0.02,0.13 3M7D,GLU_19,6.3,3.49,-1.8,0.13 4E6S,GLU_78,4.82,0.18,0,0.13 1PGV,GLU_240,4.57,0.33,0,-0.25 100X,LYS_92,10.25,-0.41,0,0.16 3CGW,ARG_99,13.08,-3.06,0.36,3.26 1SNT,CYS_352,12.7,-0.3,0.36,3.63 1XKR,GLU_155,4.01,0.21,-0.25,-0.45

2X5Y,ARG 871,13,11,-0,28,0,53,0,36 100H,ASP 206,3.94,-0.56,0.1,0.6 2FXT,GLU_247,4.76,0.09,0,0.16 3IL3,ASP_233,3.77,-0.39,-0.02,0.38 1RI5,TYR_194,10.78,-0.57,-0.6,1.96 1UJ8,HIS 5,5.83,-0.15,0,-0.51 1UJ8,ASP_74,3.1,-0.63,-0.34,0.26 1ZCU,LYS_201,10.34,-0.16,0,0 4AF2,LYS_67,10.49,-0.26,0,0.25 3GFP,LYS 305,10,13,-0,26,0,-0,11 1DTO.GLU 48.4.11.0.25.-0.31.-0.33 1QZN,GLU_8,4.91,0.48,0,-0.07 2HP7,LYS 153,10.26,-0.2,0,-0.03 1R53,ASP_166,4.3,-0.47,0.11,0.86 3BB7.LYS 114,10.33,-0.18,0,0.01 3HQX,ASP_7,3.4,-0.68,-0.02,0.3 3S0A,GLU_93,3.02,0.53,-1.58,-0.43 2W0G,ASP_196,3.49,-0.8,-0.38,0.87 4FH3,ARG_286,12.4,-0.15,0,0.05 1UCH,GLU_124,3.58,0.43,-0.85,-0.5 109G,LYS_95,10.29,-0.27,0,0.06 10YI.HIS 379.6.33.-0.34.0.0.17 3BJV,TYR_153,10.45,0,0.29,0.16 2XHC,ARG 126,12.42,-0.08,0,0 2B78.HIS 90.6.35.-0.13.0.-0.02 1UOH,GLU_21,4.63,0.17,0,-0.04 1EV8,LYS_229,10.37,-0.2,0,0.07 1Q2Y,ASP_14,3.68,-0.85,-0.03,0.76 3DB9,ARG 189,12.28,-0.22,0,0 3EJG,GLU_135,4.78,0.24,0,0.04 3IVF,GLU_34,4.48,0.25,-0.06,-0.22 1V8E,LYS_140,10.36,-0.08,0,-0.06 4H86,GLU_29,4.58,0.17,0,-0.09 1MJS,GLU_266,4.57,0.19,0,-0.11 2AZP,ARG_291,12.33,-0.38,0,0.21 2C2Y,ASP_42,3.92,-0.1,0.06,0.17 1R6Y,GLU_94,4.61,0.19,0,-0.08 1R5Q,ARG 69,12.42,-0.08,0,0 2R51,LYS_91,10.38,-0.18,0,0.06 2IDC,TYR_22,13.69,-0.16,0.16,3.69 3RJX,TYR_315,12.14,-0.29,-1.21,3.64 2HNG,GLU 90,4.59,0.25,-0.07,-0.09 3EGN/LYS 494/10.14/-0.21/0/-0.15 2CXA,TYR_210,10.52,0,0.2,0.32 1ZBP,LYS_232,12.12,-0.43,1.23,0.82 2PGX,LYS_51,10.45,-0.05,0,0 3COU,GLU_11,4.29,0.33,-0.3,-0.24 2BT8,ASP 176,3.93,-0.21,0.0.34 1BYI,GLU_48,4.45,0.12,0,-0.18 1EYH,ASP_138,4.17,0,0.22,0.15 1YLN,LYS_67,10.71,-0.27,0.17,0.3 2IDC,ASP 154,2.51,-1.59,-0.49,0.8 2QDJ,CYS_169,11.78,0,0.13,2.65 1NFN,LYS 95,10,45,-0.05,0,0 1SIG,TYR_394,10,-0.21,-0.44,0.66 3IBT,TYR_142,10.12,0,-0.13,0.26 3M16,TYR 52,12.26,-0.72,0.68,2.3 4GCO,ARG_183,13.48,-1.73,1.63,1.09 2QV2,ARG_278,11.79,-0.5,0,-0.21 1RKA,GLU_300,3.95,0.84,-0.82,-0.57 1PGV.ARG 385,12.55,-0.29,0.17,0.17 4EZB,ARG_150,12.25,-0.85,0,0.59 3RJZ,LYS 218,10.53,-0.46,0.0.49 2EFK,TYR_53,10.17,0,0,0.17 3RFY,ASP_367,3.93,0,0,0.13 20HT.GLU 108.4.72.0.33.0.-0.11 1XEU,TYR_277,10.24,0,0.05,0.19 2CXC,ARG_144,12.23,-0.3,0,0.03 1T3Y,HIS_47,6.46,-0.29,0,0.25

3P51,ARG 51,13.3,-0.34,0.79,0.35 2B02,TYR_456,10.43,-0.01,-0.06,0.49 4FZR,ARG_378,13.26,-0.31,0.66,0.41 2YX0,GLU_137,4.57,0.21,0,-0.13 1DUP,TYR_23,10.77,0,0,0.77 2D7U,GLU 28,3.59,0.34,-0.85,-0.39 1J7G.LYS 112.9.99.-1.0.0.49 2AHE,TYR_244,11.94,0,0.02,1.92 3TMO, ARG_244, 12.39, -0.25, 0, 0.13 3L3P,GLU_280,3.63,1.04,-1.47,-0.43 2AXO, ASP 159, 3.56, -0.47, 0, 0.23 3C5V.LYS 338.10.19.-0.31.0.0 3F7M,ARG_230,11.77,-0.59,0,-0.14 1RSS,GLU_129,4.68,0.26,0,-0.07 1XWM.TYR 213.11.82.-0.79.0.77.1.84 1RHS/HIS 120,4.71,-2.55,0.8,-0.04 3OKQ,GLU_611,4.66,0.16,0,0 3EX9,GLU_154,4.61,0.11,0,0 10IS,ARG_294,12.35,-0.22,0,0.08 3FK5,ARG_249,12.3,-0.2,0,0 3EYE,ARG 134,13.07,-0.32,0.51,0.39 4H4J,HIS_44,6.38,-0.34,0,0.22 3IL3,GLU_49,4.24,1.15,-1.63,0.23 1C3K.LYS 60.10.21.-0.29.0.0 2AHE,GLU 92,5.91,2.2,-0.32,-0.47 1V43,LYS_353,11.33,-0.25,0.76,0.32 2AH5,HIS_144,6.14,-0.51,0,0.15 2R51,LYS_186,10.25,-0.22,0,-0.02 1LN4,GLU_98,3.51,0.41,-1.41,0 2D7J.HIS 155.5.16.-1.28.0.-0.06 3M70,GLU_152,4.6,0.1,0,0 1YR6,GLU_172,4.88,0.39,0,-0.02 1NAF.ASP 285,4.12,0.0.0.32 2FM9,LYS 151,10.22,-0.16,0,-0.13 2I88, ARG_409, 12.01, -0.63, 0, 0.14 3PZ9,GLU_250,2.58,0.6,-2.52,0 2Q07,LYS_284,10.37,-0.19,0,0.06 3SMD,GLU_65,5.85,1.85,-0.72,0.23 105T,HIS_129,2.58,-2.74,0,-1.19 1QQE,ARG_110,12.93,-0.28,0.1,0.6 2D0A,ARG_308,12.38,-0.21,0,0.08 1P1L,ARG_17,12.75,-0.22,0.06,0.41 2WB8,LYS 664,10.38,-0.12,0,0 2FPN,ASP_58,3.96,0,-0.27,0.42 3GEC,ARG_266,12.71,-0.11,0.03,0.3 3UX2,GLU_74,4.92,0.12,0,0.3 2YX0,TYR_199,11.31,-0.55,-1.42,3.27 2B61,ASP 236,3.71,-0.07,-0.17,0.15 2AD1,GLU_279,4.29,0.16,0,-0.37 2PGX,ASP_28,3.22,-0.57,-0.44,0.43 3BPP,LYS_229,10.37,-0.16,0,0.02 1YDL,HIS 2,6.43,-0.07,0,0 1SQW,LYS_62,10.47,-0.11,0,0.08 4EKU,CYS_44,10.38,-0.08,-0.33,1.79 3H6Q,GLU_168,4.56,0.06,0,0 2Z0M,ARG_175,12.36,-0.71,0.12,0.45 3L3P.GLU 446.3.04.1.91.-1.98.-1.39 1TD6,LYS_61,10.51,-0.18,0,0.2 3US6.ARG 8.12.25,-0.29.0.0.03 2EFK,ARG_113,11.63,-1.1,0,0.23 1D2K,LYS 97,11.1,-0.2,0.11,0.69 1R5O,LYS 38,10.62,-0.12,0,0.24 3MTT,LYS_589,10.53,-0.06,0,0.09 1TUL,TYR_81,10.08,0,-0.11,0.19 1VSM,ARG_137,12.27,-0.34,0,0.11 2P0L,LYS_171,10.37,-0.1,0,-0.03 2FBQ,ASP_73,3.19,-0.61,-0.38,0.37 3QKY,ARG_30,12.56,-0.1,0,0.15 1TLV,ASP_99,4.75,0,-0.01,0.96

2YLF,ARG 197,12.37,-0.18,0,0.06 2Q99,GLU_90,3.49,1.66,-1.85,-0.81 2A6B,ASP_59,4.26,0,-0.13,0.59 1ZBP,GLU_193,4.1,0.33,-0.39,-0.34 2AD1.GLU 210.4.52.0.32.-0.1.-0.2 3V55.GLU 588.4.59.0.09.0.0 2IQT,LYS_31,10.36,-0.22,0,0.08 10IS,GLU_288,4.06,0.54,-0.32,-0.65 3V3T,HIS_137,5.72,-1.55,0.72,0.06 1FHL.GLU 18.4.74.0.23.0.0.01 1GVP,ARG_80,12.29,-0.46,0,0.23 20EW.GLU 79.5.74.1.87.0.-0.64 3FHF,LYS_21,11.33,-0.3,0.85,0.28 1XWM.ARG 188.12.56.-0.23.0.0.29 2AHE,ARG 219,11.52,-1.04,0.0.06 3PP8,ASP_218,2.81,-0.86,-0.39,0.26 3HUE,HIS_47,5.62,-2.02,0.81,0.33 3LJI,LYS_202,10.42,-0.06,0,-0.01 10ZN.ARG 102.12.81.-0.37.0.31.0.38 1DTO,GLU_141,4.26,0.28,-0.45,-0.07 4AM1,CYS_23,8.26,-1.69,-0.15,1.11 1MN3,CYS_432,9.51,0,0.01,0.5 1UJ8.HIS 7,6.79,-0.41,0.36,0.35 3FS3,ARG 105,13.3,-0.31,0.51,0.6 2HXB,TYR_56,10.6,0,0.03,0.57 3IO0,LYS_163,10.53,-0.53,0,0.55 1WXQ,ARG_156,12.33,-0.31,0,0.14 3P51,TYR 91,13.69,-0.85,1.52,3.02 1T3Y,GLU_40,3.46,1.32,-1.65,-0.71 4E8B,LYS_127,9.93,-0.49,0,-0.09 1R6Y,HIS_16,7.06,-0.46,0.85,0.17 1SQH,GLU_265,4.41,0.17,0,-0.25 2RFA.ARG 180.12.96.-0.33.0.19.0.6 2IRM,CYS_93,9.97,-0.07,0,1.04 3KEY,HIS_435,6.41,-0.21,0,0.12 3KT9,LYS_80,10.4,-0.24,0,0.14 2GYZ,GLU_76,4.51,0.29,-0.01,-0.26 1ZP2.HIS 147.6.91.-0.16.0.15.0.41 3T5B,GLU_179,4.45,1.04,-0.64,-0.45 2JHY,ASP_93,2.48,-1.7,-0.04,0.42 3GT0.GLU 141.4.66.0.08.0.0.07 1RWZ,ARG 155,12,22,-0,33,0,0.05 2V5B,HIS_96,3.75,-2.47,0.8,-1.08 1LFP.ARG 114,12,22,-0,3,0,0,02 3GS9,GLU_316,4.78,0.28,0,0 2W1R,GLU_114,4.91,0.39,0,0.02 2X4L,ASP 173,4,11,0,-0.07,0.38 4DBX,ASP_179,4.02,0,-0.09,0.31 3LJN,LYS_195,10.48,-0.02,0,0 1ZHV.ARG 58,12,13,-0,19,0,-0,17 3L7N,TYR 129,10.5,0,-0,12,0,61 1J74,ARG_123,11.63,-1.09,0,0.22 2D7U,TYR_155,10.61,0,-0.25,0.85 3CAX,LYS_272,10.97,-0.64,0.58,0.54 2ZTY,GLU_5,4.55,0.12,0,-0.07 1RAJ,ASP_406,3.51,-0.63,0,0.34 4F85,HIS_86,5.58,-0.71,0,-0.2 1X91,CYS 136,12.27,0,0.02,3.25 1IAP,ARG_191,12.35,-0.39,0,0.24 1X9G,ASP_174,2.13,-2.21,-0.31,0.84 2EJB,ARG_37,12.56,-0.18,0,0.24 1LFP,LYS_217,10.5,-0.19,0,0.19 2D2S,GLU_617,5,0.79,0,-0.3 3ASA,ARG_369,11.49,-3.48,0,2.47 30IP.GLU 25,4,19,0,27,-0,2,-0,38 3UX2,CYS_99,9.27,-0.01,0,0.29 3L7N,LYS_110,10.6,-0.34,0.09,0.35 2D7U,ARG 273,12.29,-0.1,0,-0.11 2P0L,GLU_232,3.23,0.44,-1.32,-0.4

1TR9.LYS 309.10.21.-0.4.0.0.11 100X,TYR_65,11.1,0,0.23,0.87 2CL3,TYR_202,10.3,0,0.17,0.12 1FO9,LYS_248,10.15,-0.35,0,0 1A8Q,ASP_229,3.43,-0.45,-0.33,0.4 2B0A,LYS 117,10.59,-0.07,0,0.17 1YB2,GLU_226,3.95,0.15,-0.7,0 3GV0,GLU_170,3.29,0.81,-1.14,-0.89 3TIR,ASP_24,4.03,0,-0.08,0.31 2FL4.ARG 120.12.27.-0.23.0.0 2X4L,ASP_300,4.03,0,0,0.23 3CJW,ARG 371,13.88,-0.8,1.22,0.96 1SJ8,LYS_687,10.39,-0.11,0,0 1FKM.GLU 475.4.68.0.22.0.-0.04 3HVM,LYS_212,10.52,-0.4,0,0.41 1V6T,ASP_123,3.37,-0.66,-0.12,0.35 2H85,HIS_18,6.16,-0.3,0,-0.04 105T,CYS_225,12.26,-0.09,0.12,3.23 2ZQ5,ASP_14,3.78,0,-0.21,0.18 2FM9.HIS 243.6.6.-0.09.0.0.19 3H04,CYS_217,11.62,-0.28,0.59,2.3 1Q42,TYR_38,10.92,-0.74,-0.7,2.36 1KN3,GLU_16,3.81,0.68,-0.39,-0.98 2EFK.ARG 179,12.66,-0.27,0,0.44 2X4J,TYR_83,12.84,0,0.02,2.82 3VHJ,ASP_27,2.95,-1.04,0,0.19 3HVM,LYS_179,10.62,-0.16,0,0.28 3FS3,TYR 71,9.86,-0.33,0,0.2 3BJV.GLU 124.4.84.0.34.0.0 2EFK,ARG_196,12.56,-0.12,0,0.17 3EYE,GLU_97,3.68,0.46,-0.85,-0.43 300P.GLU 104.4.69.0.29.0.-0.1 2CN1,TYR 48,10.17,0,-0.07,0.23 1O3X,LYS_206,10.39,-0.12,0,0.02 2RIK,GLU_161,3.09,0.38,-1.51,-0.27 3EZ7,TYR_41,11.05,0,0.09,0.96 1NJ4,ARG 198,11.81,-0.74,0,0.05 1AIL,ASP_2,3.91,0,0,0.11 3JRT,HIS_42,6.1,-0.44,0,0.04 1CHD.GLU 213.4.56.0.99.-0.85.-0.09 2VGM,LYS_303,10.65,-0.12,0,0.28 1YOY, LYS 125, 10.23, -0.36, 0, 0.09 3CGW,GLU_23,4.9,0.96,-0.35,-0.22 3K1H,GLU_65,4.33,0.33,-0.74,0.24 4DBX,ASP_175,3.15,-0.64,-0.43,0.42 3ULX,ARG_34,12.25,-0.36,0,0.11 3N2T,LYS 255,10.62,-0.32,0,0.43 1QQE,TYR_47,10.93,0,0.2,0.73 2EA9,TYR 108,12.6,0,79,0.8,1.01 3V3T,GLU_82,4.54,0.21,0,-0.16 1JSX,HIS 19,6.22,-0.28,0,0 4EKU,LYS_225,10.32,-0.12,0,-0.06 1YR6,LYS_40,10.57,-0.15,0,0.22 3E0H,ASP_126,4.04,0,-0.05,0.3 3E7P,HIS_236,6.38,-0.35,0,0.23 3BQE,HIS_337,5.16,-1.7,0,0.35 2NSN,TYR_97,10.26,0,0.13,0.12 3UC9,ARG_93,12.88,-0.34,0.03,0.69 1V43,ARG_310,12.22,-0.36,0,0.09 2IF4,ASP_212,4.1,0,0.12,0.18 3O48,GLU 105,4,49,0,22,0,-0,22 3CS1,GLU_138,4.69,0.41,0,-0.21 3RLE,GLU_15,4.74,0.31,0,-0.07 3MTT,ARG_559,12.67,-0.17,0,0.34 3FRR,ARG_164,12.35,-0.29,0,0.14 3ETU,LYS_195,9.61,-0.74,0,-0.15 3NR5,LYS_40,10.46,-0.04,0,0 3K8J,ASP_134,4.12,-0.7,-0.47,1.49 1QZN,ASP_168,3.99,-0.18,0,0.37

3H13,GLU 277,4,73,0.54,-0.35,0.05 2VGM,HIS 325,4.97,-2.48,0.74,0.23 3V3T,HIS_48,5.45,-0.72,0.11,-0.44 1T6L,ASP_106,2.67,-1.59,-0.44,0.92 1ZHV.ARG 39.12.12.-0.42.0.0.04 2AD1,HIS 176,3.64,-3.61,0.82,-0.07 2W1R,LYS 60,11.38,-0.23,0.55,0.55 2AXO,HIS 79,3,44,-3,06,0,0 1059,GLU_99,4.47,2.79,-1.62,-1.2 4AM1,HIS 262,5.37,-1.25,0.0.12 30IP.LYS 222,10,48,-0,17,0,0,15 1RWZ,GLU_159,4.48,0.15,0,-0.16 2G5X,TYR_210,11.37,-0.11,0.11,1.38 1HF8,GLU_65,4.61,0.19,0,-0.08 4DIU,HIS 234,4.49,-1.85,0,-0.16 1AD6,HIS_555,6.23,-0.37,0,0.09 3EJG,LYS_96,10.47,-0.03,0,0 3IBT,GLU_184,5.42,1.67,-0.79,0.03 208P.ASP 28.2.98.-0.85.-0.54.0.57 2NRK,ARG_72,12.5,-0.19,0,0.19 2EFK,GLU_156,4.64,0.23,-0.2,0.11 2FBI,ARG 115,12,38,-0.23,0,0,11 30DJ,ARG_52,12.63,-1.14,0.71,0.56 3ETV,ARG 279,13.22,-1.11,0.84,0.99 3CX2,HIS 210,6.55,-0.24,0,0.3 3F6F,LYS_20,10.5,-0.15,0,0.15 3R87,LYS_43,11.15,-0.27,0.4,0.52 20BI,GLU_87,4.61,0.1,0,0.01 4DBX,ASP 42,4.12,0,-0.03,0.35 3BQW,GLU_167,4.56,0.09,0,-0.03 100L,LYS 100,10,53,-0,3,0,0,33 2YT4,GLU_596,4.86,0.21,0,0.15 3EVZ,GLU 100,4.35,1.09,-1.23,-0.01 1RKA,GLU_203,4.02,0.17,-0.43,-0.23 2G9D,ASP_145,3.69,0,-0.36,0.25 3RFY,ARG_230,12.44,-0.11,0,0.04 3T5B,ASP_157,3.09,-0.83,-0.66,0.79 3GG6,GLU 109,3.94,1.16,-1.08,-0.63 2H2Z,ASP_92,3.25,-0.84,-0.15,0.45 2H85,ARG_90,12.56,-0.77,0.37,0.45 1ZP2,TYR_182,11.1,0,0.16,0.94 3VJ8,ARG 52,12.24,-0.29,0,0.04 1J33,ARG 72,12,39,-0,37,0,0,25 1XIP,ARG_153,12.55,-0.08,0,0.13 2B3M,ASP_139,4.23,0,-0.03,0.47 2BDV,HIS_145,7.08,-0.6,0.85,0.32 2H2Z,HIS 80,6.47,-0.79,0.76,0 3P28,HIS 121,3.8,-2.69,0,-0.01 2GS5,GLU_66,4.14,0.43,-0.79,0 2QEV,GLU_1,3.75,0.4,-0.85,-0.29 1D2K,TYR_342,10.74,-0.44,0,1.18 1T3Y,ASP 97.3.12,-1.6,-0.29,1.22 1RI6,GLU_206,5.28,0.55,0,0.24 1TR9.ARG 313.12.91.-0.65.0.65.0.41 3DHN,GLU_30,4.21,0.3,0,-0.6 4DBX,GLU_26,4.25,0.4,-0.49,-0.17 4H4J.LYS 184.11.49.-0.3.0.85.0.44 1X9G,LYS_53,10.81,-1,0.85,0.45 3BWT,TYR_603,10.39,0,0.21,0.17 3OBS,TYR_42,10.43,0,-0.26,0.69 3BOW.ASP 112,3.42,-0.8,-0.01,0.43 1UAJ,LYS_45,10.46,-0.04,0,0 3UAH, ASP 217, 3, 28, -0, 89, -0, 26, 0, 64 1Q46,ASP_76,3.34,-0.89,-0.01,0.44 1XIP,ASP_15,3.96,0,-0.09,0.25 3V55,ASP 716,3.04,-0.84,-0.31,0.38 3ADO,GLU_205,4.76,0.86,-0.32,-0.28 3KT9,GLU_32,4.7,0.2,0,0 3ETU,GLU_332,3.66,0.46,-0.85,-0.45

2R0S,GLU_309,4.19,0.29,-0.6,0 2R0S,TYR 38,12.77,0.63,0.61,1.52 1X04,ASP_107,4.13,0,0,0.32 3GEC,LYS_485,10.37,-0.17,0,0.04 2ZCX,ARG_62,12.46,-0.09,0,0.05 1YTQ,ARG 159,12.41,-0.09,0,0 1PDB.TYR 182,11.7.0.06.0.04,1.6 1SNT,HIS_300,6.14,-0.52,0,0.15 1YTD,ASP_68,2.66,-0.83,-0.62,0.31 2EHG,LYS_91,10.2,-0.3,0,0 4DIU,CYS_115,12.89,-0.65,0.85,3.68 3G9G,ARG_174,13.36,-0.7,1.12,0.44 1L2F,ARG_117,12.51,-0.49,0.13,0.37 1D2K,LYS_403,10.42,-0.08,0,0 1LN4,GLU_31,4.57,0.07,0,0 100L.GLU 87.5.55.1.27.0.-0.21 1P2F,LYS_88,10.7,-0.22,0,0.41 3GFP,ASP_319,4.05,-0.18,0.09,0.34 1H4U,GLU_521,4.65,0.31,0,-0.16 1WPA,GLU 473,4.15,0.24,-0.59,0 3K8U.TYR 77.10.43.0.0.25.0.19 2I88,LYS_406,11.39,-0.25,0.79,0.34 1C3K,TYR_107,12.05,0.79,0.39,0.86 3H04,ASP 267,4.03,0,-0.12,0.34 3Q1C,ASP_256,3.95,-0.39,-0.21,0.75 307K,GLU_50,4.73,0.25,0,-0.02 2VAN, ARG_328, 12.3, -0.69, 0.09, 0.41 1ZYL,ARG_144,11.45,-3.48,0,2.42 2FC3,GLU 108,4.48,0.41,0,-0.43 4EZB,TYR_279,11.4,0.15,-0.03,1.3 2D59,LYS_88,10.44,-0.08,0,0.02 2Q07,LYS_355,10.47,-0.14,0,0.11 3G9T,LYS 68,9,94,-0.57,0,0.01 10I7,HIS 140,6.17,-0.27,0,-0.06 3OIP,TYR_209,10.7,0,0,0.7 3KV0,GLU_17,3.69,0.21,-0.64,-0.38 3I0C, ARG_279, 13.12, -0.28, 0.45, 0.44 2B78,LYS_308,10.32,-0.2,0,0.02 2FZ4.HIS 203.6.5.-0.37.0.0.37 3EVZ,LYS_231,10.17,-0.36,0,0.03 3G9T,LYS_252,11.08,-0.31,0.47,0.41 2EDM,LYS_145,10.53,-0.35,0.14,0.24 3LJI,LYS 103,10.73,-0.17,0,0.4 3IPZ,GLU_121,4.71,0.21,0,0 1IDK,TYR_343,10.21,0,0,0.21 2EJB,TYR_130,10.61,0,-0.01,0.62 1AT0,GLU_364,3.97,0.32,-0.57,-0.27 2Z84,HIS 35,7.29,-0.31,0.85,0.24 109G,ASP_244,4,0,-0.22,0.42 100X,GLU_93,4.1,0.33,-0.8,0.07 1Z3X,ARG_209,11.85,-0.58,0,-0.07 2VGY,TYR 52,10.31,0,0.05,0.26 2PGX,HIS_176,5.75,-0.64,0,-0.11 1V43,HIS_98,6.63,-0.15,0.28,0 1R5Q,HIS_91,7.61,-0.52,1.17,0.46 20EW,ASP_316,3.95,0,-0.15,0.31 3N0K,ARG_124,13.17,-0.52,0.65,0.54 3T8R,ARG_106,12.29,-0.21,0,0 105J,GLU_91,4.03,0.34,-0.81,0 1JT9,GLU_10,3.98,0.36,-0.33,-0.56 1NAR,TYR_178,10.32,-0.77,-0.55,1.63 1YW5.GLU 23.4.16.0.88.-0.7.-0.53 1DZF,CYS_83,10.62,-0.8,0.43,2 1JSX,GLU_118,4.39,0.7,-0.37,-0.44 3E5T,ARG_198,12.59,-0.23,0,0.31 1QQE,GLU_75,4.79,0.21,0,0.09 3CAX,ASP_279,3.91,0,-0.22,0.33 1BKB.GLU 13.5.11.0.23.0.0.38 2D2S,GLU_626,4.58,0.26,0,-0.19

2CIU.LYS 211,10.39,-0.08,0,-0.03 2PLQ,GLU_173,3.7,0.82,-1.61,-0.01 2E3C,LYS_331,10.01,-0.37,0,-0.13 2ATR,ASP_127,3.93,0,0,0.13 2CN1.LYS 95.9.77.-1.01.0.0.27 1DUP.ASP 61.2.31.-1.5.-0.38.0.39 1X8F,GLU_161,4.39,0.25,0,-0.36 1L3K,GLU_114,4.08,0.34,-0.68,-0.08 3MIX,ASP_551,3.63,-0.99,0.2,0.63 3PP8,ARG_169,12.77,-0.3,0.19,0.39 1LPL,GLU_223,5.04,0.24,0,0.3 1UAJ,GLU_18,4.49,0.35,0,-0.36 2DG7,ASP_169,2.42,-1.8,0,0.41 3UV9.LYS 319,10.24,-0.26,0,0 1DZF.GLU 67.4.48.0.16.0.-0.18 1V43,GLU_134,4.95,0.2,0,0.24 2BAA,HIS_17,8.01,-0.88,1.76,0.62 2ZCX,CYS_116,12.29,0,0.15,3.15 2JHYLYS 113,10,09,-0,55,0,0,14 2FBI,GLU_118,4.68,0.22,0,-0.05 1MML,ASP_209,3.8,0,-0.24,0.24 1YTD, ASP_9, 3.96, -0.01, -0.1, 0.28 2P1W,GLU_215,4.13,0.67,-0.31,-0.74 2WOZ.ASP 294.3.93.0.0.0.13 3MTT,TYR_505,10.44,0,0.33,0.11 3UX2,HIS_112,6.22,-0.43,0.2,-0.05 2CN1,ARG_71,13.11,-0.48,0.61,0.48 2Z61, ASP 64, 3.47, -0.83, -0.51, 1.02 10LR,CYS_206,11.04,-2.83,0.13,4.74 109G,GLU_109,3.43,0.85,-1.17,-0.75 3K8J,ARG_167,12.44,-0.13,0,0.07 1AD6.GLU 465.4.07.0.42.-0.85.0 3ETV,GLU_130,4.09,1.03,-0.85,-0.59 3HQX,CYS_104,12.12,0.42,0.75,1.96 1SI7.LYS 251.9.64.-0.94.0.0.08 3RKV,GLU_232,4.66,0.16,0,0 2PLQ,LYS_181,10.55,-0.6,0,0.65 3E5T,HIS 214,5.63,-0.96,0.0.08 2WOZ,GLU_531,4.97,0.25,0,0.22 3PAC, ASP_146, 3.97, -0.82, 0.09, 0.9 30KY,ARG 261,13,25,-0,45,0,72,0,47 3UC9.HIS 109.5.69.-1.06.0.34.-0.09 3PU6,ASP_78,2.69,-1.41,-0.05,0.35 1YTD, ASP_232, 1.5, -2.42, -0.79, 0.91 2EJB,LYS_172,10.57,-0.19,0,0.25 3DZ1,CYS 163,12.09,-0.1,-0.32,3.51 105T.TYR 420.12.65,-0.91,1.12,2.44 1R6Y,GLU_64,6.55,2.89,-0.84,0 1JKS,GLU_84,1.18,1.18,-3.55,-0.96 3EYE, ARG_139, 12.21, -0.33, 0, 0.04 3UPD,LYS 88,10,48,-0.08,0,0.05 2VAN, ARG_333, 12.66, -2.86, 1.73, 1.31 2H85,GLU_68,5.96,2.85,-0.88,-0.52 1AM2,ARG_181,13.04,-0.36,0.27,0.64 2Q98,TYR 185,12.11,-0.23,0.22,2.13 30IPLYS 50,10.19,-0.29,0,-0.03 2NRK,GLU_17,4.68,0.22,0,-0.04 3FFM,ASP_132,4.12,-0.77,-0.02,1.1 3K8J,GLU_264,4.77,0.31,0,-0.03 3BPP.LYS 195,10.23,-0.43,0,0.16 3NR5,ASP_95,4.02,0,0,0.23 3JRT,ARG_86,12.2,-0.96,0,0.66 2YWX,GLU_41,4.18,0.45,-0.81,0.04 3D9H,GLU 42,3.96,0.41,-0.53,-0.42 10TM,GLU_74,3,0.61,-1.73,-0.38 1SIG,ARG_363,12.38,-0.14,0,0.03 3A7L,GLU_113,4.64,0.12,0,0.03 2E3I,ARG_59,12.56,-0.21,0,0.27 2AHE,CYS_100,9.11,-0.26,0,0.38

2P0L.TYR 210.11.81.0.0.34.1.48 3ZXY,ASP 243,3,23,-1,32,-0,15,0,9 2B61,TYR_80,11.24,-0.02,-0.42,1.69 1EQ6,CYS_195,11.43,0,0.06,2.37 2H30,LYS 111,10,33,-0,17,0,0 3ZTA, ASP_24, 3.51, -0.46, -0.02, 0.19 2FB6,LYS_6,10.93,-1.01,0.85,0.59 1V8E,ARG 183,13.03,-0.8,0.85,0.49 3K8J,LYS_69,10.35,-0.12,0,-0.03 3BCH,TYR_139,10.24,0,0.13,0.11 4HDE,LYS 112,11,41,-0.32,0.85,0.38 2Q99,LYS_113,10.4,-0.1,0,0 1UAJ,CYS_35,11.1,0,-0.03,2.12 1X04,ASP_186,3.94,0,-0.12,0.26 3M70,GLU_259,3.5,0.82,-1.6,-0.23 2D7U,GLU_266,4.62,0.39,-0.17,-0.11 3MIX,TYR_399,12.06,0,0.21,1.86 2FZ4,ARG_104,12.3,-0.2,0,0 3ILC,ARG 6,11.8,-0.7,0,0 20RX.TYR 165.10.13.0.0.0.13 2AZL,ASP_102,4.09,0,0,0.29 4H89,LYS_136,10.36,-0.14,0,0 3CX2,HIS 257,7,37,-0,33,0,85,0,35 4AM1.LYS 33,11.45,-0.23,0.8,0.38 2FC3,ASP_106,3.94,0,-0.08,0.22 3RNV,GLU_449,3.52,0.25,-0.74,-0.49 2QEV,HIS_124,6.17,-0.21,0,-0.12 3MIX,ASP_593,3.77,0,-0.27,0.24 20EW,LYS 11,10,26,-0,24,0,0 3EJG,HIS_9,6.3,-0.38,0,0.18 2B3M,ASP_69,3.09,-0.98,-0.1,0.37 3GW3,GLU_97,4.63,0.18,0,-0.05 1XTD.TYR 29,10.32,0,0,0.32 1KCM,TYR_48,12.68,0.85,0.35,1.47 3G9B,LYS_63,10.57,-0.22,0,0.28 3P51,GLU_143,4.69,0.19,0,0 2E3H,TYR_262,9.99,-1.22,0.36,0.84 3LJI,HIS_77,1.94,-2.18,0,-2.38 1DCF,TYR_133,10.93,0,0.86,0.06 1BKB.GLU 111,3.55,0.3,-0.85,-0.4 2JHY,LYS_186,10.38,-0.06,0,-0.06 2GZQ,LYS_39,9.74,-0.93,0,0.18 4EKU.GLU 34,4,79,0,15,0,0,13 3LQE,GLU_456,3.92,1.91,-2.5,0 1YM5,CYS_173,13.1,0,0.26,3.84 3JV1,HIS_181,6.36,-0.25,0.08,0.03 20GQ,ASP_416,2.17,-2.38,-0.32,1.07 3KEY,GLU_406,4.47,0.22,0,-0.24 3CO1.TYR 32.11.93.-0.1.0.01.2.02 1XIP,GLU_236,4.47,0.3,-0.26,-0.06 2B61,HIS 268,4.32,-2.18,0,0 3H13.TYR 464,10.11.0.-0.27.0.38 1ZKZ,GLU_33,3.39,0.67,-1.59,-0.19 1SI7,LYS_213,10.3,-0.22,0,0.01 2BLL,ARG_418,13.29,-0.38,0.76,0.41 3FK5,ARG_163,12.57,-0.56,0,0.64 109G,ARG 5,13.39,-0.36,0.69,0.57 3SMD,GLU_31,4.56,0.06,0,0 1NRI,ASP_25,3.93,-0.31,-0.01,0.45 2EA9,ARG_26,12.67,-0.66,0.06,0.77 4FZR.ARG 25.12.12.-0.39.0.0.01 10I7,ASP_274,3.04,-0.72,-0.35,0.32 1QYI,LYS_333,10.14,-0.61,0,0.26 1FKM,ASP_438,2.58,-1.74,-0.41,0.93 1SJY,ARG 150,12.84,-0.32,0.31,0.34 3H5T,ARG_174,12.79,-0.21,0,0.5 3IL3,GLU_205,4.83,0.22,0,0.11 1RHS,ARG_44,12.31,-0.25,0,0.06 300P,ARG_2,12.44,-0.06,0,0

2AZP.ARG 5.12.45.-0.47.0.2.0.22 2H14,LYS 291,10,33,-0.22,0,0.05 3BQE,ASP_285,4.01,-0.69,-0.29,1.2 3OAV.ASP 31.3.61,-0.19,-0.25,0.26 1AK1,HIS_70,5.9,-0.87,0,0.27 3NZL,HIS 8,5.81,-0.46,0,-0.22 1P1L,GLU_99,4.93,0.21,0,0.23 1N81.ASP 171.3.95.0.0.0.15 3ONH,GLU_467,4.59,0.19,0,-0.1 1AD6,TYR 403,12,27,0.85,0.52,0.9 1YOY,ASP 115,1.67,-1.83,-0.76,0.46 2H85,GLU_339,3.99,0.35,-0.4,-0.45 200K,TYR_87,10.74,-0.4,0.38,0.76 4DEZ,ASP 120,3.58,-0.67,0.0.44 3O16.TYR 231,10.51,0,0.29,0.22 3M70,LYS_207,10.69,-0.12,0,0.31 2H85,LYS 334,10.67,-0.11,0,0.27 100X,ASP_230,3.34,-1.08,0.21,0.4 3LPZ.LYS 260.10.17.-0.59.0.0.26 2XHC.TYR 113,11,92,-0.57,0.89,1.6 1YTD, ASP_132, 3.58, -0.23, -0.16, 0.18 3P28,HIS 91,6.45,-0.91,0.89,-0.03 3JSN,ARG_99,13.59,-0.3,0.73,0.66 1VSM,LYS 129,10.43,-0.29,0,0.22 3UV9,ARG 325,12,29,-0,21,0,0 30DJ,ARG_129,13.01,-1.27,0.84,0.93 3V55,GLU_696,4.55,0.05,0,0 1PZC,ASP_47,3.74,0,-0.32,0.26 3FTT,HIS 119,6.2,-0.29,0,-0.01 2GEN,HIS_44,6.35,-0.13,0,-0.02 2V4U,HIS 439,6.18,-0.27,0,-0.04 3PU6,ARG_24,13.65,-0.51,0.86,0.81 3EAZ.LYS 76,10.42,-0.12,0,0.04 2D7U,ARG 34,10.98,-2.95,0,1,43 1ILW,ARG_62,12.26,-0.24,0,0 1V43,TYR_70,10.56,0,0.18,0.37 2BDD,GLU_42,4.48,0.36,0,-0.38 2X5Y,GLU 808,5.83,4.38,-2.61,-0.43 2YLF,ARG_81,13.56,-0.38,0.68,0.76 2EHG,ARG_141,12.57,-0.08,0,0.15 1XFK,HIS_185,5.95,-0.68,0.15,-0.02 1SJ8,GLU 759,4.8,0.22,0,0.07 2FL4,TYR 86,11.62,0.85,0.38,0.39 2D0A,LYS_50,11.14,-0.61,0.85,0.4 2IF4,LYS_104,10.35,-0.17,0,0.03 3ASA,CYS_148,12.07,-0.43,0.21,3.29 2Q12,GLU_27,3.26,0.89,-1.68,-0.45 1GOE.ASP 79.4.1.0.0.0.3 2XMZ,GLU_217,4.11,0.31,-0.63,-0.08 2Q13,ARG_275,13.41,-0.34,0.67,0.58 1VSM,ASP_174,3.89,0,-0.23,0.32 4ETX.TYR 204.12.13.0.0.23.1.9 3DZ1,ARG_190,11.8,-1.03,0,0.33 3AU3,ASP_512,3.73,-0.87,-0.06,0.85 2IDC, ASP_52, 3.85, 0, -0.13, 0.18 2FZ4,TYR_179,13.9,0,0.92,2.97 1X91,ASP 109,3,16,-0.85,-0.39,0.6 1QQE,LYS_271,10.5,-0.09,0,0.08 1WYC,HIS_346,6.11,-1.31,0.83,0.09 4FH3,CYS_105,10.6,-0.79,-0.11,2.5 1R3F.GLU 211,3.96,0.3,-0.74,-0.11 30IP,ASP_23,4.43,-0.3,0.03,0.9 3IBT.GLU 207.3.92.0.52.-0.73.-0.38 3EZ7,ARG_96,13.37,-0.4,0.89,0.38 3L3P,ASP_384,4.32,0,-0.19,0.7 10LR.TYR 37,10.28.0,-0.2.0.47 1T07,LYS_64,10.4,-0.1,0,0 2E3C,LYS_336,10.51,-0.16,0,0.17 1YB2,ASP_126,4.07,0,0.11,0.17

1IDK.TYR 34,10.48,0.0.14,0.34 3US6,HIS 79,5.86,-0.27,0,-0.37 2QOP,HIS_15,6.17,-0.36,0.02,0.01 2l6l,GLU_20,3.97,0.54,-1.03,-0.04 2B61,LYS_137,10.13,-0.55,0,0.18 2V4U,LYS 417,10.19,-0.34,0,0.03 3U2R.ARG 68.12.33.-0.22.0.0.05 3FXH,HIS_25,6.02,-0.41,0,-0.07 3BCH,ASP_31,3.88,-0.7,-0.09,0.86 1ZBS,GLU_40,4.86,0.43,-0.4,0.32 1U3Y,GLU 293,3.52,0.43,-0.8,-0.61 3ERF,CYS_206,10.82,0,0.54,1.28 1YM5,ASP_129,3.87,0,-0.25,0.32 1LTU,HIS_126,6.33,-0.33,0,0.16 3I4T,ARG 18,12,49,-0,12,0,0,1 2WB3,LYS_385,10.33,-0.17,0,0 1FHL,TYR_22,13.61,0,0.69,2.93 1U53,ASP_4,3.86,0,-0.04,0.1 1WYC, ASP_72, 3.96, 0, -0.06, 0.23 2EFK,GLU_12,3.66,0.37,-0.65,-0.57 1EV8.ARG 225.12.76.-0.39.0.29.0.36 2A4D,LYS_205,10.45,-0.05,0,0 2OB5,ASP_12,2.84,-0.72,-0.51,0.28 2OZO.ARG 116.12.43.-0.1.0.03.0 2007.HIS 278,4.04,-2.45,0.81,-0.82 3IDW,ARG_21,12.31,-0.27,0,0.08 3I47,TYR_149,10.67,-0.38,-0.04,1.09 4DIU,LYS_156,9.89,-0.53,0,-0.08 2YWX,LYS_75,11.34,-0.28,0.75,0.38 1RI5.LYS 115.10.53.-0.1.0.0.14 2QV2,HIS_185,5.02,-1.53,0.01,0.05 4F8A,TYR_684,10.56,0,0.14,0.42 4DVD.GLU 109.4.59.0.09.0.0 1G5Z.ASP 124.2.88.-0.7.-0.68.0.47 1GXN,ARG_346,12.87,-0.98,0.73,0.62 2C2Y,ARG 202,12,47,-0.35,0,0.32 3PP8,HIS_25,6.21,-0.36,0,0.07 2FD5,LYS_94,10.36,-0.19,0,0.06 1Z9L,LYS 19,10.81,-0.12,0.0.42 1RHS,ASP_219,3.7,0,-0.38,0.28 2XMZ,GLU_126,4.79,0.26,0,0.03 3CBN,ARG_100,12.75,-0.35,0.02,0.58 2FL7,ASP 46,1.6,-2.36,-0.38,0.54 4AE7,LYS_208,11.18,-0.27,0.24,0.7 1WXQ,LYS_158,11.35,-0.38,0.85,0.38 1DUN,GLU_117,4.58,0.08,0,0 20PJ,CYS_47,10.26,-0.23,-0.45,1.95 2X4L.LYS 90,10.25,-0.48,0.0.23 1ZCU,GLU_154,4.01,0.18,-0.32,-0.35 3AU3,CYS_420,10.28,-0.87,0.14,2.01 2NMU,GLU_23,2.99,1.48,-2.87,-0.11 2NRK,ASP_106,3.16,-1.09,0,0.45 2GKG,HIS_92,4.94,-1.44,0,-0.13 1PSW,TYR_114,9.14,-0.8,-0.44,0.39 2BV9,GLU_29,4.69,0.26,0,-0.07 2FD4,LYS_521,10.69,-0.23,0,0.41 1ZBM,LYS_44,12.24,-0.39,1.19,0.94 3BQE,LYS_343,10.29,-0.62,0,0.42 4DBX,HIS 195,5,46,-3,28,0,87,1,38 3MIX,ASP_654,4.07,-0.12,-0.25,0.65 106D,ARG 139,12.58,-0.18,0,0.27 1RI5.GLU 255.4.93.0.27.0.0.16 1TR9,TYR_36,12.32,-0.01,0.27,2.05 4ETX,ASP_378,3.96,-0.18,0.02,0.32 1WNH,ASP_44,3.83,0,-0.26,0.29 4AE7,ASP_112,2.9,-0.8,-0.25,0.16 3IVF,HIS_250,5.32,-1.21,0,0.02 3QAV,GLU_146,5.07,1.92,-1.17,-0.19 4EZB,GLU_236,3.66,1.27,-0.85,-1.25

1JKS,HIS 137,5,44,-3,29,0,87,1,35 3V3T,GLU_244,4.38,0.58,-0.17,-0.53 1DOV,ASP_185,3.34,-0.54,-0.39,0.46 1WRU,ASP_301,2.71,-1.3,-0.23,0.44 1ZBP.GLU 203.4.84.0.19.0.15.-1.39E-17 3HVW,ASP_302,3.79,0,-0.28,0.28 1MN3,ASP_424,2.84,-1.26,0,0.3 3CCY,ASP_119,3,-1,-0.07,0.27 4FD6,LYS_17,10.47,-0.06,0,0.03 3P28.GLU 84.4.28.0.24.-0.6.0.14 3LPZ,ASP_275,4.03,0,-0.13,0.36 2V5B.CYS 40.12.41.0.-0.1.3.51 1NAF,ASP_272,3.66,-0.08,-0.4,0.33 3CJW.TYR 191.10.59.0.0.02.0.57 1KCM,TYR 63,12.04,0.23,0.8,1 1ZKZ,TYR_86,10.14,-0.47,0.3,0.31 2D2S,GLU_553,4.49,0.19,0,-0.19 3CBN,HIS_33,7.05,-0.58,0.85,0.29 30A7.TYR 549.10.13.0.0.06.0.07 1LTU,GLU_85,4.62,0.21,0,-0.08 3H8Y,ARG_34,12.15,-0.31,0,-0.04 3C38,ARG_170,12.65,-1.79,1.19,0.75 3BJV,GLU 24,3.73,0.32,-0.82,-0.28 3LJI.ARG 138,12,24,-0.35,0,0,1 3QAV,LYS_191,10.36,-0.14,0,0 3CRM,LYS_286,10.27,-0.12,0,-0.11 3PBH,LYS_127,10.47,-0.09,0,0.06 2Y2T,GLU 22,4.99,0.5,0,0 1ZBS,LYS_160,10.46,-0.08,0,0.04 2F8H,ARG_293,13.8,-0.71,1.6,0.41 2RIS,GLU_71,4.56,0.25,0,-0.19 3FWU.GLU 35,4.33,0.43,-0.09,-0.49 2BLL.GLU 338.4.49.0.42.-0.22.-0.19 3PP8,ARG_134,12.16,-0.39,0,0.06 3M66,GLU_411,4.7,0.25,0,-0.04 2RGY,TYR_305,10.51,0,0.26,0.25 1XFK,GLU 277,4.6,0.1,0,0 1TD6.HIS 93.5.59.-2.07.0.72.0.43 3L7N,GLU_37,3.79,0.5,-0.85,-0.36 2V4U,CYS_299,11.62,0,0.37,2.24 1W24,TYR 48,11,86,0,0,1,86 1TLV.ARG 107.12.27.-0.32.0.0.09 3PBH,LYS_39,10.37,-0.36,0,0.23 1WRU,GLU_206,4.83,0.33,0,0 3R2E,ASP_19,3.77,-0.17,0,0.13 3RKV,ARG_240,13.42,-0.27,0.69,0.5 3CJW,ASP 240,3.2,-1.49,-0.03,0.91 2VGY,HIS_67,6.23,-0.32,0,0.04 2GKG,ASP_110,4.17,0,0.19,0.18 4ACJ,GLU_801,4.72,0.59,-0.83,0.46 1XIP,ARG_104,11.75,-1.1,0,0.34 1ZCE,GLU_127,4.61,0.23,0,-0.11 2RIK,TYR_75,10.28,0,-0.01,0.29 1TD6,LYS_17,10.39,-0.11,0,0 1P1L,LYS 71,10.31,-0.19,0,0.01 2R51,GLU_242,4.15,0.38,-0.73,0 3EUR,TYR_13,11.26,0,0,1.26 2P5D,LYS 17,10.6,-0.15,0,0.26 3IL3,ARG_144,11.98,-0.88,0,0.35 2P65,GLU 152,3.63,0.59,-1.07,-0.4 4FZR,GLU_68,4.72,0.09,0,0.12 2FXT,LYS_241,10.32,-0.2,0,0.02 3C0C,ASP_316,3.07,-0.8,-0.38,0.45 2CL3,TYR_54,10.25,0,0.08,0.17 3U4K,GLU_154,4.66,0.51,-0.15,-0.2 1KCM,ASP_187,3.94,0,-0.02,0.16 2YYO, ASP_105, 2.44, -1.67, -0.33, 0.63 2AXO,HIS 266,6,72,-0.03,0,25,0 1FQI,LYS_416,10.58,-0.1,0,0.18

3BWT.HIS 576.6.17.-0.26.0.-0.08 3IVF,HIS 255,5.03,-1.11,0,-0.35 2B78,ASP_25,3.37,-0.85,-0.53,0.95 3V55,TYR_669,11.17,-0.47,0.52,1.12 2P0L,ASP 126,3.95,-0.56,-0.25,0.95 3BOE, ASP 298, 3, 31, -0, 75, -0, 09, 0, 35 2RFA,ASP_226,4.2,0.02,0.12,0.27 3GS3.GLU 182.5.33.2.35.-0.78.-0.74 3LJC,GLU_227,4.67,0.17,0,0 3RJX.LYS 250.10.67.-0.12.0.0.3 1R53,ASP 169,3,75,-0.64,0.01,0.59 2IRM,ASP_192,3.18,-1.08,0,0.46 2RIK,HIS_24,6.48,-0.41,0,0.38 1P4X.LYS 2.10.08,-0.29,0,-0.13 109G.ARG 10.12.47.-0.07.0.0.04 3ETV,GLU_344,4.48,0.31,-0.05,-0.27 2Q07,ARG_421,12.52,-0.06,0,0.08 3LJI,TYR_79,11.29,-0.01,0.16,1.14 3RE9,ASP_85,2.7,-1.52,-0.02,0.44 208I,ARG_157,12.24,-1.42,0.59,0.58 3RLE,HIS_200,5.96,-0.51,0,-0.02 2ZQ5,HIS_318,7.19,-0.36,0.39,0.67 2EJX,LYS_3,10.73,-0.15,0,0.38 20KT,TYR 280,12.45,0,0.15,2.3 3IVF,ARG_74,12.61,-0.09,0,0.2 3IPZ,ASP_73,3.91,0,-0.11,0.23 3LH5,ARG_635,12.33,-0.56,0,0.38 1JYH,TYR_94,10.16,-1.02,-0.56,1.74 3DTE,ARG 165,12.6,-0.51,0.04,0.57 2CWY,ARG_53,12.31,-0.38,0,0.19 3LD1,LYS_312,9.94,-0.38,0,-0.19 1XAW,LYS_511,10.17,-0.21,0,-0.12 2F9F.CYS 93.12.97.-0.47.0.6.3.84 4H4J,TYR_112,13.97,0.85,1.09,2.02 1MTZ,CYS_66,13.11,-0.19,0.6,3.71 3KEY,TYR_489,12.29,-0.04,0.49,1.84 3GS3,ASP 77,2.57,-1.68,-0.5,0.95 2FD5,ARG_23,13.27,-0.45,0.62,0.61 2P0L,ARG_237,12.28,-0.6,0,0.38 20EW,LYS_268,10.46,-0.07,0,0.03 1DZF,LYS_94,10.33,-0.17,0,0 3O48,TYR 69,10.48,-0.06,-0.36.0.91 2Z0M,ASP_281,3.83,0,-0.24,0.27 1TLV,LYS_244,10.47,-0.38,0.09,0.25 3GYW,LYS_59,10.52,-0.14,0,0.16 3IVF.GLU 384,4.92,0.42,0.0 2IOT.ARG 54,10.26,-2.44,0.0.2 3G9G,TYR_119,9.98,-0.22,-0.31,0.5 20DJ.CYS 221,12,4,-0.04,0.29,3,15 2H2Z,ASP_155,3.26,-0.43,-0.34,0.23 2IRM,HIS 68,4.51,-2.34,0,0.35 1M5I,LYS_212,10.58,-0.19,0,0.27 3IU5,ARG_148,12.03,-0.7,0,0.23 1MHN,GLU_135,4.79,0.24,0,0.05 1DVO,LYS_35,10.47,-0.03,0,0 2V1L,GLU_121,4.66,0.23,0,-0.07 2Q5X,ASP_870,2.86,-1.09,-0.77,0.93 1JB3.GLU 24.3.86.0.27.-0.58.-0.32 1ANU,ASP_93,2.86,-1.29,-0.15,0.5 2E3S,ASP_496,3.29,-0.82,0,0.31 3CJW.CYS 314.12.64.0.0.24.3.4 2QRX,ARG_183,12.31,-0.19,0,0 4AM1,GLU_341,4.8,1.61,-0.81,-0.5 2Z0M,LYS_200,11.54,-0.32,0.59,0.77 1YTD,LYS 320,10.96,-0.79,0.74,0.52 2Q07,LYS_509,10.06,-0.3,0,-0.14 2Z0M,LYS_205,10.45,-0.12,0,0.08 3L7N,LYS_82,10.15,-0.21,0,-0.14 1QYI,HIS_365,5.75,-0.67,0.02,-0.1

1JSX,LYS_10,10.44,-0.34,0,0.28 2P4D.TYR 142,11.96,-0.09,0.24,1.81 3ASA,ARG_3,12.34,-0.16,0,0 2NRR/HIS 420,5.62,-0.37,0,-0.49 3RFY,ASP 276,4.06,-1.56,0.11,1.71 2GEN.ARG 34.13.7.-0.34.0.86.0.69 1T95.GLU 39.4.82.1.35.-0.26.-0.77 1R3F,TYR_76,11.23,-0.21,-1.04,2.47 3L3P,TYR_487,10.39,0,0.04,0.35 1SNT,ASP_254,3.07,-0.79,-0.36,0.42 1F2V,ASP_151,2.26,-1.62,-0.38,0.46 3TIR,GLU_15,4.75,0.29,0,-0.04 3RLE,ASP_169,3.69,-0.38,0,0.28 1XFK.TYR 282.11.99.0.0.04.1.95 2V1L,GLU_75,4.81,0.83,-0.63,0.1 2BV9,TYR_276,12.9,-0.85,-0.02,3.77 3BWT.HIS 876.5.93.-0.47.0.-0.1 2NRR,ARG_415,12.21,-0.3,0,0.02 1PBV.LYS 159,10.42,-0.43,0.0.34 20EW,ASP_226,4.57,0,-0.08,0.86 2RIS,ASP_92,3.61,-1.65,-0.38,1.84 3UV9,GLU_449,4.04,0.31,-0.85,0.06 4H86,HIS_-3,6.43,-0.21,0.14,0 3JZ9,GLU 361,3.92,0.48,-0.85,-0.21 4EZB.TYR -4.10.17.0.0.06.0.12 1ZP2,ARG_47,12.46,-0.06,0,0.03 3H13,TYR_449,10.8,0,0.26,0.54 4ANN,TYR_154,13.3,-0.19,0.11,3.38 1T95.GLU 149.3.98.0.42.-0.76.-0.17 3GS3,CYS_94,12.23,0,0.06,3.18 3ZXY,CYS 140,11,99,-0.04,0.05,2.98 3AUF,GLU_146,4.71,0.23,0,-0.02 3ETV.LYS 101,10.35,-0.09,0,-0.05 1RZ2.LYS 212,9.94,-0.53,0,-0.02 3HNX,ARG_96,12.24,-0.32,0,0.06 2IXM,LYS_76,10.52,-0.28,0,0.29 1P2F,HIS_45,5.61,-0.57,0,-0.32 4ETX,GLU 290,4.79,0.29,0,0 2B3M,GLU_38,4.61,0.2,0,-0.08 2E3H,ARG_217,13.31,-0.29,0.84,0.26 1QQE,GLU_82,3.42,0.95,-1.2,-0.82 3LQE,TYR 477,12.41,-0.77,0.19,2.99 3T5B,ARG 17,12.4,-0.13,0.0.03 3JRT,LYS_34,10.72,-0.33,0.01,0.55 1MML,ARG_44,13.03,-0.42,0.3,0.65 2QDJ,ASP_145,3.45,-0.74,0,0.39 3EIZ,ASP_133,3.96,0,-0.13,0.28 2FC3.LYS 73.10.56.-0.3.0.0.36 4ANN,GLU_177,4.6,0.21,0,-0.11 3PP8,ASP_287,2.91,-0.84,-0.38,0.33 2PIM,GLU_119,4.61,0.45,0,-0.34 2PPN, ARG 18, 12, 48, -0, 22, 0, 0, 19 1YOY,TYR_160,10.94,-0.39,0.15,1.18 3F6F,LYS 121,10.31,-0.19,0.0 3DHN,CYS_65,11.46,0,0.1,2.36 1AD6,ASP_421,2.94,-0.82,-0.44,0.41 3V46,ASP 297,3.86,-0.97,-0.17,1.2 1AT0, ARG_366, 13.41, -0.35, 0.57, 0.69 4FZR,GLU_30,4.47,0.5,0,-0.52 1RHS,GLU_277,5.25,2.14,-1.36,-0.04 2X4G,ARG 166,12,36,-1,59,0,46,0,99 1PSW,ARG_80,12.5,-0.07,0,0.07 3EJC.TYR 8.10.19.0.0.0.19 2R51,GLU_11,5.07,0.24,0.1,0.22 3LMO,GLU_14,4.53,0.36,-0.37,0.04 4FD6,ARG_178,12.39,-0.11,0,0 3F1X,ARG_250,12.38,-0.12,0,0 1N81,LYS_112,10.26,-0.29,0,0.04 1V6T,LYS_26,10.69,-0.29,0,0.47

3ANJ,ASP 65,3.04,-1.14,-0.08,0.46 2CI3,TYR 208,12.47,-0.09,0.4,2.16 2BV9,ASP_174,3.17,-0.8,-0.26,0.44 3SMD,CYS_107,11.82,0,0.08,2.74 3M66,TYR_371,10.18,0,0.03,0.15 2C2Y,ARG 31,12.17,-0.33,0,0 2H85,ASP_282,2.69,-2.08,-0.45,1.42 3BWT,ASP_755,4.02,-1.46,-0.02,1.7 2FBI,GLU_34,3.09,0.77,-1.3,-0.87 1L2F,ASP_277,4.01,0,-0.08,0.29 3H9W,TYR 38,10.28,0,-0.11,0.39 3CJW,ASP_324,2.7,-1.1,-0.36,0.36 4AM1,LYS_28,10.27,-0.57,0,0.34 3V1Q,ASP_508,2.18,-1.64,-0.78,0.8 4GCO.TYR 180.11.23.0.-1.39E-17.1.22 1YR6.GLU 239,4.64,0.31,0,-0.16 3HVM,GLU_180,4.65,0.87,0,-0.73 106D,ASP_55,3.29,-0.85,-0.63,0.97 1DZF,ARG_207,12.44,-0.06,0,0 1SNT,HIS 163,6.42,-2.87,0.88,1.91 3U2R,ASP_134,2.4,-1.17,-0.8,0.58 3N0K,GLU_50,4.74,0.23,0,0.01 2Z84,LYS_13,10.4,-0.28,0,0.18 3DSH,GLU_277,4.75,0.16,0,0.09 1YR6,TYR 241,12.88,-0.81,0.45,3.25 3KEY,TYR_493,10.59,0,0.09,0.5 208PLYS 138,11.19,-0.94,0.85,0.77 2IQT,ARG_195,12.92,-0.36,0.2,0.58 3CGW,TYR_74,10.41,0,0.07,0.33 1MN3.ASP 411.3.9.0.-0.09.0.19 3PZ9,LYS_162,12.24,-0.93,1.7,0.98 1DUP,GLU_134,4.5,0.13,-0.13,0 3RNV,LYS 366,10,39,-0,22,0,0,12 4DBX,HIS_251,5.6,-0.56,0,-0.34 2GS5,ASP_154,4.07,-0.69,0.25,0.7 3T57,LYS_276,11,-0.71,0.55,0.66 2ZQ5,LYS_279,10.35,-0.26,0,0.11 3G9T,ARG_292,12.04,-0.62,0,0.16 2CW4,GLU_61,3.87,0.49,-0.61,-0.5 3VHJ,LYS_120,10.35,-0.28,0,0.13 3BWT,LYS_850,10.98,-0.25,0.34,0.38 1R3F,GLU_224,4.8,0.15,0,0.15 3016,GLU 142,4.5,0.19,-0.25,0.06 3GOZ,ASP_149,3.89,-0.64,-0.05,0.77 3E7P,ARG_159,11.57,-1.11,0,0.17 3GA2,LYS_149,10.54,-0.16,0,0.2 2P52,LYS_162,9.85,-0.45,0,-0.2 1SNT.ARG 83,12.92,-0.39,0.32,0.49 3U2R,GLU_138,3.18,0.39,-1.25,-0.46 4EZB,GLU_50,4.5,0.19,0,-0.19 1P6F,TYR_37,11.79,-0.58,0.24,2.13 2E3I,GLU 62,2.96,0.56,-1.32,-0.78 1P2F,ASP_177,3.93,0,-0.03,0.16 1WXQ,ARG_377,12.23,-0.44,0,0.17 3M7G,GLU_213,4.35,0.26,-0.23,-0.18 3IU5,ARG_66,13.24,-0.33,0.66,0.4 2WZ9,LYS_96,10.23,-0.28,0,0.01 3FNI,CYS_57,11.7,0,0.05,2.65 2H2Z,HIS_64,6.27,-0.22,0,-0.01 1UW7,LYS_81,10.47,-0.03,0,0 4FLE,GLU_168,3.53,0.62,-1.49,-0.1 2WOZ,HIS 440,3,33,-3,11,0.02,-0.09 3JZN,CYS_324,9.52,-1.42,0.34,1.59 3LPZ,ASP_116,1.96,-1.35,-1.09,0.59 3CS1,GLU_160,4.08,0.33,-0.37,-0.38 3BB7.ARG 267.12.71.-3.55.1.18.2.59 1YTD,ASP_302,4.02,0,-0.06,0.28 20HT.GLU 54.4.36.0.17.-0.31.0 1GPP,TYR_154,10.26,0,-0.15,0.42

2I88,HIS 440,6.38,-0.28,0,0.16 1SNT,LYS_370,10.62,-0.19,0,0.31 1U3Y,GLU_341,4.64,0.16,0,-0.03 1J33,ARG_199,12.47,-0.24,0,0.21 3DZ1.LYS 70.10.24.-0.26.0.0 3L7N,LYS 79,10,49,-0,31,0,0,31 3OIP,ASP_102,3.44,-0.64,-0.05,0.33 2OJQ,ASP_591,4.09,0,0,0.29 2IRM,ASP_36,3.9,0,-0.1,0.2 3BZT.LYS 321.11.2.-0.5.0.7.0.49 2IN0, ARG_43, 13.28, -0.41, 0.74, 0.46 3EVN,ASP_79,4.18,0,-0.53,0.9 3CAN,LYS_116,11.69,-0.33,0.85,0.67 3KB5.LYS 317.10.43.-0.07.0.0 1Y2O.GLU 69.4.7.0.29.0.-0.09 1EDG,ARG_172,12.64,-2.09,0.63,1.6 2Q13,ARG_154,12.45,-0.05,0,0 2F8H,ARG_244,13.32,-0.36,0.73,0.45 3GEC.TYR 335.10.-0.09.-0.33.0.43 1I60,LYS_265,10.06,-0.48,0,0.04 2B0J,ASP_56,3.41,-0.36,-0.27,0.24 2Z61,LYS_59,11.01,-0.46,0.24,0.74 105T,ARG_388,12.28,-0.4,0,0.18 3CZC,LYS 3,10.87,-0.18,0,0.56 2QVT,ASP_140,4.18,0,-0.05,0.42 3V55,LYS_702,10.96,-0.28,0,0.74 2O4D,ARG_41,12.42,-1.5,0.86,0.56 2NYC, ARG 264, 13.02, -0.84, 0.63, 0.73 2R0S,GLU_305,4.38,0.27,-0.06,-0.33 2P4D,LYS_51,10.48,-0.23,0,0.21 3JRT,HIS_105,5.61,-0.89,0,0 3LJN,LYS 66,11.39,-0.27,0.57,0.58 1LZL.GLU 10.4.25.0.35,-0.82.0.22 1VJG,GLU_75,4.47,0.14,0,-0.17 3FS3,ASP_80,3.74,0,-0.43,0.37 3KEY,TYR_337,10.89,0,-0.03,0.92 2B0A,LYS 67,9.74,-1.09,0,0.32 4DBX,ASP_174,2.91,-0.85,-0.48,0.44 1DTO,TYR_87,10.13,-0.75,0.14,0.75 4D8L,TYR_239,11.82,0.65,0.08,1.09 2ZTY,ARG 13,12.27,-0.25,0,0.02 2ZCX.ARG 128.12.77.-0.17.0.44.0 4ACJ,TYR_769,10.44,0,0.03,0.41 2IQT,ARG_153,12.71,-0.21,0,0.42 3C2E,LYS_292,10.36,-0.37,0,0.24 1UCH,CYS_95,11.29,-0.83,0.19,2.92 2D7U.HIS 331.5.97.-0.83.0.0.31 1GQE,ARG_60,12.33,-0.38,0,0.21 2FL4,HIS_145,6.52,-0.35,0,0.36 1RSS,ASP_140,2.01,-1.49,-0.79,0.49 3CNU,LYS 109,10,27,-0,14,0,-0.09 3RLE,ASP_148,2.31,-2.26,0,0.78 3O16, ASP_94, 3.04, -1.36, -0.35, 0.95 3IU5,TYR_60,10.04,-0.08,-0.28,0.41 2WB8,HIS 746,4.2,-1.96,0.13,-0.46 1R3F.TYR 199,10.6.0.-0.25.0.85 3M70,LYS_117,10.91,-0.22,0.21,0.42 3GYW,TYR 53,10.74,0.1,0.44,0.2 2YWJ,ARG_106,12.35,-0.19,0,0.04 3FK5,GLU 172,4.58,0.13,0,-0.05 1X8F,ARG 168,11.4,-1.94,0,0.84 3CSR,LYS_120,10.1,-0.37,0,-0.03 1SI7,HIS_82,6.19,-0.18,0,-0.12 3CCY,LYS_122,10.3,-0.12,0,-0.08 2FBQ,LYS_21,10.29,-0.3,0,0.1 3R2E,GLU_8,4.61,0.16,0,-0.05 2R0S, ASP_299, 2.46, -1.39, -0.38, 0.43 2PGX,ASP_201,3.28,-0.82,-0.13,0.43 3SMD,LYS_132,10.48,-0.53,0.13,0.38

4FD6.LYS 215.10.08.-0.46.0.0.03 3IVF,ASP_110,3.7,-0.26,-0.26,0.42 2P4D,LYS_128,10.25,-0.37,0,0.12 1TUL,LYS_94,10.73,-0.1,0,0.33 1RI5,ARG 64,12,25,-0,13,0,-0,12 3OBS,CYS_73,10.4,-0.85,-0.1,2.36 3LOD,HIS_116,6.31,-0.19,0,0 2NYC,ASP_197,3.95,0,-0.05,0.2 1YTQ,ARG_190,13.43,-0.44,0.72,0.66 1ZP2,CYS_82,12.62,0,0,3.62 2EA9,GLU_74,4.24,0.28,-0.54,0 2VAN,GLU_154,5.22,1.07,0,-0.35 1X04,GLU_166,3.59,0.28,-0.73,-0.46 2013.LYS 119.10.67,-0.3.0.0.47 1X04.LYS 205.10.57.-0.16.0.0.23 3ZTA,GLU_143,4.69,0.19,0,0 1RI5,ARG 183,11.79,-1.87,0.57,0.58 3SMD,GLU_69,4.3,0.76,-0.77,-0.18 3Q1C,TYR 67,12.52,0,0.12,2.4 2Z61,ASP_112,3.88,-0.14,0.01,0.22 1XKR,GLU_35,3.47,0.24,-0.82,-0.44 3IL3,GLU_41,4.92,0.56,0,-0.13 2X4G,GLU_230,4.24,1.04,-0.71,-0.59 4EZB.HIS 87,6.51,-0.47,0.33,0.16 1JYH,ASP_56,3.94,0,0,0.14 2W2S,GLU_48,4.59,0.09,0,0 1I60,LYS_138,9.82,-0.5,0,-0.18 3RE9,GLU 199,4.47,0.13,0,-0.16 3GS9,ASP_4,3.88,0,-0.18,0.26 3RLN,LYS_621,9.78,-0.85,0,0.13 1PSW,CYS_186,12.63,-0.2,0.52,3.32 3BB7,GLU_72,4.69,0.19,0,0 4AF2,GLU 156,4.06,0.49,-0.79,-0.15 1RAJ,HIS_320,6.68,-0.31,0,0.5 3CXS,TYR_84,10.48,0,0.09,0.38 3PP8,ARG_266,12.25,-0.25,0,0 1EYH,HIS 15,6.47,-0.05,0,0.02 3B7X,GLU_45,4.83,0.3,0,0.03 20KT,GLU_174,3.85,1.51,-0.85,-1.3 3HYQ,GLU_87,5.91,3.03,-0.79,-0.82 2FG1,TYR_5,11.68,0.12,0.28,1.28 20PJ,HIS 274,6.35,-0.15,0,0 1NWA, ARG 147, 13, 17, -0, 5, 0, 47, 0, 7 3JSN,GLU_51,3.95,0.47,-0.74,-0.28 1KN3,ARG_26,12.6,-0.38,0,0.48 2R0S,ASP_67,3.26,-0.85,-0.43,0.74 3RRQ,TYR_121,12.19,-0.01,-0.31,2.51 1WNH,GLU_191,4.27,0.25,-0.48,0 2R0S.LYS 57.10.46.-0.11.0.0.07 2X4L,GLU_277,4.22,0.26,-0.68,0.14 1H4U,ASP_511,2.52,-1.43,-0.45,0.59 2PP6.GLU 73.4.61.0.28.0.-0.17 2B3M,LYS_27,9.77,-0.68,0,-0.04 3DZ1,HIS_168,4.22,-2.38,0.11,-0.01 2G9D,TYR_260,11.61,0,0.02,1.59 3EUR,GLU_89,3.87,0.44,-0.72,-0.34 2YT4,GLU_534,4.6,0.1,0,0 2Q98,HIS_180,5.95,-0.59,0,0.04 10IS,TYR_170,9.82,-1.55,0.45,0.92 3AU3,CYS_607,11.18,-0.12,-0.07,2.36 2AZL,ASP 62,4,16,-0,17,-0,03,0,55 2W2S,ARG_87,12.42,-0.45,0,0.37 3GW3,GLU_167,4.57,1.47,-1.13,-0.26 3BZT,CYS_269,12.34,-0.42,0.13,3.63 1XEU,GLU_221,4.54,0.17,0,-0.13 3DZ1,LYS_73,10.39,-0.08,0,-0.03 1SIG,HIS_180,6.32,-1.54,0.85,0.51 2O4D,GLU_66,3.16,0.39,-1.35,-0.38 1ZYL,ARG_305,12.45,-0.3,0,0.24

2CXA.LYS 83,10.4,-0.1.0.0 3ANJ.GLU 83,4.72,2.89,-1.98,-0.7 208P,LYS_61,10.37,-0.15,0,0.02 2GZQ,CYS_187,11.81,0,-0.06,2.86 2YX0.ARG 265.12.46.-0.46.0.0.41 2CXA.GLU 17.3.86.0.17.-0.69.-0.12 2D0A,HIS_78,6.49,-0.31,0,0.3 3HNX,HIS_0,6.73,-0.4,0.82,-0.19 3S0A,GLU_4,3.77,0.32,-0.85,-0.2 2IXM.TYR 199,12.32.0.0.05,2.27 20V2.TYR 64.10.11.0.0.06.0.05 3PZ9,TYR_366,10.55,0,-0.06,0.61 3EOD.HIS 72.6.31.-0.3.0.0.11 3F1X,ASP 32,3,93,0,0,03,0,1 2D7U,GLU_216,5.54,0.98,0,0.06 2B6P,ASP 150,1.58,-2.68,-0.95,1.41 2BQQ,ASP_134,5.13,0,0.34,1 1UAJ,LYS_206,10.79,-0.24,0,0.53 2F9F,LYS_130,10.44,-0.11,0,0.05 1DUP,LYS_8,10.33,-0.17,0,0 3P2F,TYR_22,12.17,-0.89,0.74,2.33 3CGW.GLU 242.4.72.0.26.0.-0.04 1FO9,ARG_179,12.36,-0.19,0,0.05 1XFK,ARG 24,11.9,-0.6,0,0 3IO0.HIS 156.4.35.-2.38.0.0.23 3LQE,ASP_313,2.4,-1.82,-0.01,0.43 1CHD,LYS_340,10.36,-0.35,0,0.22 2Q13,GLU_14,3.89,0.22,-0.85,0.02 1PV5,GLU 21,3.74,0.24,-0.61,-0.38 1YR6,ARG_117,13.3,-0.27,0.69,0.37 4DBX,GLU_129,4.29,0.6,-0.43,-0.38 1AT0,GLU_277,4.01,0.26,-0.42,-0.32 3RLE.GLU 78,4.64,0.21,0,-0.07 3G9G,ASP 178,3.05,-1.12,-0.44,0.81 2Q34,HIS_220,6.41,-0.15,0,0.07 2E3C,GLU_337,4.86,0.92,-0.02,-0.55 2ILR,LYS_491,10.32,-0.19,0,0.01 1IAP,GLU 132,4.56,0.2,0,-0.13 2CL3,TYR_24,10.03,0,0,0.03 3M66,GLU_296,4.81,0.31,0,0 2A6B,GLU_161,4.5,0,0,0 1ILW,TYR 149,11.91,0.85,0.56,0.49 3I4T.GLU 201.3.46.1.37.-2.29.-0.12 2CWC,TYR_220,12.2,0.85,0.41,0.94 2HRZ,HIS_227,4.27,-3.03,0.8,0 105J,GLU_98,4.64,0.24,0,-0.11 3EVZ,GLU_115,4.67,0.22,-0.09,0.04 1RHS,GLU_172,4.53,0.21,0,-0.18 2CXA,LYS_183,10.34,-0.16,0,0 10LR,HIS_188,4.73,-1.3,0,-0.48 1R9W,HIS_306,6.22,-0.28,0,0 2E3I,LYS 123,10.28,-0.16,0,-0.06 4FCU,ASP_171,3.04,-1.02,0,0.26 3EVZ.LYS 229,10.57,-0.33,0,0,4 1R3D,HIS_135,5.1,-1.2,0,-0.21 1ZBP,ARG_222,11.9,-0.63,0,0.03 20K1.ASP 457.3.2.-0.79.-0.59.0.77 3OKQ,HIS_630,6.18,-0.35,0,0.03 1R9W,LYS_299,10.31,-0.25,0,0.06 1FO9,ARG_387,11.64,-1.03,0,0.17 3H8Y,ARG 38,12,34,-0.37,0.0.21 3I4T,LYS_51,10.35,-0.36,0,0.22 2XMZ.GLU 8.4.49.0.35.0.-0.37 1JT9,ASP_113,3.22,-0.73,-0.18,0.32 3OBS,LYS_14,10.48,-0.09,0,0.07 3C6B,TYR 38,10,79,0,-0,04,0,83 2C2Y,ASP_196,3.75,-0.15,-0.2,0.29 3RFY,ASP_186,3.56,-0.2,-0.4,0.36 2YX0,ASP_220,2.65,-1.23,-0.49,0.58

4ACJ.GLU 714.4.5.0.0.0 3IU5.GLU 86.4.86.0.15.0.0.21 2IQT,LYS_145,10.57,-0.33,0,0.39 3AUF,ASP_201,4.05,0,0.15,0.1 3V55,GLU_568,4.54,0.1,0,-0.06 2Z61,ASP 114,2.64,-1.58,-0.65,1.06 3LH5,ARG 645,10.06,-2,45,0,0.01 4E8B,ARG_30,13.35,-0.51,0.95,0.41 1SI7,ASP_100,3.99,-0.16,0,0.34 3A7L,HIS_13,5.34,-1.23,0,0.08 2CBE,LYS 225,10.61,-0.26,0,0.36 4F8A,ASP_675,3.57,0,-0.5,0.26 1PV5,GLU_55,4.78,0.28,0,-0.01 109G,ARG_74,11.59,-0.94,0,0.03 20KT.GLU 134,4.17,0.27,-0.28,-0.31 2OK1.LYS 551.10.32.-0.2.0.0.03 2OB5,TYR_110,11.21,0,0,1.21 2H85,GLU_326,4.08,0.28,-0.31,-0.38 3MTT,HIS_450,5.12,-1.08,0,-0.29 2C2Y,HIS 245,6.41,-0.43,0,0.35 4GCO,ARG_205,12.49,-0.29,0,0.28 1ES9,HIS_195,6.7,-1.06,0.85,0.41 1KCM,HIS_226,2.41,-3.14,0,-0.95 1XTZ.ARG 83.12.28.-0.22.0.0 3LOD,CYS 62,12,05,0,-0,07,3,12 3ASA,TYR_71,10.06,0,-0.01,0.07 2IF4.ASP 247.4.0.0.0.2 1TUL,LYS_36,10.6,-0.06,0,0.16 3CNU,GLU 44,4.83,0.52,0.03,-0.22 2ZTY,TYR_31,10.77,0,0.03,0.74 20EW,TYR_29,10.5,-0.54,0.39,0.65 1C3K,ASP_66,3.14,-0.68,-0.16,0.19 2W2S,LYS 60,10.57,-0.26,0,0.33 3PP8.LYS 32.11.06.-0.19.0.36.0.38 1NFN,ARG_119,12.01,-0.52,0,0.02 2EJX,ASP_100,3.2,-0.83,-0.21,0.43 3VJ8,ARG_148,12.44,-0.37,0,0.31 2BLL,CYS_420,12.53,-0.05,-0.05,3.63 3GYW,ASP_275,4.17,0,0.01,0.36 2CXC,LYS_59,10.43,-0.08,0,0.01 1RKA,ARG_131,12.06,-0.77,0,0.33 2BQQ,ARG_102,12.37,-0.38,0,0.25 3BCY,HIS 108,6.48,-0.26,0,0.25 2AXO,LYS_196,11.39,-0.26,0.75,0.39 2QOP,GLU_64,4.73,0.22,0,0.01 3H5T,GLU_257,4.05,0.32,-0.44,-0.34 3GYW,TYR_79,11.57,0,0.06,1.49 3GW3.CYS 66.10.13.-0.8.-0.02.1.96 1GPP,ARG_94,13.3,-0.27,0.65,0.42 1N81,LYS_147,10.48,-0.06,0,0.04 3OKQ, ASP_658, 4.05, 0, 0, 0.25 3HVM,HIS 130,6.03,-0.68,0,0.22 2CXC,ASP_112,3.89,0,-0.04,0.13 3CAX,LYS_206,9.65,-0.62,0,-0.23 2QDJ,ARG_320,12.85,-0.33,0.26,0.43 3RFF,ARG_155,12.43,-0.41,0,0.34 4ESS,GLU_141,3.77,0.41,-0.64,-0.49 2V4U,ARG_479,12.3,-0.2,0,0 3P28.HIS 188.6.22.-0.23.0.-0.05 20PJ,ARG_288,12.82,-0.22,0,0.54 2FG1,GLU 48,3.84,0.26,-0.84,-0.1 2BDD,LYS 79,10.6,-0.12,0,0.22 1YLN,CYS_56,11.11,0,-0.02,2.14 3V55,GLU_437,3.81,0.23,-0.85,-0.06 2CIU,ARG_152,12.03,-0.47,0,0 2EDM,ASP_196,3.66,-0.53,0,0.39 2P4D,GLU_131,4.58,0.08,0,0 1F2V.ARG 29.11.79.-0.83.0.0.12 1J33,ARG_207,12.41,-0.19,0,0.1

3ASA,ASP 341,3.97,0,-0.12,0.29 2HP7,ARG_94,13.26,-0.14,0.62,0.29 3M3P,ASP_40,3.17,-0.85,-0.21,0.43 2J8A,LYS_273,10.34,-0.24,0,0.08 1YR6.CYS 244.10.95.0.84.0.4.0.71 4FCU,ARG_170,12.45,-0.15,0,0.09 3AU3,GLU_422,4.66,0.16,0,0 1HUF,ASP_22,3.45,-0.54,-0.24,0.44 3IL3,TYR_87,10.04,0,0,0.04 3COU.HIS 109.3.59.-2.46.0.-0.45 1OXZ,TYR_253,12.04,0.65,0.38,1.01 1J33,GLU_196,4.28,0.1,0,-0.32 1FO9,ARG_117,12.84,-0.23,0,0.57 1WXO.LYS 114.10.52.-0.25.0.0.26 1R53.GLU 64.4.67.0.23.0.-0.06 1KCM,ARG_245,12.69,-0.32,0.16,0.36 1PVT,HIS_92,6.67,-0.9,0.63,0.45 3D9H,HIS_69,5.78,-0.42,0,-0.31 4H89.HIS 155.5.68.-0.66.0.-0.15 1TR9,CYS_267,12.53,0,0.51,3.02 1XIP,LYS_195,11.2,-0.42,0.74,0.38 20KT,LYS_261,11.43,-0.37,0.85,0.44 1W7B,LYS 310,11.31,-0.65,0.85,0.6 2EHG.GLU 133.4.55.0.34.0.-0.3 4DEZ,GLU_85,4.6,0.14,0,-0.04 1YTD, ASP_70, 3.48, -0.71, -0.67, 1.07 1QQE,GLU_128,4.27,1.87,-1.43,-0.67 1AD6,ARG 467,13.98,-0.32,1.42,0.38 3CX2,LYS_244,10.42,-0.08,0,0 3RLE,GLU_110,4.56,0.25,0,-0.2 3ADO,ARG_314,11.75,-0.84,0,0.09 3CAX.GLU 268.4.84.0.3.0.0.04 3G9G,GLU 20.3.64.0.37,-0.85,-0.38 3O16,LYS_223,10.48,-0.13,0,0.12 3FRR,CYS_125,10.35,-0.4,-0.15,1.91 1D2K,LYS_358,11.41,-0.28,0.68,0.51 1H09,ASP 234,3.25,-1.61,-0.13,1.18 20PJ.CYS 54.12.84.0.0.22.3.62 3K1H,ASP_68,2.97,-1.19,-0.03,0.39 1RWZ,ARG_26,12.23,-0.77,0.14,0.36 1FHL.TYR 57,11.57,-0.82,-0.19,2.57 3IDW,LYS 2,10,49,-0.01,0,0 1WRU,ARG_265,13.39,-1.41,1.42,0.88 3MEW,GLU_231,4.54,0.12,0,-0.08 3IVF,LYS_274,10.44,-0.06,0,0 3ERF,ARG_219,13.01,-1.45,0.88,1.07 3V46,LYS 368,10,44,-0.09,0,0.03 1NRI,CYS_254,8.69,-0.68,0,0.37 3G9T,ASP_182,3.89,0,-0.08,0.17 3LOD,TYR 124,12,49,0,0,2,49 3B4D,ARG 172,13,21,-0.34,0.68,0.37 2VGM,LYS_293,10.47,-0.24,0,0.22 3RVC,LYS_175,10.66,-0.34,0,0.49 2Q98,ARG_16,12.5,-0.2,0,0.2 3ULX,TYR 137,12.96,0.05,0.23,2.68 3RE9,GLU_243,4.76,0.24,-0.01,0.03 1X8F,GLU_278,4.56,0.06,0,0 2FZ4,GLU 163,3.42,1.19,-1.46,-0.81 3H13,TYR_360,13.1,-0.82,1.09,2.83 1GQE,GLU 94,4.58,0.08,0,0 1SIG,GLU 124,5.92,1.99,-0.22,-0.36 2Z61,ASP_141,3.04,-0.85,-0.41,0.49 3L3P,GLU_476,4.1,0.77,-0.55,-0.62 1G5Z,GLU 132,4.55,0.24,0,-0.18 2OJQ,ASP_376,4.09,0,-0.05,0.34 1LN4,HIS_44,5.48,-0.59,0,-0.43 1WLY,GLU_73,3.92,0.51,-0.62,-0.46 2V1L,LYS_7,10.35,-0.1,0,-0.05 1WP5,LYS_50,10.26,-0.46,0,0.22

1TXJ.ASP 28.3.8.0.-0.15.0.16 1XWM.TYR 137.12.94.0.0.26.2.68 2R51,TYR_77,12.87,0.16,0.49,2.23 3RFY,LYS_248,10.58,-0.37,0,0.45 3KEY,ARG 454,12,41,-0.77,0.0.68 3PU6,ARG 80,12,42,-0.08,0,0 3G9G,ARG_205,13.1,-0.57,0.49,0.68 3H5T,ASP_46,3.56,-0.61,-0.04,0.41 4F85,LYS_130,10.25,-0.42,0,0.17 3BB7.TYR 264.10.99.-0.29.0.58.0.7 1D2K,ASP 152,4,41,0,-0.08,0.69 4H4J,ASP_59,4.08,0,0.08,0.2 1WYC,ARG_274,11.11,-1.31,0,-0.08 2IXM,GLU_75,4.76,0.22,0,0.04 1F2V.GLU 79.4.49.0.43.-0.01.-0.43 3EVZ,TYR_119,10.35,-0.16,0.05,0.46 1RAJ,ARG_402,12.34,-0.19,0,0.04 3K8U,GLU_64,4.58,0.15,0,-0.06 1WXF,TYR_33,10.72,0,0.36,0.36 2V4U,LYS 309,10,11,-0,12,0,-0,28 1ZKZ,ASP_48,4.39,0.12,0.28,0.18 2J8A,GLU_282,4.85,0.52,0,-0.17 3I47,ASP_41,4.05,0,-0.02,0.28 2E3H,ASP_235,3.28,-0.78,0,0.25 3GFP,ARG_423,9.65,-3.24,0,0.39 3DZ1,ARG_94,13.22,-0.46,0.69,0.49 2VGM,GLU_261,3.3,0.49,-1.55,-0.14 3M66,GLU 304,3.9,0.43,-0.62,-0.41 1PBV.GLU 165.4.47.0.45.-0.75.0.27 1X04,LYS_155,10.44,-0.06,0,0 3OKQ,LYS_619,10.56,-0.17,0,0.23 20JQ,GLU_597,4.54,0.12,0,-0.09 1KW4,LYS 55,10.41,-0.12,0,0.04 3IRA,GLU_157,3.52,0.25,-0.85,-0.38 3M7G,LYS_184,10.05,-0.89,0,0.43 2CXA,GLU_70,4.23,0.53,-0.8,0 3OKQ,ASP 671,3.86,-0.25,0,0.31 1XIP,ARG_68,12.25,-0.81,0,0.56 1Q42,ASP_159,3.65,-0.09,-0.4,0.34 3B21,ARG 210,13,12,-0,17,0,17,0.63 2FL4,LYS_101,11.23,-0.39,0.58,0.53 2ZQ5,HIS 153,6.14,-0.6,0.19,0.07 3ASA,HIS 163,7,26,-0.37,0.81,0.32 2IQT,LYS_67,11.52,-0.5,0.85,0.66 2C2Y,GLU_183,2.89,1.7,-2.38,-0.92 2IXM,LYS_194,12.09,-0.84,1.7,0.73 3FFM,LYS_24,10.31,-0.29,0,0.1 2EHG,GLU_33,4.3,0.61,-0.41,-0.39 1P6F,ARG_56,12.44,-0.06,0,0 2NRR,GLU_349,4.71,0.54,0,-0.32 1DUP,HIS 58,6.26,-0.42,0,0.18 2EJB.ARG 178,12,39,-0,17,0,0,06 1SNT,GLU_376,4.1,0.6,-0.69,-0.31 2IXM,GLU_234,4.39,0.24,0,-0.35 1FKM,LYS_320,10.48,-0.15,0,0.12 2OKT,LYS_252,10.89,-0.59,0.5,0.48 1QQE,ASP 264,3.19,-0.78,-0.3,0.47 2CIU,ASP_163,1.5,-2.37,-0.62,0.69 1CBY,HIS_59,5.83,-1.08,0.46,-0.04 2XHC,LYS 130,10.43,-0.07,0,0 2EEY,LYS 43,11.55,-0.36,0.84,0.56 2RGY,ARG_116,12.37,-0.47,0,0.34 3M9A,ARG_77,12.47,-0.03,0,0 3IVF,LYS_334,10.6,-0.12,0,0.22 2H8O, ARG_63, 11.92, -0.72, 0, 0.14 3A4C,CYS_453,8.25,-1.13,0.02,0.36 3ZSL,LYS_227,10.44,-0.13,0,0.07 1WYC,ARG_293,13.28,-0.45,0.77,0.46 4DVD,HIS_78,6.15,-0.22,0,-0.13

3T5B,HIS_178,3.77,-2.94,0,0.21 2BDV.CYS 2,11.59,-0.28,-0.96,3.83 3O48, ARG_77, 12.34, -0.27, 0, 0.11 1L3K.LYS 87.10.69.-0.38.0.14.0.44 1XTD.CYS 43.10.32.0.0.13.1.19 2E3C,GLU 340,3.91,0.4,-0.75,-0.24 3LD1,GLU 314,4,35,0,23,-0,05,-0,32 3IDW,ASP_53,3.46,-1.17,-0.33,1.14 2FM9,ASP_161,4.05,0,-0.05,0.3 1LN4.GLU 90.4.45.0.25.0.-0.29 3HUE,ARG 304,12,47,-0.06,0,0.03 1PZC,TYR_82,11.69,0,0,1.69 3F5D,ASP_73,4.14,0,0.01,0.33 3P2F,GLU_101,7.34,4.29,-1.04,-0.4 1NJ4,ASP 307,2.65,-0.66,-0.9,0.42 106D,HIS 114,5.71,-0.59,0,-0.2 2NRK,TYR_120,11.85,0.83,0.41,0.61 3GW3,ARG_184,12.37,-0.39,0,0.26 3V55,LYS_644,10.93,-0.13,0,0.55 1SJ8,LYS 533,10.61,-0.2,0,0.31 2B61,TYR_249,10.34,-0.01,-0.36,0.71 2AZP,GLU_146,4.17,0.39,-0.34,-0.38 1RWZ,ASP_146,2.86,-0.85,-0.52,0.43 3CCY,LYS 127,11.45,-0.39,0.85,0.49 1RKA,LYS 269,11.49,-0.5,0.91,0.59 3RJX,LYS_159,10.36,-0.38,0,0.24 1MUF,TYR_122,11.32,0,0.07,1.25 1PVT,ASP_206,5.19,0,0.39,1 1QYI,GLU 355,4.68,0.18,0,0 1WYC,HIS_108,6.31,-2.35,1.68,0.48 2YX0,LYS 120,11.15,-0.61,0.79,0.46 2WB8,ARG_779,12.31,-0.28,0,0.09 2IQT,ARG 251,13.06,-0.3,0.3,0.55 2ZCX,ARG 91,12.68,-0.31,0.0.48 3C38,ASP_216,3.99,0,-0.04,0.22 1DOV,ARG_137,13.2,-0.35,0.69,0.36 3GE9,ARG_193,12.9,-1.81,1.43,0.78 3GG6,TYR_145,10.4,0,0,0.4 3ONT,TYR_8,10.08,0,0,0.08 3I4T,LYS_269,10.49,-0.01,0,0 1UAJ,GLU_130,4.94,1.15,-0.85,0.14 3V1Q,GLU 543,4.65,0.36,0,-0.21 2R51.GLU 177.3.85.0.35.-0.77.-0.24 1V43,GLU_16,4.68,0.34,0,-0.16 2V5B,ARG_99,12.4,-1.03,0.43,0.5 2PP6,LYS_50,11.11,-0.27,0.39,0.49 2FBQ,ARG 139,12.67,-0.33,0.2,0.29 1G5Z.GLU 140.3.3.0.6,-1.07,-0.72 2E0T,GLU_177,3.92,0.3,-0.87,-0.01 2GKG,CYS_66,11.42,0,-0.21,2.63 4DNU,LYS_269,10.4,-0.32,0,0.21 1R3D,CYS 43,11,4,0,0,2,4 1XFK,TYR_301,13.59,0.66,0.56,2.37 2YWJ,LYS 177,10,55,-0,3,0,0,34 3OBS,LYS_16,10.51,-0.1,0,0.11 4FZN,ARG_176,11.74,-0.76,0,0 1W7B.GLU 66.4.64.0.17.0.-0.03 1ZHV,GLU_129,4.57,0.09,0,-0.03 2E3C,ASP_292,4.09,0,0,0.29 2F9F,GLU_56,3.1,0.4,-1.46,-0.34 1AKO.GLU 34,4,2,2,34,-1,64,-0,99 3CRM,GLU_275,4.54,0.18,0,-0.14 3GW3,ASP 117,2.29,-1.77,-0.41,0.67 2Q34,ARG_211,12.68,-0.72,0.52,0.38 1YW5,HIS_106,5.16,-1.44,0,0.1 3RKV,LYS 229,10,45,-0.05,0,0 2A0J,GLU_27,4.31,0.31,0,-0.5 2AXO,CYS_234,11.84,-0.03,-0.02,2.89 1EDG,LYS_363,10.31,-0.43,0,0.24

3M7G,GLU 15,3.88,0.49,-0.78,-0.34 2I88,LYS_510,9.95,-0.46,0,-0.09 2Q13,GLU_131,4.72,0.25,0,-0.04 3IL3,GLU_148,4.76,0.63,-0.01,-0.36 2V5B,ARG_208,10.67,-1.92,0,0.09 3V55,CYS 667,9.87,-0.43,-0.02,1.31 1LTU,LYS 82,10.61,-0.13,0.0.24 2VGM,LYS_238,10.36,-0.27,0,0.15 20BI,TYR_96,12.22,0.85,0.38,0.99 3IO0, ARG_172, 12.46, -0.12, 0, 0.07 1NFN,GLU 66,2.96,0.51,-1.4,-0.65 1L2F,ASP_241,3.42,-0.78,0,0.39 105Z.GLU 620.3.77.0.24.-0.59.-0.38 1SIG,GLU_381,4.76,0.31,0,-0.05 2B2H.GLU 183,4.69,0.24,-0.04,0 3TOW.TYR 189,11.17,-0.24,0.48,0.93 2EFK,HIS_177,6.14,-0.24,0,-0.12 1JYH,GLU_82,4.56,0.08,0,-0.02 1X91,ARG_63,12.32,-0.22,0,0.05 3JZN,TYR_387,9.59,-1.33,-0.2,1.12 3F5D,ASP 127,3.26,-0.85,0.0.31 4EKU,GLU_69,4.17,0.45,-0.68,-0.1 4HDE,LYS_141,11.23,-0.32,0.85,0.2 2AXO,LYS 231,10.14,-0.33,0,-0.04 300P.ASP 124.2.6.-1.49.0.0.3 2W1R,ASP_68,4.21,0,0.13,0.28 3GA2,TYR_195,10.93,-0.03,-0.2,1.16 2A0J,ASP_16,3.41,-0.31,-0.46,0.38 1YTQ,GLU 42,4.66,0.16,0,0 1NRI,ASP_40,4.2,0,-0.01,0.42 1G8P,ARG_253,11.51,-0.84,0,-0.14 3IU5,LYS_154,10.5,0,0,0 3AU3.HIS 672.6.4,-0.1.0.0 2HRZ.GLU 330.4.12.1.17.-0.85.-0.7 1DUN,ASP_72,3.88,-0.12,-0.04,0.24 1CHD,ARG_202,12.37,-0.13,0,0 3BQE,LYS_355,10.26,-0.22,0,-0.02 1CBY,ASP_151,3.93,0,-0.1,0.24 1ZCE.CYS 92.10.38.0.0.11.1.27 2QDJ,ARG_167,12.38,-0.27,0,0.15 3UAH,TYR_385,12.04,0,0.29,1.75 3BCH,TYR_39,9.82,0,-0.27,0.1 3BA1,ARG 28,13.9,-0.52,1.22,0.69 4DVD,ARG_84,13.92,-0.54,1.03,0.93 1SIG,LYS_296,10.76,-0.17,0.12,0.3 1V6T,ARG_50,12.74,-0.29,0.53,0.01 2FBQ,ARG_75,12.81,-0.64,0.68,0.27 3IVF.CYS 236.11.39.-0.04.-0.11.2.55 2RFA,GLU_108,4.38,0.61,-0.15,-0.58 3U4K,TYR_155,11.08,-0.39,-0.22,1.69 1WRU,LYS_53,10.8,-0.19,0.1,0.39 1GXN.LYS 418.10.05.-0.46.0.0.01 3CRM,GLU_211,5.06,0.19,0,0.37 3LJI,TYR_33,10.35,0,0,0.35 1P4X,LYS_151,9.93,-0.3,0,-0.27 2CBE,LYS_9,10.78,-0.15,0.23,0.21 20EW,HIS_320,6.78,-0.25,0.42,0.1 1PSW,GLU_53,4.28,0.31,-0.24,-0.29 1ZCU,LYS 75,10.02,-0.32,0,-0.16 2PGE,ASP_38,4.35,0,-0.34,0.88 1W24,LYS_43,10.76,-0.16,0,0.43 4ECC,ASP 39,3.87,0,0,0.07 2QRX,LYS_15,10.44,-0.06,0,0 2Z84,GLU_168,3.85,0.44,-0.96,-0.13 3FK5,LYS_239,11.41,-0.32,0.85,0.38 4FD6.TYR 19.10.69.0.0.03.0.66 2XHC,LYS_32,10.37,-0.14,0,0.01 1KCM.GLU 6.5.32.2.61,-0.82,-0.97 3P28,GLU_63,3.82,0.36,-0.49,-0.56

2B61.TYR 282.12.28.0.82.0.21.1.26 2Z84,CYS_101,12.77,-0.34,1.04,3.07 4E8B,GLU_10,4.58,0.2,0,-0.12 1L3K,GLU_66,4.81,0.11,0,0.2 3LH5.GLU 746.4.55.0.07.0.-0.02 1TXJ.ASP 130.4.16.0.0.09.0.28 4FCU,GLU_217,3.78,0.94,-1.52,-0.15 2P1W,ASP_60,2.77,-1.28,-0.02,0.26 2FL7,ARG_21,12.45,-0.05,0,0 109G.ARG 135.13.12.-0.39.0.56.0.46 1ES9,LYS_10,10.82,-0.44,0.44,0.33 3B7H,GLU_14,4.38,0.28,-0.15,-0.25 2EYI,GLU_30,3.79,0.41,-0.45,-0.68 1T07.ASP 78.3.91.0.0.0.11 2B61,HIS 337,6.83,-3,16,0.85,2.63 1R53,LYS_73,10.38,-0.12,0,0 3M16,GLU_317,4.96,1.68,-1.32,0.09 4EKU,GLU_142,4.74,0.25,0,-0.02 3OIP,ARG_15,12.62,-1.15,0.76,0.51 2GEN,ASP_149,4.04,0,0.08,0.16 3FFM,LYS_137,10.39,-0.29,0,0.18 3E7P,ARG_138,12.04,-0.81,0,0.36 2FD5,GLU_129,4.65,0.21,0,-0.06 2ZCO.LYS 231,10.41,-0.09,0.0 3CXS,CYS_157,9.89,0,0.02,0.87 1TR9,TYR_305,13.34,0.54,0.91,1.89 2JKF,ASP_45,4.15,0,0,0.35 3BJV,GLU 87,4.66,0.16,0,0 3I4T,ASP_84,3.26,-1.38,-0.34,1.17 3RE9,TYR_214,10.39,-0.17,-0.07,0.62 1J33,HIS_110,6.05,-0.48,0.09,-0.05 1TLV.HIS 189,5.45,-0.72,0.06,-0.4 4EZB.GLU 239.5.75.1.2.0.0.06 2WOZ,GLU_323,4.15,0.37,-0.85,0.13 2IN0,GLU_411,4.46,0.3,0,-0.34 4FH3,ASP_253,3.59,-0.77,-0.09,0.65 2YT4,ARG_522,12.51,-0.39,0.14,0.26 3A7L.GLU 94.4.12.0.3.-0.68.0 2D7U,GLU_330,3.72,0.4,-0.86,-0.32 1UCH,HIS_112,5.73,-0.44,0,-0.33 3C5V.TYR 285,10.43,-0.02,0.02,0.43 3ETU.GLU 76.4.74.0.24.0.0 2FI9,LYS_94,10.48,-0.19,0,0.17 2B78,LYS_343,10.28,-0.2,0,-0.02 2CI3,LYS_119,10.58,-0.13,0,0.21 2JEO,TYR_205,9.17,-0.44,-0.78,0.39 4AM1.CYS 127.10.81.0.-1.58.3.39 2Z0M,ASP_126,2.7,-1.35,-0.16,0.41 1WNH,CYS_20,12.71,0,0,3.71 1L3K.ASP 139.2.09.-1.88.-0.12.0.3 4DVD,ARG 43,12,42,-0.08,0.0 1WYC,ARG_12,11,-2.14,0.4,0.24 1WNH,LYS_97,10.46,-0.04,0,0 3F5D,LYS_92,9.68,-0.94,0,0.12 1RAJ,ASP_71,2.9,-1.8,-0.5,1.41 4EVF,LYS_194,10.34,-0.42,0,0.26 1G5Z,GLU_173,4.82,0.83,0,-0.52 2IRM,HIS 336,4.75,-1.22,0,-0.53 3G9B,LYS_149,10.49,-0.16,0,0.15 3F1X,HIS 202,6.19,-0.66,0,0.34 2FXT,HIS_292,5.3,-1.43,0,0.22 1A8Q,ASP_129,3.87,0,-0.02,0.09 1DCF,ARG_130,12.51,-0.15,0,0.16 2A4D,GLU_93,4.67,0.25,0,-0.08 3RJX.GLU 66.4.8.0.28.0.0.02 3US6,ARG_114,12.48,-0.26,0,0.23 1Z9L,HIS_86,5.12,-1.12,0,-0.26 1N81,GLU_26,4.8,0.3,0,0.01 3L7N,HIS_107,6.64,-0.22,0,0.36

1YLN.CYS 158.12.3.0.0.14.3.16 2FL4,LYS 106,10.53,-0.19,0,0.21 1JKS,ASP_259,2.43,-1.14,-0.76,0.53 1YLN,ARG_227,12.38,-0.33,0,0.22 2FZP,ASP 222,3,24,-0.84,0,0.29 3BWT.LYS 698.11.11.-0.23.0.38.0.46 10TM,ASP_68,3.09,-0.97,-0.2,0.46 3NBI,LYS_130,10.37,-0.37,0,0.24 3IVF,GLU_132,4.6,0.3,0,-0.2 2RJD.GLU 311.4.63.0.59.-0.14.-0.32 105J.LYS 20.10.2.-0.3.0.-0.01 2PGE,TYR_287,10.9,0,-0.02,0.92 2OJQ,LYS_374,9.94,-0.6,0,0.04 1PZC,HIS 6,6.27,-0.44,0.0.21 1YTD.LYS 32.10.43.-0.07.0.0 4FZN,TYR_24,12.01,-0.46,0.24,2.22 1TXJ,GLU_103,4.76,0.24,0,0.02 1H09,LYS_203,9.66,-0.45,0,-0.38 3ETU,LYS 69,11.58,-0.49,0.85,0.72 1WLY,ARG 102,10,17,-3,0,0.67 2X4G,ASP_249,3.24,-0.54,-0.35,0.33 1YM5,TYR_279,10.45,-0.08,-0.13,0.67 1X7F,TYR_150,10.93,-1.07,0.07,1.93 3I4T, ASP 154, 2.97, -0.86, -0.41, 0.44 3BB7,TYR_331,10.22,-1.54,0.43,1.34 2ZCO,TYR_10,11.99,0.5,0.4,1.08 1JT9,HIS_96,6.84,-0.41,0.72,0.03 2V4U,LYS 344,11.45,-0.28,0.85,0.38 3FXH.GLU 109.2.43.0.72,-1.97,-0.81 1CHD,TYR_295,10.16,0,0,0.16 2D7U,TYR_22,12.59,0.61,0.38,1.59 3DZ1,LYS_185,10.35,-0.13,0,-0.01 10IS,HIS 338,5.68,-0.64,0,-0.18 3EJG,CYS_141,11.5,0,-0.16,2.66 3FK5,ARG_93,12.03,-0.93,0,0.46 4DNU,ARG_146,12.37,-0.74,0,0.61 1JYH,LYS 62,10.42,-0.08,0,0 3T57,LYS_163,10.91,-0.43,0.18,0.65 1VSM,HIS_142,5.69,-1.67,1.02,-0.16 1MTZ,ASP_120,3.83,0,-0.16,0.19 2HP7,GLU_221,4.68,0.35,0,-0.17 3EVP,CYS 228,12.13,-0.82,-0.09,4.04 3BOE,ARG 354,13,28,-0.26,0.41,0.64 1Z3X,ARG_94,12.37,-0.24,0,0.11 2VGY,TYR_68,10.18,0,0.03,0.15 4FH3,TYR_220,12.22,0,0.09,2.13 1SI7,TYR_304,11.46,-0.37,0,1.83 3RAZ,ASP_30,2.67,-1.54,-0.09,0.5 2FBO,ARG 29,12,25,-0,25,0,0 2QZQ,LYS_112,10.02,-0.27,0,-0.22 3CAX,LYS_468,10.33,-0.17,0,0 2IOT.GLU 122.4.37.0.24,-0.16,-0.21 3NR5,ARG_73,13.5,-0.28,0.73,0.55 3GW3,GLU_27,3.54,0.57,-0.85,-0.68 1PBV,GLU_241,4.28,0.27,0,-0.5 3BCY,GLU_32,5.79,1.02,0,0.26 3A0X,GLU 623,4.61,0.33,0,-0.21 2CBE,LYS_113,10.21,-0.29,0,0 3ZSL,TYR_118,10.33,0,0,0.33 2Z84,GLU_10,4.61,0.15,0,-0.04 2BCF,CYS 100,9.01,-0.21,0.05,0.17 1Q46,LYS_117,11.19,-0.39,0.32,0.75 3A4C,HIS_510,5.29,-1.58,0.83,-0.46 3GE9,ARG_129,13.06,-0.31,0.55,0.32 1J33,ARG 80,12.21,-0.26,0,-0.03 3M7D,LYS_347,11.45,-0.49,0.85,0.59 3JRT,LYS_73,9.74,-0.42,0,-0.34 3H6Q,LYS_34,11.25,-0.64,0.85,0.54 3F6F,ARG_37,12.2,-0.3,0,0

2Q13,GLU_252,5.12,0.25,0.38,0 1G5Z.LYS 138.10.72.-0.25.0.0.47 3COU,GLU_76,5.87,1.69,-0.75,0.45 3EJG,ARG 85,12,44,-0,42,0,0,36 2D0A,TYR_213,9.25,-0.85,-0.36,0.46 109G,CYS 59,13.45,-0.49,1.87,3.07 1YDL, ASP_39, 2.97, -0.86, -0.23, 0.27 1MML,GLU_117,2.73,0.37,-1.39,-0.75 2IRM,LYS_152,10.42,-0.08,0,0 4AM1,HIS_185,6.35,-0.22,0,0.07 10YI.GLU 353,4.84,0.51,0,-0.17 1JSX,LYS_206,10.28,-0.36,0,0.15 3HUE,CYS 231,11.5.0.0.05,2.45 3A4C,HIS_525,6.13,-0.24,0,-0.13 1NAR,LYS 115,11.34,-0.5,0.78,0.57 1SFE,ARG_92,12.82,-0.32,0.07,0.57 3DZ1,ASP_287,3.6,-0.13,-0.26,0.19 3G9T,ASP_27,2.81,-0.88,-0.42,0.31 1T6L.TYR 103,10.05,-0.55,0.22,0.39 3V75,ASP_232,3.41,-0.78,0,0.39 1JYH,GLU_46,3.54,2.02,-2.09,-0.89 3H13.GLU 263.4.95.3.07.-2.65.0.04 1I60,HIS_146,5.87,-0.76,0,0.14 3KEY,LYS 402,9.71,-0.79,0,-0.01 4E9E,LYS 458,10.38,-0.41,0.0.29 1DCF,HIS_29,6.18,-0.21,0,-0.11 2Q13,CYS_183,9.28,-0.15,0.01,0.42 3L3P,GLU_307,4.67,0.22,0,-0.05 3T57,LYS 133,10.57,-0.07,0,0.15 2XHC,LYS_108,10.14,-0.47,0,0.1 2J8A,GLU_322,4.54,0.45,0,-0.41 1TUL,CYS_73,10.71,-0.68,0,2.39 208P,LYS 150,10.96,-0.66,0.69,0.43 1Z3X.ARG 181.12.41.-0.26.0.0.17 1TWU,GLU_24,4.75,0.27,0,-0.03 2GAU,TYR_180,11.88,0.85,0.35,0.67 1WLY,TYR_243,12.44,-0.42,0.09,2.77 4E6S,HIS 70,6.44,-0.1,0.04,0 1SQH,ASP_23,4.01,0,-0.12,0.32 3TRE,GLU_28,4.85,0.22,0,0.12 3F1X,GLU_255,4.08,0.34,-0.72,-0.04 1VSM,ARG 161,12.62,-0.21,0,0.33 2G3A,LYS 135,10.87,-0.8,0.85,0.31 3IRA,GLU_83,5.31,0.51,0,0.29 2E3S,GLU_400,3.83,0.24,-0.55,-0.37 2DFL,ASP_193,4.13,0,0,0.33 1R53,GLU_160,4.62,0.13,0,-0.01 3ETU,ASP_300,3.91,0,-0.12,0.23 1AT0, ARG_387, 13.4, -0.2, 0.78, 0.32 2PGE,TYR_300,10.97,-0.08,-0.33,1.37 1T6L, ARG_208, 13.25, -0.41, 0.79, 0.37 2RGY,LYS 264,10,42,-0,1,0,0,02 2QZQ,LYS_142,10.31,-0.17,0,-0.01 1MUF,LYS_286,10.41,-0.14,0,0.05 2ZCO,ARG_224,12.49,-0.32,0,0.3 1SNT,ASP_345,2.25,-2.53,-0.17,1.15 4FZR,ARG 91,11.95,-1.33,0.47,0.3 1X9G,GLU_70,4.36,0.23,-0.37,0 1NFN,GLU_77,4.65,0.19,0,-0.04 3JRT,GLU_137,4.77,0.14,0,0.13 3ZXY,ASP_201,3.87,-0.13,-0.09,0.28 2CL3,CYS_144,9.66,-0.38,-0.25,1.3 2E3S,ARG 520,13,55,-1,14,1,3,0,89 3OKQ,ASP_578,4.24,0,0.12,0.33 20EW,LYS_19,10.56,-0.09,0,0.14 1ZP2.LYS 110.10.46.-0.04.0.0 1BN6,TYR_90,13.15,0,0.53,2.61 2P4D,ASP_79,3.18,-1.58,-0.2,1.16 3LPZ,TYR_25,10.26,0,0.07,0.19

4DIU,GLU_153,4.83,0.23,0,0.1 3DSH,LYS 402,11.3,-1.18,0.79,1.19 3I47,LYS_222,10.42,-0.08,0,0 3UAH,ARG_418,12.62,-0.76,0,0.88 3IV4.TYR -3.10.06.0.0.06 20EW, ASP 182, 3.9, -0.05, -0.38, 0.53 2P0Y.ASP 314.3.04.-1.23.-0.18.0.64 3M16,CYS_174,12.59,-0.19,0,3.78 4E8B,GLU_165,4.14,0.22,-0.45,-0.13 2RIS,HIS_104,7.2,-0.31,0.85,0.16 3GG6,HIS_99,5.9,-0.28,0,-0.32 3M70,ASP 84,2.92,-1.1,-0.16,0.37 3PP8,GLU_261,4.04,0.19,-0.65,0 1ZBM,LYS_95,10.45,-0.3,0,0.24 2YYO,TYR_80,13.09,0.46,0.78,1.85 2G2D.HIS 130.5.02,-1.44.0.31,-0.33 3ILC,ARG_165,12.18,-0.32,0,0 1NAR,LYS_176,11.52,-0.41,0.81,0.61 3FTT,ASP_166,3.57,-0.75,-0.06,0.57 2X4L,LYS 124,11.41,-0.23,0.63,0.5 1R53.GLU 206.4.53.0.32.0.-0.28 1SNT,CYS_332,12.13,-0.36,0.38,3.09 2FC3,TYR_20,11.03,-0.78,0.08,1.73 4H4J.LYS 167.10.33.-0.15.0.-0.02 1WRU.CYS 96.10.03.0.0.46.0.57 2P0L,HIS_50,2.78,-3.64,0,-0.08 3JRT,ASP 165,3.02,-0.63,-0.54,0.4 1FQI,TYR_337,10.15,-0.23,0.1,0.29 3HKX,ASP_94,3.77,-0.03,-0.39,0.39 3T57.GLU 150.3.16.0.44,-1.27,-0.51 2I6I,LYS_57,11.44,-0.38,0.85,0.47 2EYI,TYR_215,9.56,-0.3,-0.4,0.25 3V3T.GLU 132.5.38.0.53.0.23.0.11 2Z14,GLU 94,4.63,0.3,0,-0.16 1Y0K,ARG_105,12.13,-0.14,0,-0.24 1G8P,CYS_78,8.69,-2.54,-0.15,2.38 1W7B,LYS_249,10.42,-0.1,0,0.02 3JZ9,HIS_496,5.6,-0.72,0,-0.18 2FL7,ARG_92,11.65,-1.84,0.01,0.96 2VGM,GLU_23,3.91,0.63,-0.54,-0.68 1ZKZ,GLU_18,5.03,0.14,0,0.39 2E3C,LYS_245,10.81,-0.25,0,0.57 2HRZ,HIS 229,1.87,-3.36,0,-1.27 3ETV,LYS_102,10.08,-0.39,0,-0.02 105T,ARG_321,11.71,-2.04,0.61,0.63 3A7L,TYR_96,11.8,-0.84,0.17,2.47 1WYC,ARG_50,12.1,-0.15,0,-0.25 1Y2O.GLU 24.3.93.1.78.-1.65.-0.7 3OKQ,ARG_556,13.56,-0.36,0.79,0.63 1NWA,ASP_133,4,0,-0.07,0.27 10IS,LYS_304,11.11,-0.75,0.85,0.51 2D0A, ARG 47, 11.8, -0.63, 0, -0.07 3NZL,HIS_19,6.04,-0.36,0,-0.1 2B61,TYR_56,10.78,0,0.3,0.48 1WRU,GLU_151,3.86,0.35,-1.01,0.03 2IF4,LYS_289,10.96,-0.17,0.26,0.37 1Q2Y,LYS_25,11.5,-0.54,0.58,0.96 2YX0,GLU_191,3.63,0.31,-0.83,-0.34 1GVP.CYS 33.11.15.0.0.2.15 2CBE,ASP_85,3.89,0,-0.1,0.18 3ADO,ARG_298,12.2,-0.39,0,0.09 30DJ.TYR 120,10.3,0,0,0.3 3LJN,ARG_106,11.88,-0.93,0.03,0.27 1MIX,ARG_207,12.13,-0.33,0,-0.04 3DHN,TYR_85,10.76,0,0.76,0 3RJX,LYS_297,10.54,-0.23,0,0.27 2CI3,ARG_31,12.24,-0.55,0,0.29 2V4U,ASP_350,3.58,-0.38,-0.21,0.36 3PM2,LYS_152,11.45,-0.24,0.81,0.38

3G9G,ASP 102,3.64,-0.5,-0.38,0.72 4DEZ,HIS_99,5.53,-0.87,0,-0.1 3ZXY,GLU 128,2.67,0.61,-2.45,0 3IVF,GLU_237,4.86,1.2,-0.39,-0.45 1YR6,ASP 184,4.45,0,0.08,0.56 2XWS.HIS 10.5.3.-0.93.0.-0.27 3LJN,LYS_104,10.41,-0.22,0,0.12 3BWT,HIS_795,5.6,-0.9,0,1.04E-17 2J8A,LYS_299,10.89,-0.26,0,0.65 4EKU,HIS 106.6.15.-2.34.1.12.0.87 3CAX,GLU_465,4.66,0.16,0,0 1T3Y.GLU 103.3.79.0.3.-0.6.-0.4 3ZTA,GLU_57,4.33,0.35,-0.24,-0.29 100X.GLU 245,4.15,0.15,-0.14,-0.36 3L3P.ARG 508.12.34,-0.2.0.0.04 4D8L,ARG_98,12.22,-1.38,0.53,0.58 1JSX,GLU_157,4.44,0.1,0,-0.16 2Z0M,LYS_151,11,-0.38,0.47,0.41 2AZL.GLU 21.5.02.0.35.0.0.17 1VSM,LYS_119,9.22,-1.37,0,0.09 2FGG,ASP_21,4.09,0,-0.05,0.34 1RL0,ASP_81,1.81,-2.32,-0.28,0.61 1DVO.TYR 149,10.43,0,0.34,0.09 3PM2.HIS 131.6.15,-1.31.0.51.0.45 208P,HIS_163,6.21,-0.42,0,0.14 3M3P,ARG_47,12.52,-0.19,0,0.21 3G9T,HIS_268,7.4,-2.69,0.85,2.74 1Q46,ASP 166,3.3,-0.31,-0.6,0.41 3V1Q,ARG_535,12.1,-0.52,0,0.11 208P,GLU_42,4.02,0.49,-0.66,-0.3 1GPP,GLU_103,3.1,0.54,-1.5,-0.43 2FBO,ARG 127,12.38,-0.16,0,0.04 3N2T,ASP 34,3,28,-0.65,-0.17,0.31 2FZP,LYS_283,10.2,-0.33,0,0.03 3COU,GLU_169,4.45,0.65,-0.5,-0.21 2RIS,TYR_57,10.51,0,0.21,0.31 1YG2,TYR 129,10.97,0,-0.05,1.02 3TMO,HIS 282,6,23,-0,28,0,0,01 2E3H,ASP_247,3.11,-0.84,-0.26,0.4 1YR6,GLU_52,4.68,1.59,-1.28,-0.12 1GOE, ARG 117, 12, 43, -0, 36, 0, 0, 29 3E7P.ARG 26.11.89.-2.05.0.01.1.43 2B0J,GLU_59,3.95,0.66,-0.42,-0.79 1PSW,ARG_134,11.51,-1.06,0,0.07 3CIV,ASP_60,3.65,-0.83,-0.1,0.78 1NIJ,ARG 213,12.46,-0.17,0,0.13 2GEN,ASP 148,2,99,-0,49,-0,72,0,39 1X8F,GLU_29,4.46,1.12,-0.69,-0.48 1SUU,LYS_668,10.43,-0.37,0,0.3 2CVB.GLU 162,4,27,0,34,-0,18,-0,39 1AM2,HIS 197,6.24,-1.17,0.85,0.06 3O48,GLU_32,1.79,0.6,-3.26,-0.04 4DNU,ASP_326,3.45,-0.33,-0.23,0.2 3HUE,LYS_45,10.16,-0.14,0,-0.2 2X4L,GLU 88,4.27,0.3,0,-0.54 1JKS,HIS_272,6.09,-1.45,0.85,0.19 3HUE,GLU_239,5.94,1.08,0,0.36 1G5Z,LYS 120,11.39,-0.22,0.63,0.48 1ZBS,TYR_66,12.88,-0.26,-0.04,3.19 3UAH, ASP 261, 2.12, -1.69, -0.38, 0.39 2D7U,ASP_215,3.29,-0.88,-0.21,0.58 1XWM,LYS_211,10.51,-0.07,0,0.09 1RZ2,ARG_133,12.58,-0.61,0.17,0.53 1GXN,TYR 526,10.4,-0.08,-0.68,1.17 4H89.GLU 117.4.19.0.3.-0.46.-0.16 2X5Y,LYS_816,10.28,-0.32,0,0.1 1X7F,LYS_140,10.19,-0.31,0,0 3EYE, ARG_93, 13.91, -0.52, 1.3, 0.63 1RI6,ARG_66,13.02,-0.38,0.58,0.32

2B61.LYS 21.10.38.-0.12.0.0 1AT0,CYS_400,10.41,-1.48,0.01,2.89 1KCM,LYS_68,10.28,-0.38,0,0.16 3GS9,TYR_52,10.05,0,0,0.05 1Z3X.ASP 97.2.91,-1.02,-0.29.0.42 3ADO,CYS 305,9,48,-0.04,-0.07,0.6 2DFL,LYS_200,10.45,-0.1,0,0.05 1SJY.GLU 53.4.83.0.22.0.0.1 1MTZ,HIS_271,7.2,-2.97,0.85,2.82 2JHY,TYR_156,10.34,0,-0.3,0.64 1BN6.GLU 132.4.0.42,-0.8,-0.12 3D9H,ARG_53,12.29,-0.21,0,0 3FHF,LYS_11,10.77,-0.6,0.52,0.35 2GEN.ARG 107.13.19.-0.47.0.46.0.69 2WOZ.GLU 377.4.7.0.13.0.0.06 1X9G,GLU_22,3.85,0.29,-0.85,-0.09 1SNT,ASP_58,3.8,-0.42,-0.19,0.6 2H01,HIS_156,6.1,-0.3,0,-0.1 3MEW, ASP_139, 3.33, -0.77, 0, 0.3 2B2H,GLU_375,4.98,0.53,0,-0.06 1XIP,LYS_246,11.19,-0.78,0.81,0.64 3PAC, ASP_92, 3.82, 0, -0.2, 0.22 1UJ8,GLU_24,4.08,0.76,-0.85,-0.34 3F1X.GLU 85,4.17,0.6,-0.54,-0.4 20GQ,LYS_492,10.21,-0.53,0,0.24 2GEN,ARG_170,12.2,-0.29,0,-0.01 1QYI,TYR_302,12.72,0.32,0.8,1.6 2OJQ,GLU_682,4.48,0.22,0,-0.24 2B61.GLU 330.4.03.0.42.-0.85.-0.04 1HUF,GLU_36,3.85,0.22,-0.3,-0.57 2AH5,HIS_123,5.75,-0.51,0.07,-0.31 1TP6,ARG_25,12.43,-0.12,0,0.04 3016.LYS 77.10.26.-0.28.0.0.04 3BZT,TYR_271,11.85,0.85,0.38,0.61 1WPA,LYS_504,10.72,-0.18,0.01,0.38 2R2Y,LYS_97,9.77,-0.35,0,-0.39 1QQL,ARG 13,11.93,-0.44,0,-0.13 3RLN,GLU_660,4.54,0.08,0,-0.04 3GOZ,ASP_28,3.02,-1.62,-0.18,1.03 3M7G,ASP_182,2.51,-1.84,-0.35,0.9 3RKV,HIS_307,7.06,-0.52,0.83,0.26 3GS9,CYS_281,9.81,0,0.19,0.62 2GS5,ARG 180,13,21,-1,38,1,34,0,75 2QDJ,GLU_323,4.15,0.27,-0.26,-0.37 2QDJ,GLU_79,4.59,0.37,-0.22,-0.06 1AM2.TYR 163,12.88,0,0,24,2,65 2EJX,GLU_49,4.61,0.24,0,-0.13 4GCO,LYS_212,10.67,-0.72,0.85,0.05 1RL0,LYS_157,10.67,-0.4,0.36,0.2 3M3P,HIS_246,6.38,-0.12,0,0 2YX0,LYS 62,10.62,-0.55,0.07.0.6 2R0S,ASP_204,2.67,-1.59,-0.02,0.47 2ZQ5,ASP_308,3.25,-0.84,-0.02,0.31 3H5T,LYS_191,10.82,-0.2,0.2,0.32 3ILC,TYR_15,11.98,0.78,0.48,0.72 2IQT,ARG_232,10.91,-1.59,0,0 1AT0,ASP 318,3.43,-0.69,-0.24,0.55 3GS3.LYS 218.10.39.-0.12.0.0.01 2FZP,GLU_248,4.87,0.24,0,0.14 2JHY,ARG 117,12.2,-0.3,0,0 1V6TLYS 137,10.54,-0.13,0,0.16 2IXM,GLU_298,4.63,0.47,0,-0.34 1QYI,ARG_370,13.14,-0.43,0.71,0.36 1ILW,GLU_80,4.35,0.3,-0.06,-0.38 10TM,LYS 131,10.41,-0.09,0,0 2R0S,LYS_201,10.46,-0.04,0,0 1YTD,HIS_144,6.13,-0.37,0,0 3RLE,TYR_72,11.42,0,0.06,1.36 20EW,ASP_235,3.62,0,-0.37,0.19

3ANJ.TYR 334.10.55.0.0.2.0.34 3T57.GLU 266.4.18.0.52.-0.82.-0.02 1X6J,HIS_30,6.85,-0.31,0.64,0.03 1W7B.ARG 245.12.56.-0.5.0.1.0.47 1PBV.ASP 236.3.97.0.-0.21.0.38 1WP5,HIS 68,5.92,-0.5,0,-0.08 3T8R.ARG 81.14.-0.45.1.29.0.65 2V1L,ASP_118,3.63,0,-0.42,0.25 4FLE,TYR_111,10.12,0,0,0.12 3DB9,HIS_256,5.67,-1.2,0.29,0.09 1T3Y,ASP 123,3.85,0,-0,14,0,19 1R9W,CYS_276,9.12,-1.32,0.03,1.4 3JV1,ARG_93,12.36,-0.55,0,0.41 1YW5.GLU 44.4.73.0.09.0.0.14 1PGV.ARG 253.12.71.-0.38.0.07.0.52 3PP8.GLU 135.3.94.0.26.-0.82.0 1R29,LYS 123,10,37,-0,13,0,0 1UOH,GLU_54,4.65,0.25,0,-0.1 1TXJ,ASP_73,3.43,-0.63,-0.27,0.52 4DEZ,ARG 64,12,42,-0.08,0.0 1NRI,HIS_134,6.31,-0.16,0,-0.03 2CWY,ARG 63,12.04,-0.31,0,-0.16 1Y0K.GLU 48.3.47.0.37.-1.56.0.16 3EGN,GLU 403,4.77,0.27,0,0 1SI7.GLU 264.4.63.0.13.0.0 1KN3,GLU_19,4.06,0.3,-0.49,-0.24 3ZSL,ASP_241,3.83,0,-0.27,0.29 3CRM,ARG_219,11.85,-0.68,0,0.03 2YT4,TYR 609,9.25,-0.77,-0.41,0.42 2XHC,ASP_47,3.43,-0.21,-0.46,0.3 3VJ8,HIS_101,5.66,-0.94,0.26,-0.16 3P2F,ARG_95,12.33,-0.21,0,0.05 3ADO.ARG 254,12.5,-0.26,0.04,0.23 1R3F.ASP 185.3.11.-1.43.-0.5.1.23 4DBX,LYS_158,11.4,-0.34,0.85,0.39 3GV0,ARG_139,12.63,-2.35,1.32,1.15 1N81,TYR_51,10.25,0,0.08,0.17 3V75,ARG 242,12.37,-0.32,0,0.2 2IRM,GLU_101,4.52,0.49,-0.09,-0.38 3ERF,HIS_58,4.74,-1.51,0,-0.25 4H89,HIS_167,5.67,-0.61,0,-0.22 2D0A,GLU 148,4.66,0.16,0,0 2X5Y,ASP 865,3.98,-0.81,-0.16,1.16 3JV1,GLU_161,3.92,0.24,-0.85,0.03 1YW5,TYR_39,10.05,0,0,0.05 3ADO,ASP_191,3.89,0,-0.11,0.2 1P2F,LYS 21,11.39,-0.37,0.85,0.4 1X7F.GLU 232.3.49.0.43.-0.85.-0.58 3Q1C,GLU_263,4.35,0.24,-0.33,-0.07 3RNV,TYR_396,11.71,0.57,0.38,0.76 3FS3,TYR_53,10.61,0.05,0.38,0.19 10YI.LYS 2.10.63.-0.33.0.0.46 4FZR,ARG_95,12.42,-0.45,0,0.37 2JKF,ASP 49,3.78,-0.35,-0.03,0.36 3FXH,HIS_80,6.09,-1.01,0.47,0.12 2CI3,GLU_84,4.65,0.34,-0.35,0.16 2GEN, ASP 98, 3.67, -0.32, -0.28, 0.47 10I7,ARG_236,13.2,-0.43,0.72,0.4 2IRM,ARG_347,12.49,-0.21,0,0.2 3FXH,LYS_54,10.58,-0.12,0,0.2 3CAN,LYS 48,10,28,-0,12,0,-0,11 2V4U,TYR_314,11.56,-0.66,0.45,1.77 1SBX.GLU 118.4.62.0.25.0.-0.13 1EDG,ASP_356,2.53,-1.46,-0.75,0.94 4DEZ,ARG_42,12.47,-0.03,0,0 3GEC.ARG 525.12.53.-0.09.0.0.12 200K,LYS_184,10.22,-0.33,0,0.05 1NFN,LYS_69,10.6,-0.25,0,0.34 3F6M,HIS_5,7.25,-0.42,0.85,0.32

1KN3.GLU 135.3.76.1.27.-1.83.-0.17 2GAU,CYS_222,9.12,-0.65,-0.2,0.96 1CBY,ASP_209,2.79,-1.44,-0.01,0.44 3IU5,ASP 142,3,19,-0.61,-0.4,0.39 3GS3,HIS_103,6.32,-0.61,0.21,0.22 1RL0,ASP 120,3,-1.08,-0.14,0.42 1ES5.LYS 107.10.-0.51.0.0.01 1ZCE,GLU_27,4.42,1.11,-0.85,-0.34 3JZ9,TYR_529,10.08,0,-0.04,0.11 2P5D,CYS_9,13.32,0,0,4.32 3V55,HIS 415,4.6,-2.2,0.91,-0.62 2GAU,LYS_31,10.64,-0.1,0,0.24 2YWX,LYS_132,10.64,-0.09,0,0.23 4ACJ,GLU_730,4.52,0.14,-0.07,-0.06 3IV4.GLU 105.4.92.1.13.-0.38.-0.33 2HXB.GLU 84.4.61.0.11.0.0 1L2H,TYR_24,9.39,-0.85,0.01,0.22 1SNT,ARG_241,12.27,-0.23,0,0 2R57,HIS_258,4.95,-1.16,0,-0.39 2P65,GLU_100,3.74,0.58,-0.83,-0.51 3GOZ.ASP 290.3.29,-1.02,-0.14,0.65 1CBY,GLU_178,4.48,0.3,-0.43,0.11 2QEV,LYS_68,10.44,-0.06,0,0.01 3CN5.ARG 118.12.74.-1.37.0.7.0.91 3BA1.TYR 186.10.61.0.0.08.0.53 3RLE,ARG_47,11.25,-1.3,0,0.05 1NRI,LYS 41,11.09,-0.22,0.45,0.36 2GAU,ARG_72,12.31,-0.19,0,0 3QKY,TYR 177,10.18,0,-0.01,0.19 2CW4,ASP 37,2.9,-1.24,-0.02,0.36 3LJI,GLU_64,3.86,0.34,-0.75,-0.23 2GZR,GLU_108,4.4,0.21,0,-0.32 3N2T.GLU 165.4.95.0.22.0.0.24 1ZBP,ASP 83,3.7,-0.49,-0.13,0.52 2EYI,TYR_193,12.78,0,0.58,2.2 3LJN,ARG_33,13.07,-0.23,0.21,0.59 3E5T,ASP_206,3.31,-0.71,-0.04,0.26 1059,TYR_119,10.32,-0.07,0,0.39 2098, ARG 43, 12, 93, -0.37, 0.45, 0.35 106D,GLU_135,3.9,0.44,-0.85,-0.19 4EZB,GLU_183,5.25,3.55,-1.86,-0.95 3RKV,ASP_258,3.5,-0.83,-0.15,0.68 2D2S,GLU 673,4.73,0.47,0,-0.23 2EFK,GLU_170,4.59,0.22,0,-0.13 2Q98,TYR_147,10.25,0,0.07,0.18 3KV0,GLU_185,4.9,0.23,0,0.17 1NIJ,ASP_232,3.8,0,-0.23,0.24 2Z84.CYS 107.11.92.0.0.38.2.54 2GS5,ARG_34,12.09,-0.48,0,0.07 2FL7,TYR_207,10.25,0,-0.38,0.63 4EVF,GLU_158,3.66,1.28,-1.5,-0.62 3IBT,GLU 106,3.99,0.69,-0.64,-0.56 2WZ9,LYS_31,10.5,0,0,0 3JSN,GLU_292,4.92,0.33,0,0.1 2D2S,GLU_563,5.64,1.62,-0.19,-0.29 3CAN,GLU_130,3.83,0.41,-0.63,-0.47 2EYI,ARG_197,12.91,-0.13,0.1,0.45 3B79,LYS_53,10.36,-0.13,0,-0.01 2HP7,TYR 69,12.02,-0.02,0.23,1.81 2CN1,GLU_161,5.18,1.61,-0.85,-0.09 4ECC,CYS 182,11.59,-0.06,0.39,2.26 1PNE.CYS 70.11.54.0.-0.1.2.64 3R87,GLU_116,4.85,0.3,-0.25,0.29 2JKF,LYS_70,10.39,-0.11,0,0 3RLE,ASP_171,2.89,-1.7,-0.6,1.39 3A4C,LYS_482,10.54,-0.2,0,0.23 2QDJ,LYS_65,11.42,-0.35,0.84,0.43 2IDC,ASP_102,2.92,-0.64,-0.55,0.31 3EAZ,LYS_169,11.46,-0.27,0.85,0.38

2WB8,TYR 736,13,59,0,0,92,2,67 3M66,HIS_338,6.56,-0.77,0.79,0.04 1U3Y,ASP_318,3.32,-0.76,-0.1,0.38 1L2F,GLU_301,4.5,0.11,0,-0.11 3V10.LYS 577.11.18.-0.34.0.7.0.33 2A0J.ARG 69,11.94,-0.58,0.0.02 2XHC,TYR_255,9.93,0,-0.27,0.21 2EFK,GLU_240,2.99,0.45,-1.58,-0.38 2Q13,TYR_36,10.19,0,0,0.19 3COU.ASP 150.2.59.-1.68.0.0.47 3GG6,ARG_77,12.67,-0.27,0.04,0.41 2R51,LYS 192,10.2,-0.3,0,0 3BA1,LYS_177,10.48,-0.16,0,0.14 4ETX.TYR 208,9.88,0,-0.19,0.08 1T3Y.TYR 45.13.62.0.0.53.3.09 3FRR,ARG_147,12.46,-0.09,0,0.06 2NSN,HIS_19,7.54,-0.52,0.85,0.72 2YWJ,ASP_11,3.77,0,-0.21,0.17 2BDV.LYS 87.10.28.-0.22.0.0 3ELI,GLU_123,4.85,0.15,0,0.2 2IDC,ARG_104,13.11,-0.5,0.64,0.47 3HVM,LYS_239,10.98,-0.24,0.26,0.47 1YTD,ASP_264,3.08,-0.96,-0.4,0.63 3E7P,ASP 13,4.01,0.0.0.21 3IBT,ASP_200,3.63,0,-0.58,0.4 4FD6,HIS_211,5.69,-1.1,0.17,0.12 3CRM,TYR_263,10.35,0,0.03,0.32 2ZCX.GLU 161,4.44,0.15,0,-0.21 3BWT,GLU_642,4.75,0.41,0,-0.16 3RLN,CYS_737,10.88,-0.29,-0.82,3 3EYE,LYS_94,10.49,-0.27,0,0.26 3ILC,LYS 20,10,15,-0,44,0,0.09 100X.LYS 253,11.2,-0.2,0.42,0.48 2IRM,ARG_330,12.54,-0.54,0.11,0.48 2GQV,GLU_60,3.19,0.56,-1.57,-0.29 3F1X,TYR_70,10.08,0,0,0.08 1R6Y,ASP_58,4.01,0,-0.22,0.43 1RHS.TYR 36,12,66,-0.92,1,31,2,28 1ZYL,GLU_319,4.63,0.13,0,0 3PBH,ARG_85,12.28,-0.34,0,0.12 1BKR.TYR 103.10.13.0.-0.09.0.22 3M3P,LYS 196,10.63,-0.17,0.0.3 2R0S,LYS_172,10.3,-0.27,0,0.08 2CL3,ASP 133,3.06,-0.79,-0.34,0.39 1A8Q,ARG_113,13.27,-0.34,0.26,0.85 4EKU,GLU 315,4.51,0.08,0,-0.08 3O16,TYR 29,12,58,-1,67,0,4,25 3IVF,LYS_254,10.36,-0.14,0,0 1X91,ASP_93,2.59,-1.4,-0.24,0.43 1Y0K,ARG_117,12.22,-0.43,0,0.15 3MIX.GLU 664.3.95.0.39.-0.67.-0.26 4E8B,ASP_202,3.91,0,-0.02,0.14 3FHF,ARG_97,11.41,-1.32,0,0.22 2AXO,ARG_123,11.43,-1.04,0,-0.03 3C2E,ARG 15,13.19,-0.33,0.61,0.41 4DIU,LYS_212,10.18,-0.62,0,0.3 3IVF,LYS_66,11.02,-0.33,0,0.84 20YZ,LYS 55,10.38,-0.41,0,0.3 3D9H,ASP_192,3.65,-0.67,-0.06,0.58 2D8N,TYR 86,11.33,-0.72,0.19,1.86 1ZKZ,GLU_106,4.44,0.23,0,-0.28 3N0K,HIS_18,6.97,-1.03,0.85,0.65 1SQW,LYS_75,10.49,-0.06,0,0.06 2BCF,ARG 185,12.21,-0.6,0,0.31 2H2W,GLU_123,4.25,1.05,-1.3,0 4H86,HIS_66,2.57,-3.37,0.16,-0.72 3CAX,ARG_222,13.32,-0.31,0.61,0.52 2IRM,ASP 249,2.96,-0.99,-0.45,0.6 3O16,LYS_23,10.08,-0.47,0,0.05

1X91.GLU 3.4.54.0.21.0.-0.18 2V81.GLU 20.4.37.0.56.-0.68.-0.01 4DNU,ARG_234,12.13,-2.12,0.76,1 1NJ4,LYS_306,10.36,-0.41,0,0.27 1ZHV.GLU 113.4.78.0.16.0.0.12 2VGY.ARG 80.11.77.-0.95.0.0.22 3EOD, ASP_24, 2.91, -1.45, 0, 0.56 1X8F,ASP_10,2.82,-0.91,-0.35,0.29 3HYQ,ARG_181,12.77,-0.25,0.02,0.49 2HRZ.GLU 270.4.08.0.28.-0.45.-0.26 3LD1,LYS 244,10.98,-0.13,0.24,0.37 3FXH,TYR_57,9.68,-0.7,0.02,0.36 3GS3,ASP_206,3.61,-0.89,-0.16,0.86 2CVB,ARG_27,12.66,-0.26,0,0.42 3DSH,GLU_293,4.8,0.13,0,0.16 3I4T,ASP_235,3.98,0,-0.3,0.49 1YM5,GLU_240,3.41,0.8,-0.96,-0.93 2ZQ5,CYS_210,9.64,-0.37,-0.04,1.05 2H8O, ARG_177, 12.19, -0.35, 0, 0.04 2Q13,GLU_220,4.56,0.06,0,0 3A0X,ARG_643,12.76,-0.28,0,0.54 3GS3,GLU_65,4.47,0.24,0,-0.27 3I0C,ARG_199,11.98,-0.32,0,-0.19 3ASA.CYS 227,11.94,0,0.09,2.86 3NJM,CYS_34,10.45,0.36,0.3,0.79 1F2V,GLU_126,4.56,0.12,-0.02,-0.03 2D7U,TYR_190,10.13,0,0,0.13 1RZ2,TYR 110,12.49,0,0.54,1.94 1T3Y.GLU 122.5.04.0.7.0.-0.16 2D7J,ARG_144,13.31,-0.24,0.59,0.46 2RJD,TYR_211,13.56,0.85,0.85,1.86 2FD4.LYS 546.10.32.-0.19.0.0.01 1NIJ,HIS 187,6.41,-0.13,0,0.04 1X9G,ARG_43,13.48,-1.07,1.3,0.75 2BDD,HIS_22,6.37,-0.36,0.3,-0.07 200K,ASP_115,2.76,-1.05,-0.47,0.47 1YB2,ASP_133,2.9,-0.86,-0.39,0.35 3U2A,GLU_84,4.39,0.18,0,-0.3 3FFM,ARG_18,12.71,-0.8,0.58,0.43 4F3J,ASP_126,2.42,-2.19,-0.3,1.12 1X7F,HIS_172,6.47,-0.61,0.63,-0.05 2P0L,TYR 121,11.27,-0.01,0.08,1.2 4EVF.ASP 163.4.72.0.0.13.0.79 3SMD,LYS_8,10.32,-0.18,0,0 3O48,TYR_18,10.05,0,0,0.05 1GQE,ASP_208,2.78,-1.12,-0.3,0.39 1JYH,TYR_52,13.18,0.85,0.73,1.61 1P6F,GLU_21,4.57,0.18,0,-0.1 3PZ9,HIS 302,3.33,-4.77,1.63,-0.03 1J33,GLU_329,2.45,0.47,-1.87,-0.64 2C2Y,LYS 9,10.38,-0.21,0,0.1 4F8A,LYS 640,10.51,-0.1,0,0.11 2QK1,LYS_410,10.46,-0.85,0.52,0.29 3F1X,GLU_188,4.87,0.54,0,-0.17 4ANN,TYR_112,10.9,-0.19,-0.52,1.61 3JRT,GLU_121,3.74,0.32,-0.83,-0.26 2B02,CYS_380,10.99,-0.24,0.19,2.03 3HUE,ARG_46,12.19,-0.31,0,0 3R87, ASP_75, 2.72, -1.76, -0.83, 1.51 1XEU,ARG_241,12.72,-0.09,0,0.3 1WOU.ASP 79.3.21.-0.83.-0.16.0.4 2GZR,TYR_204,11.84,-0.08,-0.01,1.93 2PLQ,ARG_324,12.21,-0.3,0,0.01 2XWS,ARG_27,12.27,-0.3,0,0.07 3CS1,LYS_47,10.35,-0.32,0,0.18 1WXF,ARG_105,12.24,-0.26,0,0 3CAX,HIS_207,5.72,-3.78,1.6,1.4 3M7G,ARG_249,13.49,-0.58,1.07,0.5 2VGM,LYS_243,10.4,-0.21,0,0.12

3PZ9,LYS 120,11.16,-0.66,0.85,0.47 3M3PHIS 19.6.42,-1.27,0.85,0.33 1DVO,ASP_184,3.75,-0.57,0.2,0.33 3BWT.GLU 736.4.62.0.12.0.0 106D,LYS_91,11.38,-0.35,0.85,0.38 2R0S,ASP 114,4.02,0,-0.02,0.23 2Z0M,ARG_303,12.18,-3.23,1.6,1.31 3EVZ,ARG_126,12.78,-0.82,0.47,0.63 3RFY,TYR_433,10.67,0,0.33,0.34 1AIL,LYS_41,9.94,-0.51,0,-0.04 2CL3.GLU 51.4.71.0.21.0.0 3GE9,ARG_87,12.25,-0.25,0,0 3UPD.GLU 307.5.02.0.45.0.0.08 3M7G,GLU 89,4,53,0,18,0,-0,16 1G8P,ARG 187,11.96,-0.55,0,0.01 3Q9P,LYS_171,10.47,-0.03,0,0 3ZSL,ASP_154,3.43,-0.71,-0.18,0.53 2G5X,LYS_100,10.43,-0.45,0,0.38 3NR5.CYS 156.12.9,-0.06,-0.01,3.97 2G5X.ARG 184.12.09.-0.49.0.0.08 1R9W,ARG_330,12.37,-0.33,0,0.2 20KT.GLU 69.3.88.0.56.-0.85.-0.33 2G3A,LYS_15,11.16,-0.19,0.85,0 3RLN,HIS 755,3.81,-1.86,0,-0.82 3I4T,LYS 168,10,49,-0.01,0,0 3IPZ,ASP_116,2.25,-2.08,-0.45,0.99 3C38,LYS_163,10.13,-0.7,0,0.33 3Q6L,GLU_62,4.54,0.23,0,-0.2 3CS1,LYS 104,10.59,-0.13,0,0.22 1TD6,LYS_271,10.23,-0.55,0,0.27 3EVN.GLU 170.4.79.0.15.0.0.13 1RZ2,HIS_247,2.91,-3.54,0,-0.05 1PGV.ASP 235,1.59,-2.3,-0.47,0.56 3EVZ,ARG 37,11.94,-0.45,0,-0.1 3H13,ARG_435,11.9,-0.55,0,-0.04 3FFM,HIS_27,5.7,-0.75,0,-0.04 3EZ7,LYS_73,9.76,-0.66,0,-0.08 20BI,HIS 114,4.82,-2.01,0.34,-0.01 1DUN,ASP_33,4.02,0,-0.1,0.32 2G2D,ARG_32,12.03,-0.63,0,0.15 3ETV,ARG_328,12.32,-0.39,0,0.21 1NAR,HIS 75,5.62,-0.68,0.04,-0.24 3R2E,ASP 37,2.52,-1.18,-0.54,0.45 1O3X,LYS_198,10.37,-0.13,0,0 1SI7,TYR_114,9.67,-0.85,0.21,0.32 4D8L,GLU_14,4.61,0.25,0,-0.14 1AM2,ASP_20,2.98,-0.92,-0.38,0.48 3V55.LYS 709.10.3.-0.3.0.0.1 1ZBS,LYS_189,11.09,-0.24,0.46,0.37 3UAH,ARG_500,13.56,-0.2,0.72,0.53 2H85,GLU_228,4.32,0.37,-0.39,-0.17 1R3F.ARG 212,12,46,-0,15,0,0,11 2IF4,GLU_260,4.89,0.48,-0.21,0.13 1TXD,LYS_949,10.72,-0.17,0,0.38 1RZ2,ASP_64,3.94,0,0,0.14 1WYC,GLU_176,4.76,1.19,-1.27,0.34 1L3K.GLU 28,4.03,0.26,-0.86,0.14 2Q99,LYS_181,10.75,-0.11,0,0.36 4F8A,ASP_616,4.03,-0.33,-0.26,0.82 3V1Q,LYS_640,10.43,-0.04,0,-0.03 3ADO,LYS 287,10.69,-0.57,0.46,0.3 1WRU,ASP_202,3.76,0,-0.32,0.28 20K1.HIS 314.6.72.-0.09.0.31.0 1QYI,GLU_368,3.34,0.61,-1.34,-0.41 3DHN,ARG_171,13.61,-0.37,0.8,0.69 3UV9.GLU 395,3.49,1.33,-1.51,-0.83 1NWA,LYS_123,10.59,-0.15,0,0.24 3E0H,HIS_156,6.56,-0.29,0,0.34 2OGQ,TYR_510,9.64,-0.74,-0.65,1.03 3K8J,ARG_152,13,-0.77,0.7,0.58 2EYI,ASP_192,3.6,-0.2,-0.36,0.36 3F6M,GLU_151,3.69,0.34,-0.85,-0.31 1WPA, ARG 468, 12, 32, -0, 18, 0, 0 1RI6,ASP_71,3.26,-1.06,0.07,0.44 3EGN,GLU 462,4.42,1.22,-0.84,-0.45 3EYE,LYS 116,11.35,-0.87,0.85,0.87 2IF4,LYS_162,10.91,-0.25,0.28,0.38 3O48,GLU_15,4.26,0.27,-0.38,-0.13 1PSW,ASP_253,4.05,-0.62,-0.09,0.95 4AE7,TYR 70,11.48,0,0.13,1.35 2H2Z,TYR_154,10.07,0,0.01,0.06 3IL3,TYR_271,12.5,0.66,0.41,1.44 2Q13,LYS_375,10.4,-0.13,0,0.03 2GZR,HIS_287,5.51,-0.85,0,-0.14 3ANJ,TYR 278,10.17,-1.46,-0.26,1.91 3C2E,TYR_167,10.94,0,-0.39,1.33 2YT4,ARG_527,12.39,-0.11,0,0 4H86,LYS_32,11.04,-0.27,0.29,0.51 2Q5X,ARG 800,11.51,-1.12,0,0.13 3GW3.TYR 164.11.94.0.0.23.1.7 1RAJ,GLU_337,3.99,0.28,-0.64,-0.15 2Q34,LYS_228,10.48,-0.3,0,0.28 3E5T.ARG 95.12.31.-0.19.0.0 1DVO.LYS 125.9.95.-0.18.0.-0.38 3HQX,LYS_36,9.89,-0.8,0,0.18 3EX9.ARG 139.11.8.-1.0.0.3 1XTZ,HIS_259,5.92,-0.22,0,-0.36 1Q2Y,LYS_125,10.37,-0.24,0,0.11 3EOD,ARG 117,12.3,-0.25,0.0.05 2CE6,CYS_42,9.14,0,0.01,0.13 2AZL,GLU_269,4.53,0.2,0,-0.17 4ETX.GLU 418.2.62.0.89.-2.31.-0.46 2B0J,TYR_218,10.32,0,-0.05,0.37 3ETV,LYS_207,10.07,-0.58,0,0.15 1YW5,HIS_20,6.36,-0.14,0,0 1BN6,ARG_265,13.32,-0.5,0.84,0.48 2WB3,LYS_288,10.44,-0.06,0,0 2QDJ,ARG_73,12.24,-0.33,0,0.07 1JT9,TYR_74,10.05,-0.82,0.25,0.62 3LH5,GLU_568,4.45,0.34,0,-0.38 3EVZ,TYR_58,12.07,-0.09,-0.09,2.25 3HQX,GLU_98,4.76,0.15,0,0.11 1BN6,ASP_209,4.04,0,-0.6,0.84 1UAJ,ARG_92,13,-0.45,0.29,0.66 3FHF,ARG_152,13.3,-0.21,0.66,0.35 3DHN,GLU_60,4.52,0.43,-0.69,0.29 1X7F.ASP 254.3.89.0.-0.03.0.12 2W0G,GLU_200,4.32,0.27,-0.2,-0.25 2Q12,ARG_171,11.6,-0.76,0,-0.14 1QQL,TYR_64,10.14,-0.04,-0.5,0.68 3EAZ,GLU 93,4.57,0.46,0,-0.39 1Z3X,TYR_64,11.64,0,0,1.64 4EZB,ASP_90,3.31,-0.4,-0.32,0.23 2BV9,HIS_287,6.3,-0.19,0,-0.02 1AK1,HIS_262,4.46,-2.55,0.35,0.17 3K1H,LYS_60,10.47,-0.22,0,0.2 3CGW,GLU_269,4.59,0.18,0,-0.09 3CX2,ASP_228,3.79,-0.08,-0.23,0.3 1WXQ,ASP_361,3.74,-0.06,-0.23,0.23 1F2V,GLU 178,4.82,0.22,0,0.1 3DTE,TYR 234,10.91,-0.06,0.04,0.94 1N81,LYS_173,10.66,-0.2,0,0.37 2ZCO,LYS_16,10.43,-0.19,0,0.12 4AM1,TYR_211,12.23,-0.07,0.1,2.2 2GZR,HIS_264,6.24,-0.34,0,0.08 2AHE,ASP_28,2.24,-1.99,0,0.43 3GEC,TYR_264,12.26,-0.69,-0.33,3.28 2Q07,LYS_286,9.94,-0.34,0,-0.21

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3M70,LYS 26,10,29,-0,35,0,0,14 2EEY,HIS_156,6.91,-0.37,0.79,-0.01 4ETX,ASP_271,3.99,0,-0.3,0.49 3G9T,LYS_39,10.43,-0.07,0,0 4E6S.ARG 75.12.19.-0.38.0.0.07 1XIP.ASP 244.3.53,-0.61,-0.13.0.48 3LJI,ARG_285,12.48,-0.74,0.42,0.3 2A6B,ASP_73,1.83,-2.13,-0.43,0.59 3F7M,ARG_122,12.43,-0.28,0,0.21 2Q5X,ARG_834,12.81,-0.48,0.24,0.55 3FFM,HIS_77,6.22,-0.39,0,0.12 3EVZ,GLU_188,4.64,0.28,0,-0.14 3AU3,HIS_668,5.68,-1.53,0.72,0 3KB5.ARG 278.12.71.-0.28.0.16.0.33 2P52.GLU 282.4.69.1.7.-0.82.-0.69 1A8Q,GLU_99,3.92,4.25,-1.36,-3.46 3V3T,HIS_51,5.88,-0.53,0.16,-0.25 2R0S,TYR_247,12.81,0.01,0.67,2.13 1RZ2.LYS 249.10.58.-0.51.0.0.59 3QYB,LYS_917,11.54,-0.36,0.85,0.55 2B61,TYR_24,10.28,0,0.11,0.16 2X5Y,GLU_852,2.88,0.48,-1.76,-0.33 2W2S,ASP_30,3.03,-0.85,0,0.08 1A80,ARG 86,12,17,-0.26,0,-0.07 2BT8, ASP_215, 3.92, 0, -0.21, 0.34 1JYH,LYS_155,10.48,-0.31,0,0.3 3QAV,ARG_101,12.19,-1.75,0.38,1.07 1FQI,ASP 286,2.37,-1.53,-0.41,0.51 1SQH,GLU_160,3.82,0.27,-0.9,-0.06 3V55,TYR_367,10.79,-0.4,0.3,0.88 3FS3,TYR_276,10.18,-0.72,-0.17,1.08 2DFL.ARG 66.12.47.-0.13.0.0.1 1VSM.LYS 166.10.18.-0.31.0.-0.01 3JZ9,CYS_446,12.09,-0.01,0.28,2.83 3HZO.GLU 4.4.59.0.09.0.0 2F4Q,ARG_78,12.26,-0.41,0,0.18 1QQL,GLU_62,4.48,0.25,0,-0.27 2WB3.LYS 336.10.15.-0.4.0.0.06 1X04,TYR_203,10.31,-0.85,-0.16,1.31 2H01,ASP_145,3.84,0,-0.22,0.26 1SUU.LYS 787.10.35.-0.17.0.0.02 2BDD.TYR 130.11.97.0.85.0.51.0.6 2Q98,GLU_143,4.56,0.14,0,-0.08 2ILR,GLU_517,4.63,0.23,0,-0.1 1LPL,LYS_183,10.56,-0.43,0,0.5 4AM1,ARG 208,10.68,-3.03,0.03,1.18 2C2Y.GLU 250.4.46.0.12.0.-0.15 1R7J,LYS 84,10.43,-0.12,0.0.05 1PVT,LYS_191,10.41,-0.27,0,0.19 1NWA,ASP_64,2.69,-1.61,-0.33,0.82 3V3T,ARG 252,13,13,-0,19,0,52,0,3 1X8EGLU 223.4.65.0.26.0.-0.11 1TUL,TYR_57,10.6,-0.8,0.21,1.18 3I47,LYS_160,10.49,-0.22,0,0.21 1HF8,HIS_84,4.75,-1.75,0,-1.39E-17 2ZQ5,TYR_313,12.4,0.85,0.44,1.1 1TR9,GLU_247,4,0.55,-0.75,-0.29 2APL,GLU_83,4.93,0.34,0,0.09 1ZCU,ASP_44,3.75,0,-0.22,0.17 1SUU,ASP_679,3.9,0,-0.28,0.38 2YX0.ASP 327.2.85.-1.05.-0.62.0.72 4FLE,HIS 31,5.68,-0.69,0,-0.12 2D0A,TYR_104,12.21,-0.85,0.33,2.72 3HVM,LYS_48,10.46,-0.12,0,0.08 3C38,LYS 240,10,53,-0,26,0,0,29 2R2Y,ASP_53,3.85,-0.06,-0.01,0.12 3LH5,ARG_752,12.49,-0.19,0,0.18 3Q6L,GLU_55,4.49,0.27,0,-0.28 1V43,ASP_120,2.4,-1.52,-0.34,0.46 3N0K,HIS 89,6.05,-0.73,0.35,-0.08 3E5T.GLU 185.3.1.0.24.-1.64.0 2IIA,TYR_60,11.75,-0.01,0.33,1.43 105T,ARG_300,12.58,-0.52,0,0.61 106D,LYS_16,10.23,-0.14,0,-0.14 1ANU,CYS 33,12.88,0,0.18,3.71 3T57,GLU_289,4.74,0.16,0,0.09 4FZR,GLU_304,5.34,0.86,0,-0.02 3NR5,CYS_34,11.26,-0.11,-0.1,2.47 3G6S,ARG_56,12.5,-0.36,0,0.36 3I4T,LYS 73,11.39,-0.34,0.85,0.38 3ADO,ASP_219,4.03,0,-0.01,0.23 2HXB,ASP_49,3.07,-1.02,0,0.28 3VJ8,TYR_304,12.68,-0.01,0.3,2.38 3COU,CYS 23,12.65,-0.02,0.28,3.39 2GZR,HIS_238,4.61,-2.21,0.08,0.24 1F2V,ASP_9,3.58,-0.51,0,0.28 3JV1,ARG_83,12.07,-0.9,0.11,0.36 1DUN,GLU 15,4.24,0.28,-0.66,0.12 1ES9,HIS 180.6.52,-0.31,0.0.33 3A2Z,ASP_77,4.07,0,-0.39,0.65 1ZBS,GLU_144,3.84,1.55,-1.8,-0.41 3DZ1,LYS_55,10.62,-1.22,0.78,0.55 1MTZ,LYS_139,10.37,-0.25,0,0.13

2188.GLU 394.5.26.0.85.0.-0.08 3UX2,ARG_106,12.34,-0.16,0,0 2CWC,TYR_294,9.83,-0.36,-0.74,0.92 3ERF,ASP_78,3.88,0,-0.02,0.11 1ES5.LYS 197.10.37.-0.13.0.0 4EUG.GLU 13.4.6.0.11.0.-0.01 3CSR,CYS_36,11.98,0,-0.07,3.04 2B6P,ARG_156,12.47,-0.03,0,0 10IS,GLU_246,4.63,0.13,0,0 3JZN.GLU 131.2.93.0.46.-1.38.-0.64 1V6T,LYS_216,10.37,-0.35,0,0.23 2GYZ,ARG_38,12.46,-0.04,0,0 1QQL,TYR_97,13.84,0,0.58,3.26 3ILC.CYS 151,12.61.0.0.3.61 3M16.GLU 156.3.96.0.59.-0.75.-0.38 3B7H,LYS_2,11.53,-0.32,0.85,0.5 2H30,LYS_55,10.46,-0.12,0,0.08 2RIK,LYS_184,9.93,-0.33,0,-0.23 3B4D,ARG_248,12.92,-0.37,0.34,0.45 3EJG.ARG 99.12.61.-0.31.0.0.41 3DTE,TYR_205,9.26,-0.59,-0.31,0.15 1YLN,HIS_113,6.31,-0.38,0,0.19 3EZ7,GLU_354,4.58,0.15,0,-0.06 3CJW,HIS_333,6.33,-0.46,0,0.29 3C6B,ARG_232,12.8,-0.51,0.07,0.74 3H5T,HIS_117,6.47,-0.29,0,0.26 2B2H,TYR_129,13.89,-0.1,0.12,3.87 2GS5.ASP 31.4.12.0.0.0.32 3RJX.GLU 317.8.38.4.37.-0.78.0.29 2I88,LYS_420,10.65,-0.07,0,0.22 2QHT,ASP_160,4.29,0,0.08,0.4 2PPN,GLU_60,4.04,1.07,-1.44,-0.09 3HNX,GLU 86,4.59,0.2,0,-0.11 1SJY,TYR 139,10.24,-0.03,0.05,0.21 2YX0,HIS_292,6.32,-1.24,0.85,0.21 1J85,CYS_22,12.72,0,0.13,3.6 2YLF,TYR_196,13.22,0,0.87,2.35 1XTD,GLU_81,4.44,0.2,0,-0.26 2YLF,LYS_142,10.74,-0.14,0.38,0 2APL,GLU_85,3.97,0.41,-0.85,-0.09 3HNX,HIS_88,7.3,-0.44,0.85,0.4 1MML,GLU 123,4.12,0.3,-0.52,-0.15 1JT9.GLU 261.4.73.0.25.-0.02.0 1Z3X,TYR_165,13.89,0,0.74,3.15 2GAU,GLU_184,4.18,0.27,-0.57,-0.01 20VT.TYR 38.11.26.0.-0.05.1.31

3BCY,ASP 65,3,49,-0,73,-0.03,0,45 3JZN,TYR 365,12.95,-0.08,-0.62,3.65 3KB5,GLU_399,4.6,0.09,0,0.01 1P2F,LYS_149,10.16,-0.62,0,0.27 2CXC,ASP_77,3.26,-0.8,-0.12,0.37 3CGW.GLU 83.447.032-038.003 1UJ8,TYR_27,10.68,0,0.44,0.23 2RIK,HIS_112,6.5,-0.25,0,0.26 2GAU,CYS_96,10.39,-0.06,-0.18,1.62 2P65,ASP_74,3.74,-0.01,-0.22,0.16 2WZ9,LYS_79,11.04,-0.35,0.33,0.56 3GT0,LYS_24,10.27,-0.28,0,0.05 2AH5,LYS_41,10.32,-0.12,0,-0.06 2CWC,ARG_106,12.65,-0.09,0,0.25 2RJD,ARG 321,12,29,-0,21,0,0 1ZBM,ASP 151,2.46,-1.37,-0.39,0.43 1WOU,ARG_85,11.92,-0.63,0,0.06 1NRI,GLU_238,4.65,0.15,0,0 1059,LYS_2,10.5,0,0,0 2I88,LYS 369,10.62,-0.11,0,0.23 2BLL,ARG_355,10.95,-1.11,0,-0.44 3EJG,TYR_106,13.35,-1.57,0.7,4.22 3N0K,ASP_52,4,-0.06,-0.25,0.5 1CBY,LYS 208,10.5,-0.05,0.0.05 1ES5.ARG 30.12.58.-0.38.0.02.0.44 20YZ,ASP_85,3.98,0,-0.04,0.22 208I,ARG_99,12.2,-0.26,0,-0.05 2FI9,GLU_64,4.7,0.28,0,-0.08 4DIU,ARG_16,13.2,-0.54,0.28,0.96 2B2H,GLU_85,4.66,0.28,0,-0.12 2D0A,LYS_206,10.23,-0.47,0,0.2 2G2D,ARG_133,11.28,-1.14,0,-0.08 2VGM.TYR 255,10.09,0,-0.09,0.19 1P1L.LYS 26.10.31.-0.3.0.0.11 2QVO,GLU_16,4.58,0.52,-0.21,-0.24 1ES5,TYR_222,10.09,0,-0.1,0.2 1TLV,ASP_91,3.52,-0.06,-0.47,0.25 4DNU,GLU_189,4.42,0.42,0,-0.5 2XMZ,LYS 79,11.36,-0.29,0.58,0.57 200K,ARG_86,11.86,-1.86,0.26,0.96 3EUR,LYS_63,10.41,-0.14,0,0.05 3CIV.ASP 74.4.05.0.0.04.0.21 3CJW,ASP_290,3.14,-0.58,-0.42,0.34 3C2E,TYR_135,12.48,-0.02,0.68,1.82 3RNV,LYS_362,10.44,-0.06,0,0 2W0G,HIS_180,5.81,-0.85,0.36,-0.2