

# 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]

Stefano M. Marino, İnanç Soylu

Akdeniz University, Department of Agricultural Biotechnology, Antalya

RESULTS of ppka1 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_147,2.76,0.56,-1.6,0	2E3S,GLU_494,4.5,0,0,0	2QHT,GLU_203,4.5,0,0,0	3ASA,GLU_349,3.84,0.14,-0.8,0
4FD6,LYS_106,10.43,-0.07,0,0	1O9G,ARG_34,11.1,-1.4,0,0	2D7J,LYS_174,10.5,0,0,0	2FM9,LYS_133,10.29,-0.21,0,0
3Q1C,HIS_155,1.49,0.33,-0.45,-4.89	2O0K,ASP_242,3.47,0.07,-0.4,0	4E9E,ASP_568,3.85,0.14,-0.09,0	2H14,CYS_334,8.67,-0.39,0,0.07
3K8J,ASP_114,3.87,0.07,0,0	3U2A,ARG_88,12.22,-0.28,0,0	2V4U,GLU_356,4.71,0.21,0,0	2X5Y,CYS_798,10.15,-0.03,0,1.18
1MUF,ARG_103,12.22,-0.28,0,0	2O8P,GLU_10,4.06,0.28,-0.72,0	1MHN,ARG_133,12.5,0,0,0	4H4J,ARG_139,12.22,-0.28,0,0
1AK1,HIS_88,0.98,0.3,-1.97,-3.85	4F85,ASP_154,3.36,0.28,-0.71,0	2YYO,ASP_14,3.87,0.07,0,0	2B02,LYS_394,10.36,-0.14,0,0
3Q1C,ARG_156,12.01,-0.49,0,0	3M16,LYS_323,10.43,-0.07,0,0	2WB8,CYS_762,8.72,-0.28,0,0	2P5D,ARG_123,12.5,0,0,0
1XFK,ARG_313,11.8,-0.7,0,0	2W0G,GLU_207,3.66,0.14,-0.99,0.9	2GAU,HIS_74,3.25,0,-1.77,-1.48	2Q34,ARG_85,12.22,-0.28,0,0
3AUF,ASP_20,3.41,0.56,-0.95,0	2GKG,GLU_114,4.57,0.07,0,0	2IQT,LYS_164,10.36,-0.14,0,0	3UAH,GLU_276,4.57,0.07,0,0
1JKS,GLU_18,3.84,0.14,-0.8,0	2XJ4,HIS_262,6.5,0,0,0	1RZ2,LYS_55,10.29,-0.21,0,0	2RIS,TYR_87,11.58,0,-0.01,1.6
1NJ4,LYS_186,10.36,-0.14,0,0	1SQW,HIS_77,6.43,0,0,-0.07	3FHF,ASP_20,3.29,0.35,-0.86,0	1RI6,ASP_70,3.28,0.14,-0.66,0
1OTM,GLU_150,6.13,1.13,-1.17,1.67	2E3S,ARG_406,12.08,-0.42,0,0	2ZOM,ASP_78,3.28,0.28,-0.8,0	1XKR,LYS_33,10.15,-0.35,0,0
1O6D,GLU_54,4.23,0.7,-0.97,0	2OSA,ASP_335,2.73,0.63,-1.7,0	4H89,HIS_154,6.43,0,0,-0.07	1MUF,GLU_220,4.78,0.28,0,0
3V55,ARG_374,10.54,-1.96,0,0	3RFF,TYR_122,9.99,0.21,-0.22,0.0	3M66,LYS_299,10.5,0,0,0	1Q42,ASP_89,3.97,0.42,-0.25,0
2EDM,TYR_69,10.39,0.52,-0.13,0	3PZ9,TYR_291,10.07,0.07,0,0	2IF4,LYS_117,10.22,-0.28,0,0	1ILW,LYS_121,10.36,-0.14,0,0
4H4J,LYS_222,10.36,-0.14,0,0	1FO9,TYR_185,9.22,0.14,-1.99,1.07	1HF8,TYR_222,11.72,0.21,-0.64,2.15	2ZCO,TYR_24,10.14,0.14,0,0
1UAJ,GLU_116,4.64,0.14,0,0	3KT9,ARG_18,12.15,-0.35,0,0	1WYC,HIS_191,6.43,0,0,-0.07	4DNU,HIS_258,1.24,0.45,-1.64,-4.08
2QZQ,HIS_163,6.76,0.41,0,-0.14	2BLL,GLU_412,4.12,0.42,-0.8,0	3JZN,ASP_438,2.1,0.7,-2.4,0	2B0A,LYS_65,10.5,0,0,0
1T6L,ARG_218,12.22,-0.28,0,0	1ES9,HIS_106,6.36,0,0,-0.14	3EOD,ARG_115,11.94,-0.56,0,0	3G9T,TYR_125,11.41,1.41,0,0
2W1R,ASP_78,1.54,0.63,-2.89,0	3ZTA,GLU_77,3.86,0.35,-0.99,0	3FXH,GLU_34,4.39,0.07,-0.18,0	1ZP2,ASP_148,4.14,0.49,-0.15,0
2IRM,GLU_80,4.57,0.07,0,0	3CRM,GLU_237,4.5,0,0,0	2G5X,LYS_125,10.29,-0.21,0,0	2APL,GLU_17,3.98,0.28,-0.8,0
3FWU,HIS_14,6.43,0,0,-0.07	3ETV,LYS_234,10.22,-0.28,0,0	2X4G,TYR_154,10.75,0.55,0,0.2	2YLF,ASP_93,2.98,0.28,-1.1,0
3EVP,HIS_297,4.7,0.29,0,-2.09	1T95,ASP_11,2.72,0.07,-1.15,0	3DZ1,LYS_2,10.5,0,0,0	1XEU,GLU_195,4.92,0.42,0,0
3SMD,LYS_142,10.29,-0.21,0,0	4DNU,LYS_115,10.5,0,0,0	1OXZ,ASP_285,3.95,0.28,-0.13,0	3CE7,TYR_23,10,0,0,0
3HVM,CYS_28,8.6,-0.4,0,0	2AZL,LYS_217,10.5,0,0,0	3SMD,TYR_92,9.52,0.05,-0.53,0	2C2Y,HIS_160,6.48,0.05,0,-0.07
3IL3,TYR_203,10.96,0.07,0,0.89	2IXM,GLU_115,3.78,0.07,-0.79,0	3GV0,GLU_175,3.98,0.28,-0.8,0	1QQE,GLU_282,4.5,0,0,0
3BCH,ARG_186,12.01,-0.49,0,0	3COU,HIS_99,4.16,0.08,0,-2.42	2AHE,CYS_35,5.11,-5.33,-0.22,1.67	1YM5,GLU_245,4.5,0,0,0
1XFK,HIS_117,6.97,0.69,0,-0.21	2B6P,ARG_153,11.73,-0.77,0,0	4H4J,CYS_58,8.93,-0.61,0,0.54	1XIP,GLU_303,4.78,0.28,0,0
3LJI,LYS_62,10.5,0,0,0	4EKU,ARG_39,11.66,-0.84,0,0	3MEW,ARG_202,12.01,-0.49,0,0	3EJC,ARG_107,12.43,-0.07,0,0
1IAP,HIS_200,6.42,0.06,0,-0.14	3OOP,LYS_17,10.43,-0.07,0,0	1LZL,ASP_34,3.85,0.14,-0.09,0	3PP8,GLU_300,4.64,0.14,0,0
1JT9,LYS_248,10.36,-0.14,0,0	3GE9,ASP_22,3.11,0.14,-0.82,0	3M7G,GLU_262,4.64,0.14,0,0	3B21,ASP_198,3.33,0.14,-0.61,0
1JKS,LYS_50,10.5,0,0,0		2EHG,ASP_142,4.0,0.21,-0.01,0	

2HXB,LYS\_52,10.43,-0.07,0,0  
 1X7F,TYR\_22,10.39,2.18,-1.79,0  
 3IOO,LYS\_245,10.5,0,0,0  
 4FZN,GLU\_4,4.57,0.07,0,0  
 1P6F,TYR\_173,11.76,0.14,-0.79,2.4  
 3IBT,ASP\_67,3.27,0.42,-0.95,0  
 3ILC,HIS\_0,6.22,0,0,-0.28  
 3TOW,ARG\_153,11.94,-0.56,0,0  
 4AF2,ASP\_37,3.41,0.35,-0.74,0  
 1BYI,GLU\_12,4.5,0,0,0  
 1U3Y,ASP\_297,3.87,0.07,0,0  
 1NAF,ASP\_247,3.8,0,0,0  
 1FKM,ARG\_460,12.29,-0.21,0,0  
 3CGW,GLU\_170,4.13,0.49,-0.86,0  
 2DFL,ASP\_16,3.8,0,0,0  
 1OGL,ARG\_9,12.5,0,0,0  
 2EFK,LYS\_66,10.22,-0.28,0,0  
 3DB9,ASP\_117,3.13,0.14,-0.81,0  
 1YTD,TYR\_361,11.15,1.55,-0.28,-0.11  
 1BN6,HIS\_199,6.48,0.12,0,-0.14  
 3AU3,GLU\_582,2.62,0.84,-2.71,0  
 2PGX,ARG\_112,12.22,-0.28,0,0  
 1UXQ,ARG\_46,12.29,-0.21,0,0  
 3JSN,ARG\_172,11.59,-0.91,0,0  
 2RFA,GLU\_68,4.64,0.14,0,0  
 4AE7,TYR\_149,10,0,0,0  
 1DTO,ARG\_27,12.29,-0.21,0,0  
 3C38,HIS\_120,6.43,0,0,-0.07  
 1YTD,ARG\_378,13.02,-2.28,0,2.8  
 1Y2Q,ARG\_108,11.73,-0.77,0,0  
 3BCY,HIS\_85,4.9,0,0,-1.6  
 2EYI,GLU\_143,4.5,0,0,0  
 1NAF,HIS\_235,7.44,0.94,0,0  
 1DVO,LYS\_35,10.5,0,0,0  
 2ZTY,GLU\_96,3.67,0.35,-1.18,0  
 3FTT,GLU\_123,4.85,0.35,0,0  
 3TMO,ASP\_236,3.36,0.42,-0.86,0  
 2EEY,CYS\_124,10.05,0,0,1.05  
 2VGM,LYS\_2,10.29,-0.21,0,0  
 3N2T,HIS\_149,6.95,0.59,0,-0.14  
 2VGM,GLU\_304,3.63,0.21,-1.08,0  
 2V1L,HIS\_108,6.5,0,0,0  
 1R53,LYS\_237,10.43,-0.07,0,0  
 3UOV,ARG\_117,11.31,-1.19,0,0  
 1P4X,HIS\_153,6.5,0,0,0  
 4FH3,ARG\_293,10.93,-1.57,0,0  
 3KT9,LYS\_39,10.5,0,0,0  
 1MHN,ASP\_96,3.29,0.7,-1.22,0  
 3ZSL,ASP\_215,3.28,0.28,-0.8,0  
 1O9G,TYR\_4,10.07,0.07,0,0  
 3MIX,GLU\_507,4.57,0.07,0,0  
 4AE7,LYS\_191,10.43,-0.07,0,0  
 3NZL,ASP\_32,3.94,0.14,0,0  
 2CXY,LYS\_89,10.29,-0.21,0,0  
 1NAR,ASP\_20,2.95,0.28,-1.14,0  
 3DZ1,ASP\_237,3.71,0,-0.09,0  
 3KEY,LYS\_363,10.43,-0.07,0,0  
 3Q9P,HIS\_90,6.43,0,0,-0.07  
 4FCU,ASP\_43,2.98,0.49,-1.3,0  
 4AF2,CYS\_95,9.44,-0.09,0,0.53  
 3GT0,GLU\_158,4.57,0.07,0,0  
 1OSJ,GLU\_44,4.5,0,0,0  
 2AZL,GLU\_141,4.5,0,0,0  
 2NRR,HIS\_488,6.43,0,0,-0.07  
 1JKS,GLU\_187,0.69,2.05,-3.46,-2.4  
 3CQ1,ARG\_46,11.87,-0.63,0,0  
 3GVO,GLU\_78,4.05,1.28,-1.73,0  
 3H6Q,LYS\_97,10.22,-0.28,0,0  
 2F4Q,TYR\_77,12.83,1.2,0,1.63  
 4GCO,LYS\_155,10.5,0,0,0  
 2G2D,GLU\_101,4.0,21,-0.71,0  
 4DVD,LYS\_59,10.36,-0.14,0,0  
 2X5Y,LYS\_882,10.15,-0.35,0,0  
 3CS1,LYS\_64,10.01,-0.49,0,0  
 3I4T,LYS\_13,10.5,0,0,0  
 3IOO,ASP\_98,2.9,0.35,-1.25,0  
 2JKF,GLU\_107,3.82,0.21,-0.89,0  
 3CIV,CYS\_147,8.99,-3.31,-0.97,4.26  
 2FPN,TYR\_37,10.84,0,-0.21,1.04  
 3R87,ARG\_77,11.59,-0.91,0,0  
 2OJQ,LYS\_583,10.29,-0.21,0,0  
 3V1Q,HIS\_594,6.36,0,0,-0.14  
 3BCY,ASP\_117,4.12,0.35,-0.03,0  
 1JKS,ASP\_268,2.17,0.28,-1.91,0  
 3KV0,ARG\_140,12.08,-0.42,0,0  
 1DUN,ASP\_116,3.03,0.56,-1.33,0  
 2FL4,LYS\_37,10.5,0,0,0  
 3N2T,ASP\_93,2.78,0.77,-1.79,0  
 3JSN,ARG\_252,12.15,-0.35,0,0  
 2E3C,ASP\_206,1.75,0.7,-2.75,0  
 3LQE,ASP\_231,3.72,0.21,-0.29,0  
 3FXH,HIS\_33,7.1,0.67,0,-0.07  
 1GXN,TYR\_573,10,0,0,0  
 4D8L,ASP\_207,1.22,0.56,-3.14,0  
 3M3P,HIS\_176,12.1,5.2,5.52,-5.13  
 2FC3,LYS\_74,10.5,0,0,0  
 2CE6,ASP\_12,1.78,0.84,-2.87,0  
 1YM5,GLU\_15,4.71,0.21,0,0  
 3I47,ASP\_186,1.26,0.63,-3.17,0  
 4EF5,ARG\_310,13.25,-1.05,0,1.8  
 2YX0,TYR\_274,10,0,0,0  
 2CBE,TYR\_128,13.06,0.14,0.52,2.4  
 1YOY,TYR\_141,10,0,0,0  
 3DTE,ARG\_241,12.22,-0.28,0,0  
 3H04,LYS\_11,10.5,0,0,0  
 2NRK,GLU\_61,4.5,0,0,0  
 3RFY,ASP\_193,3.86,0.21,-0.15,0  
 3ONH,ARG\_466,11.73,-0.77,0,0  
 3CCY,ARG\_75,11.66,-0.84,0,0  
 1SFE,ARG\_172,11.58,-1.35,0,0.43  
 3BJV,GLU\_42,4.85,0.35,0,0  
 3JZ9,LYS\_382,10.29,-0.21,0,0  
 1DZF,ARG\_17,11.66,-0.84,0,0  
 1XTZ,TYR\_99,10.07,0.07,0,0  
 1AD6,ARG\_544,12.22,-0.28,0,0  
 2RGY,HIS\_164,4.72,0,0,-1.78  
 1ZCE,TYR\_7,12.24,2.24,0,0  
 1WP5,HIS\_321,7.2,0.78,0,-0.07  
 3ADO,LYS\_307,10.08,-0.42,0,0  
 3GOZ,ASP\_316,2.13,0.63,-2.31,0  
 1QYI,HIS\_357,6.36,0,0,-0.14  
 4F3J,ASP\_120,3.8,0,0,0  
 1TD6,LYS\_34,10.5,0,0,0  
 3ETV,LYS\_301,10.43,-0.07,0,0  
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 2HP7,GLU\_145,4.35,0.07,-0.22,0  
 2B0J,LYS\_185,10.29,-0.21,0,0  
 1R7J,ARG\_39,12.43,-0.07,0,0  
 3I4T,CYS\_98,9.13,0,0,0.13  
 1YW5,GLU\_165,4.05,0.35,-0.8,0  
 3R2E,ARG\_85,12.36,-0.14,0,0  
 1X1E,GLU\_118,4.5,0,0,0  
 1RH5,HIS\_51,2.84,0,0,-3.66  
 1XTZ,GLU\_257,3.91,0.21,-0.8,0  
 4FD6,GLU\_114,3.53,0.63,-1.6,0  
 4F85,HIS\_57,4.14,1.39,0,-3.75  
 3IBT,CYS\_52,10.08,-0.92,-0.08,2.08  
 1A8Q,HIS\_52,4.51,1.99,1.69,-5.67  
 3H8Y,GLU\_69,4.85,0.07,0.28,0  
 4EKU,CYS\_61,7.82,-1.51,0,0.33  
 1KN3,GLU\_33,4.78,0.28,0,0  
 2X4J,ASP\_33,1.83,0.28,-2.25,0  
 3IOO,ASP\_295,3.93,0.14,-0.01,0  
 3P28,TYR\_103,10,0,0,0  
 1WYC,TYR\_13,9.14,0.14,-1.05,0.05  
 1R3F,LYS\_265,10.22,-0.28,0,0  
 1ZYL,GLU\_262,4.89,1.73,-1.34,0  
 1OXZ,LYS\_213,10.43,-0.07,0,0  
 4DND,LYS\_16,10.5,0,0,0  
 1T95,LYS\_160,10.5,0,0,0  
 1PZC,GLU\_4,4.57,0.07,0,0  
 3OKQ,TYR\_558,13.41,0.21,0.8,2.4  
 1X04,GLU\_56,4.78,0.28,0,0  
 2V4U,ARG\_477,12.08,-0.42,0,0  
 3FNI,ARG\_149,11.94,-0.56,0,0  
 3IU5,ASP\_59,2.1,0.7,-2.4,0  
 3LPZ,ARG\_98,12.22,-0.28,0,0  
 1GQE,TYR\_244,11.37,1.03,-1.04,1.38  
 4EVF,GLU\_63,5.04,0.94,-1.33,0.92  
 1SIG,ARG\_122,11.87,-0.63,0,0  
 4ETX,ARG\_381,11.94,-0.56,0,0  
 1YB2,TYR\_190,10.28,0.13,0,0.15  
 4DBX,ASP\_286,3.8,0,0,0  
 1XTD,LYS\_169,10.08,-0.42,0,0  
 3EX9,ASP\_96,3.24,0.56,-1.12,0  
 3BWT,ARG\_788,11.87,-0.63,0,0  
 3HZQ,GLU\_36,4.5,0,0,0  
 4F8A,ASP\_631,3.74,0.35,-0.41,0  
 2FM9,GLU\_153,4.57,0.07,0,0  
 3ETV,GLU\_158,4.26,0.56,-0.8,0  
 2QK0,ASP\_66,1.92,0.56,-2.44,0  
 1XEU,GLU\_269,4.57,0.07,0,0  
 1TD6,GLU\_53,4.57,0.07,0,0  
 1DTO,CYS\_140,10.25,0,0,1.25  
 1L2F,TYR\_35,9.62,0,-0.38,0  
 3G9B,TYR\_42,12.98,1.5,-1.08,2.56  
 2P5D,LYS\_73,10.36,-0.14,0,0  
 3M7G,GLU\_169,4.77,0.35,-0.08,0  
 3H13,LYS\_245,10.5,0,0,0  
 4FH3,GLU\_124,3.96,0.21,-0.75,0  
 3V1Q,HIS\_503,7.18,0.75,0,-0.07  
 3F1X,LYS\_31,10.36,-0.14,0,0  
 3G9G,TYR\_8,13.38,0.07,0.46,2.85  
 3G59,ASP\_22,3.82,0.56,-0.54,0  
 3H8Y,ASP\_73,3.87,0.07,0,0  
 2ZQ5,TYR\_169,11.03,0,0,1.03  
 3H5T,GLU\_348,4.57,0.07,0,0  
 1AK1,LYS\_205,10.15,-0.35,0,0  
 3RRQ,GLU\_136,4.49,0,-0.01,0  
 2OPJ,ARG\_113,12.95,-1.43,0,1.88  
 1YLN,GLU\_117,4.64,0.14,0,0  
 1YM5,GLU\_161,4.67,0.28,-0.11,0  
 3QKY,TYR\_146,11.44,0.07,0,1.37  
 4EUG,GLU\_211,4.71,0.21,0,0  
 2RH3,GLU\_164,4.5,0,0,0  
 3G59,GLU\_111,4.5,0,0,0  
 3COU,ASP\_66,1.22,1.05,-3.63,0  
 2Q5X,GLU\_761,4.5,0,0,0  
 3H13,ASP\_343,2.61,0.49,-1.69,0  
 4EVF,LYS\_37,10.5,0,0,0  
 3ONH,ASP\_530,3.94,0.14,0,0  
 1WRU,GLU\_278,4.4,0.83,-0.8,-0.13  
 3C38,LYS\_225,10.08,-0.42,0,0  
 1ZYL,ARG\_58,13.85,-2.0,3.35  
 1RLO,LYS\_235,10.43,-0.07,0,0  
 1E59,HIS\_53,5.25,0,0,-1.25  
 1RKA,GLU\_172,4.57,0.07,0,0  
 3CS1,LYS\_92,10.5,0,0,0  
 3PM2,GLU\_26,4.71,0.21,0,0  
 3RFY,ASP\_141,3.94,0.14,0,0  
 200K,ARG\_30,11.87,-0.63,0,0  
 3LH5,GLU\_675,4.62,0.28,-0.16,0  
 3GFP,TYR\_325,11.63,2.43,-0.8,0  
 1R3D,HIS\_186,6.43,0,0,-0.07  
 2AZP,ASP\_202,1.97,0.49,-2.32,0  
 2D8N,TYR\_158,11.27,0,0,1.27  
 1RAJ,ASP\_381,0.83,1.05,-4.02,0  
 1FO9,TYR\_390,11.83,1.83,0,0  
 1XAW,TYR\_517,13.55,0.35,0.8,2.4  
 2CXY,GLU\_13,3.13,0.56,-1.94,0  
 3IOC,ASP\_194,1.68,0.28,-2.4,0  
 1HF8,ARG\_125,11.8,-0.7,0,0  
 2FBQ,GLU\_25,4.5,0,0,0  
 2X4J,ARG\_42,4.48,0,-0.42,0,0  
 1ZP2,LYS\_112,10.5,0,0,0  
 2BDV,ARG\_4,10.46,-2.04,0,0  
 1X6J,ASP\_37,3.7,0.07,-0.17,0  
 3RUX,LYS\_214,10.5,0,0,0  
 3PM2,HIS\_167,3.46,0.05,-3.09  
 3CCY,LYS\_42,4.48,0,-0.02,0  
 3MIX,TYR\_643,10,0,0,0  
 1DTO,CYS\_195,5.47,-3.53,0,0  
 2D7J,GLU\_156,4.92,0.42,0,0  
 1R3F,GLU\_106,4.45,0,-0.05,0  
 2FXT,GLU\_407,4.5,0,0,0  
 2P0L,CYS\_227,9,0,0,0  
 3JZN,ARG\_313,11.72,-3.18,0,2.4  
 1MTZ,CYS\_269,10.95,-0.02,1.55,0.42  
 1LTU,LYS\_86,10.08,-0.42,0,0  
 3PP8,ASP\_214,3.9,0.21,-0.11,0  
 1X7F,HIS\_147,1.02,0,0,-5.48  
 1WRU,ARG\_115,12.01,-0.49,0,0  
 2RGY,TYR\_309,10,0,0,0  
 2FZP,GLU\_235,4.0,28,-0.78,0  
 1ZP2,CYS\_27,6.59,-1.39,-2.18,1.15  
 1IDK,CYS\_161,9.7,-0.8,0,1.5  
 2B0J,LYS\_116,10.36,-0.14,0,0  
 3IVF,LYS\_306,10.5,0,0,0  
 3MIX,ASP\_517,2.28,0.21,-1.73,0  
 2IRM,GLU\_111,2.51,2.4,-1.99,-2.4  
 1AKO,ARG\_116,11.94,-0.56,0,0  
 2EHG,GLU\_100,4.64,0.14,0,0  
 2D7J,GLU\_177,4.57,0.07,0,0  
 3KFS,GLU\_171,4.57,0.07,0,0  
 2B61,LYS\_316,10.29,-0.21,0,0  
 1DOV,GLU\_110,4.5,0,0,0  
 1X9G,HIS\_78,6.36,0,0,-0.14  
 2ZTY,LYS\_82,10.22,-0.28,0,0  
 3RFF,CYS\_80,9.09,-0.05,0,0.14  
 1O17,GLU\_215,1.81,0.98,-3.67,0  
 2PPN,GLU\_102,4.55,0.07,-0.02,0  
 3EGN,TYR\_443,13.66,1.11,0.15,2.4  
 2BV9,HIS\_288,6.15,0,0,-0.35  
 2OSA,HIS\_380,6.73,0.23,0,0  
 2POY,ARG\_30,12.15,-0.35,0,0  
 3LJC,GLU\_124,4.5,0,0,0  
 1QQH,LYS\_88,10.22,-0.28,0,0  
 2G5X,LYS\_227,10.5,0,0,0  
 1EYH,ARG\_141,12.5,0,0,0  
 3AU3,ASP\_491,2.75,0.42,-1.47,0  
 1O6D,GLU\_17,4.5,0,0,0  
 1D2K,LYS\_274,10.29,-0.21,0,0  
 2IXM,ARG\_173,12.29,-0.21,0,0  
 3IOC,TYR\_126,11.45,0,0,1.45  
 2B0J,HIS\_123,4.26,0,0,-2.24  
 3GEC,ARG\_533,11.94,-0.56,0,0

1NAR,HIS\_19,6,5,0,0,0  
2PP6,ARG\_80,12.15,-0.35,0,0  
3FRR,ARG\_61,11.87,-0.63,0,0  
3JZN,LYS\_375,10.5,0,0,0  
2IRM,ARG\_308,12.36,-0.14,0,0  
2CL3,LYS\_167,10.5,0,0,0  
1YB2,ASP\_169,2.23,0.28,-1.85,0  
3EVN,GLU\_115,4.5,0,0,0  
1MIX,LYS\_324,10.5,0,0,0  
1J85,GLU\_117,3.55,0.07,-1.01,0  
2BT8,HIS\_158,6.36,0,0,-0.14  
1FHL,TYR\_258,10,0,0,0  
4DNU,LYS\_252,10.5,0,0,0  
1H4U,ARG\_488,8.46,-4.18,0,0.14  
1O59,ARG\_339,11.94,-1.88,0,1.32  
3K9I,GLU\_89,4.71,0.21,0,0  
3LOD,HIS\_118,6.73,0.37,0,-0.14  
1AK1,LYS\_307,10.43,-0.07,0,0  
1BKR,GLU\_83,4.5,0,0,0  
3EVP,LYS\_69,10.43,-0.07,0,0  
2D7U,LYS\_144,10.22,-0.28,0,0  
1GQE,LYS\_30,10.22,-0.28,0,0  
1MTZ,GLU\_186,4.52,0.14,-0.12,0  
1RZ2,GLU\_41,4.64,0.14,0,0  
4EKU,GLU\_314,4.52,0.14,-0.12,0  
2G55,ARG\_12,11.87,-0.63,0,0  
3K9I,ARG\_91,12.5,0,0,0  
1K95,HIS\_141,6.43,0,0,-0.07  
3CNU,LYS\_108,10.5,0,0,0  
3ETV,GLU\_167,3.86,0.14,-0.78,0  
3H04,LYS\_7,10.36,-0.14,0,0  
3IBT,LYS\_38,10.15,-0.35,0,0  
3EUR,TYR\_106,11.53,1.81,-0.35,0.06  
3H9W,LYS\_55,10.43,-0.07,0,0  
1Z3X,LYS\_192,10.5,0,0,0  
3N2T,ASP\_47,3.2,0.21,-0.81,0  
1A8Q,LYS\_40,10.29,-0.21,0,0  
2FBQ,TYR\_44,10,0,0,0  
2CBE,TYR\_51,11.75,2.55,-0.8,0  
3FTT,GLU\_3,2.96,0.42,-1.96,0  
2PPN,ASP\_32,2.77,0.42,-1.45,0  
4FH3,HIS\_41,4.72,0,0,-1.78  
2CWC,TYR\_266,9.65,0,-1.02,0.67  
2YWX,HIS\_64,6.43,0,0,-0.07  
3DSH,ARG\_252,12.43,-0.07,0,0  
2IRM,ARG\_278,12.22,-0.28,0,0  
1P6F,LYS\_136,9.73,-0.77,0,0  
3GOZ,TYR\_213,10.24,0.29,-0.05,0  
2IRM,TYR\_44,10,0,0,0  
3E0H,GLU\_82,4.5,0,0,0  
1OXZ,GLU\_199,4.71,0.21,0,0  
3ETV,LYS\_27,10.15,-0.35,0,0  
3Q1C,GLU\_352,4.5,0,0,0  
2EYI,LYS\_95,9.66,-0.84,0,0  
1R6Y,GLU\_34,5.47,1.12,-0.15,0  
1X8F,LYS\_79,10.22,-0.28,0,0  
3EVP,LYS\_259,10.43,-0.07,0,0  
3CGW,LYS\_214,9.66,-0.84,0,0  
2W2S,ASP\_183,3.9,0.7,-0.6,0  
2GAU,GLU\_166,4.5,0,0,0  
3RKV,GLU\_200,4.57,0.07,0,0  
3BCY,TYR\_129,9.34,0.14,-0.8,0  
1HF8,LYS\_149,10.5,0,0,0  
3JV1,LYS\_94,10.29,-0.21,0,0  
2OOK,CYS\_179,11.8,0,0,2.8  
2GEN,GLU\_111,4.05,0.28,-0.73,0  
3RJZ,LYS\_110,10.36,-0.14,0,0  
2CXC,ARG\_129,12.01,-0.49,0,0  
3GV0,ARG\_117,12.43,-0.07,0,0  
2FC3,GLU\_17,2.38,0.28,-2.4,0  
2DVK,ASP\_154,3.71,0,-0.09,0  
3RE9,HIS\_152,1.7,0.98,-1.28,-4.5  
1UOH,ARG\_184,11.73,-0.77,0,0  
2CL3,ARG\_68,12.22,-0.28,0,0  
3P2F,TYR\_47,12.94,0.28,0.1,2.56  
3IPZ,GLU\_165,4.5,0,0,0  
2E3C,GLU\_396,4.38,0.34,0,-0.46  
2QRX,GLU\_110,4.12,0.42,-0.8,0  
3M70,GLU\_51,4.5,0,0,0  
3LOD,ARG\_110,11.52,-0.98,0,0  
4EVF,LYS\_40,10.5,0,0,0  
2Q98,HIS\_59,3.5,0.26,0.61,-3.87  
2ZCX,ARG\_197,12.29,-0.21,0,0  
2PLQ,LYS\_321,10.5,0,0,0  
3RJX,ARG\_189,12.43,-2.47,0,2.4  
2H30,CYS\_68,4.28,-4.86,0,0.14  
1ZCE,LYS\_20,9.94,-0.56,0,0  
3GOZ,CYS\_184,8.99,-0.01,0,0  
4EKU,LYS\_98,10.01,-0.49,0,0  
2V81,LYS\_198,10.29,-0.21,0,0  
4FH3,ARG\_349,12.08,-0.42,0,0  
1G8P,ARG\_202,11.38,-1.12,0,0  
1AKO,ARG\_170,12.01,-0.49,0,0  
3HUE,ASP\_178,3.34,0.07,-0.53,0  
1O0X,GLU\_120,4.02,1,-0.71,0  
3OBS,ASP\_123,2.92,0.56,-1.44,0  
1QQE,CYS\_208,10.38,-0.4,0.1,78  
2IF4,ASP\_169,3.63,0.21,-0.38,0  
3EZ7,GLU\_31,4.13,0.14,-0.51,0  
2QVT,ARG\_122,12.36,-0.14,0,0  
2D7U,CYS\_131,5.52,-4.96,0,1.48  
3GOZ,HIS\_297,6.43,0,0,-0.07  
3C6B,GLU\_251,4.35,0.84,-0.99,0  
3EVP,LYS\_71,10.22,-0.28,0,0  
2FL7,LYS\_129,10.22,-0.28,0,0  
2D59,TYR\_109,9.54,0,-1.82,1.37  
3A4C,CYS\_498,7.02,-1.98,0,0  
3GA2,GLU\_161,4.5,0,0,0  
3CAX,ASP\_472,3.8,0,0,0  
4ETX,GLU\_178,4.71,0.21,0,0  
2AHE,ASP\_180,1.15,1.05,-3.7,0  
2QDJ,CYS\_278,8.87,-0.2,0,0.07  
1R29,ARG\_122,12.29,-0.21,0,0  
2Q34,GLU\_22,3.91,0.21,-0.8,0  
3HYQ,GLU\_114,4.5,0,0,0  
1NWA,LYS\_104,10.43,-0.07,0,0  
2Q12,GLU\_255,4.5,0,0,0  
1QQH,HIS\_188,7.02,0.8,0,-0.28  
1NJ4,HIS\_146,6.36,0,0,-0.14  
1TD6,GLU\_69,4.19,0.42,-0.73,0  
4EF5,ARG\_284,11.8,-0.7,0,0  
3PP8,LYS\_298,10.43,-0.07,0,0  
3PU6,ASP\_143,3.3,0.49,-0.99,0  
1SIG,GLU\_152,4.62,0.49,-0.37,0  
3M7D,LYS\_244,10.5,0,0,0  
3NR5,GLU\_109,4.57,0.07,0,0  
4AM1,TYR\_168,8.92,0.07,-1.16,0  
3BB7,GLU\_263,4.03,0.28,-0.75,0  
1R53,HIS\_271,7.2,0.85,0,-0.14  
2A4D,GLU\_197,4.09,0.35,-0.76,0  
1PV5,ARG\_247,12.15,-0.35,0,0  
2OJQ,GLU\_474,4.5,0,0,0  
2ZTY,ASP\_85,2.52,0.7,-1.98,0  
3M66,ARG\_181,12.08,-0.42,0,0  
3OIP,LYS\_22,10.29,-0.21,0,0  
1VJG,GLU\_130,4.25,0.56,-0.81,0  
2B61,CYS\_167,11.86,-0.81,1.05,2.62  
2R51,LYS\_230,10.5,0,0,0  
2FZ4,ARG\_152,11.82,-0.68,0,0  
1L2H,TYR\_68,10.26,0.26,0,0  
1BKB,LYS\_60,10.5,0,0,0  
3ELI,HIS\_147,7.12,0.9,0,-0.28  
2EJB,LYS\_56,10.36,-0.14,0,0  
3GEC,LYS\_446,10.22,-0.28,0,0  
3TOW,HIS\_195,6.51,0.07,0,-0.07  
1DZF,GLU\_102,4.5,0,0,0  
3EUR,GLU\_74,3.25,0.42,-1.67,0  
2OGQ,TYR\_462,12.77,0.07,0.53,2.17  
2OKT,GLU\_303,4.55,0.14,-0.09,0  
1XEU,LYS\_185,10.36,-0.14,0,0  
2G2D,ARG\_137,12.5,0,0,0  
3LD1,CYS\_110,8.58,-0.49,0,0.07  
3RJX,ARG\_106,13.45,-1.45,0,2.4  
3IBT,ARG\_56,11.45,-1.05,0,0  
3S0A,ASP\_58,2.24,0.84,-2.4,0  
4EZB,GLU\_236,1.36,0.77,-0.8,-3.11  
2OKT,HIS\_165,6.43,0,0,-0.07  
3BQE,LYS\_363,10.08,-0.42,0,0  
2P52,HIS\_230,4.72,0,0,-1.78  
1G5Z,GLU\_109,4.71,0.21,0,0  
3IBT,ARG\_167,12.08,-0.42,0,0  
3LJN,GLU\_300,4.71,0.21,0,0  
3RVC,ARG\_200,12.5,0,0,0  
4EKU,ASP\_37,4.15,0.35,0,0  
3IOO,ASP\_169,4.01,0.21,0,0  
1XEU,LYS\_217,10.5,0,0,0  
1ZCE,GLU\_10,4.36,0.42,-0.56,0  
2Q13,ASP\_49,4.07,0.28,-0.01,0  
1X7F,LYS\_288,10.5,0,0,0  
1W24,LYS\_21,10.08,-0.42,0,0  
3MIX,GLU\_668,4.5,0,0,0  
3BB7,HIS\_179,6.29,0,0,-0.21  
1NKD,LYS\_3,10.5,0,0,0  
1RAJ,ARG\_379,11.8,-0.7,0,0  
1PVT,ARG\_2,12.5,0,0,0  
1NJ4,ARG\_304,11.45,-1.05,0,0  
2G9D,ASP\_298,3.9,0.14,-0.04,0  
3Q6L,ASP\_3,3.72,0,-0.08,0  
3F7M,GLU\_345,2.59,0.49,-2.4,0  
1SQH,ARG\_72,11.45,-1.05,0,0  
3E5T,GLU\_145,0.54,3.29,-2.65,-4.61  
3CE7,ASP\_66,3.96,0.28,-0.12,0  
3Q9P,CYS\_137,9.14,0,0,0.14  
1UXO,HIS\_161,7.08,0.72,0,-0.14  
3T57,GLU\_147,4.16,0.14,-0.48,0  
3CIV,ARG\_33,12.08,-0.42,0,0  
3GEC,LYS\_512,10.29,-0.21,0,0  
1AKO,GLU\_95,4.57,0.07,0,0  
1YR6,GLU\_174,3.04,0.21,-1.67,0  
3KEY,TYR\_438,10,0,0,0  
1Q8B,CYS\_48,8.87,-0.27,0.14  
3PAC,ASP\_143,2.8,0.63,-1.63,0  
1SJY,ARG\_64,11.52,-0.98,0,0  
3C2E,LYS\_84,10.36,-0.14,0,0  
1Q42,ASP\_110,1.58,0.63,-2.84,0  
3MIX,GLU\_321,4.5,0,0,0  
1SQH,ASP\_15,3.92,0.42,-1.47,1.17  
3M16,LYS\_226,10.36,-0.14,0,0  
1NKD,HIS\_44,6.99,0.49,0,0  
3I47,TYR\_8,11.46,0.21,0,1.25  
3QKY,GLU\_93,4.06,0.94,-1.38,0  
2B61,ASP\_334,3.27,0.35,-0.88,0  
1J7G,LYS\_41,10.22,-0.28,0,0  
3ANJ,LYS\_88,10.08,-0.42,0,0  
1S7K,ARG\_147,12.5,0,0,0  
2F61,LYS\_146,9.94,-0.56,0,0  
3DTE,ARG\_75,12.22,-0.28,0,0  
2O8P,GLU\_184,4.37,0.14,-0.26,0  
1WRU,GLU\_133,3.58,0.42,-1.34,0  
2EFK,ARG\_226,11.94,-0.56,0,0  
3FXH,HIS\_11,6.5,0,0,0  
3GW3,GLU\_63,2.45,0.35,-2.4,0  
2H30,LYS\_80,10.43,-0.07,0,0  
2GAU,ASP\_173,1.2,0.77,-3.37,0  
3H5T,CYS\_274,12.7,0,0,3.7  
2B78,HIS\_259,6.61,0.18,0,-0.07  
1V43,GLU\_62,4.16,0.35,-0.69,0  
3LMF,HIS\_40,8.32,1.96,0,-0.14  
3G69,GLU\_152,4.5,0,0,0  
1JB3,LYS\_38,9.66,-0.84,0,0  
3T57,GLU\_296,4.69,0.77,-0.58,0  
2BLL,HIS\_361,7.23,0.8,0,-0.07  
4ECC,ASP\_75,3.73,0.07,-0.14,0  
15JY,GLU\_65,4.99,0.76,-0.27,0  
1YM5,TYR\_64,12.45,0.07,0,2.38  
1U53,LYS\_68,10.5,0,0,0  
2AH5,TYR\_71,11.9,1.9,0,0  
4FH3,TYR\_52,10.27,0.27,0,0  
3G53,GLU\_221,4.5,0,0,0  
1Z3X,ARG\_193,11.94,-0.56,0,0  
4AM1,LYS\_303,10.5,0,0,0  
2G9D,HIS\_295,6.5,0,0,0  
3AUF,ARG\_189,11.8,-0.7,0,0  
2H2W,GLU\_83,3.5,0.07,-1.07,0  
2Z0M,ARG\_257,12.08,-0.42,0,0  
2H2Z,ARG\_217,12.29,-0.21,0,0  
2OKT,ARG\_321,12.43,-0.07,0,0  
2Q99,GLU\_11,3.36,2.75,-2.62,-1.27  
1O9G,ASP\_153,3.39,0.63,-1.04,0  
3COU,ARG\_67,12.5,0,0,0  
3BCY,HIS\_60,6.43,0.07,0,-0.14  
3EOD,LYS\_8,10.43,-0.07,0,0  
3TOW,ARG\_190,12.08,-0.42,0,0  
4FZN,ARG\_163,12.15,-0.35,0,0  
3L7N,LYS\_62,10.29,-0.21,0,0  
1O17,GLU\_19,4.5,0,0,0  
1ILW,CYS\_133,12.42,-0.59,1.25,2.76  
3DTE,ARG\_54,12.29,-0.21,0,0  
1V43,GLU\_66,4.29,0.07,-0.28,0  
1QZN,ASP\_151,4.02,1,-0.01,0  
3ETV,LYS\_182,10.5,0,0,0  
3CZC,HIS\_62,7.05,0.69,0,-0.14  
3TMO,LYS\_253,10.43,-0.07,0,0  
2RJD,GLU\_214,4.85,0.35,0,0  
3ONH,GLU\_534,4.5,0,0,0  
2BQQ,TYR\_70,12.49,0.45,-0.36,2.4  
2FG1,ASP\_88,1.83,1.19,-3.16,0  
4ANN,ASP\_60,3.2,0.21,-0.81,0  
2VGM,LYS\_25,10.29,-0.21,0,0  
3D9H,ARG\_54,12.45,0.49,-0.48,0  
2W1R,GLU\_100,3.89,0.07,-0.68,0  
2G9D,ARG\_90,13.08,-1.82,0,2.4  
3S0A,ASP\_77,1.87,0.49,-2.42,0  
2JKF,GLU\_149,4.5,0,0,0  
3BWT,HIS\_783,6.5,0,0,0  
2XJ4,ARG\_44,12.01,-0.49,0,0  
1NWA,GLU\_101,4.01,0.21,-0.7,0  
2JEO,CYS\_40,12.04,-0.25,0.84,2.45  
3EVP,ARG\_254,8.4,-4.1,0,0  
1VJG,HIS\_182,4.19,0.8,0,-3.11  
1YTD,LYS\_230,10.29,-0.21,0,0  
2GD7,ARG\_242,13.56,-1.34,0,2.4  
3RNV,ASP\_410,2.18,0.56,-2.18,0  
3DSH,ASP\_239,4.08,0.28,0,0  
3DSH,CYS\_340,9.09,-0.09,0.18  
2DG7,TYR\_47,11,0.28,-0.02,0.75

3ERF,CYS\_86,8.65,-0.66,-2.15,2.46  
3G9B,ARG\_46,12.01,-0.49,0,0  
3AU3,LYS\_523,10.36,-0.14,0,0  
1R5Q,CYS\_45,9.04,-0.03,0,0,0  
3GS9,TYR\_212,10,0,0,0  
1P1L,GLU\_102,4.81,0.56,-0.25,0  
3CX2,ASP\_245,4.22,0.42,0,0  
3LD1,CYS\_212,10,-0.07,0,1.07  
2HRZ,ARG\_22,12.29,-0.21,0,0  
3JZ9,GLU\_344,4.71,0.21,0,0  
3CAX,LYS\_126,9.94,-0.56,0,0  
2EDM,ARG\_67,12.08,-0.42,0,0  
3LJN,GLU\_307,4.64,0.14,0,0  
3K8J,GLU\_67,4.5,0,0,0  
1G8P,ARG\_262,11.66,-0.84,0,0  
1DCF,LYS\_95,10.5,0,0,0  
2FI9,GLU\_85,4.5,0,0,0  
3DSH,ASP\_323,2.96,0.49,-1.33,0  
2BAA,ARG\_110,11.8,-0.7,0,0  
3VJ8,GLU\_113,4.13,0,-0.37,0  
1VSM,GLU\_187,4.5,0,0,0  
3RJX,LYS\_274,10.5,0,0,0  
3JZ9,ASP\_388,2.92,0.35,-1.23,0  
1PGV,HIS\_266,6.15,0,0,-0.35  
1D2K,TYR\_219,13.46,0.26,0.8,2.4  
2AD1,LYS\_72,10.43,-0.07,0,0  
1RI6,LYS\_297,10.5,0,0,0  
2X4L,LYS\_56,10.29,-0.21,0,0  
1DUN,LYS\_42,10.43,-0.07,0,0  
1SNT,TYR\_59,10.14,0.14,0,0  
2ZOM,HIS\_199,4.36,0.39,0,-2.53  
2ZCO,ARG\_271,12.5,0,0,0  
3CNU,CYS\_12,12.1,-0.13,2.4,0.83  
2QEV,LYS\_15,10.36,-0.14,0,0  
2VAN,GLU\_172,4.57,0.07,0,0  
3IVF,ASP\_27,3.68,0.49,-0.61,0  
3M16,ARG\_135,11.52,-0.98,0,0  
1YTQ,HIS\_106,7.02,0.66,0,-0.14  
2ZQ5,LYS\_22,10.5,0,0,0  
1MUF,GLU\_279,3.99,0,-0.51,0  
1EYH,TYR\_101,10,0,0,0  
1YG2,TYR\_137,13.84,0.07,1.37,2.4  
2P52,HIS\_176,6.97,0.47,0,0  
1XIP,TYR\_243,12.95,1.26,-0.64,2.33  
1AD6,LYS\_548,10.15,-0.35,0,0  
1YTQ,TYR\_163,9.87,0.14,-0.27,0  
2D7U,LYS\_65,10.22,-0.28,0,0  
2OGQ,LYS\_589,10.5,0,0,0  
3IRA,GLU\_64,4.64,0.14,0,0  
1PVT,TYR\_71,12.56,0.07,0.09,2.4  
4ECC,CYS\_151,9.07,0,0,0,0  
2WOZ,LYS\_602,10.29,-0.21,0,0  
3H04,CYS\_77,11.32,-0.3,2.35,0.26  
3EX9,GLU\_36,4.57,0.07,0,0  
2ZCX,GLU\_133,4.03,0.28,-0.75,0  
3LD1,GLU\_128,4.69,0.28,-0.09,0  
1WPS,ARG\_248,11.66,-0.84,0,0  
2BLL,CYS\_383,10.09,-0.19,0.08,1.2  
1OIS,LYS\_236,10.29,-0.21,0,0  
3TRE,ARG\_54,12.29,-0.21,0,0  
2PLQ,ASP\_303,3.6,0,-0.2,0  
3IL3,ARG\_17,11.36,-1.14,0,0  
1IDK,TYR\_254,10.75,0,0,0.75  
1O17,GLU\_278,3.57,0.49,-1.41,0  
2IQT,GLU\_190,2.35,2.47,-2.22,-2.4  
1RWZ,LYS\_233,10.5,0,0,0  
4FZR,LYS\_79,10.43,-0.07,0,0  
1NAR,HIS\_133,8.59,0.65,1.44,0  
1XIP,TYR\_108,10.07,0.07,0,0  
2RJD,TYR\_255,12.65,1.23,0,1.42  
3ETV,LYS\_145,10.43,-0.07,0,0  
3HUE,ARG\_250,12.5,0,0,0  
2WB8,ASP\_703,2.43,0.35,-1.72,0  
1W7B,LYS\_206,10.5,0,0,0  
3ONT,GLU\_137,3.74,0.35,-1.11,0  
1LTU,LYS\_167,10.22,-0.28,0,0  
3ASA,ASP\_378,3.67,0.14,-0.27,0  
3CIV,HIS\_113,6.36,0,0,-0.14  
3JZN,ASP\_237,3.14,0.28,-0.94,0  
2WB8,ARG\_590,11.73,-0.77,0,0  
3ADO,TYR\_255,9.96,0,-0.04,0  
2OEW,GLU\_144,4.5,0,0,0  
1IAP,ARG\_152,12.08,-0.42,0,0  
3OA7,TYR\_534,10.46,0,0,0.46  
1NJ4,GLU\_230,4.78,0.28,0,0  
3IVF,HIS\_124,6.36,0,0,-0.14  
2WZ9,GLU\_75,3.66,0.28,-1.12,0  
3K1H,GLU\_130,4.71,0.21,0,0  
1V6T,GLU\_23,4.5,0,0,0  
1FKM,ARG\_303,12.43,-0.07,0,0  
1KCM,GLU\_102,4.05,0.35,-0.8,0  
3RNV,GLU\_375,4.05,0.35,-0.8,0  
1QQE,LYS\_261,10.5,0,0,0  
3ELI,ARG\_8,11.87,-0.63,0,0  
2HNG,GLU\_127,4.5,0,0,0  
1V43,LYS\_370,10.5,0,0,0  
2DG7,ASP\_139,2.25,0.56,-2.11,0  
1SJV,ARG\_24,12.15,-0.35,0,0  
3CRM,GLU\_272,3.05,0.28,-1.72,0  
1EW4,HIS\_58,6.86,0.57,0,-0.21  
1AD6,ARG\_418,12.25,-1.84,0,1.59  
3H6Q,ASP\_113,3.68,0,-0.12,0  
1IAP,GLU\_169,4.17,0.49,-0.82,0  
3GE9,HIS\_69,6.5,0,0,0  
1UOH,LYS\_206,10.29,-0.21,0,0  
1ZCU,CYS\_88,11.29,-0.92,0.3,2.1  
3GYW,TYR\_127,10,0,0,0  
1QYI,TYR\_27,8.55,0.33,-0.27,-1.51  
1PGV,ARG\_312,12.29,-0.21,0,0  
1YB2,GLU\_20,3.73,0.28,-1.05,0  
3RLE,ARG\_101,12.15,-0.35,0,0  
2H01,GLU\_19,4.78,0.28,0,0  
3N2T,LYS\_228,10.5,0,0,0  
3F1X,LYS\_122,10.29,-0.21,0,0  
2AD1,LYS\_202,10.15,-0.35,0,0  
1PV5,ARG\_28,12.43,-0.07,0,0  
1L2F,ARG\_119,12.43,-0.07,0,0  
3QKY,ARG\_52,12.08,-0.42,0,0  
1TR9,HIS\_108,4.24,1.59,0,-3.85  
3BA1,GLU\_240,4.12,0.42,-0.79,0  
3JV1,GLU\_114,4.57,0.07,0,0  
1DOV,ASP\_114,3.28,0.28,-0.8,0  
3GS3,TYR\_131,12.76,2.45,-0.8,1.11  
2Q34,CYS\_103,6.88,-2.08,-1.65,1.61  
3IRA,ARG\_128,12.29,-0.21,0,0  
2FZP,ARG\_231,12.36,-0.14,0,0  
2CW4,ARG\_51,11.59,-0.91,0,0  
3EGN,LYS\_437,10.5,0,0,0  
2NRK,GLU\_18,4.5,0,0,0  
2BDD,LYS\_144,10.29,-0.21,0,0  
3RFF,ASP\_112,3.36,0.28,-0.72,0  
3P2F,GLU\_81,3.98,0.28,-0.8,0  
1SQW,LYS\_100,10.36,-0.14,0,0  
2ZCO,GLU\_180,4.5,0,0,0  
3EVN,GLU\_60,4.57,0.07,0,0  
3OA7,TYR\_501,10,0,0,0  
3MIX,TYR\_501,10,0,0,0  
2RIS,LYS\_204,10.5,0,0,0  
2Q99,ARG\_52,12.01,-0.49,0,0  
2FG1,TYR\_97,9.09,0.14,-1.05,0  
3JSN,TYR\_35,11,1,0,0  
2VGM,GLU\_132,4.33,0.52,-0.69,0  
2VGM,GLU\_333,4.57,0.07,0,0  
2E3S,TYR\_435,10.06,0.07,-0.01,0  
3U2A,ARG\_79,11.94,-0.56,0,0  
2X4L,ASP\_158,2.89,0.21,-1.12,0  
2IDC,ASP\_20,3.25,0.63,-1.18,0  
1PSW,GLU\_249,4.27,0,-0.23,0  
3GFP,HIS\_441,6.22,0,0,-0.28  
2WB8,TYR\_667,10.1,0.64,-0.54,0  
1Z9L,TYR\_78,10,0,0,0  
3KB5,GLU\_365,4.5,0,0,0  
3P2F,ARG\_44,12.36,-0.14,0,0  
3P28,GLU\_165,2.77,0.77,-2.5,0  
3L3P,ARG\_445,12.08,-0.42,0,0  
3HKX,HIS\_37,6.22,0,0,-0.28  
2QVT,ARG\_123,12.36,-0.14,0,0  
3BWT,ASP\_610,1.71,0.28,-2.37,0  
1W7B,LYS\_302,10.08,-0.42,0,0  
3H6Q,TYR\_103,10.39,0,-0.01,0.39  
1S7K,ASP\_101,1.19,1.19,-3.8,0  
2W2S,ARG\_73,12.29,-0.21,0,0  
2OKT,LYS\_147,10.5,0,0,0  
1WXF,GLU\_137,4.57,0.07,0,0  
2WOZ,ASP\_421,3.05,0.63,-1.38,0  
2FD4,GLU\_537,4.57,0.07,0,0  
1NIJ,GLU\_42,4.28,0,-0.22,0  
1ZBP,GLU\_10,4.64,0.14,0,0  
2H14,ARG\_154,11.87,-0.63,0,0  
2Q99,LYS\_215,10.08,-0.42,0,0  
1TLV,TYR\_202,9.87,0,-0.69,0.56  
3M70,GLU\_86,4.57,0.07,0,0  
2ZQ5,ARG\_66,12.08,-0.42,0,0  
3JSN,TYR\_52,10.46,0,-0.19,0.65  
3CGW,GLU\_142,4.64,0.14,0,0  
3OIP,TYR\_95,13.41,0.21,0.8,2.4  
1AM2,HIS\_187,7.34,0.98,0,-0.14  
1L2F,LYS\_179,10.29,-0.21,0,0  
2PP6,LYS\_23,10.29,-0.21,0,0  
1TP6,ARG\_66,11.87,-0.63,0,0  
3TOW,ASP\_67,3.73,0.07,-0.14,0  
1ZCU,TYR\_94,13.64,0.39,0.8,2.45  
1ZP2,LYS\_66,10.5,0,0,0  
2V4X,LYS\_70,10.43,-0.07,0,0  
2ATR,LYS\_5,10.5,0,0,0  
2H01,TYR\_160,9.63,0,-0.37,0  
4FZN,TYR\_13,13.26,2.42,-0.08,0.92  
1L2F,LYS\_173,10.5,0,0,0  
1N81,ARG\_92,11.94,-0.56,0,0  
2FBI,GLU\_122,3.36,0,-1.14,0  
2WOZ,LYS\_575,10.22,-0.28,0,0  
2R57,GLU\_321,3.5,2.68,-3.68,0  
2IF4,GLU\_192,4.5,0,0,0  
3NR5,ASP\_62,2.59,0.56,-1.77,0  
3GG6,GLU\_79,4.73,0.35,-0.12,0  
2X4G,GLU\_246,4.62,0.14,-0.02,0  
2R51,GLU\_98,5.01,0.56,-0.04,0  
4F85,GLU\_94,3.92,0.21,-0.79,0  
3ASA,ARG\_268,11.94,-0.56,0,0  
3DTE,TYR\_103,10.87,0,-0.08,0.94  
3U4K,TYR\_113,11.16,1.44,0,-0.28  
2D7U,GLU\_162,1.58,1.08,-1.6,-2.4  
2WB8,GLU\_530,3.77,0.07,-0.8,0  
3BQW,LYS\_184,9.8,-0.7,0,0  
1Y2Q,LYS\_18,10.5,0,0,0  
3M3P,ARG\_82,12.29,-0.21,0,0  
3L7N,ARG\_231,11.87,-0.63,0,0  
3M70,GLU\_58,3.98,0.28,-0.8,0  
2GS5,TYR\_78,7.76,0.43,-0.27,-2.4  
3M70,ASP\_268,2.98,0.63,-1.45,0  
4D8L,ARG\_121,8.51,-1.65,0,-2.34  
3UV9,ASP\_447,2.93,0.56,-1.43,0  
1NIJ,ASP\_189,3.94,0.14,0,0  
1X8F,LYS\_130,10.5,0,0,0  
1T95,ASP\_143,3.32,0.63,-1.11,0  
2FG1,GLU\_141,3.46,0.56,-1.6,0  
2Q99,LYS\_368,10.5,0,0,0  
2PLQ,TYR\_171,12.38,0.31,0,2.07  
1MJS,GLU\_346,5.11,0.77,-0.16,0  
3RHE,HIS\_114,6.5,0,0,0  
3QAV,ASP\_33,3.52,0.35,-0.63,0  
3Q1C,HIS\_186,6.6,0.1,0,0  
2C2Y,GLU\_106,3.77,0.42,-1.15,0  
2W2S,LYS\_115,10.15,-0.35,0,0  
2YT4,GLU\_574,4.2,0.07,-0.37,0  
3PP8,GLU\_136,2.6,0.56,-2.45,0  
1RWZ,LYS\_130,10.29,-0.21,0,0  
1L2F,LYS\_269,10.08,-0.42,0,0  
1U3Y,LYS\_312,10.43,-0.07,0,0  
157K,ASP\_165,4.01,0.21,0,0  
2AHE,CYS\_234,10.51,0,0,1.51  
1Q5Z,GLU\_603,4.64,0.14,0,0  
2QOP,ARG\_168,11.22,-1.28,0,0  
1X91,ASP\_106,3.83,0.07,-0.04,0  
3C38,ARG\_72,12.08,-0.42,0,0  
1AIL,GLU\_26,4.5,0,0,0  
2CXC,GLU\_33,4.02,0.21,-0.69,0  
3JZN,ASP\_362,3.01,0.35,-1.14,0  
2IXM,HIS\_318,7.22,0.86,0,-0.14  
2QDJ,GLU\_315,4.59,0.14,-0.05,0  
2QEV,LYS\_34,10.01,-0.49,0,0  
2WB8,LYS\_771,10.5,0,0,0  
4H4J,GLU\_47,0.48,1.27,-3.2,-2.1  
1FKM,HIS\_473,6.87,0.51,0,-0.14  
3HVM,GLU\_161,3.63,0.77,-1.65,0  
1QZN,ASP\_83,2.16,0.7,-2.34,0  
3RLE,LYS\_50,10.5,0,0,0  
1X1E,CYS\_173,6.99,-3.2,0,1.19  
1M5I,ARG\_232,12.22,-0.28,0,0  
2BAA,LYS\_109,10.36,-0.14,0,0  
1U3Y,ARG\_252,12.5,0,0,0  
1NKD,GLU\_5,3.38,0.42,-1.54,0  
2BT8,ARG\_282,11.38,-1.12,0,0  
2YX0,TYR\_158,10,0,0,0  
3U0V,LYS\_163,10.5,0,0,0  
4ANN,ARG\_153,11.87,-0.63,0,0  
2BT8,ARG\_316,12.15,-0.35,0,0  
2F8H,ARG\_298,12.29,-0.21,0,0  
2DFL,ARG\_180,11.8,-0.7,0,0  
3EX9,ARG\_121,12.29,-0.21,0,0  
2HXB,ASP\_7,1.98,0.28,-2.1,0  
4EVF,LYS\_169,10.5,0,0,0  
1QQE,GLU\_224,4.91,0.63,-0.22,0  
3Q2C,GLU\_92,4.09,0.21,-0.62,0  
3H8Y,CYS\_68,8.32,-0.68,0,0  
2Z84,CYS\_186,9,0,0,0  
1X8F,ASP\_243,3.76,0.49,-0.53,0  
2E3S,GLU\_409,4.04,0,-0.46,0  
4HDE,HIS\_158,10.74,4.67,2.78,-3.22  
3CSV,ARG\_369,12.22,-0.28,0,0  
1WXQ,LYS\_241,10.5,0,0,0  
1NJ4,LYS\_246,10.29,-0.21,0,0  
2RJD,LYS\_442,10.08,-0.42,0,0  
1BYI,GLU\_44,4.78,0.28,0,0  
1R53,LYS\_183,10.43,-0.07,0,0  
3O48,ASP\_12,2.23,0.28,-1.85,0



1JKS, TYR\_83, 13.49, 0.21, 0.46, 2.83  
1YR6, TYR\_238, 10.26, 0.0, 0.26, 0  
3M7G, ASP\_178, 3.69, 0.0, -0.11, 0  
1WPA, GLU\_419, 4.64, 0.14, 0.0  
2F19, TYR\_45, 10.61, 0.21, -1.11, 1.51  
3G6S, LYS\_35, 10.36, -0.14, 0.0  
1CHD, HIS\_270, 6.5, 0.0, 0  
1NRI, HIS\_114, 6.75, 0.46, 0.0, -0.21  
1P6F, LYS\_186, 10.5, 0.0, 0  
3ODJ, LYS\_88, 9.94, -0.56, 0.0  
1W7B, ARG\_178, 12.36, -0.14, 0.0  
3F7M, ARG\_120, 11.45, -1.05, 0.0  
3ULX, GLU\_26, 3.28, 0.28, -1.51, 0  
3RLE, CYS\_192, 10.02, 0.0, 1.02  
1EV8, TYR\_209, 13.81, 0.07, 0.59, 3.15  
3OOP, ARG\_106, 11.66, -0.84, 0.0  
3IOC, TYR\_71, 12.98, 0.0, 3.2, 6.8  
3Q1C, HIS\_40, 6.72, 0.29, 0.0, -0.07  
1TWU, GLU\_121, 4.05, 0.21, -0.66, 0  
1SFE, TYR\_16, 10.37, 0.0, -0.09, 0.45  
2BDD, ASP\_120, 1.56, 1.12, -3.37, 0  
3BA1, GLU\_44, 4.07, 0.28, -0.71, 0  
3CGW, LYS\_176, 10.36, -0.14, 0.0  
2G9D, ASP\_336, 4.01, 0.21, 0.0  
2H8O, ARG\_44, 11.94, -0.56, 0.0  
2NYC, TYR\_272, 10.14, 0.14, 0.0  
4F85, HIS\_124, 7.24, 0.95, 0.0, -0.21  
2DOA, LYS\_132, 10.22, 0.28, 0.0  
1OST, TYR\_248, 10.0, 0.0, 0  
2IQT, LYS\_203, 10.43, -0.07, 0.0  
2YX0, CYS\_81, 9.8, -3.49, 2.16, 2.14  
1TXJ, TYR\_134, 12.85, 0.58, 0.2, 2.27  
3BA1, GLU\_272, 1.93, 0.63, -3.2, 0  
3GW3, GLU\_270, 4.5, 0.0, 0  
2Z61, TYR\_308, 9.1, 2.6, -1.53, -1.97  
1ZBS, TYR\_277, 10.36, 0.14, -0.81, 1.02  
2BV9, HIS\_137, 7.16, 0.8, 0.0, -0.14  
3CIV, TYR\_247, 10.4, 0.51, -0.11, 0  
3T57, ARG\_259, 12.29, -0.21, 0.0  
1OIS, TYR\_358, 10.14, 0.14, 0.0  
1T95, LYS\_139, 10.15, -0.35, 0.0  
1PBV, ARG\_152, 12.43, -0.07, 0.0  
3GEC, ARG\_460, 11.8, -0.7, 0.0  
1X1E, ASP\_51, 3.03, 0.63, -1.41, 0  
1HUFG, GLU\_118, 3.34, 0.49, -1.65, 0  
1XTZ, ASP\_63, 3.21, 0.63, -1.22, 0  
4EKU, GLU\_301, 4.02, 0.21, -0.7, 0  
2W0G, TYR\_248, 10.59, 0.53, 0.0, 0.06  
2GZQ, ASP\_87, 3.86, 0.21, -0.15, 0  
2R2Y, HIS\_58, 6.77, 0.48, 0.0, -0.21  
4HDE, GLU\_120, 4.5, 0.0, 0  
2B61, HIS\_327, 6.85, 0.77, 0.0, -0.42  
3QKY, LYS\_85, 10.43, -0.07, 0.0  
3UAH, TYR\_396, 9.27, 0.07, -0.8, 0  
2POL, LYS\_187, 10.08, -0.42, 0.0  
1YOY, GLU\_41, 3.22, 0.21, -1.49, 0  
1XWM, LYS\_102, 10.43, -0.07, 0.0  
2C13, TYR\_223, 10.45, 0.49, -0.04, 0  
2BQQ, ARG\_56, 12.08, -0.42, 0.0  
1O59, LYS\_140, 10.36, -0.14, 0.0  
2O8PH, HIS\_62, 7.02, 0.8, 0.0, -0.28  
2XJ4, GLU\_94, 4.5, 0.28, -0.28, 0  
2H30, LYS\_157, 10.5, 0.0, 0  
2RIK, LYS\_193, 10.43, -0.07, 0.0  
3VHJ, ASP\_104, 3.94, 0.14, 0.0  
1LZL, ASP\_233, 3.94, 0.14, 0.0  
2P52, HIS\_211, 3.35, 0.13, 0.0, -3.28  
1WXQ, LYS\_295, 10.5, 0.0, 0  
2P1W, GLU\_199, 4.5, 0.0, 0  
1Q42, ASP\_66, 2.41, 0.98, -2.37, 0  
2P52, LYS\_136, 10.43, -0.07, 0.0  
1R5S, ARG\_143, 11.8, -0.7, 0.0  
2PGX, ASP\_87, 3.8, 0.0, 0  
2FD4, TYR\_547, 10.17, 0.07, 0.0, 1  
3IBT, ASP\_161, 2.8, 0.42, -1.42, 0  
2IQT, ASP\_48, 3.9, 0.21, -0.11, 0  
4AE7, CYS\_142, 10.37, -2.18, 0.3, 5.6  
2HP7, GLU\_111, 4.57, 0.07, 0.0  
3IV4, LYS\_4, 10.5, 0.0, 0  
3T5B, GLU\_389, 4.36, 0.14, -0.28, 0  
1ZBS, ARG\_230, 12.5, 0.0, 0  
2ATR, GLU\_8, 4.5, 0.0, 0  
1HUF, CYS\_23, 8.92, -0.08, 0.0  
1R29, HIS\_116, 6.5, 0.0, 0  
1WRU, ARG\_244, 11.94, -0.56, 0.0  
2AZL, LYS\_53, 10.08, -0.42, 0.0  
1NWA, TYR\_98, 10.56, 0.0, 0.56  
2ZCO, CYS\_11, 10.63, -0.19, 0.1, 8.2  
2E3S, ASP\_385, 2.85, 0.56, -1.51, 0  
1BN6, ASP\_167, 3.77, 0.14, -0.17, 0  
3P51, GLU\_139, 4.05, 0.35, -0.8, 0  
2RFA, GLU\_164, 3.72, 1.23, -2.66, 0.64  
2NMM, HIS\_29, 6.43, 0.0, -0.07  
3T57, GLU\_248, 4.57, 0.07, 0.0  
2XMX, HIS\_243, 5.41, 1.76, 2.11, -4.96  
1RWZ, TYR\_197, 13.05, 0.07, 0.57, 2.4  
3N0K, TYR\_136, 9.99, 0.0, -0.01, 0  
1S17, ARG\_56, 11.44, -1.06, 0.0  
3CNU, ARG\_102, 12.5, 0.0, 0  
1RIS, ARG\_113, 12.43, -0.07, 0.0  
3F53, ARG\_222, 11.66, -0.84, 0.0  
1NKD, ARG\_52, 12.29, -0.21, 0.0  
1NRI, GLU\_99, 3.39, 0.28, -1.39, 0  
4DNU, GLU\_138, 3.34, 0.21, -1.38, 0  
3EJC, ARG\_9, 12.5, 0.0, 0  
2XHC, LYS\_25, 9.87, -0.63, 0.0  
1RHS, TYR\_70, 11.24, 0.14, 0.1, 1  
2R57, CYS\_193, 9.33, -0.13, 0.0, 4.6  
3P51, GLU\_115, 4.57, 0.07, 0.0  
2EYI, HIS\_88, 7.22, 0.79, 0.0, -0.07  
2GAU, ASP\_221, 2.76, 0.63, -1.68, 0  
3O16, ARG\_176, 12.08, -0.42, 0.0  
2AHE, ARG\_227, 12.01, -0.49, 0.0  
3DSH, ARG\_249, 11.94, -0.56, 0.0  
3M66, ASP\_202, 2.92, 0.14, -1.02, 0  
2D7J, LYS\_28, 10.5, 0.0, 0  
3ZXY, GLU\_200, 4.64, 0.14, 0.0  
1Y0K, ARG\_46, 12.29, -0.21, 0.0  
1YW5, ARG\_132, 12.15, -0.35, 0.0  
1U7U, GLU\_402, 4.03, 0.28, -0.75, 0  
2ZCX, GLU\_152, 3.62, 0.28, -1.16, 0  
3IDW, LYS\_59, 10.5, 0.0, 0  
1U3Y, ASP\_277, 2.53, 0.84, -2.11, 0  
1W24, GLU\_178, 3.04, 0.14, -1.6, 0  
3G9B, TYR\_27, 13.86, 0.74, 0.69, 2.43  
3LPZ, GLU\_23, 4.64, 0.14, 0.0  
1XTZ, TYR\_170, 10.0, 0.0, 0  
3LJN, LYS\_165, 10.08, -0.42, 0.0  
1V6T, LYS\_47, 10.92, -0.07, 0.0, 4.9  
2OBI, GLU\_50, 3.98, 0.28, -0.8, 0  
2F19, ARG\_61, 11.94, -0.56, 0.0  
2XHC, GLU\_15, 1.77, 0.91, -3.64, 0  
1FQI, LYS\_308, 10.15, -0.35, 0.0  
1QQE, HIS\_109, 6.64, 0.15, 0.0  
3FNI, LYS\_2, 10.5, 0.0, 0  
1O5T, GLU\_115, 4.71, 0.21, 0.0  
1EV8, ARG\_49, 12.36, -0.14, 0.0  
3L7N, HIS\_4, 3.08, 0.0, -3.42  
3KB5, ARG\_356, 13.78, -0.64, 0.1, 9.2  
1LZL, TYR\_134, 10.19, 0.07, -0.83, 0.95  
2EFK, LYS\_51, 10.5, 0.0, 0  
3LE4, GLU\_323, 4.5, 0.0, 0  
3Q6L, GLU\_130, 3.89, 0.28, -0.9, 0  
2IXM, GLU\_90, 4.14, 0.42, -0.78, 0  
3K9I, LYS\_62, 10.5, 0.0, 0  
2HP7, LYS\_46, 10.5, 0.0, 0  
1JKS, GLU\_237, 4.64, 0.14, 0.0  
1UCH, ARG\_5, 11.24, -1.26, 0.0  
2QQZ, HIS\_169, 6.29, 0.0, -0.21  
1ZKZ, LYS\_87, 10.43, -0.07, 0.0  
3H13, ASP\_441, 3.92, 0.21, -0.09, 0  
3V75, ARG\_169, 12.5, 0.0, 0  
2YLF, LYS\_189, 10.5, 0.0, 0  
1NAR, ARG\_74, 12.22, -0.28, 0.0  
3ILC, HIS\_113, 7.33, 1.04, 0.0, -0.21  
2V1L, ARG\_100, 12.43, -0.07, 0.0  
1XKR, ASP\_134, 3.87, 0.07, 0.0  
3M70, GLU\_269, 4.5, 0.0, 0  
3EAZ, GLU\_143, 4.5, 0.0, 0  
2BLI, HIS\_618, 6.63, 0.13, 0.0  
3M70, LYS\_95, 10.5, 0.0, 0  
157K, GLU\_160, 4.64, 0.14, 0.0  
3PM2, GLU\_127, 2.54, 0.91, -2.86, 0  
1Q2Y, LYS\_115, 10.43, -0.07, 0.0  
2V4U, ARG\_532, 12.29, -0.21, 0.0  
3HYQ, GLU\_135, 5.03, 0.49, -1.31, 1.34  
1VJG, GLU\_109, 4.5, 0.0, 0  
2CXA, GLU\_118, 4.71, 0.21, 0.0  
2ZTY, LYS\_12, 10.5, 0.0, 0  
2RIS, ASP\_180, 3.75, 0.28, -0.33, 0  
1DTO, TYR\_43, 11.43, 0.31, -0.7, 1.82  
4DBX, LYS\_156, 10.29, -0.21, 0.0  
2GKG, ARG\_93, 11.94, -0.56, 0.0  
2CXA, HIS\_180, 7.21, 0.71, 0.0  
4DVD, GLU\_74, 4.64, 0.14, 0.0  
2E3C, ARG\_426, 11.84, -1.12, 0.0, 4.6  
2Q5X, ASP\_813, 0.79, 0.56, -3.57, 0  
2GEN, ARG\_129, 12.01, -0.49, 0.0  
3G5S, LYS\_51, 10.5, 0.0, 0  
3U2A, CYS\_55, 8.87, -0.53, 0.0, 4  
4FZR, HIS\_0, 6.5, 0.0, 0  
1QQE, GLU\_34, 4.62, 0.14, -0.02, 0  
4H4J, ASP\_100, 2.63, 0.42, -1.59, 0  
1SUU, ASP\_631, 3.95, 0.28, -0.13, 0  
4FCU, ARG\_53, 12.36, -0.14, 0.0  
3H6Q, HIS\_114, 7.67, 1.38, 0.0, -0.21  
2H2W, LYS\_17, 10.5, 0.0, 0  
3G69, ASP\_123, 2.51, 0.49, -1.78, 0  
1GSZ, LYS\_48, 10.5, 0.0, 0  
3LJI, ARG\_31, 11.66, -0.84, 0.0  
3M3P, HIS\_108, 6.26, 0.04, 0.0, -0.28  
1U53, ARG\_23, 8.51, -3.99, 0.0  
3C2E, HIS\_295, 6.5, 0.0, 0  
2Q13, TYR\_190, 10.0, 0.0, 0  
1BN6, ARG\_157, 11.66, -0.84, 0.0  
2V8C, CYS\_47, 8.98, -0.09, 0.0, 0.07  
1XTZ, ARG\_158, 11.94, -0.56, 0.0  
2YX0, ASP\_326, 3.45, 0.77, -1.12, 0  
3G6S, TYR\_13, 9.86, 0.0, -0.6, 0.46  
1NFN, ARG\_134, 11.52, -0.98, 0.0  
1ILW, ARG\_173, 12.22, -0.28, 0.0  
3BWT, LYS\_583, 10.22, -0.28, 0.0  
3G9G, LYS\_162, 10.5, 0.0, 0  
2PWQ, LYS\_92, 10.5, 0.0, 0  
3IVF, ASP\_261, 3.48, 0.35, -0.67, 0  
1AK1, GLU\_19, 4.71, 0.21, 0.0  
2BV9, TYR\_87, 12.11, 1.8, -0.36, 0.67  
4DNU, GLU\_43, 3.77, 0.07, -0.8, 0  
4EVF, GLU\_49, 4.5, 0.0, 0  
2VGM, LYS\_84, 10.29, -0.21, 0.0  
2ZCO, ARG\_181, 12.69, -0.84, 0.1, 0.3  
2JEO, ARG\_172, 13.44, -1.33, 0.2, 2.27  
3FXH, LYS\_48, 10.36, -0.14, 0.0  
1PSW, LYS\_79, 10.29, -0.21, 0.0  
1BN6, ARG\_133, 11.59, -0.91, 0.0  
3A7L, GLU\_61, 4.57, 0.07, 0.0  
1TR9, GLU\_104, 3.23, 2.3, -3.57, 0  
2Z84, ASP\_25, 3.94, 0.14, 0.0  
3H9W, GLU\_81, 4.64, 0.14, 0.0  
4D8L, HIS\_33, 3.96, 2.46, 1.75, -6.75  
3M7G, ARG\_231, 13.57, -1.33, 0.2, 4  
2ZCX, GLU\_68, 2.87, 0.49, -2.12, 0  
3TRE, ASP\_18, 3.8, 0.0, 0  
3HUE, ARG\_308, 4.06, 0.21, -0.65, 0  
3PZ9, ASP\_362, 1.33, 0.98, -3.45, 0  
3CZC, LYS\_45, 10.22, -0.28, 0.0  
3RFF, ARG\_50, 11.59, -0.91, 0.0  
1QYI, HIS\_160, 6.43, 0.0, -0.07  
2YLF, GLU\_55, 3.2, 0.49, -1.79, 0  
3M7D, GLU\_13, 4.5, 0.0, 0  
1PSW, HIS\_74, 6.75, 0.46, 0.0, -0.21  
2J8A, HIS\_340, 6.5, 0.0, 0  
1ZP2, LYS\_198, 10.5, 0.0, 0  
2AD1, GLU\_175, 4.69, 0.26, -0.07, 0  
1MIX, LYS\_334, 10.43, -0.07, 0.0  
4F8A, ARG\_583, 12.36, -0.14, 0.0  
3DB9, ASP\_72, 3.79, 0.0, -0.01, 0  
3M66, GLU\_256, 4.5, 0.0, 0  
3QAV, GLU\_70, 4.5, 0.0, 0  
2RJD, LYS\_216, 10.36, -0.14, 0.0  
2V4U, GLU\_513, 4.66, 2.77, -2.61, 0  
3H6Q, ARG\_100, 3.91, 0.21, -0.8, 0  
2QOP, ASP\_186, 2.91, 0.7, -1.59, 0  
2IXM, ASP\_175, 3.16, 0.14, -0.78, 0  
2IRM, LYS\_35, 10.36, -0.14, 0.0  
3RLE, GLU\_117, 3.91, 0.21, -0.8, 0  
1J85, LYS\_81, 10.5, 0.0, 0  
3CAX, ARG\_253, 12.08, -0.42, 0.0  
2GZR, LYS\_109, 10.29, -0.21, 0.0  
2OBI, ASP\_6, 2.51, 0.77, -2.05, 0  
3EGN, ARG\_392, 12.43, -0.07, 0.0  
3S0A, GLU\_33, 3.91, 0.21, -0.8, 0  
3CRM, LYS\_317, 10.5, 0.0, 0  
2P4D, TYR\_166, 11.35, 0.34, -0.07, 1.08  
1TR9, GLU\_88, 4.5, 0.0, 0  
3CX2, GLU\_223, 4.46, 0.21, -0.25, 0  
2ZQ5, ASP\_147, 3.94, 0.14, 0.0  
2AZL, ARG\_150, 12.29, -0.21, 0.0  
2G9D, ARG\_261, 12.15, -0.35, 0.0  
1KCM, TYR\_141, 11.04, 0.14, -0.8, 1.7  
2CXA, HIS\_130, 2.77, 0.19, -0.02, -3.91  
2DG7, ASP\_163, 3.92, 0.28, -0.16, 0  
2FPN, LYS\_71, 10.5, 0.0, 0  
3EVN, ASP\_61, 3.88, 0.21, -0.13, 0  
1EQ6, TYR\_199, 13.15, 0.92, -0.17, 2.4  
3CNU, GLU\_40, 5.13, 0.63, 0.0  
3GT0, LYS\_142, 10.22, -0.28, 0.0  
4ANN, ASP\_75, 4.15, 0.35, 0.0  
2Q99, TYR\_119, 12.81, 1.12, 0.6, 1.09  
3RAZ, ASP\_86, 3.8, 0.0, 0  
1MTZ, ARG\_206, 12.01, -0.49, 0.0  
2E3C, ARG\_314, 12.5, 0.0, 0  
2EYI, LYS\_157, 10.43, -0.07, 0.0  
1UAJ, HIS\_46, 6.5, 0.0, 0  
2FD5, ASP\_74, 3.22, 0.56, -1.14, 0  
1JYH, GLU\_140, 4.64, 0.14, 0.0

2B2H, TYR\_92, 11.86, 2.9, -1.04, 0  
 3I4T, CYS\_119, 8.7, -0.85, 0, 0.55  
 3F53, ASP\_34, 3.94, 0.14, 0, 0  
 2OB5, ASP\_24, 4.08, 0.28, 0, 0  
 2D59, ASP\_76, 3.16, 0.28, -0.92, 0  
 3LPZ, ARG\_107, 12.52, -1.01, 0, 1.03  
 1J33, HIS\_56, 4.41, 1.65, 2.4, -6.14  
 2AHE, LYS\_130, 10.5, 0, 0, 0  
 2V81, HIS\_90, 6.43, 0, 0, -0.07  
 2CL3, TYR\_191, 12.01, 0.52, 0, 1.49  
 2EJX, TYR\_111, 9.4, 0.07, -0.67, 0  
 2FZ4, ARG\_221, 7, -3.11, 0, -2.39  
 3HST, ASP\_130, 3.2, 0.28, -0.88, 0  
 1NUJ, ASP\_85, 1.66, 0.42, -2.56, 0  
 4FH3, LYS\_133, 10.5, 0, 0, 0  
 4F3J, TYR\_160, 10, 0, 0, 0  
 2RH3, GLU\_176, 4.71, 0.21, 0, 0  
 1V6T, CYS\_35, 9.59, -1.95, 0, 2.54  
 3AUF, GLU\_164, 3.89, 0.28, -0.89, 0  
 2RIS, ASP\_170, 1.57, 0.21, -2.44, 0  
 1ZBP, TYR\_235, 9.85, 0.07, -0.22, 0  
 3CXS, LYS\_73, 10.5, 0, 0, 0  
 2CIU, ASP\_121, 3.21, 0.21, -0.8, 0  
 2GZQ, TYR\_171, 11.97, 0, 1.97  
 1P4X, HIS\_70, 6.99, 0.56, 0, -0.07  
 3HZQ, LYS\_62, 10.22, -0.28, 0, 0  
 2BDD, GLU\_92, 4.71, 0.21, 0, 0  
 2QK1, LYS\_342, 10.5, 0, 0, 0  
 1RKA, GLU\_93, 3.87, 0.35, -0.98, 0  
 2P0Y, GLU\_235, 4.7, 1.27, -1.07, 0  
 1X04, GLU\_159, 4.29, 0.42, -0.63, 0  
 3ONH, CYS\_442, 9.07, 0, 0, 0.07  
 2W0G, ARG\_270, 11.87, -0.63, 0, 0  
 3Q1C, HIS\_148, 6.43, 0, 0, -0.07  
 3KT9, GLU\_101, 4.19, 0.07, -0.38, 0  
 3PBH, LYS\_86, 10.36, -0.14, 0, 0  
 2E0T, GLU\_64, 3.35, 0.21, -1.36, 0  
 2FPN, CYS\_130, 9, 0, 0, 0  
 2X4J, ASP\_52, 3.42, 0.07, -0.45, 0  
 1SIG, HIS\_338, 7.85, 1.56, 0, -0.21  
 3CCY, ARG\_47, 12.29, -0.21, 0, 0  
 1O3X, ARG\_258, 12.08, -0.42, 0, 0  
 1YTQ, TYR\_136, 12.12, 0.85, 0, 1.28  
 1GXN, GLU\_396, 4.85, 3.22, -2.86, 0  
 1V8E, TYR\_69, 12.37, 0.19, 0, 2.18  
 1MML, ASP\_28, 3.99, 0.21, -0.62, 0  
 3JZ9, ARG\_506, 11.87, -0.63, 0, 0  
 2JKF, LYS\_50, 10.15, -0.35, 0, 0  
 4ETX, ASP\_182, 3.24, 0.42, -0.98, 0  
 1J85, GLU\_56, 4.78, 0.28, 0, 0  
 3KTR, TYR\_55, 11.39, 0, 1.39  
 3GA2, GLU\_74, 2.37, 0.98, -3.11, 0  
 3HVM, HIS\_167, 6.36, 0, -0.14  
 1GVP, TYR\_61, 9.83, 0.14, -0.31, 0  
 1O6D, ASP\_83, 3.82, 0.07, -0.05, 0  
 3HVM, GLU\_174, 3.21, 0.28, -1.57, 0  
 1PNE, ASP\_8, 3.81, 0.21, -0.2, 0  
 1OLR, ASP\_172, 3.42, 0.42, -0.8, 0  
 3M66, GLU\_396, 3.76, 0.42, -1.16, 0  
 2R51, GLU\_175, 4.92, 0.42, 0, 0  
 2QV2, ASP\_324, 3.36, 0.14, -0.58, 0  
 3EAZ, ARG\_94, 12.5, 0, 0, 0  
 4DBX, ARG\_2, 12.36, -0.14, 0, 0  
 4D8L, LYS\_196, 10.29, -0.21, 0, 0  
 1ILW, ARG\_116, 11.94, -0.56, 0, 0  
 1EDG, ASP\_290, 3.3, 0.28, -0.78, 0  
 2YX0, ARG\_119, 11.93, -0.57, 0, 0  
 3CAX, LYS\_153, 10.43, -0.07, 0, 0  
 1V8E, ARG\_215, 12.36, -0.14, 0, 0  
 2D59, TYR\_50, 11.03, 1.03, 0, 0  
 2RFA, ASP\_90, 3.28, 0.28, -0.8, 0  
 1NWA, LYS\_81, 10.5, 0, 0, 0  
 2NRK, TYR\_149, 10.62, 0.66, -0.04, 0  
 1YM5, GLU\_35, 4.64, 0.21, -0.07, 0  
 3LJN, ASP\_237, 2.72, 1.26, -2.33, 0  
 1HUF, ARG\_28, 12.5, 0, 0, 0  
 2G7O, ARG\_110, 11.8, -0.7, 0, 0  
 2AZL, GLU\_94, 4.08, 0.28, -0.7, 0  
 2X4J, LYS\_64, 10.5, 0, 0, 0  
 1L2F, LYS\_81, 10.29, -0.21, 0, 0  
 2RGY, TYR\_301, 9.37, 2.34, -1.09, -1.88  
 1JKS, ASP\_88, 2.9, 0.7, -1.6, 0  
 2R51, GLU\_85, 3.84, 0.21, -0.87, 0  
 1M5I, ASP\_156, 3.88, 0.14, -0.06, 0  
 3IVF, LYS\_263, 10.5, 0, 0, 0  
 1UAJ, GLU\_203, 4.5, 0, 0, 0  
 1ES9, ARG\_206, 12.43, -0.07, 0, 0  
 3I82, ARG\_8, 11.59, -0.91, 0, 0  
 1AM2, HIS\_143, 6.82, 0.46, 0, -0.14  
 3BA1, GLU\_216, 4.57, 0.07, 0, 0  
 2FG1, LYS\_42, 10.01, -0.49, 0, 0  
 3T57, GLU\_91, 4.5, 0, 0, 0  
 1SFE, ASP\_59, 2.57, 0.21, -1.44, 0  
 3LPZ, LYS\_112, 10.43, -0.07, 0, 0  
 3U4K, LYS\_137, 9.59, -0.91, 0, 0  
 1SIG, LYS\_324, 10.43, -0.07, 0, 0  
 2EFK, GLU\_189, 4.54, 0.07, -0.03, 0  
 3VJ8, ASP\_194, 3.23, 0.28, -0.85, 0  
 1H09, ASP\_333, 3.8, 0, 0, 0  
 2QK1, LYS\_361, 10.15, -0.35, 0, 0  
 2V4U, GLU\_347, 3.98, 0.28, -0.8, 0  
 2OJQ, LYS\_621, 10.5, 0, 0, 0  
 2I6I, ASP\_69, 3.53, 0.28, -0.55, 0  
 2I88, HIS\_427, 4.66, 0.55, 0, -2.39  
 3JRT, LYS\_100, 10.43, -0.07, 0, 0  
 1DTO, GLU\_149, 4.57, 0.07, 0, 0  
 2OYZ, GLU\_5, 4.5, 0, 0, 0  
 3EGN, GLU\_417, 4.5, 0, 0, 0  
 2YLF, ARG\_188, 12.36, -0.14, 0, 0  
 2IDC, LYS\_71, 10.22, -0.28, 0, 0  
 1O5J, GLU\_16, 4.02, 0.28, -0.76, 0  
 2E0T, ASP\_184, 3.36, 0.42, -0.86, 0  
 1GVP, ASP\_50, 3.14, 0.49, -1.16, 0  
 1MIX, LYS\_272, 10.5, 0, 0, 0  
 2EDM, ARG\_57, 12.36, -0.14, 0, 0  
 1V43, ASP\_117, 3.56, 0.07, -0.31, 0  
 2OKT, TYR\_108, 10.22, 0.22, 0, 0  
 2ZCX, ASP\_144, 4.01, 0.21, 0, 0  
 2B3M, ARG\_117, 11.59, -0.91, 0, 0  
 3M70, CYS\_232, 5.71, -3.43, 0, 0.14  
 1TJE, ASP\_161, 1.8, 0.42, -2.42, 0  
 1UAJ, GLU\_120, 4.57, 0.07, 0, 0  
 2R57, CYS\_333, 11.16, -0.05, 1.29, 0.92  
 1RSS, GLU\_142, 3.67, 0.42, -1.25, 0  
 3GW3, TYR\_133, 9.82, 1.35, 0, -1.53  
 1UOH, HIS\_52, 7.01, 0.72, 0, -0.21  
 2B61, TYR\_313, 13.41, 0.21, 0.8, 2.4  
 3IUS, TYR\_84, 10.42, 0.42, 0, 0  
 3F6F, GLU\_136, 4.64, 0.14, 0, 0  
 3V3T, ASP\_221, 2.2, 0.42, -2.02, 0  
 3F7M, ASP\_288, 2.33, 0.91, -2.38, 0  
 1DTO, TYR\_115, 10.1, 0.1, 0, 0  
 3Q6L, ASP\_99, 3.9, 0.14, -0.04, 0  
 1O0X, LYS\_19, 10.22, -0.28, 0, 0  
 1J85, ARG\_121, 12.22, -0.28, 0, 0  
 3L3P, GLU\_509, 4.57, 0.07, 0, 0  
 3ANJ, LYS\_8, 10.5, 0, 0, 0  
 1X04, GLU\_219, 4.57, 0.07, 0, 0  
 1MIX, CYS\_236, 9.65, -0.04, 0, 0.69  
 1DCF, HIS\_51, 3.53, 0.4, 0, -3.37  
 2B78, GLU\_346, 3.32, 0.42, -1.6, 0  
 2PGX, ASP\_221, 4.02, 0.42, -0.21, 0  
 3GOZ, ASP\_120, 3.94, 0.14, 0, 0  
 1T6L, HIS\_248, 6.69, 0.19, 0, 0  
 2D59, GLU\_92, 4.92, 0.42, 0, 0  
 1YTD, ARG\_335, 12.15, -0.35, 0, 0  
 2IXM, TYR\_68, 10.38, 0.38, 0, 0  
 3TOW, GLU\_157, 4.09, 0.14, -0.55, 0  
 4ACJ, LYS\_695, 10.5, 0, 0, 0  
 2A1V, HIS\_140, 6.56, 0.06, 0, 0  
 2P65, GLU\_135, 4.64, 0.14, 0, 0  
 3ERF, ARG\_156, 11.94, -0.56, 0, 0  
 3K1H, ARG\_80, 12.08, -0.42, 0, 0  
 1TR9, ASP\_284, 3.99, 0.21, -0.02, 0  
 2TRD, ARG\_374, 11.96, -2.25, 0, 1.71  
 2XHC, ARG\_229, 12.29, -0.21, 0, 0  
 1RAJ, GLU\_76, 4.71, 0.21, 0, 0  
 3T5B, GLU\_23, 4.26, 1.81, -2.05, 0  
 3ON1, HIS\_79, 6.5, 0, 0, 0  
 1U3Y, LYS\_275, 10.36, -0.14, 0, 0  
 2FG1, GLU\_91, 4.5, 0, 0, 0  
 2BLL, GLU\_374, 4.5, 0, 0, 0  
 1HF8, GLU\_249, 4.57, 0.07, 0, 0  
 2RFA, TYR\_154, 12.38, 0, 2.38  
 3B79, ARG\_56, 12.36, -0.14, 0, 0  
 2DVK, ARG\_111, 12.01, -0.49, 0, 0  
 1BYI, HIS\_184, 7.23, 0.8, 0, -0.07  
 3PP8, GLU\_131, 4.85, 0.35, 0, 0  
 2P52, TYR\_199, 10.13, 0, 0.13  
 2YWK, GLU\_7, 3.77, 0.21, -0.94, 0  
 2W0G, LYS\_273, 10.5, 0, 0, 0  
 3FFM, GLU\_66, 4.5, 0, 0, 0  
 4DBX, HIS\_50, 7.3, 1.01, 0, -0.21  
 1N81, GLU\_134, 5.69, 0.97, 0, 0.22  
 3UC9, HIS\_157, 7.36, 0.93, 0, -0.07  
 2QDJ, TYR\_155, 10.61, 1.39, -0.8, 0.02  
 1Q46, GLU\_78, 4.57, 0.07, 0, 0  
 3V55, ASP\_662, 3.83, 0.21, -0.18, 0  
 2PLQ, ARG\_24, 11.8, -0.7, 0, 0  
 2OB5, ASP\_100, 2.51, 0.56, -1.85, 0  
 2B02, TYR\_386, 9.46, 0.07, -0.75, 0.14  
 4E9E, GLU\_552, 3.46, 0.56, -1.6, 0  
 3UV9, ARG\_484, 13.48, -1.62, 0.26  
 1I60, TYR\_54, 11.99, 0.35, 0, 1.64  
 2Y2T, ASP\_74, 3.87, 0.07, 0, 0  
 3A4C, GLU\_506, 3.2, 0.35, -1.65, 0  
 1AKO, ARG\_224, 11.73, -0.77, 0, 0  
 3VHJ, TYR\_47, 11.97, 0.07, 0.09, 1.81  
 3ETV, LYS\_71, 10.29, -0.21, 0, 0  
 2RIS, CYS\_165, 6.17, -6.49, 1.98, 1.7  
 3BB7, ASP\_58, 4.15, 0.35, 0, 0  
 1O17, GLU\_159, 4.64, 0.14, 0, 0  
 2O8I, ASP\_90, 3.16, 0.28, -0.92, 0  
 1YLN, ARG\_108, 11.94, -0.56, 0, 0  
 3K9I, GLU\_137, 4.12, 0.35, -0.73, 0  
 4H4J, LYS\_35, 10.15, -0.35, 0, 0  
 3EJC, ASP\_20, 3.96, 0.21, -0.05, 0  
 2APL, HIS\_11, 6.43, 0, 0, -0.07  
 1WLY, HIS\_141, 7.68, 1.64, 2.48, -2.94  
 3V75, ARG\_268, 12.01, -0.49, 0, 0  
 1SQW, LYS\_115, 10.08, -0.42, 0, 0  
 3CIV, ASP\_211, 3.71, 0.14, -0.23, 0  
 2P52, ARG\_155, 13.68, -1.22, 0.24  
 1IDK, TYR\_215, 10.53, 0.62, -0.07, -0.02  
 1NIJ, GLU\_230, 3.62, 0.72, -1.6, 0  
 4DNU, GLU\_170, 3.97, 0.14, -0.67, 0  
 1NKD, ASP\_31, 3.28, 0.07, -0.59, 0  
 1R16, TYR\_65, 10.8, 0.8, 0, 0  
 2P0L, TYR\_136, 10, 0, 0, 0  
 2FBI, GLU\_50, 2.94, 0.84, -2.41, 0  
 1D2K, LYS\_346, 10.5, 0, 0, 0  
 3RLE, GLU\_81, 4.09, 0.21, -0.62, 0  
 3ADO, TYR\_152, 12.8, 0.61, 0.13, 2.06  
 1P6F, ASP\_101, 2.58, 0.35, -1.57, 0  
 1X7F, GLU\_234, 2.04, 1.61, -3.44, -0.63  
 3QAV, TYR\_10, 12.81, 0.07, 0.34, 2.4  
 3CS1, LYS\_197, 10.69, -0.28, 0.47  
 1UW7, ASP\_25, 3.2, 0, -0.6, 0  
 2CBE, TYR\_114, 10.39, 0.39, 0, 0  
 1BKB, ARG\_136, 12.5, 0, 0, 0  
 1ATO, ARG\_304, 12.15, -0.35, 0, 0  
 3DZ1, ASP\_244, 3.79, 0.14, -0.15, 0  
 3R2E, GLU\_113, 3.44, 0.42, -1.48, 0  
 1ZBM, ASP\_235, 3.7, 0, -0.1, 0  
 2VGM, TYR\_196, 12.93, 0.14, 0.38, 2.4  
 3BJV, TYR\_57, 9.9, 0.78, -0.88, 0  
 3LJN, ASP\_201, 2.97, 0.49, -1.32, 0  
 2Z0M, ASP\_118, 3.29, 0.56, -1.07, 0  
 2Q98, TYR\_168, 12.36, 1, 0.136  
 2YWK, GLU\_20, 12.01, -0.49, 0, 0  
 3BQE, ASP\_257, 3.31, 0.84, -1.33, 0  
 1ESS, TYR\_206, 9.47, 0.49, -1.02, 0  
 1R53, HIS\_338, 6.31, 0.02, 0, -0.21  
 3ETU, LYS\_89, 10.5, 0, 0, 0  
 4EZB, GLU\_194, 3.98, 0.28, -0.8, 0  
 1O5T, CYS\_274, 4.65, -4.35, 0, 0  
 2FBI, GLU\_48, 4.64, 0.14, 0, 0  
 3RLN, LYS\_597, 10.43, -0.07, 0, 0  
 4E8B, ARG\_33, 12.08, -0.42, 0, 0  
 3GFP, ASP\_458, 3.87, 0.07, 0, 0  
 3ETU, CYS\_245, 8.54, -0.53, 0, 0.07  
 2O0K, GLU\_326, 4.57, 0.07, 0, 0  
 2D8N, ARG\_71, 10.01, -2.49, 0, 0  
 1V43, ASP\_174, 2.68, 0.42, -1.54, 0  
 2OKT, HIS\_58, 6.49, 0.06, 0, -0.07  
 1OLR, ARG\_159, 12.15, -0.35, 0, 0  
 3O48, TYR\_14, 10.47, 0.14, 0, 0.33  
 2QRX, GLU\_40, 4.45, 0, -0.05, 0  
 2A4D, ASP\_175, 2.89, 0.84, -1.76, 0  
 3G9B, LYS\_99, 10.5, 0, 0, 0  
 4AM1, LYS\_43, 10.36, -0.14, 0, 0  
 3RAZ, LYS\_65, 10.5, 0, 0, 0  
 2HNG, CYS\_103, 9.29, -0.23, 0.52  
 3HXK, HIS\_219, 5.4, 2.74, 2.4, -6.24  
 3B21, TYR\_76, 13, 0.07, 0.61, 2.31  
 4F8A, ARG\_573, 11.94, -0.56, 0, 0  
 1ILW, LYS\_171, 10.5, 0, 0, 0  
 2A4D, GLU\_112, 4.09, 0.35, -0.76, 0  
 1ZYL, TYR\_42, 9.78, 0.02, -0.24, 0  
 2IRK, HIS\_206, 2.99, 1.6, -0.32, -4.79  
 1RHS, ARG\_20, 12.01, -0.49, 0, 0  
 1T3J, LYS\_731, 10.5, 0, 0, 0  
 2BQQ, GLU\_137, 4.5, 0, 0, 0  
 3E7P, TYR\_241, 12.82, 0.79, 0.203  
 2EEY, LYS\_108, 9.87, -0.63, 0, 0  
 2AHE, TYR\_204, 10.43, -0.07, 0, 0  
 2R51, TYR\_270, 9.14, 2.32, -1.94, -1.25  
 1X7F, TYR\_129, 13.65, 1.22, 0.03, 2.4  
 3DZ1, ASP\_26, 4.01, 0.35, -0.14, 0  
 3E0H, ARG\_86, 12.15, -0.35, 0, 0  
 3P28, TYR\_97, 11.91, 2.44, -0.53, 0  
 3EOD, GLU\_118, 4.18, 0.35, -0.67, 0  
 3AU3, GLU\_633, 4.19, 0.49, -0.8, 0  
 1YM5, ARG\_213, 13.46, -2.18, 0.314  
 3FHF, ARG\_98, 11.87, -0.63, 0, 0  
 3UAH, LYS\_260, 10.22, -0.28, 0, 0

1C3K,LYS\_51,10.5,0,0,0  
 1YR6,LYS\_87,10.15,-0.35,0,0  
 3ONH,GLU\_526,4.12,0.28,-0.66,0  
 3M7D,GLU\_194,3.93,0.21,-0.78,0  
 2F4Q,ARG\_15,11.52,-0.98,0,0  
 1ZBS,CYS\_106,9.98,0,0.09,0.89  
 1RL0,GLU\_125,1.5,0.78,-1.95,-1.82  
 3S0A,GLU\_39,4.64,0.14,0,0  
 3BPP,GLU\_54,3.97,0.59,-1.12,0  
 4FH3,CYS\_48,10.38,-0.14,0,1.52  
 1T3J,LYS\_713,10.36,-0.14,0,0  
 2EJB,HIS\_157,6.5,0,0,0  
 4E9E,LYS\_562,10.43,-0.07,0,0  
 2P5D,GLU\_29,3.41,0.42,-1.51,0  
 2Q13,ARG\_171,12.22,-0.28,0,0  
 2H30,TYR\_118,9.65,0,-0.35,0  
 2CW4,CYS\_75,8.23,-1.79,0,1.02  
 3ODJ,TYR\_40,10.07,0.07,0,0  
 2R51,HIS\_111,6.5,0,0,0  
 2D7J,GLU\_113,2.64,0.52,-0.98,-1.4  
 3TIR,ARG\_125,11.17,-1.33,0,0  
 3UX2,ASP\_135,2.27,0.42,-1.95,0  
 1R29,ASP\_29,2.64,0.42,-1.58,0  
 2BT8,ARG\_321,12.5,0,0,0  
 1T6L,CYS\_117,8.98,-0.02,0,0  
 1MUF,GLU\_177,4.5,0,0,0  
 4DBX,TYR\_177,11.79,1.26,-0.8,1.33  
 4DVD,ARG\_82,12.01,-0.49,0,0  
 3FWU,CYS\_88,9.41,0,0,0.41  
 1T3J,ASP\_685,3.53,0.21,-0.48,0  
 3QKY,ARG\_160,11.73,-0.77,0,0  
 2ZCO,HIS\_148,6.36,0,-0.14  
 3MIX,ARG\_367,11.52,-0.98,0,0  
 1P2F,LYS\_193,10.22,-0.28,0,0  
 3EYE,ASP\_44,3.59,0.07,-0.28,0  
 3CZC,ARG\_27,11.87,-0.63,0,0  
 3HUE,TYR\_112,10.42,0.07,0,0.35  
 1FKM,ASP\_403,3.94,0.14,0,0  
 2E3H,CYS\_265,8.73,-0.34,0,0.07  
 1GPP,ASP\_116,2.15,0.63,-0.27,0  
 1XEU,LYS\_100,10.67,-0.00,0,0  
 3FWU,ASP\_36,3.24,0.14,-0.7,0  
 1AK1,LYS\_5,10.43,-0.07,0,0  
 3BPV,ARG\_70,12.15,-0.35,0,0  
 3VHJ,GLU\_152,3.67,0.56,-1.4,0  
 3J5N,GLU\_47,4.5,0,0,0  
 1V6T,TYR\_86,11.69,0,0,1.69  
 1JB3,ASP\_75,3.33,0.28,-0.75,0  
 1MUF,GLU\_142,4.47,0.28,-0.31,0  
 2OBI,HIS\_25,7.44,1.08,0,-0.14  
 2Z84,ARG\_93,11.94,-0.56,0,0  
 3KB5,CYS\_313,8.17,-1.07,-0.42,0.66  
 3GOZ,HIS\_226,7.18,0.95,0,-0.28  
 3NBI,GLU\_28,4.32,0.07,-0.25,0  
 2GAU,LYS\_40,10.36,-0.14,0,0  
 2G2D,GLU\_83,4.35,0,-0.15,0  
 3GW3,HIS\_331,7.09,0.8,0,-0.21  
 1AD6,CYS\_407,7.77,-1.3,0,0.07  
 1J8B,CYS\_52,8.67,-0.33,0,0  
 1EV8,TYR\_4,11.97,1.98,-0.01,0  
 1XIP,GLU\_7,4.69,0.21,-0.02,0  
 1DUN,TYR\_75,9.88,0.07,-0.19,0  
 1NKD,ASP\_38,3.84,0.07,-0.03,0  
 1MTZ,ASP\_277,3.28,0.28,-0.8,0  
 1P1L,LYS\_45,9.8,-0.7,0,0  
 1MML,ARG\_80,11.87,-0.63,0,0  
 1TUL,HIS\_43,6.84,0.69,0,-0.35  
 3J5N,GLU\_21,4.78,0.28,0,0  
 2D0A,ARG\_141,11.94,-0.56,0,0  
 1P4X,LYS\_24,10.5,0,0,0  
 1UUA,GLU\_142,3.39,1.79,-2.89,0  
 1CHD,ASP\_249,3.18,0.21,-0.83,0  
 3JZN,ARG\_264,12.5,-1.13,0,1.13  
 3US6,ASP\_51,3.77,0.14,-0.17,0  
 2BCF,ARG\_250,11.94,-0.56,0,0  
 1X1E,HIS\_115,6.43,0,0,-0.07  
 3GT0,LYS\_112,10.5,0,0,0  
 1YLN,HIS\_154,6.31,0.02,0,-0.21  
 2Z0W,TYR\_39,10,0,0,0  
 2CIU,LYS\_139,10.5,0,0,0  
 3FK5,GLU\_141,4.19,0.49,-0.8,0  
 1LTU,ARG\_58,12.01,-0.49,0,0  
 1PVT,HIS\_104,3.58,1.6,-1.47,-5.99  
 2ATR,TYR\_45,10.63,0.21,-0.2,0.62  
 2D0A,ASP\_136,2.9,0.42,-1.31,0  
 2XJ4,ARG\_167,11.35,-1.15,0,0  
 1X9G,GLU\_46,4.26,0.56,-0.8,0  
 1PSW,ARG\_22,11.66,-0.84,0,0  
 3A4C,LYS\_537,10.22,-0.28,0,0  
 3TMO,HIS\_315,6.5,0,0,0  
 3ZTA,LYS\_67,10.15,-0.35,0,0  
 1RKA,GLU\_236,4.5,0,0,0  
 3M7G,GLU\_259,4.57,0.07,0,0  
 3I4T,ASP\_210,2.8,0.35,-1.35,0  
 3U2R,ARG\_141,12.15,-0.35,0,0  
 3V1Q,LYS\_614,10.43,-0.07,0,0  
 1RZ2,ASP\_156,2.56,0.35,-1.59,0  
 3EX9,CYS\_145,8.99,-0.01,0,0  
 3ETV,CYS\_257,2.25,-6.88,0,0.14  
 1YTD,ARG\_262,11.52,-0.98,0,0  
 2JEO,LYS\_69,10.22,-0.28,0,0  
 2D59,TYR\_68,10.32,0.07,0,0.25  
 3H8Y,GLU\_22,4.57,0.07,0,0  
 4FD6,ARG\_134,12.83,-2.71,0,3.03  
 2RFA,GLU\_177,4.78,0.28,0,0  
 3V3T,LYS\_260,10.29,-0.21,0,0  
 3ULX,ARG\_19,12.01,-0.49,0,0  
 1MML,ARG\_187,11.62,-0.88,0,0  
 1YTD,LYS\_218,10.08,-0.42,0,0  
 3UAH,ASP\_275,3.7,0,-0.1,0  
 2CN1,GLU\_276,4.02,0.14,-0.62,0  
 1DOV,ASP\_96,3.63,0.14,-0.31,0  
 3CAX,ARG\_156,12.22,-0.28,0,0  
 2BDV,ARG\_81,12.29,-0.21,0,0  
 3KEY,LYS\_410,10.43,-0.07,0,0  
 4E8B,ASP\_120,3.11,0.21,-0.9,0  
 3ELI,HIS\_98,4.45,0.02,0,-2.07  
 1KN3,ASP\_144,3.25,0.07,-0.63,0  
 3VJ8,CYS\_172,10.61,-0.05,-0.75,2.4  
 2FPN,LYS\_59,10.36,-0.14,0,0  
 1EYH,GLU\_90,4.5,0,0,0  
 3C5V,GLU\_353,5.79,3.65,-2.36,0  
 3RNV,CYS\_389,11.22,-0.11,0,2.33  
 3ZRI,LYS\_58,10.5,0,0,0  
 1O5T,GLU\_121,4.57,0.07,0,0  
 3M7D,ASP\_124,1.8,0.56,-2.56,0  
 3F1X,HIS\_167,3.82,0.09,0,-2.77  
 2IDC,ARG\_49,12.15,-0.35,0,0  
 4ETX,ARG\_205,12.15,-0.35,0,0  
 1BYI,ASP\_110,3,0.7,-1.5,0  
 2QVT,HIS\_85,7.61,1.18,0,-0.07  
 1D2K,LYS\_60,10.36,-0.14,0,0  
 1Q42,ARG\_116,11.94,-2.84,0,2.28  
 2G3A,HIS\_55,6.43,0,0,-0.07  
 3LPZ,ARG\_292,12.5,0,0,0  
 1NJ4,TYR\_312,13.27,0.07,0.8,2.4  
 3P2F,HIS\_14,6.36,0,0,-0.14  
 3EX9,ASP\_57,3.19,0.07,-0.67,0  
 3CGW,LYS\_183,10.08,-0.42,0,0  
 2NYC,ARG\_294,11.38,-1.12,0,0  
 3LH5,LYS\_564,10.5,0,0,0  
 1AD6,LYS\_462,10.01,-0.49,0,0  
 2G55,GLU\_41,4.57,0.07,0,0  
 1TLV,ARG\_203,12.5,0,0,0  
 2H85,ASP\_260,3.95,0.21,-0.06,0  
 3BWT,HIS\_639,7.08,0.65,0,-0.07  
 2GAU,GLU\_159,3.52,0.53,-1.51,0  
 3CJW,ARG\_385,12.5,0,0,0  
 3BB7,TYR\_120,13.55,0.35,0.8,2.4  
 2EEY,LYS\_106,10.29,-0.21,0,0  
 3FHF,ARG\_84,12.29,-0.21,0,0  
 2A0J,ASP\_90,3.6,0.21,-0.41,0  
 3I82,ASP\_118,2.73,0.21,-1.28,0  
 3JZN,ASP\_140,1.97,0.84,-2.67,0  
 3CGW,ARG\_60,11.94,-0.56,0,0  
 2E3S,TYR\_404,10.55,0.07,0,0.48  
 1RAJ,GLU\_396,4.03,0.21,-0.68,0  
 4EZB,ASP\_220,3.18,0.49,-1.12,0  
 3O7K,LYS\_122,10.22,-0.28,0,0  
 4DBX,HIS\_251,6.36,0,0,-0.14  
 2DFL,HIS\_186,6.5,0,0,0  
 1J7G,GLU\_34,3.51,0.21,-1.2,0  
 3GEC,ASP\_238,3.57,0.21,-0.44,0  
 3G9T,LYS\_225,10.5,0,0,0  
 3GFP,LYS\_382,10.43,-0.07,0,0  
 3ETV,GLU\_202,4,0.21,-0.71,0  
 1CHD,CYS\_207,9.18,-0.06,0,0.24  
 2Q98,ASP\_17,3.71,0,-0.09,0  
 3ASA,LYS\_96,10.5,0,0,0  
 1WPA,GLU\_449,4.71,0.21,0,0  
 2Q99,ASP\_361,4.05,0.35,-0.1,0  
 1IDK,HIS\_232,4.65,0.79,0,-2.64  
 3I0O,LYS\_179,10.43,-0.07,0,0  
 2IDC,GLU\_25,4.64,0.14,0,0  
 2X4L,GLU\_340,4.5,0,0,0  
 2E3I,TYR\_108,8.18,0.14,-1.96,0  
 3M70,TYR\_8,9.34,0.14,-0.8,0  
 1NAR,LYS\_106,10.22,-0.28,0,0  
 2ZCX,GLU\_65,3.9,0.7,-1.3,0  
 1P6FLY,LYS\_59,10.08,-0.42,0,0  
 3TOW,HIS\_106,6.5,0,0,0  
 2D59,ARG\_5,12.5,0,0,0  
 3RE9,GLU\_118,4.5,0,0,0  
 3B2I,GLU\_80,4.31,0.28,-0.47,0  
 4FH3,ARG\_294,12.08,-0.42,0,0  
 2RJD,HIS\_291,3.01,0.16,0,-3.65  
 3OKQ,ASP\_579,3.9,0.14,-0.04,0  
 3JZN,TYR\_308,10.93,0,0,0.93  
 2E3C,CYS\_296,9.15,-0.32,0,0.47  
 2C2Y,HIS\_147,4.56,0,0,-1.94  
 1XAW,ASP\_426,3.09,0.14,-0.85,0  
 2NRR,ARG\_484,12.29,-0.21,0,0  
 1BYI,LYS\_182,10.5,0,0,0  
 2X4L,LYS\_198,10.29,-0.21,0,0  
 1Q42,ARG\_48,11.87,-0.63,0,0  
 1R3F,HIS\_43,4.49,0.02,0,-2.03  
 4E9E,TYR\_509,11.19,0,0,1.19  
 1AT0,GLU\_337,2.79,0.77,-2.48,0  
 3DHN,ARG\_36,12.5,0,0,0  
 3F53,ARG\_83,12.01,-0.49,0,0  
 2CXV,GLU\_71,4.5,0,0,0  
 4H4J,TYR\_41,13.62,0.59,-0.78,3.82  
 3V4G,GLU\_142,4.44,0.07,-0.13,0  
 1O17,HIS\_62,7.61,1.18,0,-0.07  
 2XMX,CYS\_235,9.65,0,0,0.65  
 2DG7,CYS\_173,8.51,-0.49,0,0  
 3R2E,HIS\_63,7.15,0.79,0,-0.14  
 1M5I,GLU\_136,4.71,0.21,0,0  
 2R57,CYS\_376,9,0,0,0  
 4F85,ARG\_268,13.12,-1.68,0,2.3  
 3G53,GLU\_169,4.5,0,0,0  
 2PGE,ARG\_72,12.22,-0.28,0,0  
 2RJD,ASP\_420,3.77,0,-0.03,0  
 3CIV,LYS\_111,10.5,0,0,0  
 2V4U,LYS\_353,10.5,0,0,0  
 1Y2Q,GLU\_107,4.12,0.42,-0.8,0  
 3U0V,HIS\_53,6.22,0,0,-0.28  
 3ODJ,LYS\_131,10.5,0,0,0  
 1JB3,HIS\_32,7.09,0.8,0,-0.21  
 2O8P,TYR\_222,9.85,0.14,-0.47,0.18  
 2BCF,TYR\_233,10,0,0,0  
 2AZP,HIS\_208,4.65,1.94,2.06,-5.84  
 4EUG,CYS\_200,3.36,-6.1,-0.66,1.12  
 1WNH,LYS\_114,10.5,0,0,0  
 2H85,TYR\_88,8.29,0.43,-0.35,-1.8  
 4FLE,ASP\_138,3.64,0,-0.16,0  
 3PP8,GLU\_79,4.11,0.49,-0.88,0  
 1QQE,LYS\_199,10.29,-0.21,0,0  
 2IQT,ARG\_95,11.59,-0.91,0,0  
 1517,ARG\_188,12.5,0,0,0  
 1G5Z,ASP\_105,4.08,0.28,0,0  
 4ANN,GLU\_164,4.5,0,0,0  
 1AKO,ARG\_78,12.01,-0.49,0,0  
 1ZBS,ARG\_226,12.29,-0.21,0,0  
 1OGL,GLU\_265,4.5,0,0,0  
 3MIX,LYS\_318,4.5,0,0,0  
 1IAP,ARG\_137,12.29,-0.21,0,0  
 2IDC,LYS\_129,10.5,0,0,0  
 1DZF,ARG\_55,13.46,-1.44,0,2.4  
 1WNH,CYS\_144,11.16,-0.55,0,2.71  
 3GT0,GLU\_106,4.12,0.42,-0.8,0  
 2CXY,LYS\_192,10.36,-0.14,0,0  
 1JB3,GLU\_126,4.5,0,0,0  
 3LJC,GLU\_191,4.5,0,0,0  
 2ZQ5,ARG\_72,13.62,-2.9,0,4.02  
 4EVF,GLU\_76,3.93,0.14,-0.71,0  
 1R3F,ARG\_81,12.22,-0.28,0,0  
 2X4G,ASP\_66,3.13,0.28,-0.95,0  
 1TD6,GLU\_226,4.34,0.07,-0.23,0  
 1BKB,GLU\_19,4.57,0.07,0,0  
 4DIU,LYS\_86,10.5,0,0,0  
 3B4D,ASP\_180,0.49,0.63,-3.93,0  
 3KB5,TYR\_429,9.64,0.34,-0.7,0  
 2O8P,LYS\_119,10.5,0,0,0  
 3GT0,GLU\_145,3.91,0.21,-0.8,0  
 2O0K,ASP\_201,3.6,0.21,-0.41,0  
 2YWX,LYS\_151,10.5,0,0,0  
 3F53,ARG\_82,11.23,-1.94,0,0.67  
 2EEY,TYR\_129,10.07,0.07,0,0  
 1WP5,ARG\_114,11.07,-0.63,0,0  
 1JT9,GLU\_122,2.47,1.73,-3.76,0  
 2YX0,GLU\_230,4.05,0.35,-0.8,0  
 1T95,GLU\_62,4.64,0.14,0,0  
 2YLF,TYR\_217,13.57,0.72,-0.1,2.95  
 3V3T,LYS\_304,10.5,0,0,0  
 3CJW,HIS\_291,6.89,0.67,0,-0.28  
 2WB8,GLU\_461,4.57,0.07,0,0  
 2Q12,TYR\_147,10,0,0,0  
 3M66,HIS\_309,6.76,0.33,0,-0.07  
 3CN5,LYS\_64,10.5,0,0,0  
 1X1E,ARG\_198,12.22,-0.28,0,0  
 2QDJ,LYS\_192,10.29,-0.21,0,0  
 1F09,GLU\_215,4.31,0.63,-0.82,0  
 1T07,ASP\_18,3.29,0.14,-0.64,0  
 1TR9,TYR\_84,12.57,2.57,0,0  
 2Q07,ASP\_396,2.72,0.42,-1.5,0

3RRQ,CYS\_93,4.56,-4.51,0,0,0,0  
3BCH,LYS\_166,10.5,0,0,0  
1XEU,ASP\_256,3.94,0.14,0,0  
2FBI,CYS\_59,9,0,0,0  
2B6P,ARG\_85,13.6,-0.93,0,2,0,3  
3DHN,GLU\_129,4.5,0,0,0  
2EJB,GLU\_46,2.93,0.49,-2.06,0  
1TWU,ASP\_78,4.15,0.35,0,0  
1AKO,HIS\_118,6.6,0.31,0,-0.21  
1A8Q,ASP\_44,3.26,0.28,-0.82,0  
1YTD,LYS\_313,10.43,-0.07,0,0  
3JRT,LYS\_115,10.43,-0.07,0,0  
1ILW,GLU\_42,4.57,0.07,0,0  
3OA7,ARG\_556,12.22,-0.28,0,0  
1R7J,LYS\_4,10.43,-0.07,0,0  
1GVP,ASP\_79,2.55,0.35,-1.6,0  
4FCU,ASP\_164,3.11,0.35,-1.05,0  
2BDD,ARG\_100,12.29,-0.21,0,0  
1BN6,GLU\_268,4.5,0,0,0  
1YB2,GLU\_45,4.05,0.35,-0.8,0  
3P28,LYS\_65,10.29,-0.21,0,0  
2WB8,LYS\_663,10.5,0,0,0  
2YX0,ASP\_329,3.05,0.56,-1.31,0  
2AXO,LYS\_230,10.15,-0.35,0,0  
2EDM,TYR\_46,9.81,0.28,-0.47,0  
1F09,GLU\_104,4.02,0,-0.48,0  
3L7N,LYS\_172,10.15,-0.35,0,0  
1WXF,HIS\_260,6.92,0.49,0,-0.07  
1J7G,ASP\_135,3.86,0.07,-0.01,0  
3MTT,GLU\_543,4.36,0.21,-0.35,0  
3IL3,ASP\_238,3.21,0.63,-1.22,0  
2ZCX,ARG\_218,11.94,-0.56,0,0  
1G5Z,GLU\_51,4.23,0.14,-0.41,0  
1T95,TYR\_189,13.41,0.21,0.8,2.4  
1GVP,LYS\_46,10.15,-0.35,0,0  
1ES9,HIS\_144,6.43,0,0,-0.07  
1QQ,GLU\_91,4.5,0,0,0  
2HXB,TYR\_90,8.44,0.07,-1.65,0.02  
3GV0,TYR\_99,11.48,0,1,48  
2F19,GLU\_79,4.64,0.14,0,0  
2QXR,TYR\_141,10.33,0.66,-0.33,0  
2HNG,ASP\_38,3.26,0.42,-0.97,0  
2D25,LYS\_613,9.8,-0.7,0,0  
3CRM,ARG\_54,12.5,0,0,0  
1TD6,ARG\_144,12.15,-0.35,0,0  
1PDB,ASP\_186,2.75,0.84,-1.9,0  
4DNU,HIS\_268,6.37,0.01,0,-0.14  
1SNT,TYR\_359,7.5,0.81,-0.8,-2.51  
1WLY,GLU\_107,4.5,0,0,0  
3T5B,ARG\_11,11.63,-1.15,0,0.28  
3PZ9,ASP\_158,2.32,0.77,-2.25,0  
3V3T,LYS\_271,9.94,-0.56,0,0  
3IVF,LYS\_57,10.43,-0.07,0,0  
2EFK,LYS\_30,10.29,-0.21,0,0  
3H5T,ARG\_41,12.08,-0.42,0,0  
2FC3,GLU\_120,3.91,0.21,-0.8,0  
1T07,GLU\_52,4.5,0,0,0  
3CAX,ARG\_193,11.52,-0.98,0,0  
1OTM,GLU\_129,4.78,0.28,0,0  
2BT8,ARG\_225,11.45,-1.05,0,0  
2V5B,GLU\_134,3.35,0.49,-1.63,0  
3G59,TYR\_179,13.05,1.19,0.06,1.81  
1LTU,ASP\_154,3.9,0.14,-0.04,0  
3RKV,LYS\_328,10.5,0,0,0  
2DBN,LYS\_119,9.73,-0.77,0,0  
1RSQ,ASP\_6,3.26,0.42,-0.95,0  
1HF8,TYR\_118,9.46,0.07,-0.61,0  
2EFK,GLU\_15,3.84,0.14,-0.8,0  
1V43,TYR\_259,11.29,0,-0.78,2.06  
3LQE,HIS\_270,4.09,0,0,-2.41  
3IOC,GLU\_242,4.78,0.49,-0.21,0  
2XWS,HIS\_74,6.43,0,0,-0.07  
1F2V,LYS\_155,10.43,-0.07,0,0  
1O0X,CYS\_155,8.95,-0.56,0,0.51  
1MN3,ARG\_438,12.5,0,0,0  
2WB8,CYS\_792,9.07,0,0,0.07  
3M66,ARG\_257,12.29,-0.21,0,0  
2AD1,HIS\_142,6.84,0.41,0,-0.07  
1U53,CYS\_152,9.47,0,0,0.47  
1K95,TYR\_86,12.47,0.14,0.38,1.95  
2AD1,GLU\_161,2.59,0.49,-2.4,0  
1R29,ARG\_44,11.73,-0.77,0,0  
2E3C,ARG\_252,12.15,-0.35,0,0  
1F2V,LYS\_69,10.5,0,0,0  
1LZL,HIS\_283,7.02,0.8,0,-0.28  
1Z9L,LYS\_87,10.01,-0.49,0,0  
3V1Q,HIS\_634,6.27,0.33,0,-0.56  
2EJX,ARG\_118,11.94,-0.56,0,0  
3N2T,ASP\_36,3.13,0.28,-0.94,0  
3E5T,ARG\_230,12.43,-0.07,0,0  
3RHE,HIS\_61,6.5,0,0,0  
3PP8,GLU\_21,14.5,0,0,0  
2FGG,ASP\_49,3.8,0.14,-0.14,0  
1OI7,GLU\_216,3.84,0.14,-0.8,0  
4EZB,GLU\_208,4.57,0.07,0,0  
2PPN,GLU\_5,4.43,0.14,-0.21,0  
3OA7,GLU\_565,4.5,0,0,0  
1EV8,ARG\_107,12.08,-0.42,0,0  
2YT4,LYS\_659,10.36,-0.14,0,0  
4F85,ASP\_65,3.1,0.49,-1.19,0  
3CX5,GLU\_120,5.77,0.45,-0.32,1.15  
3G65,ASP\_71,2.04,0.77,-2.53,0  
2BT8,GLU\_194,4.5,0,0,0  
3JZN,GLU\_347,3.67,0.35,-1.18,0  
1ZCU,TYR\_194,10.07,0.07,0,0  
3OA7,GLU\_518,4.86,0.42,-0.06,0  
3RUX,TYR\_181,11.37,1.37,0,0  
3CNU,LYS\_5,10.01,-0.49,0,0  
1RSS,CYS\_47,9.46,-0.67,0,1.13  
2G2D,ASP\_61,3.93,0.21,-0.08,0  
3RUX,GLU\_239,4.51,0.28,-0.26,0  
2VAN,TYR\_142,13.17,0.29,0.48,2.4  
3M66,LYS\_329,10.5,0,0,0  
1SUU,ASP\_578,3.59,0.56,-0.77,0  
3CE7,LYS\_30,10.5,0,0,0  
1SQW,LYS\_148,10.5,0,0,0  
1Z9L,GLU\_103,4.5,0,0,0  
1HF8,LYS\_24,10.43,-0.07,0,0  
1PGV,GLU\_268,4.58,0.21,-0.13,0  
3K8J,ARG\_221,12.15,-0.35,0,0  
2OBI,ARG\_69,11.8,-0.7,0,0  
2GZQ,ASP\_22,2.98,0.35,-1.17,0  
4GCO,HIS\_165,7.16,0.8,0,-0.14  
2ZQ5,GLU\_84,3.93,0.56,-1.13,0  
1H09,LYS\_330,10.5,0,0,0  
3GV0,LYS\_205,10.29,-0.21,0,0  
1DUN,CYS\_83,10.03,0,1,0.3  
1KN3,HIS\_86,1.8,1.15,0.74,-6.59  
1SIG,LYS\_121,10.5,0,0,0  
3G9G,ARG\_128,12.08,-0.42,0,0  
2QEV,LYS\_140,10.43,-0.07,0,0  
1TLV,ARG\_238,12.36,-0.14,0,0  
2X5Y,LYS\_761,10.29,-0.21,0,0  
1J33,ARG\_269,11.87,-0.63,0,0  
1WP5,ARG\_234,11.73,-0.77,0,0  
3GV0,GLU\_178,4.64,0.14,0,0  
1YW5,GLU\_119,4.57,0.07,0,0  
2Q13,GLU\_120,4.57,0.07,0,0  
3VJ8,GLU\_222,4.5,0,0,0  
2VAN,LYS\_168,10.22,-0.28,0,0  
3GA2,CYS\_60,11.03,-0.48,0.25,2.26  
2C13,ARG\_11,12.08,-0.42,0,0  
3IOC,TYR\_259,10,0,0,0  
2OSA,LYS\_453,10.22,-0.28,0,0  
2EA9,HIS\_79,6.42,0.06,0,-0.14  
2D25,LYS\_534,10.5,0,0,0  
3V3T,GLU\_300,4.57,0.07,0,0  
1TWU,TYR\_66,11.46,0,-0.27,1.73  
3GW3,LYS\_178,10.36,-0.14,0,0  
3IVF,ARG\_194,11.46,-1.04,0,0  
3LD1,HIS\_329,4.99,1.34,0,-2.84  
3M16,LYS\_71,10.22,-0.28,0,0  
2FD5,ARG\_121,12.29,-0.21,0,0  
2C2Y,TYR\_94,10.28,1.25,-1.05,0.07  
1W24,HIS\_88,3.76,0,-0.07,-2.67  
2XWS,TYR\_71,12.46,0.42,-0.36,2.4  
3TMO,GLU\_241,4.37,0,-0.13,0  
1XEU,GLU\_187,3.84,0.14,-0.8,0  
3NOK,GLU\_9,3.91,0.21,-0.8,0  
1TJE,ASP\_8,1.97,0.42,-2.25,0  
1NIJ,HIS\_294,6.43,0,0,-0.07  
2Q34,ASP\_34,1.61,0.7,-2.9,0  
3PU6,HIS\_119,6.8,0.3,0,0  
2F19,ARG\_118,12.36,-0.14,0,0  
2IDC,TYR\_117,8.96,0.07,-1.11,0  
2AZP,CYS\_49,10.14,0,-0.93,2.07  
3L7N,TYR\_67,10.85,0.14,-0.8,1.51  
4DIU,GLU\_128,4.78,0.28,0,0  
1OIS,ASP\_195,3.85,0.07,-0.02,0  
2AZL,GLU\_61,4.5,0,0,0  
3G53,GLU\_267,4.5,0,0,0  
3CAX,LYS\_403,10.29,-0.21,0,0  
3ULX,GLU\_11,4.5,0,0,0  
2B02,ASP\_410,2.9,0.28,-1.18,0  
3K9I,ASP\_141,1.68,0.63,-2.75,0  
1L2H,LYS\_94,10.36,-0.14,0,0  
4D8L,ASP\_134,3.8,0,0,0  
4EF5,CYS\_309,10.75,0,1.75  
2GAU,ARG\_128,12.5,0,0,0  
2VAN,ASP\_145,2.32,0.35,-1.84,0  
1AM2,LYS\_98,10.08,-0.42,0,0  
1RI5,HIS\_163,3.6,0.85,0,-3.75  
1XWM,ARG\_21,12.08,-0.42,0,0  
2OOK,LYS\_31,10.01,-0.49,0,0  
2P5D,LYS\_95,10.08,-0.42,0,0  
4EF5,CYS\_292,9.83,-0.46,0,1.29  
3HUE,CYS\_222,9.73,-0.07,0,0.8  
3H9W,LYS\_78,10.43,-0.07,0,0  
3ANJ,TYR\_260,10,0,0,0  
3FHF,GLU\_130,3.5,1.99,-2.1,-0.9  
1X7F,GLU\_255,3.91,0.28,-0.86,0  
3MTT,LYS\_477,9.66,-0.84,0,0  
3ZXY,HIS\_179,6.61,0.11,0,0  
3EJC,GLU\_112,2.9,0.28,-1.88,0  
2X4G,ARG\_223,12.98,-0.74,0,1.23  
2F9F,GLU\_119,3.99,0.28,-0.79,0  
3M16,GLU\_176,3.57,1.05,-1.98,0  
1XIP,ASP\_254,3.8,0,0,0  
2EHG,LYS\_108,10.5,0,0,0  
2QXR,ARG\_154,12.01,-0.49,0,0  
1C44,GLU\_21,4.57,0.07,0,0  
3CJW,LYS\_389,10.5,0,0,0  
1C44,GLU\_25,4.5,0,0,0  
3BA1,LYS\_137,10.08,-0.42,0,0  
3NOK,GLU\_140,4.5,1.16,-1.16,0  
2FXT,GLU\_390,4.57,0.07,0,0  
2NRK,LYS\_162,10.5,0,0,0  
2V81,ARG\_95,11.87,-0.63,0,0  
3M7G,GLU\_41,4.62,0.28,-0.16,0  
2Q5X,ASP\_747,2.5,0.49,-1.79,0  
1NIJ,ASP\_285,3.07,0.35,-1.08,0  
4AM1,GLU\_18,4.64,0.14,0,0  
4DBX,CYS\_192,7.9,0,-2.2,1.1  
1SQH,TYR\_82,12.01,3.61,-1.6,0  
2H8O,ARG\_144,12.22,-0.28,0,0  
3ZSL,GLU\_184,3.69,0.28,-1.09,0  
3EJG,HIS\_9,6.43,0,0,-0.07  
2DFL,GLU\_307,3.33,0.69,-0.36,-1.5  
2WB8,GLU\_735,3.6,0.7,-1.6,0  
2PP6,GLU\_91,4.76,0.28,-0.02,0  
1NIJ,ARG\_175,11.73,-0.77,0,0  
2E3I,ASP\_57,3.81,0.07,-0.06,0  
2P65,CYS\_155,11.81,-0.47,0,3.28  
2RGY,ASP\_178,3.53,0,-0.27,0  
2YT4,GLU\_626,3.87,0.21,-0.84,0  
1N81,ARG\_83,12.01,-0.49,0,0  
3MIX,LYS\_573,10.5,0,0,0  
4DVD,ARG\_23,10.65,-0.83,0,-1.02  
1N81,HIS\_22,6.71,0.42,0,-0.21  
2BAA,TYR\_96,13.41,0.21,0.8,2.4  
3O7K,ARG\_120,11.94,-0.56,0,0  
3RUX,LYS\_94,10.5,0,0,0  
1R3D,TYR\_156,9.01,2.05,-0.8,-2.24  
3TOW,GLU\_132,4.5,0,0,0  
2IRM,LYS\_100,10.29,-0.21,0,0  
2OOK,HIS\_176,2.53,0.29,0,-4.22  
3CIV,ARG\_140,12.29,-0.21,0,0  
1OTM,LYS\_109,10.29,-0.21,0,0  
3CSR,LYS\_95,10.43,-0.07,0,0  
3G9G,GLU\_172,4.49,0.35,-0.36,0  
3V46,TYR\_392,9.96,0.81,0,-0.85  
2A6B,ARG\_204,10.87,-1.63,0,0  
3CS1,ASP\_26,2.96,0.28,-1.12,0  
1T6L,LYS\_224,10.5,0,0,0  
4AM1,LYS\_351,10.43,-0.07,0,0  
2P65,GLU\_61,4.0,0.28,-0.78,0  
2E3C,HIS\_392,6.38,0.09,0,-0.21  
3EVN,ASP\_265,2.87,0.35,-1.29,0  
2VAN,ARG\_149,11.8,-0.7,0,0  
2GEN,GLU\_55,2.24,0.94,-3.2,0  
2AHE,GLU\_16,3.16,0.56,-1.91,0  
4DND,GLU\_65,2.66,0.56,-2.4,0  
2E0T,ARG\_80,11.87,-0.63,0,0  
1RH6,LYS\_136,4.26,0.56,-0.8,0  
4FD6,LYS\_118,10.5,0,0,0  
3T5B,TYR\_290,9.01,1.29,-0.32,-1.96  
3UAH,LYS\_366,10.22,-0.28,0,0  
3GFP,TYR\_405,11.53,0.91,0,0.62  
2A1V,ASP\_11,2.39,0.21,-1.61,0  
2QZQ,GLU\_39,4.78,0.28,0,0  
1O0X,LYS\_126,10.08,-0.42,0,0  
2B0A,LYS\_60,10.29,-0.21,0,0  
1AK1,GLU\_90,1.52,0.42,-3.4,0  
3I47,TYR\_196,9.45,0.07,-0.62,0  
1RAJ,TYR\_195,10.07,0.07,0,0  
1YR6,LYS\_166,10.15,-0.35,0,0  
3I82,HIS\_127,3.73,0.07,0,-2.84  
1SNT,GLU\_319,3.82,0.35,-1.03,0  
1YIB,TYR\_217,11.67,0.06,1.62  
3K8J,ARG\_112,12.08,-0.42,0,0  
2RGY,ARG\_191,12.15,-0.35,0,0  
1E55,GLU\_249,4.14,0.49,-0.85,0  
1R53,GLU\_239,4.1,0.71,-1.11,0  
3UV9,GLU\_317,4.5,0,0,0  
3CS1,TYR\_67,9.86,0.21,-0.35,0  
1XTD,TYR\_41,10,0,0,0



2Z61,ASP\_90,3.14,0.07,-0.73,0  
 1J33,TYR\_66,10,0,0,0  
 2CVB,ARG\_127,10.88,-1.62,0,0  
 2Q99,LYS\_357,10.5,0,0,0  
 3IPZ,ASP\_152,3.67,0,-0.13,0  
 3GMS,ARG\_92,11.48,-1.66,0,0.64  
 2BAA,CYS\_223,9.76,-0.42,-0.03,1.21  
 2RJD,ARG\_521,12.22,-0.28,0,0  
 2DVK,GLU\_169,4.64,0.14,0,0  
 3ETU,LYS\_99,10.5,0,0,0  
 1R15,TYR\_124,11.38,2.98,-1.6,0  
 3R87,ARG\_33,12.15,-0.35,0,0  
 3LJI,GLU\_187,4.03,1.13,-1.6,0  
 2B78,LYS\_12,10.43,-0.07,0,0  
 2C2Y,ARG\_166,11.87,-0.63,0,0  
 2D7U,HIS\_110,6.5,0.14,0,-0.14  
 2IXM,CYS\_167,10.54,0,0,1.54  
 2BDV,HIS\_82,6.72,0.36,0,-0.14  
 2JHY,LYS\_200,10.43,-0.07,0,0  
 1OLR,ARG\_186,11.87,-0.63,0,0  
 4DVD,TYR\_142,10,0,0,0  
 2BT8,ARG\_201,12.43,-0.07,0,0  
 1JKS,ASP\_169,4.01,0.21,0,0  
 3LJC,CYS\_39,9.07,0,0,0.07  
 2H2Z,TYR\_101,13.86,0.05,0.1,3.71  
 3T5B,ARG\_379,11.87,-0.63,0,0  
 3FWU,ARG\_24,11.59,-0.91,0,0  
 2Y2T,LYS\_66,10.5,0,0,0  
 1R3D,HIS\_259,6.36,0,0,-0.14  
 1WP5,GLU\_104,4.5,0,0,0  
 3RJX,ARG\_262,11.94,-0.56,0,0  
 1PSW,ARG\_244,12.15,-0.35,0,0  
 2BV9,GLU\_238,4.21,0.42,-0.71,0  
 1UOH,ARG\_222,12.5,0,0,0  
 157K,ARG\_174,11.94,-0.56,0,0  
 3D9H,HIS\_162,7.04,0.61,0,-0.07  
 1OOX,GLU\_127,4.19,0.28,-0.59,0  
 2H14,HIS\_300,4.72,1.67,1.13,-4.58  
 2AXO,ARG\_143,12.43,-0.07,0,0  
 1NRI,GLU\_15,4.78,0.28,0,0  
 3KV0,ARG\_165,11.24,-1.26,0,0  
 4EZB,ASP\_58,2.69,0.35,-1.46,0  
 1J33,ARG\_149,12.08,-0.42,0,0  
 1NWA,GLU\_115,3.6,0.21,-1.11,0  
 3COU,ARG\_114,12.43,-0.07,0,0  
 3B79,ARG\_14,11.38,-1.12,0,0  
 1PBV,ASP\_113,3.94,0.14,0,0  
 2RIK,GLU\_124,4.64,0.14,0,0  
 2YT4,LYS\_582,10.36,-0.14,0,0  
 2YX0,GLU\_270,3.44,3.79,-2.29,-2.56  
 1ZYL,ARG\_190,11.38,-1.12,0,0  
 3T5B,GLU\_361,4.57,0.07,0,0  
 2BT8,ASP\_325,3.32,0.28,-0.76,0  
 2POY,ASP\_184,3.38,0.42,-0.84,0  
 2O8P,LYS\_35,10.22,-0.28,0,0  
 2GZR,LYS\_171,10.29,-0.21,0,0  
 2Q12,TYR\_41,11.1,0,-0.03,1.13  
 3U2A,ASP\_12,1.66,0.49,-2.62,0  
 2I88,LYS\_470,10.5,0,0,0  
 2RJD,ARG\_267,11.07,-2.64,0,1.21  
 1O59,HIS\_214,6.98,0.55,0,-0.07  
 3B7X,ARG\_36,12.22,-0.28,0,0  
 3HVM,HIS\_323,3.35,3.2,0.29,-6.65  
 3SOA,LYS\_64,10.36,-0.14,0,0  
 3FHF,HIS\_83,2.07,0.91,-1.87,-3.48  
 2EYI,ASP\_98,3.9,0.14,-0.04,0  
 1EV8,LYS\_96,9.94,-0.56,0,0  
 2JHY,ASP\_185,3.87,0.07,0,0  
 3VHJ,TYR\_129,10,0,0,0  
 3EX9,HIS\_32,6.5,0,0,0  
 1V6T,HIS\_62,3.02,1.6,1.52,-6.6  
 3CIV,GLU\_31,3.27,0.07,-1.3,0  
 2B6P,TYR\_149,12.18,2.18,0,0  
 3AU3,GLU\_428,4.57,0.07,0,0  
 3U4K,ARG\_102,12.22,-0.28,0,0  
 2X4G,HIS\_207,6.48,0.12,0,-0.14  
 1SNT,HIS\_64,6.65,0.28,0,-0.14  
 3DSH,HIS\_453,6.5,0,0,0  
 3F1X,ARG\_127,12.08,-0.42,0,0  
 3B21,HIS\_199,6.49,0.06,0,-0.07  
 1H09,CYS\_239,8.89,-0.59,0,0.48  
 2V1L,HIS\_58,13.76,5.2,4.11,-2.05  
 1OIS,ASP\_339,2.54,0.56,-1.82,0  
 1NJ4,ASP\_127,3.8,0.07,-0.07,0  
 3N2T,LYS\_192,10.5,0,0,0  
 2R0S,HIS\_230,5.33,0.8,0,-1.97  
 2GYZ,ARG\_15,12.15,-0.35,0,0  
 1P4X,HIS\_219,7.31,0.81,0,0  
 3BCY,ASP\_27,2.92,0.35,-1.24,0  
 1X9G,HIS\_45,3.98,0.81,0,-3.33  
 1OTM,LYS\_120,10.5,0,0,0  
 1H09,TYR\_137,10.79,0.14,-1.47,2.11  
 2QK1,LYS\_460,9.94,-0.56,0,0  
 4DBX,LYS\_209,10.5,0,0,0  
 3ZXY,HIS\_61,3.49,1.54,0,-4.56  
 1SIG,ARG\_339,12.36,-0.14,0,0  
 1R9W,ARG\_320,12.5,0,0,0  
 2YYO,GLU\_44,3.6,0.63,-1.53,0  
 1KW4,ASP\_21,2.08,0.21,-1.93,0  
 3FXH,GLU\_37,4.5,0,0,0  
 3P2F,GLU\_63,4.5,0,0,0  
 3CAX,LYS\_215,10.5,0,0,0  
 3V46,ASP\_365,3.58,0.35,-0.57,0  
 2OJQ,TYR\_660,9.54,0.34,-0.8,0  
 1RLO,GLU\_70,4.12,0.42,-0.8,0  
 2D8N,ASP\_165,3.26,0.56,-1.1,0  
 3MIX,GLU\_588,3.52,0.63,-1.61,0  
 2CXC,ARG\_80,12.22,-0.28,0,0  
 2PWQ,GLU\_124,4.59,0.14,-0.05,0  
 3OBS,ARG\_23,12.08,-0.42,0,0  
 2B78,HIS\_265,3.51,0,0,-2.99  
 1CHD,LYS\_246,10.08,-0.42,0,0  
 2QDJ,LYS\_122,10.22,-0.28,0,0  
 2OEW,TYR\_223,9.7,0.5,-0.8,0  
 3GMS,CYS\_134,11.25,0,0,2.25  
 1NIJ,GLU\_307,4.5,0,0,0  
 2EEY,TYR\_145,10.07,0.07,0,0  
 1OOX,LYS\_63,10.36,-0.14,0,0  
 4FCU,ARG\_165,12.5,0,0,0  
 2O8P,GLU\_47,1.76,0.7,-3.44,0  
 1ZCE,ARG\_33,11.1,-1.4,0,0  
 3ULX,LYS\_35,10.29,-0.21,0,0  
 2B0A,HIS\_50,3.34,0.08,-1.09,-2.15  
 1RLO,ASP\_152,3.48,0.14,-0.46,0  
 2ZQ5,GLU\_135,3.82,0.42,-1.1,0  
 1ATO,LYS\_379,10.01,-0.49,0,0  
 4FCU,ASP\_135,3.67,0,-0.13,0  
 2OQG,HIS\_382,6.5,0,0,0  
 3I47,LYS\_254,10.5,0,0,0  
 2QHT,CYS\_138,11.04,-1.29,0,3.33  
 1MML,ASP\_108,2.8,0.07,-1.07,0  
 2CWY,LYS\_64,10.36,-0.14,0,0  
 3MEW,GLU\_198,4.57,0.07,0,0  
 2C13,CYS\_177,11.73,-0.12,0,2.85  
 2WB3,HIS\_369,6.43,0,0,-0.07  
 4FCU,ASP\_71,3.36,0.21,-0.65,0  
 1J33,TYR\_97,13.41,0.21,0.8,2.4  
 1OOX,GLU\_137,4.5,0,0,0  
 2ZTY,GLU\_81,4.13,0.14,-0.51,0  
 2V4U,LYS\_490,10.29,-0.21,0,0  
 3ONH,ARG\_443,12.08,-0.42,0,0  
 3JZN,ASP\_279,3.87,0.07,0,0  
 3TMO,ASP\_221,3.87,0.07,0,0  
 1W24,ARG\_60,12.22,-0.28,0,0  
 1AK1,ASP\_149,3.26,0.07,-0.61,0  
 1OOX,ARG\_133,11.48,-1.02,0,0  
 3JZN,ARG\_439,12.08,-0.42,0,0  
 2WB8,GLU\_548,4.5,0,0,0  
 2A1V,ASP\_18,4.04,0.28,-0.04,0  
 1EQ6,ASP\_62,3.39,0.07,-0.48,0  
 1EYH,HIS\_146,7.27,0.84,0,-0.07  
 3C01,HIS\_29,6.72,0.22,0,0  
 1MJS,ARG\_242,11.45,-1.05,0,0  
 3EVZ,HIS\_59,6.3,0.08,0,-0.28  
 1X7F,ARG\_271,11.45,-1.05,0,0  
 1YW5,ASP\_131,3.66,0.21,-0.35,0  
 3LPZ,LYS\_119,10.5,0,0,0  
 2EOT,HIS\_129,7.27,0.91,0,-0.14  
 1JSX,GLU\_179,3.88,0.49,-1.11,0  
 1OST,LYS\_458,10.29,-0.21,0,0  
 2R15,TYR\_53,10.54,0,-0.13,0.67  
 1HF8,ASP\_43,3.5,0.42,-0.72,0  
 1H4U,ASP\_606,3.26,0.28,-0.82,0  
 2IDC,ASP\_118,3.2,0.7,-1.3,0  
 1ZYL,ARG\_50,12.43,-0.07,0,0  
 1X91,ASP\_113,3.83,0.07,-0.04,0  
 2X4L,LYS\_67,9.73,-0.77,0,0  
 3G59,ASP\_285,3.16,0.56,-1.2,0  
 2BDV,GLU\_12,3.81,0.21,-0.9,0  
 1A8Q,ASP\_84,2.91,0.07,-0.96,0  
 2OJQ,GLU\_460,4.64,0.14,0,0  
 3EX9,CYS\_104,6.35,-3.6,0,0.95  
 3CXS,ASP\_10,2.64,0.35,-1.51,0  
 3CGW,ARG\_161,12.08,-0.42,0,0  
 2EYI,LYS\_147,10.22,-0.28,0,0  
 3JZ9,TYR\_403,10.16,0.16,0,0  
 4EZB,ARG\_201,12.5,0,0,0  
 1TD6,LYS\_23,10.5,0,0,0  
 2AZP,ARG\_221,12.22,-0.28,0,0  
 1OTM,GLU\_55,3.91,0.21,-0.8,0  
 1DVO,CYS\_135,8.4,-0.67,0,0.07  
 1E55,ASP\_65,3.94,0.42,-0.28,0  
 3ULX,TYR\_120,10.05,0.07,-0.02,0  
 3M70,GLU\_79,3.87,0.21,-0.84,0  
 3BQW,LYS\_97,10.5,0,0,0  
 2QRX,HIS\_49,7.37,1.6,1.88,-2.61  
 2R51,ARG\_240,12.43,-0.07,0,0  
 1ZBS,ASP\_83,3.8,0,0,0  
 1V6T,HIS\_107,1.13,1.01,0,-6.38  
 1V43,GLU\_39,2.28,1.63,-1.67,-2.18  
 1U53,ASP\_168,3.98,0.21,-0.03,0  
 2X4L,LYS\_307,10.29,-0.21,0,0  
 3CAX,LYS\_462,10.43,-0.07,0,0  
 3O16,ARG\_175,12.66,-1.88,0,2.04  
 2YLF,ARG\_76,12.5,0,0,0  
 2G9D,ASP\_78,3.76,0.07,-0.11,0  
 3U56,CYS\_104,9.46,0,0,0.46  
 1I60,CYS\_149,6.49,-4.16,0,1.64  
 1VJG,LYS\_74,10.5,0,0,0  
 2FZ4,GLU\_103,4.64,0.14,0,0  
 2PWQ,GLU\_131,4.65,0.21,-0.06,0  
 2B0J,GLU\_306,3.52,0.07,-1.05,0  
 3BCY,TYR\_53,11.01,1.71,-0.7,0  
 1R7J,CYS\_17,9.87,0,0,0.87  
 1NAR,GLU\_107,4.5,0,0,0  
 2O8P,LYS\_166,10.5,0,0,0  
 3D9H,ASP\_161,3.13,0.49,-1.16,0  
 3MTT,GLU\_466,4.57,0.07,0,0  
 1W7B,GLU\_253,4.85,0.35,0,0  
 1YLN,CYS\_168,10.55,-0.54,0,2.09  
 1X8F,GLU\_75,4.64,0.14,0,0  
 3BF7,GLU\_216,3.33,0.49,-1.66,0  
 3DSH,ASP\_227,3.77,0,-0.03,0  
 3RJZ,CYS\_213,7.52,-1.55,0,0.07  
 2R2Y,TYR\_48,10.94,0.07,0.58,0.29  
 1MD6,GLU\_93,4.71,0.21,0,0  
 1VJG,ARG\_139,11.52,-0.98,0,0  
 1RWZ,GLU\_92,4.13,0.21,-0.58,0  
 3EJG,CYS\_123,10.37,-0.13,0,37.1.13  
 2YWK,HIS\_59,6.36,0,0,-0.14  
 2CN1,ASP\_140,3.32,0.35,-0.83,0  
 3ONT,HIS\_126,6.5,0,0,0  
 2H8O,ARG\_136,13.48,-1.42,0,2.4  
 2Q0K,ASP\_54,2.99,0.28,-1.08,0  
 3T5B,ARG\_41,12.08,-0.42,0,0  
 2JKF,LYS\_133,10.15,-0.35,0,0  
 1JYH,GLU\_23,3.72,0,-0.78,0  
 3ILC,ARG\_100,11.94,-0.56,0,0  
 2Q13,GLU\_239,4.78,0.28,0,0  
 2R05,TYR\_126,10.14,0.14,0,0  
 4ECC,ASP\_90,3.87,0.07,0,0  
 2POL,ASP\_109,4.08,0.28,0,0  
 2GAU,ARG\_144,10.32,-2.18,0,0  
 2ZCO,GLU\_220,2.83,0.57,-0.79,-1.45  
 3EZ7,ARG\_104,12.01,-0.49,0,0  
 2D7U,GLU\_169,4.85,0.35,0,0  
 2ZCO,TYR\_105,13.91,0.71,0.8,2.4  
 3G9G,GLU\_222,4.64,0.14,0,0  
 1J7G,CYS\_113,9.81,-0.85,0,1.66  
 2CBE,ASP\_71,1.79,0.35,-2.37,0  
 3ERF,GLU\_109,2.82,0.56,-2.24,0  
 2A1V,HIS\_84,6.29,0,0,-0.21  
 1KCM,HIS\_85,7.16,0.8,0,-0.14  
 3RE9,GLU\_129,3.32,0.42,-1.6,0  
 3IBT,ASP\_82,3.87,0.07,0,0  
 1H4U,GLU\_491,3.91,0.21,-0.8,0  
 3FXH,ASP\_22,3.8,0,0,0  
 3O48,ASP\_101,3.24,0.28,-0.84,0  
 3G9G,HIS\_147,1.65,0,-2,-2.85  
 1WRU,ARG\_160,11.22,-1.28,0,0  
 1YW5,GLU\_114,3.45,0.42,-1.47,0  
 2CBE,ARG\_227,11.3,-1.2,0,0  
 3A4C,ASP\_520,3.86,0.07,-0.01,0  
 3C38,ARG\_146,12.29,-0.21,0,0  
 1LZL,ARG\_211,11.8,-0.7,0,0  
 2BLL,GLU\_377,3.86,0.35,-0.99,0  
 2A4D,CYS\_145,11.55,0.92,1.64  
 4ESS,LYS\_134,10.15,-0.35,0,0  
 2GAU,GLU\_93,4.5,0,0,0  
 2JKF,ASP\_165,4.13,0.72,-1.1,0  
 2BLL,GLU\_586,4.05,0.35,-0.8,0  
 2H2Z,LYS\_97,10.5,0,0,0  
 3CBN,ARG\_25,11.94,-0.56,0,0  
 3BZT,ASP\_342,2.79,0.35,-1.37,0  
 3MIX,ARG\_372,11.8,-0.7,0,0  
 2CVB,GLU\_155,3.71,0.35,-1.14,0  
 3UAH,ASP\_173,3.94,0.14,0,0  
 1DTO,ARG\_47,12.15,-0.35,0,0  
 3FWU,HIS\_13,6.5,0,0,0  
 3BWT,LYS\_786,10.36,-0.14,0,0  
 3LQE,GLU\_342,3.83,0.49,-1.16,0  
 2FZ4,ARG\_62,11.66,-0.84,0,0  
 1A8Q,LYS\_177,10.22,-0.28,0,0  
 2Q13,TYR\_168,10.45,0,0,0.45  
 1GXN,TYR\_635,10.62,2.07,0,-1.45  
 2W2S,ARG\_118,12.36,-0.14,0,0

1YB2,HIS\_210,4.24,0,0,-2.26  
3RKV,GLU\_297,3.42,0.35,-1.43,0  
3F6M,LYS\_31,10.22,-0.28,0,0  
3CO1,LYS\_83,10.5,0,0,0  
2NSN,LYS\_70,10.5,0,0,0  
3UPD,ARG\_96,11.8,-0.7,0,0  
2XMZ,LYS\_36,10.29,-0.21,0,0  
4D8L,LYS\_48,10.5,0,0,0  
3H9W,ASP\_85,3.16,0.63,-1.26,0  
2NRK,TYR\_168,10,0,0,0  
1YOK,GLU\_191,4.5,0,0,0  
3K8U,ARG\_66,12.22,-0.28,0,0  
3LJC,GLU\_151,4.5,0,0,0  
4E8B,ARG\_151,11.87,-0.63,0,0  
2W2S,GLU\_58,4.39,0.42,-0.53,0  
1X6J,HIS\_30,7.19,0.69,0,0  
3RRQ,ARG\_115,12.08,-0.42,0,0  
3CCY,GLU\_31,4.5,0,0,0  
2FM9,HIS\_209,6.5,0,0,0  
2X4G,GLU\_204,4.5,0,0,0  
3H5T,GLU\_49,4.5,0,0,0  
1ZCE,CYS\_85,9.29,-0.06,0,0.35  
2A0J,LYS\_23,10.43,-0.07,0,0  
3U0V,TYR\_58,11.79,1.79,0,0  
2G9D,ASP\_342,3.8,0,0,0  
3LJN,GLU\_236,4.78,0.28,0,0  
1DUP,GLU\_115,3.63,0.28,-1.15,0  
3GFP,ASP\_395,3.32,0.28,-0.76,0  
1XDZ,TYR\_64,10.07,0.07,0,0  
3B21,TYR\_115,11.75,0.29,-0.54,2  
2H14,TYR\_35,12.97,0.89,-0.38,2.46  
3E0H,GLU\_157,4.5,0,0,0  
2OEW,LYS\_151,10.5,0,0,0  
2XWS,ARG\_3,12.08,-0.42,0,0  
1AD6,TYR\_454,12.15,1.34,0,0.81  
1E59,ARG\_83,13.67,-3.46,0,4.63  
3K8J,GLU\_175,4.54,0.21,-0.17,0  
2E0T,ASP\_73,1.77,0.84,-2.87,0  
3ONH,ASP\_544,3.28,0.21,-0.73,0  
2ZQ5,HIS\_164,4.48,0.04,0,-2.06  
1W7B,TYR\_316,10,0,0,0  
2B61,ASP\_325,3.56,0.56,-0.81,0  
1AKO,TYR\_52,10.47,0.47,0,0  
2CXA,ASP\_32,1.72,0.7,-2.78,0  
2OKT,TYR\_194,11.33,1.89,-0.19,-0.38  
2D7J,ARG\_95,12.5,0,0,0  
2AD1,LYS\_223,10.5,0,0,0  
3DB9,ARG\_87,11.94,-0.56,0,0  
1O59,HIS\_194,6.5,0,0,0  
3EIZ,HIS\_137,6.43,0,0,-0.07  
2Q98,GLU\_145,4.5,0,0,0  
1FKM,ASP\_330,3.35,0.77,-1.22,0  
1EYH,GLU\_143,3.72,0.35,-1.12,0  
3ASA,LYS\_83,9.87,-0.63,0,0  
2CWY,GLU\_22,4.57,0.07,0,0  
2EJB,GLU\_127,3.56,0.14,-1.08,0  
1S1Y,GLU\_151,3.91,0.21,-0.8,0  
4ETX,GLU\_356,4.02,1,-0.71,0  
2FL4,LYS\_97,10.5,0,0,0  
1SNT,GLU\_72,4.05,0.07,-0.52,0  
3EYE,ARG\_62,12.15,-0.35,0,0  
3K1H,GLU\_129,4.5,0,0,0  
2F4Q,LYS\_172,10.5,0,0,0  
3CJW,GLU\_339,4.5,0,0,0  
2EHG,GLU\_87,4.64,0.14,0,0  
3F5D,LYS\_4,9.94,-0.56,0,0  
3EZ7,LYS\_331,10.36,-0.14,0,0  
1MD6,ARG\_47,11.87,-0.63,0,0  
3IPZ,GLU\_168,4.57,0.07,0,0  
3GE9,LYS\_6,10.43,-0.07,0,0  
3CBN,ASP\_140,2.26,0.7,-2.23,0  
2JEO,GLU\_196,4.05,0.35,-0.8,0  
1UAJ,GLU\_243,4.12,0.42,-0.8,0  
2CE6,ASP\_26,2.81,0.42,-1.41,0  
2D7U,GLU\_307,4.47,0.21,-0.24,0  
3JZ9,ASP\_445,3.84,0.28,-0.24,0  
2YX0,GLU\_54,4.52,0.21,-0.19,0  
3RUX,LYS\_147,10.29,-0.21,0,0  
2IXM,GLU\_262,4.78,0.28,0,0  
1R53,HIS\_174,6.5,0,0,0  
1NRI,LYS\_175,10.5,0,0,0  
1PVT,GLU\_209,3.48,0.35,-1.37,0  
2V4X,GLU\_21,4.64,0.14,0,0  
3ON1,GLU\_3,4.5,0,0,0  
3A0X,LYS\_682,10.22,-0.28,0,0  
1J33,LYS\_115,9.87,-0.63,0,0  
1P1L,TYR\_76,13.73,0.42,0.8,2.51  
3EVN,TYR\_8,11.27,2.07,-0.8,0  
3GA2,GLU\_212,4.64,0.14,0,0  
3VJ8,HIS\_268,5.52,1.08,0,-2.06  
2FG1,LYS\_73,10.36,-0.14,0,0  
4F85,GLU\_181,6.86,4.22,-1.86,0  
1JKS,LYS\_108,10.29,-0.21,0,0  
3C5V,LYS\_296,10.22,-0.28,0,0  
1YB2,ASP\_140,3.1,0.21,-0.91,0  
1UAJ,CYS\_112,13.11,-0.1,1.78,2.43  
1M5I,ASP\_170,4.02,0.35,-0.13,0  
1WYC,CYS\_216,8.93,-3.3,0.64,2.58  
2YWX,GLU\_136,4.85,0.35,0,0  
4ETX,HIS\_338,4.2,0.05,-2.35  
1GVP,LYS\_69,9.8,-0.7,0,0  
3DHN,LYS\_42,10.29,-0.21,0,0  
1K95,GLU\_116,3.84,0.14,-0.8,0  
2O0K,LYS\_112,10.22,-0.28,0,0  
1KCM,GLU\_41,3.84,0.14,-0.8,0  
3KB5,ARG\_408,12.43,-0.07,0,0  
1U3Y,ASP\_276,3.8,0.42,-0.42,0  
2H85,GLU\_220,3.95,0.07,-0.62,0  
1RHS,ASP\_200,4.17,0.28,0.09,0  
3PU6,ARG\_99,11.66,-0.84,0,0  
2CVB,TYR\_47,10,0,0,0  
2AZP,ARG\_313,12.29,-0.21,0,0  
2D0A,HIS\_180,1.68,0.57,0,-5.39  
3LJN,CYS\_50,9.19,-0.28,0.47  
3ETU,ARG\_316,12.5,0,0,0  
3MTT,LYS\_529,10.5,0,0,0  
3EGN,CYS\_420,8.27,-0.72,0,0  
1L3K,GLU\_132,4.78,0.28,0,0  
3Q2C,LYS\_42,10.29,-0.21,0,0  
3FK5,GLU\_173,4.35,0.42,-0.56,0  
3BWT,TYR\_615,9.62,0.07,-0.45,0  
2A68,GLU\_102,4.5,0,0,0  
2E3C,ARG\_330,10.69,-1.84,0,0.03  
1HF8,ARG\_126,11.87,-0.63,0,0  
3U0V,GLU\_180,4.5,0,0,0  
1QYI,GLU\_16,3.1,0.91,-0.8,-1.5  
2G9D,ASP\_16,3.23,0.42,-0.99,0  
2OJQ,GLU\_597,4.5,0,0,0  
1Q42,GLU\_36,4.5,0,0,0  
1RKA,ASP\_306,3.81,0.14,-0.13,0  
3ETV,GLU\_88,4.57,0.07,0,0  
3ELI,ARG\_111,12.15,-0.35,0,0  
2X5Y,LYS\_748,10.43,-0.07,0,0  
1DZF,LYS\_152,10.43,-0.07,0,0  
1DVO,ARG\_111,11.87,-0.63,0,0  
1YR6,GLU\_94,4.78,0.28,0,0  
1LTU,GLU\_39,4.64,0.14,0,0  
3CO1,CYS\_45,10.89,-0.1,0,1.99  
1UJ8,ASP\_18,2.65,0.84,-1.98,0  
1FHL,LYS\_166,10.29,-0.21,0,0  
1GPP,TYR\_146,10.04,0.61,-0.9,0.33  
2AHE,LYS\_177,10.5,0,0,0  
3EUR,LYS\_132,10.5,0,0,0  
2AZL,LYS\_265,9.59,-0.91,0,0  
3G53,ARG\_113,11.87,-0.63,0,0  
2C2Y,LYS\_9,10.43,-0.07,0,0  
3RFY,LYS\_411,9.52,-0.98,0,0  
1TR9,ARG\_276,13.74,-0.92,0.2,1.6  
1GPP,LYS\_128,10.36,-0.14,0,0  
2EHG,ASP\_28,3.36,0,-0.44,0  
1UXO,ASP\_136,1.31,0.84,-3.33,0  
2H01,ASP\_109,3.94,0.14,0,0  
4D8L,CYS\_78,9.68,-0.9,1.58  
2C2Y,ARG\_267,12.59,-1.75,0,1.84  
2QK1,GLU\_476,3.3,1.2,-2.4,0  
3M3P,HIS\_152,5.21,1.46,0,-2.75  
1DTO,TYR\_154,9.25,0.07,-0.83,0  
2J8A,CYS\_248,7.51,-1.49,0,0  
4GA2,GLU\_73,4.48,0.28,-0.3,0  
3OKQ,GLU\_585,3.52,0.28,-1.26,0  
3RVC,TYR\_89,10,0,0,0  
3M3P,ASP\_219,3.85,0.07,-0.02,0  
2EJB,LYS\_158,10.5,0,0,0  
2A6B,TYR\_127,12.02,0.07,-0.34,2.29  
3CIV,GLU\_5,4.67,0.35,-0.18,0  
1R53,GLU\_15,4.41,0.07,-0.17,0  
2QD1,GLU\_112,4.57,0.07,0,0  
1Q5Z,LYS\_617,10.36,-0.14,0,0  
1LTU,ASP\_257,3.06,0.42,-1.16,0  
1DZF,ARG\_14,12.22,-0.28,0,0  
1Q42,CYS\_67,8.58,-0.49,0,0.07  
2OPJ,ARG\_169,11.59,-0.91,0,0  
1WXF,LYS\_257,10.5,0,0,0  
1TD6,ARG\_288,12.36,-0.14,0,0  
2OKT,ARG\_160,11.51,-0.99,0,0  
4ACJ,HIS\_653,7.09,0.66,0,-0.07  
2Q34,LYS\_33,10.43,-0.07,0,0  
1BKB,LYS\_10,10.5,0,0,0  
1WNH,GLU\_43,4.13,0.35,-0.72,0  
2WB8,ARG\_616,11.94,-0.56,0,0  
1T95,LYS\_153,10.29,-0.21,0,0  
1X04,GLU\_188,4.5,0,0,0  
1TWU,GLU\_67,4.54,0.07,-0.03,0  
3GEC,ARG\_316,12.08,-0.42,0,0  
1WPC,CYS\_118,12.18,-0.62,0.3,8  
1GPP,GLU\_141,4.78,0.35,-0.07,0  
3G59,LYS\_71,10.29,-0.21,0,0  
1A8Q,GLU\_262,3.22,0.7,-1.98,0  
2P5D,ASP\_74,2.01,0.42,-2.22,0  
1V6T,ARG\_168,11.76,-0.85,0.0,1.1  
2OB5,CYS\_126,10.35,0,0,1.35  
2G2D,ARG\_185,12.5,0,0,0  
3T5B,ASP\_130,3.59,0.21,-0.42,0  
3LQE,ASP\_272,2.13,0.42,-2.09,0  
3C0C,GLU\_324,3.79,0.49,-1.2,0  
3FRR,ARG\_10,12.22,-0.28,0,0  
1DTO,HIS\_53,6.34,0.05,0,-0.21  
2D7U,ARG\_138,11.74,-0.76,0,0  
4FCU,LYS\_114,10.29,-0.21,0,0  
3LQE,ARG\_238,11.8,-0.7,0,0  
1SQW,LYS\_94,10.36,-0.14,0,0  
1L2F,GLU\_122,4.5,0,0,0  
3JRT,LYS\_152,10.15,-0.35,0,0  
2QK1,TYR\_376,11.57,2.25,-0.68,0  
4ANN,ARG\_134,11.66,-2.6,0,1.76  
3J5N,GLU\_187,4.07,0.14,-0.57,0  
2NRR,LYS\_389,10.36,-0.14,0,0  
2R05,CYS\_130,7.47,-2.3,0,0.77  
1YTD,LYS\_170,10.5,0,0,0  
3H5T,ARG\_23,12.5,0,0,0  
4AE7,ARG\_92,12.36,-0.14,0,0  
3LMF,ARG\_23,12.5,0,0,0  
1EQ6,ASP\_73,3.33,0.07,-0.54,0  
4FH3,HIS\_336,3.86,0,0,-2.64  
2ZQ5,ASP\_323,3.41,0.42,-0.81,0  
4DEZ,TYR\_83,13.5,0.36,-0.21,3.35  
2OEW,ARG\_56,12.36,-0.14,0,0  
3G53,ASP\_167,3.8,0,0,0  
1QQE,ASP\_151,3.89,0.28,-0.19,0  
1L2F,ASP\_278,3.57,0.49,-0.72,0  
3V55,ARG\_467,12.01,-0.49,0,0  
3V75,ASP\_267,3.53,0.49,-0.76,0  
1RZ2,TYR\_168,12.74,2.81,-0.07,0  
1XEU,ARG\_67,3.98,0.28,-0.8,0  
3IL3,HIS\_243,2.31,1.34,0,-5.53  
1NJ4,GLU\_278,3.98,0.28,-0.8,0  
1JB3,ASP\_58,3.94,0.14,0,0  
3VJ8,GLU\_344,3.86,0.21,-0.85,0  
1BYI,TYR\_74,9.35,0.24,-1.13,0.24  
1X9G,ARG\_84,12.5,0,0,0  
2Q99,ASP\_40,3.99,0.28,-0.09,0  
3LPZ,LYS\_4,10.43,-0.07,0,0  
2X4L,CYS\_331,11.19,-0.55,0,2.74  
2XJ4,ARG\_198,12.36,-0.14,0,0  
3TIR,ARG\_21,12.5,0,0,0  
1X9G,ARG\_84,12.5,0,0,0  
1WYC,ASP\_193,0.98,0.77,-3.58,0  
1X04,GLU\_112,4.64,0.14,0,0  
1X8F,GLU\_83,4.05,0.35,-0.8,0  
4FCU,ASP\_242,3.36,0.49,-0.93,0  
3B21,GLU\_174,4.5,0,0,0  
3B21,TYR\_200,10.43,1.23,-0.8,0  
3RVC,ARG\_140,12.29,-0.21,0,0  
1G8P,TYR\_147,12.35,2.35,0,0  
2C13,ARG\_144,12.49,-1.7,0,1.69  
1T3Y,LYS\_72,10.22,-0.28,0,0  
3V75,ARG\_74,12.29,-0.21,0,0  
1ZBP,GLU\_214,4.48,0,-0.02,0  
2XWS,GLU\_36,4.29,0.21,-0.42,0  
3EIZ,LYS\_132,10.01,-0.49,0,0  
3H8Y,LYS\_94,10.5,0,0,0  
3T5B,GLU\_66,4.74,1.33,-1.09,0  
3LPZ,ASP\_26,3.21,0.21,-0.98,0  
1WPC,LYS\_215,11.52,-0.8,0,0  
4DIU,GLU\_15,4.35,0.28,-0.43,0  
3KT9,GLU\_99,4.05,0.35,-0.8,0  
3COU,ARG\_5,12.29,-0.21,0,0  
3P2F,ASP\_170,3.87,0.07,0,0  
2EFK,ASP\_82,3.47,0.21,-0.54,0  
1S1Y,ASP\_126,3.38,0.14,-0.56,0  
3BQW,ARG\_101,12.15,-0.35,0,0  
2A1V,HIS\_139,6.5,0,0,0  
1Y2Q,TYR\_13,10.63,0.67,-0.04,0  
3A2Z,ASP\_49,3.87,0.07,0,0  
3GVO,ASP\_248,1.75,1.05,-3.1,0  
1KCM,GLU\_250,4.5,0,0,0  
1E59,GLU\_126,4.71,0.21,0,0  
3C5V,ARG\_325,12.43,-0.07,0,0  
3CRM,ASP\_244,1.19,0.49,-3.1,0  
3Q2C,GLU\_68,3.53,0.35,-1.32,0  
3M7G,GLU\_266,4.64,0.14,0,0  
4F8A,CYS\_568,8.96,-0.11,0,0.07  
3F5D,ASP\_168,3.94,0.14,0,0  
1SUU,LYS\_648,10.5,0,0,0  
3IV4,HIS\_26,3.59,0,0,-2.91  
1KW4,ARG\_27,12.29,-0.21,0,0

1UOH,ASP\_181,3.21,0.21,-0.8,0  
2J8A,HIS\_294,4.31,0.68,0,-2.87  
3CO1,TYR\_119,10.72,0.42,-0.19,0.49  
2AZL,GLU\_268,4.57,0.07,0,0  
3FRR,TYR\_165,12.72,0.51,0.79,1.42  
3ETV,LYS\_111,10.5,0,0,0  
2X4J,LYS\_30,10.5,0,0,0  
3NR5,LYS\_2,10.5,0,0,0  
3C5V,ARG\_106,11.73,-0.77,0,0  
1JKS,ASP\_14,4.21,0.42,-0.01,0  
1RHS,ASP\_195,3.94,0.14,0,0  
157K,TYR\_95,13.27,0.07,0.8,2.4  
3KEY,GLU\_461,3.68,0.21,-1.03,0  
2RJD,ARG\_467,13.65,-0.94,0.2,0.09  
2OKT,ARG\_76,11.94,-0.56,0,0  
2ILR,ARG\_365,11.83,-0.67,0,0  
2BV9,TYR\_54,10.0,0,0,0  
3G9G,GLU\_23,4.11,0.56,-0.95,0  
2Q5X,LYS\_865,10.22,-0.28,0,0  
2XHC,ARG\_272,12.5,0,0,0  
1H09,LYS\_236,10.5,0,0,0  
2W0G,ASP\_196,3.26,0.42,-0.96,0  
3H13,HIS\_417,7.1,0.66,0,-0.07  
4DBX,HIS\_131,6.93,1.6,3.91,-5.08  
3RJZ,LYS\_90,10.5,0,0,0  
1XTZ,LYS\_65,10.36,-0.14,0,0  
3GYW,HIS\_120,7.41,1.19,0,-0.28  
1T95,LYS\_228,10.5,0,0,0  
1SQH,GLU\_20,3.91,0.21,-0.8,0  
3L7N,LYS\_111,10.36,-0.14,0,0  
1OTM,GLU\_194,4.56,0.07,-0.01,0  
1LFP,LYS\_119,10.08,-0.42,0,0  
1P4X,LYS\_54,9.52,-0.98,0,0  
3I82,TYR\_70,10.59,0,-0.42,1.02  
2C2Y,ARG\_150,11.94,-0.56,0,0  
4ECC,HIS\_160,6.5,0,0,0  
3ANJ,TYR\_187,11.01,0,0,1.01  
2E0T,ASP\_75,3.79,0,-0.01,0  
3PP8,HIS\_109,6.43,0,0,-0.07  
2EYI,GLU\_113,3.73,0.28,-1.05,0  
3IVF,HIS\_188,6.43,0,0,-0.07  
3ONH,ARG\_522,11.45,-1.05,0,0  
3K8J,TYR\_49,11.04,0.47,-0.8,1.37  
1PZC,ASP\_37,3.18,0.56,-1.18,0  
2F4Q,GLU\_228,1.48,1.1,-2.4,-1.72  
2D7J,LYS\_138,10.5,0,0,0  
1ZP2,GLU\_70,4.18,0.07,-0.39,0  
1UCH,HIS\_179,7.07,0.1,0,-0.21  
1W7B,LYS\_81,10.5,0,0,0  
2ZCO,LYS\_9,10.5,0,0,0  
2HRZ,HIS\_86,0.84,0.22,-0.66,-5.21  
3DTE,TYR\_160,9.6,0,-0.4,0  
1J85,LYS\_42,10.5,0,0,0  
1OIS,LYS\_271,10.36,-0.14,0,0  
1TXJ,GLU\_66,4.9,0.63,-0.23,0  
3EZ7,GLU\_301,4.12,0.42,-0.8,0  
2Q98,GLU\_39,3.55,0.35,-1.3,0  
4DIU,ARG\_62,12.08,-0.42,0,0  
3EX9,ARG\_117,12.29,-0.21,0,0  
1L3K,ASP\_80,2.69,0.49,-1.6,0  
3EJC,GLU\_87,3.98,0.28,-0.8,0  
3QAV,LYS\_119,10.01,-0.49,0,0  
1XAW,TYR\_443,9.98,0,-0.02,0  
1YTQ,GLU\_122,3.88,0.21,-0.83,0  
1IAP,ARG\_136,12.29,-0.21,0,0  
3G6S,ARG\_26,10.13,-2.69,0,0.32  
3CAX,LYS\_137,10.29,-0.21,0,0  
3V3T,ASP\_133,3.6,0.07,-0.27,0  
2GZR,ARG\_167,11.87,-0.63,0,0  
2JKF,TYR\_35,9.34,0.14,-0.8,0  
1G8P,HIS\_159,7.52,1.16,0,-0.14  
1BN6,CYS\_139,12.58,0,0.48,3.1  
3ADO,GLU\_52,5.12,0.75,-0.13,0  
3D9H,HIS\_103,4.38,0,0,-2.12  
1MML,GLU\_171,4.78,0.28,0,0  
1FQI,LYS\_319,10.5,0,0,0  
2BLL,ARG\_317,12.22,-0.28,0,0  
1DZF,GLU\_6,4.5,0,0,0  
1P1L,HIS\_2,6.31,0.09,0,-0.28  
2B78,TYR\_222,10.27,1.8,-0.85,-0.67  
3K9I,ARG\_111,12.08,-0.42,0,0  
3RLN,GLU\_592,3.38,0.98,-2.1,0  
1SQH,TYR\_288,11.36,2.16,-0.8,0  
2X5Y,ASP\_803,1.88,0.56,-2.48,0  
2Q34,LYS\_205,10.5,0,0,0  
2AZL,ARG\_46,12.29,-0.21,0,0  
1O59,HIS\_76,6.36,0,0,-0.14  
2CVB,GLU\_17,4.07,0.35,-0.78,0  
1YR6,GLU\_41,4.5,0,0,0  
3NR5,ASP\_39,3.82,0.07,-0.05,0  
2ATR,CYS\_128,8.94,-0.06,0,0  
3JV1,CYS\_147,8.59,-0.79,0,0.38  
3E0H,ASP\_114,3.87,0.07,0,0  
1ZBP,HIS\_205,4.59,0.61,0,-2.52  
2CWC,ARG\_107,12.29,-0.21,0,0  
3KEY,ASP\_375,3.62,0.21,-0.39,0  
1OXZ,GLU\_257,3.96,0.35,-0.89,0  
3COU,GLU\_8,4.5,0,0,0  
2YWX,LYS\_17,10.22,-0.28,0,0  
3ADO,HIS\_145,6.75,1.89,1.56,-3.2  
4FZR,GLU\_77,4.5,0,0,0  
1R3F,ASP\_90,3.44,0.91,-1.27,0  
1NAF,LYS\_226,10.5,0,0,0  
2YX0,GLU\_297,4.57,0.07,0,0  
3M7G,GLU\_123,4.5,0,0,0  
2RIS,LYS\_191,10.5,0,0,0  
1WJG,ARG\_61,11.94,-0.56,0,0  
1O0X,ASP\_151,2.24,0.63,-2.19,0  
3RJZ,ARG\_60,11.87,-0.63,0,0  
1NKD,ASP\_45,3.87,0.14,-0.07,0  
2ZCX,TYR\_63,10.07,0.07,0,0  
1NJ4,LYS\_309,10.43,-0.07,0,0  
3T8R,GLU\_43,4.04,0.07,-0.53,0  
1P2F,LYS\_16,10.43,-0.07,0,0  
2V4U,ASP\_341,4.1,0.42,-0.12,0  
3K8J,LYS\_237,10.36,-0.14,0,0  
4EKU,LYS\_249,10.5,0,0,0  
4DBX,ARG\_296,11.94,-0.56,0,0  
2OJQ,ASP\_452,3.93,0.14,-0.01,0  
1R3F,TYR\_208,12.28,2.12,-0.8,0.96  
3GW3,GLU\_315,4.57,0.07,0,0  
3GYW,ARG\_68,12.29,-0.21,0,0  
1TD6,TYR\_128,13.41,0.21,0.8,2.4  
4HDE,ARG\_188,11.8,-0.7,0,0  
3CO1,GLU\_36,4.56,0.07,-0.01,0  
2E3C,LYS\_415,10.22,-0.28,0,0  
1KCM,GLU\_113,0.23,1.57,-1.28,-4.57  
1GPP,LYS\_148,10.22,-0.28,0,0  
3V3T,ASP\_41,4.05,0.42,-0.17,0  
2FXT,TYR\_305,11.67,1.5,-0.12,0.28  
1UJ8,HIS\_44,7.89,1.53,0,-0.14  
2RFA,ARG\_134,12.15,-0.35,0,0  
2O8P,ARG\_136,12.67,-0.65,0,0.82  
3N2T,GLU\_305,2.8,0.77,-2.46,0  
2ATR,ASP\_62,0.75,1.05,-4.1,0  
1V6T,HIS\_38,4.68,1.6,1.46,-4.88  
4ETX,TYR\_427,10.09,0.14,-0.05,0  
1WRU,TYR\_100,12.96,0.07,0.49,2.4  
1AKO,ASP\_143,3.87,0.07,0,0  
3OBS,CYS\_87,11.29,0,0.2,2.9  
1F09,ARG\_121,12.29,-0.21,0,0  
1PDB,ARG\_70,10.22,-2.28,0,0  
4ETX,ASP\_318,2.73,0.42,-1.49,0  
2D59,GLU\_115,3.77,0.07,-0.8,0  
1Z9L,LYS\_31,10.36,-0.14,0,0  
2FG1,LYS\_44,9.87,-0.63,0,0  
2J8A,LYS\_366,10.22,-0.28,0,0  
3CIV,HIS\_136,6.43,0,0,-0.07  
2GZQ,LYS\_11,10.15,-0.35,0,0  
1Ri6,TYR\_53,11.86,1.05,0,0.81  
2FXT,LYS\_330,10.5,0,0,0  
3K85,GLU\_290,4.5,0,0,0  
2QZQ,LYS\_151,10.5,0,0,0  
4E8B,CYS\_115,3.98,-5.16,0.14  
2BDD,TYR\_128,10.2,0,0.2  
3G9G,ARG\_175,12.08,-0.42,0,0  
2D0A,ASP\_40,3.94,0.14,0,0  
2P4D,ASP\_100,1.29,0.84,-3.35,0  
1Ri5,GLU\_257,4.27,0.07,-0.3,0  
2EJB,HIS\_81,6.61,0.18,0,-0.07  
2Y74,HIS\_632,6.5,0,0,0  
4H89,ARG\_45,12.29,-0.21,0,0  
2X4L,GLU\_154,3.91,0.21,-0.8,0  
3K8J,HIS\_141,6.5,0,0,0  
1ZCE,CYS\_134,9.62,-0.24,0.86  
3C38,GLU\_176,4.57,0.07,0,0  
3FKS,HIS\_271,4.15,0,0,-2.35  
2Q98,GLU\_107,4.71,0.21,0,0  
3EVN,TYR\_81,13.41,0.21,0.8,2.4  
1AD6,GLU\_464,2.38,0.28,-2.4,0  
1FHL,TYR\_113,12.68,2.68,0,0  
2FZP,GLU\_201,4.5,0,0,0  
2FD5,GLU\_72,4.5,0,0,0  
4AM1,HIS\_212,4.25,0.77,0,-3.02  
1VSM,GLU\_172,4.34,0.35,-0.5,0  
3HUE,LYS\_71,10.36,-0.14,0,0  
1AK1,LYS\_135,10.36,-0.14,0,0  
2X4G,GLU\_312,4.57,0.07,0,0  
1ZP2,ASP\_61,10.4,-3.11,0,1.01  
1DVO,ARG\_49,12.01,-0.49,0,0  
4F3J,ASP\_137,2.64,0.63,-1.79,0  
1ZP2,HIS\_178,6.84,0.48,0,-0.14  
3DZ1,ASP\_226,3.85,0.07,-0.02,0  
3ODJ,GLU\_45,4.65,0.28,-0.13,0  
3HUE,LYS\_84,10.43,-0.07,0,0  
1WRU,GLU\_184,4.34,0.07,-0.23,0  
2ZCO,GLU\_178,4.05,0.35,-0.8,0  
3K9I,GLU\_129,4.39,0.35,-0.46,0  
1L3K,GLU\_135,4.64,0.14,0,0  
1QYI,GLU\_183,0.52,1.44,-3.91,-1.51  
1P2F,ARG\_27,12.5,0,0,0  
3QKY,GLU\_268,3.44,0.42,-1.48,0  
1XEU,HIS\_192,6.37,0.15,0,-0.28  
4E8B,ASP\_72,3.42,0.49,-0.87,0  
2P65,ASP\_171,2.32,0.63,-2.11,0  
1QZN,TYR\_101,10.79,0.45,-1.18,1.52  
2FM9,LYS\_164,10.36,-0.14,0,0  
2B78,TYR\_356,13.59,0.47,0.72,2.4  
2QEV,LYS\_117,10.36,-0.14,0,0  
3G6S,LYS\_73,10.5,0,0,0  
2IQT,GLU\_44,4.5,0,0,0  
1NAR,LYS\_69,10.08,-0.42,0,0  
3A4C,ARG\_526,12.5,0,0,0  
2GZR,TYR\_219,8.62,0.21,-1.59,0  
1PNE,ARG\_88,11.66,-0.84,0,0  
3E7P,TYR\_244,13.5,0.35,0.75,2.4  
2CYG,LYS\_302,10.5,0,0,0  
2CN1,TYR\_170,13.25,0.43,0.42,2.4  
2ZQ5,HIS\_255,8.01,1.77,2.61,-2.87  
1KN3,LYS\_156,10.43,-0.07,0,0  
3IL3,GLU\_64,4.64,0.14,0,0  
1ZCE,TYR\_53,10.07,0.07,0,0  
2QK1,TYR\_369,9.84,0.45,-0.61,0  
3M66,GLU\_218,4.12,0.42,-0.8,0  
2P4D,LYS\_87,10.43,-0.07,0,0  
3V75,ASP\_33,3.35,0.28,-0.73,0  
2RJD,GLU\_352,2.73,1.76,-3.53,0  
2B78,LYS\_66,10.5,0,0,0  
3FTT,GLU\_34,4.29,0.28,-0.49,0  
2IRM,GLU\_193,4.5,0,0,0  
1WRU,ASP\_258,1.84,0.49,-2.45,0  
1Z3X,GLU\_123,4.19,0.49,-0.8,0  
1Y0K,ARG\_36,10.58,-1.92,0,0  
2W1R,TYR\_128,10.07,0.07,0,0  
3AUF,ARG\_94,12.15,-0.35,0,0  
1Ri5,GLU\_97,4.5,0,0,0  
1J85,LYS\_92,10.15,-0.35,0,0  
3BCH,ASP\_200,3.79,0.35,-0.35,0  
1V6T,ASP\_173,1.99,0.49,-2.29,0  
2BAA,TYR\_123,10.07,0.07,0,0  
4DNU,TYR\_241,10.08,0.07,0,0.01  
1XFK,ARG\_173,11.87,-0.63,0,0  
2Q13,LYS\_361,10.15,-0.35,0,0  
3HKX,GLU\_172,3.7,0.28,-1.08,0  
1UAJ,ASP\_177,3.69,0.14,-0.25,0  
2Q34,CYS\_52,9.45,0,0.0,45  
2WB8,ASP\_519,3.7,0.28,-0.38,0  
2RJD,TYR\_490,9.27,0.07,-0.8,0  
2YX0,LYS\_62,10.22,-0.28,0,0  
1TD6,LYS\_78,10.43,-0.07,0,0  
1GQE,LYS\_292,10.22,-0.28,0,0  
3RFY,ARG\_280,12.36,-0.14,0,0  
3MEW,TYR\_245,10.21,0,0.21,0  
3EOD,ARG\_117,12.01,-0.49,0,0  
3RFY,LYS\_170,10.5,0,0,0  
1SJ8,CYS\_750,9.6,0,0.6  
3L3P,GLU\_383,4.57,0.07,0,0  
3BQW,ARG\_119,11.94,-0.56,0,0  
1X04,HIS\_135,7.05,0.69,0,-0.14  
3JSN,LYS\_53,10.15,-0.35,0,0  
2ZQ5,ASP\_33,3.1,0.14,-0.84,0  
3K1H,CYS\_54,10.36,0,0.136  
3G9G,HIS\_169,7.76,1.26,0,0  
3ONJ,ARG\_49,10.15,-0.35,0,0  
2J8A,GLU\_249,4.11,0.35,-0.74,0  
1UXO,HIS\_62,8.5,2.14,0,-0.14  
1EYH,GLU\_21,3.28,0.42,-1.64,0  
3LMF,GLU\_106,4.36,0.07,-0.21,0  
2PGX,ASP\_136,2.28,0.56,-2.08,0  
3PB8,LYS\_150,10.5,0,0,0  
3CAX,TYR\_433,10.0,0,0,0  
4ESS,ASP\_17,1.15,0.56,-3.21,0  
2CIU,GLU\_188,3.86,0.56,-1.2,0  
3ADO,TYR\_251,10.0,0,0,0  
2V5B,LYS\_53,9.87,-0.63,0,0  
1TXJ,CYS\_14,8.74,-1.96,0.17  
1MUF,CYS\_119,6.56,-2.84,-0.36,0.76  
4H4J,ARG\_259,11.73,-0.77,0,0  
1P1L,GLU\_16,4.78,0.28,0,0  
1U7U,ARG\_342,11.3,-1.2,0,0  
1NAF,LYS\_174,10.29,-0.21,0,0  
3CIV,GLU\_257,3.06,0.63,-2.07,0  
3H04,ASP\_12,0.45,0.49,-3.84,0  
2RIK,ASP\_68,1.6,0.91,-3.12,0  
2H85,ASP\_183,3.59,0.42,-0.63,0  
2FGG,GLU\_22,4.25,0.35,-0.6,0

2CL3,GLU\_70,3.98,0.56,-1.08,0  
 2VGM,ASP\_241,4.18,0.49,-0.11,0  
 3LMF,HIS\_107,7.0,5,0,0  
 1MUF,CYS\_303,9.44,-0.65,0,1.1  
 3HST,GLU\_330,4.42,0.14,-0.22,0  
 2IN0,ARG\_96,11.8,-0.7,0,0  
 1BN6,ASP\_93,3.84,0.07,-0.03,0  
 2XMZ,ARG\_73,12.43,-0.07,0,0  
 1O6D,GLU\_147,2.45,0.35,-2.4,0  
 1QZN,LYS\_117,10.29,-0.21,0,0  
 3I82,GLU\_27,4.5,0,0,0  
 1Q2Y,TYR\_17,11.83,0,0.06,1.77  
 2YYO,ARG\_34,12.36,-0.14,0,0  
 1WXQ,TYR\_323,12.54,1.26,0,1.28  
 2GZR,ARG\_161,12.4,-3.06,0,2.97  
 1TXJ,GLU\_86,4.57,0.07,0,0  
 1X7F,GLU\_208,4.55,1.11,-1.06,0  
 2V4X,ARG\_58,11.87,-0.63,0,0  
 1WRU,LYS\_304,10.5,0,0,0  
 3A0X,LYS\_723,10.5,0,0,0  
 2EFK,ARG\_222,12.01,-0.49,0,0  
 3ADO,LYS\_264,10.5,0,0,0  
 200K,LYS\_192,10.5,0,0,0  
 2CL3,LYS\_182,10.5,0,0,0  
 1NUJ,ARG\_257,8.93,-3.93,0,0.36  
 2OJQ,GLU\_442,4.57,0.07,0,0  
 3OKQ,LYS\_632,10.5,0,0,0  
 1TD6,LYS\_134,10.5,0,0,0  
 3LJI,TYR\_290,10.0,0,0,0  
 3F6F,LYS\_188,10.08,-0.42,0,0  
 1OOX,ASP\_122,1.05,0.7,-3.45,0  
 1RL0,GLU\_199,4.05,0.35,-0.8,0  
 2H85,LYS\_264,10.29,-0.21,0,0  
 2GZQ,LYS\_106,10.5,0,0,0  
 3M70,ASP\_251,2.8,0.42,-1.42,0  
 3BWT,LYS\_751,10.5,0,0,0  
 3Q2C,TYR\_35,8.01,0.07,-2.06,0  
 4DVD,GLU\_56,4.64,0.14,0,0  
 1YLN,GLU\_142,4.5,0,0,0  
 1V43,ASP\_357,3.27,0.56,-1.09,0  
 3AU3,ARG\_499,12.22,-0.28,0,0  
 3PZ9,LYS\_167,10.29,-0.21,0,0  
 2P65,ASP\_112,4.03,0.28,-0.05,0  
 2JEO,ARG\_22,12.22,-0.28,0,0  
 2QOP,GLU\_111,4.87,0.68,-0.31,0  
 1QQH,ASP\_205,2.11,0.42,-2.11,0  
 2XWS,ASP\_81,1.82,0.49,-2.47,0  
 2HP7,ASP\_108,2.03,0.42,-2.2,0  
 1ZCE,ASP\_60,4.28,0.56,-0.08,0  
 4EVF,GLU\_277,4.25,0.07,-0.32,0  
 1PVT,LYS\_167,10.43,-0.07,0,0  
 4ECC,GLU\_104,3.84,0.14,-0.8,0  
 1SJV,HIS\_3,6.5,0,0,0  
 3L7N,TYR\_105,10.17,0.14,-2.11,2.14  
 1AK1,HIS\_28,6.91,0.41,0,0  
 2CWC,ARG\_295,11.94,-0.56,0,0  
 1SFE,ARG\_72,11.73,-0.77,0,0  
 3CN5,ASP\_241,2.2,0.63,-2.22,0  
 3H13,HIS\_334,6.22,0.0,-0.28  
 3UOV,CYS\_87,6.33,-2.67,0,0  
 2VAN,CYS\_239,10.68,-0.6,0,2.28  
 3CNU,LYS\_54,10.22,-0.28,0,0  
 3AUF,ARG\_30,12.36,-0.14,0,0  
 3EAZ,LYS\_137,10.36,-0.14,0,0  
 3QAV,GLU\_27,2.17,1.67,-1.6,-2.4  
 1S7K,HIS\_62,4.59,1.86,-0.32,-3.46  
 1SJB,ASP\_515,2.79,0.42,-1.43,0  
 1QQH,LYS\_66,10.5,0,0,0  
 3ONH,TYR\_471,11.29,1.29,0,0  
 3BCY,HIS\_83,6.6,0.17,0,-0.07  
 2PGE,ARG\_74,12.5,0,0,0  
 4F3J,TYR\_136,10.29,1.35,-1.06,0  
 3ULX,LYS\_123,10.36,-0.14,0,0  
 1O17,LYS\_33,9.94,-0.56,0,0  
 3RKV,ARG\_220,12.01,-0.49,0,0  
 1R9W,CYS\_273,9.89,0,0,0.89  
 1NRI,CYS\_110,8.74,-0.26,0,0  
 1YM5,ASP\_169,2.23,0.63,-2.2,0  
 2CBE,HIS\_3,6.43,0,0,-0.07  
 3Q9P,ASP\_93,3.79,0.21,-0.22,0  
 3ULX,ASP\_141,3.35,0.35,-0.8,0  
 3M3P,LYS\_238,10.5,0,0,0  
 1GVPT,TYR\_56,8.63,0.1,-1.52,0.04  
 3BA1,ARG\_118,11.48,-1.02,0,0  
 2ZCO,TYR\_75,10.07,0.07,0,0  
 2QEF,GLU\_25,4.41,0.7,-0.79,0  
 3BQW,GLU\_24,3.42,0.28,-1.36,0  
 1CBY,HIS\_30,6.57,0.07,0,0  
 3GMS,GLU\_272,4.85,0.35,0,0  
 1YW5,ARG\_94,13.91,-0.58,0,1.99  
 1PBV,ASP\_206,3.87,0.07,0,0  
 2P5D,TYR\_31,9.99,0.07,-0.08,0  
 2A6B,LYS\_101,10.5,0,0,0  
 2O8I,GLU\_23,4.05,0.35,-0.8,0  
 2W0Z,CYS\_451,8.09,-3.6,0,2.69  
 3H8Y,GLU\_89,4.1,0.28,-0.68,0  
 3UAH,LYS\_288,10.43,-0.07,0,0  
 3IDW,GLU\_7,4.25,0.21,-0.46,0  
 2P52,GLU\_204,4.57,0.07,0,0  
 3ANJ,TYR\_383,12.04,2.43,-0.39,0  
 1G8P,GLU\_125,4.13,0.14,-0.51,0  
 1WP5,TYR\_131,13.27,0.07,0.8,2.4  
 1XIP,GLU\_83,4.58,0.35,-0.27,0  
 1MJS,LYS\_340,10.15,-0.35,0,0  
 1PDB,ASP\_141,3.88,0.28,-0.2,0  
 3U2R,LYS\_94,10.43,-0.07,0,0  
 3EST,ASP\_196,3.21,0.21,-0.8,0  
 2Z61,HIS\_33,9.22,2.32,2.4,-2  
 3BJV,HIS\_11,6.47,0.04,0,-0.07  
 3H13,GLU\_414,4.57,0.07,0,0  
 2CXA,CYS\_228,7.71,-1.36,0,0.07  
 1RZ2,TYR\_40,10.0,0,0,0  
 2H14,TYR\_228,10.62,0,0,0.62  
 2A6B,GLU\_36,3.53,0.63,-1.6,0  
 2XMK,HIS\_3,5.04,0.16,0.32,-1.95  
 200K,GLU\_16,4.92,0.42,0,0  
 2OYZ,GLU\_43,4.92,0.71,-0.29,0  
 2X4G,ARG\_233,11.87,-0.63,0,0  
 2VAN,GLU\_144,1.39,0.42,-3.53,0  
 2BLL,GLU\_407,4.85,0.35,0,0  
 4H89,ARG\_168,11.87,-0.63,0,0  
 2V4U,ARG\_411,13.45,-0.88,0,1.83  
 3E7P,ASP\_157,3.43,0.28,-0.65,0  
 1L2F,GLU\_264,2.13,1.32,-1.8,-1.89  
 2ATR,HIS\_40,6.36,0,0,-0.14  
 1UCH,GLU\_40,4.5,0,0,0  
 3ANJ,TYR\_391,13.41,0.21,0.8,2.4  
 3IU5,ASP\_62,1.71,1.19,-3.29,0  
 1UCH,ASP\_79,3.87,0.07,0,0  
 3US6,GLU\_40,4.78,0.28,0,0  
 1O5J,LYS\_13,10.29,-0.21,0,0  
 4EVF,ARG\_187,11.66,-0.84,0,0  
 2W1R,GLU\_166,3.84,0.14,-0.8,0  
 1TUE,HIS\_89,6.43,0,0,-0.07  
 1RIS,CYS\_223,11.7,0.25,2.33,0.12  
 4EVF,ARG\_278,12.08,-0.42,0,0  
 2B2H,HIS\_305,0.37,0,0,-6.13  
 3E0H,LYS\_51,10.22,-0.28,0,0  
 1WP5,GLU\_295,4.36,0.21,-0.35,0  
 1UJ8,ASP\_49,3.94,0.14,0,0  
 2EJB,GLU\_26,4.57,0.07,0,0  
 1O59,ARG\_78,4.5,0,0,0  
 3P51,GLU\_16,12.36,-0.14,0,0  
 3HKX,ARG\_112,10.96,-1.54,0,0  
 3ELI,ASP\_121,3.6,0.7,-0.9,0  
 3JZ9,LYS\_464,10.22,-0.28,0,0  
 1WOU,CYS\_110,9.61,-0.35,0,0.96  
 2XWS,ARG\_123,12.5,0,0,0  
 2D59,ASP\_37,3.67,0,-0.13,0  
 3A2Z,LYS\_127,10.5,0,0,0  
 1W7B,TYR\_24,10.0,0,0,0  
 3GOZ,TYR\_259,11.73,0.03,0,1.7  
 2OGQ,CYS\_544,6.42,-3.18,0,0.6  
 2IXM,HIS\_308,5.05,0,0,-1.45  
 3FHF,GLU\_91,4.36,0.07,-0.21,0  
 1SUU,ASP\_762,3.87,0.07,0,0  
 1YLN,ARG\_194,12.36,-0.14,0,0  
 3LOD,GLU\_13,3.02,0.35,-1.83,0  
 1JT9,ARG\_18,11.87,-0.63,0,0  
 1RL0,LYS\_254,10.22,-0.28,0,0  
 3G53,LYS\_29,10.5,0,0,0  
 1J33,HIS\_271,3.2,0,0,-3.3  
 3GW3,ARG\_247,12.01,-0.49,0,0  
 1XAW,TYR\_432,9.62,0.42,-0.8,0  
 1U3Y,ASP\_271,4.08,0.28,0,0  
 2P52,GLU\_283,3.46,0.56,-1.6,0  
 1SJB,ARG\_589,11.87,-0.63,0,0  
 2YLF,CYS\_221,10.61,-0.14,0,1.75  
 3LH5,GLU\_530,3.43,0.35,-1.42,0  
 3AU3,LYS\_670,10.29,-0.21,0,0  
 1VJG,HIS\_173,6.5,0,0,0  
 1R3D,HIS\_78,6.65,0.22,0,-0.07  
 2QEV,ASP\_67,0.88,0.63,-3.55,0  
 2IRM,TYR\_34,7.62,0.86,-1.36,-1.88  
 1MTZ,GLU\_279,3.62,0.14,-1.02,0  
 1SUU,ARG\_735,12.15,-0.35,0,0  
 2C13,LYS\_252,10.15,-0.35,0,0  
 2V1L,GLU\_137,4.5,0,0,0  
 4FD6,LYS\_5,10.43,-0.07,0,0  
 1KCM,ASP\_238,4.08,0.28,0,0  
 2POL,ASP\_257,3.28,0.07,-0.59,0  
 2B78,TYR\_286,9.49,1.09,-1.6,0  
 4FZR,GLU\_251,4.58,0.56,-0.48,0  
 2DOA,TYR\_46,10.35,0.38,-0.03,0  
 2B61,TYR\_252,10.0,0,0,0  
 1G8P,ARG\_230,11.87,-0.63,0,0  
 2HXB,ASP\_135,3.59,0,-0.21,0  
 1R53,ASP\_273,4.04,0.28,-0.04,0  
 2VAN,TYR\_322,10.87,0.21,0,0.66  
 1YTD,ASP\_175,3.8,0,0,0  
 3ONT,HIS\_118,6.93,0.5,0,-0.07  
 3UX2,ASP\_49,1.39,0.77,-3.18,0  
 1NJ4,ASP\_204,1.53,0.63,-2.9,0  
 1TUL,CYS\_90,9,0,0,0  
 1RHS,ARG\_146,12.36,-0.14,0,0  
 3M66,TYR\_149,10,0,0,0  
 1O17,LYS\_25,10.43,-0.07,0,0  
 3BB7,TYR\_212,10,0,0,0  
 3F5D,CYS\_100,10.1,-2.31,2.42,0.99  
 1ZBP,HIS\_73,6.93,0.57,0,-0.14  
 3CX5,TYR\_170,10.88,1.68,-0.8,0  
 2AD1,CYS\_26,6.9,-2.24,0,0.14  
 3HKX,ASP\_255,3.63,0.63,-0.8,0  
 1XDZ,LYS\_13,10.43,-0.07,0,0  
 4GA2,GLU\_136,4.57,0.07,0,0  
 4EKU,ASP\_100,4.03,0.63,-0.4,0  
 3ZSL,HIS\_217,6.41,0.12,0,-0.21  
 3COU,GLU\_119,3.4,0.28,-1.38,0  
 3IRA,TYR\_91,10.98,0.98,0,0  
 1ZBM,ASP\_65,2.91,0.42,-1.31,0  
 3UOV,GLU\_189,3.72,0.28,-1.06,0  
 1XU7,HIS\_262,7.55,1.05,0,0  
 1FQI,LYS\_283,10.5,0,0,0  
 4DEZ,ASP\_72,3.87,0.07,0,0  
 3OBS,TYR\_32,10,0,0,0  
 1O17,GLU\_208,3.1,0.54,-0.01,-1.93  
 3CAN,GLU\_53,3.48,0.28,-1.29,0  
 2F4Q,ASP\_276,3.87,0.07,0,0  
 3IVF,LYS\_106,10.5,0,0,0  
 3G9T,LYS\_16,10.5,0,0,0  
 1L2F,GLU\_158,4.08,0.14,-0.56,0  
 2QEV,ASP\_33,3.67,0.84,-0.97,0  
 2GZQ,ASP\_48,3.76,0,-0.04,0  
 3DZ1,GLU\_20,9.39,-1.46,-2.4,0  
 1WLY,ARG\_269,11.87,-0.63,0,0  
 3GG6,ARG\_37,12.5,0,0,0  
 4EZB,GLU\_163,4.5,0,0,0  
 1LFP,LYS\_202,10.29,-0.21,0,0  
 1XTZ,GLU\_254,4.16,0.28,-0.62,0  
 2CBE,TYR\_40,10.5,0,0,0  
 2FPN,LYS\_44,10.43,-0.07,0,0  
 1RIG,ASP\_161,2.78,0.63,-1.65,0  
 2DFL,ASP\_70,3.87,0.07,0,0  
 3CAN,GLU\_22,4.5,0,0,0  
 2ILR,CYS\_421,8.67,-1.6,0,1.27  
 3LD1,CYS\_20,9.39,-1.46,-0.13,1.98  
 1RAJ,LYS\_250,10.5,0,0,0  
 2VAN,GLU\_335,4.5,0,0,0  
 3RUX,HIS\_264,3.35,0,-3.15  
 2IQT,GLU\_281,4.57,0.07,0,0  
 2R51,ARG\_60,12.29,-0.21,0,0  
 1PVT,GLU\_226,12.5,0,0,0  
 4HDE,LYS\_88,10.5,0,0,0  
 2QVT,ASP\_60,1.77,1.26,-3.29,0  
 2R57,CYS\_277,8.36,-0.71,0,0.07  
 2E0T,TYR\_166,9.75,0.55,-0.8,0  
 2H2W,GLU\_208,4.16,0.35,-0.69,0  
 1WNH,ARG\_214,12.29,-0.21,0,0  
 2Y2T,ARG\_32,11.73,-0.77,0,0  
 1DUN,ASP\_26,2.74,0.28,-1.33,0  
 3M66,ARG\_302,12.29,-0.21,0,0  
 3OOP,LYS\_75,9.8,-0.7,0,0  
 3LJC,GLU\_62,3.94,0.21,-0.77,0  
 2LHV,HIS\_157,6.29,0.0,-0.21  
 2EDM,ASP\_158,3.21,0.28,-0.87,0  
 3EYE,CYS\_86,11.49,-0.12,0,2.61  
 1ZBM,ARG\_102,12.36,-0.14,0,0  
 1L3K,ARG\_146,12.22,-0.28,0,0  
 3ASA,TYR\_327,9.65,2.36,-0.8,-1.91  
 2NRK,LYS\_167,10.29,-0.21,0,0  
 1Q5Z,ARG\_571,10.84,-1.66,0,0  
 1TR9,LYS\_236,10.5,0,0,0  
 3IDW,CYS\_19,9.03,-0.11,0,0.14  
 2EEY,GLU\_116,5.14,1.45,-0.81,0  
 3L7N,TYR\_34,10.14,0,0,0.14  
 4H4I,ASP\_136,3.35,0.42,-0.87,0  
 4E8B,HIS\_15,7.2,0.7,0,0  
 3CX5,CYS\_45,4.64,-5.51,0.64,0.51  
 2YWJ,LYS\_118,10.29,-0.21,0,0  
 3FWU,ARG\_61,12.36,-0.14,0,0  
 2AZL,ARG\_44,11.43,-2.91,0,1.84  
 1CBY,TYR\_168,11.71,0,0,1.71  
 2V5B,GLU\_186,4.46,0.14,-0.18,0  
 2HNG,GLU\_113,4.32,0.28,-0.46,0  
 1X8F,ASP\_32,3.08,0.14,-0.86,0  
 3L3P,ARG\_378,13.72,-1.18,0,2.4



1UOH,GLU\_187,4.06,0.56,-0.99,0  
 1S17,GLU\_97,4.5,0,0,0  
 3K8J,ASP\_166,2.27,0.35,-1.88,0  
 3BQW,ASP\_321,3.87,0.07,0,0  
 3RLN,TYR\_591,10,0,0,0  
 1Z9L,GLU\_124,4.57,0.07,0,0  
 3GYW,ARG\_222,11.8,-0.7,0,0  
 2B61,HIS\_130,6.43,0,0,-0.07  
 1N1J,LYS\_253,10.15,-0.35,0,0  
 2FL4,GLU\_44,4.52,0.21,-0.19,0  
 2HRZ,ASP\_124,2.63,0.56,-1.73,0  
 3LQE,GLU\_407,5.2,0.7,0,0  
 1PNE,TYR\_6,10,0,0,0  
 2YLF,ARG\_70,12.36,-0.14,0,0  
 1L3K,CYS\_43,9.82,0,0,0.82  
 1YR6,ARG\_227,11.73,-0.77,0,0  
 1O17,LYS\_226,10.29,-0.21,0,0  
 1MML,TYR\_222,10.25,0,0.25,0  
 3E7P,ARG\_225,12.36,-0.14,0,0  
 1MSI,ASP\_149,3.28,0.28,-0.8,0  
 2B3M,LYS\_16,10.29,-0.21,0,0  
 1NRI,GLU\_31,2.38,0.28,-2.4,0  
 1WXF,GLU\_239,4.61,0.56,-0.98,0.54  
 3RKV,GLU\_192,3.53,0.28,-1.25,0  
 2HP7,TYR\_89,10.06,1.16,-1.52,0.43  
 3T57,LYS\_159,10.22,-0.28,0,0  
 4EZB,GLU\_228,4.78,0.28,0,0  
 4FZR,GLU\_83,4.82,0.35,-0.03,0  
 2Q5X,GLU\_796,4.78,0.28,0,0  
 1PSW,GLU\_68,4.71,0.21,0,0  
 4DND,GLU\_101,4.5,0,0,0  
 1MUF,GLU\_132,4.5,0,0,0  
 3K8J,GLU\_224,4.12,0.42,-0.8,0  
 1TXJ,HIS\_123,6.43,0,0,-0.07  
 3COC,GLU\_320,4.71,0.21,0,0  
 1BN6,ARG\_32,11.87,-0.63,0,0  
 1PGV,GLU\_290,4.78,0.28,0,0  
 2CBE,ASP\_130,2.63,0.63,-1.8,0  
 1ZYL,GLU\_155,4.91,0.07,0.34  
 4ANN,LYS\_41,10.43,-0.07,0,0  
 3BA1,GLU\_69,3.25,0.35,-1.6,0  
 1MHN,GLU\_134,2.55,0.98,-2.93,0  
 2XJ4,LYS\_35,10.08,-0.42,0,0  
 1OOX,GLU\_245,4.39,0.14,-0.25,0  
 1UCH,TYR\_137,11.63,0.21,0,1.42  
 3EUR,ASP\_85,4.08,0.42,-0.14,0  
 1RAJ,ASP\_412,3.82,0.28,-0.26,0  
 1S18,LYS\_592,10.29,-0.21,0,0  
 2QV2,GLU\_26,4.69,0.42,-0.23,0  
 3ELI,HIS\_37,6.43,0,0,-0.07  
 1MN3,GLU\_451,4.71,0.21,0,0  
 2VGM,LYS\_124,9.8,-0.7,0,0  
 3CSR,ASP\_149,3.01,0.14,-0.93,0  
 3LOD,LYS\_149,10.08,-0.42,0,0  
 3MEW,TYR\_273,11.53,0,1.53  
 1A8Q,LYS\_130,10.43,-0.07,0,0  
 1LN4,ASP\_55,2.19,0.49,-2.1,0  
 2YLF,ASP\_138,3.85,0.07,-0.02,0  
 2B61,LYS\_349,10.29,-0.21,0,0  
 3UX2,GLU\_51,3.33,0.35,-1.53,0  
 2POL,ASP\_214,3.17,0.56,-1.19,0  
 1JKS,GLU\_192,4.64,0.14,0,0  
 1SBX,CYS\_153,9.72,-0.04,0.5,0.26  
 2CVB,TYR\_79,10,0,0,0  
 3CX2,ASP\_152,3.77,0.07,-0.1,0  
 2RGY,LYS\_169,10.29,-0.21,0,0  
 1J7G,LYS\_95,9.94,-0.56,0,0  
 3H13,CYS\_310,12.26,0,0.3,26  
 1P4X,ARG\_208,12.29,-0.21,0,0  
 1X6J,GLU\_48,4.5,0,0,0  
 3E5T,HIS\_197,6.74,3.2,1.57,-4.52  
 1X7F,ASP\_293,3.34,0.28,-0.74,0  
 2ATR,GLU\_35,4.5,0,0,0  
 1YB2,HIS\_211,4.32,0.45,0,-2.63  
 1WPS,LYS\_124,10.36,-0.14,0,0  
 3ONT,LYS\_10,10.5,0,0,0  
 1XIP,GLU\_11,4.48,0.21,-0.23,0  
 3O48,GLU\_107,4.71,0.28,-0.07,0  
 2CN1,ASP\_128,3.87,0.07,0,0  
 2BV9,ARG\_143,12.15,-0.35,0,0  
 1RWZ,ASP\_62,2.95,0.35,-1.2,0  
 3C2E,GLU\_61,4.0,0.77,-1.27,0  
 1K9S,ARG\_186,13.26,-0.64,0,1.4  
 1C44,LYS\_14,10.29,-0.21,0,0  
 4DEZ,GLU\_123,4.57,0.07,0,0  
 1C3K,HIS\_91,6.5,0,0,0  
 1T07,GLU\_41,3.91,0.21,-0.8,0  
 1AKO,ASP\_40,3.43,0.14,-0.51,0  
 2Q13,LYS\_193,10.43,-0.07,0,0  
 3IBT,GLU\_141,4.5,0,0,0  
 3MTT,GLU\_537,4.64,0.14,0,0  
 2QDJ,LYS\_294,10.29,-0.21,0,0  
 2EHG,LYS\_40,10.5,0,0,0  
 1YTQ,GLU\_166,4.64,0.14,0,0  
 4F8A,LYS\_679,10.5,0,0,0  
 3M66,ARG\_365,10.66,-1.84,0,0  
 3OKQ,CYS\_643,9,0,0,0  
 2QVO,LYS\_53,10.36,-0.14,0,0  
 1FO9,GLU\_298,3.8,0.35,-1.05,0  
 2A6B,TYR\_55,13.02,0.3,0.02,2.7  
 4EVF,ASP\_275,2.76,0.56,-1.6,0  
 4FH3,ARG\_78,11.66,-0.84,0,0  
 2QK1,ARG\_344,11.59,-0.91,0,0  
 1TWU,LYS\_36,10.29,-0.21,0,0  
 2W0G,LYS\_202,10.43,-0.07,0,0  
 2X4G,GLU\_71,4.78,0.28,0,0  
 2NMU,ARG\_12,12.08,-0.42,0,0  
 4F8A,CYS\_658,8.85,-0.29,0.14  
 1X6J,ASP\_38,3.55,0.07,-0.32,0  
 1Q42,TYR\_88,13.08,0.14,0.54,2.4  
 2POL,ASP\_223,3.96,0.28,-0.12,0  
 3EVZ,LYS\_226,10.5,0,0,0  
 2DG7,ARG\_117,11.94,-0.56,0,0  
 3ELI,ASP\_44,3.48,0.21,-0.53,0  
 2VGM,LYS\_45,10.08,-0.42,0,0  
 3I47,LYS\_13,10.5,0,0,0  
 1ZBP,LYS\_59,10.5,0,0,0  
 1EQ6,HIS\_210,6.47,0.18,0,-0.21  
 3LH5,TYR\_669,10.82,0.82,0,0  
 3GEC,TYR\_414,11.22,1.22,0,0  
 2CXA,ARG\_80,12.43,-0.07,0,0  
 1AD6,GLU\_413,4.5,0,0,0  
 2P5D,LYS\_142,10.43,-0.07,0,0  
 1X9G,LYS\_26,10.5,0,0,0  
 3TMO,LYS\_211,10.01,-0.49,0,0  
 2R51,LYS\_180,10.22,-0.28,0,0  
 3M7D,ARG\_37,12.37,-1.66,0,1.53  
 3CS1,ASP\_177,2.01,0.98,-2.78,0  
 1XTZ,HIS\_263,7.89,1.6,0,-0.21  
 3I82,ARG\_35,11.66,-0.84,0,0  
 1R9W,ARG\_349,12.29,-0.21,0,0  
 2GZQ,GLU\_13,3.98,0.28,-0.8,0  
 3LJI,GLU\_74,3.97,2.54,-0.79,-2.29  
 1DZF,HIS\_99,6.5,0,0,0  
 2IXM,LYS\_103,10.5,0,0,0  
 2V81,LYS\_142,10.15,-0.35,0,0  
 2FBI,CYS\_101,9.11,0,0,0.11  
 3H6Q,TYR\_93,10.16,0,0,0.16  
 2HRZ,ARG\_309,11.78,-0.72,0,0  
 1QQE,GLU\_73,4.67,0.21,-0.04,0  
 3EOD,ARG\_20,11.45,-1.05,0,0  
 2W0G,LYS\_242,10.22,-0.28,0,0  
 2Z61,ARG\_347,11.34,-3.24,0,2.08  
 4ANN,LYS\_180,10.5,0,0,0  
 1CBY,GLU\_112,4.5,0,0,0  
 3V4G,ARG\_22,11.94,-0.56,0,0  
 2A0J,GLU\_18,4.08,0.14,-0.56,0  
 3M70,ARG\_199,11.87,-0.63,0,0  
 2PGE,TYR\_351,10.89,0.89,0,0  
 3JSN,ARG\_177,12.08,-0.42,0,0  
 1R3F,GLU\_235,4.71,0.21,0,0  
 3PU6,ARG\_50,11.94,-0.56,0,0  
 1ZHV,CYS\_65,4.8,-3.9,-1.85,1.56  
 3K8U,CYS\_17,3.42,-5.96,-1.6,1.97  
 1RKA,CYS\_63,9.68,-0.28,0.96  
 1OIS,TYR\_270,10.62,0.01,0,0.61  
 3LD1,LYS\_335,10.43,-0.07,0,0  
 2AXQ,ARG\_106,11.73,-0.77,0,0  
 2QEY,GLU\_20,4.26,0.56,-0.8,0  
 3TMO,CYS\_247,9.24,0,0.24  
 3FHF,LYS\_6,10.43,-0.07,0,0  
 2O0K,HIS\_264,6.5,0,0,0  
 2FGG,ASP\_46,4.16,0.63,-0.27,0  
 1ANU,ASP\_133,3.05,0.49,-1.24,0  
 2Q12,LYS\_63,10.5,0,0,0  
 3HST,HIS\_143,3.17,0.06,0,-3.39  
 3TRR,ARG\_100,12.29,-0.21,0,0  
 1UJ8,TYR\_30,10,0,0,0  
 2P5D,TYR\_72,11.17,0.14,0,1.03  
 1D2K,ASP\_337,3.31,0.28,-0.77,0  
 1BGF,LYS\_73,10.5,0,0,0  
 1X04,HIS\_125,7.3,0.8,0,0  
 1ZP2,GLU\_157,4.3,0.07,-0.27,0  
 1J74,LYS\_66,10.36,-0.14,0,0  
 3GMS,ARG\_287,11.94,-0.56,0,0  
 2P4D,TYR\_35,9.86,0.07,-0.21,0  
 2FZP,GLU\_245,3.8,0.56,-1.26,0  
 1ZCU,ASP\_129,3.94,0.14,0,0  
 1XKR,GLU\_104,4.5,0,0,0  
 3CAN,ARG\_127,11.45,-1.05,0,0  
 1QQE,GLU\_237,4.05,0.35,-0.8,0  
 1DUP,ASP\_6,3.72,0,-0.08,0  
 2IF4,GLU\_102,1.5,1.13,-1.73,-2.4  
 1OTM,LYS\_102,10.15,-0.35,0,0  
 2RIS,LYS\_186,10.43,-0.07,0,0  
 3BB7,ASP\_248,4.07,0.28,-0.01,0  
 1YLN,HIS\_64,6.43,0,0,-0.07  
 3EVN,ARG\_25,12.29,-0.21,0,0  
 2IIA,TYR\_51,10.14,0.14,0,0  
 3N2T,GLU\_254,4.5,0,0,0  
 1UOH,GLU\_186,4.57,0.07,0,0  
 2YLF,GLU\_127,3.84,0.14,-0.8,0  
 2NRK,CYS\_31,8.96,-0.7,0.0,66  
 1O17,TYR\_53,9.34,0.14,-0.8,0  
 4E9E,TYR\_566,12.17,0.88,0,1.29  
 1EW4,GLU\_85,4.46,0.14,-0.18,0  
 2ZOM,ARG\_255,11.38,-1.12,0,0  
 3BB7,LYS\_146,10.5,0,0,0  
 2B78,HIS\_283,6.5,0,0,0  
 3CAX,LYS\_223,10.36,-0.14,0,0  
 3CIV,GLU\_81,4.41,0,-0.09,0  
 3EVZ,GLU\_82,2.12,0.98,-3.36,0  
 1YJH,LYS\_6,10.5,0,0,0  
 3GG6,LYS\_40,10.5,0,0,0  
 2PLQ,HIS\_281,6.82,0.74,0,-0.42  
 3LJI,GLU\_261,4.5,0,0,0  
 4EUG,HIS\_67,6.36,0,0,-0.14  
 2BDV,HIS\_46,3.36,0,0,-3.14  
 1X9G,LYS\_147,10.5,0,0,0  
 4E9E,GLU\_533,2.93,0.63,-2.2,0  
 3L7N,ASP\_196,3.02,0.14,-0.92,0  
 2RIS,ARG\_177,12.15,-0.35,0,0  
 3CXS,ASP\_83,4.28,0.56,-0.08,0  
 1RIS,ARG\_162,11.52,-0.98,0,0  
 1TR9,GLU\_232,4.37,0.42,-0.55,0  
 1PSW,ASP\_150,3.34,0.77,-1.23,0  
 1XFK,HIS\_15,6.95,0.59,0,-0.14  
 2RIS,ARG\_177,12.15,-0.35,0,0  
 2X4G,ARG\_44,12.29,-0.21,0,0  
 3EUR,CYS\_40,5.59,-3.47,0.0,0.07  
 3HQX,TYR\_18,10,0,0,0  
 3NBI,GLU\_200,4.57,0.07,0,0  
 2BCF,GLU\_82,4.12,0.42,-0.8,0  
 3CSR,TYR\_153,10.79,0.07,0,0  
 2D2S,LYS\_721,10.5,0,0,0  
 2FZ4,TYR\_87,12.04,0,0.2,0.4  
 2OGQ,ARG\_584,11.94,-0.56,0,0  
 1VSM,ASP\_165,2.85,0.35,-1.3,0  
 1XEU,LYS\_162,10.29,-0.21,0,0  
 4E8B,GLU\_203,2.55,1.05,-3,0  
 1PVT,LYS\_176,9.87,-0.63,0,0  
 2FC3,ASP\_56,3.02,0.84,-1.62,0  
 3ONT,LYS\_64,10.29,-0.21,0,0  
 2CW4,GLU\_116,5.13,0.63,0,0  
 2YXO,ARG\_70,11.59,-0.91,0,0  
 2NMU,CYS\_128,3.14,-6,0.0,14  
 1O17,GLU\_196,3.98,0.28,-0.8,0  
 3G9G,ASP\_197,3.87,0.07,0,0  
 2EFK,ASP\_26,2.49,0.42,-1.73,0  
 2CXV,LYS\_67,10.43,-0.07,0,0  
 2A4D,TYR\_189,10,0,0,0  
 1AK1,TYR\_253,12.92,1.79,-0.8,1.93  
 1T95,ARG\_238,12.08,-0.42,0,0  
 1AK1,ASP\_228,3.94,0.14,0,0  
 3G6S,LYS\_235,10.01,-0.49,0,0  
 1ZCE,GLU\_132,2.71,0.49,-2.28,0  
 1X9G,HIS\_7,6.88,0.59,0,-0.21  
 1Q46,LYS\_34,10.36,-0.14,0,0  
 2Q07,TYR\_272,11.41,0.65,-0.59,1.35  
 2FL7,ARG\_195,12.01,-0.49,0,0  
 1OIS,GLU\_335,2.59,0.49,-2.4,0  
 3CGW,GLU\_185,4.19,0.56,-0.87,0  
 3M9A,LYS\_97,10.5,0,0,0  
 3ETU,TYR\_82,10.79,0.07,-0.8,1.52  
 1XAW,ASP\_479,3.42,0.42,-0.8,0  
 3K1H,ASP\_66,4.01,0.21,0,0  
 1Y2Q,LYS\_47,10.08,-0.42,0,0  
 3QAV,ARG\_55,12.5,0,0,0  
 3P2F,ASP\_50,1.83,0.49,-2.46,0  
 2P0Y,ARG\_214,12.22,-0.28,0,0  
 3QKY,GLU\_95,4.37,0,-0.13,0  
 2AD1,ASP\_278,3.39,0.49,-0.9,0  
 1H09,TYR\_287,11.44,0.04,0,1.4  
 3GV0,GLU\_319,4.71,0.21,0,0  
 2B61,ASP\_62,4.08,0.28,0,0  
 2R57,CYS\_123,7.38,-4.2,0.2,58  
 3PAC,ASP\_70,3.67,0.28,-0.41,0  
 1JSX,HIS\_110,6.5,0,0,0  
 1V43,GLU\_297,4.05,0.35,-0.8,0  
 2QHT,GLU\_26,3.91,0.21,-0.8,0  
 3L3P,ASP\_388,3.42,0.49,-0.87,0  
 3FK5,CYS\_123,7.38,-4.2,0.2,58  
 1J85,ARG\_43,12.15,-0.35,0,0  
 2RJD,LYS\_408,10.43,-0.07,0,0  
 1MTZ,ASP\_73,2.17,0.28,-1.9,0  
 1MHN,LYS\_93,10.43,-0.07,0,0

1ZCU,ARG\_116,11.73,-0.77,0,0  
1OLR,CYS\_216,8.22,-3.48,0.18,2.52  
2HXB,ASP\_25,3.77,0.07,-0.1,0  
3JRT,ASP\_20,3.93,0.21,-0.08,0  
2Q07,LYS\_432,10.5,0,0,0  
1AK1,ARG\_128,13.84,-1.06,0,2.4  
2F8H,ASP\_205,3.88,0.14,-0.06,0  
2Q12,LYS\_172,10.5,0,0,0  
3G6S,ARG\_214,11.94,-0.56,0,0  
1RKA,LYS\_215,10.29,-0.21,0,0  
2F4Q,ARG\_74,12.15,-0.35,0,0  
2R51,LYS\_23,10.36,-0.14,0,0  
4AM1,GLU\_87,4.57,0.07,0,0  
2FXT,ARG\_272,12.29,-0.21,0,0  
2F8H,ARG\_174,12.01,-0.49,0,0  
3VHJ,TYR\_16,10,0,0,0  
1EDG,ASP\_92,3.09,0.35,-1.06,0  
3TRE,HIS\_83,6.29,0,0,-0.21  
2QZQ,LYS\_78,9.87,-0.63,0,0  
2YLF,GLU\_122,3.65,0.49,-1.34,0  
2YT4,TYR\_530,10.65,0.65,0,0  
2WOZ,HIS\_493,4.05,0.8,-0.67,-2.58  
1O59,GLU\_255,4.57,0.07,0,0  
1R5Q,GLU\_52,4.64,0.14,0,0  
3N2T,ASP\_310,3.2,0.35,-0.96,0  
1OTM,LYS\_139,10.5,0,0,0  
1BN6,ASP\_277,3.25,0.49,-1.04,0  
3T8R,LYS\_20,10.29,-0.21,0,0  
2Q5X,ARG\_840,12.29,-0.21,0,0  
1VSM,LYS\_191,10.29,-0.21,0,0  
3F53,LYS\_51,10.43,-0.07,0,0  
1QZN,ASP\_132,3.07,0.35,-1.07,0  
2F9F,ARG\_162,12.01,-0.49,0,0  
3HYQ,LYS\_149,10.5,0,0,0  
3LJC,LYS\_218,10.29,-0.21,0,0  
4AF2,ASP\_57,3.43,0.42,-0.79,0  
2F8H,ASP\_149,3.94,0.21,-0.07,0  
3B21,CYS\_70,11.24,-0.69,0,2.93  
3V5S,LYS\_557,10.43,-0.07,0,0  
2BAA,TYR\_125,8.66,1.98,-0.92,-2.4  
2EFK,ASP\_218,3.25,0.21,-0.76,0  
1DUP,ASP\_32,3.28,0.28,-0.8,0  
2VAN,ASP\_321,3.89,0.14,-0.05,0  
3RE9,GLU\_242,4.5,0,0,0  
3ZXV,ASP\_92,2.27,0.56,-2.09,0  
1SUU,LYS\_773,10.22,-0.28,0,0  
1L2F,LYS\_274,10.15,-0.35,0,0  
1XIP,TYR\_277,13.43,3.01,-0.05,0.47  
1DVO,ARG\_122,11.87,-0.63,0,0  
1JYH,ASP\_53,1.56,0.98,-3.21,0  
2A6B,HIS\_137,3.07,0.57,-1.65,-2.35  
3PBH,TYR\_151,11.99,1.67,-0.02,0.34  
2POY,ASP\_127,3.66,0,-0.14,0  
4ESS,LYS\_40,9.73,-0.77,0,0  
1ZBP,TYR\_116,10.07,0.07,0,0  
4DND,ARG\_55,12.08,-0.42,0,0  
1KCM,TYR\_190,10,0,0,0  
1SNT,ARG\_172,11.8,-0.7,0,0  
1LZL,GLU\_176,4.64,0.14,0,0  
3Q1C,CYS\_279,9.07,0,0,0.07  
2E3S,LYS\_402,10.43,-0.07,0,0  
2I6I,LYS\_155,10.5,0,0,0  
2A4D,TYR\_219,8.76,0.21,-1.45,0  
4ETX,ARG\_207,11.8,-0.7,0,0  
4DIU,GLU\_149,3.91,0.21,-0.8,0  
1PVT,GLU\_216,4.64,0.14,0,0  
3DSH,LYS\_299,10.43,-0.07,0,0  
3PU6,ARG\_13,12.08,-0.42,0,0  
3CZC,GLU\_35,4.71,0.21,0,0  
2Q12,ASP\_29,3.35,0.35,-0.8,0  
3IV4,ASP\_48,3.8,0,0,0  
1XKR,GLU\_89,4.18,0.21,-0.53,0  
3LMF,GLU\_54,4.5,0,0,0  
2V81,CYS\_170,10.29,-0.18,0,1.47  
1V43,ARG\_138,12.22,-0.28,0,0  
4ETX,ARG\_423,12.15,-0.35,0,0  
2AHE,ASP\_152,2.56,0.98,-2.22,0  
1Ri6,GLU\_262,4.5,0,0,0  
2QV2,TYR\_189,10,0,0,0  
3M7D,GLU\_89,4.41,0.28,-0.37,0  
1M5I,ARG\_141,12.22,-0.28,0,0  
3B21,CYS\_212,6.84,-2.3,0,0.14  
3Q1C,GLU\_47,4.85,0.42,-0.07,0  
2Y2T,CYS\_29,9,0,0,0  
1RAJ,HIS\_413,7.35,0.92,0,-0.07  
2H14,LYS\_207,9.8,-0.7,0,0  
4DEZ,ARG\_20,11.87,-0.63,0,0  
1MUF,GLU\_151,4.5,0,0,0  
1FO9,TYR\_228,10.36,0.28,0,0.08  
1P1L,CYS\_30,8.37,-0.77,0,0.14  
3CS1,LYS\_79,10.36,-0.14,0,0  
2FL4,GLU\_138,4.82,1.12,-0.8,0  
1X9G,HIS\_110,6.36,0,-0.14  
2R57,ARG\_234,9.83,-2.67,0,0  
1LZL,GLU\_64,3.64,0.07,-0.93,0  
1X1E,HIS\_76,2.38,1.09,-0.04,-5.17  
1TXJ,LYS\_116,10.43,-0.07,0,0  
3R2E,LYS\_40,10.29,-0.21,0,0  
3AU3,LYS\_534,10.5,0,0,0  
1X7F,ARG\_168,11.66,-0.84,0,0  
1FHL,TYR\_214,12.8,1.78,0,1.02  
3H8Y,GLU\_87,4.5,0,0,0  
1QE,LYS\_186,10.5,0,0,0  
1WLJ,LYS\_114,10.5,0,0,0  
1LN4,GLU\_42,3.85,0.14,-0.79,0  
1WRU,CYS\_64,12.63,0.32,1.32,1.98  
3B79,GLU\_97,2.83,0.14,-1.81,0  
2B78,GLU\_178,1.91,3.1,-2.48,-3.21  
4E6S,CYS\_34,9,0,0,0  
3JRT,LYS\_45,10.5,0,0,0  
3ADO,LYS\_54,10.36,-0.14,0,0  
1YG2,ARG\_93,12.36,-0.14,0,0  
1Y0K,ARG\_170,13.72,-1.18,0,2.4  
4HDE,CYS\_73,6.96,-3.6,0.22,1.34  
1WXQ,LYS\_347,10.01,-0.49,0,0  
3B21,ASP\_40,3.8,0,0,0  
1JYH,GLU\_132,5.22,2.77,-2.04,0  
2Q99,ARG\_366,11.87,-0.63,0,0  
2D7J,LYS\_98,10.36,-0.14,0,0  
2QOP,CYS\_117,7.6,-1.85,0,0.45  
1O5T,TYR\_329,9.55,0.7,-1.15,0  
1UCH,LYS\_74,10.08,-0.42,0,0  
2B6P,TYR\_89,9.71,1.32,-0.9,-0.71  
3ELI,ASP\_89,3.81,0.14,-0.13,0  
1NFN,ARG\_92,12.08,-0.42,0,0  
1TP6,TYR\_118,12.55,0.07,0.38,2.11  
1XFK,HIS\_184,4.36,0,0,-2.14  
3ANJ,TYR\_222,10,0,0,0  
3GYW,LYS\_45,10.5,0,0,0  
2DG7,GLU\_53,3.39,0.35,-1.47,0  
3BQE,CYS\_349,7.11,-2.25,0,0.37  
3CIV,CYS\_98,9.34,0,0,0.34  
3F7M,ASP\_202,1.71,1.05,-3.14,0  
3US6,LYS\_82,10.43,-0.07,0,0  
2IF4,LYS\_165,10.5,0,0,0  
1AD6,LYS\_475,10.5,0,0,0  
3RVC,ASP\_139,3.48,0.21,-0.53,0  
3EVZ,LYS\_185,9.8,-0.7,0,0  
2EEY,LYS\_82,10.43,-0.07,0,0  
4F85,ARG\_147,12.08,-0.42,0,0  
3V3T,TYR\_238,11.67,1.67,0,0  
1UOH,TYR\_199,13.27,0.07,0.8,2.4  
4DBX,TYR\_186,11.26,0,-0.16,1.42  
2D0A,ARG\_182,11.86,-0.64,0,0  
3RJZ,LYS\_229,10.01,-0.49,0,0  
1GXN,ARG\_413,11.66,-0.84,0,0  
3NBI,LYS\_183,10.01,-0.49,0,0  
2E3I,LYS\_115,10.22,-0.28,0,0  
1O59,LYS\_305,10.29,-0.21,0,0  
2NYC,ARG\_219,12.08,-0.42,0,0  
2BOJ,ASP\_164,3.23,0.28,-0.85,0  
4H4J,LYS\_251,10.43,-0.07,0,0  
1KCM,ASP\_107,3.94,0.14,0,0  
3LPZ,ASP\_213,3.35,0.35,-0.8,0  
3T57,CYS\_138,7.44,-0.88,-1.12,0.43  
1EDG,TYR\_325,10.3,0.56,-0.26,0  
3I47,TYR\_175,10,0,0,0  
3AU3,CYS\_447,9.21,0,0,0.21  
1MML,LYS\_258,10.43,-0.07,0,0  
2HP7,GLU\_147,2.9,0.77,-2.37,0  
1ZP2,TYR\_139,10.34,1.99,-1.65,0  
3BB7,LYS\_205,10.43,-0.07,0,0  
3EVP,LYS\_284,10.43,-0.07,0,0  
2BCF,ARG\_114,12.15,-0.35,0,0  
2AZL,LYS\_34,10.01,-0.49,0,0  
2IN0,GLU\_434,4.52,1.64,-1.62,0  
3IL3,GLU\_74,4.53,0.49,-0.45,0  
2YWX,ARG\_32,12.22,-0.28,0,0  
3EVN,HIS\_252,6.36,0,0,-0.14  
1X1E,ASP\_233,2.05,0.91,-2.66,0  
1ZBS,HIS\_239,3.77,0,0,-2.73  
3G9T,ASP\_242,2.57,0.49,-1.72,0  
3D9H,ASP\_133,3.47,0.28,-0.61,0  
3JZN,ARG\_287,12.08,-0.42,0,0  
1RWZ,ARG\_222,13.83,-1.07,0,2.4  
2H8O,HIS\_143,6.59,0.44,0,-0.35  
4AM1,LYS\_42,10.15,-0.35,0,0  
2IN0,GLU\_86,3.97,0.14,-0.67,0  
1SIG,LYS\_220,10.15,-0.35,0,0  
4F3J,TYR\_218,9.88,0,-0.12,0  
1TR9,HIS\_161,2.6,1.6,-1.41,-4.09  
4H4J,GLU\_53,4.5,0,0,0  
3M3P,ASP\_202,2.99,0.35,-1.16,0  
2F8H,HIS\_51,9.33,3.6,1.98,-2.75  
1IAP,LYS\_90,10.5,0,0,0  
1N81,LYS\_149,9.8,-0.7,0,0  
3I0C,GLU\_215,4.71,0.21,0,0  
2AZP,ASP\_126,1.23,0.63,-3.2,0  
4EKU,GLU\_342,3.81,1.54,0,-2.23  
3GW3,CYS\_308,8.74,-0.33,0,0.07  
3LPZ,ASP\_299,3.69,0.42,-0.53,0  
1DVO,LYS\_118,10.5,0,0,0  
1XTZ,ASP\_176,3.49,0.56,-0.87,0  
3LH5,LYS\_553,10.36,-0.14,0,0  
3G9G,ASP\_66,3.11,0.49,-1.18,0  
4F85,ARG\_149,12.01,-0.49,0,0  
2O4D,ARG\_135,12.01,-0.49,0,0  
1RL0,ARG\_60,12.15,-0.35,0,0  
3MIX,ASP\_416,3.31,0.07,-0.56,0  
2P5D,GLU\_98,4.57,0.07,0,0  
2YT4,CYS\_535,7.53,-1.47,0,0  
3E5T,HIS\_216,6.63,0.2,0,-0.07  
1EV8,ARG\_53,12.08,-0.42,0,0  
1VJG,LYS\_6,10.29,-0.21,0,0  
3E5T,ASP\_223,3.72,0,-0.08,0  
3BB7,ASP\_200,3.15,0.35,-1.0  
1G8P,GLU\_157,3.91,0.21,-0.8,0  
1T95,ARG\_63,12.29,-0.21,0,0  
2H8O,ARG\_187,12.43,-0.07,0,0  
3PZ9,ARG\_160,11.87,-0.63,0,0  
3KEY,GLU\_394,3.93,0.21,-0.78,0  
1Z3X,ASP\_180,3.76,0,-0.04,0  
3ETV,TYR\_93,11.01,1.01,0,0  
2P4D,ASP\_61,3.49,0.28,-0.59,0  
4FD6,LYS\_38,10.01,-0.49,0,0  
1TLV,ASP\_113,3.85,0.07,-0.02,0  
2FG1,LYS\_55,10.5,0,0,0  
2B61,ASP\_161,3.21,0.21,-0.8,0  
1Q46,LYS\_66,10.15,-0.35,0,0  
1Q2Y,LYS\_75,10.5,0,0,0  
3EJC,CYS\_142,9.71,-0.56,0,1.27  
2Q34,LYS\_63,9.94,-0.56,0,0  
1V43,ASP\_83,4.12,0.35,-0.03,0  
2YWX,LYS\_351,12.15,-0.35,0,0  
1AD6,GLU\_466,4.5,0,0,0  
3BA1,ARG\_117,12.43,-0.07,0,0  
3CX5,ASP\_91,4.21,0.49,-0.08,0  
3U4K,ASP\_43,3.54,0.07,-0.33,0  
2QV2,ARG\_11,12.5,0,0,0  
4FH3,LYS\_117,10.36,-0.14,0,0  
3AU3,HIS\_492,6.59,0.09,0,0  
3OKQ,LYS\_602,10.29,-0.21,0,0  
3J1V,ASP\_82,2.91,0.14,-1.04,0  
3ERF,GLU\_150,4.5,0,0,0  
2ZCO,HIS\_92,5.29,0,0,-1.21  
1EYH,LYS\_117,10.36,-0.14,0,0  
3CIV,CYS\_254,5.66,-3.34,0,0  
2X4G,ARG\_279,12.5,0,0,0  
1OTM,LYS\_143,10.22,-0.28,0,0  
3LJC,LYS\_223,10.5,0,0,0  
1P2F,ARG\_182,12.5,0,0,0  
1WXQ,LYS\_346,10.22,-0.28,0,0  
4FCU,HIS\_3,5.03,1.6,0,-3.07  
4F3J,TYR\_152,10,0,0,0  
2R4Q,LYS\_234,10.08,-0.42,0,0  
1XKR,GLU\_158,5.22,0.49,0.23,0  
1DZF,GLU\_85,4.64,0.14,0,0  
2AZL,ARG\_88,11.8,-0.7,0,0  
1VJG,HIS\_73,6.43,0,0,-0.07  
2E3C,LYS\_293,10.5,0,0,0  
3PM2,GLU\_115,4.23,0.21,-0.48,0  
2H14,LYS\_227,10.36,-0.14,0,0  
3ZTA,ASP\_47,2.75,1.12,-2.17,0  
4H89,ARG\_79,12.29,-0.21,0,0  
1AD6,GLU\_428,4.71,0.21,0,0  
1X9G,LYS\_125,10.01,-0.49,0,0  
2Z0M,LYS\_32,10.22,-0.28,0,0  
3I47,ASP\_224,2.46,0.42,-1.76,0  
3KT2,HIS\_69,6.5,0,0,0  
1BGF,LYS\_93,10.22,-0.28,0,0  
1KCM,LYS\_50,10.36,-0.14,0,0  
3FFM,ASP\_89,3.94,0.14,0,0  
3GV0,LYS\_310,10.29,-0.21,0,0  
2R0S,TYR\_94,10,0,0,0  
1R7J,ASP\_46,4.01,0.35,-0.14,0  
2EFK,ARG\_199,12.29,-0.21,0,0  
1V43,GLU\_133,3.85,0.28,-0.93,0  
2BLL,HIS\_379,3.69,0,0,-2.81  
2ZQ5,GLU\_259,3.88,0.42,-1.04,0  
2JHY,TYR\_128,10.82,2.42,-1.6,0  
3TRE,LYS\_108,10.15,-0.35,0,0  
1U7U,GLU\_258,4.71,0.21,0,0  
3LH5,TYR\_588,10,0,0,0  
3K8J,TYR\_128,9.27,0.07,-0.8,0  
1T07,ARG\_53,12.08,-0.42,0,0  
1R7J,ARG\_51,12.01,-0.49,0,0

1X9G,GLU\_97,4.71,0.21,0,0  
2A6B,HIS\_31,4.4,0.8,0,-2.9  
3M7G,LYS\_116,10.01,-0.49,0,0  
4FCU,HIS\_132,6.43,0,0,-0.07  
2E0T,LYS\_183,10.43,-0.07,0,0  
3EJC,LYS\_48,10.36,-0.14,0,0  
1H4U,HIS\_536,7.16,0.8,0,-0.14  
2D59,LYS\_119,10.08,-0.42,0,0  
2QVO,LYS\_69,9.87,-0.63,0,0  
1QQH,GLU\_171,2.73,0.63,-2.4,0  
2WOZ,GLU\_395,4.33,1.31,-1.48,0  
3M7D,HIS\_260,7.23,0.8,0,-0.07  
2OJQ,ASP\_467,4.02,0.49,-0.27,0  
1XDZ,LYS\_202,10.15,-0.35,0,0  
3EVZ,TYR\_178,9.66,0,-0.34,0  
3DTE,ASP\_106,3.2,0.07,-0.67,0  
3K9I,LYS\_157,10.22,-0.28,0,0  
1Q8B,LYS\_76,10.5,0,0,0  
3OKQ,LYS\_641,10.29,-0.21,0,0  
3BCY,HIS\_46,6.29,0,0,-0.21  
3B4D,LYS\_213,10.5,0,0,0  
1EDG,LYS\_373,10.36,-0.14,0,0  
2CW4,TYR\_16,8.03,0.14,-2.11,0  
1XTD,LYS\_150,10.5,0,0,0  
3GYW,GLU\_61,4.71,0.21,0,0  
3EVN,ARG\_7,11.94,-0.56,0,0  
1YR6,GLU\_92,4.36,0.66,-0.8,0  
3HUE,ASP\_213,3.71,0,-0.09,0  
3H04,LYS\_137,10.22,-0.28,0,0  
3Q2C,HIS\_36,5.6,0.2,0,-1.1  
1R5Q,TYR\_96,9.31,0,-0.69,0  
4DND,ASP\_84,3.91,0.14,-0.03,0  
3ANJ,ARG\_22,12.01,-0.49,0,0  
1UXO,LYS\_127,10.36,-0.14,0,0  
2YWJ,ASP\_39,2.92,0.35,-1.23,0  
2Q13,LYS\_70,10.29,-0.21,0,0  
1TR9,TYR\_213,8.65,0.14,-1.49,0  
2HXB,HIS\_128,4.68,0.88,0,-2.7  
1RHS,GLU\_165,2.76,0.42,-2.16,0  
3ETU,ASP\_174,3.46,0.49,-0.83,0  
1P6F,GLU\_83,4.64,0.14,0,0  
3BA1,ARG\_127,12.29,-0.21,0,0  
3T5B,ASP\_135,3.72,0,-0.08,0  
1OSJ,LYS\_61,10.08,-0.42,0,0  
1X04,GLU\_104,4.6,0.14,-0.04,0  
3C6B,TYR\_119,10.62,0.21,0,0.41  
2F8H,ARG\_95,11.8,-0.7,0,0  
2YYO,ARG\_91,12.43,-0.07,0,0  
1WXF,ARG\_263,11.94,-0.56,0,0  
3UAH,HIS\_228,5.45,0.1,-2.15  
3E5T,HIS\_118,6.36,0,0,-0.14  
1EV8,LYS\_235,10.29,-0.21,0,0  
3UOV,HIS\_138,3.74,0,0,-2.76  
1TD6,ARG\_66,11.87,-0.63,0,0  
3M66,GLU\_292,4.57,0.07,0,0  
2G3A,ARG\_35,12.01,-0.49,0,0  
1UAJ,ARG\_220,12.36,-0.14,0,0  
3MIX,ASP\_609,3.8,0,0,0  
2G2D,ASP\_40,3.87,0.07,0,0  
1XIP,LYS\_81,10.5,0,0,0  
1WJG,ARG\_57,12.43,-0.07,0,0  
1TD6,GLU\_221,4.71,0.21,0,0  
3LD1,LYS\_78,10.29,-0.21,0,0  
4H4J,ARG\_122,11.59,-0.91,0,0  
2CL3,HIS\_87,7.16,0.8,0,-0.14  
2ZCX,ARG\_208,12.36,-0.14,0,0  
3AU3,TYR\_486,10.42,0.21,0,0.2  
1FQI,GLU\_302,4.19,0.14,-0.45,0  
3E5T,LYS\_25,10.5,0,0,0  
3H5T,ARG\_32,12.08,-0.42,0,0  
1FKM,ARG\_329,12.5,0,0,0  
2OGQ,ARG\_396,12.22,-0.28,0,0  
4F85,CYS\_129,8.82,-0.82,0,0.64  
1WYC,ARG\_99,11.73,-0.77,0,0  
1P4X,GLU\_16,3.22,1.92,-0.8,-2.4  
2Z61,TYR\_185,10,0,0,0  
3F6F,GLU\_185,3.91,0.21,-0.8,0  
1TLV,ARG\_252,12.43,-0.07,0,0  
1MTZ,TYR\_170,9.39,0.99,-1.6,0  
2VGM,LYS\_243,10.43,-0.07,0,0  
3T5B,ARG\_221,12.22,-0.28,0,0  
3EZ7,LYS\_240,9.45,-1.05,0,0  
2OKT,HIS\_339,7.24,0.74,0,0  
1X7F,GLU\_342,4.5,0,0,0  
3BWT,GLU\_642,4.57,0.07,0,0  
2XHC,LYS\_73,10.5,0,0,0  
2CXA,GLU\_176,3.86,0.42,-1.06,0  
3FTT,TYR\_71,9.16,1.11,-0.3,-1.66  
4F3J,ASP\_213,3.8,0,0,0  
2NRK,ARG\_122,9.18,-0.99,0,-2.33  
3T8R,GLU\_91,4.5,0,0,0  
4H4J,GLU\_160,4.59,0.14,-0.05,0  
1SNT,ARG\_314,12.29,-0.21,0,0  
3P51,ASP\_103,2.95,0.63,-1.48,0  
3M66,HIS\_172,6.76,0.61,0,-0.35  
1LN4,HIS\_10,6.37,0.01,0,-0.14  
3LJN,LYS\_19,10.36,-0.14,0,0  
1IAP,ARG\_183,12.22,-0.28,0,0  
1A8Q,GLU\_150,3.14,0.7,-2.06,0  
1ZCE,ARG\_119,12.43,-0.07,0,0  
1HF8,ARG\_261,11.94,-0.56,0,0  
1T07,LYS\_37,10.36,-0.14,0,0  
4DEZ,ARG\_69,12.29,-0.21,0,0  
1ZYL,ARG\_40,12.29,-0.21,0,0  
1TD6,GLU\_68,5.61,1.11,0,0  
1RKA,LYS\_154,10.36,-0.14,0,0  
3GS9,TYR\_160,13.82,1.18,-0.17,2.81  
1Q8B,GLU\_67,5.5,1.73,-0.73,0  
3CO1,LYS\_98,10.43,-0.07,0,0  
2AXO,LYS\_171,10.5,0,0,0  
1QYI,LYS\_64,10.43,-0.07,0,0  
2GZQ,TYR\_69,10,0,0,0  
1NRI,TYR\_226,12.74,0.07,0.57,2.1  
1DUP,HIS\_76,6.5,0,0,0  
2GQV,TYR\_69,10.35,0.35,0,0  
3T5B,ARG\_244,12.29,-0.21,0,0  
1FQI,LYS\_290,10.01,-0.49,0,0  
3GE9,ARG\_190,11.94,-0.56,0,0  
1ILW,GLU\_63,4.52,0.28,-0.26,0  
2IF4,CYS\_253,9.41,-0.05,-0.72,1.18  
1GXN,LYS\_485,10.5,0,0,0  
3P28,ARG\_74,11.87,-0.63,0,0  
2G2D,TYR\_107,10.53,0.28,0,0.25  
3V55,LYS\_466,10.22,-0.28,0,0  
1AKO,GLU\_34,2.48,2.1,-1.87,-2.25  
2H2Z,CYS\_16,10.45,0,0,1.45  
3P28,LYS\_78,10.43,-0.07,0,0  
2GYZ,ARG\_6,12.08,-0.42,0,0  
1TJE,LYS\_137,10.29,-0.21,0,0  
3ASA,ARG\_244,12.43,-0.07,0,0  
3K8U,GLU\_40,4.5,0,0,0  
2CBE,ASP\_165,3.8,0,0,0  
2WB8,ASP\_709,3.77,0,-0.03,0  
1O6D,CYS\_30,10.05,0,0,1.05  
1X1E,ARG\_212,12.08,-0.42,0,0  
3HUE,GLU\_263,4.5,0,0,0  
1IDK,ARG\_236,13.8,-2.11,0,3.4  
4FLE,TYR\_124,10.02,0,0,0.02  
3B4D,ASP\_233,2.87,0.42,-1.35,0  
3RRQ,GLU\_141,4.14,0.42,-0.78,0  
2OPJ,GLU\_151,4.5,0,0,0  
1O9G,ARG\_215,11.94,-0.56,0,0  
1WP5,GLU\_225,4.64,0.14,0,0  
2H2W,TYR\_240,9.97,0,-0.03,0  
4DIU,ASP\_198,2.69,0.49,-1.6,0  
2X5Y,GLU\_795,4.5,0,0,0  
2NRR,ARG\_410,12.15,-0.35,0,0  
4DNU,GLU\_375,4.57,0.07,0,0  
3RFY,LYS\_158,10.5,0,0,0  
2CL3,ARG\_221,12.08,-0.42,0,0  
3LMO,GLU\_58,4.5,0,0,0  
2W25,LYS\_176,10.5,0,0,0  
4FLE,ASP\_102,4.01,0.21,0,0  
1R3F,GLU\_171,3.52,0.42,-1.4,0  
1PSW,ASP\_293,3.22,0.14,-0.72,0  
2E3I,ARG\_63,11.59,-0.91,0,0  
2Z84,TYR\_41,10.68,0.35,-1.7,2.01  
3BPV,ARG\_95,12.43,-0.07,0,0  
1V8E,GLU\_176,4.5,0,0,0  
4GCO,TYR\_166,10.91,0.84,-0.8,0.87  
1R29,GLU\_99,3.56,0.28,-1.21,0  
3DSH,ASP\_430,3.8,0,0,0  
3RFY,ARG\_393,12.22,-0.28,0,0  
1AIL,ASP\_29,2.9,0.42,-1.33,0  
2F4Q,ASP\_296,3.92,0.28,-0.16,0  
1ZBM,HIS\_-2,6.29,0,0,-0.21  
1TR9,GLU\_180,4.05,0.35,-0.8,0  
1SNT,HIS\_132,6.15,0,0,-0.35  
1UOH,LYS\_189,10.5,0,0,0  
2DFL,LYS\_163,10.5,0,0,0  
3A0X,CYS\_721,9.22,-1.38,0,1.59  
2F4Q,TYR\_51,11.13,0,0,1.13  
2A0J,ARG\_84,11.8,-0.7,0,0  
3UAH,ASP\_200,2.59,0.49,-1.7,0  
3CNS,CYS\_132,8.85,-0.22,0,0.07  
3JV1,ARG\_149,11.52,-0.98,0,0  
1U3Y,LYS\_249,10.22,-0.28,0,0  
3RKV,GLU\_209,3.95,0.42,-0.97,0  
3BQW,LYS\_90,10.22,-0.28,0,0  
4DIU,LYS\_230,10.15,-0.35,0,0  
3CXS,HIS\_34,6.5,0,0,0  
1NWA,ARG\_-1,12.5,0,0,0  
1Ri6,GLU\_176,4.5,0,0,0  
3ADO,LYS\_104,10.5,0,0,0  
3C5V,GLU\_239,4.5,0,0,0  
3CAN,LYS\_86,10.43,-0.07,0,0  
2ZCX,HIS\_200,6.5,0,0,0  
1R9W,ASP\_228,3.74,0.28,-0.34,0  
3K8J,LYS\_91,10.5,0,0,0  
4E9E,LYS\_480,10.43,-0.07,0,0  
3GEC,ARG\_394,11.94,-0.56,0,0  
1NJ4,ASP\_337,3.56,0.56,-0.8,0  
3AU3,HIS\_464,6.56,0.06,0,0  
2OBI,LYS\_151,10.15,-0.35,0,0  
4DEZ,ARG\_150,12.31,-2.32,0,2.13  
2F8H,ASP\_229,3.46,0.28,-0.62,0  
1TWU,ASP\_23,3.85,0.07,-0.02,0  
2A1V,LYS\_126,10.5,0,0,0  
2PWQ,GLU\_21,3.74,0.28,-1.05,0  
2ZQ5,TYR\_317,9.75,0,-0.25,0  
2F4Q,ASP\_82,3.6,0.21,-0.41,0  
3M66,LYS\_168,10.22,-0.28,0,0  
2Q34,TYR\_125,13.13,1.84,-0.01,1.31  
1D2K,LYS\_369,10.5,0,0,0  
1NAF,ARG\_299,12.5,0,0,0  
1N81,ARG\_100,12.07,-3.51,0,3.08  
4DNU,ASP\_380,2.86,0.49,-1.43,0  
2AZL,TYR\_39,10.41,0.3,-0.69,0.81  
1U7U,ASP\_203,3.43,1.26,-1.63,0  
2YWJ,GLU\_112,3.98,0.28,-0.8,0  
2FG1,HIS\_114,7.27,0.84,0,-0.07  
2BQQ,LYS\_140,10.5,0,0,0  
2GAU,LYS\_39,10.43,-0.07,0,0  
1WRU,GLU\_171,4.28,0.42,-0.63,0  
100X,LYS\_220,10.22,-0.28,0,0  
2C13,CYS\_221,9.73,-2.17,0,2.9  
3EGN,LYS\_425,10.36,-0.14,0,0  
2ILR,ARG\_290,12.22,-0.28,0,0  
1X04,ARG\_38,12.01,-0.49,0,0  
3RJX,HIS\_226,5.75,1.6,4.72,-7.08  
3OA7,HIS\_563,6.43,0,0,-0.07  
1O59,LYS\_237,10.29,-0.21,0,0  
3OOP,LYS\_100,10.5,0,0,0  
3AU3,GLU\_460,4.5,0,0,0  
1T3Y,CYS\_10,8.71,-0.78,0,0.49  
2F19,ASP\_19,3.75,0.21,-0.27,0  
3M70,TYR\_249,11.61,2.43,-0.82,0  
3H6Q,ARG\_160,11.66,-0.84,0,0  
1X04,ASP\_147,2.05,0.63,-2.38,0  
3RFF,GLU\_49,4.31,0.56,-0.76,0  
2WB8,ASP\_592,3.25,0.49,-1.05,0  
1J74,GLU\_17,4.58,0.21,-0.13,0  
2FM9,LYS\_146,10.29,-0.21,0,0  
3H13,GLU\_241,4.02,0.21,-0.69,0  
3I4T,GLU\_70,3.98,0.28,-0.8,0  
4E8B,ASP\_51,3.69,0.28,-0.39,0  
3RFF,HIS\_17,2.01,0,0,-4.49  
1ZBM,ASP\_133,3.94,0.14,0,0  
3T8R,TYR\_9,10,0,0,0  
2V4X,LYS\_23,10.43,-0.07,0,0  
3A2Z,HIS\_152,3.66,0,0,-2.84  
1TR9,ASP\_142,4.83,0.8,0,-2.47  
3F5D,LYS\_87,10.5,0,0,0  
1PSW,TYR\_200,10,0,0,0  
3NZL,TYR\_73,11.3,0.07,0,1.23  
2HXB,ASP\_10,3.86,0.14,-0.08,0  
1G8P,ARG\_142,12.22,-0.28,0,0  
2WOZ,GLU\_577,4.42,0.14,-0.22,0  
3P51,HIS\_25,7.28,0.85,0,-0.07  
1IAP,CYS\_77,12,0,1.11,1.89  
1F2V,ASP\_26,2.89,0.14,-1.04,0  
1ZBM,TYR\_232,11.95,2.09,-0.63,0.48  
3TMO,GLU\_323,3.98,0.28,-0.8,0  
2XWS,LYS\_99,9.87,-0.63,0,0  
2FBI,LYS\_97,10.36,-0.14,0,0  
1G8P,GLU\_176,3.89,0.14,-0.74,0  
3GW3,ASP\_239,3.22,0.35,-0.93,0  
2XJ4,LYS\_168,10.5,0,0,0  
2FG1,GLU\_58,4.64,0.14,0,0  
2B2H,LYS\_83,10.5,0,0,0  
2PLQ,ASP\_40,3.84,0.14,-0.1,0  
1R3D,GLU\_66,4.57,0.07,0,0  
1P6F,ASP\_93,2.87,0.49,-1.42,0  
4AM1,GLU\_254,4.64,0.14,0,0  
2H01,HIS\_157,6.36,0,0,-0.14  
3ZXY,ASP\_27,2.64,0.77,-1.94,0  
2AHE,ARG\_250,12.36,-0.14,0,0  
3LPZ,ASP\_321,3.86,0.07,-0.01,0  
3GEC,GLU\_431,4.62,0.14,-0.02,0  
2YX0,ARG\_38,11.8,-0.7,0,0  
4HDE,LYS\_85,10.5,0,0,0  
1R5Q,TYR\_81,10,0,0,0  
3JRT,ARG\_62,11.73,-0.77,0,0  
2IF4,TYR\_246,12.84,0.07,0.37,2.4  
2D59,ARG\_21,12.08,-0.42,0,0  
1PBV,HIS\_127,6.43,0,0,-0.07

1S1G,LYS\_393,10.36,-0.14,0,0  
 3ADO,GLU\_212,4.5,0,0,0  
 3DZ1,ASP\_115,3.66,0.14,-0.28,0  
 200K,ARG\_202,11.83,-0.67,0,0  
 2CIU,TYR\_213,13.13,0.21,0.52,2.4  
 2F8H,CYS\_137,3.21,-8.07,0.47,1.81  
 1N81,GLU\_148,2.52,0.42,-2.4,0  
 1T3Y,ASP\_6,2.81,0.35,-1.34,0  
 3K8J,GLU\_181,3.76,0.86,-1.6,0  
 1W7B,LYS\_119,10.5,0,0,0  
 2X5Y,GLU\_781,3.05,0.28,-1.73,0  
 2Q07,LYS\_525,10.15,-0.35,0,0  
 1X1E,GLU\_193,4.57,0.07,0,0  
 2FZ4,ARG\_104,12.29,-0.21,0,0  
 3ONH,ASP\_451,1.94,0.77,-2.64,0  
 2QOP,ARG\_106,12.79,-2.11,0.2,4  
 3L0D,ASP\_141,3.8,0,0,0  
 1PBV,ARG\_239,12.5,0,0,0  
 3FFM,ARG\_146,11.94,-0.56,0,0  
 2CVB,LYS\_78,10.36,-0.14,0,0  
 2OSA,ASP\_440,2.54,0.35,-1.61,0  
 2PPN,ARG\_40,13.3,-1.6,0,2.4  
 4F8A,ARG\_674,12.08,-0.42,0,0  
 2Q5X,TYR\_849,10.38,0.39,-0.01,0  
 2IRM,ASP\_37,3.34,0.42,-0.88,0  
 1O59,GLU\_72,4.57,0.71,-0.64,0  
 3GT0,ARG\_197,11.87,-0.63,0,0  
 3F1X,GLU\_286,4.23,0.21,-0.48,0  
 1ZP2,LYS\_67,10.01,-0.49,0,0  
 3L3P,ASP\_363,1.88,0.63,-2.55,0  
 1JKS,GLU\_113,2.4,0.63,-2.72,0  
 3FXH,LYS\_92,10.29,-0.21,0,0  
 2P65,HIS\_125,4.19,0.07,0,-2.38  
 3J5N,ASP\_186,3.87,0.07,0,0  
 1PDB,GLU\_183,4.78,0.28,0,0  
 3I47,ASP\_46,3.27,0.63,-1.16,0  
 4H4J,TYR\_179,12.28,0,2.28  
 3CJW,HIS\_175,6.36,0,0,-0.14  
 1NIJ,ASP\_236,2.94,0.91,-1.76,0  
 2CXI,LYS\_3,10.5,0,0,0  
 1WP5,HIS\_322,7.02,0.8,0,-0.28  
 3E5T,HIS\_72,5.65,2.19,1.08,-4.12  
 1G8P,GLU\_347,4.71,0.42,-0.21,0  
 3LH5,LYS\_629,10.5,0,0,0  
 2F9F,CYS\_88,8.22,-0.81,-2.32,2.35  
 1QYI,ARG\_58,13.69,-0.32,0,1.51  
 1YR6,ASP\_168,3.0,84,-1.65,0  
 2A6B,ASP\_134,2.48,0.56,-1.88,0  
 3E5T,ASP\_31,3.35,0.35,-0.8,0  
 3IRA,GLU\_65,4.64,0.14,0,0  
 2D8N,TYR\_32,10,0,0,0  
 2I6I,LYS\_151,10.5,0,0,0  
 4EVF,TYR\_214,10.15,0.15,0,0  
 4H86,LYS\_47,10.29,-0.21,0,0  
 1PVT,TYR\_39,12.54,0.21,0.8,1.53  
 2QEV,TYR\_127,11.51,0.12,0,1.39  
 1YDL,LYS\_32,9.94,-0.56,0,0  
 3F6M,GLU\_14,4.5,0,0,0  
 3GT0,LYS\_43,10.29,-0.21,0,0  
 3C6B,ASP\_92,3.73,0.07,-0.14,0  
 2BT8,TYR\_295,11.52,1.64,-0.12,0  
 3G9G,ARG\_58,12.01,-0.49,0,0  
 3LJN,ASP\_221,2.27,0.28,-1.81,0  
 1NRI,GLU\_48,4.5,0,0,0  
 3G53,ARG\_198,12.5,0,0,0  
 3HUE,HIS\_241,7.58,1.08,0,0  
 3EX9,LYS\_136,10.08,-0.42,0,0  
 3V3T,HIS\_120,1.21,0.44,-1.3,-4.42  
 2D59,ARG\_16,11.87,-0.63,0,0  
 3RNV,LYS\_433,10.36,-0.14,0,0  
 1O9G,ARG\_137,11.87,-0.63,0,0  
 2Q99,LYS\_32,10.22,-0.28,0,0  
 3ETV,TYR\_136,9.42,0,-0.58,0  
 1NJ4,LYS\_143,10.5,0,0,0  
 1X7F,GLU\_233,3.97,0.14,-0.67,0  
 1XIP,GLU\_117,4.23,0.07,-0.34,0  
 3F5D,TYR\_193,12.96,0.07,0.56,2.33  
 1T95,LYS\_166,10.36,-0.14,0,0  
 1C3K,ASP\_78,4.29,0.49,0,0  
 3H5T,LYS\_175,10.43,-0.07,0,0  
 2Q13,GLU\_336,3.42,0.49,-1.57,0  
 1DZF,LYS\_122,10.5,0,0,0  
 1ZP2,ASP\_201,3.98,0.28,-0.1,0  
 3BQW,ARG\_127,12.08,-0.42,0,0  
 1JT9,CYS\_228,7.21,-1.78,0,0  
 3BJV,LYS\_149,10.15,-0.35,0,0  
 1TUL,LYS\_97,10.29,-0.21,0,0  
 1P2F,TYR\_213,11.83,0.33,-0.44,1.94  
 1W24,ASP\_95,3.35,0.35,-0.8,0  
 3M16,ARG\_235,13.41,-1.57,0,2.48  
 2G9D,TYR\_341,9.97,0,-0.03,0  
 3UPD,TYR\_5,10,0,0,0  
 3PP8,HIS\_25,6.5,0,0,0  
 3JZN,ARG\_306,12.5,0,0,0  
 1AM2,GLU\_14,4.5,0,0,0  
 3L3P,GLU\_321,4.5,0,0,0  
 4ANN,LYS\_91,10.43,-0.07,0,0  
 2CL3,HIS\_93,3.81,0.09,0,-2.78  
 3GW3,GLU\_45,1.6,0.63,-3.53,0  
 4GA2,ASP\_145,3.75,0,-0.05,0  
 3E7P,GLU\_239,4.71,0.21,0,0  
 2B0J,LYS\_107,10.43,-0.07,0,0  
 2GYZ,ARG\_37,12.5,0,0,0  
 3H04,GLU\_134,4.32,0.35,-0.53,0  
 3C2E,LYS\_75,10.5,0,0,0  
 2EDM,ARG\_56,10.75,-1.75,0,0  
 2CXA,CYS\_102,9.27,-1.14,0,1.41  
 1VJG,ARG\_97,11.66,-0.84,0,0  
 3DZ1,ARG\_236,12.22,-0.28,0,0  
 1H09,GLU\_24,4.57,0.07,0,0  
 4ECC,HIS\_152,7.04,0.61,0,-0.07  
 1M5I,ARG\_216,11.94,-0.56,0,0  
 1D2K,LYS\_187,10.29,-0.21,0,0  
 2CWC,ARG\_49,12.5,0,0,0  
 3L3P,ASP\_434,2.88,0.49,-1.41,0  
 2G9D,LYS\_329,10.36,-0.14,0,0  
 1NIJ,LYS\_32,10.36,-0.14,0,0  
 4D8L,LYS\_18,10.36,-0.14,0,0  
 3Q1C,LYS\_56,10.15,-0.35,0,0  
 1IDK,TYR\_286,11.79,0.21,-0.83,2.42  
 1CHD,GLU\_201,4.55,0.28,-0.23,0  
 3N2T,ARG\_143,12.43,-0.07,0,0  
 3ILC,ARG\_102,12.43,-0.07,0,0  
 4EKU,GLU\_357,4.5,0,0,0  
 1R3F,GLU\_221,4.71,0.21,0,0  
 3L0D,HIS\_107,7.21,1.06,0,-0.35  
 4DEZ,CYS\_47,5.99,-3.41,-1.19,1.59  
 3M66,HIS\_346,6.36,0,0,-0.14  
 2WOZ,LYS\_459,10.5,0,0,0  
 3EVP,ARG\_267,12.01,-0.49,0,0  
 3KVO,ARG\_136,11.87,-0.63,0,0  
 1DZF,TYR\_46,11.69,0.44,0,1.25  
 1TD6,GLU\_273,4.64,0.14,0,0  
 1YLN,ARG\_217,11.94,-0.56,0,0  
 3BQW,GLU\_172,4.57,0.07,0,0  
 3IRA,ASP\_86,0.94,0.77,-3.63,0  
 1ZBS,ASP\_90,3.43,0.07,-0.44,0  
 3I0O,ASP\_236,3.4,0.35,-0.75,0  
 1HF8,ASP\_111,1.3,0.63,-3.13,0  
 1SJY,GLU\_69,6.49,1.84,-1,1.15  
 2FXT,ASP\_412,4.01,0.21,0,0  
 1D2K,TYR\_322,13.4,0.64,-0.03,2.8  
 2JHY,ASP\_143,3.35,0.63,-1.08,0  
 3JZ9,LYS\_533,10.43,-0.07,0,0  
 3EGN,LYS\_477,10.5,0,0,0  
 3CAX,ASP\_154,2.44,0.42,-1.78,0  
 3Q1C,LYS\_53,10.15,-0.35,0,0  
 2QOP,LYS\_55,10.29,-0.21,0,0  
 3GMS,HIS\_56,6.5,0,0,0  
 1PSW,HIS\_300,6.5,0,0,0  
 2RGY,ASP\_108,3.43,0.28,-0.65,0  
 2CXA,ARG\_8,12.29,-0.21,0,0  
 3V55,GLU\_607,1.33,2.43,-3.2,-2.4  
 3LH5,LYS\_673,10.5,0,0,0  
 3S0A,ASP\_40,2.02,0.56,-2.34,0  
 1J74,TYR\_63,10.52,0.74,-0.22,0  
 1YB2,ARG\_254,12.29,-0.21,0,0  
 3ANJ,ARG\_104,10.91,-2.59,0,1  
 1RSS,LYS\_35,10.43,-0.07,0,0  
 3GA2,TYR\_165,11.04,0,-0.11,1.15  
 3EUA,LYS\_41,6.5,0,0,0  
 3GE9,ARG\_95,12.15,-0.35,0,0  
 3A7L,ARG\_17,11.87,-0.63,0,0  
 1X91,ASP\_122,1.93,0.7,-2.57,0  
 3JZ9,CYS\_446,10.17,-0.05,0,1.22  
 3R87,ARG\_118,12.01,-0.49,0,0  
 1ZP2,GLU\_76,3.52,0.49,-1.47,0  
 1YTD,LYS\_195,10.36,-0.14,0,0  
 3BPP,LYS\_167,10.36,-0.14,0,0  
 1XIP,CYS\_300,8.77,-2.29,0,2.06  
 3EVP,GLU\_163,4.57,0.07,0,0  
 1G8P,GLU\_258,4.23,0.35,-0.62,0  
 4D8L,ARG\_230,11.87,-0.63,0,0  
 1PV5,HIS\_3,6.29,0,0,-0.21  
 1DCF,LYS\_52,10.43,-0.07,0,0  
 1WP5,LYS\_191,10.5,0,0,0  
 1LTU,ASP\_6,2.95,0.35,-1.2,0  
 2WB8,LYS\_462,10.5,0,0,0  
 3LJC,LYS\_49,10.36,-0.14,0,0  
 2A4D,GLU\_206,4.78,0.28,0,0  
 2Q07,HIS\_404,2.7,0.8,-0.7,-3.9  
 1QVI,CYS\_125,9,0,0,0  
 1PSW,GLU\_126,4.5,0,0,0  
 1PGV,LYS\_327,9.87,-0.63,0,0  
 3RFY,ARG\_153,11.73,-0.77,0,0  
 1IDK,TYR\_24,10.46,0,0,0.46  
 3GV0,HIS\_108,6.43,0,0,-0.07  
 2WOZ,GLU\_584,4.5,0,0,0  
 2Q5X,GLU\_836,4.58,0.35,-0.27,0  
 2CIU,TYR\_196,10,0,0,0  
 2XMZ,ASP\_249,3.09,0.28,-0.99,0  
 2H2W,ASP\_266,3.94,0.14,0,0  
 1J85,GLU\_102,1.88,1.36,-3.99,0  
 1WXF,LYS\_275,10.5,0,0,0  
 3EVP,GLU\_126,0.75,0.77,-4.52,0  
 2Q13,TYR\_302,11.81,0.67,0,1.14  
 1D7O,ASP\_173,3.86,0.14,-0.08,0  
 3ADO,ARG\_116,12.43,-0.07,0,0  
 1KW4,GLU\_28,4.57,0.07,0,0  
 2CW4,ASP\_44,2.13,0.49,-2.15,0  
 2OEW,LYS\_313,10.5,0,0,0  
 1WP5,ARG\_279,12.5,0,0,0  
 2CE6,TYR\_81,8.26,0.14,-1.95,0.06  
 2VAN,LYS\_280,10.5,0,0,0  
 3VJ8,ARG\_348,11.59,-0.91,0,0  
 2BQQ,LYS\_66,10.5,0,0,0  
 1WYC,LYS\_246,10.29,-0.21,0,0  
 3EVN,HIS\_197,6.36,0,0,-0.14  
 3RNV,TYR\_422,10,0,0,0  
 3IVF,GLU\_269,1.29,0.93,-1.74,-2.4  
 1X04,LYS\_28,10.5,0,0,0  
 1J5X,ASP\_171,3.72,0,-0.08,0  
 2A0J,GLU\_46,4.64,0.14,0,0  
 1X1E,ARG\_63,11.8,-0.7,0,0  
 3H9W,CYS\_76,5.1,-3.74,-1.19,1.03  
 3LME,LYS\_39,10.36,-0.14,0,0  
 2OSA,GLU\_381,4.39,0.21,-0.32,0  
 3PU6,LYS\_104,10.08,-0.42,0,0  
 3FK5,TYR\_144,10.03,0,0,0.03  
 2GEN,HIS\_160,3.75,0,0,-2.75  
 2Q98,ASP\_20,3.81,0.35,-0.34,0  
 2RFA,ASP\_188,3.22,0.49,-1.07,0  
 3MEW,GLU\_197,4.5,0,0,0  
 2G3A,ARG\_58,11.66,-0.84,0,0  
 3CE7,ARG\_97,12.08,-0.42,0,0  
 3HQX,ARG\_66,12.22,-0.28,0,0  
 3K9I,TYR\_119,10,0,0,0  
 2AXO,ASP\_246,1.96,0.56,-2.4,0  
 3DB9,HIS\_199,6.38,0.09,0,-0.21  
 2DG7,ARG\_104,10.32,-2.45,0,0.28  
 3GEC,TYR\_468,10.11,0.47,-0.36,0  
 3ADO,ASP\_253,3.92,0.14,-0.02,0  
 3US6,GLU\_44,4.85,0.35,0,0  
 1TJE,LYS\_91,10.36,-0.14,0,0  
 2F4Q,ARG\_330,11.8,-0.7,0,0  
 1P4X,HIS\_246,6.38,0.09,0,-0.21  
 2YWJ,TYR\_24,11.58,0.07,-0.21,1.72  
 1V6T,LYS\_238,10.36,-0.14,0,0  
 1Y2Q,LYS\_51,10.22,-0.28,0,0  
 2B0A,LYS\_25,10.5,0,0,0  
 3ZXY,ARG\_103,11.87,-0.63,0,0  
 1E55,LYS\_3,10.22,-0.28,0,0  
 3QKY,GLU\_150,4.5,0,0,0  
 1ZBP,GLU\_22,4.55,0.14,-0.09,0  
 3E5T,GLU\_47,4.64,0.14,0,0  
 1JT9,LYS\_183,10.5,0,0,0  
 1MML,HIS\_161,6.29,0,0,-0.21  
 2FG1,LYS\_125,8.17,-0.83,0,0  
 2BV9,HIS\_285,6.43,0,0,-0.07  
 1QZN,GLU\_85,4.5,0,0,0  
 1X6J,ASP\_53,3.87,0.07,0,0  
 1RAJ,TYR\_450,10.56,0.04,-0.65,1.17  
 1O6D,GLU\_89,4.92,0.42,0,0  
 2HG,ARG\_126,11.94,-0.56,0,0  
 1Q5Z,LYS\_518,10.5,0,0,0  
 2WB3,LYS\_338,10.36,-0.14,0,0  
 3LJN,ARG\_283,11.8,-0.7,0,0  
 2QV2,LYS\_132,10.29,-0.21,0,0  
 3GT0,LYS\_213,10.22,-0.28,0,0  
 1ZB5,CYS\_189,10.29,-0.21,0,0  
 1MTZ,ARG\_278,11.87,-0.63,0,0  
 3RFY,LYS\_236,10.5,0,0,0  
 2XHC,TYR\_143,10.31,0.14,0,0.17  
 1ZBM,ARG\_181,11.59,-0.91,0,0  
 3D9H,ASP\_101,3.87,0.07,0,0  
 3GW3,ARG\_142,11.41,-1.09,0,0  
 2IRM,GLU\_293,0.28,2.18,-2.36,-4.04  
 4EKU,ARG\_306,11.8,-0.7,0,0  
 1V6T,ARG\_73,12.01,-0.95,0.46  
 1EV8,LYS\_10,10.29,-0.21,0,0  
 3M66,GLU\_170,4.85,0.35,0,0  
 3ADO,ARG\_19,11.33,-1.17,0,0  
 3RAZ,GLU\_59,4.56,0.73,-0.67,0  
 2B3M,HIS\_67,6.08,0,0,-0.42  
 3HYQ,GLU\_91,4.12,0.42,-0.8,0  
 1X1E,GLU\_20,4.57,0.07,0,0



3GW3,GLU\_114,4.5,0,0,0  
3I47,GLU\_243,2.88,1.26,-2.88,0  
3K8U,LYS\_118,10.5,0,0,0  
1MD6,LYS\_34,10.01,-0.49,0,0  
1YTD,GLU\_252,3.98,0.28,-0.8,0  
3V1Q,LYS\_571,10.5,0,0,0  
3H6Q,LYS\_148,10.43,-0.07,0,0  
3MEW,LYS\_189,10.5,0,0,0  
2H01,ARG\_106,12.15,-0.35,0,0  
2IF4,HIS\_83,6.87,0.44,0,-0.07  
3FNI,TYR\_15,12.84,0.42,-1.26,3.68  
1W7B,ARG\_63,13.51,-1.39,0,2.4  
1O9G,ARG\_113,12.01,-0.49,0,0  
2P0L,ARG\_255,12.5,0,0,0  
1R5S,LYS\_53,10.22,-0.28,0,0  
3M7D,ARG\_131,8.51,-3.64,0,-0.35  
2B0A,GLU\_54,4.5,0,0,0  
2JKF,GLU\_62,5.08,0.63,-0.05,0  
3K8U,LYS\_124,10.22,-0.28,0,0  
4FCU,ARG\_181,13.67,-1.23,0,2.4  
1FO9,ARG\_303,11.02,-1.48,0,0  
2YLF,ARG\_74,12.5,0,0,0  
2CWY,ARG\_68,12.08,-0.42,0,0  
1Z9L,LYS\_118,10.5,0,0,0  
2H01,ARG\_119,12.08,-0.42,0,0  
3PU6,GLU\_51,4.5,0,0,0  
1ZCE,ARG\_42,11.73,-0.77,0,0  
3IL3,ARG\_40,12.29,-0.21,0,0  
3LQE,ARG\_390,12.01,-0.49,0,0  
3SMD,LYS\_97,9.8,-0.7,0,0  
1D2K,TYR\_106,13.46,0.21,0.58,2.66  
1SBX,ASP\_95,3.68,0,-0.12,0  
1K9S,GLU\_126,4.57,0.07,0,0  
3M66,HIS\_152,6.97,0.68,0,-0.21  
1C3K,GLU\_55,4.64,0.14,0,0  
3CBN,TYR\_26,13.41,0.21,0.8,2.4  
1LZL,LYS\_66,10.08,-0.42,0,0  
3UUV,LYS\_400,10.22,-0.28,0,0  
1T6L,TYR\_92,8.97,0.21,-1.24,0  
1P6F,ARG\_124,12.29,-0.21,0,0  
2PGE,GLU\_176,4.49,0.49,0,0  
1GSZ,LYS\_161,10.5,0,0,0  
1L2H,LYS\_97,10.29,-0.21,0,0  
1O59,GLU\_260,4.03,0.21,-0.68,0  
1ZBM,TYR\_149,9.1,0,-0.9,0  
3F6M,CYS\_150,10.32,-0.45,0,1.76  
4FZR,ASP\_58,3.94,0.14,0,0  
3H04,LYS\_264,10.36,-0.14,0,0  
3FNI,LYS\_134,10.5,0,0,0  
2QV2,GLU\_95,4.57,0.07,0,0  
1X04,ASP\_119,3.38,0.56,-0.98,0  
2EYI,ARG\_82,12.29,-0.21,0,0  
2HRZ,GLU\_72,4.43,0.14,-0.21,0  
2OJQ,HIS\_633,5.14,0.26,0.08,-1.71  
2OEW,ASP\_206,4.06,0.35,-0.09,0  
1GPP,HIS\_170,7.23,0.8,0,-0.07  
3BZT,LYS\_261,10.43,-0.07,0,0  
3F1X,ARG\_269,12.29,-0.21,0,0  
1FKM,ASP\_317,3.2,0.35,-0.95,0  
2C2Y,ARG\_112,11.8,-0.7,0,0  
1WYC,ASP\_132,2.99,0.42,-1.23,0  
3EX9,ARG\_129,12.08,-0.42,0,0  
1Z3X,GLU\_100,4.64,0.14,0,0  
3RFY,ARG\_361,12.5,0,0,0  
1UW7,TYR\_89,10.77,0.84,-0.64,0.57  
2IF4,ASP\_159,3.69,0.28,-0.39,0  
1P4X,LYS\_25,10.43,-0.07,0,0  
4ACJ,ARG\_681,12.29,-0.21,0,0  
1DZF,ARG\_11,12.22,-0.28,0,0  
1WXF,CYS\_60,11.85,0,0,2.85  
1Z3X,GLU\_139,3.09,0.56,-1.97,0  
3L3P,HIS\_461,3.93,0.84,0,-3.41  
2QZQ,GLU\_90,3.7,0.77,-1.57,0  
1DCF,ASP\_94,2.03,0.49,-2.26,0  
1QYI,LYS\_68,10.5,0,0,0  
3TOW,GLU\_138,4.5,0,0,0  
3KEY,ASP\_366,3.61,0.28,-0.47,0  
3D9H,ARG\_23,12.08,-0.42,0,0  
1HF8,HIS\_281,6.5,0,0,0  
1P6F,HIS\_108,6.36,0,0,-0.14  
2ATR,ASP\_49,3.28,0.28,-0.8,0  
3LH5,ASP\_667,3.8,0,0,0  
3VJ8,LYS\_160,9.87,-0.63,0,0  
1SJV,ASP\_4,3.94,0.21,-0.07,0  
3FRR,LYS\_23,10.5,0,0,0  
3KEY,HIS\_486,6.68,0.25,0,-0.07  
2Q98,GLU\_101,4.71,0.21,0,0  
2XWS,ARG\_44,12.29,-0.21,0,0  
4AM1,ARG\_329,13.64,-1.06,0,2.2  
3U0V,LYS\_70,10.5,0,0,0  
3GS9,GLU\_128,4.05,0.35,-0.8,0  
3H13,ARG\_243,12.08,-0.42,0,0  
2EFK,LYS\_52,10.43,-0.07,0,0  
2QK1,LYS\_500,10.15,-0.35,0,0  
2YWJ,LYS\_155,10.08,-0.42,0,0  
1FHL,TYR\_20,11.45,0.07,0,1.38  
2C2Y,CYS\_140,11.74,-0.85,1.16,2.43  
3UPD,ARG\_100,12.5,0,0,0  
1JKS,ARG\_47,11.8,-0.7,0,0  
1SJB,GLU\_601,4.15,0.42,-0.77,0  
1TD6,GLU\_70,5.02,0.52,0,0  
2P1W,GLU\_233,4.25,0.43,-0.78,0.1  
2IRM,GLU\_84,4.07,3,-1.22,0  
1P2F,LYS\_88,10.43,-0.07,0,0  
2GAU,GLU\_32,4.64,0.14,0,0  
2P65,GLU\_184,4.5,0,0,0  
3N2T,GLU\_244,3.91,0.42,-1.01,0  
4GA2,TYR\_116,9.99,0,-0.01,0  
3DB9,ARG\_17,12.43,-0.07,0,0  
2RGY,CYS\_186,7.93,-3.6,0.6,1.93  
1GQE,LYS\_177,10.29,-0.21,0,0  
3RJK,LYS\_154,10.29,-0.21,0,0  
2GKG,GLU\_124,4.5,0,0,0  
4AM1,ARG\_245,10.7,-1.8,0,0  
2CIU,LYS\_179,10.43,-0.07,0,0  
1WRU,TYR\_121,10.14,0.14,0,0  
4FD6,GLU\_153,4.71,0.21,0,0  
2BV9,TYR\_176,12.02,0,0,2.02  
4ACJ,LYS\_677,10.5,0,0,0  
1QQH,LYS\_178,10.29,-0.21,0,0  
3CQ1,ARG\_98,12.29,-0.21,0,0  
1MML,TYR\_133,9.75,0,-0.25,0  
2HP7,ARG\_75,12.08,-0.42,0,0  
1D2K,ARG\_147,11.31,-1.19,0,0  
2EDM,LYS\_192,9.73,-0.77,0,0  
3NBI,GLU\_128,4.78,0.28,0,0  
2NRK,LYS\_148,10.5,0,0,0  
2XHC,TYR\_84,10.07,0.07,0,0  
1R6Y,CYS\_46,9,0,0,0  
2XHC,TYR\_6,10.07,0.07,0,0  
3B79,GLU\_23,4.5,0,0,0  
2V4U,LYS\_297,10.01,-0.49,0,0  
3P2F,ARG\_49,11.8,-0.7,0,0  
3FFM,HIS\_118,7.13,0.84,0,-0.21  
3G9T,LYS\_257,10.5,0,0,0  
2F4Q,ARG\_158,12.01,-0.49,0,0  
2O0K,ARG\_349,11.87,-0.63,0,0  
3BWT,GLU\_664,4.54,0.14,-0.1,0  
2FD4,ARG\_449,11.1,-1.4,0,0  
1H4U,ASP\_473,3.16,0.49,-1.14,0  
2QDJ,LYS\_341,10.5,0,0,0  
1M5I,GLU\_138,3.54,0.49,-1.45,0  
3V1Q,HIS\_638,6.9,0.54,0,-0.14  
1ILW,HIS\_71,6.49,2.78,1.24,-4.03  
1X7F,LYS\_16,10.22,-0.28,0,0  
3ULX,ASP\_58,4.08,0.28,0,0  
3H5T,LYS\_334,10.43,-0.07,0,0  
3LMF,ARG\_68,12.22,-0.28,0,0  
3U0V,LYS\_114,10.29,-0.21,0,0  
1RL0,ARG\_166,12.08,-0.42,0,0  
1GSZ,LYS\_127,10.29,-0.21,0,0  
3M7G,LYS\_28,10.15,-0.35,0,0  
1T6L,HIS\_212,6.29,0,0,-0.21  
3F5D,HIS\_84,6.43,0,0,-0.07  
3CQY,ASP\_180,3.68,0.28,-0.4,0  
2OSA,LYS\_368,10.43,-0.07,0,0  
1WOU,HIS\_59,6.5,0,0,0  
2P0L,ASP\_263,4.07,0.35,-0.08,0  
3EX9,TYR\_120,11.32,1.32,0,0  
2APL,ASP\_116,3.94,0.14,0,0  
2ROS,TYR\_73,10.38,0.38,0,0  
1JT9,GLU\_257,4.71,0.21,0,0  
1O0X,ASP\_170,3.79,0.14,-0.15,0  
1SOH,LYS\_242,10.36,-0.14,0,0  
2EHG,GLU\_39,3.41,0.42,-1.51,0  
2FB6,CYS\_78,8.87,-0.2,0,0.07  
1TP6,ASP\_112,1.62,1.33,-3.51,0  
4F85,HIS\_99,5.29,1.1,0,-2.31  
2O8I,ARG\_124,11.87,-0.63,0,0  
1QSZ,GLU\_607,3.82,0.21,-0.89,0  
3K8J,HIS\_66,6.36,0,0,-0.14  
4E6S,TYR\_17,10.1,0.07,-0.07,0.1  
3UUV,ASP\_318,2.93,0.42,-1.29,0  
2GKG,ARG\_25,11.87,-0.63,0,0  
2RJD,HIS\_512,13.89,8.38,2.56,-3.55  
3PBH,TYR\_140,12.5,0.71,0.68,1.11  
1T07,ASP\_29,1.75,0.35,-2.4,0  
2JEO,LYS\_81,10.43,-0.07,0,0  
2Q5X,CYS\_818,8.24,-0.75,0,0  
1QQ,ARG\_119,12.08,-0.42,0,0  
3CBN,GLU\_152,3.44,0,-1.06,0  
1Q46,ARG\_175,12.5,0,0,0  
3JZN,LYS\_293,10.29,-0.21,0,0  
3BQE,LYS\_310,10.5,0,0,0  
2B0J,GLU\_86,4.71,0.21,0,0  
2AZL,ARG\_249,11.87,-0.63,0,0  
3IV4,GLU\_28,4,0.28,-0.78,0  
1LPL,ARG\_163,11.66,-0.84,0,0  
3PBH,CYS\_240,2.94,-4.02,-3.37,1.34  
2X4G,LYS\_14,10.22,-0.28,0,0  
1BN6,ARG\_144,10.5,-2,0,0  
2FD5,ARG\_67,11.59,-0.91,0,0  
2QHT,ARG\_208,12.08,-0.42,0,0  
2W88,ARG\_695,11.94,-0.56,0,0  
2H85,ARG\_126,13.09,-1.81,0,2.4  
3GW3,LYS\_289,10.43,-0.07,0,0  
3CX2,GLU\_258,4.5,0,0,0  
2P5D,ARG\_134,12.08,-0.42,0,0  
2Q13,LYS\_91,10.43,-0.07,0,0  
1RH5,ASP\_65,3.18,0.56,-1.18,0  
3KB5,ARG\_386,12.15,-0.35,0,0  
2GZG,HIS\_93,2.99,0.91,0.57,-4.99  
2VGM,TYR\_311,10,0,0,0  
4FZN,ASP\_184,1.89,0.49,-2.4,0  
3GEC,LYS\_457,10.43,-0.07,0,0  
3HQX,CYS\_23,8.88,-0.8,0,0.68  
1L2F,ARG\_199,12.08,-0.42,0,0  
3ETU,LYS\_270,10.29,-0.21,0,0  
2B78,LYS\_65,10.5,0,0,0  
3UAH,ASP\_421,3.89,0.14,-0.05,0  
1DUN,GLU\_11,3.91,0.21,-0.8,0  
2NRK,ARG\_118,13.05,-1.51,0,2.06  
3NR5,GLU\_115,1.99,0.56,-3.07,0  
3GV0,ASP\_275,2.95,0.56,-1.41,0  
2ZCX,ARG\_154,11.45,-1.05,0,0  
2Q07,TYR\_245,11.53,0,0,1.53  
2RGY,LYS\_264,10.5,0,0,0  
1RHS,ARG\_186,11.69,-1.85,0,1.05  
3LJI,ASP\_278,2.85,0.35,-1.3,0  
2AZL,ARG\_55,11.87,-0.63,0,0  
3N2T,ARG\_109,11.66,-0.84,0,0  
2QEV,HIS\_35,3.03,0.04,0,-3.51  
2HXB,ARG\_58,12.36,-0.14,0,0  
1J33,GLU\_28,4.46,0.14,0,-0.18  
2YX0,GLU\_316,4.5,0,0,0  
2RJD,HIS\_233,6.5,0,0,0  
2CXA,HIS\_121,6.72,0.22,0,0  
3L7N,ASP\_42,4.01,0.21,0,0  
1D70,TYR\_44,11.54,0,0,1.54  
3TMO,ASP\_231,3.35,0.35,-0.8,0  
3U2R,GLU\_40,4.5,0,0,0  
1MN3,ASP\_430,3.78,0.14,-0.16,0  
2P0L,ARG\_129,12.15,-0.35,0,0  
1PGV,GLU\_379,3.98,0.28,-0.8,0  
3UPD,LYS\_55,9.95,-0.35,0,-0.2  
1TP6,ASP\_112,1.62,1.33,-3.51,0  
1I60,HIS\_46,7.7,1.63,0,-0.42  
3LPZ,ARG\_197,11.8,-0.7,0,0  
1OLR,ARG\_146,12.22,-0.28,0,0  
1NWA,TYR\_65,11.5,1.5,0,0  
2FCU,ARG\_69,11.87,-0.63,0,0  
4F4Q,ASP\_140,3.64,0.07,-0.23,0  
1ZCU,GLU\_118,4.66,2.15,-1.99,0  
1MTZ,ASP\_287,3.35,0.35,-0.8,0  
4DIU,GLU\_123,4.9,0.49,-0.09,0  
3MIX,LYS\_565,10.43,-0.07,0,0  
3B7X,LYS\_85,10.36,-0.14,0,0  
1JT9,HIS\_81,6.29,0,0,-0.21  
2V5B,ARG\_227,12.43,-0.07,0,0  
3CRM,ARG\_258,12.01,-0.49,0,0  
2AHE,TYR\_205,10.47,0.35,-0.13,0.26  
2V1L,TYR\_50,9.18,0.28,-1.1,0  
3CBN,ASP\_57,3.86,0.56,-0.5,0  
1RAJ,GLU\_426,4.64,0.14,0,0  
1RIS,LYS\_132,10.22,-0.28,0,0  
4EUG,ARG\_105,12.08,-0.42,0,0  
3A4C,GLU\_488,4.5,0,0,0  
1RWZ,LYS\_158,10.5,0,0,0  
3COU,ARG\_20,12.01,-0.49,0,0  
1WNH,ASP\_155,4.01,0.21,0,0  
2FL7,LYS\_209,10.29,-0.21,0,0  
4E88,HIS\_17,6.96,0.82,0,-0.35  
350A,GLU\_4,3.91,0.21,-0.8,0  
2OB5,ASP\_51,3.8,0.28,-0.28,0  
3LE4,TYR\_319,9.68,0,-0.31,0  
3BB7,ARG\_353,12.18,-0.75,0,0.43  
3ZXY,ARG\_82,12.22,-0.28,0,0  
2JHY,CYS\_79,5.26,-3.81,0,0.07  
2ATR,TYR\_78,13.34,0.14,0.8,2.4  
3I47,ARG\_173,12.22,-0.28,0,0  
1YM5,LYS\_202,10.22,-0.28,0,0  
3VJ8,HIS\_269,0.01,0,-2.4,-4.09  
3Q6L,ASP\_18,3.6,0.63,-0.83,0  
3UC9,GLU\_77,4.38,0.07,-0.19,0  
3LJN,CYS\_57,11,-0.23,0,2.23  
1YG2,TYR\_136,10,0,0,0

3F1X,GLU\_135,4.71,0.21,0,0  
4E5S,ASP\_138,2.58,0.14,-1.36,0  
4HDE,LYS\_53,10.5,0,0,0  
1V8E,LYS\_89,9.8,-0.7,0,0  
2PLQ,ASP\_95,3.07,0.07,-0.8,0  
2AH5,GLU\_94,4.64,0.14,0,0  
1DCF,ASP\_117,3.72,0,-0.08,0  
3RFY,LYS\_246,10.22,-0.28,0,0  
1L2H,LYS\_92,10.01,-0.49,0,0  
3FFM,LYS\_131,10.5,0,0,0  
2QVO,ARG\_5,12.43,-0.07,0,0  
1D2K,LYS\_271,10.36,-0.14,0,0  
1ZBP,LYS\_5,10.5,0,0,0  
2CBE,LYS\_76,10.15,-0.35,0,0  
2RIK,LYS\_236,10.5,0,0,0  
1FHL,GLU\_323,4.59,0.14,-0.05,0  
3Q2C,TYR\_73,10.59,0.81,-0.22,0  
2B2H,ASP\_66,3.18,1.12,-1.73,0  
1U3Y,GLU\_264,3.71,0.42,-1.21,0  
3A7L,GLU\_122,4.57,0.07,0,0  
1BN6,TYR\_35,11.09,0.02,0.1,0.07  
1V43,LYS\_112,10.43,-0.07,0,0  
1GQE,ARG\_262,11.87,-0.63,0,0  
2DG7,GLU\_60,2.52,1.04,-0.62,-2.4  
1WRU,GLU\_27,2.78,1.06,-0.38,-2.4  
2HRZ,GLU\_290,4.5,0,0,0  
1RL0,ARG\_182,12.15,-0.35,0,0  
3PZ9,HIS\_90,7.69,3.2,3.51,-5.52  
3ETU,GLU\_202,4.5,0,0,0  
1RZ2,LYS\_72,10.43,-0.07,0,0  
1RSS,ARG\_41,12.08,-0.42,0,0  
3MEW,ARG\_157,12.5,0,0,0  
2IQT,GLU\_110,4.71,0.21,0,0  
1JB3,LYS\_48,10.5,0,0,0  
2P5D,TYR\_141,10.2,0.2,0,0  
2DG7,ARG\_42,12.5,0,0,0  
3F7M,ASP\_221,3.04,0.84,-1.6,0  
1NAF,GLU\_220,3.86,0.14,-0.78,0  
3ODJ,ARG\_82,12.22,-0.28,0,0  
3Q9P,ARG\_136,11.73,-0.77,0,0  
4EKU,CYS\_310,11.11,0.0,0.94,1.17  
2Q99,ASP\_100,3.35,0.35,-0.8,0  
2AHE,ARG\_61,12.5,0,0,0  
1G8P,GLU\_291,4.67,0.35,-0.18,0  
1O5J,GLU\_64,4.71,0.21,0,0  
1V6T,HIS\_162,2.91,0,0,-3.59  
1SIG,GLU\_136,4.42,0.71,-0.79,0  
2B0J,LYS\_160,10.5,0,0,0  
3GYW,ARG\_132,13.47,-1.31,0,2.28  
3EVP,HIS\_82,2.09,0,0,-4.41  
2D2S,LYS\_747,10.5,0,0,0  
3OOP,HIS\_20,6.5,0,0,0  
3KT9,GLU\_78,4.92,0.42,0,0  
2R0S,ASP\_269,2.23,0.42,-1.99,0  
2NRR,GLU\_444,3.43,0.42,-1.49,0  
1LZL,ASP\_60,3.87,0.07,0,0  
2FL4,ASP\_40,3.87,0.07,0,0  
2EJX,LYS\_102,10.5,0,0,0  
1AK1,HIS\_183,3.54,1.18,0,-4.14  
1MD6,GLU\_39,3.87,0.52,-1.15,0  
2YT4,HIS\_660,7.13,0.77,0,-0.14  
3BPP,TYR\_179,11.24,0,0,1.24  
2Q07,TYR\_453,10,0,0,0  
1R29,HIS\_14,6.43,0,0,-0.07  
1YTD,GLU\_275,0.9,0.89,-1.91,-2.58  
3RKV,ARG\_316,11.8,-0.7,0,0  
2FZ4,TYR\_28,12.31,0,0,12.2.19  
2HRZ,ARG\_104,12.15,-0.35,0,0  
1LFP,ARG\_50,11.59,-0.91,0,0  
4E8B,ARG\_188,11.66,-0.84,0,0  
2QDJ,TYR\_292,11.26,0,0,1.26  
1S7K,CYS\_74,9,0,0,0  
3IL3,GLU\_301,7.4,3.45,-0.55,0  
1OLR,ARG\_127,11.9,-0.6,0,0  
2A0J,HIS\_67,3.75,0,0,-2.75  
3V4G,LYS\_19,10.43,-0.07,0,0  
3H5T,ARG\_148,12.01,-0.49,0,0  
1YB2,LYS\_248,10.43,-0.07,0,0  
2D0A,ARG\_309,12.08,-0.42,0,0  
3EZ7,TYR\_105,10,0,0,0  
3NBI,GLU\_54,4.64,0.14,0,0  
2NRK,TYR\_103,10.61,1.21,-0.23,-0.37  
3ULX,ARG\_155,12.29,-0.21,0,0  
2G5X,ARG\_26,12.29,-0.21,0,0  
3U0V,LYS\_228,10.01,-0.49,0,0  
1O6D,LYS\_38,10.43,-0.07,0,0  
2OGQ,ARG\_581,12.01,-0.49,0,0  
3M7D,GLU\_171,4.19,0.47,-0.78,0  
2YWX,LYS\_143,9.87,-0.63,0,0  
1NAR,GLU\_29,4.5,0,0,0  
1G5Z,GLU\_44,4.49,0.14,-0.15,0  
3HVM,TYR\_27,10,0,0,0  
3EAZ,TYR\_112,10,0,0,0  
3GMS,LYS\_322,9.38,-1.12,0,0  
1TUL,GLU\_30,3.87,0.21,-0.85,0  
1RI6,GLU\_225,4.5,0,0,0  
2RJD,HIS\_477,6.23,0.01,0,-0.28  
1NFN,GLU\_109,4.49,0.21,-0.22,0  
1J33,GLU\_137,4.71,0.21,0,0  
1XFK,LYS\_225,10.36,-0.14,0,0  
1Y2Q,GLU\_36,4.27,0.07,-0.3,0  
1WXQ,LYS\_51,10.36,-0.14,0,0  
2V1L,TYR\_133,10,0,0,0  
2OGQ,ASP\_447,1.18,0.7,-3.33,0  
2H01,LYS\_93,10.36,-0.14,0,0  
1RIS,ARG\_59,12.29,-0.21,0,0  
1BN6,ARG\_129,13.33,-1.57,0,2.4  
3E7P,GLU\_91,4.64,0.14,0,0  
3G9G,CYS\_221,9,0,0,0  
3EYE,ASP\_126,3.07,7,-1.57,0  
2FPN,HIS\_203,6.43,0,0,-0.07  
3EIZ,TYR\_142,13.54,2.0,0.03,1.5  
1YTQ,GLU\_22,3.52,0.21,-1.19,0  
3FRR,ASP\_122,3.32,0.35,-0.83,0  
3LH5,ARG\_742,11.31,-1.19,0,0  
3EZ7,ASP\_322,3.8,0,0,0  
2G5X,LYS\_159,10.5,0,0,0  
3IPZ,GLU\_156,4.5,0,0,0  
2EJX,ARG\_78,11.94,-0.56,0,0  
3LMF,HIS\_20,6.43,0,0,-0.07  
2H2W,LYS\_255,10.5,0,0,0  
3UV9,TYR\_389,10.07,0.07,0,0  
1RAJ,TYR\_350,13.88,0.41,0.8,2.67  
3EVP,TYR\_301,7.09,0.7,-1.21,-2.4  
3I0C,GLU\_276,3.99,0.28,-0.79,0  
2RGY,HIS\_115,6.5,0,0,0  
2OBI,ASP\_23,3.34,0.35,-0.81,0  
3RVC,GLU\_142,4.27,0.28,-0.51,0  
1T3Y,LYS\_98,10.15,-0.35,0,0  
2YT4,GLU\_604,4.78,0.28,0,0  
3CIV,CYS\_143,8.84,-1.62,-0.48,1.94  
1H09,LYS\_128,10.08,-0.42,0,0  
1MTZ,LYS\_158,10.43,-0.07,0,0  
3EJC,GLU\_164,4.71,0.21,0,0  
4D8L,ARG\_288,11.74,-0.76,0,0  
3PZ9,GLU\_252,4.57,0.07,0,0  
3RLN,HIS\_719,6.48,0.05,0,-0.07  
1FHL,GLU\_326,4.5,0,0,0  
2AZL,GLU\_14,4.85,0.35,0,0  
2CBE,GLU\_238,3.91,0.21,-0.8,0  
4ECC,ASP\_179,3.73,0.56,-0.63,0  
2E0T,GLU\_210,4.5,0,0,0  
1JT9,ASP\_141,2.05,0.56,-2.32,0  
1SIG,TYR\_228,10.07,0.07,0,0  
3P28,HIS\_189,7.53,1.03,0,0  
3M9A,GLU\_13,4.11,0.07,-0.46,0  
2R0S,LYS\_239,10.43,-0.07,0,0  
3RVC,ARG\_193,12.5,0,0,0  
1O0X,LYS\_138,10.22,-0.28,0,0  
1OIS,GLU\_280,4.64,0.14,0,0  
3A7L,ASP\_127,3.8,0,0,0  
3FK5,ARG\_231,12.29,-0.21,0,0  
1YM5,GLU\_168,4.57,0.07,0,0  
3RFY,TYR\_223,11.37,0,0,1.37  
2RJD,LYS\_302,10.29,-0.21,0,0  
3CGW,LYS\_123,10.29,-0.21,0,0  
4EKU,GLU\_205,4.16,0.56,-0.9,0  
3V75,ASP\_258,2.62,0.49,-1.67,0  
2XHC,ARG\_279,11.45,-1.05,0,0  
2D7U,TYR\_186,10.61,0,0,0.61  
3OIP,ASP\_178,3.11,0.49,-1.17,0  
1DOV,TYR\_245,10,0,0,0  
3M7G,TYR\_226,9.84,2.38,-0.85,-1.7  
2H2W,LYS\_295,11.01,-0.14,0,0.65  
2EYI,LYS\_106,10.5,0,0,0  
3F1X,HIS\_66,6.84,0.41,0,-0.07  
3BA1,ARG\_36,12.22,-0.28,0,0  
4FLE,ARG\_121,11.87,-0.63,0,0  
2B0J,HIS\_201,7.94,1.6,4.44,-4.59  
2Z14,ARG\_100,12.5,0,0,0  
4EZB,ARG\_45,12.22,-0.28,0,0  
2H14,HIS\_128,4.49,1.63,1.21,-4.84  
2O0K,ARG\_278,12.5,0,0,0  
2VGM,GLU\_189,3.65,0.7,-1.55,0  
3FHF,GLU\_153,0.29,0.59,-2.4,-2.4  
2OJQ,LYS\_471,10.43,-0.07,0,0  
1YR6,GLU\_183,4.16,0.63,-0.97,0  
2V1L,ARG\_120,12.22,-0.28,0,0  
2AXO,ARG\_65,12.29,-0.21,0,0  
3UV9,TYR\_466,9.27,0.07,-0.8,0  
3I00,ARG\_282,13.48,-1.15,0,2.13  
1YM5,HIS\_283,5.42,0.45,0,-1.53  
1YDL,LYS\_6,10.5,0,0,0  
3HXQ,ASP\_71,3.94,0.14,0,0  
2CXC,ARG\_53,12.5,0,0,0  
3U56,CYS\_112,8.75,-0.32,0,0.07  
2NMU,HIS\_6,6.5,0,0,0  
1ZBM,HIS\_22,6.99,0.63,0,-0.14  
3I47,LYS\_221,10.01,-0.49,0,0  
3PP8,GLU\_182,3.92,0.49,-1.07,0  
3LJI,ASP\_115,4.08,0.35,-0.07,0  
1DVO,ARG\_143,13.38,-0.56,0,1.44  
2ILR,GLU\_318,4.5,0,0,0  
2FD5,ARG\_170,12.5,0,0,0  
3ANJ,TYR\_204,13.27,0.07,0.8,2.4  
1TWU,GLU\_31,4.54,0.07,-0.03,0  
3BJV,GLU\_155,4.57,0.07,0,0  
1TJE,LYS\_130,10.29,-0.21,0,0  
3LD1,LYS\_13,9.94,-0.56,0,0  
3EST,GLU\_200,4.43,0.14,-0.21,0  
3A4C,ARG\_528,12.5,0,0,0  
2Q12,LYS\_152,10.36,-0.14,0,0  
3AUF,ARG\_167,12.15,-0.35,0,0  
2CWC,HIS\_48,6.44,0.01,0,-0.07  
3I00,ASP\_243,3.87,0.07,0,0  
3L7N,HIS\_141,1.49,1.08,-0.43,-5.66  
1TXJ,ASP\_111,3.73,0,-0.07,0  
1FKM,ARG\_482,12.39,-1.32,0,1.21  
3COU,ASP\_52,1.95,0.91,-2.77,0  
2D59,LYS\_23,9.87,-0.63,0,0  
3P28,GLU\_197,3.01,0.85,-1.02,-1.32  
2DG7,ASP\_141,3.74,0,-0.06,0  
1I60,TYR\_42,11.3,0.14,0,1.16  
3PM2,ASP\_98,3.98,0.28,-0.1,0  
4DVD,ARG\_68,12.19,-0.31,0,0  
3E7P,GLU\_229,4.05,0.35,-0.8,0  
3EAZ,ASP\_159,3.73,0.35,-0.42,0  
2QRX,LYS\_75,10.43,-0.07,0,0  
2Q5X,ASP\_763,3.87,0.07,0,0  
3V55,TYR\_620,10.77,0,0,0.77  
2EEY,ASP\_136,2.96,0.21,-1.06,0  
2D2S,GLU\_681,4.5,0,0,0  
2P65,LYS\_77,10.15,-0.35,0,0  
1RH5,ASP\_110,11.64,-4.35,0,3.49  
3AU3,GLU\_601,3.03,0.28,-1.75,0  
3A0X,GLU\_645,4.71,0.21,0,0  
1U53,LYS\_41,10.29,-0.21,0,0  
3T5B,ARG\_199,11.1,-1.4,0,0  
1P6F,ARG\_70,12.22,-0.28,0,0  
1NRI,ARG\_26,12.29,-0.21,0,0  
2R51,LYS\_28,10.22,-0.28,0,0  
2OSA,CYS\_391,9.55,0,0,0.55  
2FL4,TYR\_51,10,0,0,0  
2W2S,ARG\_88,11.94,-0.56,0,0  
1O59,GLU\_311,4.5,0,0,0  
1C3K,ASP\_136,3.8,0,0,0  
4FH3,ARG\_66,12.15,-0.35,0,0  
1XKR,ASP\_127,3.82,0.14,-0.12,0  
3BQW,GLU\_194,4.5,0,0,0  
3LJC,ARG\_97,12.65,-2.25,0,2.4  
3I47,GLU\_78,4.5,0,0,0  
2XHC,ASP\_303,3.23,0.49,-1.05,0  
2QV2,GLU\_126,3.44,0.21,-1.27,0  
4FZR,ASP\_167,3.73,0,-0.07,0  
2CWC,TYR\_112,13.39,0.21,0.78,2.4  
2GZQ,LYS\_124,10.22,-0.28,0,0  
3O16,GLU\_69,4.57,0.07,0,0  
1ZP2,ARG\_115,12.15,-0.35,0,0  
2PIM,ASP\_32,2.68,0.28,-1.4,0  
2E3S,LYS\_488,10.08,-0.42,0,0  
2AZL,GLU\_184,4.07,0.28,-0.71,0  
2OYZ,LYS\_84,10.5,0,0,0  
3EZ7,TYR\_41,10.07,0.07,0,0  
2H30,ASP\_45,0.21,0.63,-4.23,0  
2BAA,ARG\_55,12.76,-1.03,0,1.29  
1MTZ,TYR\_152,11.83,0.07,0,1.76  
4H89,ARG\_116,11.87,-0.63,0,0  
1W7B,ARG\_37,12.5,0,0,0  
3ANJ,GLU\_10,1.79,0.49,-3.2,0  
3GG6,TYR\_169,11.37,0,0,1.37  
3OIP,GLU\_172,3.19,0.14,-1.45,0  
2G9D,LYS\_249,10.5,0,0,0  
4ETX,GLU\_254,4.64,0.14,0,0  
2OJQ,GLU\_617,4.57,0.07,0,0  
1FO9,GLU\_258,3.18,0.56,-1.88,0  
1OGL,ASP\_187,3.87,0.07,0,0  
2GEN,ARG\_74,12.5,0,0,0  
1Y2Q,ARG\_2,11.94,-0.56,0,0  
4GA2,LYS\_115,10.29,-0.21,0,0  
2O8P,ASP\_9,1.52,0.35,-2.64,0  
2EDM,LYS\_59,10.36,-0.14,0,0  
1LN4,GLU\_38,4.01,0.28,-0.77,0  
2EDM,ASP\_170,3.61,0.21,-0.39,0  
2JEO,GLU\_111,4.02,0.07,-0.55,0  
3CX5,ASP\_126,4.08,0.28,0,0  
3G59,ASP\_201,3.07,0.56,-1.29,0

2D7U,GLU\_14,3.37,4.88,-3.54,-2.47  
 2FL7,TYR\_101,11.15,0.81,0,0.34  
 3M66,ASP\_165,1.79,0.56,-2.57,0  
 1R15,ARG\_126,12.5,0,0,0  
 2BDV,LYS\_63,10.22,-0.28,0,0  
 2B02,LYS\_432,10.29,-0.21,0,0  
 3E7P,LYS\_100,10.5,0,0,0  
 2I88,LYS\_469,9.94,-0.56,0,0  
 3DTE,ASP\_98,3.87,0.14,-0.07,0  
 1WOU,LYS\_89,10.5,0,0,0  
 2GKG,ARG\_115,12.01,-0.49,0,0  
 2O0K,TYR\_77,12.92,0.07,0.45,2.4  
 1YG2,HIS\_5,6.19,0.04,0,-0.35  
 1R16,ARG\_141,12.15,-0.35,0,0  
 3BCH,ASP\_44,2.95,0.42,-1.28,0  
 3CN5,CYS\_127,10.26,0,0,1.26  
 3B21,HIS\_145,6.97,1.62,2.3,-3.36  
 2ZCO,GLU\_250,1.68,0.35,-1.5,-1.68  
 1WXQ,ASP\_47,3.93,0.14,-0.01,0  
 3AU3,ASP\_432,3.62,0.21,-0.39,0  
 1RKA,ARG\_129,11.94,-0.56,0,0  
 1WNH,ARG\_171,11.8,-0.7,0,0  
 3G69,GLU\_231,4.5,0,0,0  
 3CN5,TYR\_90,10,0,0,0  
 3DSH,ARG\_328,12.23,-1.49,0,1.22  
 2POL,ASP\_134,3.62,0.07,-0.24,0  
 3OA7,ARG\_528,12.36,-0.14,0,0  
 1YLN,ARG\_140,12.22,-0.28,0,0  
 1NAR,HIS\_234,6.43,0,0,-0.07  
 2H2Z,ASP\_245,3.76,0,-0.04,0  
 1E59,ARG\_154,12.15,-0.35,0,0  
 1R29,HIS\_46,6.78,0.42,0,-0.14  
 1L2F,GLU\_15,4.5,0,0,0  
 1ZHV,GLU\_23,4.05,0.28,-0.73,0  
 3R87,ASP\_42,3.79,0,-0.01,0  
 2X4L,LYS\_264,10.08,-0.42,0,0  
 1D2K,TYR\_418,10.8,0.52,0,0.28  
 2RIK,LYS\_82,10.5,0,0,0  
 2GAU,TYR\_140,10.51,0,0,0.51  
 1ZHV,ASP\_41,3.85,0.35,-0.3,0  
 2HRZ,GLU\_304,4.45,0.21,-0.26,0  
 4AE7,LYS\_231,10.5,0,0,0  
 3I4T,TYR\_125,10,0,0,0  
 1MTZ,LYS\_23,10.5,0,0,0  
 2I6I,TYR\_2,11.75,1.63,0,0.12  
 2ZTY,CYS\_147,7.45,-3.51,0,1.96  
 2AD1,LYS\_86,10.36,-0.14,0,0  
 3GE9,HIS\_91,6.5,0,0,0  
 3RKV,ASP\_331,3.93,0.14,-0.01,0  
 2IXM,ARG\_193,12.06,-3.21,0,2.78  
 1D2K,TYR\_350,10.48,0.73,-0.25,0  
 2AZL,GLU\_18,3.91,0.21,-0.8,0  
 1R16,HIS\_237,5.81,2.38,2.4,-5.48  
 1C3K,LYS\_67,9.94,-0.56,0,0  
 2H01,LYS\_126,10.29,-0.21,0,0  
 2IXM,LYS\_62,9.8,-0.7,0,0  
 2W0G,ASP\_170,3.92,0.21,-0.09,0  
 3PP8,LYS\_170,10.22,-0.28,0,0  
 1XEU,HIS\_103,6.5,0.8,1.42,-2.22  
 2AXO,ARG\_137,12.01,-0.49,0,0  
 1U7U,ASP\_375,3.8,0.35,-0.35,0  
 2CBE,ASP\_190,2.83,0.35,-1.31,0  
 2I6I,TYR\_50,10.46,0,0,0.46  
 1GQE,ARG\_150,11.94,-0.56,0,0  
 3J5N,ASP\_76,3.54,0.42,-0.68,0  
 1W7B,ARG\_78,12.43,-0.07,0,0  
 2YT4,GLU\_642,4.83,0.21,0,1.2  
 2PPN,LYS\_105,10.29,-0.21,0,0  
 3EX9,GLU\_146,4.04,0.21,-0.67,0  
 2ZCX,GLU\_81,2.52,0.42,-2.4,0  
 1Y2Q,GLU\_55,3.37,0.84,-1.97,0  
 4H4J,ASP\_91,3.89,0.14,-0.05,0  
 2P0Y,ASP\_316,3.53,0.07,-0.34,0  
 3NBI,ASP\_195,3.87,0.07,0,0  
 3BB7,GLU\_44,4.78,0.28,0,0  
 2FZ4,ARG\_110,10.58,-1.92,0,0  
 1XIP,GLU\_288,4.57,0.07,0,0  
 3QAV,ASP\_127,2.93,0.35,-1.22,0  
 3QKY,ARG\_175,12.15,-0.35,0,0  
 1RHS,ARG\_121,11.66,-0.84,0,0  
 2CN1,GLU\_136,3.71,0.49,-1.28,0  
 1J33,GLU\_280,4.07,2.23,-0.93,-1.73  
 2O0K,ASP\_131,3.94,0.14,0,0  
 2Q99,ASP\_159,3.57,0.14,-0.38,0  
 2IN0,ARG\_54,11.87,-0.63,0,0  
 3FK5,HIS\_113,7.23,0.8,0,-0.07  
 2GAU,ARG\_15,12.22,-0.28,0,0  
 1L2H,LYS\_16,9.66,-0.84,0,0  
 3V46,TYR\_341,10.54,1.79,-0.8,-0.45  
 1RKA,LYS\_160,10.5,0,0,0  
 3JZN,LYS\_106,9.94,-0.56,0,0  
 1VJG,ARG\_63,13.16,-1.66,0.2,3.2  
 3PBH,TYR\_136,12.68,0.28,0.2,4  
 3BQW,GLU\_273,4.5,0,0,0  
 2R05,LYS\_188,10.5,0,0,0  
 1XDZ,ASP\_30,3.8,0.14,-0.14,0  
 350A,LYS\_18,10.43,-0.07,0,0  
 1JSX,GLU\_130,4.5,0,0,0  
 4FLE,HIS\_33,6.5,0,0,0  
 1X6J,ARG\_74,12.43,-0.07,0,0  
 2PGX,ARG\_74,12.15,-0.35,0,0  
 2RIK,LYS\_126,10.5,0,0,0  
 1SIG,ARG\_232,12.15,-0.35,0,0  
 1UXO,ASP\_110,3.51,0.56,-0.85,0  
 2YLF,HIS\_80,7.41,0.98,0,-0.07  
 2DG7,ASP\_74,3.03,0.35,-1.12,0  
 3RFY,GLU\_302,4.5,0,0,0  
 2PLQ,HIS\_107,6.15,0,0,-0.35  
 1T3Y,GLU\_44,4.57,0.07,0,0  
 1XEU,LYS\_236,10.29,-0.21,0,0  
 1WYC,GLU\_199,3.76,0.42,-1.16,0  
 3F1X,HIS\_207,6.29,0,0,-0.21  
 2AZL,GLU\_213,4.64,0.14,0,0  
 3DZ1,LYS\_268,10.5,0,0,0  
 2WB8,LYS\_773,10.22,-0.28,0,0  
 2G9D,GLU\_29,4.5,0,0,0  
 3HVM,CYS\_312,9.56,-1.97,0.1,2.44  
 1EW4,ASP\_29,3.99,0.21,-0.02,0  
 3EVP,LYS\_79,10.43,-0.07,0,0  
 1ZCU,LYS\_208,10.29,-0.21,0,0  
 2BCF,HIS\_178,9.72,1.63,3.64,-2.05  
 1U3Y,ASP\_302,2.59,0.49,-1.7,0  
 3ADO,ASP\_221,3.45,0.21,-0.56,0  
 2B61,LYS\_308,10.29,-0.21,0,0  
 3FHF,HIS\_0,7.09,0.66,0,-0.07  
 2D7J,CYS\_186,10.36,-0.2,0,1.56  
 2CN1,LYS\_117,10.36,-0.14,0,0  
 3LPZ,GLU\_26,4.5,0,0,0  
 2B78,HIS\_354,8.2,1.98,0,-0.28  
 3EGN,GLU\_433,4.57,0.07,0,0  
 3I4T,LYS\_234,10.36,-0.14,0,0  
 2EYI,GLU\_30,3.48,0.35,-1.38,0  
 1QCV,CYS\_123,9.92,0.43,0,0.49  
 1PDB,ARG\_32,11.94,-0.56,0,0  
 3GFP,ASP\_363,3.57,0.28,-0.51,0  
 2F9F,HIS\_54,6.5,0,0,0  
 1FO9,ARG\_363,12.29,-0.21,0,0  
 2FZP,HIS\_312,6.29,0,0,-0.21  
 2PGX,ASP\_48,3.06,0.42,-1.16,0  
 3CJW,LYS\_362,10.43,-0.07,0,0  
 1GVP,LYS\_87,10.5,0,0,0  
 3M7D,GLU\_372,3.91,0.21,-0.8,0  
 2PIM,CYS\_114,7.64,-1.36,0,0  
 3EUR,GLU\_75,4.64,0.14,0,0  
 3UPD,HIS\_149,6.58,1.6,1.77,-3.28  
 3OBS,ASP\_104,1.8,1.19,-3.18,0  
 1R2Z,TYR\_53,12.95,1.35,0,1.6  
 2X4G,LYS\_151,10.43,-0.07,0,0  
 3E7P,HIS\_68,7.21,0.92,0,-0.21  
 2PPN,LYS\_35,10.08,-0.42,0,0  
 2YWJ,LYS\_135,10.15,-0.35,0,0  
 2B61,GLU\_54,3.64,0.35,-1.2,0  
 1EV8,HIS\_57,6.29,0,0,-0.21  
 2OPJ,ARG\_128,13.47,-3.48,0.4,4.5  
 1MTZ,TYR\_9,11.16,0,-0.09,1.25  
 2BQQ,TYR\_103,10,0,0,0  
 3GS9,ASP\_102,3.9,0.14,-0.04,0  
 3SMD,GLU\_12,4.78,0.28,0,0  
 1WLJ,ARG\_279,11.08,-1.42,0,0  
 3U2R,GLU\_135,4.92,0.42,0,0  
 3U2R,HIS\_56,6.34,0.05,0,-0.21  
 3RJK,CYS\_319,8.75,0,-1.58,1.33  
 2HP7,GLU\_154,2.03,0.73,-3.2,0  
 1YTD,GLU\_23,4.5,0,0,0  
 1J7G,GLU\_104,4.46,0.14,-0.18,0  
 1MTZ,HIS\_181,3.02,0.8,-0.29,-4  
 3ONH,LYS\_457,10.36,-0.14,0,0  
 3V75,ARG\_173,11.94,-0.56,0,0  
 3PBH,TYR\_214,9.15,0.15,-0.08,-0.92  
 3T5B,GLU\_345,4.5,0,0,0  
 2FB6,GLU\_109,3.53,0.63,-1.6,0  
 4F8A,ASP\_587,3.65,0,-0.15,0  
 2PWO,GLU\_3,3.32,0.42,-1.6,0  
 3EZ7,GLU\_65,4.6,0.14,-0.04,0  
 1UXO,ASP\_179,4.01,0.21,0,0  
 1KN3,ASP\_134,2.49,0.28,-1.59,0  
 3IV4,ASP\_50,3.87,0.07,0,0  
 2FD5,ARG\_66,11.84,-2.22,0,1.56  
 3EVZ,ASP\_55,3.94,0.35,-0.21,0  
 1IAP,ARG\_232,12.43,-0.07,0,0  
 2E0T,ARG\_112,12.43,-0.07,0,0  
 3LPZ,ARG\_14,12.43,-0.07,0,0  
 3EJG,ASP\_139,3.79,0.28,-0.29,0  
 2PPN,ASP\_41,3.06,0.28,-1.01,0  
 3LJN,HIS\_210,2.68,0,0,-3.82  
 2ZCO,ARG\_34,11.87,-0.63,0,0  
 3ETV,ARG\_104,12.22,-0.28,0,0  
 3V3T,GLU\_61,4.5,0,0,0  
 2H80,LYS\_206,9.73,-0.77,0,0  
 2B0A,GLU\_19,3.94,0.07,-0.63,0  
 3M7G,ARG\_108,12.15,-0.35,0,0  
 2B78,ARG\_200,13.62,-2.09,0.3,2.1  
 3RLE,GLU\_154,4.5,0,0,0  
 1MML,ASP\_235,3.77,0.07,-0.1,0  
 1NIJ,GLU\_171,4.53,0.07,-0.03,0  
 2X4L,LYS\_250,10.22,-0.28,0,0  
 3BCY,HIS\_156,7.24,0.88,0,-0.14  
 2AZP,ARG\_272,11.73,-0.77,0,0  
 3E7P,ASP\_19,4.12,0.63,-0.31,0  
 3C01,LYS\_76,10.5,0,0,0  
 3GV0,LYS\_65,10.5,0,0,0  
 1PV5,GLU\_208,4.85,0.35,0,0  
 3Q9P,ARG\_140,12.22,-0.28,0,0  
 1OGL,LYS\_251,10.01,-0.49,0,0  
 1SFE,ASP\_42,3.28,0.28,-0.8,0  
 3P29,LYS\_205,9.45,-1.05,0,0  
 3BA1,ARG\_146,11.66,-0.84,0,0  
 1Z9L,ARG\_51,11.66,-0.84,0,0  
 2WB8,ASP\_578,3.39,0.42,-0.83,0  
 3M70,ASP\_114,3.47,0.14,-0.47,0  
 2VGM,HIS\_290,7.73,1.44,0,-0.21  
 2OKT,LYS\_40,10.43,-0.07,0,0  
 2IQT,TYR\_240,8.35,0.14,0,-1.79  
 3GV0,GLU\_274,4.5,0,0,0  
 2H2W,ARG\_56,12.7,-1.65,0,1.85  
 1YM5,CYS\_88,10.64,-0.19,0,1.83  
 2EEY,ARG\_158,12.22,-0.28,0,0  
 2D7U,GLU\_313,1.67,0.55,-1.66,-1.72  
 3ETU,GLU\_78,4.71,0.21,0,0  
 1JYH,GLU\_124,4.72,0.28,-0.06,0  
 1U7U,CYS\_274,12.06,0.0,1.3,2.93  
 1A8Q,CYS\_195,7.63,-3.6,-0.44,2.67  
 2YX0,LYS\_133,10.43,-0.07,0,0  
 3V55,ASP\_645,4.25,0.49,-0.04,0  
 1UCH,ARG\_215,11.11,-1.9,0,0.51  
 1O17,LYS\_222,10.43,-0.07,0,0  
 1Q46,GLU\_124,4.64,0.14,0,0  
 1O59,HIS\_228,6.5,0,0,0  
 2EA9,HIS\_61,6.53,0.45,0,-0.42  
 3CCY,CYS\_41,8.66,-0.34,0,0  
 3RAZ,GLU\_142,4.4,0.14,-0.24,0  
 3H13,TYR\_463,10,1.03,-1.03,0  
 3LMO,ARG\_20,11.94,-0.56,0,0  
 1SIG,ARG\_260,11.93,-0.57,0,0  
 1PVT,HIS\_125,2.22,0.35,-1.65,-2.99  
 3TRE,TYR\_76,10.78,0.14,0,0.64  
 1WJG,ARG\_108,12.01,-0.49,0,0  
 3ZTA,LYS\_22,10.43,-0.07,0,0  
 1QQE,ASP\_252,2.65,0.63,-1.78,0  
 1RKA,ARG\_276,12.08,-0.42,0,0  
 2IXM,ARG\_148,12.01,-0.49,0,0  
 3PB8,CYS\_164,8.01,-1.44,0,0.45  
 2H14,LYS\_296,10.5,0,0,0  
 1UXO,HIS\_83,6.5,0,0,0  
 2JKF,TYR\_101,11.65,1.65,0,0  
 1R6Y,GLU\_35,4.64,0.14,0,0  
 15I7,LYS\_293,10.5,0,0,0  
 2SPWQ,ASP\_13,3.34,0.35,-0.81,0  
 2Z0W,GLU\_15,2.94,0.42,-1.98,0  
 3RAZ,ARG\_103,12.01,-0.49,0,0  
 3QAV,ASP\_124,3.63,0.28,-0.45,0  
 3GFP,GLU\_356,4.5,0,0,0  
 4DIU,GLU\_206,4.45,0.28,-0.33,0  
 2LJN,HIS\_480,5.79,2.194,-4.65  
 4ECC,HIS\_31,6.36,0,0,-0.14  
 2Z61,ASP\_86,3.03,0,-0.77,0  
 3G6S,GLU\_145,3.91,0.21,-0.8,0  
 3GA2,GLU\_159,3.87,0.07,-0.7,0  
 2AD1,ASP\_30,3.76,0.07,-0.11,0  
 3FHF,LYS\_30,10.15,-0.35,0,0  
 1PSW,LYS\_92,10.36,-0.14,0,0  
 4H4J,LYS\_233,10.43,-0.07,0,0  
 3PB8,ARG\_55,11.66,-0.84,0,0  
 4EKU,LYS\_198,10.5,0,0,0  
 2ATR,HIS\_17,7.46,1.1,0,-0.14  
 3VJ8,GLU\_229,4.77,0.27,0,0  
 1L2F,LYS\_134,10.22,-0.28,0,0  
 1N81,TYR\_49,11.82,0.53,-0.57,1.86  
 1X7F,GLU\_343,3.68,0.28,-1.1,0  
 3EYE,GLU\_55,4.5,0,0,0  
 1O5T,LYS\_96,10.5,0,0,0  
 2RJD,TYR\_275,10,0,0,0  
 2CN1,GLU\_185,3.8,0.42,-1.12,0  
 2IF4,ASP\_285,3.5,0.14,-0.44,0  
 3CX2,HIS\_206,6.57,0.28,0,-0.21  
 1JSX,CYS\_151,10.62,0,0,1.62

1P6F,GLU\_137,4.03,0.35,-0.82,0  
1YTD,ARG\_127,12.31,-2.27,0,2.07  
1PZC,LYS\_24,9.8,-0.7,0,0  
2CXY,LYS\_65,10.43,-1.07,0,0  
2IF4,CYS\_239,8.62,-1.03,0,0.65  
1PDB,HIS\_130,7.33,1.04,0,-0.21  
1J85,HIS\_86,4.14,0.19,0,-2.55  
1JT9,GLU\_73,2.54,1.69,-3.11,-0.54  
4FZR,GLU\_159,4.36,0.21,-0.35,0  
1X04,ARG\_142,11.87,-0.63,0,0  
2CIU,HIS\_175,4.01,0.39,0,-2.88  
1PZC,LYS\_117,10.29,-0.21,0,0  
2OKT,LYS\_88,10.43,-0.07,0,0  
3EJC,GLU\_28,3.58,0.28,-1.2,0  
2PP6,ARG\_19,12.22,-0.28,0,0  
1LTU,ASP\_105,3.54,0.18,-0.54,0  
1LTU,ARG\_226,10.8,-1.7,0,0  
3L7N,CYS\_162,2.61,-7.42,-0.34,1.37  
1TP6,CYS\_127,8.96,-0.04,0,0  
3JZN,HIS\_185,6.5,0,0,0  
2B6P,HIS\_122,6.42,0.06,0,-0.14  
3S0A,GLU\_73,4.57,0.07,0,0  
3G53,ARG\_27,12.36,-0.14,0,0  
1OST,LYS\_432,10.5,0,0,0  
1P4X,LYS\_8,9.66,-0.84,0,0  
4AM1,ASP\_41,3.08,0.21,-0.93,0  
3ADO,CYS\_141,10.64,-0.01,0.11,1.55  
2B02,ARG\_379,11.59,-0.91,0,0  
3A7L,ASP\_86,3.94,0.14,0,0  
2FBI,LYS\_139,10.5,0,0,0  
3B7X,HIS\_67,6.5,0,0,0  
1WNH,ASP\_186,1.78,1.05,-3.08,0  
2YT4,ARG\_570,12.08,-0.42,0,0  
2EHG,GLU\_120,4.71,0.21,0,0  
3SMD,ASP\_96,2.75,0.77,-1.82,0  
1OLR,HIS\_138,6.36,0,0,-0.14  
3CX2,CYS\_249,9,0,0,0  
1RWZ,LYS\_199,10.29,-0.21,0,0  
1KN3,ASP\_96,4.05,0.63,-0.37,0  
3DB9,LYS\_100,10.29,-0.21,0,0  
1TD6,LYS\_185,10.5,0,0,0  
1G8P,ARG\_229,12.5,0,0,0  
2QK0,ARG\_80,11.45,-1.05,0,0  
1ZBM,LYS\_24,10.36,-0.14,0,0  
2R57,CYS\_359,8.59,-0.46,-1.41,1.46  
1ZBS,GLU\_80,4.03,0.28,-0.75,0  
4H86,GLU\_45,4.78,0.28,0,0  
3ASA,GLU\_377,4.5,0,0,0  
2YWJ,TYR\_104,13.61,0.41,0.8,2.4  
3P29,LYS\_265,10.43,-0.07,0,0  
3FFM,GLU\_143,4.57,0.07,0,0  
1XWM,GLU\_91,6.56,0.79,-0.69,1.95  
4DBX,ARG\_178,11.8,-0.7,0,0  
3BZT,TYR\_272,10,0,0,0  
2ZQ5,GLU\_172,5.76,2.57,-1.75,0.44  
3O16,GLU\_172,4.78,0.28,0,0  
3UC9,ASP\_55,2.59,0.7,-1.91,0  
2O4D,GLU\_22,3.13,0.85,-1.65,-0.57  
1R22,GLU\_59,3.93,0.63,-1.2,0  
4EVF,HIS\_146,2.76,0,-0.17,-3.57  
1TR9,GLU\_307,3.22,0.28,-1.57,0  
3B4D,LYS\_223,10.5,0,0,0  
1T6L,HIS\_145,7.95,1.6,2.4,-2.55  
3LJ,HIS\_180,7.5,1.07,0,-0.07  
3SMD,LYS\_73,10.5,0,0,0  
3K8J,ARG\_61,11.87,-0.63,0,0  
2BV9,CYS\_158,11.18,-1.61,1.79,1.99  
1ZBS,TYR\_248,10.53,1.7,-1.17,0  
3F1X,ARG\_164,12.9,-2.83,0,3.23  
1XIP,ASP\_74,3.31,0.28,-0.77,0  
4DBX,ASP\_237,3.72,0.07,-0.15,0  
3I4T,ASP\_225,2.8,0.56,-1.56,0  
3LJC,LYS\_239,10.43,-0.07,0,0  
3OIP,LYS\_147,10.29,-0.21,0,0  
3CN5,ARG\_265,12.22,-0.28,0,0  
1OI7,ARG\_117,11.92,-0.63,0,0.05  
1J74,ASP\_99,3.08,0.77,-1.5,0  
1TD6,HIS\_140,6.29,0,-0.21  
1S7K,CYS\_134,9.25,-0.08,0,0.33  
3EJC,LYS\_6,10.5,0,0,0  
1ES9,CYS\_205,13.57,0.47,2.4,1.7  
2H85,LYS\_109,10.5,0,0,0  
2CWY,ARG\_13,11.94,-0.56,0,0  
1UAJ,ARG\_183,12.5,0,0,0  
2FM9,ASP\_223,2.75,0.63,-1.68,0  
3EVZ,LYS\_244,9.94,-0.56,0,0  
1XFK,TYR\_248,10.54,0,0,0.54  
2R51,TYR\_194,11.44,0,0,1.44  
2FL4,LYS\_14,10.36,-0.14,0,0  
3FTT,LYS\_127,10.15,-0.35,0,0  
2EYI,HIS\_170,6.04,0.03,0,-0.49  
2PGX,ASP\_58,2.76,0.63,-1.67,0  
3CN5,HIS\_260,6.3,0.01,0,-0.21  
1SQH,ARG\_207,12.01,-0.49,0,0  
1YTD,ASP\_49,3.52,0.07,-0.35,0  
1V8E,ARG\_54,11.41,-1.09,0,0  
3N0K,ARG\_33,12.36,-0.14,0,0  
2EEY,HIS\_97,6.15,0,0,-0.35  
1MUF,ARG\_323,12.01,-0.49,0,0  
2DFL,ARG\_242,12.29,-0.21,0,0  
1CHD,GLU\_156,4.15,0.21,-0.56,0  
3CN5,TYR\_122,9.22,1.59,-0.8,-1.57  
3SMD,TYR\_7,10.73,0.07,-0.27,0.92  
3U2R,ASP\_11,3.08,0.07,-0.79,0  
2EFK,ARG\_35,12.36,-0.14,0,0  
1HF8,ASP\_263,4.15,0.35,0,0  
2AD1,ASP\_280,3.49,0.49,-0.8,0  
2CN1,TYR\_103,12.09,2.61,-0.52,0  
3EVZ,ARG\_40,11.87,-0.63,0,0  
2W1R,GLU\_159,4.92,0.42,0,0  
2AHE,GLU\_241,4.93,0.49,-0.06,0  
1JB3,ARG\_84,11.59,-0.91,0,0  
1J85,GLU\_53,1.68,0.77,-3.59,0  
3G9G,LYS\_152,9.94,-0.56,0,0  
2NRK,GLU\_14,4.64,0.14,0,0  
1P1L,ARG\_88,12.5,0,0,0  
3M3P,GLU\_135,4.79,1.09,-0.8,0  
3MEW,ARG\_208,12.43,-0.07,0,0  
2B78,ARG\_281,12.01,-0.49,0,0  
2WZ9,ARG\_114,12.08,-0.42,0,0  
2P52,TYR\_160,10.84,0.92,-1.11,1.04  
4AE7,GLU\_179,4.57,0.42,0,0  
4EF5,HIS\_332,2.52,0.78,-1.87,-2.89  
4F3J,HIS\_237,6.69,0.26,0,-0.07  
3CS1,LYS\_165,10.08,-0.42,0,0  
2QV2,TYR\_51,10.07,0,0,0.07  
3LJN,GLU\_119,3.91,0.21,-0.8,0  
2I6I,ARG\_127,12.08,-0.42,0,0  
2ATR,LYS\_110,10.29,-0.21,0,0  
2H85,TYR\_278,12.7,1.09,0,1.61  
3M7G,GLU\_186,4.02,0.14,-0.62,0  
3LJC,HIS\_24,6.29,0,-0.21  
4EZB,ARG\_289,11.87,-0.63,0,0  
4ETX,ARG\_376,12.08,-0.42,0,0  
4HDE,TYR\_183,10.22,0.28,-0.06,0  
1F2V,ARG\_87,12.01,-0.49,0,0  
2ATR,LYS\_89,10.5,0,0,0  
3OIP,TYR\_70,12.6,1.94,-0.05,0.7  
1EQ6,ASP\_126,3.49,0.49,-0.8,0  
2BCF,LYS\_106,10.43,-0.07,0,0  
1RI6,TYR\_51,9.98,0.07,-0.8,0.71  
1UOH,ASP\_68,3.85,0.14,-0.09,0  
2GZQ,ARG\_190,12.22,-0.28,0,0  
4D8L,TYR\_49,10,0,0,0  
3NR5,GLU\_70,2.83,0.7,-2.37,0  
1ILW,ARG\_135,12.15,-0.35,0,0  
2IRM,ARG\_173,12.36,-0.14,0,0  
3LQE,ARG\_322,13.6,-0.38,0,1.48  
1RL0,ASP\_134,2.12,0.63,-2.31,0  
3H5T,ARG\_222,13.85,-0.86,0,2.21  
1KN3,ASP\_174,1.44,1.05,-3.4,0  
3EIZ,TYR\_130,10,0,0,0  
3DSH,ARG\_396,12.5,0,0,0  
1PDB,GLU\_78,4.43,0.28,-0.35,0  
2H2Z,ASP\_216,3.24,0.42,-0.97,0  
2H14,GLU\_322,3.56,0.14,-1.08,0  
1NIJ,HIS\_170,6.36,0,0,-0.14  
2PGE,ARG\_80,12.08,-0.42,0,0  
1XTD,GLU\_109,4.5,0,0,0  
1WLY,CYS\_89,11.58,-0.35,-0.06,2.99  
1D70,HIS\_56,6.43,0,0,-0.07  
3GV0,GLU\_121,4.5,0,0,0  
3CAX,ARG\_394,12.08,-0.42,0,0  
3J5N,ASP\_135,1.93,0.77,-2.64,0  
3LQE,GLU\_292,4.85,0.35,0,0  
1K95,ARG\_145,11.8,-0.7,0,0  
1WXQ,ASP\_98,3.75,0.49,-0.55,0  
3DHN,HIS\_47,6.43,0,0,-0.07  
1ES9,TYR\_191,12.09,0.07,0,2.02  
2WZ9,LYS\_111,10.22,-0.28,0,0  
2OSA,GLU\_334,4.64,0.14,0,0  
1AT0,GLU\_307,3.98,0.28,-0.8,0  
1MTZ,TYR\_159,13.29,0.14,0.75,2.4  
3IVF,GLU\_252,3.84,0.14,-0.8,0  
3ADO,HIS\_294,7.02,0.8,0,-0.28  
2X4L,ASP\_262,3.28,0.28,-0.8,0  
1LZL,GLU\_307,3.53,0.63,-1.6,0  
3T57,HIS\_119,6.43,0,0,-0.07  
2X4G,ASP\_38,4.08,0.28,0,0  
3PM2,ARG\_74,11.73,-0.77,0,0  
2OOK,LYS\_99,10.29,-0.21,0,0  
4EVF,ASP\_16,4.11,0.35,-0.04,0  
2IXM,ASP\_113,3.94,0.14,0,0  
2DG7,ASP\_5,1.42,0.42,-2.8,0  
1NIJ,ARG\_115,4.5,0,0,0  
1ZCE,LYS\_13,10.36,-0.14,0,0  
1SFE,GLU\_111,4.57,0.07,0,0  
1OST,HIS\_387,7.23,0.73,0,0  
3T8R,GLU\_33,4.71,0.21,0,0  
2OKT,ARG\_100,12.99,-1.91,0,2.4  
1RI5,ASP\_203,3.87,0.07,0,0  
3F53,LYS\_170,10.36,-0.14,0,0  
1DCF,HIS\_81,6.43,0,0,-0.07  
2PLQ,TYR\_227,10.32,0.32,0,0  
3F6F,ARG\_35,12.5,0,0,0  
1RI5,GLU\_202,4.5,0,0,0  
2H85,GLU\_41,4.37,0.28,-0.41,0  
1NAF,HIS\_186,6.5,0,0,0  
1Y2Q,LYS\_59,9.8,-0.7,0,0  
2F9F,GLU\_79,3.04,0.14,-1.6,0  
2FZP,CYS\_291,9.95,-0.51,1.08,0.38  
2ZCO,HIS\_78,6.44,0.22,0,-0.28  
1X04,GLU\_68,4.12,0.42,-0.8,0  
1ZHV,LYS\_114,10.43,-0.07,0,0  
2B3M,ARG\_111,12.29,-0.21,0,0  
2ROS,HIS\_177,6.52,0.09,0,-0.07  
2C2Y,ARG\_12,11.66,-0.84,0,0  
1ZHV,HIS\_124,3.99,0.6,0,-3.11  
1YLN,ARG\_94,12.36,-0.14,0,0  
1WYC,HIS\_38,7.01,0.86,0,-0.35  
1X7F,CYS\_165,8.95,-0.85,0,0.8  
3GA2,ARG\_180,11.24,-1.26,0,0  
2E35,ARG\_582,12.22,-0.28,0,0  
1OLR,ARG\_84,12.5,0,0,0  
3OIP,CYS\_124,10.79,0,0,1.79  
3CQ1,GLU\_22,4.64,0.14,0,0  
3CJW,ASP\_235,3.8,0,0,0  
3CBN,ARG\_118,11.74,-0.76,0,0  
2E0T,HIS\_119,6.5,0,0,0  
2W0G,GLU\_201,4.5,0,0,0  
1XTZ,LYS\_185,10.43,-0.07,0,0  
2V1L,GLU\_40,4.5,0,0,0  
3P28,GLU\_94,3.5,0.28,-1.28,0  
1WXF,ASP\_94,8.38,-0.69,0,0.07  
2OYZ,TYR\_93,11.71,0,0,0.7,1.64  
3KT9,TYR\_94,13.19,0.21,0.58,2.4  
2AXO,GLU\_47,3.6,3.87,-2.37,-2.4  
4GCO,ASP\_241,2.56,0.63,-1.87,0  
1N81,LYS\_150,10.5,0,0,0  
2JEO,ASP\_156,3.55,0.21,-0.45,0  
2Q12,TYR\_48,10.07,0.07,0,0  
2D0A,HIS\_226,4.81,0,0,-1.69  
2FGG,LYS\_9,10.5,0,0,0  
3AU3,ASP\_397,3.06,0,-0.74,0  
3SMD,LYS\_9,10.5,0,0,0  
3J5N,CYS\_202,12.15,-0.35,0,0  
1J33,ASP\_14,3.86,0.21,-0.15,0  
3EIZ,LYS\_136,10.29,-0.21,0,0  
1ZBS,ARG\_103,13.99,-1.36,0,2.85  
2AHE,HIS\_196,1.76,0.01,-1.57,-3.18  
3CRM,ASP\_302,3.18,0.91,-1.53,0  
3U2A,ARG\_150,12.22,-0.28,0,0  
3IL3,GLU\_57,3.98,0.28,-0.8,0  
1Z3X,ARG\_189,11.45,-1.05,0,0  
1JK5,TYR\_129,9.12,0.14,-1.02,0  
4DVD,GLU\_103,4.12,0.42,-0.8,0  
2QVO,GLU\_56,4.5,0,0,0  
3U4K,TYR\_117,9.94,0,-0.06,0  
3EX9,CYS\_80,9.07,0,0,0.07  
2AZL,ASP\_35,3.28,0.7,-1.22,0  
2Q07,LYS\_470,10.5,0,0,0  
1O59,GLU\_129,3.32,0.42,-1.6,0  
1HF8,LYS\_221,9.8,-0.7,0,0  
4AM1,ARG\_256,11.73,-0.77,0,0  
1XIP,ARG\_181,11.38,-1.12,0,0  
3M66,LYS\_275,10.5,0,0,0  
2PWQ,GLU\_42,4.72,0.28,-0.06,0  
2GZQ,ARG\_84,12.5,0,0,0  
2H80,ARG\_42,12.08,-0.42,0,0  
3P29,TYR\_114,13.41,0.21,0.8,2.4  
1WRU,LYS\_257,10.5,0,0,0  
4FZR,ASP\_200,3.75,0.56,-0.61,0  
3ONH,ASP\_479,1.62,0.84,-3.03,0  
3V46,GLU\_374,3.87,0.07,-0.7,0  
1XIP,GLU\_320,4.34,0.07,-0.23,0  
2WB8,GLU\_516,3.62,0.77,-1.65,0  
2PP6,CYS\_31,8.77,-0.38,0,0.15  
3K8U,LYS\_43,10.36,-0.14,0,0  
2YWJ,CYS\_75,4.68,-3.95,-2.4,2.03  
3FTT,HIS\_114,6.48,0.05,0,-0.07  
3JZ9,ASP\_512,3.21,0.21,-0.8,0  
4DBX,LYS\_155,10.5,0,0,0  
3UX2,GLU\_137,3.91,0.21,-0.8,0  
2CIU,LYS\_118,10.5,0,0,0  
1OGL,LYS\_60,10.43,-0.07,0,0  
2CIU,HIS\_221,7.33,0.97,0,-0.14



3DHN,TYR\_92,10.89,0.89,0,0  
2C2Y,ASP\_105,3.12,0.35,-1.04,0  
2G3A,LYS\_80,10.5,0,0,0  
1X9G,LYS\_185,10.22,-0.28,0,0  
3F7M,HIS\_173,12.42,5.2,4.5,-3.78  
3V75,GLU\_272,4.78,0.28,0,0  
1R5Q,LYS\_35,10.29,-0.21,0,0  
3G9T,HIS\_74,0.69,0.92,-1.21,-5.52  
3IV4,LYS\_19,10.29,-0.21,0,0  
2VAN,ASP\_130,3.36,0.42,-0.86,0  
4FCU,LYS\_169,10.5,0,0,0  
3V75,GLU\_191,4.57,0.07,0,0  
3CIV,ASP\_30,3.68,0,-0.12,0  
2CWC,ARG\_176,12.1,-0.4,0,0  
4D8L,GLU\_7,3.6,0.21,-1.11,0  
3C5V,GLU\_225,4.05,0.35,-0.8,0  
1AK1,GLU\_23,3.84,0.14,-0.8,0  
2C2Y,ARG\_195,12.5,0,0,0  
1J33,ARG\_12,11.59,-0.91,0,0  
3P28,TYR\_58,11.73,2.53,-0.8,0  
2H8O,ARG\_137,12.15,-0.35,0,0  
1DTO,GLU\_74,4.5,0,0,0  
1ES9,HIS\_28,6.45,0.09,0,-0.14  
3IL3,LYS\_234,10.15,-0.35,0,0  
2B3M,GLU\_151,4.0,0.21,-0.71,0  
3EZ7,ARG\_54,12.22,-0.28,0,0  
2C2Y,ASP\_27,3.14,0.14,-0.8,0  
2E0T,GLU\_117,4.62,0.14,-0.02,0  
3ELI,ARG\_93,11.31,-1.19,0,0  
3ETU,ARG\_269,11.06,-1.44,0,0  
2PIM,GLU\_39,3.5,0.49,-1.49,0  
3DHN,ASP\_181,3.94,0.14,0,0  
3C6B,TYR\_123,13.46,1.43,0.01,2.01  
1X91,GLU\_74,4.78,0.28,0,0  
1EV8,ASP\_89,3.29,0.28,-0.78,0  
1YDL,TYR\_22,10,0,0,0  
1ZP2,TYR\_84,11.79,0.14,-0.2,1.85  
2AOJ,ARG\_35,12.5,0,0,0  
3ERF,GLU\_204,4.88,0.21,0.17,0  
2QOP,HIS\_51,6.5,0,0,0  
1BKR,LYS\_2,10.43,-0.07,0,0  
1YB2,ASP\_195,3.74,0,-0.06,0  
3G53,ASP\_194,3.94,0.14,0,0  
1UXO,LYS\_24,10.43,-0.07,0,0  
1SJY,GLU\_68,4.45,0.35,-0.4,0  
1G5Z,LYS\_92,10.22,-0.28,0,0  
3HO4,LYS\_29,10.01,-0.49,0,0  
1JSX,ARG\_106,12.36,-0.14,0,0  
1JKS,GLU\_17,3.91,0.14,-0.73,0  
4ETX,ARG\_239,12.36,-0.14,0,0  
1S7K,GLU\_153,2.45,0.35,-2.4,0  
3IL3,LYS\_132,9.87,-0.63,0,0  
3LH5,ASP\_547,3.04,0.35,-1.11,0  
2E3C,LYS\_435,9.94,-0.56,0,0  
3RLN,LYS\_627,10.5,0,0,0  
1ES5,LYS\_61,10.43,-0.07,0,0  
3LMO,ASP\_42,3.94,0.14,0,0  
1MUF,ARG\_312,10.71,-2.22,0.43  
1XEU,LYS\_175,10.43,-0.07,0,0  
1QYI,GLU\_259,4.5,0,0,0  
3E7P,HIS\_205,6.77,0.41,0,-0.14  
1ZHV,ASP\_111,3.66,0.42,-0.56,0  
2FBQ,GLU\_20,4.0,0.28,-0.78,0  
1ZCU,CYS\_97,8.93,-1.87,0,1.8  
2CWY,ASP\_4,2.78,0.49,-1.51,0  
3M7G,TYR\_238,12.35,0.49,-0.68,2.54  
2PP6,ASP\_3,4.13,0.35,-0.02,0  
3EZ7,LYS\_316,10.5,0,0,0  
1YR6,ARG\_155,11.94,-0.56,0,0  
2P5D,GLU\_66,4.3,0.42,-0.62,0  
2Z0M,ARG\_230,11.87,-0.63,0,0  
1W7B,LYS\_204,10.29,-0.21,0,0  
3ETU,GLU\_155,3.83,0.21,-0.88,0  
2VAN,ASP\_332,3.42,0.42,-0.8,0  
1KCM,GLU\_249,4.64,0.14,0,0  
1YG2,CYS\_55,8.96,-0.04,0,0  
1YOY,ARG\_166,12.29,-0.21,0,0  
1NIJ,LYS\_220,10.5,0,0,0  
2OPJ,ARG\_170,11.87,-0.63,0,0  
3K8J,TYR\_127,9.83,0,-0.17,0  
4D8L,ASP\_241,3.2,0.21,-0.81,0  
1H4U,LYS\_407,10.01,-0.49,0,0  
1ZYL,TYR\_128,9.69,0,-0.31,0  
1YB2,LYS\_115,10.5,0,0,0  
2Z61,LYS\_280,10.5,0,0,0  
3P51,TYR\_46,9.29,0,-0.71,0  
1SJY,GLU\_40,4.57,0.42,-0.35,0  
4AM1,ARG\_129,11.34,-3.63,0.2,47  
1ZHV,ARG\_18,12.15,-0.35,0,0  
1V43,LYS\_187,10.5,0,0,0  
1TR9,LYS\_47,10.5,0,0,0  
2PLQ,LYS\_278,10.22,-0.28,0,0  
1SQH,ARG\_47,12.5,0,0,0  
1R3F,CYS\_193,7.11,-2.1,0.0,2  
2OEW,GLU\_174,4.5,0,0,0  
2F8H,ARG\_360,11.58,-0.98,0.0,0.06  
1RLO,ASP\_21,3.42,0.21,-0.59,0  
2IF4,GLU\_43,3.66,0.07,-0.91,0  
1JB3,HIS\_122,6.56,0.06,0,0  
1GXN,LYS\_592,10.5,0,0,0  
1ZCE,LYS\_82,10.36,-0.14,0,0  
2I6I,ARG\_130,12.22,-0.28,0,0  
3ONT,ASP\_39,4.01,0.21,0,0  
3DHN,TYR\_219,10.58,0.21,-2.03,2.4  
4GCO,LYS\_189,10.36,-0.14,0,0  
3C2E,CYS\_255,8.26,-0.74,0,0  
2GAU,GLU\_142,4.78,0.28,0,0  
1JSX,GLU\_196,3.79,0.35,-1.06,0  
3ASA,GLU\_283,3.3,0.35,-1.55,0  
2HRZ,GLU\_216,4.14,0.21,-0.57,0  
1ZHV,ARG\_4,12.29,-0.21,0,0  
2FD5,GLU\_118,4.63,0.21,-0.08,0  
1AIL,LYS\_62,10.15,-0.35,0,0  
2H85,LYS\_289,10.22,-0.28,0,0  
2H8O,LYS\_178,9.52,-0.98,0,0  
1RIS,GLU\_133,4.63,0.21,-0.08,0  
1JKS,GLU\_100,6.42,0.55,0,1.37  
1CHD,TYR\_243,10.23,0.15,-0.43,0.5  
1XFK,CYS\_246,9.53,-0.68,0,1.2  
2BLL,ARG\_426,11.34,-2.85,0,1.69  
3RLE,ASP\_106,3.82,0.07,-0.05,0  
2AHE,TYR\_128,13.24,0.64,0.8,1.8  
3EAZ,ASP\_141,1.36,0.91,-3.36,0  
3DSH,LYS\_401,10.5,0,0,0  
3PP8,GLU\_233,3.66,0.67,-1.51,0  
3KV0,TYR\_186,11.25,1.79,-0.54,0  
3IOO,GLU\_80,3.86,0.35,-1,0  
3EVP,LYS\_237,10.15,-0.35,0,0  
3O48,GLU\_73,4.5,0,0,0  
4FCU,ASP\_64,3.21,0.28,-0.87,0  
2B2H,ASP\_268,1.66,0.56,-2.71,0  
1ZBM,LYS\_66,10.43,-0.07,0,0  
3A4C,GLU\_516,4.85,0.35,0,0  
3FK5,TYR\_33,9.84,0.7,-1.9,1.05  
3CO1,HIS\_57,6.5,0,0,0  
2F8H,LYS\_202,10.29,-0.21,0,0  
3P51,GLU\_109,3.98,0.28,-0.8,0  
4EF5,CYS\_257,11.68,0,0,2.68  
2HRZ,ARG\_176,12.43,-0.07,0,0  
1IAP,CYS\_78,10.31,-0.19,0,1.5  
2VGM,ARG\_332,12.86,-2.04,0,2.4  
3CAX,ASP\_365,3.22,0.56,-1.14,0  
1WP5,ARG\_23,12.36,-0.14,0,0  
1YG2,ARG\_42,11.73,-0.77,0,0  
4DIU,LYS\_80,10.5,0,0,0  
2H8O,ARG\_299,11.94,-0.56,0,0  
3IRA,GLU\_37,4.5,0,0,0  
3M7G,ARG\_193,11.66,-0.84,0,0  
3BB7,HIS\_305,5.55,1.61,1.87,-4.42  
3GW3,LYS\_242,10.5,0,0,0  
2H14,LYS\_165,10.01,-0.49,0,0  
2IXM,HIS\_31,6.76,0.33,0,-0.07  
1XDZ,LYS\_186,10.43,-0.07,0,0  
2QV2,GLU\_148,3.77,0.35,-1.08,0  
2YX0,HIS\_69,3.6,0.8,-0.49,-3.21  
3FFM,ASP\_150,3.99,0.49,-0.31,0  
2PGX,LYS\_2,10.43,-0.07,0,0  
1Z3X,GLU\_200,1.64,0.63,-3.49,0  
2WB3,LYS\_304,10.43,-0.07,0,0  
1EW4,CYS\_80,1.63,-7.37,0,0  
2JKF,TYR\_89,11.93,0.01,1.93  
2RGY,GLU\_135,4.35,0.28,-0.43,0  
1TJE,ARG\_72,11.45,-1.05,0,0  
3ANJ,ASP\_241,2.96,0.07,-0.91,0  
2A1V,LYS\_122,10.5,0,0,0  
1YM5,GLU\_118,4.47,0,-0.03,0  
2XMZ,GLU\_144,4.49,0,-0.01,0  
1ANU,LYS\_7,10.36,-0.14,0,0  
2PLQ,ARG\_264,11.94,-0.56,0,0  
3GYW,GLU\_84,4.56,0.14,-0.08,0  
1EYH,ARG\_25,11.73,-0.77,0,0  
2GYZ,ARG\_71,12.43,-0.07,0,0  
1YW5,ARG\_175,13.2,-2.74,0.3,44  
1OTM,LYS\_187,10.5,0,0,0  
3ZSL,GLU\_185,3.91,0.21,-0.8,0  
3LJN,GLU\_31,3.98,0.28,-0.8,0  
2D7J,ASP\_130,4.01,0.21,0,0  
3VJ8,TYR\_174,13.34,0.14,0.8,2.4  
3HVM,TYR\_137,11.39,0,0,1.39  
3G9G,GLU\_45,4.57,0.07,0,0  
2OYZ,TYR\_89,10.92,0.71,0.0,21  
3E7P,ARG\_85,12.08,-0.42,0,0  
1WOU,CYS\_69,10.08,-0.47,0,1.55  
1PNE,LYS\_69,9.66,-0.84,0,0  
2EYI,ASP\_138,3.32,0.28,-0.76,0  
3M70,LYS\_164,10.22,-0.28,0,0  
4F85,ARG\_204,11.7,-0.8,0,0  
4AE7,LYS\_53,10.5,0,0,0  
1M5I,ARG\_168,12.22,-0.28,0,0  
3V46,ASP\_348,3.34,0.35,-0.81,0  
3EYE,TYR\_57,10.07,0.07,0,0  
3IVF,LYS\_322,10.5,0,0,0  
2EA9,ASP\_56,3.93,0.21,-0.08,0  
2W0G,HIS\_148,6.43,0,0,-0.07  
1FQI,LYS\_368,10.5,0,0,0  
3ONH,TYR\_489,12.73,0.0,2.74  
1FHL,ASP\_60,3.74,0,-0.06,0  
1QQE,ASP\_171,3.49,0.28,-0.59,0  
1QQH,TYR\_159,9.72,0.07,-0.35,0  
2PGX,GLU\_49,3.69,0.7,-1.51,0  
1KCM,LYS\_117,10.29,-0.21,0,0  
4FZR,ASP\_375,2.11,0.77,-2.46,0  
2D8N,ASP\_110,3.13,1.19,-1.85,0  
2D25,GLU\_593,4.67,0.28,-0.11,0  
1ZP2,CYS\_190,8.79,-0.35,0.0,14  
1QQE,ASP\_58,4.03,0.28,-0.05,0  
2EJX,GLU\_5,4.71,0.21,0,0  
2G9D,CYS\_91,11.83,-0.01,0.2,84  
1EDG,ASP\_268,4.0,0.21,-0.01,0  
2X4L,GLU\_128,4.5,0,0,0  
2H85,GLU\_254,4.64,0.14,0,0  
2P65,ARG\_154,10.8,-1.7,0,0  
1NIJ,HIS\_114,6.5,0,0,0  
3Q9P,ASP\_149,2.49,0.63,-1.94,0  
2QDJ,ARG\_355,11.38,-1.12,0,0  
3CRM,ARG\_311,12.22,-0.28,0,0  
1VJG,LYS\_116,10.5,0,0,0  
4DND,CYS\_298,5.55,-0.52,0.0,0.07  
2QHT,GLU\_134,4.71,0.35,-0.14,0  
2BV9,ASP\_201,3.28,0.28,-0.8,0  
1AK1,ARG\_3,11.52,-0.98,0,0  
1EV8,ASP\_13,3.85,0.35,-0.29,0  
3H5T,LYS\_139,9.87,-0.63,0,0  
2EYH,ASP\_115,3.86,0.07,-0.01,0  
2PP6,ARG\_70,12.43,-0.07,0,0  
2W0G,GLU\_185,2.93,0.35,-1.92,0  
3EUR,LYS\_7,10.15,-0.35,0,0  
2Q13,CYS\_335,9.0,0,0,0  
3LH5,TYR\_550,10,0,0,0  
2NYC,ARG\_291,12.5,0,0,0  
2QEV,TYR\_94,11.96,1.96,0,0  
2D7U,ARG\_257,11.59,-0.91,0,0  
3FHF,GLU\_14,4.5,0,0,0  
4DNU,GLU\_140,4.05,0.14,-0.59,0  
4EKU,LYS\_229,10.29,-0.21,0,0  
1RIS,LYS\_115,3.86,0.07,0,0  
3CAX,LYS\_237,10.5,0,0,0  
2BAA,TYR\_31,10.15,0.21,-0.06,0  
2D7J,GLU\_111,3.57,0.14,-1.07,0  
2CXC,GLU\_46,4.16,0.35,-0.69,0  
1KCM,TYR\_48,13.48,0.28,0.8,2.4  
2QDJ,LYS\_130,10.29,-0.21,0,0  
2E3S,HIS\_378,7.11,4.39,0,-3.78  
3PBH,HIS\_7,7.48,1.12,0,-0.14  
1TJE,ARG\_183,12.01,-0.49,0,0  
2FXT,GLU\_269,4.5,0,0,0  
3H5T,ARG\_312,12.29,-0.21,0,0  
2H85,GLU\_44,4.64,0.14,0,0  
3CXS,LYS\_80,10.5,0,0,0  
2F8H,ASP\_121,3.48,0.42,-0.74,0  
1X1E,LYS\_54,10.36,-0.14,0,0  
2Q98,GLU\_162,4.7,0.35,-0.15,0  
1BKB,TYR\_132,9.54,0.07,-0.65,0.12  
2W0G,GLU\_198,4.34,0.28,-0.44,0  
1F09,ARG\_358,11.73,-0.77,0,0  
1O5T,LYS\_249,10.43,-0.07,0,0  
2IXM,LYS\_111,10.5,0,0,0  
1DVO,GLU\_52,4.5,0,0,0  
3EVN,GLU\_292,4.71,0.21,0,0  
3F6F,LYS\_79,10.5,0,0,0  
2YT4,TYR\_621,9.92,0,-0.08,0  
1XKR,LYS\_196,10.22,-0.28,0,0  
3EVN,GLU\_238,4.71,0.21,0,0  
3PZ9,HIS\_152,7.21,2.68,1.65,-3.62  
3LJN,ARG\_175,12.7,-2.29,0.2,49  
1P2F,LYS\_191,10.29,0.36,-0.14,0  
3CIV,ASP\_308,3.79,0.07,-0.08,0  
1XTD,ASP\_129,1.05,0.49,-3.24,0  
1XDZ,LYS\_53,10.22,-0.28,0,0  
1RHS,GLU\_218,4.5,0,0,0  
2HNG,GLU\_49,4.5,0,0,0  
3C2E,LYS\_191,10.43,-0.07,0,0  
1RAJ,ARG\_408,12.5,0,0,0  
3ASA,ASP\_306,2.91,0.56,-1.44,0  
2OB5,LYS\_143,10.15,-0.35,0,0  
1WLY,HIS\_193,6.29,0,-0.21

1R6Y,HIS\_71,6.47,0.11,0,-0.14  
1R2Z,LYS\_111,10.22,-0.28,0,0  
1X1P,ARG\_321,11.45,-1.05,0,0  
3PP8,ASP\_82,2.12,0.08,-1.96,0  
1DUN,GLU\_95,4.57,0.27,0,0  
2Q13,TYR\_147,10,0,0,0  
1OXZ,LYS\_206,10.08,-0.42,0,0  
3BPV,HIS\_18,11.92,3.22,4.59,-2.39  
1SQW,CYS\_69,1.54,-6.16,-1.96,0.65  
1WJG,ARG\_96,11.8,-0.7,0,0  
2HRZ,ARG\_285,12.01,-0.49,0,0  
21QT,HIS\_182,6.59,0.09,0,0  
2AXO,TYR\_135,13.38,0.21,0.77,2.4  
3GEC,ASP\_260,3.94,0.14,0,0  
21F4,LYS\_103,10.01,-0.49,0,0  
4DBX,GLU\_14,4.5,0,0,0  
3EVN,GLU\_313,3.23,0.63,-1.89,0  
3MTT,ASP\_552,3.85,0.28,-0.23,0  
3M9A,GLU\_72,3.95,0.63,-1.17,0  
2B0J,GLU\_94,4.12,0.42,-0.8,0  
1YR6,LYS\_205,10.29,-0.21,0,0  
3LH5,ARG\_561,13.91,-0.94,0.235  
2D7U,ARG\_269,12.08,-0.42,0,0  
3EIZ,ASP\_11,3.94,0.14,0,0  
1PSW,GLU\_65,3.99,0.07,-0.58,0  
2EA9,CYS\_100,9.07,0,0,0,0  
1X1E,TYR\_192,9.68,0,-0.57,0.25  
3COU,ARG\_6,11.87,-0.63,0,0  
3CBN,GLU\_141,4.16,0.35,-0.69,0  
1N81,LYS\_62,10.36,-0.14,0,0  
1X6J,ASP\_33,3.16,0.21,-0.85,0  
3TMO,HIS\_246,6.49,0.06,0,-0.07  
3RVC,ASP\_173,2.26,0.42,-1.96,0  
21QT,HIS\_227,7.02,0.8,0,-0.28  
4HDE,ASP\_185,3.67,0.28,-0.41,0  
2VGM,LYS\_44,10.43,-0.07,0,0  
4D8L,ARG\_130,12.43,-0.07,0,0  
1T07,LYS\_44,10.29,-0.21,0,0  
1S17,ARG\_247,12.08,-0.42,0,0  
2CN1,GLU\_85,6.02,1.85,0,-0.33  
1NJ4,ARG\_40,11.48,-1.02,0,0  
1X7F,GLU\_361,4.71,0.21,0,0  
2AHE,GLU\_93,4.64,0.14,0,0  
3DB9,LYS\_18,10.5,0,0,0  
1S7K,ARG\_123,12.43,-0.07,0,0  
2G5X,ARG\_93,12.5,0,0,0  
1MML,HIS\_143,7.28,0.92,0,-0.14  
3HVM,GLU\_236,4.58,0.49,-0.41,0  
3PU6,LYS\_3,9.94,-0.56,0,0  
1LZL,GLU\_258,2.85,0.35,-2,0  
1T6L,CYS\_175,8.81,-0.19,0,0  
1ZCU,TYR\_196,10,0,0,0  
1A8Q,GLU\_190,4.33,0.56,-0.73,0  
1G8PLYS\_133,10.29,-0.21,0,0  
3F7M,ARG\_251,11.66,-0.84,0,0  
2A1V,HIS\_22,7.25,0.96,0,-0.21  
3JZN,ASP\_339,3.17,0.14,-0.77,0  
3ASA,GLU\_142,4.57,0.07,0,0  
3V4G,ASP\_128,3.36,0.28,-0.72,0  
2FB6,ASP\_17,3.8,0,0,0  
2XJ4,LYS\_197,10.29,-0.21,0,0  
1ES9,ARG\_141,11.38,-1.12,0,0  
2DFL,ARG\_291,12.29,-0.21,0,0  
4FCU,GLU\_200,3.46,0,-1.04,0  
2NYC,ASP\_227,2.28,0.98,-2.51,0  
2FL4,ARG\_80,12.08,-0.42,0,0  
1G8P,GLU\_76,4.57,0.07,0,0  
1XDZ,TYR\_51,13.7,1.1,0.2,2.4  
3EVN,ARG\_247,12.29,-0.21,0,0  
2FPN,LYS\_124,10.5,0,0,0  
3JSN,ASP\_257,3.12,0.14,-0.82,0  
1Z9L,ASP\_24,3.19,0.35,-0.96,0  
3CIV,ARG\_217,12.08,-0.42,0,0  
1P6F,GLU\_13,4.02,0.14,-0.62,0  
3F53,LYS\_47,10.5,0,0,0  
3CX2,ASP\_198,2.36,0.35,-1.79,0  
4ECC,ASP\_148,3.97,0.35,-0.18,0  
3U2A,GLU\_73,2.59,0.49,-2.4,0  
3DTE,ASP\_131,3.4,0.42,-0.83,0  
3K85,GLU\_396,3.3,0.7,-1.9,0  
3LPZ,ASP\_254,3.38,0.07,-0.49,0  
2PGE,ASP\_40,1.85,0.49,-2.44,0  
1ES9,LYS\_35,10.5,0,0,0  
2V4U,GLU\_528,5.53,3.01,-1.98,0  
2CXC,ARG\_62,12.01,-0.49,0,0  
3LJI,ASP\_93,4.08,0.28,0,0  
1WRU,ASP\_239,3.37,0.21,-0.64,0  
1GVP,GLU\_51,4.5,0,0,0  
3VJ8,ASP\_62,3.01,0.35,-1.14,0  
4F85,GLU\_231,4.5,0,0,0  
3FRR,ARG\_21,12.08,-0.42,0,0  
3PP8,ARG\_308,11.52,-0.98,0,0  
1Q46,GLU\_28,4.5,0,0,0  
2ZQ5,HIS\_154,6.5,0,0,0  
2F19,GLU\_128,4.5,0,0,0  
3EGN,ARG\_505,12.5,0,0,0  
3OA7,ARG\_531,12.01,-0.49,0,0  
2PWQ,LYS\_2,10.36,-0.14,0,0  
3OA7,CYS\_567,9,0,0,0  
3MTT,GLU\_526,4.5,0,0,0  
3I4T,TYR\_86,10.07,0.07,0,0  
3EUR,TYR\_94,10.07,0.07,0,0  
3L3P,GLU\_517,4.09,0.21,-0.62,0  
1GXN,LYS\_645,9.94,-0.56,0,0  
1TLV,HIS\_200,6.5,0,0,0  
2P52,GLU\_177,3.98,0.28,-0.8,0  
1PV5,GLU\_145,4.71,0.21,0,0  
3C6B,LYS\_77,10.36,-0.14,0,0  
3IRA,TYR\_18,10,0,0,0  
3CX5,GLU\_90,4.09,0.35,-0.76,0  
1XKR,GLU\_179,4.57,0.07,0,0  
1L3K,GLU\_67,2.49,1.19,-3.21,0  
1TD6,TYR\_32,10.07,0.07,0,0  
3BPP,ASP\_39,3.77,0.07,-0.1,0  
1PV5,GLU\_16,4.64,0.14,0,0  
2B61,ARG\_271,11.94,-0.56,0,0  
2B3M,GLU\_125,4.19,0.49,-0.8,0  
2AZL,ASP\_188,3.68,0,-0.12,0  
1WRU,LYS\_89,10.15,-0.35,0,0  
310C,ASP\_154,2.7,0.84,-1.94,0  
3O16,ASP\_40,2.36,0.56,-2,0  
3HVM,HIS\_93,6.5,0,0,0  
3CBN,ARG\_148,12.15,-0.35,0,0  
1YB2,ASP\_161,3.38,0.42,-0.84,0  
1X7F,GLU\_120,4.06,3.57,-0.94,-3.07  
2AXO,GLU\_96,3.91,0.28,-0.87,0  
3G65,ARG\_201,12.43,-0.07,0,0  
2PIM,GLU\_107,4.01,0.28,-0.77,0  
1WXQ,GLU\_238,4.78,0.28,0,0  
3ONT,HIS\_125,6.4,0.04,0,-0.14  
3K1H,LYS\_67,10.36,-0.14,0,0  
2FZ4,ARG\_95,12.36,-0.14,0,0  
4FCU,ARG\_14,12.29,-0.21,0,0  
3N2T,ARG\_222,12.29,-0.21,0,0  
3N2T,ASP\_229,3.78,0,-0.02,0  
2Q13,HIS\_140,6.5,0,0,0  
3PZ9,LYS\_264,10.36,-0.14,0,0  
3VHJ,LYS\_68,10.5,0,0,0  
1BN6,HIS\_24,6.76,0.26,0,0  
1T3Y,ASP\_32,3.87,0.07,0,0  
1MSI,TYR\_158,10.98,0.07,-0.27,1.18  
1Y2Q,TYR\_10,10,0,0,0  
1T3J,GLU\_693,4.64,0.14,0,0  
2YWK,ARG\_45,12.5,0,0,0  
1MUF,ASP\_270,2.29,0.49,-1.99,0  
2FGG,ASP\_14,3.47,0.14,-0.47,0  
2R51,HIS\_83,6.5,0,0,0  
1AKO,HIS\_201,6.51,0.01,0,0  
3K8J,HIS\_196,7.23,0.8,0,-0.07  
1GPP,ARG\_147,12.36,-0.14,0,0  
1YG2,ARG\_151,11.94,-0.56,0,0  
3FHF,GLU\_73,4.71,0.21,0,0  
1QQH,GLU\_175,3.8,0.56,-1.26,0  
1CBY,TYR\_242,11.71,0,0,1.71  
3RKY,LYS\_189,10.5,0,0,0  
4EVF,GLU\_36,4.15,0.14,-0.49,0  
2DFL,ARG\_107,11.94,-0.56,0,0  
1JKS,ASP\_220,3.86,0.07,-0.01,0  
2AD1,LYS\_184,10.43,-0.07,0,0  
1YTD,ARG\_318,12.5,0,0,0  
3RVC,ARG\_148,13.74,-0.94,0.2,1.8  
2AD1,GLU\_158,3.3,0.28,-1.49,0  
1FQI,LYS\_342,10.22,-0.28,0,0  
3MIX,ARG\_400,10.78,-1.06,0,-0.66  
2D0A,LYS\_174,10.01,-0.49,0,0  
3ASA,GLU\_160,4.5,0,0,0  
1WJG,ARG\_58,11.8,-0.7,0,0  
2GZQ,ARG\_12,11.94,-0.56,0,0  
2HRZ,ARG\_192,11.21,-1.29,0,0  
1PSW,CYS\_171,9.31,0,0,0,31  
3MIX,GLU\_576,4.64,0.14,0,0  
4DNU,ASP\_107,2.56,0.14,-1.38,0  
3MEW,ASP\_172,3.87,0.07,0,0  
3ASA,GLU\_151,4.71,0.21,0,0  
1NAF,ARG\_260,12.15,-0.35,0,0  
4AM1,HIS\_99,2.09,0,0,-4.41  
1XWM,CYS\_104,8.88,-0.55,0,0.43  
2YXO,GLU\_164,4.71,0.21,0,0  
21F4,ARG\_121,12.15,-0.35,0,0  
1Q42,ARG\_169,12.15,-0.35,0,0  
4GA2,GLU\_74,4.28,0.07,-0.29,0  
3VJ8,ASP\_200,1.98,0.84,-2.66,0  
1IAP,GLU\_195,3.77,0.7,-1.42,0  
2FB6,TYR\_96,13.52,0.07,-0.16,3.61  
1YB2,LYS\_66,10.5,0,0,0  
3LJI,ASP\_92,4.47,0.49,0.18,0  
1XDZ,GLU\_180,4.5,0,0,0  
3Q2C,HIS\_69,6.5,0,0,0  
2FD5,TYR\_45,9.94,0,-0.06,0  
1L2F,ARG\_36,12.22,-0.28,0,0  
2YWK,GLU\_28,4.64,0.14,0,0  
3EVN,TYR\_186,12.4,2.54,-0.14,0  
4F85,GLU\_170,4.5,0,0,0  
1IAP,ARG\_196,12.22,-0.28,0,0  
1YB2,ASP\_124,2.68,0.56,-1.68,0  
3L3P,ARG\_374,12.01,-0.49,0,0  
1ZYL,LYS\_138,10.22,-0.28,0,0  
3BB7,GLU\_232,3.98,0.28,-0.8,0  
1L2F,LYS\_164,10.29,-0.21,0,0  
1X7F,LYS\_53,10.01,-0.49,0,0  
2F19,ASP\_117,4.01,0.21,0,0  
2OPJ,CYS\_253,9.98,-1.09,0.2,0.8  
1UAJ,ARG\_215,11.87,-0.63,0,0  
2D59,ASP\_51,3.35,0.28,-0.73,0  
21QT,GLU\_206,4.64,0.14,0,0  
2DFL,TYR\_178,13.03,0.21,0.42,2.4  
2Q34,GLU\_134,2.69,0.91,-2.73,0  
3LMF,HIS\_32,6.54,0.04,0,0  
3BZT,ARG\_313,12.29,-0.21,0,0  
1PSW,TYR\_287,13.72,1.27,0.14,2.31  
2EJX,ASP\_75,3.36,0.42,-0.86,0  
3OBS,ASP\_34,4.01,0.21,0,0  
2OQG,ARG\_392,11.24,-1.26,0,0  
3N2T,ARG\_188,13.51,-1.39,0.2,4  
1G5Z,LYS\_167,10.22,-0.28,0,0  
2QDJ,LYS\_153,10.22,-0.28,0,0  
4EVF,TYR\_215,10,0,0,0  
3H6Q,TYR\_140,10.63,0,0,0.63  
3V1Q,ARG\_534,12.01,-0.49,0,0  
1N81,ASP\_164,3.37,0.49,-0.92,0  
1XTZ,LYS\_243,10.22,-0.28,0,0  
1W24,CYS\_41,5.05,-4.19,-0.4,0.64  
1O5J,GLU\_62,3.98,0.28,-0.8,0  
3RVS,ASP\_189,4.01,0.21,0,0  
3V75,HIS\_255,6.77,0.27,0,0  
3ONH,LYS\_468,10.22,-0.28,0,0  
1FQI,LYS\_375,10.5,0,0,0  
3LJC,GLU\_93,4.64,0.14,0,0  
3F6F,TYR\_209,9.56,0.11,-0.55,0  
3R9Y,TYR\_223,10.07,0.07,0,0  
1R6Y,ARG\_98,12.43,-0.07,0,0  
1RWZ,ASP\_76,3.87,0.07,0,0  
3QKY,GLU\_172,4.07,-0.57,0  
3FFM,ARG\_35,12.01,-0.49,0,0  
1U3Y,GLU\_350,4.57,0.07,0,0  
2YWJ,LYS\_21,10.5,0,0,0  
1160,GLU\_24,3.13,0.91,-2.28,0  
4ANN,ASP\_141,3.92,0.21,-0.09,0  
1S1Y,HIS\_46,3.86,0.91,-3.55  
1P1L,ARG\_67,11.87,-0.63,0,0  
3ADO,HIS\_173,6.44,0.15,0,-0.21  
2QDJ,HIS\_69,6.5,0,0,0  
4H89,HIS\_164,6.36,0,-0.14  
4F85,ASP\_187,2.7,0.63,-1.73,0  
2DG7,ASP\_32,2.12,0.42,-2.1,0  
2PGE,ARG\_244,12.5,0,0,0  
3COU,GLU\_160,4.45,0,-0.05,0  
3BPV,ARG\_132,12.5,0,0,0  
2G55,GLU\_28,4.5,0,0,0  
3ASA,GLU\_196,4.5,0,0,0  
1O3X,ARG\_207,12.01,-0.49,0,0  
3EJG,TYR\_52,9.74,0.07,-0.56,0.22  
1J74,GLU\_21,4.05,0.35,-0.8,0  
1U7U,ASP\_250,3.47,0.56,-0.89,0  
2AXO,ASP\_213,1.97,0.28,-2.12,0  
3BQE,GLU\_250,6.37,2.9,-1.02,0  
2CBE,GLU\_214,3.32,0.7,-1.88,0  
1QQE,ASP\_38,3.8,0,0,0  
3JV1,ARG\_193,11.38,-1.12,0,0  
3V4G,GLU\_153,2.02,0.35,-2.83,0  
1MTZ,HIS\_179,6.29,0,0,-0.21  
2INO,GLU\_426,4.64,0.14,0,0  
2E3C,GLU\_425,4.18,2.69,-3.01,0  
3BB7,LYS\_167,10.01,-0.49,0,0  
2P5D,LYS\_32,10.29,-0.21,0,0  
2B02,GLU\_403,3.84,0.14,-0.8,0  
2O4D,ARG\_97,11.87,-0.63,0,0  
2PPN,GLU\_54,3.01,0.49,-1.98,0  
2PPN,ARG\_13,12.5,0,0,0  
1T6L,ASP\_120,3.94,0.14,0,0  
3QAV,ARG\_95,12.15,-0.35,0,0  
1YQY,LYS\_47,10.29,-0.21,0,0  
1NJ4,TYR\_52,12.16,0.57,0.159  
4ANN,ASP\_169,3.76,0.07,-0.11,0  
1PDB,TYR\_121,12.96,2.96,0,0  
1SQH,GLU\_175,4.5,0,0,0

3GT0,LYS\_88,10.29,-0.21,0,0  
1XAW,ASP\_516,2.63,0.42,-1.59,0  
3V75,GLU\_80,4.78,0.28,0,0  
2QK1,ASP\_490,3.94,0.14,0,0  
3K8J,ARG\_260,12.15,-0.35,0,0  
2B0J,ASP\_280,3.94,0.14,0,0  
3HVM,GLU\_9,2.08,1.12,-3.54,0  
3GMS,HIS\_265,5.07,0,0,-1.43  
3E5T,LYS\_188,10.5,0,0,0  
1OST,LYS\_153,10.5,0,0,0  
1V43,LYS\_314,10.5,0,0,0  
4ACJ,CYS\_776,4.08,-5.84,0,0.92  
3GA2,LYS\_104,10.43,-0.07,0,0  
1X6J,ARG\_45,11.94,-0.56,0,0  
3CAX,GLU\_382,4.5,0,0,0  
1D7O,GLU\_162,4.64,0.14,0,0  
2HRZ,HIS\_-5,7.07,0.57,0,0  
2OEW,ASP\_222,3.35,0.21,-0.66,0  
2EA9,HIS\_87,6.08,0,0,-0.42  
2O8P,ASP\_49,1.87,0.84,-2.78,0  
3ELI,ARG\_5,12.15,-0.35,0,0  
2HRZ,GLU\_150,3.87,0.28,-0.9,0  
3MTT,ARG\_527,11.87,-0.63,0,0  
4EF5,TYR\_186,9.67,0.35,-1.29,0.61  
1YB2,ARG\_220,12.43,-0.07,0,0  
1BN6,GLU\_234,4.64,0.14,0,0  
2QZQ,LYS\_158,10.36,-0.14,0,0  
3CIV,HIS\_249,7.84,1.62,0,-0.28  
2FBI,ARG\_44,11.87,-0.63,0,0  
3H13,ARG\_303,12.36,-0.14,0,0  
2Q13,LYS\_191,10.15,-0.35,0,0  
2W0G,LYS\_160,10.43,-0.07,0,0  
2XJ4,ARG\_242,12.22,-0.28,0,0  
3HYQ,GLU\_116,2.88,0.37,0,-1.99  
2OKT,TYR\_291,9.62,0.07,-0.45,0  
3B79,LYS\_74,10.15,-0.35,0,0  
4DNU,GLU\_364,4.5,0,0,0  
3HUE,ASP\_97,3.94,0.14,0,0  
4F8A,GLU\_578,4.64,0.14,0,0  
2GEN,CYS\_17,7.78,-1.29,0,0.07  
1MUF,HIS\_181,6.36,0,0,-0.14  
3T8R,LYS\_29,10.5,0,0,0  
2H14,GLU\_292,3.91,0.21,-0.8,0  
3H13,HIS\_443,3.06,0.19,0,-3.63  
3GEC,ASP\_381,3.99,0.49,-0.3,0  
3F53,LYS\_93,10.5,0,0,0  
2QOP,ASP\_84,2.64,0.49,-1.65,0  
2PP6,ASP\_30,3.25,0.28,-0.83,0  
3PZ9,ASP\_56,3.41,0.56,-0.95,0  
2QOP,ASP\_157,3.29,0.56,-1.06,0  
1TD6,LYS\_158,10.29,-0.21,0,0  
1O6D,ASP\_12,3.68,0,-0.12,0  
4GA2,TYR\_70,10,0,0,0  
3M66,ASP\_278,3.39,0.49,-0.9,0  
1EQ6,ASP\_53,2.74,0.77,-1.83,0  
2WOZ,GLU\_564,2.95,0.63,-2.18,0  
3RFF,ARG\_90,11.52,-0.98,0,0  
3H9W,ASP\_89,2.03,0.63,-2.4,0  
2YX0,ARG\_325,12.55,-1.22,0,1.27  
2XJ4,ARG\_196,12.15,-0.35,0,0  
1YLN,ARG\_161,12.29,-0.21,0,0  
3C6B,LYS\_25,10.5,0,0,0  
2V4X,ARG\_9,11.66,-0.84,0,0  
3GOZ,LYS\_189,10.5,0,0,0  
4FD6,CYS\_189,9.99,-1.15,0,0.14  
1J74,LYS\_85,10.15,-0.35,0,0  
1SNT,ARG\_55,11.45,-1.05,0,0  
1R3D,HIS\_22,1.33,0.82,-0.74,-5.25  
2EJB,LYS\_140,10.43,-0.07,0,0  
3GA2,LYS\_13,10.15,-0.35,0,0  
2CXA,ARG\_44,12.01,-0.49,0,0  
1MIX,ARG\_220,13.31,-0.8,0,1.61  
1X8F,LYS\_284,10.15,-0.35,0,0  
1LZL,GLU\_108,4.56,0.07,-0.01,0  
1O6D,LYS\_93,10.36,-0.14,0,0  
2FXT,ASP\_345,4.01,0.21,0,0  
1Q5Z,TYR\_640,11.35,0.07,-0.07,1.35  
2AXO,LYS\_155,10.5,0,0,0  
1KCM,GLU\_38,4.64,0.14,0,0  
4H86,GLU\_147,4.01,0.21,-0.7,0  
1Ri6,ASP\_241,2.11,0.77,-2.46,0  
3MTT,GLU\_486,4.5,0,0,0  
3F53,ASP\_192,3.85,0.28,-0.23,0  
1F2V,GLU\_32,4.5,0,0,0  
2B0J,LYS\_113,10.5,0,0,0  
3NBI,GLU\_65,4.5,0,0,0  
3PBH,ARG\_1,12.22,-0.28,0,0  
1DCF,GLU\_41,4.5,0,0,0  
2E3C,GLU\_222,3.98,0.14,-0.66,0  
3BQW,TYR\_275,10,0,0,0  
3LQE,TYR\_435,9.96,0,-0.04,0  
2QK1,ARG\_454,12.5,0,0,0  
1PV5,GLU\_167,4.64,0.14,0,0  
3M7G,ARG\_267,12.01,-0.49,0,0  
2OKT,GLU\_319,4.85,0.35,0,0  
1HUF,ASP\_7,3.35,0.42,-0.87,0  
1NIJ,ARG\_270,10.82,-1.68,0,0  
3BQW,GLU\_56,4.85,0.35,0,0  
2P1W,GLU\_232,4.5,0,0,0  
3JZ9,LYS\_380,10.5,0,0,0  
2CL3,HIS\_171,4.6,0.8,0,-2.7  
3RFY,GLU\_175,4.57,0.07,0,0  
1YM5,ARG\_257,11.66,-0.84,0,0  
1EV8,TYR\_94,11.73,2.07,-0.45,0.11  
3M7D,HIS\_281,6.88,0.66,0,-0.28  
2D59,LYS\_33,10.5,0,0,0  
2XJ4,LYS\_155,10.43,-0.07,0,0  
3CNU,ASP\_70,3.79,0.07,-0.08,0  
3B4D,ASP\_206,3.94,0.14,0,0  
1J85,GLU\_64,4.64,0.14,0,0  
2GAU,ARG\_230,12.5,0,0,0  
2AHE,TYR\_225,11.58,1.5,-0.8,0.88  
3H13,LYS\_247,10.29,-0.21,0,0  
1SQH,HIS\_61,7.82,1.74,0,-0.42  
1R5S,ARG\_155,12.08,-0.42,0,0  
3J5N,LYS\_44,10.5,0,0,0  
3IOC,TYR\_150,11.34,0.82,0,0.52  
2QHT,LYS\_21,10.29,-0.21,0,0  
3M7D,ARG\_351,12.08,-0.42,0,0  
2V81,CYS\_105,11.55,0,0,2.55  
2QOP,ARG\_90,11.87,-0.63,0,0  
3Q6L,LYS\_80,10.15,-0.35,0,0  
3L0D,ASP\_11,2.93,0.35,-1.23,0  
2QDJ,ARG\_150,11.77,-0.73,0,0  
3AUF,CYS\_135,10.63,-0.89,1.33,1.18  
1U7U,GLU\_336,4.75,0.42,-0.17,0  
2EFK,LYS\_247,9.73,-0.77,0,0  
1U53,TYR\_144,12.29,0.21,0.18,1.9  
1LPL,ARG\_162,11.52,-0.98,0,0  
3T57,GLU\_255,4.46,0.21,-0.25,0  
2IF4,GLU\_105,3.81,0.21,-0.9,0  
1HF8,ARG\_150,12.01,-0.49,0,0  
4FH3,TYR\_49,9.68,0.12,-0.44,0  
3A0X,LYS\_732,10.5,0,0,0  
2DG7,ASP\_175,3.87,0.14,-0.07,0  
1S17,ARG\_291,11.24,-1.26,0,0  
3K85,TYR\_416,12.16,0.07,-0.58,2.67  
2QV2,ASP\_72,3.89,0.28,-0.19,0  
3I47,ARG\_37,12.01,-0.49,0,0  
1QYI,ASP\_124,3.97,0.21,-0.04,0  
2FBQ,CYS\_65,9.87,0,0,0.87  
3QKY,GLU\_55,4.0,0.07,-0.57,0  
1HF8,ARG\_100,11.87,-0.63,0,0  
1V8E,ARG\_139,11.52,-0.98,0,0  
3V46,ARG\_235,12.5,0,0,0  
1F2V,ASP\_174,3.35,0.35,-0.8,0  
4EVF,LYS\_119,10.5,0,0,0  
3F1X,GLU\_125,3.89,0.14,-0.75,0  
1P6F,TYR\_63,10.14,0.14,0,0  
1XEU,TYR\_254,9.31,0.21,-1.02,0.12  
3F6F,LYS\_46,10.5,0,0,0  
3P2F,ASP\_89,4.08,0.28,0,0  
1L2F,ASP\_50,1.62,0.63,-2.82,0  
1J8B,ASP\_64,3.94,0.14,0,0  
2P65,LYS\_80,10.29,-0.21,0,0  
1NAR,CYS\_246,11.1,0,0,2.1  
4ACJ,ASP\_789,3.83,0.07,-0.04,0  
2CBE,LYS\_213,10.22,-0.28,0,0  
3H04,TYR\_194,10.04,0.07,-0.03,0  
2EJX,TYR\_84,12.34,0.07,0.05,2.23  
1PDB,LYS\_176,10.43,-0.07,0,0  
2WB3,LYS\_384,10.5,0,0,0  
2BLL,HIS\_593,6.29,0,0,-0.21  
3EYE,ARG\_10,12.39,-2.85,0,2.74  
1FKM,LYS\_265,10.22,-0.28,0,0  
2RIK,GLU\_148,4.5,0,0,0  
2WB3,GLU\_382,4.71,0.21,0,0  
1Ri6,HIS\_333,7.16,0.79,0,-0.14  
2IQT,GLU\_43,4.57,0.07,0,0  
3FHF,LYS\_27,10.15,-0.35,0,0  
3LQE,ASP\_255,2.95,0.84,-1.69,0  
2Z61,ARG\_287,12.15,-0.35,0,0  
2B78,TYR\_129,11.58,0,-0.16,1.74  
3M70,GLU\_163,4.5,0,0,0  
3EVP,LYS\_127,10.5,0,0,0  
2OYZ,ARG\_56,11.8,-0.7,0,0  
3KV0,ASP\_133,3.13,0.14,-0.82,0  
3CO1,LYS\_60,10.43,-0.07,0,0  
2X4L,LYS\_347,10.5,0,0,0  
1RAJ,ARG\_415,12.08,-0.42,0,0  
3CXS,GLU\_5,4.19,0.49,-0.8,0  
2F9F,GLU\_129,4.57,0.07,0,0  
2CN1,GLU\_20,4.64,0.14,0,0  
1DZF,GLU\_40,4.5,0,0,0  
3V55,ARG\_576,11.8,-0.7,0,0  
2RIK,GLU\_54,4.5,0,0,0  
2E3C,GLU\_261,4.57,0.07,0,0  
2Z84,LYS\_88,10.22,-0.28,0,0  
2FPN,GLU\_123,3.98,0.28,-0.8,0  
3ETV,GLU\_309,4.57,0.07,0,0  
1R7J,TYR\_40,10,0,0,0  
1YR6,GLU\_228,4.57,0.07,0,0  
1FHL,ASP\_91,3.51,0.35,-0.64,0  
1LZL,ARG\_303,12.15,-0.35,0,0  
3GMS,ARG\_283,11.87,-0.63,0,0  
3RFY,TYR\_109,13.86,0.69,0.8,2.37  
3CBN,LYS\_119,10.43,-0.07,0,0  
1SIG,HIS\_242,6.53,0.03,0,0  
1D2K,HIS\_66,2.02,1.6,-1,-5.08  
4DIU,HIS\_176,6.92,0.49,0,-0.07  
2RJD,GLU\_472,4.85,0.35,0,0  
1TUL,LYS\_105,9.73,-0.77,0,0  
3IVF,ARG\_30,12.43,-0.07,0,0  
3LJI,TYR\_250,11.37,0.59,0,0.78  
2B78,ARG\_132,11.73,-0.77,0,0  
3IOC,LYS\_131,10.29,-0.21,0,0  
1OIS,GLU\_255,4.92,0.42,0,0  
3GOZ,GLU\_15,3.91,0.21,-0.8,0  
1WXQ,ARG\_258,13.42,-1.48,0,2.4  
2EFK,LYS\_138,10.43,-0.07,0,0  
3RFY,ASP\_409,3.94,0.14,0,0  
1AKO,ARG\_184,10.47,-2.03,0,0  
2OGQ,ARG\_563,12.08,-0.42,0,0  
3M66,ASP\_388,2.63,0.42,-1.59,0  
3M70,GLU\_211,4.85,0.35,0,0  
1NIJ,GLU\_306,1.9,0.45,-0.8,-2.25  
2GAU,LYS\_121,10.22,-0.28,0,0  
2YLF,GLU\_148,4.57,0.07,0,0  
3DHN,CYS\_62,9,0,0,0  
1RWZ,LYS\_32,9.94,-0.56,0,0  
157K,LYS\_92,10.36,-0.14,0,0  
3CSR,LYS\_116,10.22,-0.28,0,0  
3VJ8,HIS\_98,6.43,0.07,0,-0.14  
1R3F,ASP\_230,3.8,0,0,0  
3GS9,ASP\_216,2.07,0.91,-2.64,0  
3M3P,CYS\_159,8.98,-2.28,0.74,1.53  
3HUE,GLU\_203,4.5,0,0,0  
2D7U,GLU\_240,4.27,0.56,-0.79,0  
2ZQ5,ASP\_341,3.69,0.07,-0.18,0  
22QY,GLU\_60,10.5,0,0,0  
3CQ1,ARG\_91,12.15,-0.35,0,0  
1DOV,LYS\_246,10.5,0,0,0  
2IF4,LYS\_39,10.15,-0.35,0,0  
4AM1,LYS\_15,10.08,-0.42,0,0  
1H4U,GLU\_558,4.5,0,0,0  
2OGQ,ASP\_402,2.75,0.84,-1.89,0  
1TR9,GLU\_295,4.57,0.07,0,0  
1LFP,ARG\_68,12.29,-0.21,0,0  
1O9G,CYS\_60,12.5,-0.66,2.44,1.72  
3IO0,LYS\_183,9.87,-0.63,0,0  
3KB5,ARG\_447,12.22,-0.28,0,0  
2CIU,TYR\_171,12.8,0.4,2.4  
3PM2,TYR\_166,9.82,0.35,-0.53,0  
2FZ4,LYS\_150,10.15,-0.35,0,0  
3EZZ,ARG\_378,11.94,-0.56,0,0  
3U0V,HIS\_20,6.71,0.49,0,-0.28  
1NRI,LYS\_241,10.43,-0.07,0,0  
3M70,GLU\_71,4.39,0.28,-0.39,0  
3B4D,GLU\_224,4.5,0,0,0  
4AM1,LYS\_340,10.29,-0.21,0,0  
3LMF,GLU\_35,4.78,0.28,0,0  
2O0K,GLU\_122,4.05,0.35,-0.8,0  
3F53,LYS\_198,10.36,-0.14,0,0  
1JKS,GLU\_239,4.57,0.07,0,0  
4ECC,CYS\_98,5.62,-3.45,0,0.07  
3L3P,GLU\_400,4.67,0.14,0.03,0  
3QKY,GLU\_238,4.5,0,0,0  
1AK1,ASP\_76,3.94,0.14,0,0  
2R57,ASP\_215,2.39,0.91,-2.31,0  
3EX9,GLU\_28,4.18,0.42,-0.74,0  
3DHN,ASP\_203,3.29,0.35,-0.86,0  
2Q98,LYS\_69,10.29,-0.21,0,0  
1MUF,GLU\_166,4.57,0.07,0,0  
1WXF,TYR\_231,9.1,0.62,0,-1.53  
3SMD,GLU\_17,4.06,0.07,-0.51,0  
3GG6,ARG\_65,12.5,0,0,0  
1TD6,GLU\_266,3.78,0.14,-0.86,0  
2EA9,ARG\_40,11.87,-0.63,0,0  
1KN3,ASP\_56,3.73,0,-0.07,0  
3P28,ARG\_186,12.15,-0.35,0,0  
1ZCU,HIS\_70,7.36,1.14,0,-0.28  
3HYQ,CYS\_37,13.81,0.2,2.24,2.57  
4DVD,ARG\_121,11.8,-0.7,0,0  
2XJ4,GLU\_87,4.57,0.07,0,0  
2B0J,LYS\_232,10.22,-0.28,0,0  
2QEV,ARG\_23,11.73,-0.77,0,0

1SIG,LYS\_426,10.36,-0.14,0,0  
 1MIX,LYS\_316,10.43,-0.07,0,0  
 35MD,TYR\_6,10,0,0,0  
 1MIX,CYS\_286,9.39,0,0,0.39  
 3EJG,LYS\_62,10.5,0,0,0  
 1SJ8,GLU\_780,5.69,1.38,-0.19,0  
 3D9H,HIS\_166,6.5,0,0,0  
 1P4X,ARG\_101,11.8,-0.7,0,0  
 3ZXV,GLU\_122,3.4,0.28,-1.38,0  
 1ZBM,GLU\_256,4.64,0.14,0,0  
 1RI6,LYS\_289,10.29,-0.21,0,0  
 3MTT,ARG\_510,12.29,-0.21,0,0  
 3GS9,GLU\_184,4.5,0,0,0  
 3NZL,LYS\_27,10.5,0,0,0  
 3CNU,LYS\_9,10.29,-0.21,0,0  
 2GAU,LYS\_136,10.5,0,0,0  
 3FS3,LYS\_44,10.22,-0.28,0,0  
 3DSH,LYS\_449,10.29,-0.21,0,0  
 3HVV,TYR\_324,10,0,0,0  
 1SQW,GLU\_7,3.98,0.28,-0.8,0  
 3C6B,ASP\_153,3.4,0.14,-0.54,0  
 1SOH,HIS\_35,1.24,0,0,-5.26  
 4EKU,CYS\_267,9.69,-0.3,0.21,0.77  
 1BN6,ASP\_175,4.01,0.28,-0.07,0  
 1ILW,ASP\_153,2.84,0.7,-1.66,0  
 4ECC,ASP\_114,3.87,0.14,-0.07,0  
 1PVT,GLU\_151,4.71,0.21,0,0  
 1GPP,GLU\_69,4.5,0,0,0  
 1NIJ,GLU\_97,2.82,1.45,-2.4,-0.73  
 1BN6,ASP\_150,2.88,0.14,-1.06,0  
 3JZN,ASP\_142,3.12,0.63,-1.31,0  
 1R53,GLU\_36,2.74,0.42,-2.18,0  
 2OJQ,GLU\_596,2.07,0.77,-3.2,0  
 2O8P,CYS\_161,9.99,0,0,0.99  
 2VAN,GLU\_147,2.52,0.42,-2.4,0  
 2NRR,GLU\_384,4.82,0.35,-0.03,0  
 4E8B,HIS\_27,6.43,0,0,-0.07  
 4ACJ,LYS\_787,10.5,0,0,0  
 4FH3,LYS\_63,10.5,0,0,0  
 2IRM,TYR\_247,10.28,0.28,0,0  
 2B78,TYR\_150,13.15,0.35,-0.37,3.17  
 2EJB,TYR\_156,10,0,0,0  
 3GG6,GLU\_62,0.1,1.48,-1.44,-4.44  
 1RAJ,ARG\_437,12.15,-0.35,0,0  
 2VAN,CYS\_267,10.55,0,0,1.55  
 3VHJ,ASP\_62,3.35,0.63,-1.08,0  
 3I4T,TYR\_268,13.99,0,0,1.3.89  
 2R57,ASP\_247,1.39,0.91,-3.32,0  
 2RFA,HIS\_201,3.27,1.08,0,-4.31  
 2XMZ,LYS\_236,10.36,-0.14,0,0  
 2OBI,CYS\_66,9,0,0,0  
 3D9H,HIS\_81,6.87,0.79,0,-0.42  
 2V4U,LYS\_560,10.43,-0.07,0,0  
 2GAU,ASP\_213,3.34,0.28,-0.74,0  
 2GKG,LYS\_3,10.15,-0.35,0,0  
 4E8B,ARG\_174,12.5,0,0,0  
 1X91,ASP\_39,3.56,0.63,-0.87,0  
 1AK1,ASP\_171,2.97,0.21,-1.04,0  
 2OYZ,ARG\_44,12.08,-0.42,0,0  
 3Q1C,ARG\_106,12.29,-0.21,0,0  
 2AHS,TYR\_197,11.1,0.07,-0.41,1.44  
 2ZCO,TYR\_41,11.79,2.26,-0.23,-0.24  
 1OLR,TYR\_11,12.82,0.21,0.22,2.4  
 2CL3,LYS\_23,10.43,-0.07,0,0  
 2NRR,LYS\_390,10.29,-0.21,0,0  
 2IRM,GLU\_264,4.5,0,0,0  
 1OGL,LYS\_92,10.29,-0.21,0,0  
 3EVN,TYR\_157,11.69,1.69,0,0  
 1BK6,GLU\_72,4.62,0.35,-0.23,0  
 2OKT,TYR\_44,11.56,0,0,1.56  
 1TWU,TYR\_59,10,0,0,0  
 3IOO,LYS\_283,10.5,0,0,0  
 1PV5,GLU\_49,4.61,0.21,-0.1,0  
 4F3J,LYS\_109,10.15,-0.35,0,0  
 1A8Q,ARG\_20,10.95,-1.55,0,0  
 2JKF,ARG\_14,12.15,-0.35,0,0  
 4FZR,ARG\_362,11.8,-0.7,0,0  
 3ZTA,GLU\_14,4.5,0,0,0  
 2RFA,ARG\_139,11.73,-0.77,0,0  
 2H30,ASP\_56,4.01,0.21,0,0  
 2JEO,LYS\_78,10.5,0,0,0  
 1SNT,ARG\_134,12.08,-0.42,0,0  
 3O7K,ARG\_41,11.59,-0.91,0,0  
 2E3C,GLU\_247,1.92,0.62,-0.8,-2.4  
 1LTU,ARG\_123,11.64,-2.98,0,2.12  
 3LJC,LYS\_219,10.01,-0.49,0,0  
 1WRU,TYR\_67,10.39,0,0,0.39  
 1X8F,ASP\_107,3.5,0.35,-0.65,0  
 1XDZ,LYS\_224,10.36,-0.14,0,0  
 3RNV,LYS\_414,10.5,0,0,0  
 1W7B,HIS\_224,6.39,1.62,1,-2.73  
 4DNU,ASP\_96,3.85,0.28,-0.23,0  
 3BPP,GLU\_162,4.64,0.14,0,0  
 3PAC,LYS\_135,10.29,-0.21,0,0  
 3NBI,GLU\_75,4.5,0,0,0  
 2Z0M,ASP\_220,3.15,0.21,-0.86,0  
 3GV0,ARG\_185,11.24,-1.26,0,0  
 1SJ8,ASP\_600,3.87,0.07,0,0  
 2G5X,LYS\_212,10.29,-0.21,0,0  
 1H4U,LYS\_500,10.15,-0.35,0,0  
 1YTQ,TYR\_61,9.41,0.21,-0.8,0  
 3I47,LYS\_59,10.5,0,0,0  
 2QZQ,TYR\_141,13.41,0.21,0.8,2.4  
 3VJ8,GLU\_234,4.78,0.28,0,0  
 1ES9,HIS\_166,6.51,0.22,0,-0.21  
 2PGE,ARG\_212,12.89,-3.02,0,3.41  
 1J7G,GLU\_18,4.5,0,0,0  
 2GQV,GLU\_75,4.12,0.42,-0.8,0  
 1WRU,ARG\_108,12.08,-0.42,0,0  
 1A8Q,LYS\_274,10.29,-0.21,0,0  
 3E5T,CYS\_222,6.61,-2.39,0,0  
 3LPZ,LYS\_92,10.15,-0.35,0,0  
 1Q46,ASP\_83,3.28,0.28,-0.8,0  
 2AZL,LYS\_17,10.43,-0.07,0,0  
 1QZN,TYR\_58,9.77,1.03,-1.26,0  
 2RGY,GLU\_230,4.25,0.42,-0.67,0  
 3E7P,GLU\_173,2.36,0.84,-1.67,-1.3  
 1Q46,CYS\_5,9.22,-0.31,0,0.53  
 3ELI,GLU\_9,4.15,0.07,-0.42,0  
 1MML,ASP\_174,3.24,0.84,-1.4,0  
 3NZL,ASP\_28,3.87,0.07,0,0  
 2B61,ARG\_291,11.73,-0.77,0,0  
 2O8I,ASP\_132,3.87,0.07,0,0  
 3COC,TYR\_344,10.07,0.07,0,0  
 2X4L,ASP\_336,3.46,0.42,-0.76,0  
 1V43,ARG\_74,12.08,-0.42,0,0  
 3M7G,GLU\_129,5.11,1.97,-1.36,0  
 2Z0M,ARG\_309,12.01,-0.49,0,0  
 1WP5,GLU\_308,3.98,0.28,-0.8,0  
 1Q46,GLU\_9,4.46,0.35,-0.39,0  
 1R6Y,GLU\_7,4.01,0.14,-0.63,0  
 3M16,LYS\_277,10.22,-0.28,0,0  
 4FZN,ARG\_228,12.29,-0.21,0,0  
 1VJG,LYS\_95,10.5,0,0,0  
 2R2Y,ARG\_27,12.29,-0.21,0,0  
 1A8Q,ARG\_48,12.15,-0.35,0,0  
 3GV0,ASP\_245,3.42,0.42,-0.8,0  
 3RNV,CYS\_344,7.52,-1.48,0,0  
 3KEY,LYS\_340,10.5,0,0,0  
 2POY,HIS\_328,7.29,0.79,0,0  
 1LFP,LYS\_23,10.15,-0.35,0,0  
 2O8P,ARG\_99,12.01,-0.49,0,0  
 1NRI,GLU\_227,4.21,0.28,-0.57,0  
 1KN3,LYS\_47,10.5,0,0,0  
 4FZR,TYR\_117,10.78,1.98,-0.4,-0.81  
 1OST,ARG\_162,10.06,-2.44,0,0  
 2A1V,ASP\_132,3.43,0.21,-0.58,0  
 3K8U,HIS\_87,4.82,1.05,0,-2.73  
 3ASA,ASP\_161,4.01,0.21,0,0  
 2FXT,ARG\_347,12.5,0,0,0  
 1GPP,LYS\_4,10.5,0,0,0  
 3GYW,ASP\_73,3.87,0.07,0,0  
 3MEW,HIS\_250,6.43,0,0,-0.07  
 3K8U,LYS\_27,10.43,-0.07,0,0  
 1O9G,TYR\_178,9.61,0.02,-0.81,0.41  
 1R9W,ARG\_287,12.01,-0.49,0,0  
 3FNI,ASP\_150,3.48,0.35,-0.67,0  
 3EOD,GLU\_45,4.5,0,0,0  
 3FS3,LYS\_81,10.5,0,0,0  
 1XEU,ARG\_39,12.43,-0.07,0,0  
 3B7X,ASP\_141,3.22,0.49,-1.06,0  
 2ATR,GLU\_90,4.5,0,0,0  
 1W7B,TYR\_317,10,0,0,0  
 1Z3X,ARG\_91,12.29,-0.21,0,0  
 3F6F,GLU\_38,3.68,0.35,-1.17,0  
 2CYG,TYR\_141,10,0,0,0  
 3RKY,LYS\_278,10.5,0,0,0  
 3H6Q,ARG\_81,9.56,-2.94,0,0  
 2CYG,LYS\_51,10.29,-0.21,0,0  
 3RE9,TYR\_87,9.92,0,-0.08,0  
 1O59,HIS\_312,4.81,1.38,0,-3.07  
 1IAP,LYS\_106,10.5,0,0,0  
 3L3P,GLU\_507,4.5,0,0,0  
 1P2F,ARG\_117,12.22,-0.28,0,0  
 3BWT,GLU\_606,4.5,0,0,0  
 3EJC,ARG\_80,12.01,-0.49,0,0  
 1PV5,ARG\_9,11.8,-0.7,0,0  
 2RGY,HIS\_117,6.57,0.07,0,0  
 2X4G,ARG\_308,12.36,-0.14,0,0  
 3NBI,HIS\_19,6.29,0,0,-0.21  
 3UC9,LYS\_149,10.22,-0.28,0,0  
 2FC3,GLU\_72,4.57,0.07,0,0  
 3V55,LYS\_538,10.29,-0.21,0,0  
 1Z9L,ARG\_55,12.5,0,0,0  
 4E2B,ASP\_277,3.45,0.56,-0.91,0  
 3IVF,LYS\_318,10.29,-0.21,0,0  
 1KN3,LYS\_93,10.43,-0.07,0,0  
 3JRT,GLU\_125,4.49,0.56,-0.57,0  
 3HUE,ASP\_221,3.45,0.07,-0.43,0  
 1GXN,GLU\_384,4.5,0,0,0  
 1XFK,HIS\_127,2.18,0.94,1.83,-7.09  
 3RLN,LYS\_683,10.43,-0.07,0,0  
 1R6Y,LYS\_89,10.22,-0.28,0,0  
 3I47,ASP\_187,3.81,0.07,-0.06,0  
 2A6B,ASP\_221,3.8,0,0,0  
 1VJG,ASP\_179,1.3,1.05,-3.54,0  
 4FH3,GLU\_50,4.71,0.21,0,0  
 3ASA,GLU\_384,4.5,0,0,0  
 3CAX,ASP\_208,3.31,0.28,-0.78,0  
 1PGV,GLU\_308,3.69,0.56,-1.38,0  
 2EFK,HIS\_266,6.5,0,0,0  
 3LJN,CYS\_61,8.95,-0.12,0,0.07  
 1O59,ARG\_238,12.5,0,0,0  
 3DSH,HIS\_452,6.43,0,0,-0.07  
 2IF4,ARG\_284,12.36,-0.14,0,0  
 2OEW,LYS\_285,10.5,0,0,0  
 1MUF,HIS\_252,7.32,0.89,0,-0.07  
 2PLQ,LYS\_106,10.08,-0.42,0,0  
 4AM1,HIS\_284,8.16,1.6,1.6,-1.54  
 1PBV,ARG\_98,12.29,-0.21,0,0  
 1WYC,ARG\_130,12.01,-0.49,0,0  
 2Q5X,ASP\_731,3.66,0,-0.14,0  
 4E9E,LYS\_565,10.36,-0.14,0,0  
 3ON1,TYR\_59,10,0,0,0  
 3NR5,GLU\_5,4.5,0,0,0  
 1J33,TYR\_25,10.78,0.9,-0.86,0.73  
 3GE9,CYS\_215,11.46,0,0,2.46  
 2Q98,HIS\_46,6.36,0,0,-0.14  
 1PV5,ARG\_101,11.34,-1.16,0,0  
 3F7M,TYR\_163,10.07,0.07,0,0  
 1JSX,ARG\_87,11.71,-0.79,0,0  
 3M7D,LYS\_335,10.01,-0.49,0,0  
 3HVM,LYS\_30,10.5,0,0,0  
 1WJG,ARG\_17,12.01,-0.49,0,0  
 1OTM,LYS\_64,10.5,0,0,0  
 2D2S,TYR\_739,10.57,0.07,0,0.5  
 2H2Z,CYS\_156,9,0,0,0  
 2JEO,ARG\_66,11.05,-1.45,0,0  
 2ATR,GLU\_109,4.5,0,0,0  
 1GPP,ASP\_429,3.0,1.4,-0.94,0  
 1M5I,CYS\_207,9,0,0,0  
 2NRR,LYS\_447,10.22,-0.28,0,0  
 2XJ4,ARG\_213,11.94,-0.56,0,0  
 2GZR,ASP\_99,2.31,0.63,-2.11,0  
 3OKQ,GLU\_622,4.71,0.21,0,0  
 3GE9,ARG\_199,11.66,-0.84,0,0  
 3RFF,ARG\_23,12.01,-0.49,0,0  
 2C2Y,ASP\_237,3.78,0,-0.02,0  
 3ONH,ARG\_497,12.15,-0.35,0,0  
 3LH5,ASP\_701,3.8,0,0,0  
 2BLL,ASP\_445,2.65,0.91,-2.07,0  
 3ETV,LYS\_282,10.5,0,0,0  
 3FRR,LYS\_7,10.5,0,0,0  
 1ZBS,CYS\_15,7.28,-2.36,0,0.64  
 3T57,LYS\_126,10.5,0,0,0  
 3BJV,GLU\_147,4.05,0.35,-0.8,0  
 1T3Y,ASP\_19,3.06,0.49,-1.23,0  
 3ETV,LYS\_282,10.5,0,0,0  
 2Z14,LYS\_121,10.5,0,0,0  
 1F2V,GLU\_171,3.33,0.63,-1.8,0  
 4ECC,GLU\_30,4.37,1.66,0,-1.79  
 3DB9,ASP\_98,3.87,0.07,0,0  
 1BGF,ARG\_114,11.94,-0.56,0,0  
 2QV2,GLU\_155,4.24,0.7,-0.96,0  
 2CI3,GLU\_243,4.11,0.28,-0.67,0  
 1RKA,ARG\_239,12.15,-0.35,0,0  
 2OJQ,GLU\_439,4.64,0.14,0,0  
 3HNX,HIS\_47,6.29,0,0,-0.21  
 4D8L,ASP\_88,3.62,0.56,-0.74,0  
 2FPN,ASP\_104,3.75,0,0,-0.05,0  
 3Q1C,GLU\_52,3.28,0.14,-1.37,0  
 3B7X,ARG\_24,12.15,-0.35,0,0  
 4H86,ASP\_163,3.59,0.49,-0.7,0  
 1O5T,LYS\_418,10.5,0,0,0  
 1C3K,LYS\_105,10.29,-0.21,0,0  
 1O6D,GLU\_46,3.6,0.14,-1.04,0  
 2B0A,LYS\_170,10.5,0,0,0  
 3U0V,TYR\_158,11.4,1.23,-0.72,0.89  
 4EUG,LYS\_15,10.15,-0.35,0,0  
 4EKU,ARG\_79,12.01,-0.49,0,0  
 2WB8,GLU\_451,4.57,0.07,0,0  
 2G9D,TYR\_211,12.26,0.55,0,1.71  
 3EAZ,GLU\_142,4.64,0.14,0,0  
 2CI3,GLU\_239,4.06,0.35,-0.79,0  
 2B0A,ARG\_21,12.43,-0.07,0,0  
 2B0J,ARG\_12,13.64,-1.26,0,2.4



3BPV,ARG\_19,12.36,-0.14,0,0  
3I82,HIS\_106,5.08,0,0,-1.42  
1NRI,ARG\_34,12.22,-0.28,0,0  
1ZYL,ARG\_242,12.43,-0.07,0,0  
3IVF,ASP\_201,1.6,0.84,-3.05,0  
3RLN,CYS\_679,8.65,-0.49,0,0.14  
4FCU,TYR\_155,13.31,0.21,0.7,2.4  
2QRX,ARG\_24,11.94,-0.56,0,0  
3EJG,LYS\_104,10.5,0,0,0  
1AK1,LYS\_188,10.5,0,0,0  
1XDZ,TYR\_141,13.15,0.94,-0.78,2.98  
3RFF,ASP\_139,2.15,0.28,-1.93,0  
2XMZ,GLU\_165,3.95,0.63,-1.18,0  
2R2Y,CYS\_127,9.1,-0.04,0,0.14  
4DIU,GLU\_132,4.5,0,0,0  
2OBI,GLU\_87,4.5,0,0,0  
2O8P,ASP\_50,3.13,0.14,-0.81,0  
3ILC,ASP\_176,4.22,0.42,0,0  
2VGM,ASP\_340,3.8,0.14,-0.14,0  
2FZP,ARG\_213,12.15,-0.35,0,0  
3I0C,CYS\_209,10.88,-1.6,0.3,48  
3NJM,LYS\_12,10.43,-0.07,0,0  
1NIJ,ASP\_161,3.72,0.14,-0.22,0  
3M66,LYS\_237,10.5,0,0,0  
1RWZ,LYS\_84,10.5,0,0,0  
2GAU,GLU\_114,3.66,0.21,-1.05,0  
1AD6,LYS\_537,9.94,-0.56,0,0  
3G9T,LYS\_68,10.29,-0.21,0,0  
3GOZ,ARG\_175,12.53,-0.39,0,0.42  
3HNX,ARG\_20,12.15,-0.35,0,0  
1P6F,LYS\_118,10.5,0,0,0  
3KEY,GLU\_330,4.0,28,-0.78,0  
2ZQ5,ARG\_101,11.89,-0.61,0,0  
1KCM,ASP\_154,3.52,0.91,-1.2,0  
3BWT,ASP\_846,3.64,0.28,-0.44,0  
2FZ4,GLU\_69,4.57,0.07,0,0  
1UW7,CYS\_14,9.95,-0.25,0,1.2  
2P1W,ASP\_84,2.47,1.05,-2.38,0  
3ADO,ARG\_261,12.15,-0.35,0,0  
3ELI,ARG\_49,11.17,-1.33,0,0  
1IAP,ARG\_126,12.22,-0.28,0,0  
3GS3,GLU\_91,2.1,1.13,-1.68,-1.85  
3EYE,ASP\_147,2.29,0.42,-1.16,-0.77  
3JZN,ARG\_173,13.33,-1.08,0,1.91  
2X4J,LYS\_88,10.43,-0.07,0,0  
2QOP,GLU\_64,4.57,0.07,0,0  
2YYO,LYS\_100,10.5,0,0,0  
2Z84,CYS\_162,8.76,-0.46,0,0.22  
3M66,GLU\_270,4.56,0.14,-0.08,0  
1JT9,GLU\_148,1.58,0.56,-3.48,0  
4FH3,ASP\_109,3.21,0.77,-1.36,0  
2RGY,ASP\_182,3.86,0.28,-0.22,0  
4EZB,TYR\_222,10,0,0,0,0  
3BWT,ASP\_711,3.93,0.14,-0.01,0  
3DSH,TYR\_325,11.51,0,0,1.51  
3BWT,ASP\_853,3.41,0.07,-0.46,0  
1RLO,ASP\_49,4.07,0.35,-0.08,0  
2BLL,GLU\_333,4.44,0.59,-0.65,0  
1F2V,CYS\_98,7.39,-2.77,0.03,1.13  
2A6B,TYR\_220,13.59,0.39,0.8,2.4  
2GAU,HIS\_12,6.43,0,0,-0.07  
3IBT,GLU\_15,3.22,0.49,-1.77,0  
2CBE,LYS\_18,10.08,-0.42,0,0  
2PGE,ARG\_64,12.29,-0.21,0,0  
3LJN,ASP\_232,3.06,0.42,-1.16,0  
3QAV,LYS\_183,10.22,-0.28,0,0  
3FK5,GLU\_177,5.81,1.39,-0.08,0  
1U7U,HIS\_188,6.5,0,0,0  
3LQE,GLU\_516,4.22,0.35,-0.63,0  
3PZ9,ASP\_84,3.33,0.28,-0.75,0  
1NFN,GLU\_79,3.86,0.56,-1.2,0  
1KN3,HIS\_48,6.43,0,0,-0.07  
3H13,ARG\_337,11.52,-0.98,0,0  
2RIS,ARG\_29,12.01,-0.49,0,0  
1RKA,ASP\_175,3.18,0.21,-0.83,0  
1YOY,ARG\_34,12.5,0,0,0  
4AF2,ASP\_34,2.0,42,-2.23,0  
2P0L,GLU\_66,4.5,0,0,0  
3CGW,HIS\_278,6.5,0,0,0  
3FFM,ARG\_100,11.87,-0.63,0,0  
1SUU,ASP\_608,3.12,0.28,-0.96,0  
3EZ7,LYS\_320,10.5,0,0,0  
1E55,TYR\_108,9.11,0.28,-1.17,0  
3P28,TYR\_134,12.21,0,0,2.21  
1E55,ARG\_86,11.94,-0.56,0,0  
3VJ8,GLU\_131,2.95,0.63,-2.17,0  
2XHC,GLU\_273,3.55,0.28,-1.24,0  
1DOV,ARG\_241,11.24,-1.26,0,0  
2C2Y,LYS\_59,10.29,-0.21,0,0  
3UX2,ARG\_149,12.22,-0.28,0,0  
3IL3,CYS\_92,6.93,-2.07,0,0  
3NZL,GLU\_15,3.88,0.49,-1.11,0  
3RNV,HIS\_411,7.21,1.13,0,-0.42  
1V43,LYS\_306,10.5,0,0,0  
2B02,ASP\_404,0.92,0.56,-3.44,0  
3DHN,GLU\_221,3.84,0.14,-0.8,0  
2ZOW,LYS\_47,10.5,0,0,0  
3Q9P,TYR\_133,10,0,0,0,0  
3ERF,GLU\_57,3.23,0.63,-1.91,0  
1W24,HIS\_33,7.11,0.82,0,-0.21  
2C13,LYS\_158,10.5,0,0,0  
3UPD,GLU\_20,3.11,0.49,-1.88,0  
3M16,GLU\_267,4.59,0.21,-0.12,0  
2A6B,TYR\_110,11.61,0.83,0,0.78  
2QK1,LYS\_558,10.5,0,0,0  
4F3J,TYR\_214,11.07,0,0,1.07  
3LJI,ARG\_289,11.73,-0.77,0,0  
3IL3,ARG\_36,12.15,-0.35,0,0  
3EGN,LYS\_484,10.5,0,0,0  
3EGN,LYS\_461,10.36,-0.14,0,0  
2Q12,ASP\_241,3.66,0.14,-0.28,0  
2QVT,HIS\_81,7.18,0.75,0,-0.07  
3LJC,GLU\_227,4.5,0,0,0  
2BDV,LYS\_116,10.08,-0.42,0,0  
4ETX,ASP\_351,0.83,0.7,-3.66,0  
3DHN,ASP\_97,3.64,0.49,-0.65,0  
3EJG,GLU\_37,4.71,0.21,0,0  
3EX9,ARG\_149,12.01,-0.49,0,0  
3ASA,CYS\_168,11.74,0,0,2.74  
3E5T,ASP\_112,3.87,0.07,0,0  
1NAF,LYS\_206,10.5,0,0,0  
3R87,HIS\_7,4.14,0,0,-2.36  
3JZ9,LYS\_401,10.01,-0.49,0,0  
3M66,GLU\_221,3.91,0.21,-0.8,0  
2VGY,ARG\_105,12.08,-0.42,0,0  
3LQE,TYR\_501,9.63,0.07,-0.44,0  
4E8B,ARG\_209,12.01,-0.49,0,0  
1R9W,LYS\_299,10.29,-0.21,0,0  
2O8P,LYS\_15,10.01,-0.49,0,0  
4GA2,LYS\_5,10.36,-0.14,0,0  
1JYH,LYS\_40,10.08,-0.42,0,0  
3LJC,LYS\_113,10.36,-0.14,0,0  
3F6F,TYR\_77,13.48,0.21,0.87,2.4  
2HXB,TYR\_103,13.32,0.14,0.78,2.4  
2OSA,GLU\_291,3.98,0.28,-0.8,0  
4DIU,GLU\_58,3.23,0.49,-1.76,0  
1ZBM,TYR\_18,13.34,0.14,0.8,2.4  
3IPZ,TYR\_132,11.26,0,0,1.26  
2P5D,LYS\_116,10.29,-0.21,0,0  
1C44,LYS\_122,10.29,-0.21,0,0  
3GOZ,ASP\_98,3.49,0.07,-0.38,0  
3CCY,LYS\_45,10.43,-0.07,0,0  
1FHL,TYR\_296,11.07,3.04,-1.97,0  
2E3C,GLU\_324,1.38,2.13,-2.6,-2.64  
3GE9,GLU\_10,4.24,0.14,-0.4,0  
2QV2,ARG\_319,12.43,-0.07,0,0  
2RH3,HIS\_169,6.43,0,0,-0.07  
4F85,ARG\_238,12.5,0,0,0  
3V75,LYS\_190,4.48,0,-0.02,0  
4DVD,ARG\_166,12.01,-0.49,0,0  
2Z14,ASP\_81,3.3,0.21,-0.71,0  
1F09,LYS\_335,10.01,-0.49,0,0  
1SJ8,LYS\_745,10.5,0,0,0  
2BV9,ARG\_90,11.87,-0.63,0,0  
3BWT,ARG\_728,12.84,-0.71,0,1.05  
1PNE,GLU\_129,4.64,0.14,0,0  
1RWZ,LYS\_203,10.29,-0.21,0,0  
2EYI,GLU\_254,4.5,0,0,0  
1DZF,HIS\_147,6.22,0,0,-0.28  
4AM1,GLU\_11,4.05,0.35,-0.8,0  
1N81,TYR\_76,10,0,0,0,0  
3M7D,LYS\_116,10.22,-0.28,0,0  
3V46,HIS\_344,7.66,1.3,0,-0.14  
1FOI,HIS\_381,6.15,0,0,-0.35  
1DUPT,TYR\_93,9.78,0.07,-0.29,0  
1YTD,ASP\_274,2.03,0.77,-2.55,0  
1LZL,ASP\_150,1.99,0.84,-2.66,0  
2RIK,ASP\_205,3.25,0.56,-1.11,0  
2CXA,ASP\_192,3.73,0,-0.07,0  
2B61,ARG\_79,12.22,-0.28,0,0  
3B21,GLU\_100,4.5,0,0,0  
1SUU,TYR\_569,13.59,0.28,0.65,2.66  
4ETX,HIS\_440,6.76,0.26,0,0  
3KEY,GLU\_432,4.5,0,0,0  
4GA2,LYS\_40,10.5,0,0,0  
1V8E,HIS\_170,6.43,0,0,-0.07  
2CWY,ARG\_37,11.94,-0.56,0,0  
3GEC,GLU\_528,4.57,0.07,0,0  
2RIK,ASP\_83,2.14,0.42,-2.09,0  
3LQE,GLU\_296,4.78,0.28,0,0  
4DEZ,ASP\_209,2.59,0.28,-1.49,0  
2H85,ARG\_257,11.66,-0.84,0,0  
3IBT,GLU\_186,3.38,0.35,-1.47,0  
2P4D,TYR\_9,13.24,0.35,0.49,2.4  
3DHN,ASP\_132,4.12,0.35,-0.03,0  
2FZ4,ASP\_180,3.79,0,-0.01,0  
3FWU,GLU\_74,4.71,0.21,0,0  
1BKR,ASP\_91,2.03,0.49,-2.26,0  
4AM1,TYR\_145,8.65,1.71,-0.65,-2.4  
1JT9,ARG\_156,11.52,-0.98,0,0  
1X7F,LYS\_290,10.5,0,0,0  
2H2W,LYS\_87,10.36,-0.14,0,0  
2CWC,ARG\_156,12.01,-0.49,0,0  
2ZQ5,ARG\_131,11.22,-3.11,0,1.83  
2QV2,ASP\_76,2.71,0.84,-1.92,0  
1HF8,HIS\_32,6.43,0,0,-0.07  
2FD4,ARG\_550,12.15,-0.35,0,0  
1L3K,CYS\_175,8.07,-1.23,0,0.3  
1VSM,GLU\_68,4.29,0.95,-1.16,0  
1RSQ,ASP\_62,3.85,0.07,-0.02,0  
2IQT,LYS\_67,10.08,-0.42,0,0  
1Y2Q,ASP\_9,2.51,0.63,-1.92,0  
3E7Y,LYS\_243,10.29,-0.21,0,0  
2Q07,ARG\_244,12.5,0,0,0  
3I00,HIS\_224,6.77,1.62,4.19,-5.53  
2CW4,LYS\_107,10.5,0,0,0  
4GCO,ARG\_172,11.94,-0.56,0,0  
3H9W,ASP\_68,0.21,0.63,-4.22,0  
2P1W,HIS\_41,6.5,0,0,0  
3EIZ,HIS\_-13,6.36,0,0,-0.14  
3V75,ASP\_38,3.49,0.49,-0.8,0  
2F4Q,ARG\_116,12.5,0,0,0  
3B7X,ASP\_35,11.38,0.77,-3.18,0  
3CS1,GLU\_149,4.5,0,0,0  
2ZQ5,LYS\_91,10.5,0,0,0  
3V55,GLU\_521,4.78,0.49,-0.21,0  
1X04,HIS\_204,6.43,0,0,-0.07  
1XAW,TYR\_481,13.03,0.14,0.49,2.4  
2BAA,ASP\_20,3.55,0.56,-0.81,0  
1TJE,ASP\_167,3.43,0.21,-0.58,0  
1XEU,ARG\_153,12.29,-0.21,0,0  
3OAT,LYS\_542,10.5,0,0,0  
1OXZ,GLU\_203,4.41,0.42,-0.51,0  
2XMZ,ARG\_290,13.77,-1.13,0,2.4  
1Q46,ARG\_52,12.5,0,0,0  
1JB3,GLU\_118,4.57,0.07,0,0  
2D7U,LYS\_89,10.08,-0.42,0,0  
1L2F,LYS\_339,10.15,-0.35,0,0  
1BKB,ASP\_68,3.38,0.14,-0.56,0  
3RFY,ARG\_290,13.66,-0.84,0,0  
2OYZ,CYS\_91,12.32,0.15,2.31,0.87  
2V5B,LYS\_218,10.36,-0.14,0,0  
4EFS,ARG\_197,11.14,-1.01,0,-0.35  
2CN1,CYS\_70,8.74,-0.26,0,0  
3RKV,ARG\_305,12.15,-0.35,0,0  
3RFY,ARG\_290,13.66,-0.84,0,0  
4GA2,CYS\_82,9.96,-0.06,0,1.02  
2P4D,GLU\_104,4.2,0.49,-0.79,0  
3FNI,TYR\_11,12.02,0,0,2.02  
1I60,LYS\_87,10.43,-0.07,0,0  
3IVF,LYS\_364,10.5,0,0,0  
1LN4,TYR\_85,10.86,0.07,-0.8,1.59  
1QYI,LYS\_197,10.15,-0.35,0,0  
2D7U,TYR\_22,12.59,0.53,0.8,1.26  
3ETU,ARG\_92,12.15,-0.35,0,0  
4HDE,LYS\_91,10.5,0,0,0  
2VGM,LYS\_307,10.22,-0.28,0,0  
2RFA,TYR\_222,11.01,0.07,0.0,0.94  
1JB3,GLU\_6,4.5,0,0,0  
3JZN,ASP\_341,3.38,0.28,-0.7,0  
1YTD,LYS\_299,10.5,0,0,0  
3C6B,HIS\_122,6.17,0.02,0,-0.35  
3IVF,ASP\_69,4.07,0.49,-0.22,0  
1YM5,GLU\_33,2.05,0.77,-1.56,-1.66  
3FWU,HIS\_43,6.55,0.26,0,-0.21  
2QZQ,LYS\_132,10.22,-0.28,0,0  
2CBE,HIS\_119,5.18,1.6,3.47,-6.4  
2OEW,ASP\_182,3.78,0,-0.02,0  
1Q42,LYS\_106,10.08,-0.42,0,0  
2X4J,GLU\_116,3.84,0.14,-0.8,0  
2NYC,LYS\_276,10.5,0,0,0  
3HUE,GLU\_220,3.1,0.49,-1.89,0  
3ILC,ARG\_132,12.43,-0.07,0,0  
2CXC,ASP\_32,2.31,0.91,-2.41,0  
1AD6,GLU\_492,2.8,2.64,-2.56,-1.78  
1BN6,GLU\_171,4.64,0.14,0,0  
1YOY,GLU\_37,3.55,1.99,-1.58,-1.36  
3EZ7,GLU\_218,3.84,0.35,-1.01,0  
1MUF,GLU\_183,4.5,0,0,0  
3RJK,GLU\_308,3.98,0.28,-0.8,0  
2EFK,LYS\_166,10.5,0,0,0  
2IXM,ASP\_35,0.75,0.56,-3.62,0  
1UXO,HIS\_119,6.36,0,0,-0.14  
2OJQ,ASP\_459,3.02,0.21,-0.98,0  
1H4U,TYR\_388,10,0,0,0,0  
2XHC,TYR\_247,9.7,0,-0.3,0

2BDV,LYS\_113,10.5,0,0,0  
15QW,ARG\_174,12.08,-0.42,0,0  
3UOV,LYS\_82,10.5,0,0,0  
4FLE,LYS\_115,10.5,0,0,0  
3ONT,ARG\_106,12.5,0,0,0  
3CIV,ARG\_290,11.87,-0.63,0,0  
2E3C,GLU\_199,4.71,0.21,0,0  
2PWQ,LYS\_9,10.29,-0.21,0,0  
1XFK,ARG\_203,11.87,-0.63,0,0  
3K8J,HIS\_123,6.36,0,0,-0.14  
2FC3,GLU\_103,4.71,0.21,0,0  
1P4X,LYS\_206,10.15,-0.35,0,0  
3RLN,LYS\_743,10.08,-0.42,0,0  
1T95,HIS\_126,7.1,0.74,0,-0.14  
4ANN,HIS\_46,6.93,0.7,0,-0.28  
1EYH,ASP\_108,4.01,0.21,0,0  
3A7L,CYS\_57,10.02,0,0.27,0.75  
3OA7,TYR\_43,10,0,0,0  
3HUE,TYR\_23,11.41,1.61,-0.2,0  
1MUF,TYR\_335,10.08,0,0,0.08  
3KT9,ASP\_69,3.41,0.7,-1.09,0  
1NJ4,LYS\_92,10.36,-0.14,0,0  
1PZC,GLU\_113,4.71,0.28,0,0  
1L2F,GLU\_79,4.5,0,0,0  
3RRQ,GLU\_146,3.04,0.07,-1.54,0  
1EDG,ASP\_52,1.01,0.49,-3.27,0  
2B0J,CYS\_10,1.82,-6.28,-2.46,1.56  
2Q07,ARG\_497,12.29,-0.21,0,0  
2R51,TYR\_222,10,0,0,0  
3ADO,LYS\_33,9.73,-0.77,0,0  
1TUL,TYR\_61,12.25,0.32,0,1.93  
3EX9,ARG\_105,12.08,-0.42,0,0  
2RJD,TYR\_416,12.95,0.21,0.34,2.4  
1NJ4,ASP\_120,3.91,0.28,-0.17,0  
1GPP,ASP\_163,2.14,0.77,-2.43,0  
1QYI,LYS\_301,9.87,-0.63,0,0  
2X4G,ASP\_335,3.83,0.14,-0.11,0  
1ANU,ASP\_34,3.2,0.56,-1.16,0  
4E8B,GLU\_22,4.07,0.28,-0.71,0  
3BCY,LYS\_118,10.43,-0.07,0,0  
2B3M,LYS\_147,10.36,-0.14,0,0  
350A,LYS\_82,10.36,-0.14,0,0  
3UAH,HIS\_320,11.97,3.2,4.74,-2.47  
1AKO,ARG\_251,11.01,-1.96,0,0.47  
4FCU,ARG\_59,11.87,-0.63,0,0  
3L7N,GLU\_9,3.54,0.49,-1.45,0  
3T8R,ARG\_112,12.01,-0.49,0,0  
1N81,ARG\_78,12.15,-0.35,0,0  
3GW3,ASP\_17,3.2,0.28,-0.87,0  
1OOX,HIS\_181,3.86,0,0,-2.64  
2P5D,LYS\_109,10.01,-0.49,0,0  
1OTM,GLU\_236,4.71,0.21,0,0  
1TR9,GLU\_182,4.5,0,0,0  
3E7P,LYS\_135,10.5,0,0,0  
1RWZ,ARG\_117,12.01,-0.49,0,0  
1PZC,HIS\_40,9.74,4.4,1.87,-3.03  
3L3P,ARG\_490,12.22,-0.28,0,0  
2F4Q,TYR\_298,11.55,0.14,-0.05,1.46  
2CWC,TYR\_119,9.41,0.21,-0.8,0  
3M66,LYS\_381,10.22,-0.28,0,0  
2GYZ,ASP\_44,2.63,0.7,-1.87,0  
2EA9,ASP\_95,2.81,1.05,-2.04,0  
3C6B,HIS\_140,6.6,0,1,0,0  
1LZL,TYR\_139,11.22,0,-0.44,1.67  
2B0A,LYS\_160,10.36,-0.14,0,0  
3U4K,ARG\_69,11.8,-0.7,0,0  
3HVV,ASP\_316,3.87,0.07,0,0  
1MTZ,LYS\_283,10.5,0,0,0  
2IXM,ARG\_86,12.01,-0.49,0,0  
3IVF,HIS\_176,4.87,1,0,-2.63  
4H86,LYS\_32,10.08,-0.42,0,0  
3LJI,ASP\_106,2.38,0.7,-2.13,0  
1NAR,GLU\_61,4.5,0,0,0  
2Q34,TYR\_144,11.24,0.89,0,0.35  
4FCU,GLU\_52,4.23,0.14,-0.41,0  
1V43,GLU\_229,3.29,0.21,-1.42,0  
2JHY,LYS\_127,10.36,-0.14,0,0  
4F8A,ARG\_564,12.36,-0.14,0,0  
3H13,LYS\_430,10.22,-0.28,0,0  
3CX5,LYS\_146,10.29,-0.21,0,0  
2CXY,GLU\_112,4.5,0,0,0  
3T8R,CYS\_25,9.05,-0.09,0,0.14  
1FQI,LYS\_346,9.87,-0.63,0,0  
3JZ9,ASP\_457,3.22,0.7,-1.28,0  
1V6T,LYS\_251,10.36,-0.14,0,0  
1MN3,LYS\_435,10.29,-0.21,0,0  
3P2F,ARG\_69,13.75,-3.21,0,4.46  
3ODJ,TYR\_106,10,0,0,0  
2Z61,ASP\_172,2.73,0.35,-1.42,0  
1NAF,ARG\_191,12.43,-0.07,0,0  
2FBI,GLU\_123,4.71,0.21,0,0  
2NNU,TYR\_14,9.87,0.21,-0.8,0.46  
1BYI,LYS\_217,10.5,0,0,0  
1SFE,ARG\_165,11.37,-1.13,0,0  
2W0G,GLU\_221,4.5,0,0,0  
3OKQ,LYS\_665,10.5,0,0,0  
3GW3,GLU\_316,2.88,0.28,-1.9,0  
4GA2,LYS\_106,10.43,-0.07,0,0  
2OGQ,LYS\_475,9.87,-0.63,0,0  
1N81,GLU\_42,0.74,3.86,-3.2,-4.42  
2FL4,ARG\_92,12.22,-0.28,0,0  
1NRI,LYS\_208,10.29,-0.21,0,0  
3FHF,GLU\_184,4.86,0.21,0.15,0  
2B61,ASP\_190,2.05,1.19,-2.94,0  
3PBH,GLU\_171,8.44,4.86,-0.92,0  
3GG6,GLU\_138,4.78,0.28,0,0  
4GCC,LYS\_229,10.5,0,0,0  
1ILW,ARG\_51,11.46,-1.04,0,0  
3BQW,GLU\_78,4.47,0.77,-0.8,0  
1RWZ,GLU\_24,4.57,0.07,0,0  
2R51,GLU\_20,3.48,0,-1.02,0  
3F6F,GLU\_196,2.28,0.68,-0.57,-2.32  
3PP8,LYS\_58,10.29,-0.21,0,0  
1MIX,LYS\_343,10.5,0,0,0  
2RGY,ARG\_112,12.29,-0.21,0,0  
2YWX,GLU\_28,4.5,0,0,0  
1YB2,ARG\_89,12.5,0,0,0  
3KT9,ASP\_11,2.87,0.56,-1.48,0  
2O8I,ASP\_65,2.67,0.21,-1.34,0  
3H5T,ARG\_190,11.87,-0.63,0,0  
4E65,GLU\_32,4.13,0.14,-0.51,0  
2R4Q,LYS\_216,10.43,-0.07,0,0  
2FG1,ASP\_9,2.35,0.49,-1.94,0  
1BN6,GLU\_31,4.99,0.49,0,0  
2H14,LYS\_87,10.5,0,0,0  
4FCU,ASP\_236,2.19,0.49,-2.1,0  
3OBS,TYR\_15,9.83,1.1,-1.27,0  
1XFK,LYS\_233,10.36,-0.14,0,0  
3HUE,GLU\_193,4.57,0.07,0,0  
3RJX,GLU\_259,4.42,0.35,-0.43,0  
2Q34,LYS\_80,10.29,-0.21,0,0  
1RAJ,CYS\_212,9.88,-0.34,0,1.22  
1YB2,LYS\_30,10.5,0,0,0  
1J8B,LYS\_20,10.29,-0.21,0,0  
2O8P,LYS\_227,10.36,-0.14,0,0  
3M66,GLU\_311,3.8,0.49,-1.19,0  
1RKA,GLU\_126,4.05,0.35,-0.8,0  
1RZ2,TYR\_202,10.76,1.04,-0.28,0  
1YR6,GLU\_134,4.57,0.07,0,0  
1WNH,LYS\_64,10.5,0,0,0  
3T57,LYS\_268,10.5,0,0,0  
2OBS,HIS\_15,6.5,0,0,0  
4EKU,ASP\_116,3.9,0.49,-0.39,0  
4DVD,CYS\_123,9,0,0,0  
1PV5,CYS\_102,3.84,-3.6,-2.26,0.7  
1N81,GLU\_116,4.5,0,0,0  
3V3T,CYS\_87,8.31,-1.09,0,0.4  
2R0S,LYS\_206,10.5,0,0,0  
3PM2,HIS\_34,7.16,0.8,0,-0.14  
3R2E,GLU\_81,4.35,0.07,-0.22,0  
2AZP,ARG\_34,12.64,-1.05,0,1.19  
3GEC,TYR\_459,11.62,2.76,-1.14,0  
2BAA,TYR\_112,10.64,0.07,-1.19,1.76  
2RFA,LYS\_54,10.5,0,0,0  
2YWX,LYS\_13,10.5,0,0,0  
3KEY,ASP\_471,4.44,1.05,-0.41,0  
4EVF,LYS\_133,10.5,0,0,0  
2FPN,GLU\_35,3.21,0.42,-1.71,0  
2ZCX,GLU\_34,4.64,0.14,0,0  
3E27,LYS\_43,10.08,-0.42,0,0  
3BPB,GLU\_59,5.1,1.32,0,-0.72  
1NAR,TYR\_45,11.41,0,0,1.41  
1TD6,LYS\_122,9.87,-0.63,0,0  
3ETV,GLU\_235,3.84,0.14,-0.8,0  
3CIV,GLU\_156,3.45,2.79,-1.6,-2.24  
2CXY,LYS\_43,10.22,-0.28,0,0  
3RE9,ARG\_96,12.15,-0.35,0,0  
1V8E,GLU\_22,1.05,0.53,-0.8,-3.18  
1YTD,GLU\_96,0.6,1.35,-1.47,-3.78  
3EJC,GLU\_23,4.21,0.28,-0.57,0  
3NZL,HIS\_10,6.5,0,0,0  
4F85,GLU\_278,1.35,1.19,-4.33,0  
2CVB,ASP\_124,2.18,1.12,-2.74,0  
3IVF,LYS\_83,10.29,-0.21,0,0  
2B3M,LYS\_133,10.5,0,0,0  
3CAX,ASP\_370,1.54,0.98,-3.24,0  
2O0K,LYS\_136,10.36,-0.14,0,0  
3DHN,GLU\_204,0.53,1.3,-3.46,-1.8  
3IRM,ASP\_337,3.93,0.14,-0.01,0  
2D59,GLU\_60,4.5,0,0,0  
2BCF,HIS\_159,6.43,0,0,-0.07  
1AD6,GLU\_458,4.45,0.75,-0.8,0  
2P4D,CYS\_99,9.23,-0.14,0,0.37  
2OKT,HIS\_66,6.72,0.29,0,-0.07  
1NAR,LYS\_181,10.22,-0.28,0,0  
2V4U,CYS\_362,9.21,0,0,0.21  
2GKG,LYS\_36,10.5,0,0,0  
2Y2T,GLU\_40,4.58,0.21,-0.13,0  
3UV9,GLU\_410,4.03,0.28,-0.75,0  
3PAC,TYR\_137,8.02,0.36,-0.8,-1.54  
2RIS,ASP\_26,2.15,0.42,-2.07,0  
2NNU,HIS\_86,6.5,0,0,0  
4E8B,ARG\_114,12.01,-0.49,0,0  
1NJ4,ASP\_67,2.48,0.63,-1.95,0  
1X7F,GLU\_200,0.7,0.91,-4.71,0  
3E27,ASP\_337,2.78,0.42,-1.44,0  
4FD6,TYR\_18,9.94,0,-0.06,0  
3M66,ARG\_285,11.94,-0.56,0,0  
1YOY,GLU\_101,4.5,0,0,0  
4AF2,LYS\_167,10.5,0,0,0  
3COU,TYR\_95,9.47,0.36,-0.89,0  
2F8H,TYR\_67,10.85,0,0,0.85  
2WOZ,TYR\_291,10,0,0,0  
1SJ8,TYR\_570,10.14,0.21,-0.07,0  
1JKS,GLU\_173,4.38,0.14,-0.26,0  
2YX0,LYS\_134,9.8,-0.7,0,0  
3UV9,ARG\_441,12.08,-0.42,0,0  
1WJG,LYS\_77,10.5,0,0,0  
1EV8,GLU\_250,4.64,0.14,0,0  
3PZ9,LYS\_311,9.66,-0.84,0,0  
1MIX,LYS\_320,10.5,0,0,0  
3V46,GLU\_306,4.33,0.07,-0.24,0  
3RE9,LYS\_163,10.29,-0.21,0,0  
2GEN,ARG\_101,11.73,-0.77,0,0  
2B2H,TYR\_76,11.11,0,-0.02,1.12  
1X9G,LYS\_139,10.5,0,0,0  
4F85,ASP\_98,3.4,0.49,-0.89,0  
3LJN,ARG\_225,12.43,-0.07,0,0  
2RIK,LYS\_108,10.15,-0.35,0,0  
2C13,LYS\_266,9.73,-0.77,0,0  
3RE9,ASP\_169,2.9,0.56,-1.46,0  
1SBX,GLU\_99,3.71,0.42,-1.21,0  
1ZKZ,ASP\_89,3.7,0.07,-0.17,0  
1T07,LYS\_21,10.5,0,0,0  
1GQE,GLU\_93,4.57,0.07,0,0  
2AHE,ASP\_209,3.35,0.35,-0.8,0  
3GA2,LYS\_138,10.22,-0.28,0,0  
3HZQ,ASP\_72,4.07,0.49,-0.22,0  
2H30,ASP\_175,2.42,0.56,-1.93,0  
2E0T,HIS\_61,7.07,0.64,-0.07,0  
3A4C,ARG\_474,11.87,-0.63,0,0  
3Q2C,LYS\_5,10.29,-0.21,0,0  
2P0Y,LYS\_143,10.5,0,0,0  
3FK5,ARG\_52,12.13,-2.76,0,2.39  
2FD5,HIS\_95,0.89,0.74,-2.33,-4.02  
1N81,TYR\_118,12.0,41,0,1.59  
1JT9,LYS\_250,10.43,-0.07,0,0  
2CL3,TYR\_158,10,0,0,0  
3M3P,HIS\_245,6.5,0,0,0  
1WXQ,GLU\_63,4.01,0.28,-0.77,0  
2QV2,GLU\_241,3.57,0.65,-1.15,-0.43  
1SQH,GLU\_182,4.41,0.14,-0.23,0  
1PBV,GLU\_87,4.5,0,0,0  
2EEY,LYS\_51,10.22,-0.28,0,0  
3KB5,GLU\_342,4.31,0.42,-0.61,0  
1ZBM,TYR\_238,10,0,0,0  
2JHY,ARG\_111,11.8,-0.7,0,0  
3V55,GLU\_624,3.81,0.42,-1.11,0  
3BZT,TYR\_301,10,0,0,0  
1ANU,ARG\_38,12.43,-0.07,0,0  
2OSA,ASP\_456,3.37,0.21,-0.64,0  
1XTD,LYS\_37,10.43,-0.07,0,0  
3JSN,GLU\_110,5.81,2.98,0,-1.67  
2JEO,ARG\_57,11.8,-0.7,0,0  
4FD6,LYS\_150,10.22,-0.28,0,0  
3US6,ARG\_92,11.8,-0.7,0,0  
1LZL,GLU\_265,6.54,3.21,-2.19,1.02  
2EDM,ASP\_199,3.94,0.14,0,0  
3HVM,LYS\_232,10.01,-0.49,0,0  
2OEW,LYS\_96,10.43,-0.07,0,0  
2PIM,TYR\_6,10.07,0.07,0,0  
1PBV,GLU\_117,4.0,0.21,-0.71,0  
3E27,HIS\_327,6.5,0,0,0  
1Q5Z,HIS\_535,7.09,0.8,0,-0.21  
1AIL,ASP\_24,3.38,0.42,-0.84,0  
2B78,GLU\_205,4.5,0,0,0  
3NR5,ARG\_93,12.5,0,0,0  
3RLN,TYR\_705,12.25,0.65,-0.24,1.84  
1QYI,GLU\_153,4.23,0.07,-0.34,0  
1R7J,LYS\_61,10.43,-0.07,0,0  
1OGL,HIS\_228,6.5,0,0,0  
3M9A,ASP\_22,3.66,0,-0.14,0  
4GCO,ARG\_248,12.15,-0.35,0,0  
1WPA,ARG\_519,12.08,-0.42,0,0  
2O4D,GLU\_77,4.64,0.14,0,0  
2R57,LYS\_195,10.08,-0.42,0,0

2W1R,ASP\_127,3.29,0.21,-0.72,0  
 2IXM,ARG\_236,12.15,-0.35,0,0  
 3BB7,ARG\_254,11.73,-0.77,0,0  
 2IDC,ARG\_145,12.22,-0.28,0,0  
 1MML,LYS\_193,9.87,-0.63,0,0  
 3CJW,CYS\_326,9,0,0,0  
 2AZP,CYS\_246,11.25,-0.1,0.26,2.09  
 3QAV,LYS\_35,10.43,-0.07,0,0  
 1PGV,LYS\_239,10.36,-0.14,0,0  
 2WB3,LYS\_278,10.43,-0.07,0,0  
 3Q2C,LYS\_41,10.5,0,0,0  
 4D8L,HIS\_180,4.41,3.6,0.01,-5.71  
 1UOH,ARG\_35,12.22,-0.28,0,0  
 2A6B,ASP\_5,3.94,0.14,0,0  
 3U2A,ARG\_36,12.15,-0.35,0,0  
 1AT0,HIS\_316,6.43,0.0,-0.07  
 2OSA,GLU\_455,4.91,0.42,-0.01,0  
 3LMO,HIS\_28,6.53,0.03,0,0  
 2PWQ,LYS\_127,10.5,0,0,0  
 3CCY,CYS\_112,8.19,-1.13,0,0.32  
 1ES9,LYS\_22,10.43,-0.07,0,0  
 2E3S,CYS\_433,10.94,-0.58,0,2.52  
 2QV2,LYS\_293,12.79,0.07,0.42,2.29  
 1W7B,ARG\_77,12.5,0,0,0  
 4DEZ,LYS\_189,10.5,0,0,0  
 1OIF,LYS\_261,11.29,-1.61,0,2.4  
 3A4C,GLU\_464,4.64,0.14,0,0  
 3CSR,ASP\_57,3.62,0.28,-0.46,0  
 1GXN,LYS\_443,9.54,0.19,-0.03,-0.61  
 2WB3,LYS\_334,10.43,-0.07,0,0  
 1W24,ARG\_176,12.08,-0.42,0,0  
 2QDJ,ASP\_111,3.21,0.21,-0.8,0  
 3I4T,ARG\_97,11.87,-0.63,0,0  
 2C2Y,GLU\_14,3.98,0.28,-0.8,0  
 1NJ4,ASP\_286,3.4,0.14,-0.54,0  
 2ZCO,LYS\_77,9.34,0.14,-0.8,0  
 3G9G,GLU\_135,2.76,0.35,-2.09,0  
 1WNH,LYS\_208,10.5,0,0,0  
 1ZBM,LYS\_236,13.34,0.14,0.8,2.4  
 3P28,LYS\_233,10.5,0,0,0  
 2E0T,ARG\_158,11.52,-0.98,0,0  
 1MUF,LYS\_191,10.54,0.54,0,0  
 1YM5,LYS\_8,9.87,-0.63,0,0  
 1X9G,LYS\_10,10.36,-0.14,0,0  
 1K95,HIS\_142,6.43,0.0,-0.07  
 1W24,LYS\_180,10.22,-0.28,0,0  
 1RSQ,LYS\_66,10.43,-0.07,0,0  
 3V75,ARG\_115,12.15,-0.35,0,0  
 3GFP,LYS\_433,10.5,0,0,0  
 1YOK,ARG\_108,12.01,-0.49,0,0  
 3IDW,ASP\_34,3.12,0.28,-0.96,0  
 1Q8B,ASP\_25,3.53,0.07,-0.34,0  
 4F8A,CYS\_589,8.77,-0.74,0,0.51  
 3VHJ,GLU\_56,4.57,0.07,0,0  
 2FBQ,ARG\_113,12.15,-0.35,0,0  
 2HRZ,LYS\_75,10.29,-0.21,0,0  
 1NWA,ARG\_83,12.36,-0.14,0,0  
 2D2S,GLU\_557,4.57,0.07,0,0  
 1O3X,HIS\_235,7.37,1.01,0,-0.14  
 3R2E,ARG\_39,12.5,0,0,0  
 2EJX,ASP\_68,4.26,0.49,-0.03,0  
 1ES9,LYS\_193,9.92,0,-0.08,0  
 1VSM,HIS\_104,1.01,0.06,-0.48,-5.07  
 1LTU,ASP\_34,3.01,0.14,-0.94,0  
 3OOP,LYS\_59,10.5,0,0,0  
 3GV0,ARG\_246,12.43,-0.07,0,0  
 1WYC,LYS\_315,10.5,0,0,0  
 2Q07,ARG\_282,11.47,-2.33,0,1.3  
 2BDD,LYS\_132,10.5,0,0,0  
 3CIV,HIS\_84,9.04,2.24,3.22,-2.92  
 2B2H,LYS\_113,10.15,-0.35,0,0  
 3BA1,LYS\_29,10,0,0,0  
 3B4D,GLU\_219,4.05,0.35,-0.8,0  
 1L3K,ASP\_48,1.47,0.7,-3.04,0  
 3CXS,GLU\_127,4.37,0.21,-0.34,0  
 1I60,LYS\_274,10.43,-0.07,0,0  
 3ZXY,HIS\_114,3.57,0.13,0,-3.06  
 4FCU,ARG\_139,11.94,-0.56,0,0  
 2H8O,LYS\_49,10.5,0,0,0  
 2XMZ,ASP\_39,3.69,0.14,-0.26,0  
 3HVM,GLU\_297,3.91,0.21,-0.8,0  
 1RZZ,GLU\_207,4.56,0.21,-0.15,0  
 3EVN,LYS\_54,10.5,0,0,0  
 2PGE,LYS\_173,10.29,-0.21,0,0  
 3LE4,ARG\_341,12.5,0,0,0  
 2F9F,ASP\_53,3.48,0.28,-0.6,0  
 1NRI,GLU\_89,4.85,0.35,0,0  
 2D0A,LYS\_20,13.63,0.43,0.8,2.4  
 4DIU,LYS\_164,10.43,-0.07,0,0  
 3Q1C,LYS\_394,11.82,1.15,0.12,0.55  
 1GXN,ARG\_557,11.45,-1.05,0,0  
 2QK0,ASP\_30,3.08,0.14,-0.86,0  
 4FCU,HIS\_24,6.84,0.55,0,-0.21  
 2O0K,LYS\_19,10.5,0,0,0  
 1PSW,ARG\_69,11.87,-0.63,0,0  
 1SUU,ARG\_626,11.2,-1.3,0,0  
 2I88,LYS\_507,11.09,1.41,-0.35,0.03  
 3EZ7,CYS\_326,8.82,-0.18,0,0  
 4H89,GLU\_25,3.97,0.28,-0.81,0  
 2QK1,CYS\_443,11.15,-0.02,0.2,17  
 3KVO,ASP\_53,3.34,0.28,-0.74,0  
 2WB8,GLU\_497,1.73,2.01,-2.38,-2.4  
 3EYE,LYS\_137,10.36,-0.14,0,0  
 1JKS,LYS\_154,10.5,0,0,0  
 2D7U,GLU\_79,3.84,0.14,-0.8,0  
 3F7M,ARG\_229,12.22,-0.28,0,0  
 2A4D,ARG\_137,11.59,-0.91,0,0  
 1J7G,ASP\_14,3.11,0.77,-1.46,0  
 2R57,ASP\_337,3.52,0.28,-0.56,0  
 1AKO,GLU\_114,3.77,0.21,-0.94,0  
 3JRT,LYS\_55,11.3,0.28,0,1.02  
 2XJ4,HIS\_24,1.07,0.0,-5.43  
 2ZQ5,ARG\_304,13.88,-1.02,0,2.4  
 4ACJ,ASP\_767,3.94,0.14,0,0  
 1DVO,ARG\_170,12.15,-0.35,0,0  
 3BA1,GLU\_261,0.75,1.37,-2.72,-2.4  
 2O4D,LYS\_15,10,0,0,0  
 4ESS,GLU\_131,3.81,0.35,-1.04,0  
 3RUX,LYS\_74,10.22,-0.28,0,0  
 3G6S,CYS\_220,9.14,0,0,0.14  
 3RFY,LYS\_179,10.36,-0.14,0,0  
 2FBQ,HIS\_125,7.73,1.51,0,-0.28  
 3IVF,GLU\_342,4.64,0.14,0,0  
 1J85,ARG\_28,13.84,-1.06,0,2.4  
 3EGN,ARG\_398,11.73,-0.77,0,0  
 2A0J,LYS\_74,10.29,-0.21,0,0  
 1WLY,LYS\_182,10.29,-0.21,0,0  
 1KN3,HIS\_85,2.32,0.67,-1.11,-3.73  
 2FPN,GLU\_111,4.57,0.07,0,0  
 4FH3,LYS\_205,10,0,0,0  
 3OBS,HIS\_119,6.22,0.0,-0.28  
 2W0G,LYS\_149,10.29,-0.21,0,0  
 1A8Q,LYS\_261,10.22,-0.28,0,0  
 3ETU,LYS\_350,10.43,-0.07,0,0  
 1O59,LYS\_314,10.45,0.62,-0.17,0  
 3OKQ,LYS\_576,10.29,-0.21,0,0  
 1XKR,GLU\_176,3.84,0.14,-0.8,0  
 3ODJ,ARG\_187,12.29,-0.21,0,0  
 4DEZ,ARG\_26,11.8,-0.7,0,0  
 1RHS,LYS\_6,9.86,0.66,-0.8,0  
 1C3K,ASP\_5,2.26,0.35,-1.89,0  
 1AKO,LYS\_60,10.5,0,0,0  
 3T57,GLU\_137,4.57,0.07,0,0  
 1ZCU,LYS\_180,10.36,-0.14,0,0  
 3Q1C,LYS\_374,9.94,-0.56,0,0  
 3IV4,LYS\_37,9.54,0.32,-0.78,0  
 2AD1,GLU\_195,4.25,2.45,-2.55,-0.14  
 1RI5,GLU\_279,3.89,0.28,-0.89,0  
 1O59,GLU\_11,4.07,0.42,-0.85,0  
 3DB9,GLU\_14,4.67,0.28,-0.11,0  
 3BB7,LYS\_140,9.87,-0.63,0,0  
 2G9D,ASP\_50,2.68,0.84,-1.96,0  
 3U0V,LYS\_202,10.5,0,0,0  
 2CXA,HIS\_124,4.89,1.02,0,-2.63  
 3CBN,GLU\_156,3.55,0.49,-1.44,0  
 2E3C,CYS\_348,11.36,-0.29,0.2,65  
 1IDK,ASP\_159,3.96,0.28,-0.12,0  
 3RE9,HIS\_158,10.19,4.4,0.94,-1.65  
 1FHL,LYS\_191,9.65,0,-0.35,0  
 2YX0,LYS\_135,10.29,-0.21,0,0  
 2RH3,ARG\_196,12.43,-0.07,0,0  
 2NRK,LYS\_159,10.43,-0.07,0,0  
 3M7D,GLU\_175,2.45,0.35,-2.4,0  
 4F8A,GLU\_651,3.98,0.28,-0.8,0  
 2IQT,GLU\_75,3.18,0.28,-1.6,0  
 3CXS,CYS\_179,8.27,-0.8,0,0.07  
 3MM4,ASP\_979,4.01,0.21,0,0  
 4D8L,HIS\_31,0.9,1.6,-1.16,-6.03  
 2AZP,LYS\_84,12.65,1.11,0.46,1.08  
 1ILW,LYS\_32,10.22,-0.28,0,0  
 3RFY,LYS\_399,12.88,1.66,0,1.22  
 2W2S,ARG\_117,12.29,-0.21,0,0  
 1JKS,LYS\_154,10.5,0,0,0  
 3EUR,ASP\_16,3.27,0.49,-1.02,0  
 3I47,LYS\_209,10.29,-0.21,0,0  
 3GOZ,LYS\_94,11.05,0,0,1.05  
 3PU6,LYS\_39,11.5,0,0,1.5  
 3ONH,LYS\_551,10.5,0,0,0  
 1DZF,LYS\_71,10.29,-0.21,0,0  
 3T5B,GLU\_263,4.28,0.42,-0.64,0  
 4FCU,GLU\_129,1.85,0.52,-0.77,-2.4  
 3BQW,ASP\_94,2.42,0.56,-1.93,0  
 2EFK,GLU\_135,4.71,0.21,0,0  
 1QQE,LYS\_279,10.5,0,0,0  
 3RFY,ASP\_29,1.43,0.21,-2.57,0  
 2GKG,ASP\_30,3.35,0.35,-0.8,0  
 2Y2T,HIS\_90,6.5,0,0,0  
 2FB6,ARG\_33,12.15,-0.35,0,0  
 2POY,HIS\_251,5.01,1.62,0,-3.11  
 2ILR,ARG\_371,10.98,-1.52,0,0  
 1T9S,GLU\_198,4.64,0.14,0,0  
 1PV5,ARG\_108,11.46,-1.04,0,0  
 1R7J,GLU\_8,3.24,0.28,-1.55,0  
 2Q12,LYS\_153,10.08,-0.42,0,0  
 1JB3,ARG\_128,12.01,-0.49,0,0  
 3SMD,GLU\_99,3.94,0.49,-1.05,0  
 2IRM,ARG\_304,12.43,-0.07,0,0  
 3RVC,GLU\_97,3.04,0.56,-2.01,0  
 1ZP2,CYS\_189,7.37,-2.07,0,0.44  
 2IRM,CYS\_288,10.22,-0.37,-1.57,3.16  
 1WRU,ARG\_231,12.15,-0.35,0,0  
 3H13,LYS\_347,9.4,0.07,-0.67,0  
 1Y2Q,ASP\_17,3.75,0.07,-0.12,0  
 2XWS,ASP\_60,3.028,-1.08,0  
 2DFL,HIS\_238,6.43,0,0,-0.07  
 3CCY,HIS\_50,6.5,0,0,0  
 3I82,LYS\_65,9.59,0,-0.41,0  
 1GPP,CYS\_75,10.46,-0.54,0,1.99  
 3LJC,ARG\_216,12.08,-0.42,0,0  
 1Z3X,ASP\_93,4.01,0.21,0,0  
 3F6F,ARG\_97,10.95,-1.55,0,0  
 1IDK,ARG\_308,13.22,-1.68,0,2.4  
 2E0T,ASP\_125,2.42,0.35,-1.73,0  
 3E5T,CYS\_26,10.39,0,0,1.39  
 3EAZ,GLU\_147,3.81,0.07,-0.76,0  
 3F1X,LYS\_226,11.93,0.0,13.1,8  
 2OSA,LYS\_396,12.19,0,-0.38,2.57  
 1ZKZ,HIS\_54,6.56,0.06,0,0  
 1RSS,LYS\_44,11.33,0.14,-1.21,2.4  
 1J7G,GLU\_107,4.71,0.21,0,0  
 3ZTA,LYS\_74,10.54,0,-0.77,1.32  
 2V5B,GLU\_130,2.81,1.69,-3.38,0  
 2Q99,LYS\_358,10.5,0,0,0  
 2XHC,LYS\_14,10,0,0,0  
 1JKS,ARG\_150,12.01,-0.49,0,0  
 1H09,LYS\_225,10.36,-0.14,0,0  
 1H4U,GLU\_615,4.03,0.35,-0.82,0  
 1PBV,GLU\_229,4.71,0.21,0,0  
 2R4Q,ARG\_256,12.08,-0.42,0,0  
 3RHE,ARG\_84,12.29,-0.21,0,0  
 1F2V,ASP\_59,4.02,0.21,-0.01,0  
 1Y0K,GLU\_138,4.39,0.14,-0.25,0  
 1RAJ,LYS\_348,10.29,-0.21,0,0  
 3CCY,LYS\_134,10.17,0.21,-0.8,0.76  
 1RKA,GLU\_188,4.6,0.7,-0.6,0  
 1O5T,GLU\_199,3.28,1.67,-0.8,-2.09  
 1H09,LYS\_197,10.5,0,0,0  
 3FWU,ARG\_94,11.03,-1.47,0,0  
 1T6L,LYS\_215,10.15,-0.35,0,0  
 3FK5,LYS\_95,9.94,0.07,-0.8,0.67  
 3IL3,GLU\_23,3.96,0.42,-0.96,0  
 1CBY,GLU\_106,3.84,0.14,-0.8,0  
 1LTU,GLU\_62,3.79,0.6,-1.3,0  
 1J33,GLU\_220,4.64,0.14,0,0  
 1T07,ASP\_71,4.0,3.5,-0.15,0  
 2QK1,LYS\_382,10.5,0,0,0  
 3BCY,LYS\_106,10.08,-0.42,0,0  
 2F9F,LYS\_133,10.1,0,0,0.1  
 2GQV,LYS\_55,11.75,0.28,-0.93,2.4  
 1LFP,HIS\_120,6.5,0,0,0  
 2FBQ,LYS\_141,11.46,1.83,-0.37,0  
 3PBH,HIS\_199,6.94,4.86,2.22,-6.64  
 1N81,CYS\_46,10.33,-0.29,-1.44,3.06  
 3NBI,ASP\_71,3.87,0.07,0,0  
 2PIM,GLU\_14,4.71,0.21,0,0  
 3KB5,GLU\_289,1.01,0.45,-1.6,-2.34  
 3PM2,CYS\_54,6.58,-4.17,0,1.75  
 2VGY,LYS\_86,10.07,0.07,0,0  
 1NRI,GLU\_39,3.61,0.42,-1.31,0  
 4E8B,CYS\_160,9.77,-0.14,0,0.91  
 1SUU,LYS\_745,10.5,0,0,0  
 3LJI,GLU\_175,4.56,0.07,-0.01,0  
 2RIS,LYS\_140,10.43,-0.07,0,0  
 1RI6,LYS\_149,10.15,-0.35,0,0  
 3UAH,ASP\_234,4.01,0.21,0,0  
 3M7G,GLU\_237,4.5,0,0,0  
 3JRT,GLU\_11,3.98,0.28,-0.8,0  
 1X7F,HIS\_29,6.95,0.87,0,-0.42  
 2B78,ASP\_83,3.82,0.07,-0.05,0  
 3M3P,ASP\_217,4.01,0.21,0,0  
 1YM5,LYS\_210,12.95,1.04,0,1.91  
 2YCO,GLU\_149,3.25,0.28,-1.53,0  
 3CRM,GLU\_55,3.53,0.35,-1.32,0  
 3F1X,GLU\_47,2.4,0.69,-0.85,-1.94  
 3VJ8,HIS\_161,6.5,0,0,0  
 3EZ7,LYS\_82,12.44,0,0.04,2.4

3FRR,TYR\_75,13.23,0.64,0.18,2.4  
3GW3,TYR\_182,10.0,0,0  
2CWY,ARG\_60,12.5,0,0,0  
3ADO,ARG\_103,12.36,-0.14,0,0  
1TD6,LYS\_61,10.43,-0.07,0,0  
1VJG,ASP\_59,2.1,0.21,-1.92,0  
2D2S,ASP\_537,3.42,0.42,-0.8,0  
3RFY,ASP\_255,3.62,0.35,-0.53,0  
3B79,GLU\_108,4.5,0,0,0  
2Q12,LYS\_124,10.43,-0.07,0,0  
1R16,GLU\_305,4.52,0.14,-0.12,0  
2V5B,HIS\_48,6.5,0,0,0  
1L2H,GLU\_25,4.48,0.35,-0.37,0  
3ADO,HIS\_137,7.85,1.56,0,-0.21  
2CN1,GLU\_161,4.69,0.93,-1.09,0.35  
3GYW,TYR\_151,10.37,0,-0.22,0.6  
1EDG,ARG\_155,11.73,-0.77,0,0  
3KEY,TYR\_421,10.85,0.07,-0.8,1.58  
2Z14,ARG\_69,12.29,-0.21,0,0  
3RFY,ASP\_402,4.19,0.42,-0.03,0  
1MJS,ARG\_278,12.1,-1.26,0,0.86  
2FC3,ARG\_8,12.36,-0.14,0,0  
3RLE,LYS\_60,10.5,0,0,0  
1Z9L,GLU\_82,3.11,0.21,-1.6,0  
1ZKZ,ASP\_47,3.82,0.14,-0.12,0  
2OEW,GLU\_137,4.71,0.21,0,0  
3PZ9,ARG\_157,11.8,-0.7,0,0  
2HRZ,GLU\_267,3.37,0.28,-1.42,0  
1SNT,HIS\_185,6.43,0,0,-0.07  
2YLF,LYS\_187,10.5,0,0,0  
1JKS,LYS\_28,10.15,-0.35,0,0  
3C2E,ARG\_131,11.87,-0.63,0,0  
3D9H,HIS\_124,6.43,0,0,-0.07  
1JT9,GLU\_102,4.5,0,0,0  
3BCY,HIS\_63,6.5,0,0,0  
1KN3,ARG\_141,12.15,-0.35,0,0  
2CE6,ARG\_29,11.24,-1.26,0,0  
2GKG,ASP\_11,2.69,0.35,-1.46,0  
2R57,CYS\_372,9.96,-3.11,2.4,1.67  
1R9W,LYS\_292,10.43,-0.07,0,0  
1OST,ARG\_127,12.01,-0.49,0,0  
3F6M,LYS\_61,10.43,-0.07,0,0  
2CN1,GLU\_122,3.95,0.21,-0.76,0  
3ASA,CYS\_383,9.55,-0.1,0,0.65  
2B0J,ASP\_134,3.1,0.56,-1.26,0  
2F4Q,ARG\_336,11.94,-0.56,0,0  
2FZP,GLU\_316,4.58,0.28,-0.2,0  
3I0C,GLU\_135,4.12,0.42,-0.8,0  
2IXM,LYS\_28,10.59,-0.35,0,0.44  
2XJ4,ARG\_194,12.01,-0.49,0,0  
1DVO,CYS\_98,8.63,-0.37,0,0  
1CBY,CYS\_19,6.84,-2.17,0,0  
1AD6,GLU\_539,1.58,1.42,-1.94,-2.4  
1EYH,ASP\_31,3.49,0.49,-0.8,0  
3B4D,ARG\_227,12.5,0,0,0  
1ZCU,TYR\_145,12.06,1.12,-0.8,1.74  
3N2T,CYS\_212,9.2,-0.55,-0.84,1.6  
1DTP,GLU\_90,3.6,0.7,-1.6,0  
3PBH,TYR\_148,10,0,0,0  
1QQI,TYR\_125,12.74,0.07,0.27,2.4  
1NFN,GLU\_59,3.39,0.49,-1.6,0  
1OLR,CYS\_175,11.13,0,0,2.13  
3M7G,TYR\_38,10,0,0,0  
1SJ8,GLU\_657,4.64,0.14,0,0  
2OGQ,ARG\_560,11.8,-0.7,0,0  
1L3K,TYR\_124,8.24,0,-1.76,0  
2I88,LYS\_455,10.08,-0.42,0,0  
3KB5,LYS\_330,10.5,0,0,0  
2CN1,GLU\_19,4.5,0,0,0  
2H01,ARG\_149,11.87,-0.63,0,0  
3HVM,LYS\_258,10.5,0,0,0  
3Q6L,LYS\_53,10.43,-0.07,0,0  
3ANJ,TYR\_239,10,0,0,0  
2B78,ASP\_309,4.15,0.35,0,0  
1J33,TYR\_241,10.57,0.07,-0.16,0.65  
1IDK,HIS\_210,2.88,1.78,0,-5.4  
3GEC,CYS\_467,4.75,-4.32,0,0.07  
2P65,ARG\_32,12.43,-0.07,0,0  
1FQI,TYR\_383,10.07,0,-0.23,0.3  
1LFP,HIS\_115,7.1,0.74,0,-0.14  
4ANN,GLU\_65,3.91,0.21,-0.8,0  
3PP8,LYS\_73,10.36,-0.14,0,0  
1R53,HIS\_244,6.5,0,0,0  
1T3J,ARG\_679,12.29,-0.21,0,0  
2Q07,LYS\_431,10.5,0,0,0  
3DHN,LYS\_209,10,0,0,0  
3L7N,GLU\_73,2.95,2.45,-1.6,-2.4  
3ERF,GLU\_205,3.58,0.14,-1.06,0  
1UW7,GLU\_-7,5.27,0.77,0,0  
2DFL,LYS\_137,10.36,-0.14,0,0  
2FZ4,ASP\_39,2.73,0.84,-1.92,0  
2D59,GLU\_17,4.39,0.49,-0.6,0  
2X4G,TYR\_54,6.45,0.45,-1.6,-2.4  
2B78,ASP\_117,3.92,0.14,-0.02,0  
2R2Y,LYS\_42,10.5,0,0,0  
2BAA,HIS\_121,6.32,0.03,0,-0.21  
1O17,ARG\_263,12.08,-0.42,0,0  
3CAX,ASP\_373,2.92,0.42,-1.3,0  
1H4U,GLU\_616,4.5,0,0,0  
2IQI,TYR\_33,9.46,0.26,-0.8,0  
3HKX,GLU\_209,2.64,0.67,-0.28,-2.25  
3CCY,ARG\_87,11.45,-1.05,0,0  
3K8J,TYR\_227,10.54,0.54,0,0  
1RZ2,TYR\_191,10,0,0,0  
2XJ4,GLU\_53,4.33,0.28,-0.45,0  
2F9F,LYS\_6,10.29,-0.21,0,0  
1XKR,LYS\_86,9.94,-0.56,0,0  
2B61,GLU\_38,3.69,0.42,-1.23,0  
2Q99,HIS\_286,6.37,0.08,0,-0.21  
1BN6,ARG\_164,10.62,-1.88,0,0  
1L2F,GLU\_96,4.61,0.21,-0.1,0  
4EUG,ARG\_116,12.43,-0.07,0,0  
2EYI,ARG\_185,12.5,0,0,0  
2H85,ARG\_206,9.73,-1.19,0,-1.58  
3TIR,LYS\_29,10.43,-0.07,0,0  
4DIU,TYR\_127,10.07,0.07,0,0  
3FS3,TYR\_272,10,0,0,0  
2H85,ASP\_239,2.33,0.49,-1.96,0  
1KN3,LYS\_77,10.5,0,0,0  
1JKS,TYR\_128,9.97,0,-0.03,0  
3CGW,ARG\_266,12.36,-0.14,0,0  
2QVT,HIS\_117,6.53,0.17,0,-0.14  
3GEC,HIS\_492,6.77,0.27,0,0  
4GCO,ARG\_232,12.36,-0.14,0,0  
3P28,ASP\_81,4.08,0.28,0,0  
2CVB,ARG\_159,11.94,-0.56,0,0  
3NR5,LYS\_149,10.36,-0.14,0,0  
1X6J,GLU\_39,3.44,0.35,-1.41,0  
3H9W,GLU\_67,4.24,0.07,-0.33,0  
2QEV,ASP\_59,3.87,0.07,0,0  
1A8Q,LYS\_245,10.15,-0.35,0,0  
2QV2,LYS\_53,10.22,-0.28,0,0  
3E7P,TYR\_140,9.36,0,-0.68,0.05  
3V3T,ASP\_39,2.67,0.49,-1.63,0  
4F85,GLU\_260,4.5,0,0,0  
4F8A,ASP\_562,3.1,0.21,-0.91,0  
3I47,GLU\_136,4.74,1.45,-1.21,0  
1FO9,LYS\_301,10.29,-0.21,0,0  
1NJ4,ASP\_37,1.89,0.49,-2.4,0  
2EFK,CYS\_99,8.53,-0.55,0,0.08  
1UUA,ASP\_51,3.17,0.14,-0.77,0  
3HVM,GLU\_97,3.5,0.56,-1.56,0  
2D7Y,LYS\_184,10.43,-0.07,0,0  
3LJN,ARG\_120,12.15,-0.35,0,0  
3ETV,ARG\_13,12.43,-0.07,0,0  
2CXC,ARG\_56,12.36,-0.14,0,0  
4H4J,CYS\_63,4.78,-5.92,-0.26,1.96  
1RAJ,LYS\_359,10.5,0,0,0  
4H86,GLU\_157,2.07,1.7,-4.08,-0.04  
2WZ9,LYS\_92,10.22,-0.28,0,0  
3EOD,ASP\_42,3.94,0.21,-0.07,0  
3L3P,GLU\_411,4.5,0,0,0  
2POL,ASP\_119,2.22,0.28,-1.86,0  
3V55,HIS\_356,6.22,0,0,-0.28  
2C2Y,HIS\_191,6.29,0,0,-0.21  
3CGW,ARG\_91,12.5,0,0,0  
3ILC,ARG\_103,11.66,-0.84,0,0  
1R53,LYS\_84,10.5,0,0,0  
1TD6,GLU\_194,4.41,0.21,-0.3,0  
1YDL,ASP\_40,3.96,0.42,-0.26,0  
1C44,ASP\_77,2.82,1.12,-2.1,0  
3EVN,ASP\_192,3.28,0.28,-0.8,0  
3ILC,LYS\_87,10.36,-0.14,0,0  
3PBH,ASP\_34,2.48,0.56,-1.88,0  
2PLQ,LYS\_160,10.5,0,0,0  
1FKM,ARG\_274,11.8,-0.7,0,0  
2RH3,ARG\_117,12.43,-0.07,0,0  
2Z0M,ARG\_37,12.85,-1.44,0,1.79  
2F9F,GLU\_166,3.89,0.35,-0.96,0  
1PBV,HIS\_200,7.38,1.02,0,-0.14  
3P51,ASP\_11,2.99,0.77,-1.58,0  
2GKG,ASP\_72,2.08,0.7,-2.41,0  
2YLF,CYS\_120,8.77,-0.23,0,0  
2AZL,TYR\_190,10.57,0.57,0,0  
1SQW,ASP\_32,2.58,0.42,-1.64,0  
2Z61,LYS\_269,10.43,-0.07,0,0  
2QEV,HIS\_55,6.43,0,0,-0.07  
2D59,LYS\_144,10.5,0,0,0  
2Q99,ARG\_369,12.08,-0.42,0,0  
3Q2C,GLU\_40,3.92,0.28,-0.86,0  
1K95,ASP\_196,2.17,1.19,-2.82,0  
3EVN,LYS\_137,9.66,-0.84,0,0  
2F8H,ASP\_19,1,0.7,-3.5,0  
3IBT,ASP\_151,3.74,0.21,-0.27,0  
1SNT,LYS\_183,10.15,-0.35,0,0  
1TD6,ARG\_159,13.19,-2.72,0,3.41  
3GE9,HIS\_63,6.52,0.02,0,0  
2Q13,ARG\_287,12.22,-0.28,0,0  
3CJW,ASP\_398,3.73,0,-0.07,0  
2AHE,LYS\_203,10.15,-0.35,0,0  
2G5X,LYS\_82,10.5,0,0,0  
3BPP,TYR\_126,10.07,0.07,0,0  
3C38,CYS\_264,7.92,-1.87,0,0.79  
1P1L,GLU\_43,4.71,0.21,0,0  
2CWC,HIS\_144,6.62,0.26,0,-0.14  
1LTU,CYS\_60,9.25,-3.47,1.91,1.81  
2XHC,ARG\_228,12.43,-0.07,0,0  
2I88,TYR\_363,9.78,0.77,-0.99,0  
2H2Z,LYS\_90,10.43,-0.07,0,0  
3EST,TYR\_22,10.07,0.07,0,0  
3ILC,GLU\_98,1.64,1.14,-1.6,-2.4  
3K8J,GLU\_129,4.5,0,0,0  
1EDG,ASP\_97,3.27,0,-0.53,0  
2DVK,LYS\_63,10.43,-0.07,0,0  
3GFP,ASP\_416,2.11,0.63,-2.32,0  
3M7G,GLU\_175,4.71,0.21,0,0  
1J85,LYS\_119,10.15,-0.35,0,0  
1PV5,CYS\_134,8.51,-0.49,0,0  
1ES9,HIS\_66,6.43,0,0,-0.07  
3RLN,LYS\_578,10.15,-0.35,0,0  
1X1E,HIS\_72,3.9,0.02,0,-2.62  
3M70,TYR\_92,10.05,0.07,-0.02,0  
3BQW,GLU\_212,1.83,0.35,-3.02,0  
2OPJ,ARG\_145,11.87,-0.63,0,0  
2R0S,LYS\_208,10.36,-0.14,0,0  
3HVW,ARG\_277,11.73,-0.77,0,0  
2FC3,GLU\_61,4.64,0.14,0,0  
3RLN,GLU\_706,4.1,0.28,-0.68,0  
3JZ9,LYS\_484,10.43,-0.07,0,0  
1AT0,ARG\_366,11.73,-0.77,0,0  
4FZR,LYS\_108,10.43,-0.07,0,0  
1LZL,ASP\_8,2.99,0.35,-1.16,0  
4ANN,ARG\_125,12.5,0,0,0  
2W2S,CYS\_171,6.54,-2.96,0,0.49  
1O17,GLU\_201,3.98,0.28,-0.8,0  
3I4T,GLU\_169,3.88,0.28,-0.9,0  
1XAW,ARG\_434,12.36,-0.14,0,0  
3H13,GLU\_301,3.77,0.35,-1.08,0  
3LJN,ARG\_37,11.87,-0.63,0,0  
2B0J,LYS\_103,10.43,-0.07,0,0  
1FHL,GLU\_147,4.96,0.49,-0.03,0  
1NAF,LYS\_210,10.15,-0.35,0,0  
1MD6,HIS\_21,6.29,0,0,-0.21  
2Z84,ARG\_117,12.5,0,0,0  
1EDG,LYS\_213,10.5,0,0,0  
2AXO,TYR\_104,12.2,2.68,-0.48,0  
2APL,GLU\_87,4.57,0.07,0,0  
2NMU,ASP\_134,3.94,0.14,0,0  
1JKS,GLU\_235,4.57,0.07,0,0  
2FBQ,GLU\_15,0.23,1.47,-1.5,-4.25  
2P5D,ASP\_14,3.25,0.07,-0.62,0  
1JKS,ARG\_31,12.08,-0.42,0,0  
1J7G,GLU\_72,3.66,0.35,-1.19,0  
2V5B,ARG\_135,13.19,-1.12,0,1.81  
1R16,GLU\_25,4.64,0.14,0,0  
1YG2,LYS\_124,10.43,-0.07,0,0  
3F7M,HIS\_333,0.14,0.13,0,-6.49  
1TLV,TYR\_236,10,0,0,0  
3B21,GLU\_124,4.57,0.07,0,0  
1ES9,ASP\_182,2.07,0.49,-2.22,0  
1ZBS,GLU\_19,4.47,0,-0.03,0  
3ZSL,ARG\_129,12.22,-0.28,0,0  
3IRA,GLU\_72,4.64,0.14,0,0  
2Q98,GLU\_121,4.47,0.21,-0.24,0  
1BN6,LYS\_135,10.08,-0.42,0,0  
3JRT,GLU\_154,4.57,0.07,0,0  
1PGV,LYS\_247,10.29,-0.21,0,0  
4FLE,GLU\_53,4.64,0.14,0,0  
1H4U,TYR\_452,9.19,0.07,-1.39,0.51  
3K8J,ARG\_154,12.36,-0.14,0,0  
1XEU,LYS\_224,10.5,0,0,0  
3RJK,LYS\_289,10.22,-0.28,0,0  
3KT9,LYS\_38,10.5,0,0,0  
3EX9,TYR\_115,10,0,0,0  
1ZYI,GLU\_254,4.61,0.49,-0.38,0  
1Y2Q,ASP\_29,3.8,0,0,0  
2O8I,CYS\_45,6.24,-3.66,-0.14,1.04  
2NMU,HIS\_100,6.6,0.17,0,-0.07  
2CN1,LYS\_175,10.43,-0.07,0,0  
3EZ7,LYS\_296,10.43,-0.07,0,0  
3KVO,HIS\_146,6.22,0,0,-0.28  
1SJB,ASP\_569,2.64,0.35,-1.51,0  
2QDJ,LYS\_240,10.22,-0.28,0,0  
1LPL,LYS\_144,10.5,0,0,0  
1DCF,ARG\_120,11.8,-0.7,0,0  
1JB3,HIS\_99,7.82,1.6,0,-0.28



1GPP,LYS\_112,10.22,-0.28,0,0  
3CAX,ARG\_222,12.01,-0.49,0,0  
1ZYI,ARG\_112,11.87,-0.63,0,0  
2EYL,ARG\_34,12.08,-0.42,0,0  
3OIP,LYS\_30,10.36,-0.14,0,0  
1BN6,ASP\_94,2.35,0.42,-1.86,0  
1JYH,TYR\_3,13.37,0.21,0.76,2.4  
3T8R,TYR\_41,10.14,0.14,0,0  
1JT9,LYS\_130,10.36,-0.14,0,0  
1RHS,ASP\_102,3.44,0.14,-0.5,0  
2W2S,GLU\_141,4.28,0.56,-0.78,0  
2YLF,GLU\_43,4.64,0.14,0,0  
1YR6,GLU\_212,4.18,0.14,-0.46,0  
3BQW,ASP\_21,2.69,0.42,-1.53,0  
4AF2,LYS\_128,10.29,-0.21,0,0  
2AD1,LYS\_17,10.5,0,0,0  
2IXM,GLU\_57,4.5,0,0,0  
2BT8,TYR\_191,10,0,0,0  
1U53,LYS\_44,10.43,-0.07,0,0  
3IPZ,LYS\_108,10.22,-0.28,0,0  
1NAR,HIS\_219,6.36,0,0,-0.14  
3CCY,TYR\_29,11.87,0.35,0,-1.52  
2D7J,GLU\_26,4.11,0.14,-0.53,0  
4D8L,LYS\_96,10.5,0,0,0  
2GYZ,ARG\_28,11.73,-0.77,0,0  
2RGY,HIS\_153,4.67,0.12,-3.03  
1UOH,GLU\_20,4.57,0.07,0,0  
2EA9,TYR\_102,9.72,0.07,-0.35,0  
3UAH,ASP\_189,2.74,0.49,-1.55,0  
1L2F,ARG\_257,11.45,-1.05,0,0  
3BA1,GLU\_60,3.91,0.21,-0.8,0  
3B7X,ASP\_89,3.43,0.35,-0.71,0  
4E6S,GLU\_6,3.69,0.21,-1.02,0  
1V6T,ASP\_136,3.05,0.42,-1.17,0  
2D2S,LYS\_621,10.43,-0.07,0,0  
2B0J,GLU\_31,4.57,0.07,0,0  
3EVP,GLU\_135,6.34,2.64,-0.8,0  
3GG6,ARG\_123,12.36,-0.14,0,0  
1W7B,LYS\_227,10.22,-0.28,0,0  
2CVB,LYS\_144,10.5,0,0,0  
2Q98,ASP\_79,3.29,0.28,-0.79,0  
2OSA,GLU\_293,1.38,0.69,-1.96,-1.85  
3ASA,HIS\_260,7.16,0.8,0,-0.14  
3E7P,ARG\_219,12.5,0,0,0  
3PP8,ARG\_281,12.15,-0.35,0,0  
1WXQ,HIS\_187,6.46,0.03,0,-0.07  
2QDJ,ARG\_272,11.31,-1.19,0,0  
1L3K,LYS\_8,10.5,0,0,0  
2QK1,LYS\_489,10.5,0,0,0  
3C6B,GLU\_132,0.66,1.33,-3.89,-1.28  
2FL4,TYR\_122,12.65,1.36,0,1.29  
1H09,HIS\_60,4.39,1.62,1.7,-5.43  
1TLV,HIS\_256,7.09,0.8,0,-0.21  
1R53,ARG\_345,12.09,-0.41,0,0  
2Q98,LYS\_187,10.29,-0.21,0,0  
1P4X,ASP\_221,2.7,0.63,-1.74,0  
2JEO,ASP\_179,2.9,0.42,-1.32,0  
3T8R,ASP\_116,3.44,0.49,-0.85,0  
2OPJ,ARG\_302,13.74,-1.15,0.2,39  
3LD1,ARG\_223,12.8,-0.28,0,0.58  
3PP8,GLU\_20,4.64,0.14,0,0  
3RLE,GLU\_145,4.5,0,0,0  
1BN6,ARG\_210,11.03,-1.47,0,0  
2X4J,LYS\_126,9.87,-0.63,0,0  
2X5Y,TYR\_826,9.52,0.22,-0.8,0.1  
3BB7,ASP\_206,3.41,0.42,-0.81,0  
3ETV,GLU\_334,4.64,0.14,0,0  
3COU,GLU\_80,5.58,2.51,-1.88,0.45  
2X5Y,GLU\_766,4.57,0.07,0,0  
1X1E,LYS\_84,10.29,-0.21,0,0  
1HF8,GLU\_279,5.06,0.56,0,0  
3HYQ,TYR\_178,13.58,0.77,0.41,2.4  
4DEY,ARG\_68,12.5,0,0,0  
1ZCE,GLU\_129,3.32,0.49,-1.67,0  
1MUF,TYR\_217,13.34,0.14,0.8,2.4  
3N2T,ARG\_107,13.2,-1.63,0.2,33  
1WXF,LYS\_9,10.5,0,0,0  
2CVB,HIS\_94,6.43,0,0,-0.07  
1O3X,LYS\_250,10.5,0,0,0  
1RAJ,HIS\_389,1.87,0.8,-1.56,-3.87  
4D8L,ARG\_166,11.87,-0.63,0,0  
1AK1,TYR\_285,13.17,0.07,0.7,2.4  
2Z84,TYR\_170,11.39,0.07,0.1,32  
1OTM,ASP\_50,0.83,1.12,-4.08,0  
2O0K,LYS\_223,10.5,0,0,0  
2O8P,GLU\_52,2.22,1.26,-3.54,0  
3LJI,ARG\_48,9.73,-3.04,0.2,7  
3LJN,CYS\_117,10.38,-0.67,1.27,0.78  
1NJ4,ASP\_175,2.98,0.84,-1.66,0  
2F19,HIS\_33,6.46,0.17,0,-0.21  
1L2F,ARG\_306,12.15,-0.35,0,0  
1J85,LYS\_58,10.5,0,0,0  
2B0J,ASP\_143,3.34,0.28,-0.74,0  
1T3Y,LYS\_102,10.22,-0.28,0,0  
2H2W,LYS\_96,10.5,0,0,0  
2ZCX,GLU\_26,4.5,0,0,0  
3MIX,TYR\_603,10.5,0,0.5  
4EKU,TYR\_162,10.47,1.29,0,-0.82  
1ZBM,ASP\_162,4.03,0.28,-0.05,0  
1P2F,LYS\_12,10.5,0,0,0  
3R2E,GLU\_7,4.57,0.07,0,0  
1XEU,GLU\_73,2.37,0.63,-2.76,0  
1Q46,ASP\_39,4.43,0.63,0,0  
2XWS,LYS\_38,9.31,-1.19,0,0  
1XTD,HIS\_64,6.5,0,0,0  
3NBI,TYR\_100,9.78,0.14,-0.36,0  
3IV4,GLU\_12,3.32,0.42,-1.6,0  
3L0D,ASP\_81,2.43,0.56,-1.93,0  
3P28,HIS\_190,6.36,0,0,-0.14  
2GZQ,ARG\_191,12.22,-0.28,0,0  
3ASA,TYR\_191,10,0,0,0  
1NUJ,LYS\_292,10.5,0,0,0  
1W24,HIS\_10,9.81,3.6,3.12,-3.41  
2G2D,LYS\_160,10.29,-0.21,0,0  
1IDK,TYR\_96,10,0,0,0  
4H89,HIS\_85,6.75,0.25,0,0  
1T6L,LYS\_35,10.29,-0.21,0,0  
1QYI,ARG\_215,11.73,-0.77,0,0  
1FKM,ASP\_272,4.02,0.28,-0.06,0  
1YMS,LYS\_259,10.5,0,0,0  
4ETX,GLU\_248,3.62,0.56,-1.45,0  
3ETV,ARG\_56,12.15,-0.35,0,0  
3UC9,HIS\_18,6.37,0.2,2,-2.33  
3RE9,GLU\_93,4.57,0.07,0,0  
3M3P,HIS\_120,6.43,0,0,-0.07  
2CYG,LYS\_332,10.22,-0.28,0,0  
3MTT,ARG\_511,11.8,-0.7,0,0  
1ZBP,ARG\_190,11.45,-1.05,0,0  
1DZF,GLU\_194,1.7,1.79,-1.84,-2.75  
1T3J,GLU\_725,4.05,0.35,-0.8,0  
3MIX,GLU\_483,3.98,0.28,-0.8,0  
1O0X,ARG\_124,11.87,-0.63,0,0  
3UV9,GLU\_292,4.5,0,0,0  
3LJC,HIS\_46,7.04,0.54,0,0  
2BDV,ARG\_192,12.01,-0.49,0,0  
1JSX,ARG\_197,11.8,-0.7,0,0  
3ILC,TYR\_120,13.2,0.17,0.3,0.4  
3GMS,HIS\_236,4.76,0.8,0,-2.54  
3EVZ,ASP\_192,3.79,0,-0.01,0  
3V4G,GLU\_84,3.33,0.35,-1.52,0  
2JKF,LYS\_56,10.08,-0.42,0,0  
1YOY,GLU\_117,4.71,0.21,0,0  
3PAC,ARG\_125,13.47,-1.43,0.2,4  
1HF8,TYR\_138,13.41,0.21,0.8,2.4  
2QZQ,GLU\_130,4.6,0.1,0,0  
3LH5,LYS\_787,10.22,-0.28,0,0  
1PDB,ASP\_110,1.73,0.77,-2.84,0  
1BN6,LYS\_128,10.29,-0.21,0,0  
3EVZ,ARG\_121,11.87,-0.63,0,0  
2F9F,ASP\_99,3.88,0.21,-0.13,0  
3BQW,ARG\_73,11.73,-0.77,0,0  
3UV9,ARG\_298,12.36,-0.14,0,0  
1PDB,GLU\_161,4.85,0.35,0,0  
3I4T,TYR\_265,10,0,0,0  
1F09,GLU\_135,4.5,0,0,0  
2FZ4,ARG\_50,11.87,-0.63,0,0  
2C13,TYR\_241,12.07,1.16,-0.06,0.98  
2OEW,HIS\_259,5.73,1.6,1.34,-3.71  
1OXZ,ASP\_171,2.52,0.42,-1.7,0  
2B61,ASP\_222,3.05,0.21,-0.96,0  
1YMS,GLU\_39,3.81,0.28,-0.97,0  
4E9E,ASP\_495,2.75,0.56,-1.61,0  
3RLE,LYS\_56,10.01,-0.49,0,0  
2Q98,LYS\_78,10.01,-0.49,0,0  
2XMX,LYS\_77,10.43,-0.07,0,0  
1SUU,LYS\_633,10.5,0,0,0  
3LJC,GLU\_57,4.2,0.14,-0.44,0  
2QVT,LYS\_58,10.15,-0.35,0,0  
1JYH,LYS\_45,10.5,0,0,0  
2Q13,HIS\_363,4.88,0.51,0,-2.13  
3JRT,CYS\_106,9.01,0,0,0.01  
4EKU,HIS\_365,6.36,0,0,-0.14  
2Q99,ARG\_362,11.94,-0.56,0,0  
3SMD,LYS\_123,10.5,0,0,0  
1CHD,ARG\_238,11.31,-1.19,0,0  
3CX2,LYS\_195,10.43,-0.07,0,0  
1OGL,CYS\_115,8.25,-0.94,0,0.19  
1EQ6,ARG\_71,11.03,-1.47,0,0  
1NIJ,TYR\_31,10,0,0,0  
2RFA,CYS\_70,8.54,-0.53,0.0,0.07  
4DNU,HIS\_102,3.42,0.43,0,-3.51  
4F85,CYS\_114,10.6,-1.8,1.47,1.92  
3ILC,GLU\_124,3.84,0.14,-0.8,0  
3CS1,LYS\_19,10.5,0,0,0  
3BPP,ARG\_187,12.29,-0.21,0,0  
1GQE,ASP\_238,4.07,0.28,-0.01,0  
3RKV,GLU\_237,4.71,0.21,0,0  
3ZRI,LYS\_18,10.43,-0.07,0,0  
4FZN,ARG\_97,11.73,-0.77,0,0  
3BQW,ASP\_106,2.86,0.42,-1.36,0  
1WYMS,GLU\_237,4.57,0.07,0,0  
4EKU,GLU\_138,4.64,0.14,0,0  
3LQE,GLU\_427,0.53,1.17,-2.74,-2.4  
2V4X,GLU\_4,3.77,0.07,-0.8,0  
1SI7,CYS\_152,8.78,-0.29,0,0.07  
2OJQ,LYS\_638,10.43,-0.07,0,0  
3T57,ARG\_291,11.73,-0.77,0,0  
3EVN,ASP\_65,1.82,0.7,-2.69,0  
2FB6,LYS\_49,10.36,-0.14,0,0  
3QAV,LYS\_29,10.36,-0.14,0,0  
1ZCU,HIS\_87,8.17,2.58,2.4,-3.32  
2OKT,TYR\_300,10.39,1.19,-0.8,0  
3FFM,GLU\_67,4.5,0,0,0  
2A1V,GLU\_135,4.5,0,0,0  
2D7U,ASP\_297,3.52,0.49,-0.78,0  
3BQW,TYR\_115,13.33,0,0.03,3.3  
2POY,LYS\_305,10.5,0,0,0  
3ZXY,ARG\_273,11.8,-0.7,0,0  
2VAN,LYS\_167,10.5,0,0,0  
2A1V,ARG\_109,11.66,-0.84,0,0  
1PBV,ARG\_205,12.5,0,0,0  
3J29,LYS\_447,9.94,-0.56,0,0  
2GQV,HIS\_62,6.56,0.06,0,0  
2EJB,ASP\_163,3.94,0.14,0,0  
3M7D,ARG\_249,12.08,-0.42,0,0  
1PV5,GLU\_170,4.5,0,0,0  
1XTD,HIS\_88,6.29,0,0,-0.21  
3H9W,GLU\_117,4.64,0.14,0,0  
1W7B,LYS\_176,10.01,-0.49,0,0  
2VAN,ARG\_253,10.75,-1.75,0,0  
2B6P,HIS\_201,3.27,0,0,-3.23  
1BN6,ASP\_22,3.7,0,-0.1,0  
1R15,ARG\_119,12.29,-0.21,0,0  
1F09,GLU\_135,4.5,0,0,0  
1X1E,ARG\_164,12.5,0,0,0  
3Q9P,LYS\_114,10.5,0,0,0  
3ELI,ASP\_23,4.01,0.21,0,0  
1PDB,TYR\_33,11.33,1.33,0,0  
3RJX,LYS\_250,10.5,0,0,0  
3P51,ASP\_104,3.69,0.28,-0.39,0  
3ILC,ASP\_189,3.81,0.07,-0.06,0  
1PGV,GLU\_341,3.02,0.84,-2.32,0  
2B02,ARG\_366,11.8,-0.7,0,0  
1SQH,GLU\_221,4.66,0.21,-0.05,0  
1IAP,HIS\_58,2.91,0.12,-3.71  
3GYF,HIS\_182,6.5,0.07,0,-0.07  
3DZ1,ARG\_90,12.08,-0.42,0,0  
2QVT,LYS\_70,10.22,-0.28,0,0  
4FZR,HIS\_295,0.79,0.18,-1.59,-4.3  
1JKS,GLU\_107,3.96,0.21,-0.75,0  
2Q12,GLU\_252,4.33,0.28,-0.45,0  
3LD1,ASP\_120,3.4,0.42,-0.82,0  
2F4Q,TYR\_79,10.89,0.98,0,-0.09  
3O7K,GLU\_147,2.59,0.49,-2.4,0  
1NAR,ARG\_239,12.01,-0.49,0,0  
2Q12,LYS\_119,10.22,-0.28,0,0  
1EYH,TYR\_83,9.55,0.15,-0.6,0  
3JRT,ARG\_38,12.29,-0.21,0,0  
3BCY,GLU\_61,4.85,0.35,0,0  
2FL7,ARG\_43,11.73,-0.77,0,0  
1NAF,GLU\_209,3.84,0.14,-0.8,0  
1X6J,GLU\_31,3.6,0.56,-1.45,0  
1O9G,ASP\_12,2.53,0.28,-1.55,0  
1LTU,ARG\_69,12.29,-0.21,0,0  
3O7K,GLU\_144,0.94,1.03,-2.19,-2.4  
3EIZ,HIS\_163,6.36,0,0,-0.14  
3CIV,ASP\_116,3.44,0.14,-0.5,0  
4ECC,LYS\_91,10.5,0,0,0  
2BT8,ASP\_228,2.97,0.56,-1.39,0  
3M7D,GLU\_263,4.52,0.07,-0.05,0  
1NRI,ARG\_81,11.59,-0.91,0,0  
3ETU,GLU\_283,4.37,0.14,-0.27,0  
2G5X,ASP\_9,2.85,0.49,-1.44,0  
1LTU,ASP\_267,4.01,0.21,0,0  
4HDE,LYS\_173,10.22,-0.28,0,0  
2BHD,ARG\_33,12.08,-0.42,0,0  
2D59,ASP\_12,3.22,0.28,-0.86,0  
1MML,ARG\_253,10.86,-1.64,0,0  
2B61,TYR\_296,11.73,3.33,-1.6,0  
3E7P,ARG\_218,12.08,-0.42,0,0  
1GQE,ASP\_330,3.15,0.28,-0.93,0  
3NJM,ARG\_122,12.29,-0.21,0,0  
3U0V,GLU\_217,5.71,2.23,-1.02,0  
2E3S,ARG\_487,12.22,-0.28,0,0  
1J85,GLU\_70,3.64,0.77,-1.63,0  
2R0S,TYR\_165,10,0,0,0

3BQW, TYR\_295, 11.98, 1.98, 0,0  
2DVK, ARG\_112, 11.73, -0.77, 0,0  
1SUU, ARG\_685, 12.36, -0.14, 0,0  
2Q07, ARG\_486, 12.36, -0.14, 0,0  
2Q34, GLU\_182, 4.48, 0.14, -0.16, 0  
1EDG, CYS\_257, 10.75, 0, 0, 1.75  
1F2V, ASP\_5, 3.87, 0, 0, 0, 0  
1D2K, LYS\_362, 10.29, -0.21, 0, 0  
3C0C, ASP\_331, 3.05, 0.49, -1.24, 0  
2H2W, ARG\_192, 9.24, -3.4, 0, 0, 14  
2FD4, CYS\_477, 4.8, -5.34, 0.76, 0.39  
2IRM, ASP\_116, 4.22, 0.42, 0, 0  
3I82, LYS\_198, 10.36, -0.14, 0, 0  
1OTM, LYS\_45, 10.5, 0, 0, 0  
3ETV, ARG\_100, 11.52, -2.97, 0, 1.99  
1TD6, LYS\_58, 10.5, 0, 0, 0  
3AU3, ARG\_414, 12.01, -0.49, 0, 0  
1SFE, GLU\_50, 3.03, 0.32, -0.54, -1.26  
3GEC, ARG\_484, 12.36, -0.14, 0, 0  
1Z3X, LYS\_120, 9.87, -0.63, 0, 0  
1VSM, ARG\_179, 11.59, -0.91, 0, 0  
2D59, LYS\_86, 10.36, -0.14, 0, 0  
3EGN, ARG\_464, 12.43, -0.07, 0, 0  
4FH3, ASP\_246, 3.93, 0.14, -0.01, 0  
2HNG, GLU\_116, 3.46, 0.21, -1.25, 0  
2O8I, GLU\_142, 1.83, 1.16, -1.57, -2.26  
4H89, ARG\_24, 11.73, -0.77, 0, 0  
4ECC, LYS\_194, 10.36, -0.14, 0, 0  
3N2T, LYS\_78, 10.5, 0, 0, 0  
1OST, ARG\_133, 11.38, -1.12, 0, 0  
3I1C, ASP\_95, 1.94, 0.63, -2.49, 0  
1RZ2, LYS\_216, 10.5, 0, 0, 0  
1R53, HIS\_17, 6.43, 0, 0, -0.07  
1UW7, LYS\_86, 10.08, -0.42, 0, 0  
2IIA, HIS\_103, 7.09, 0.8, -0.21  
3PP8, HIS\_275, 9.97, 1.6, 3.79, -1.92  
2Z61, ASP\_295, 3.33, 0.14, -0.61, 0  
1AT0, GLU\_351, 4.71, 0.21, 0, 0  
3LJI, GLU\_136, 4.57, 0.07, 0, 0  
1YR6, GLU\_79, 4.71, 0.21, 0, 0  
1J33, HIS\_323, 7.16, 0.94, -0.28  
1OXZ, GLU\_251, 4.57, 0.07, 0, 0  
3FTT, ASP\_51, 2.04, 1.05, -2.81, 0  
2OSA, GLU\_431, 4.57, 0.07, 0, 0  
1LTU, ASP\_26, 2.5, 0.77, -2.07, 0  
1SIG, LYS\_377, 10.5, 0, 0, 0  
2B61, GLU\_175, 3.91, 0.21, -0.8, 0  
2F8H, GLU\_275, 3.61, 0.71, -1.6, 0  
1O6D, LYS\_112, 10.15, -0.35, 0, 0  
1GQE, LYS\_303, 10.5, 0, 0, 0  
2OEW, ARG\_276, 13.02, -1.46, 0, 1.98  
2RJD, HIS\_331, 6.5, 0, 0, 0  
2GSX, ARG\_1, 11.75, -0.75, 0, 0  
3I00, GLU\_132, 3.62, 0.72, -1.6, 0  
3L3P, ASP\_291, 3.97, 0.21, -0.04, 0  
1IAP, HIS\_206, 6.57, 0.14, 0, -0.07  
1YTD, ARG\_373, 12.29, -0.21, 0, 0  
1YR6, HIS\_178, 3.52, 0, 0, -2.98  
4FD6, HIS\_49, 4.76, 0.8, -2.54  
1NIJ, CYS\_64, 6.19, -3.89, 0, 1.08  
3OAZ, LYS\_433, 10.5, 0, 0, 0  
1BN6, GLU\_158, 4.5, 0, 0, 0  
1SI7, ARG\_47, 11.8, -0.7, 0, 0  
1WP5, ARG\_90, 12.5, 0, 0, 0  
2QVT, CYS\_83, 5.98, -3.09, 0, 0.07  
3M70, CYS\_7, 6.57, -2.5, 0, 0.07  
2POL, LYS\_160, 10.43, -0.07, 0, 0  
3GMS, ARG\_232, 11.8, -0.7, 0, 0  
4H89, GLU\_12, 4.46, 0.21, -0.25, 0  
2HRZ, HIS\_326, 3.22, 0, 0, -3.28  
1Q5Z, ASP\_556, 1.72, 0.35, -2.43, 0  
1MML, CYS\_90, 9.32, 0, 0, 0.32  
2H2W, TYR\_71, 5.76, 0.64, -2.17, -2.72  
1GXN, TYR\_456, 11.65, 1.65, 0, 0  
1JSX, LYS\_4, 10.22, -0.28, 0, 0  
3EUR, HIS\_82, 7.13, 0.7, 0, -0.07  
4GA2, GLU\_9, 4.57, 0.07, 0, 0  
2FB6, LYS\_106, 10.5, 0, 0, 0  
3I4T, ASP\_240, 3.06, 0.21, -0.95, 0  
2HRZ, ASP\_108, 3.84, 0.21, -0.17, 0  
1NKD, LYS\_25, 10.5, 0, 0, 0  
2H30, TYR\_113, 10.81, 0.94, -0.13, 0  
2GYZ, CYS\_69, 8.99, -0.01, 0, 0  
3BWT, ARG\_720, 12.29, -0.21, 0, 0  
3ETU, ARG\_88, 12.32, -2.96, 0, 2.78  
1WPA, GLU\_442, 4.85, 0.35, 0, 0  
1LZL, GLU\_117, 4.91, 1.52, -1.11, 0  
3CN5, TYR\_177, 9.98, 0, -0.02, 0  
2QRX, ARG\_98, 11.26, -1.24, 0, 0  
1O9G, TYR\_124, 10, 0, 0, 0  
3TOW, GLU\_181, 4.18, 0.49, -0.81, 0  
4GCO, GLU\_235, 4.06, 0.35, -0.79, 0  
1R3D, ARG\_169, 11.31, -1.19, 0, 0  
4ECC, GLU\_22, 3.88, 0.96, -1.58, 0  
4EKU, ARG\_228, 11.94, -0.56, 0, 0  
3GT0, TYR\_76, 9.88, 1.23, -1.35, 0  
1FKM, ARG\_316, 11.45, -1.05, 0, 0  
1SI7, ARG\_177, 12.22, -0.28, 0, 0  
3JSN, LYS\_241, 10.5, 0, 0, 0  
2RGY, GLU\_222, 4.86, 0.36, 0, 0  
4ANN, GLU\_147, 4.5, 0, 0, 0  
3H9W, GLU\_44, 3.65, 0.28, -1.13, 0  
3LPZ, ASP\_69, 3.91, 0.14, -0.03, 0  
3ASA, ARG\_348, 11.73, -0.77, 0, 0  
1ESS, LYS\_82, 9.52, -0.98, 0, 0  
2X5Y, TYR\_728, 11.76, 0, 0, 1.76  
1TLV, LYS\_191, 10.43, -0.07, 0, 0  
3TOW, HIS\_197, 6.5, 0, 0, 0  
1QYI, ARG\_299, 12.43, -0.07, 0, 0  
1NAR, ASP\_137, 3.5, 0.7, -1, 0  
1WNI, LYS\_42, 10.22, -0.28, 0, 0  
1QQE, ARG\_115, 11.66, -0.84, 0, 0  
1TWU, LYS\_139, 10.5, 0, 0, 0  
1DZF, TYR\_168, 9.82, 0.07, -0.25, 0  
3BPP, TYR\_89, 11.78, 0, -0.01, 1.8  
2R05, TYR\_275, 10.24, 0.24, 0, 0  
1EYH, GLU\_142, 4.5, 0, 0, 0  
2ZCX, ASP\_48, 3.05, 0.35, -1.1, 0  
1OTM, ASP\_156, 2.49, 0.42, -1.73, 0  
1PSW, ARG\_306, 10.89, -1.61, 0, 0  
3L3P, GLU\_264, 4.19, 0.07, -0.38, 0  
3A7L, ASP\_55, 3.01, 0.42, -1.2, 0  
2OJQ, GLU\_461, 2.79, 0.56, -2.27, 0  
3FWU, ASP\_12, 2.21, 0.7, -2.3, 0  
3A2Z, HIS\_55, 5.28, 1.48, 0, -2.7  
1T3Y, ARG\_18, 12.15, -0.35, 0, 0  
1AKO, GLU\_165, 2.45, 0.35, -2.4, 0  
1GPP, TYR\_176, 8.99, 0.14, -0.01, -1.14  
1R3F, ARG\_202, 11.84, -2.71, 0, 2.05  
4FLE, GLU\_106, 4.5, 0, 0, 0  
1WXF, HIS\_204, 7.16, 0.8, -0.14  
4FH3, GLU\_84, 4.57, 0.07, 0, 0  
2H30, TYR\_140, 10.74, 0.91, -0.17, 0  
1WXQ, HIS\_171, 5.1, 0.02, 0, -1.42  
1SQW, ASP\_152, 3.7, 0.07, -0.18, 0  
1YOK, GLU\_131, 4.57, 0.07, 0, 0  
3I1C, GLU\_153, 5.25, 0.75, 0, 0  
4ETX, TYR\_345, 11.62, 0.52, -0.61, 1.72  
1VJG, ARG\_108, 11.94, -0.56, 0, 0  
3F1X, HIS\_251, 6.41, 0.26, 0, -0.35  
1NAR, GLU\_55, 4.5, 0, 0, 0  
2FPN, LYS\_86, 10.08, -0.42, 0, 0  
3VNC, CYS\_206, 4.17, -5.85, 0.78, 0.24  
1XKR, GLU\_5, 3.91, 0.21, -0.8, 0  
1ESS, ARG\_191, 11.87, -0.63, 0, 0  
1Q2Y, LYS\_92, 10.5, 0, 0, 0  
2XJ4, ARG\_84, 12.08, -0.42, 0, 0  
3A2Z, GLU\_39, 4.71, 0.21, 0, 0  
3ZXY, HIS\_160, 3.88, 0.77, 0, -3.39  
1SNT, LYS\_263, 10.36, -0.14, 0, 0  
2IN0, LYS\_36, 10.5, 0, 0, 0  
2CVB, TYR\_131, 13.22, 1.64, -0.01, 1.59  
1Q8B, GLU\_57, 4.57, 0.07, 0, 0  
2D7J, ARG\_21, 12.36, -0.14, 0, 0  
3BZT, HIS\_320, 6.73, 0.23, 0, 0  
3P51, ARG\_71, 11.87, -0.63, 0, 0  
1UCH, HIS\_169, 10.78, 5.2, 3.25, -4.17  
3LH5, LYS\_529, 10.36, -0.14, 0, 0  
2O8I, ASP\_27, 1.71, 0.35, -2.44, 0  
2X4L, ASP\_207, 3.42, 0.42, -0.8, 0  
4FCU, GLU\_172, 4.5, 0, 0, 0  
2YT4, LYS\_614, 10.5, 0, 0, 0  
3F53, ASP\_223, 3.62, 0, -0.18, 0  
3ADO, GLU\_70, 4.57, 0.07, 0, 0  
2X4G, HIS\_12, 6.5, 0, 0, 0  
2A1V, GLU\_127, 3.91, 0.21, -0.8, 0  
3CX5, GLU\_16, 4.05, 0.35, -0.8, 0  
3JSN, GLU\_144, 4.99, 0.69, -1.01, 0.81  
1O59, ARG\_177, 9.35, -2.17, 0, -0.98  
1N81, GLU\_145, 4.5, 0, 0, 0  
3PZ9, ARG\_185, 11.94, -0.56, 0, 0  
3I00, GLU\_209, 4.26, 0.56, -0.8, 0  
1X7F, LYS\_326, 10.29, -0.21, 0, 0  
1WYC, HIS\_9, 3.79, 0.28, 0, -2.99  
1NIJ, GLU\_291, 3.39, 0.49, -1.6, 0  
3G6S, CYS\_237, 9.4, -0.82, 0, 1.22  
1MUF, GLU\_228, 3.84, 0.14, -0.8, 0  
3G9B, TYR\_130, 10.54, 0.95, -0.41, 0  
2OJQ, GLU\_426, 4.5, 0, 0, 0  
3FFM, ASP\_55, 3.63, 0.07, -0.24, 0  
2EEY, LYS\_160, 10.15, -0.35, 0, 0  
3BJV, LYS\_40, 10.43, -0.07, 0, 0  
3RRQ, ARG\_104, 12.15, -0.35, 0, 0  
3JZ9, GLU\_513, 4.5, 0, 0, 0  
2R05, LYS\_82, 10.5, 0, 0, 0  
3ON1, ARG\_69, 12.15, -0.35, 0, 0  
2VAN, GLU\_309, 4.57, 0.07, 0, 0  
2CBE, HIS\_10, 6.5, 0, 0, 0  
3H6Q, GLU\_87, 4.5, 0, 0, 0  
3E7U, LYS\_186, 10.5, 0, 0, 0  
4EKK, TYR\_155, 11.72, 2.69, 0, -0.98  
2PIM, ASP\_78, 2.56, 0.49, -1.73, 0  
2DG7, GLU\_35, 4.64, 0.14, 0, 0  
1WPS, LYS\_36, 10.29, -0.21, 0, 0  
2E3S, ARG\_471, 12.5, 0, 0, 0  
2Z14, TYR\_87, 10, 0, 0, 0  
1DUPL, LYS\_16, 10.5, 0, 0, 0  
2JHY, LYS\_99, 10.5, 0, 0, 0  
1O3X, GLU\_251, 4.49, 0.07, -0.08, 0  
3EVZ, GLU\_180, 2.69, 0.91, -2.72, 0  
1L3K, GLU\_11, 4.48, 0, -0.02, 0  
1Q4Z, LYS\_74, 10.5, 0, 0, 0  
2Q99, HIS\_115, 6.5, 0, 0, 0  
2JHY, GLU\_193, 4.7, 0.21, -0.01, 0  
4F8A, ASP\_668, 3.35, 0.35, -0.8, 0  
3KEY, CYS\_420, 7.91, -1.3, 0, 0.21  
1Q2Y, TYR\_48, 13.27, 0.07, 0.8, 2.4  
1GPP, ARG\_90, 12.08, -0.42, 0, 0  
1R3F, ARG\_302, 11.87, -0.63, 0, 0  
2D2S, ARG\_549, 11.87, -0.63, 0, 0  
1ILW, LYS\_100, 10.15, -0.35, 0, 0  
2FL7, LYS\_122, 10.29, -0.21, 0, 0  
3S0A, LYS\_69, 10.36, -0.14, 0, 0  
1W7B, TYR\_188, 10, 0, 0, 0  
2OPJ, ARG\_171, 12.08, -0.42, 0, 0  
3VJ8, ARG\_149, 12.29, -0.21, 0, 0  
3F6F, TYR\_147, 9.83, 0, -0.17, 0  
1SJJ, HIS\_8, 6.43, 0, 0, -0.07  
1QQE, ASP\_214, 2.72, 0.35, -1.43, 0  
1YOK, ARG\_194, 11.87, -0.63, 0, 0  
2R51, LYS\_67, 10.5, 0, 0, 0  
3U2A, GLU\_31, 3.02, 0.21, -1.69, 0  
2VAN, ASP\_276, 3.46, 0, -0.34, 0  
1ZBP, GLU\_48, 4.5, 0, 0, 0  
3GFP, ARG\_380, 12.22, -0.28, 0, 0  
2O8P, LYS\_216, 9.87, -0.63, 0, 0  
3JSN, ASP\_286, 2.52, 0.56, -1.84, 0  
3UPD, GLU\_54, 3.6, 1.07, -1.97, 0  
2W0G, ARG\_235, 12.01, -0.49, 0, 0  
1XDZ, GLU\_157, 3.23, 1.43, -3.6, 0  
2VAN, LYS\_113, 10.5, 0, 0, 0  
1MTZ, LYS\_117, 10.15, -0.35, 0, 0  
1WYC, ASP\_390, 1.93, 0.56, -2.43, 0  
2HRZ, ASP\_66, 1.78, 0.63, -2.66, 0  
1IAP, LYS\_53, 9.87, -0.63, 0, 0  
2IQF, GLU\_165, 4.57, 0.07, 0, 0  
3RUX, GLU\_129, 4.5, 0, 0, 0  
1L3K, GLU\_176, 4.23, 0.28, -0.55, 0  
2XMX, LYS\_119, 10.5, 0, 0, 0  
1YM5, TYR\_237, 12.28, 1.5, -0.36, 1.14  
3L3P, TYR\_480, 10, 0, 0, 0  
2H80, HIS\_79, 4.75, 1.05, 0, -2.8  
1T3Y, ASP\_55, 3.24, 0.35, -0.91, 0  
2D7U, LYS\_306, 10.15, -0.35, 0, 0  
4ECC, GLU\_129, 4.68, 0.28, -0.1, 0  
1O6D, GLU\_75, 3.98, 0.28, -0.8, 0  
2B78, LYS\_53, 10.43, -0.07, 0, 0  
3GV0, LYS\_110, 10.15, -0.35, 0, 0  
1O9G, ARG\_241, 12.22, -0.28, 0, 0  
1NAR, GLU\_213, 3.81, 0.49, -1.18, 0  
2W0G, CYS\_183, 5.75, -3.86, 0, 0.61  
2XHC, TYR\_109, 10, 0, 0, 0  
3GRY, LYS\_185, 10.5, 0, 0, 0  
2Q9X, GLU\_22, 4.5, 0, 0, 0  
2G5X, ASP\_43, 2.67, 0.35, -1.48, 0  
3PBH, ASP\_124, 3.47, 0.07, -0.4, 0  
3BQW, HIS\_332, 2, 0, -0.43, -4.07  
3PBH, TYR\_165, 10, 0, 0, 0  
1ZBS, HIS\_206, 6.29, 0, 0, -0.21  
1K2D, HIS\_62, 6.56, 1.87, 0, -0.14  
2GAU, HIS\_152, 6.5, 0, 0, 0  
2F9F, GLU\_80, 3.04, 0.42, -1.88, 0  
2V4X, GLU\_41, 3.33, 0.42, -1.59, 0  
1HUF, ARG\_49, 12.15, -0.35, 0, 0  
2B78, LYS\_342, 10.5, 0, 0, 0  
3AU3, LYS\_516, 9.94, -0.56, 0, 0  
1X04, GLU\_49, 4.03, 0.14, -0.61, 0  
1TD6, HIS\_127, 3.08, 0.76, 0, -4.18  
2D8N, LYS\_161, 10.08, -0.42, 0, 0  
1OTM, LYS\_145, 10.43, -0.07, 0, 0  
1WXQ, GLU\_328, 3.64, 0.07, -0.93, 0  
1TD6, GLU\_196, 3.66, 1.87, -0.71, -2.01  
2F4Q, LYS\_90, 10.5, 0, 0, 0  
1T07, ASP\_40, 3.95, 0.21, -0.06, 0  
3OKQ, LYS\_589, 10.43, -0.07, 0, 0  
3L7N, ASP\_69, 2.86, 0.56, -1.5, 0

2OJQ,ARG\_380,12.5,0,0,0  
 2ZCO,LYS\_20,10.01,-0.49,0,0  
 1OLR,ARG\_73,11.8,-0.7,0,0  
 2B2H,GLU\_376,1.04,0.93,-1.99,-2.4  
 1O59,LYS\_159,10.5,0,0,0  
 3E7P,TYR\_126,11.36,1.54,-0.18,0  
 2ZOM,ARG\_232,11.41,-1.38,0,0.29  
 1R5S,HIS\_122,7.13,0.77,0,-0.14  
 3RFF,ASP\_154,3.84,0.14,-0.1,0  
 3UC9,CYS\_76,9.07,0,0,0.07  
 2O4D,TYR\_80,10.14,0.21,-0.07,0  
 3AUF,ARG\_75,12.22,-0.28,0,0  
 2B0J,GLU\_299,4.64,0.14,0,0  
 2NSN,CYS\_59,9,0,0,0  
 2OSA,HIS\_407,7.15,0.79,0,-0.14  
 3I4T,HIS\_109,6.43,0,0,-0.07  
 3GOZ,GLU\_186,3.89,0.42,-1.03,0  
 2ZOM,LYS\_39,10.5,0,0,0  
 1MML,ARG\_71,11.87,-0.63,0,0  
 1PBV,GLU\_85,4.6,0.28,-0.18,0  
 1L3K,ASP\_154,4.22,0.56,-0.14,0  
 1JKS,LYS\_276,10.29,-0.21,0,0  
 3DHN,GLU\_39,3.65,0.56,-1.4,0  
 2H14,TYR\_131,10.54,0,0.54  
 2H01,TYR\_108,11.29,1.29,0,0  
 1F09,LYS\_397,9.87,-0.63,0,0  
 2IRM,ASP\_195,3.77,0.42,-0.46,0  
 2PGE,ASP\_362,3.38,0.28,-0.7,0  
 4ACJ,GLU\_708,4.6,0.14,-0.04,0  
 3BJV,GLU\_96,4.5,0,0,0  
 2BLL,CYS\_629,12.76,-0.57,3.86,0.47  
 2F8H,ASP\_302,4.11,0.35,-0.04,0  
 4GCO,GLU\_175,4.64,0.14,0,0  
 3NBI,LYS\_109,10.08,-0.42,0,0  
 2FPN,ARG\_42,11.73,-0.77,0,0  
 3GYW,TYR\_272,10,0,0,0  
 2A4D,ASP\_104,2.03,0.35,-2.12,0  
 1KCM,TYR\_7,9.97,0.94,-0.97,0  
 1R2Z,LYS\_252,10.01,-0.49,0,0  
 3A4C,LYS\_534,10.5,0,0,0  
 3GV0,GLU\_322,3.67,0.28,-1.11,0  
 1OIS,LYS\_198,10.43,-0.07,0,0  
 4GAZ,LYS\_99,10.29,-0.21,0,0  
 4GCO,GLU\_192,4.04,0.07,-0.53,0  
 2H2W,GLU\_37,4.34,0.57,-0.73,0  
 3LQE,ARG\_373,12.22,-0.28,0,0  
 3AU3,LYS\_570,9.8,-0.7,0,0  
 3EVN,HIS\_162,6.76,0.33,0,-0.07  
 1T3Y,LYS\_30,10.15,-0.35,0,0  
 2Q12,ARG\_149,12.29,-0.21,0,0  
 3BWT,LYS\_573,10.22,-0.28,0,0  
 1UAJ,ASP\_150,3.94,0.14,0,0  
 2BLL,TYR\_341,13.68,0.8,0.48,2.4  
 2DG7,ARG\_68,12.01,-0.49,0,0  
 3CZC,ASP\_33,3.43,0.28,-0.65,0  
 1YG2,ARG\_112,12.15,-0.35,0,0  
 2OEW,LYS\_60,10.43,-0.07,0,0  
 3DTE,ASP\_216,2.81,0.21,-1.19,0  
 1O5J,GLU\_23,4.78,0.28,0,0  
 1X9G,GLU\_93,4.64,0.14,0,0  
 1ZCE,ARG\_135,11.8,-0.7,0,0  
 2POL,LYS\_56,10.5,0,0,0  
 1Y0K,ASP\_135,3.45,0.42,-0.77,0  
 3PAC,HIS\_78,6.29,0,0,-0.21  
 3VHJ,LYS\_45,10.29,-0.21,0,0  
 2Q99,ASP\_227,2.36,0.7,-2.14,0  
 1WXF,LYS\_274,10.43,-0.07,0,0  
 3RFY,ARG\_259,12.08,-0.42,0,0  
 3UX2,CYS\_66,5.28,-3.94,0,0.21  
 2NRR,HIS\_370,6.65,0.22,0,-0.07  
 4ACJ,LYS\_777,10.36,-0.14,0,0  
 3GT0,CYS\_34,11.82,0.24,0.42  
 2X5Y,LYS\_760,10.15,-0.35,0,0  
 3OBS,HIS\_115,6.5,0,0,0  
 1JT9,LYS\_28,10.43,-0.07,0,0  
 4DIU,GLU\_77,4.71,0.21,0,0  
 1J33,HIS\_213,7.12,0.83,0,-0.21  
 2FM9,GLU\_111,3.9,0.35,-0.95,0  
 3V55,GLU\_572,4.64,0.14,0,0  
 3ASA,ASP\_265,3.14,0.28,-0.94,0  
 2R51,GLU\_279,4.64,0.14,0,0  
 1HF8,GLU\_65,4.5,0,0,0  
 1OXZ,ASP\_272,2.75,0.21,-1.27,0  
 3EVP,TYR\_93,9.67,0.21,-0.54,0  
 1O9G,GLU\_126,4.57,0.07,0,0  
 1R5S,LYS\_63,10.22,-0.28,0,0  
 1T3Y,LYS\_126,10.36,-0.14,0,0  
 3RFY,ARG\_317,12.29,-0.21,0,0  
 1PZC,HIS\_81,7.96,1.6,0,-0.14  
 1WYC,GLU\_96,4.21,0.63,-0.92,0  
 3CIV,ASP\_207,3,0.28,-1.09,0  
 1AK1,LYS\_190,10.36,-0.14,0,0  
 2CE6,GLU\_99,4.07,0.49,-0.92,0  
 3TMO,ARG\_294,11.66,-0.84,0,0  
 1H09,LYS\_3,10.22,-0.28,0,0  
 2H14,ARG\_196,12.01,-0.49,0,0  
 2H2Z,ASP\_34,3.21,0.28,-0.86,0  
 3ETU,LYS\_304,9.8,-0.7,0,0  
 3LH5,TYR\_527,12.41,0.14,-0.13,2.4  
 3HNX,ARG\_17,12.36,-0.14,0,0  
 3PAC,HIS\_174,6.36,0,0,-0.14  
 2IN0,ARG\_405,12.01,-0.49,0,0  
 2Q07,TYR\_408,10.68,0.68,0,0  
 1OIS,LYS\_215,9.94,-0.56,0,0  
 1LN4,ARG\_91,12.29,-0.21,0,0  
 1PDB,GLU\_30,6.06,2.36,-0.8,0  
 3CN5,LYS\_142,10.5,0,0,0  
 4ANN,GLU\_190,4.64,0.14,0,0  
 157K,GLU\_88,3.25,0.35,-1.6,0  
 3GEC,CYS\_242,9.37,-1.34,0,1.71  
 2RH3,LYS\_184,10.43,-0.07,0,0  
 3DSH,LYS\_356,10.22,-0.28,0,0  
 3RFY,LYS\_133,10.5,0,0,0  
 3BQW,LYS\_177,10.43,-0.07,0,0  
 3C6B,ASP\_275,3.11,0.28,-0.97,0  
 4E8B,GLU\_93,3.68,0.86,-1.68,0  
 1WNH,HIS\_185,7.16,0.8,0,-0.14  
 2P52,GLU\_284,4.64,0.14,0,0  
 3IOC,ASP\_103,3.83,0.07,-0.04,0  
 3C38,HIS\_166,3.88,0,0,-2.62  
 1TP6,ARG\_116,11.87,-0.63,0,0  
 2BLL,ARG\_334,11.38,-1.12,0,0  
 1F09,GLU\_280,1.72,0.42,-3.2,0  
 1KN3,TYR\_64,10.73,0.21,-1.151  
 2FD4,HIS\_476,6.43,0,0,-0.07  
 1WP5,ARG\_181,12.5,0,0,0  
 1ES9,GLU\_40,4.78,0.28,0,0  
 3FXH,GLU\_74,4.58,2.29,-2.21,0  
 1SQW,LYS\_155,10.36,-0.14,0,0  
 1LZL,ASP\_205,3.8,0.07,-0.07,0  
 2YWK,LYS\_48,10.01,-0.49,0,0  
 2XMX,ASP\_149,3.82,0.07,-0.05,0  
 1EV8,ASP\_124,3.94,0.14,0,0  
 4F85,CYS\_211,10.64,0,-0.52,2.16  
 4FZR,GLU\_134,1.77,1.62,-1.95,-2.4  
 1AD6,LYS\_412,10.5,0,0,0  
 1NFN,GLU\_80,4.5,0,0,0  
 1OIS,ASP\_239,3.97,0.21,-0.04,0  
 2OJQ,TYR\_370,9.99,0,-0.01,0  
 3T8R,LYS\_101,9.94,-0.56,0,0  
 1XEU,GLU\_35,4.5,0,0,0  
 3MEW,ARG\_255,12.15,-0.35,0,0  
 3EGN,ARG\_411,12.36,-0.14,0,0  
 2E3S,ASP\_508,3.87,0.07,0,0  
 3ANJ,LYS\_5,9.87,-0.63,0,0  
 3ASA,ARG\_302,12.83,-1.04,0,1.37  
 1RHS,TYR\_187,11.15,1.06,0,0.09  
 2A4D,ARG\_177,12.29,-0.21,0,0  
 3FK5,TYR\_157,9.24,2.57,-0.94,-2.39  
 2R51,LYS\_265,10.22,-0.28,0,0  
 3MEW,TYR\_283,10.24,0.24,0,0  
 1UW7,TYR\_32,9.25,0,-0.74,0  
 3S0A,GLU\_48,4.15,0.42,-0.77,0  
 1MML,GLU\_69,2.86,0.14,-1.77,0  
 3OOP,TYR\_5,10,0,0,0  
 1OXZ,GLU\_301,4.78,0.28,0,0  
 1LFP,LYS\_57,10.29,-0.21,0,0  
 3AZZ,TYR\_174,10,0,0,0  
 1ZBM,ASP\_207,3.15,0.28,-0.93,0  
 2V5B,ARG\_192,12.18,-2.23,0,1.91  
 2FM9,CYS\_190,9.52,-0.53,0,1.04  
 1RL0,LYS\_113,10.36,-0.14,0,0  
 2F9F,ARG\_163,11.66,-0.84,0,0  
 1PV5,HIS\_70,6.29,0,0,-0.21  
 2OEW,GLU\_44,4.64,0.14,0,0  
 2P65,ARG\_165,12.43,-0.07,0,0  
 3RLN,GLU\_701,4.64,0.14,0,0  
 3GW3,GLU\_125,4.5,0,0,0  
 2POL,LYS\_75,10.5,0,0,0  
 3DHN,ARG\_167,12.29,-0.21,0,0  
 2OJQ,GLU\_650,4.94,1.21,-0.69,-0.08  
 3BWT,LYS\_768,9.94,-0.56,0,0  
 4FH3,GLU\_242,4.64,0.14,0,0  
 2HXB,LYS\_78,10.36,-0.14,0,0  
 3O48,LYS\_70,10.5,0,0,0  
 2R51,TYR\_178,11.2,0.97,0.23  
 3HYQ,GLU\_78,3.05,0.28,-1.73,0  
 2EA9,ARG\_17,11.45,-1.05,0,0  
 1JSX,LYS\_203,9.59,-0.91,0,0  
 3CO1,ARG\_59,12.5,0,0,0  
 1ANU,LYS\_104,10.15,-0.35,0,0  
 3GYW,HIS\_72,6.43,0,0,-0.07  
 1P1L,GLU\_13,4.06,0.07,-0.51,0  
 2XWS,ASP\_35,2.83,0.42,-1.39,0  
 1BN6,GLU\_181,2.52,0.42,-2.4,0  
 2Q34,TYR\_82,9.73,0.68,-0.95,0  
 4DIU,GLU\_229,3.5,0.91,-1.91,0  
 1KCM,ARG\_74,12.5,0,0,0  
 2QK1,LYS\_340,10.29,-0.21,0,0  
 2OJQ,ARG\_702,12.5,0,0,0  
 4AM1,GLU\_142,3.84,0.14,-0.8,0  
 3F5D,TYR\_187,10,0,0,0  
 1ILW,LYS\_176,10.36,-0.14,0,0  
 2YWJ,TYR\_124,13.34,0.14,0.8,2.4  
 1WOU,LYS\_74,10.36,-0.14,0,0  
 2HXB,TYR\_156,10,0,0,0  
 3GOZ,LYS\_285,10.43,-0.07,0,0  
 2GZQ,ARG\_131,9.44,-2.13,0,-0.93  
 4ETX,ARG\_168,13.59,-1.21,0,2.3  
 3KV0,TYR\_139,9.19,0.07,-0.88,0  
 4EVF,ARG\_148,9.98,-2.52,0,0  
 3BB7,LYS\_108,10.01,-0.49,0,0  
 2JEO,LYS\_102,10.36,-0.14,0,0  
 3HUE,GLU\_315,4.5,0,0,0  
 1L3K,ARG\_47,11.87,-0.63,0,0  
 1XDZ,GLU\_206,3.86,0.35,-0.99,0  
 2ILR,TYR\_394,11.43,0.39,-1.12,2.16  
 1W24,TYR\_46,10,0,0,0  
 1Q46,TYR\_12,10,0,0,0  
 4EUG,HIS\_8,6.5,0,0,0  
 4DBX,LYS\_188,10.5,0,0,0  
 1V8E,HIS\_168,1.04,0,0,-5.46  
 2V4X,TYR\_11,12.58,0.07,0.11,2.4  
 3V75,ASP\_39,2.1,0.63,-2.33,0  
 3PZ9,TYR\_81,10.74,0.07,-0.79,1.45  
 1R29,GLU\_81,4.57,0.07,0,0  
 4HDE,ASP\_189,2.79,0.63,-1.63,0  
 2IQT,LYS\_3,10.29,-0.21,0,0  
 2HXB,LYS\_60,10.22,-0.28,0,0  
 1RAJ,ASP\_238,3.18,0.28,-0.9,0  
 3HKX,GLU\_110,4.5,0,0,0  
 3M70,LYS\_2,10.5,0,0,0  
 1SIG,ASP\_403,4.05,0.28,-0.03,0  
 2QK0,GLU\_52,4.5,0,0,0  
 1XFK,HIS\_241,6.36,0,0,-0.14  
 3IOC,HIS\_285,4.42,0,0,-2.08  
 2H01,ASP\_162,3.02,0.14,-0.92,0  
 2X4L,ARG\_59,13.54,-1.32,0.236  
 3HQX,ARG\_79,12.01,-0.49,0,0  
 2AHU,GLU\_32,4.57,0.21,-0.14,0  
 2D59,LYS\_118,10.5,0,0,0  
 3V46,ARG\_390,14,-1.07,0.257  
 2OJQ,ARG\_386,12.22,-0.28,0,0  
 2YLF,ARG\_194,12.5,0,0,0  
 1IDK,ASP\_79,3.94,0.14,0,0  
 4ACJ,GLU\_645,4.52,0.14,-0.12,0  
 3GA2,TYR\_123,10.07,0.07,0,0  
 1XTD,LYS\_27,10.43,-0.07,0,0  
 3HVM,TYR\_61,10,0,0,0  
 1O5T,GLU\_436,4.78,0.28,0,0  
 2QHT,ARG\_75,9.53,-3.18,0.0.21  
 2AZL,GLU\_146,3.5,2.2,-0.8,-2.4  
 3L7N,ASP\_217,2.16,0.35,-1.99,0  
 1LTU,LYS\_94,10.5,0,0,0  
 3CS1,LYS\_42,10.29,-0.21,0,0  
 3KB5,GLU\_348,3.62,1.19,-2.07,0  
 3UX2,TYR\_41,13.08,0.21,0.47,2.4  
 4DBX,TYR\_17,8.38,0.14,-1.75,0  
 3PBH,HIS\_239,9.3,3.6,2.4,-3.2  
 3RJK,LYS\_108,10.36,-0.14,0,0  
 1K95,ARG\_193,12.36,-0.14,0,0  
 3ELI,HIS\_43,6.7,0.34,0,-0.14  
 3G65,GLU\_261,4.57,0.07,0,0  
 2CIU,GLU\_186,3.59,0,-2.91  
 1AD6,HIS\_549,9.55,1.6,4.13,-2.68  
 2B2H,GLU\_178,4.78,0.28,0,0  
 3MTT,GLU\_515,4.57,0.07,0,0  
 3HVM,LYS\_45,10.43,-0.07,0,0  
 1YQJ,LYS\_17,10.36,-0.14,0,0  
 3OOP,ASP\_6,3.91,0.21,-0.1,0  
 2C2Y,ARG\_151,12.29,-0.21,0,0  
 3BWT,TYR\_564,10,0,0,0  
 1I60,LYS\_189,10.29,-0.21,0,0  
 2IF4,CYS\_70,10.08,0,0.1.08  
 2D0A,ARG\_222,12.15,-0.35,0,0  
 3FNI,GLU\_86,4.5,0,0,0  
 1UCH,ARG\_221,12.43,-0.07,0,0  
 1YTD,LYS\_13,10.5,0,0,0  
 1LN4,LYS\_50,10.43,-0.07,0,0  
 3LMF,HIS\_45,8.1,1.6,0,0  
 1U7U,LYS\_306,10.5,0,0,0  
 2CWC,ASP\_122,2.34,0.7,-2.16,0  
 3UV9,GLU\_392,4.18,1.86,-2.18,0  
 2OPJ,GLU\_23,3.84,0.14,-0.8,0  
 2Z14,GLU\_80,4.64,0.14,0,0  
 3EIZ,ARG\_44,12.22,-0.28,0,0

1TP6,ARG\_120,12.01,-0.49,0,0  
 1DVO,ARG\_94,11.94,-0.56,0,0  
 2QVO,HIS\_44,6.5,0,0,0  
 1G8P,GLU\_243,4.5,0,0,0  
 3N2T,ASP\_134,3.78,0,-0.02,0  
 3QKY,ARG\_179,12.01,-0.49,0,0  
 1MTZ,LYS\_53,10.5,0,0,0  
 3M9A,TYR\_65,11.86,0,0.01,1.84  
 3ULX,LYS\_167,10.5,0,0,0  
 3G9B,ARG\_73,11.59,-0.91,0,0  
 1R53,GLU\_70,4.64,0.14,0,0  
 1SQW,ASP\_157,3.23,0.77,-1.33,0  
 2OSA,LYS\_264,9.94,-0.56,0,0  
 2FPN,ASP\_137,3.4,0.07,-0.47,0  
 3FTT,HIS\_142,6.5,0,0,0  
 2CWY,ARG\_82,12.29,-0.21,0,0  
 2VGM,LYS\_201,10.22,-0.28,0,0  
 1TR9,ASP\_171,2.16,0.56,-2.2,0  
 2CN1,LYS\_260,10.5,0,0,0  
 2H8O,GLU\_95,4.51,1.61,-1.6,0  
 3U2R,ARG\_126,12.01,-0.49,0,0  
 1V8E,ARG\_202,11.87,-0.63,0,0  
 3AUF,CYS\_22,9.99,-0.18,0,1.17  
 1YM5,LYS\_148,10.15,-0.35,0,0  
 3T5B,ARG\_142,12.22,-0.28,0,0  
 1R7J,GLU\_48,4.5,0,0,0  
 2ZCO,GLU\_236,2.8,0.49,-2.19,0  
 1ZBS,ARG\_194,11.66,-0.84,0,0  
 2EYI,LYS\_89,10.43,-0.07,0,0  
 3CN5,LYS\_186,10.5,0,0,0  
 1TXJ,GLU\_104,4.5,0,0,0  
 1QZN,GLU\_20,2.4,0.56,-2.66,0  
 1P1L,GLU\_69,4.49,0.14,-0.15,0  
 3V75,ARG\_137,12.43,-0.07,0,0  
 2OGQ,CYS\_572,10.88,-0.19,1.26,0.81  
 1NAR,LYS\_275,10.43,-0.07,0,0  
 3M7D,ARG\_332,11.66,-0.84,0,0  
 3FRR,ARG\_137,11.94,-0.56,0,0  
 2CXA,GLU\_175,4.5,0,0,0  
 3IVF,ARG\_328,11.87,-0.63,0,0  
 2OSA,ASP\_320,2.36,0.84,-2.28,0  
 1RWZ,HIS\_35,6.87,1.87,1.64,-3.14  
 3V75,ARG\_87,13.5,-1.4,0,2.4  
 4GA2,LYS\_34,10.5,0,0,0  
 2OYZ,ASP\_24,3.09,0.21,-0.92,0  
 3EZ7,LYS\_48,10.5,0,0,0  
 3BWT,ASP\_739,3.87,0.42,-0.35,0  
 2CBE,TYR\_88,11.38,0.93,-1.05,1.51  
 3A2Z,TYR\_30,10.23,0.02,0,0.21  
 2X4G,TYR\_338,10.14,0.14,0,0  
 3ULX,ASP\_50,3.76,0.42,-0.46,0  
 4ETX,GLU\_428,4.57,0.07,0,0  
 3KT9,HIS\_88,6.36,0,0,-0.14  
 3ANJ,LYS\_232,10.29,-0.21,0,0  
 1MJS,CYS\_337,9.02,-0.05,0,0.07  
 3Q2C,LYS\_57,10.22,-0.28,0,0  
 2CBE,LYS\_159,10.36,-0.14,0,0  
 2ZOM,LYS\_4,10.43,-0.07,0,0  
 3EST,TYR\_117,11.5,2.69,-1.19,0  
 3LH5,TYR\_633,11.77,1.77,0,0  
 3BPP,LYS\_148,10.43,-0.07,0,0  
 3AUF,ARG\_168,12.43,-0.07,0,0  
 2E3C,GLU\_410,4.05,0.21,-0.66,0  
 1R9W,LYS\_289,10.29,-0.21,0,0  
 1M5I,ASP\_183,2.98,0.14,-0.97,0  
 2H85,LYS\_319,10.29,-0.21,0,0  
 3EX9,ARG\_20,11.59,-0.91,0,0  
 3IVF,LYS\_89,10.22,-0.28,0,0  
 2OEW,ASP\_100,3.54,0.28,-0.54,0  
 3RRQ,LYS\_78,10.43,-0.07,0,0  
 2RJD,LYS\_330,10.5,0,0,0  
 1OIS,LYS\_332,10.43,-0.07,0,0  
 4EUG,GLU\_215,4.64,0.14,0,0  
 4DNU,ASP\_260,3.14,0.42,-1.08,0  
 2X4J,GLU\_40,4.29,0.28,-0.49,0  
 2BV9,ARG\_136,11.94,-0.56,0,0  
 1PNE,LYS\_125,10.36,-0.14,0,0  
 3DSH,GLU\_384,5.13,0.63,0,0  
 2DVK,LYS\_116,10.43,-0.07,0,0  
 3R87,ASP\_17,2.12,0.56,-2.24,0  
 3PM2,LYS\_164,10.5,0,0,0  
 2B0A,LYS\_117,10.5,0,0,0  
 1K95,ASP\_134,3.94,0.14,0,0  
 2D8N,TYR\_53,11.42,1.57,-0.15,0  
 3ELI,ASP\_3,4.29,0.49,0,0  
 3GW3,LYS\_359,10.5,0,0,0  
 2OEW,LYS\_164,10.43,-0.07,0,0  
 2BV9,LYS\_25,10.29,-0.21,0,0  
 1SUU,LYS\_770,10.43,-0.07,0,0  
 3JV1,GLU\_137,4.16,0.21,-0.55,0  
 2H14,ASP\_98,1.41,0.49,-2.88,0  
 1P1L,LYS\_62,10.43,-0.07,0,0  
 3BCH,ARG\_85,12.01,-0.49,0,0  
 1UXO,ARG\_129,11.52,-0.98,0,0  
 3GOZ,ARG\_309,11.94,-0.56,0,0  
 1RHS,GLU\_42,4.57,0.07,0,0  
 3RFY,ASP\_171,3.8,0,0,0  
 2XMZ,LYS\_224,10.43,-0.07,0,0  
 4FZR,TYR\_192,10.68,1.88,-1.2,0  
 1PDB,HIS\_127,6.62,0.33,0,-0.21  
 1AM2,HIS\_56,7.42,1.13,0,-0.21  
 2GKG,LYS\_68,10.5,0,0,0  
 2X4L,ASP\_66,3.79,0,-0.01,0  
 2CVB,GLU\_85,4.5,0,0,0  
 3BB7,HIS\_287,7.37,1.6,1.72,-2.45  
 1QYI,LYS\_196,10.08,-0.42,0,0  
 1OTM,ASP\_178,2.21,0.35,-1.94,0  
 3JV1,HIS\_89,6.94,0.58,0,-0.14  
 1ZCU,ARG\_76,11.66,-0.84,0,0  
 2XJ4,TYR\_269,9.27,0.07,-0.8,0  
 1ZCU,HIS\_181,6.38,0.09,0,-0.21  
 3UV9,CYS\_493,8.35,-0.86,0,0.21  
 2ZCO,GLU\_121,3.98,0.28,-0.8,0  
 4GCO,CYS\_200,11.28,-0.19,0.94,1.53  
 2A1V,ARG\_14,12.15,-0.35,0,0  
 1P1L,ARG\_21,12.22,-0.28,0,0  
 1OTM,LYS\_230,10.5,0,0,0  
 2WB8,ASP\_789,3.12,0.49,-1.17,0  
 1PGV,ARG\_367,12.43,-0.07,0,0  
 2F4Q,GLU\_308,4.12,0.42,-0.8,0  
 2EFK,GLU\_250,4.64,0.14,0,0  
 1UAJ,LYS\_93,10.15,-0.35,0,0  
 1TLV,TYR\_126,11.35,2.15,-0.8,0  
 3NJM,GLU\_21,4.71,0.21,0,0  
 1QZN,LYS\_171,10.5,0,0,0  
 3ONT,ARG\_25,12.22,-0.28,0,0  
 2H2W,GLU\_73,4.17,0.07,-0.4,0  
 1AK1,GLU\_172,3.18,0.28,-1.6,0  
 1LTU,ARG\_219,11.44,-1.2,0,0.14  
 1XWM,GLU\_157,4.21,0.35,-0.64,0  
 2YXO,GLU\_223,3.9,0.49,-1.08,0  
 2Q13,GLU\_80,4.5,0,0,0  
 1SIG,LYS\_414,10.5,0,0,0  
 2B3M,LYS\_7,10.5,0,0,0  
 1UXO,LYS\_25,10.29,-0.21,0,0  
 1W24,ASP\_171,3.7,0.14,-0.24,0  
 2ZTY,ASP\_58,3.43,0.21,-0.58,0  
 3Q1C,GLU\_135,3.97,0.14,-0.67,0  
 2R51,LYS\_163,10.43,-0.07,0,0  
 3T5B,CYS\_42,11.28,-0.01,0,2.29  
 1DUN,LYS\_92,10.5,0,0,0  
 1X8F,LYS\_162,10.43,-0.07,0,0  
 4AE7,CYS\_113,8.01,-1,0,0  
 1JSX,ASP\_134,2.06,0.56,-2.3,0  
 3HYQ,HIS\_69,7.86,0.77,1.99,-1.41  
 3MEW,GLU\_191,4.09,0.56,-0.97,0  
 1V6T,ASP\_67,0.94,0.56,-3.42,0  
 1XTZ,ASP\_250,2.13,0.49,-2.16,0  
 3GMS,ARG\_295,12.43,-0.07,0,0  
 2BDD,LYS\_39,10.36,-0.14,0,0  
 1XIP,GLU\_371,4.12,0.28,-0.66,0  
 2H85,LYS\_155,10.43,-0.07,0,0  
 1VSM,ARG\_114,12.29,-0.21,0,0  
 1P6F,ARG\_80,11.94,-0.56,0,0  
 3UV9,HIS\_423,6.5,0,0,0  
 2E3I,ARG\_120,11.31,-1.19,0,0  
 3DSH,GLU\_368,4.57,0.07,0,0  
 2B0A,GLU\_148,4.52,3.21,-1.82,-1.37  
 2Q13,GLU\_224,4.5,0,0,0  
 1MTZ,LYS\_30,10.01,-0.49,0,0  
 1NIJ,ASP\_253,3.34,0.28,-0.74,0  
 4ECC,ARG\_195,11.87,-0.63,0,0  
 3VHJ,ASP\_118,3.51,0.14,-0.42,0  
 1TXJ,TYR\_101,9.31,0.07,-0.76,0  
 2DVK,HIS\_117,6.57,0.07,0,0  
 2F4Q,ARG\_14,12.22,-0.28,0,0  
 3TOW,ARG\_98,13.39,-0.85,0,1.74  
 2R0S,LYS\_312,10.5,0,0,0  
 3A4C,HIS\_551,6.56,0.13,0,-0.07  
 1O9G,ARG\_181,11.51,-1.19,0,0.2  
 2EA9,ARG\_22,11.45,-1.05,0,0  
 3BZT,ASP\_302,4.08,0.28,0,0  
 3FWU,GLU\_63,4.57,0.07,0,0  
 3CX2,ASP\_151,3.11,0.07,-0.76,0  
 1FKM,ASP\_325,4.08,0.28,0,0  
 1DUN,LYS\_12,9.8,-0.7,0,0  
 1O9G,GLU\_247,4.5,0,0,0  
 2Q99,TYR\_51,12.13,2.13,0,0  
 2V4U,ARG\_454,12.01,-0.49,0,0  
 2OSA,HIS\_390,3.23,0.7,-3.97  
 1R3D,LYS\_129,10.08,-0.42,0,0  
 1YLN,LYS\_238,10.43,-0.07,0,0  
 3O48,ASP\_54,2.5,0.42,-1.72,0  
 2AD1,ARG\_10,11.31,-1.19,0,0  
 2WB3,ASP\_356,3.87,0.07,0,0  
 2BDV,TYR\_62,9.61,0,-0.39,0  
 3RNV,TYR\_343,10,0,0,0  
 1Y2Q,GLU\_63,4.5,0.14,-0.14,0  
 3ULX,GLU\_61,4.65,0.28,-0.13,0  
 1ZBS,TYR\_187,10,0,0,0  
 1J74,LYS\_116,10.22,-0.28,0,0  
 3RLE,GLU\_157,2.87,0.84,-2.47,0  
 2F9F,ASP\_68,3.8,0,0,0  
 2APL,LYS\_7,10.43,-0.07,0,0  
 1SUU,TYR\_574,10.43,0,0,0.43  
 1WP5,ARG\_240,12.36,-0.14,0,0  
 3I47,GLU\_191,3.73,0.28,-1.05,0  
 4FH3,LYS\_180,10.5,0,0,0  
 2X5Y,GLU\_732,4.1,0.28,-0.68,0  
 3F1X,ASP\_32,3.79,0,-0.01,0  
 1V43,HIS\_362,2.95,0.07,-0.38,-3.24  
 1ZYL,TYR\_276,8.79,1.92,-0.26,-2.89  
 2GZR,LYS\_273,9.8,-0.7,0,0  
 2ZCX,ARG\_24,12.29,-0.21,0,0  
 3JZN,GLU\_233,4.26,0.21,-0.45,0  
 2FC3,GLU\_10,4.5,0,0,0  
 1X7F,ASP\_331,1.03,0.7,-3.47,0  
 2O0K,TYR\_142,10.79,1.65,0,-0.86  
 3B7X,ASP\_49,3.69,0,-0.11,0  
 3D9H,GLU\_212,4.64,0.14,0,0  
 2FD4,ASP\_472,3.8,0,0,0  
 1M5I,ASP\_227,3.11,0.42,-1.11,0  
 2Z61,TYR\_202,10.21,0.07,-0.8,0.94  
 3K8J,LYS\_157,10.43,-0.07,0,0  
 3RHE,ARG\_47,11.45,-1.05,0,0  
 1CHD,GLU\_235,4.13,0.56,-0.92,0  
 1R6Y,HIS\_15,7.28,1.2,0,-0.42  
 1GQE,ARG\_10,11.73,-0.77,0,0  
 1D2K,ARG\_75,12.01,-0.49,0,0  
 1JT9,GLU\_117,3.83,0.52,-1.19,0  
 4H86,ASP\_3,3.32,0.14,-0.62,0  
 2FBI,ASP\_86,3.25,0.42,-0.97,0  
 3BB7,LYS\_119,10.08,-0.42,0,0  
 3I0C,LYS\_139,10.5,0,0,0  
 3LQE,ASP\_388,3.38,0.77,-1.19,0  
 1O0X,HIS\_154,7.2,0.77,0,-0.07  
 2YWJ,CYS\_183,10.22,0,1.22  
 2Q07,ARG\_480,12.43,-0.07,0,0  
 2P1W,CYS\_197,10.2,-0.45,1.32,0.33  
 1I6O,TYR\_135,13.27,0.07,0.8,2.4  
 2BLL,ASP\_637,3.68,0,-0.12,0  
 1SNT,LYS\_329,10.5,0,0,0  
 2EFK,GLU\_101,4.25,0.14,-0.39,0  
 1FHL,HIS\_159,7.09,0.8,0,-0.21  
 1RHS,CYS\_263,9.33,0,0,0.33  
 1QQL,ASP\_26,2.76,0.42,-1.46,0  
 2BLL,HIS\_627,6.43,0,0,-0.07  
 2P52,ASP\_205,1.42,0.56,-2.94,0  
 2E3S,TYR\_586,12.22,0.07,0.19,1.96  
 1SJ8,GLU\_538,4.78,0.28,0,0  
 4EZB,ASP\_90,3.22,0.14,-0.72,0  
 2GOV,ARG\_31,2.99,-0.21,0,0  
 3G9G,TYR\_213,12.49,0.37,-0.28,2.4  
 1O0X,ARG\_130,11.87,-0.63,0,0  
 1HF8,ASP\_153,3.8,0,0,0  
 4F85,HIS\_195,1.36,0.77,0,-5.91  
 1O5T,TYR\_100,9.48,1.44,-1.97,0  
 2OBI,GLU\_88,3.2,0.28,-1.58,0  
 4EZB,GLU\_54,4.57,0.07,0,0  
 4ETX,ASP\_227,2.67,0.7,-1.83,0  
 2W1R,CYS\_77,9.96,-0.98,0.02,1.93  
 1YTD,ASP\_11,1.76,0.56,-2.6,0  
 2NMU,TYR\_93,10,0,0,0  
 3HVM,GLU\_237,3.63,1.19,-2.06,0  
 1FKM,ASP\_609,4.01,0.21,0,0  
 3MTT,ARG\_478,12.08,-0.42,0,0  
 3LQE,ASP\_385,3.5,0.07,-0.37,0  
 3LH5,LYS\_753,10.5,0,0,0  
 3G59,HIS\_75,6.41,0.05,0,-0.14  
 1X7F,GLU\_28,11.94,-0.56,0,0  
 2PLQ,LYS\_125,10.43,-0.07,0,0  
 3ILC,ASP\_193,3.89,0.14,-0.05,0  
 2VGM,ASP\_327,3.94,0.14,0,0  
 2O8I,GLU\_164,4.57,0.07,0,0  
 1JB3,ARG\_100,12.29,-0.21,0,0  
 1EV8,HIS\_255,6.22,0,0,-0.28  
 2G7O,ASP\_108,3.87,0.07,0,0  
 4DNU,ASP\_156,2.97,0.49,-1.32,0  
 3M66,LYS\_308,10.5,0,0,0  
 2CIU,CYS\_128,8.61,-0.46,0,0.07  
 2F4Q,ASP\_53,3.17,0.42,-1.05,0  
 1R16,CYS\_154,9.84,-0.35,0,1.19  
 4EUG,ARG\_80,11.87,-0.63,0,0  
 1YG2,ASP\_15,3.22,0.35,-0.93,0  
 4AM1,ARG\_330,9.72,-2.92,0,0.13  
 3JV1,GLU\_113,4.5,0,0,0



1ZBP,GLU\_132,4.5,0,0,0  
3VJ8,ARG\_317,12.15,-0.35,0,0  
1IDK,HIS\_168,7.59,2.63,2.4,-3.94  
1ZBS,GLU\_184,4.02,0.07,-0.55,0  
1J74,ASP\_28,1.97,0.35,-2.19,0  
2EYI,LYS\_31,10.5,0,0,0  
3EX9,LYS\_25,10.15,-0.35,0,0  
1OLR,TYR\_154,9.9,0.14,-0.24,0  
3M7G,ARG\_241,12.5,0,0,0  
2P0Y,ARG\_292,12.29,-0.21,0,0  
2V4U,GLU\_475,4.27,0.14,-0.37,0  
1T95,LYS\_12,10.5,0,0,0  
1L2H,LYS\_27,9.8,-0.7,0,0  
2G9D,ASP\_232,3.61,0.21,-0.4,0  
1ZHV,ASP\_42,4.15,0.35,0,0  
1NAR,ASP\_215,4.08,0.35,-0.07,0  
3HVM,HIS\_20,3.16,0.58,0,-3.93  
3FTT,ASP\_18,2.85,0.56,-1.51,0  
1G8P,ARG\_260,11.28,-1.22,0,0  
1Q2Y,LYS\_7,10.36,-0.14,0,0  
2B78,HIS\_282,6.5,0,0,0  
3G59,TYR\_228,11.29,0,0,1.29  
2FZ4,GLU\_26,3.91,0.14,-0.73,0  
1R15,LYS\_266,10.5,0,0,0  
2GYZ,ARG\_57,12.43,-0.07,0,0  
2IA,ASP\_40,3.24,0.14,-0.7,0  
1KW4,LYS\_79,10.5,0,0,0  
1L3K,GLU\_9,3.46,0.35,-1.39,0  
1D2K,ASP\_62,3.46,0.58,0,-0.62,0  
1WXF,GLU\_21,4.18,0.07,-0.39,0  
2V5B,GLU\_136,4.09,0.28,-0.69,0  
3LD1,GLU\_320,3.97,0.21,-0.74,0  
2EFK,LYS\_44,10.5,0,0,0  
1MTZ,GLU\_54,4.64,0.14,0,0  
1WXQ,HIS\_326,6.53,0.03,0,0  
1R3D,GLU\_117,3.34,4.21,-2.97,-2.4  
2FL4,ARG\_13,11.66,-0.84,0,0  
3H13,LYS\_436,10.5,0,0,0  
2VGM,GLU\_360,4.91,0.28,0.13,0  
2XW5,HIS\_166,5.9,0.16,0,-0.07  
2CYG,GLU\_275,4.05,0.35,-0.8,0  
4ACJ,LYS\_711,10.43,-0.07,0,0  
3V55,GLU\_397,5.17,0.67,0,0  
3LH5,ASP\_699,3.96,0.21,-0.05,0  
1KCM,GLU\_86,3.81,1.23,-0.5,-1.42  
1UCH,ASP\_142,3.2,0.21,-0.81,0  
2A0J,GLU\_6,4.5,0,0,0  
2OKT,HIS\_309,6.5,0,0,0  
1I60,LYS\_44,10.5,0,0,0  
2XJ4,ARG\_219,12.22,-0.28,0,0  
1UXO,CYS\_74,12.71,-0.27,0.399  
2VAN,HIS\_134,7.44,1.08,0,-0.14  
2NRK,TYR\_8,9.64,0.07,-0.43,0  
4ESS,GLU\_153,4.01,0.35,-0.84,0  
1V6T,TYR\_75,12.98,0.07,0.51,2.4  
1DTO,ARG\_37,12.15,-0.35,0,0  
1A8Q,LYS\_156,10.5,0,0,0  
1AT0,ASP\_303,3.93,0.14,-0.01,0  
3C38,ARG\_67,11.33,-1.49,0,0.32  
1MD6,HIS\_31,6.5,0,0,0  
1SQW,GLU\_176,4.91,0.04,1,0  
3EZ7,TYR\_325,10,0,0,0  
2D7J,HIS\_67,6.92,0.56,0,-0.14  
1RWZ,HIS\_214,1.82,0,-2.09,-2.58  
1R2Z,GLU\_211,4.64,0.14,0,0  
2NRK,LYS\_158,10.29,-0.21,0,0  
1K95,LYS\_184,10.5,0,0,0  
2HRZ,GLU\_287,4.08,0.35,-0.77,0  
1K95,ARG\_154,11.94,-0.56,0,0  
2CIU,GLU\_191,4.5,0,0,0  
3UPD,ARG\_59,12.36,-0.14,0,0  
2XMX,ASP\_72,1.88,1.05,-2.97,0  
3CIV,ASP\_193,1.25,0.49,-3.03,0  
3AU3,ASP\_459,2.48,0.49,-1.8,0  
2V4X,GLU\_75,4.57,0.07,0,0  
1AIL,GLU\_66,4.64,0.14,0,0  
4EVF,CYS\_137,6.24,-2.98,0,0.21  
2YT4,LYS\_673,10.36,-0.14,0,0  
2EYI,GLU\_70,3.61,0.28,-1.17,0  
3ZSL,HIS\_223,3.96,0.16,0,-2.7  
2CL3,ASP\_57,3.97,0.98,-0.81,0  
1O5J,GLU\_60,2.87,0.63,-2.27,0  
2QK1,TYR\_498,13.48,0.28,0.8,2.4  
4ESS,LYS\_28,10.01,-0.49,0,0  
1LFP,ARG\_106,12.22,-0.28,0,0  
2FG1,TYR\_50,11.08,1.2,-1.5,1.38  
3GYW,ARG\_83,11.94,-0.56,0,0  
4D8L,ASP\_82,2.9,0.21,-1.11,0  
3M7G,LYS\_47,10.5,0,0,0  
2APL,TYR\_67,10.07,0.07,0,0  
2B0J,TYR\_267,9.71,0.21,-0.5,0  
2E0T,ARG\_204,11.94,-0.56,0,0  
3GW3,LYS\_231,10.08,-0.42,0,0  
1X7F,GLU\_201,5.51,1.01,0,0  
3GYW,HIS\_115,6.43,0,0,-0.07  
3L3P,GLU\_278,3.72,0.77,-1.55,0  
2ILR,CYS\_422,9.17,0,0,0.17  
1T3J,CYS\_681,9.07,0,0,0.07  
1GPP,TYR\_431,11.34,0,0,1.34  
3RJX,GLU\_252,4.71,0.28,-0.07,0  
1S7K,GLU\_102,4.28,0.14,-0.36,0  
2X4J,GLU\_117,5.53,1.05,-0.02,0  
1UAJ,HIS\_201,6.58,0.08,0,0  
1OXZ,GLU\_279,4.58,0.56,-0.48,0  
2RIK,ARG\_40,12.5,0,0,0  
1X04,ASP\_126,2.29,0.56,-2.07,0  
2PP6,GLU\_18,4.5,0,0,0  
1YW5,ARG\_15,13.36,-1.54,0,2.4  
3EVN,ASP\_105,3.79,0,-0.01,0  
1J79,GLU\_241,4.5,0,0,0  
4EVF,HIS\_264,6.5,0,0,0  
3AU3,HIS\_408,6.83,0.4,0,-0.07  
1PV5,CYS\_260,7.3,-1.84,0,0.14  
1JKS,GLU\_62,2.98,0.42,-1.94,0  
3N2T,ASP\_295,3.84,0.14,-0.1,0  
3GEC,ARG\_494,11.38,-1.12,0,0  
2BDV,GLU\_189,3.81,0.07,-0.76,0  
2AZP,ARG\_152,12.15,-0.35,0,0  
1R3F,ARG\_220,11.87,-0.63,0,0  
2OBI,ASP\_111,3.61,0,-0.19,0  
4EF5,GLU\_336,2.56,1.52,-2.57,-0.9  
1WYC,GLU\_128,4.58,0.28,-0.2,0  
3RFF,CYS\_6,10.69,-0.25,0.194  
1YM5,GLU\_271,3.98,0.28,-0.8,0  
1PBV,LYS\_244,10.01,-0.49,0,0  
2FM9,GLU\_122,3.85,0.15,-0.8,0  
1NFN,ARG\_32,11.8,-0.7,0,0  
3BQU,GLU\_238,2.57,1.19,-3.13,0  
1JKS,GLU\_81,2.59,0.49,-2.4,0  
3LJN,TYR\_273,7.9,0.72,-1.08,-1.74  
1X9G,TYR\_60,10,0,0,0  
1UOH,TYR\_15,10,0,0,0  
2G9D,ARG\_264,12.01,-0.49,0,0  
1NRI,ASP\_23,3.98,0.28,-0.1,0  
3G9T,GLU\_57,0.4,0.7,-2.4,-2.4  
1S17,ASP\_215,4.01,0.21,0,0  
3VJ8,ARG\_360,11.87,-0.63,0,0  
4AE7,TYR\_129,8.78,2.19,-2.22,-1.19  
3A7L,HIS\_31,6.65,0.36,0,-0.21  
1LTU,GLU\_65,4.57,0.07,0,0  
3HKX,CYS\_220,9.26,-0.29,0,0.55  
1O17,LYS\_143,10.29,-0.21,0,0  
2P0Y,HIS\_313,3.81,0.77,0,-3.46  
2EEY,LYS\_21,10.15,-0.35,0,0  
2YWJ,ASP\_96,2.62,0.42,-1.6,0  
2P52,LYS\_98,10.5,0,0,0  
4ETX,ARG\_172,12.59,-0.49,0,0.58  
2OPJ,ARG\_118,11.38,-1.12,0,0  
3BWT,ASP\_776,4.18,0.49,-0.11,0  
3ZRI,HIS\_-2,7.25,0.89,0,-0.14  
3HVM,GLU\_31,4.05,0.35,-0.8,0  
1AT0,LYS\_352,10.5,0,0,0  
3EZ7,TYR\_367,8.68,0.14,-1.45,0  
3GG6,ARG\_111,11.87,-0.63,0,0  
2EEY,ASP\_53,3.14,0.56,-1.22,0  
1PVT,GLU\_166,4.64,0.14,0,0  
3IVF,ARG\_118,12.22,-0.28,0,0  
1Q42,LYS\_73,10.29,-0.21,0,0  
2QVT,ARG\_116,12.08,-0.42,0,0  
3L3P,GLU\_481,4.78,0.28,0,0  
2EY,ASP\_527,4.5,0,0,0  
2BV9,GLU\_284,3.51,0.21,-1.2,0  
4ECC,LYS\_204,10.5,0,0,0  
3O16,ASP\_216,2.98,0.28,-1.1,0  
1AKO,GLU\_239,4.64,0.14,0,0  
2POL,ARG\_264,12.08,-0.42,0,0  
1LZL,ASP\_22,3.09,0.49,-1.21,0  
2X4L,ASP\_109,3.21,0.21,-0.8,0  
1RKA,HIS\_35,6.43,0,0,-0.07  
1J79,ARG\_119,12.01,-0.49,0,0  
3MTT,GLU\_473,4.24,0.21,-0.47,0  
2OOK,CYS\_125,11.49,0,0,2.49  
1YG2,TYR\_111,9.87,0.14,-0.36,0.1  
3EVN,LYS\_15,10.36,-0.14,0,0  
2NRK,GLU\_76,4.05,0.35,-0.8,0  
2YYO,LYS\_9,10.29,-0.21,0,0  
2VGM,GLU\_91,4.57,0.07,0,0  
2IRM,HIS\_131,6.57,0.07,0,0  
1Z3X,LYS\_109,10.43,-0.07,0,0  
3B7X,LYS\_60,10.5,0,0,0  
3RFF,GLU\_146,3.66,0.35,-1.19,0  
3VJ8,GLU\_202,4.5,0,0,0  
2FZ4,ASP\_48,1.44,0.84,-3.2,0  
3F6M,ARG\_76,11.66,-0.84,0,0  
2HXB,GLU\_145,3.56,0.42,-1.36,0  
1LFP,LYS\_137,9.73,-0.77,0,0  
2FG1,TYR\_75,10,0,0,0  
3UW9,ARG\_320,12.15,-0.35,0,0  
1V43,GLU\_347,4.5,0,0,0  
1MML,GLU\_233,4.64,0.14,0,0  
3L3P,ASP\_452,3.35,0.49,-0.94,0  
2Q13,HIS\_100,7.23,0.8,0,-0.07  
2XJ4,GLU\_83,2.59,0.49,-2.4,0  
3K9I,GLU\_142,4.5,0,0,0  
1OST,LYS\_253,10.22,-0.28,0,0  
3MIX,ASP\_544,3.8,0,0,0  
2ZCX,ARG\_211,11.94,-0.56,0,0  
3ULX,ARG\_138,12.53,-1.07,0,1.11  
3T57,GLU\_282,3.37,0.42,-1.55,0  
3IPZ,CYS\_97,5.15,-4,0,0.14  
1SNT,TYR\_377,10.52,0.14,-0.15,0.53  
2IRM,LYS\_19,10.5,0,0,0  
3Q6L,LYS\_10,10.22,-0.28,0,0  
2NRK,GLU\_123,4.5,0,0,0  
2OEW,TYR\_39,10.74,0.14,-0.67,1.27  
3BPP,ARG\_43,11.66,-0.84,0,0  
1PVT,ASP\_52,3.8,0,0,0  
1L2H,ASP\_86,3.17,0.56,-1.19,0  
3EZ7,GLU\_23,4.5,0,0,0  
3M16,LYS\_8,9.8,-0.7,0,0  
3ZTA,GLU\_61,3.87,0.28,-0.91,0  
3T8R,ASP\_78,1.44,0.42,-2.78,0  
3CNU,ASP\_81,1.61,0.91,-3.1,0  
1SIG,ARG\_281,11.87,-0.63,0,0  
4FZR,GLU\_37,4.64,0.14,0,0  
2AZL,LYS\_103,10.5,0,0,0  
3VJ8,TYR\_220,10.35,1.05,-0.69,0  
1R7J,TYR\_28,10,0,0,0  
3EVP,GLU\_164,4.5,0,0,0  
3CIV,ARG\_170,13.48,-1.42,0.24  
4FCU,ASP\_240,1.28,0.77,-3.29,0  
3IVF,ASP\_341,1.23,0.49,-3.06,0  
1LN4,LYS\_80,10.22,-0.28,0,0  
1XKR,ARG\_94,12.22,-0.28,0,0  
1RSS,ASP\_126,2.76,0.56,-1.6,0  
3BA1,LYS\_267,10.5,0,0,0  
2E3C,ASP\_196,3.19,0.35,-0.96,0  
2FPN,GLU\_114,4.64,0.14,0,0  
2H14,ASP\_302,2.57,0.84,-2.07,0  
3IUS,ASP\_130,3.87,0.07,0,0  
2W2S,LYS\_187,9.73,-0.77,0,0  
2O0K,ARG\_84,12.5,0,0,0  
1UAJ,LYS\_238,10.5,0,0,0  
1LN4,GLU\_36,4.57,0.07,0,0  
3VJ8,LYS\_92,10.29,-0.21,0,0  
3TIR,LYS\_17,10.5,0,0,0  
1QQH,GLU\_177,4.64,0.14,0,0  
3BJV,LYS\_109,10.5,0,0,0  
3V55,TYR\_434,11.08,0.64,0.044  
3PM2,ASP\_83,4.01,0.21,0,0  
2IRM,ARG\_216,12.24,-1.59,0,1.33  
3M70,GLU\_263,4.17,0.28,-0.61,0  
2O8P,GLU\_77,4.57,0.07,0,0  
1DCF,CYS\_32,9.52,-0.06,0.58  
3ON1,GLU\_24,3.84,0.14,-0.8,0  
2EYI,HIS\_247,4.06,0.8,0,-3.24  
2BL,GLU\_552,2.87,0.49,-2.12,0  
3PBH,HIS\_110,3.03,0.6,0,-4.07  
2Q12,ASP\_157,3.69,0,-0.11,0  
3FTT,HIS\_120,6.5,0,0,0  
1J8B,GLU\_90,4.92,0.42,0,0  
1WRU,GLU\_197,4.5,0,0,0  
2PPN,CYS\_22,9.17,-0.26,0.43  
3BWT,LYS\_796,10.43,-0.07,0,0  
1P4X,GLU\_182,4.5,0,0,0  
1YW5,HIS\_156,3.15,0.08,1.1,-4.53  
3LOD,GLU\_98,3.45,0.86,-1.91,0  
2POL,GLU\_216,4.05,0.35,-0.8,0  
1GVP,ARG\_21,12.5,0,0,0  
2QK1,LYS\_551,10.43,-0.07,0,0  
2OYZ,GLU\_80,4.57,0.07,0,0  
1O0X,GLU\_134,3.93,0.42,-0.99,0  
3B7X,ASP\_73,3.06,0.28,-1.02,0  
1NWA,CYS\_13,8.63,-4.07,2.28,1.42  
2BAA,LYS\_54,10.22,-0.28,0,0  
2X4G,GLU\_96,4.57,0.07,0,0  
2D7U,HIS\_83,6.36,0,0,-0.14  
1PNE,ARG\_135,11.45,-1.05,0,0  
3LJI,HIS\_178,3.98,0,0,-2.52  
3PZ9,ARG\_63,12.29,-0.21,0,0  
3BWT,GLU\_599,3.15,1.05,-2.39,0  
1RHS,GLU\_46,2.52,0.42,-2.4,0  
2QHT,ARG\_186,12.15,-0.35,0,0  
3B21,GLU\_86,3.72,0.42,-1.2,0  
3H04,TYR\_6,9.51,0.07,-0.56,0  
3NBI,TYR\_85,9.94,0.07,-0.13,0

3IL3,GLU\_199,4.5,0,0,0  
3IRA,GLU\_8,4.71,0.21,0,0  
3F5D,HIS\_115,5.28,0.8,0,-2.02  
1R5S,LYS\_131,10.22,-0.28,0,0  
4E8B,GLU\_90,4.5,0,0,0  
1Q2Y,LYS\_13,10.15,-0.35,0,0  
1N81,LYS\_121,10.22,-0.28,0,0  
3BZT,LYS\_255,10.22,-0.28,0,0  
4DNU,ARG\_217,12.22,-0.28,0,0  
2WB8,HIS\_525,6.5,0,0,0  
1R3D,LYS\_252,10.5,0,0,0  
1AD6,CYS\_438,8.39,-0.75,0,0.14  
2Q07,ARG\_399,12.22,-0.28,0,0  
3F5D,LYS\_140,10.5,0,0,0  
3US6,GLU\_36,4.5,0,0,0  
3GE9,GLU\_210,5.45,0.95,0,0  
1Z9L,GLU\_113,3.42,0.56,-1.64,0  
2GKG,LYS\_94,10.29,-0.21,0,0  
3I82,HIS\_75,7.36,1.07,0,-0.21  
1QVI,TYR\_242,10,0,0,0  
2YWJ,GLU\_114,4.64,0.14,0,0  
3OA7,TYR\_572,10,0,0,0  
3HXK,ARG\_17,12.5,0,0,0  
1H09,ARG\_110,12.08,-0.42,0,0  
3CRM,ARG\_59,12.15,-0.35,0,0  
2XMZ,HIS\_103,7.16,0.8,0,-0.14  
2E3S,LYS\_470,10.22,-0.28,0,0  
3HVV,ASP\_294,4.15,0.35,0,0  
1SJ8,ARG\_692,12.01,-0.49,0,0  
2F9F,ARG\_21,12.01,-0.49,0,0  
3M66,ASP\_197,3.8,0,0,0  
2YX0,ARG\_90,12.03,-1.63,0,1.16  
2A6B,ASP\_186,3.26,0.35,-0.89,0  
3DTE,ARG\_253,12.36,-0.14,0,0  
1WXF,ARG\_134,11.66,-0.84,0,0  
1X1E,ARG\_95,12.01,-0.49,0,0  
1KCM,TYR\_155,12.96,0.28,0.28,2.4  
1SIG,ASP\_360,3.31,0.21,-0.7,0  
3CXS,LYS\_166,10.43,-0.07,0,0  
3DZ1,ARG\_154,11.73,-0.77,0,0  
3M16,ARG\_124,12.08,-0.42,0,0  
3M7D,ARG\_76,13.08,-1.47,0,2.05  
1EDG,ARG\_358,12.29,-0.21,0,0  
1SQH,GLU\_105,4.17,0.47,-0.8,0  
4AM1,TYR\_134,13.48,0.28,0.8,2.4  
2FPN,GLU\_178,4.57,0.07,0,0  
3NOK,ARG\_27,12.5,0,0,0  
1P2F,LYS\_4,10.43,-0.07,0,0  
2CXC,GLU\_79,3.98,0.14,-0.66,0  
1YTD,ARG\_24,12.29,-0.21,0,0  
1O3X,LYS\_226,10.43,-0.07,0,0  
2ZCO,GLU\_65,3.91,0.21,-0.8,0  
3GOZ,ASP\_69,3.4,0.14,-0.54,0  
2QEV,TYR\_47,12.89,0.07,0.42,2.4  
1WJG,GLU\_25,4.27,0.28,-0.51,0  
4GCO,ARG\_225,12.29,-0.21,0,0  
1A8Q,ASP\_137,3.11,0.35,-1.04,0  
1ZCU,HIS\_241,6.39,0.1,0,-0.21  
3DTE,ASP\_101,3.87,0.07,0,0  
1AK1,ASP\_95,3.09,0.42,-1.13,0  
2WZ9,GLU\_81,4.5,0,0,0  
2RJD,TYR\_319,13.78,0.58,0.8,2.4  
3ETU,LYS\_214,10.43,-0.07,0,0  
1YTD,ARG\_98,12.01,-0.49,0,0  
1V43,ASP\_359,3.48,0.49,-0.81,0  
1XTZ,ARG\_219,12.22,-0.28,0,0  
3EIZ,ASP\_157,3.13,0.21,-0.88,0  
3O16,GLU\_24,4.57,0.07,0,0  
1MSI,ASP\_147,4.2,0.7,-0.3,0  
1T6L,LYS\_237,10.43,-0.07,0,0  
3HVV,LYS\_282,9.66,-0.84,0,0  
3EX9,ARG\_67,11.45,-1.05,0,0  
2EJX,ARG\_128,12.22,-0.28,0,0  
1PGV,TYR\_378,9.81,0,-0.19,0  
3FK5,ASP\_200,3.92,0.21,-0.09,0  
1O6D,LYS\_71,9.8,-0.7,0,0  
2O8P,GLU\_147,4.5,0,0,0  
1RKA,LYS\_193,10.5,0,0,0  
2G7O,HIS\_93,6.43,0,0,-0.07  
3SMD,TYR\_100,13.6,0.67,0.53,2.4  
4FCU,GLU\_40,4.47,0,-0.03,0  
2YT4,GLU\_512,4.24,0.54,-0.8,0  
2ZCX,GLU\_85,3.53,0.28,-1.25,0  
1NIJ,GLU\_167,4.5,0,0,0  
1DVO,GLU\_158,2.52,0.49,-2.47,0  
3U0V,LYS\_222,10.43,-0.07,0,0  
1RWZ,LYS\_147,10.43,-0.07,0,0  
3GW3,ARG\_37,10.7,-2.2,0,0.4  
3K9I,ARG\_85,12.22,-0.28,0,0  
4EUG,GLU\_157,2.66,0.56,-2.4,0  
3N2T,LYS\_240,10.5,0,0,0  
3L7N,LYS\_63,10.5,0,0,0  
1AM2,CYS\_79,10.73,-0.15,0.19,1.69  
2IDC,GLU\_88,3.68,0.84,-1.66,0  
3QKY,TYR\_82,10.8,0.46,0.34  
3P2F,CYS\_67,10.14,-0.39,-0.54,2.07  
2OBI,GLU\_65,4.5,0,0,0  
4DVD,ASP\_83,3.55,0.49,-0.74,0  
3M16,ARG\_120,12.15,-0.35,0,0  
1XIPLYS\_332,10.22,-0.28,0,0  
2CBE,LYS\_112,10.22,-0.28,0,0  
2ATR,GLU\_106,4.5,0,0,0  
3BA1,GLU\_266,4.5,0,0,0  
1WYC,GLU\_176,3.06,0.42,-1.86,0  
2O4D,ASP\_116,2.62,0.56,-1.74,0  
2AXO,TYR\_178,10.97,0.79,-0.61,0.8  
1ES9,GLU\_56,4.01,0.86,-1.35,0  
1D2K,LYS\_117,10.01,-0.49,0,0  
1SJJ,CYS\_67,8.37,-0.77,0.014  
3RAZ,GLU\_145,3.56,0.21,-1.15,0  
3IU5,GLU\_63,4.5,0,0,0  
3EVP,ASP\_110,3.99,0.21,-0.02,0  
3AUF,CYS\_85,11.92,-0.25,0.317  
2EHG,TYR\_35,10.07,0.07,0,0  
1DOV,GLU\_170,4.62,0.35,-0.23,0  
2NRK,ARG\_27,3.98,0.28,-0.8,0  
3H13,LYS\_474,10.22,-0.28,0,0  
2Q07,ARG\_276,12.5,0,0,0  
1QQE,LYS\_136,10.15,-0.35,0,0  
1YR6,TYR\_204,10,0,0,0  
1Q46,GLU\_151,4.5,0,0,0  
2NRR,ARG\_362,13.1,-0.73,0,1.33  
3ODJ,HIS\_60,0.23,0.11,-1.79,-4.59  
1G8P,LYS\_265,10.43,-0.07,0,0  
2FGG,GLU\_50,4.83,0.28,0.05,0  
1QQE,ARG\_268,12.43,-0.07,0,0  
2VYG,GLU\_159,4.5,0,0,0  
1YLN,TYR\_179,10.07,0.12,-0.05,0  
2B6P,TYR\_177,10,0,0,0  
2Q13,HIS\_59,6.8,0.3,0,0  
3EX9,LYS\_40,10.5,0,0,0  
3G9T,ASP\_211,3.08,0.42,-1.14,0  
3H9W,ASP\_111,1.29,0.91,-3.42,0  
2OEW,ASP\_325,3.69,0.14,-0.25,0  
3V1Q,ARG\_647,12.15,-0.35,0,0  
3CAN,LYS\_29,10.36,-0.14,0,0  
2PWQ,GLU\_47,3.87,0.56,-1.19,0  
2JEO,ARG\_149,11.38,-1.12,0,0  
2NYC,GLU\_237,4.64,0.14,0,0  
3JV1,LYS\_153,10.5,0,0,0  
1L2F,ASP\_337,3.11,0.42,-1.11,0  
2V4U,LYS\_319,10.5,0,0,0  
3PZ9,CYS\_201,9.99,-2.53,2.4,1.12  
2BCF,ARG\_238,11.8,-0.7,0,0  
3RNV,HIS\_454,7.19,0.69,0,0  
1K95,ARG\_172,11.66,-0.84,0,0  
3TRE,TYR\_74,11.08,0.49,-0.8,1.39  
1MIX,HIS\_255,6.41,0.05,0,-0.14  
3HVV,ASP\_191,3.48,0.63,-0.95,0  
1YM5,GLU\_211,4.74,1.33,-1.09,0  
3T5B,GLU\_92,4.57,0.35,-0.28,0  
3CAN,TYR\_98,11.07,1.07,0,0  
2O0K,LYS\_51,10.5,0,0,0  
3F5D,GLU\_158,3.06,0.84,-2.28,0  
4FZR,ARG\_198,12.36,-0.14,0,0  
2BDD,LYS\_121,10.29,-0.21,0,0  
2IDC,LYS\_17,10.5,0,0,0  
4ANN,HIS\_54,7.02,0.8,0,-0.28  
3OIP,LYS\_198,10.43,-0.07,0,0  
1V6T,ARG\_126,12.01,-0.49,0,0  
2PIM,ASP\_46,3.78,0,-0.02,0  
2IRM,ARG\_219,11.87,-0.63,0,0  
1T95,LYS\_71,10.5,0,0,0  
3ANJ,TYR\_82,10,0,0,0  
1X9G,CYS\_87,7.08,-3.42,-0.66,2.16  
2EYI,ARG\_46,11.87,-0.63,0,0  
3M16,GLU\_154,0.28,2.15,-4.56,-1.81  
3GS3,ASP\_201,3.18,0.42,-1.04,0  
1HF8,GLU\_91,3.91,0.21,-0.8,0  
2POL,LYS\_268,10.5,0,0,0  
2POY,ARG\_333,12.43,-0.07,0,0  
2FD5,GLU\_122,4.64,0.14,0,0  
3LD1,ARG\_300,12.22,-0.28,0,0  
3ZRI,HIS\_-5.644,0.08,0,-0.14  
3JZN,GLU\_394,3.77,0.07,-0.8,0  
1OLR,ASP\_27,3.34,0.35,-0.81,0  
3P51,GLU\_123,4.5,0,0,0  
2FM9,LYS\_77,10.5,0,0,0  
2ZOW,GLU\_44,3.91,0.21,-0.1,0.8  
2RIK,ASP\_266,2.94,0.07,-0.93,0  
2IQT,GLU\_176,0.92,3.22,-1.04,-5.76  
3R87,TYR\_58,10.04,0,0,0.04  
2CXC,LYS\_114,10.43,-0.07,0,0  
1SJJ,ASP\_54,3.87,0.07,0,0  
2EJB,CYS\_90,11.31,0,0,2.31  
2NSN,GLU\_106,4.78,0.28,0,0  
1ILW,TYR\_103,10.68,0.63,0,0.05  
3TOW,LYS\_115,10.22,-0.28,0,0  
3ASA,LYS\_2,10.5,0,0,0  
1J7G,LYS\_44,10.5,0,0,0  
3KT9,ASP\_76,4.08,0.28,0,0  
2FXT,TYR\_274,10.29,0.29,0,0  
2Q5X,TYR\_725,10.17,0.17,0,0  
1NIJ,ARG\_278,12.01,-0.49,0,0  
3JRT,GLU\_39,3.98,0.28,-0.8,0  
1WXQ,LYS\_259,10.43,-0.07,0,0  
3RHE,TYR\_104,13.34,0.14,0.8,2.4  
2CN1,GLU\_133,4.47,0,-0.03,0  
1P2F,LYS\_169,10.43,-0.07,0,0  
1QQH,LYS\_162,10.5,0,0,0  
3ASA,ARG\_22,12,-0.5,0,0  
2OQG,TYR\_421,10,0,0,0  
3GS3,ARG\_83,11.31,-1.19,0,0  
2ZQ5,ASP\_9,3.92,0.21,-0.09,0  
2V5B,LYS\_85,10.15,-0.35,0,0  
2HP7,GLU\_177,4.4,0.7,-0.8,0  
3CX2,HIS\_225,6.68,0.25,0,-0.07  
1DVO,GLU\_45,4.17,0.07,-0.4,0  
3DTE,ASP\_42,3.8,0,0,0  
2YWX,CYS\_3,9.76,-0.25,0,1.01  
2FZ4,ARG\_229,4.59,0.0,0.09,0  
2FBI,ARG\_119,12.5,0,0,0  
1EDG,LYS\_94,10.36,-0.14,0,0  
2CE6,LYS\_17,10.15,-0.35,0,0  
1Q2Y,HIS\_134,4.29,0.08,1.67,-3.96  
2V4U,LYS\_391,10.5,0,0,0  
2GZQ,GLU\_141,3.99,0.21,-0.72,0  
2F8H,GLU\_13,4.5,0,0,0  
3COU,ASP\_63,2.98,0.77,-1.59,0  
3G9G,LYS\_131,10.36,-0.14,0,0  
1XTZ,HIS\_261,6.82,0.39,0,-0.07  
2EFK,GLU\_108,4.57,0.07,0,0  
3CGW,GLU\_79,3.91,0.07,-0.66,0  
2F8H,GLU\_13,4.5,0,0,0  
4ECC,LYS\_9,10.36,-0.14,0,0  
3V46,LYS\_385,10.36,-0.14,0,0  
4FH3,ARG\_111,12.29,-0.21,0,0  
2E3S,LYS\_581,10.5,0,0,0  
3ILC,GLU\_184,4.5,0,0,0  
2RIS,GLU\_45,3.27,0.35,-1.57,0  
1JT9,GLU\_259,1.86,0.56,-3.2,0  
3V3T,ARG\_268,12.15,-0.35,0,0  
2O8I,LYS\_120,10.5,0,0,0  
2B3M,HIS\_84,6.76,0.61,0,-0.35  
1PGV,GLU\_287,4.57,0.07,0,0  
3CBN,CYS\_117,12.13,0,0,3.13  
1X7F,TYR\_161,10.58,0.14,-0.56,0.99  
1U3Y,GLU\_338,4.45,0.14,-0.19,0  
2Q98,ARG\_125,12.43,-0.07,0,0  
4E9E,ARG\_546,11.73,-0.77,0,0  
2GZR,GLU\_139,4.2,0.98,-1.28,0  
2B61,CYS\_46,12.86,0,0,3.86  
3G9G,CYS\_202,9.37,-0.15,0,0.52  
1L2F,LYS\_156,10.08,-0.42,0,0  
4EVF,ARG\_83,11.94,-0.56,0,0  
3N2T,GLU\_304,4.5,0,0,0  
3I4T,TYR\_146,10.88,0.35,-1.86,2.4  
1QYI,LYS\_170,10.5,0,0,0  
1Z9L,ASP\_101,3.2,0.56,-1.15,0  
1X1E,GLU\_178,3.87,0.14,-0.77,0  
3RFY,TYR\_283,11.81,1.92,-0.12,0.01  
1W24,TYR\_165,10.21,0.21,0,0  
3ASA,HIS\_190,6.5,0,0,0  
2F4Q,TYR\_150,9.2,0.07,-0.87,0  
2FL4,TYR\_102,8.93,0.07,-1.43,0.28  
2Q5X,ARG\_779,11.73,-0.77,0,0  
2ZCO,LYS\_113,10.5,0,0,0  
3FHF,ARG\_87,12.36,-0.14,0,0  
3UPD,LYS\_253,10.36,-0.14,0,0  
3GT0,TYR\_178,10,0,0,0  
3BCY,LYS\_78,10.5,0,0,0  
1P2F,ARG\_113,13.23,-1.43,0,2.16  
2VGM,LYS\_193,10.43,-0.07,0,0  
3ON1,ASP\_43,2.78,0.28,-1.3,0  
2I88,ASP\_459,3.35,0.42,-0.87,0  
1O5T,ARG\_298,12.5,0,0,0  
4DBX,LYS\_280,10.5,0,0,0  
4ETX,ARG\_161,11.65,-1.09,0,0.24  
157K,ASP\_137,3.24,0.49,-1.05,0  
2D8N,GLU\_25,4.57,0.07,0,0  
2AZP,HIS\_101,6.47,0.04,0,-0.07  
1OGL,HIS\_83,1.99,0.54,-1.33,-3.72  
4F3J,HIS\_135,6.29,0,0,-0.21  
3F6F,LYS\_28,10.43,-0.07,0,0  
1LN4,LYS\_89,10.5,0,0,0  
3K8J,GLU\_131,4.57,0.07,0,0

4E8B,CYS\_216,-3.41,0,0,41  
 4EVF,GLU\_109,4.5,0,0,0  
 1V43,GLU\_351,4.57,0.07,0,0  
 4F85,ASP\_166,3.87,0.07,0,0  
 1U3Y,TYR\_348,11.8,0.07,-0.67,2.4  
 3K9I,ASP\_140,3.69,0,-0.11,0  
 3A7L,GLU\_89,3.91,0.56,-1.15,0  
 3M70,HIS\_109,3.62,0.62,-1.24,-2.25  
 1OTM,ASP\_112,3.14,0.42,-1.08,0  
 2HRZ,LYS\_279,10.5,0,0,0  
 3CX2,LYS\_218,10.5,0,0,0  
 4FD6,TYR\_113,9.72,0.07,-0.35,0  
 1BGF,HIS\_100,6.71,0.28,0,-0.07  
 2Q98,GLU\_120,4.92,0.42,0,0  
 1WPA,HIS\_499,6.43,0,-0.07  
 1X7F,GLU\_320,2.53,1.48,-3.45,0  
 1UOH,CYS\_11,8.88,-0.86,0,0.74  
 2PGX,GLU\_117,4.92,2.04,-1.83,0.22  
 3M66,LYS\_189,10.36,-0.14,0,0  
 3Q6L,ARG\_107,9.12,-3.38,0,0  
 2R51,HIS\_173,7.16,0.8,0,-0.14  
 4D8L,LYS\_129,10.29,-0.21,0,0  
 1XTZ,LYS\_137,10.15,-0.35,0,0  
 1HUF,LYS\_114,10.22,-0.28,0,0  
 1SI7,LYS\_81,10.22,-0.28,0,0  
 3I4T,ASP\_41,3.94,0.14,0,0  
 1XTZ,ARG\_172,12.01,-0.49,0,0  
 4F85,ARG\_215,12.15,-0.35,0,0  
 4D8L,HIS\_65,7.19,0.69,0,0  
 1JYH,GLU\_31,4.85,0.35,0,0  
 2JKF,ASP\_109,3.42,0.21,-0.59,0  
 1TJE,LYS\_33,10.5,0,0,0  
 3UAH,TYR\_299,9.26,0.34,-1.08,0  
 1J74,CYS\_69,11.51,-0.01,0.99,1.54  
 1KCM,TYR\_94,12.39,1.17,-0.3,1.53  
 3GS9,ARG\_99,11.73,-0.77,0,0  
 3U2R,ASP\_107,3.72,0,-0.08,0  
 1F09,TYR\_130,10.07,0.07,0,0  
 2ZCO,GLU\_242,3.58,0.68,-1.6,0  
 3O16,HIS\_107,1.7,0,0,-4.8  
 2IIA,CYS\_34,7.71,-1.28,0,0  
 3UAH,TYR\_397,8.48,0.11,0,-1.63  
 1RI5,GLU\_207,4.1,0.21,-0.61,0  
 3V3T,GLU\_220,4.57,0.07,0,0  
 2FPN,ARG\_56,12.15,-0.35,0,0  
 3JZ9,GLU\_452,4.57,0.07,0,0  
 2FM9,GLU\_170,3.98,0.28,-0.8,0  
 3D9H,CYS\_175,10.5,-0.22,0,1.72  
 1QQH,ASP\_122,2.65,0.84,-1.99,0  
 1XFK,HIS\_83,4.22,0.6,0,-2.89  
 1BKB,GLU\_122,4.57,0.07,0,0  
 2B02,ARG\_430,11.8,-0.7,0,0  
 1BKR,LYS\_108,10.29,-0.21,0,0  
 1ZBM,LYS\_87,10.15,-0.35,0,0  
 3PM2,ASP\_159,3.97,0.21,-0.04,0  
 3VHJ,TYR\_131,11.46,0.21,-1.4,2.65  
 4ACJ,ASP\_739,3.42,0.42,-0.8,0  
 2OOK,TYR\_132,10,0,0,0  
 1XDZ,GLU\_129,3.12,0.86,-2.25,0  
 1GSZ,LYS\_191,10.43,-0.07,0,0  
 3LD1,GLU\_17,3.39,0,-1.11,0  
 1OIS,ASP\_171,3.63,0.63,-0.8,0  
 1DVO,LYS\_39,10.5,0,0,0  
 2V4U,HIS\_526,3.64,0.07,0,-2.93  
 2V81,ASP\_54,3.88,0.14,-0.06,0  
 2OBI,LYS\_118,10.15,-0.35,0,0  
 3CCY,TYR\_79,10,0,0,0  
 1UOH,LYS\_116,10.36,-0.14,0,0  
 3U2A,ASP\_24,4.01,0.21,0,0  
 2RJD,ASP\_384,3.31,0.42,-0.91,0  
 3BWT,TYR\_676,10,0,0,0  
 1SUU,ARG\_776,11.66,-0.84,0,0  
 2BLL,GLU\_575,4.1,0.28,-0.68,0  
 2AXO,TYR\_199,12.51,0.74,0,1.77  
 1MTZ,HIS\_35,4.74,4.27,0.68,-6.71  
 3U2R,LYS\_114,10.5,0,0,0  
 1ZBM,ARG\_224,12.15,-0.35,0,0  
 2I6I,CYS\_96,0.47,-8.85,-1.6,1.91  
 1XTZ,ARG\_189,12.84,-2.06,0,2.4  
 1YTD,ARG\_254,12.08,-0.42,0,0  
 2D0A,HIS\_152,4.24,0.03,0,-2.29  
 1R3F,GLU\_296,4.05,0.35,-0.8,0  
 3FTT,CYS\_178,8.07,-1.05,0,0.12  
 1JKS,GLU\_70,3.91,0.21,-0.8,0  
 3P28,GLU\_124,4.85,0.35,0,0  
 2B0J,GLU\_222,4.57,0.07,0,0  
 1QZN,GLU\_131,4.71,0.21,0,0  
 2EHG,ARG\_129,12.22,-0.28,0,0  
 2AXO,ASP\_186,3.02,0.14,-0.92,0  
 3P28,LYS\_218,10.5,0,0,0  
 2GS5,HIS\_42,6.43,0,-0.07  
 1PVT,GLU\_164,2.27,0.42,-2.65,0  
 2B78,ASP\_274,4.01,0.21,0,0  
 1TD6,TYR\_258,9.74,0,-0.26,0  
 3G9T,ASP\_130,3.85,0.21,-0.16,0  
 1DUP,LYS\_77,10.43,-0.07,0,0  
 1U7U,ARG\_405,12.22,-0.28,0,0  
 1EV8,ASP\_40,4.28,0.49,-0.01,0  
 3GS9,ARG\_176,13.54,-1.7,0,2.74  
 1R9W,LYS\_259,10.43,-0.07,0,0  
 1AK1,LYS\_274,10.22,-0.28,0,0  
 3E5T,LYS\_182,9.87,-0.63,0,0  
 2FD5,HIS\_127,3.53,0.06,0,-3.03  
 1WXF,LYS\_241,10.29,-0.21,0,0  
 2R51,LYS\_55,10.5,0,0,0  
 4E9E,HIS\_557,6.36,0,0,-0.14  
 1SJ8,ARG\_634,10.02,-2.48,0,0  
 2PGX,LYS\_80,10.43,-0.07,0,0  
 4FLE,TYR\_153,10.12,0,-0.4,0.52  
 2E35,HIS\_453,6.5,0,0,0  
 4H4J,LYS\_153,10.5,0,0,0  
 1XDZ,GLU\_49,4.67,0.21,-0.04,0  
 2WB3,ASP\_374,3.71,0,-0.09,0  
 2CXC,LYS\_126,9.73,-0.77,0,0  
 1Y0K,GLU\_55,4.57,0.07,0,0  
 3PZ9,ASP\_378,1.39,0.7,-3.12,0  
 4GCO,GLU\_245,4.5,0,0,0  
 3HUE,GLU\_69,4.44,0.21,-0.27,0  
 1NRI,GLU\_187,3.74,0.35,-1.11,0  
 1CBY,GLU\_120,4.5,0,0,0  
 1ZBM,ARG\_126,12.15,-0.35,0,0  
 2V4U,ARG\_376,11.59,-0.91,0,0  
 1V43,ASP\_324,4.15,0.35,0,0  
 1GPP,LYS\_173,10.5,0,0,0  
 1Q8B,GLU\_41,3.91,0.21,-0.8,0  
 1DOV,LYS\_178,10.5,0,0,0  
 2OB5,ASP\_69,3.7,0.7,-0.8,0  
 1WYC,GLU\_310,3.5,0.28,-1.27,0  
 2QRX,TYR\_16,11.08,0.07,-0.8,1.81  
 3I4T,GLU\_138,4.5,0,0,0  
 3E7P,GLU\_131,5.08,0.35,0.23,0  
 1MJS,HIS\_248,6.5,0,0,0  
 1G8P,ARG\_299,11.96,-0.54,0,0  
 1T6L,GLU\_270,4.5,0,0,0  
 3LJN,TYR\_202,10.4,0.07,-0.42,0.75  
 3B21,GLU\_89,3.46,0.56,-1.6,0  
 1BN6,ARG\_215,12.78,-0.7,0.98  
 4FCU,GLU\_208,2.42,0.56,-2.64,0  
 1KN3,LYS\_62,10.43,-0.07,0,0  
 1JYH,LYS\_108,10.43,-0.07,0,0  
 1OST,LYS\_366,10.5,0,0,0  
 3JSN,ARG\_212,11.41,-1.09,0,0  
 2OBI,LYS\_135,9.59,-0.91,0,0  
 3ONT,ASP\_71,2.46,0.56,-1.91,0  
 1PBV,GLU\_95,4.64,0.14,0,0  
 1YR6,LYS\_93,9.66,-0.84,0,0  
 3CGW,HIS\_96,8.46,3.3,2.98,-4.32  
 1T3Y,GLU\_8,4.5,0,0,0  
 1SJY,GLU\_23,4.5,0,0,0  
 1W7B,ARG\_68,10.47,-3.28,0,1.25  
 2X4G,CYS\_59,9,0,0,0  
 3DHN,HIS\_223,6.43,0,-0.07  
 1QYI,LYS\_95,10.15,-0.35,0,0  
 1NAR,LYS\_153,10.43,-0.07,0,0  
 2GYZ,ASP\_91,3.58,0,-0.22,0  
 3ULX,ARG\_62,12.22,-0.28,0,0  
 2Q99,ARG\_372,12.01,-0.49,0,0  
 3C2E,CYS\_54,10.28,-3.21,1.96,2.53  
 3JZN,TYR\_148,10.65,0.87,-0.22,0  
 1A8Q,ARG\_111,11.24,-1.26,0,0  
 2IIA,TYR\_15,13.39,0.14,0.79,2.46  
 3HKX,ASP\_194,3.87,0.07,0,0  
 2QRX,ARG\_63,12.08,-0.42,0,0  
 2HNG,GLU\_27,3.01,0.91,-2.4,0  
 3OIP,ARG\_122,11.73,-0.77,0,0  
 2JHY,LYS\_141,9.8,-0.7,0,0  
 2WZ9,ARG\_27,12.15,-0.35,0,0  
 4H86,ASP\_13,3.94,0.14,0,0  
 1SJJ,LYS\_152,10.36,-0.14,0,0  
 2DFL,ARG\_72,12.5,0,0,0  
 3L3P,LYS\_465,10.43,-0.07,0,0  
 4ANN,LYS\_165,10.29,-0.21,0,0  
 2DG7,ARG\_127,12.08,-0.42,0,0  
 2XJ4,ARG\_187,13.75,-0.65,0.19  
 2I88,TYR\_478,10.77,0.95,-0.18,0  
 3UOV,GLU\_89,0.02,1.82,-3.58,-2.73  
 2OKT,CYS\_31,12.06,-0.73,0.42,3.37  
 3CIV,TYR\_134,11.7,1.54,-1.36,1.53  
 2F8H,TYR\_326,9.6,0.07,-0.47,0  
 4E8B,GLU\_68,3.87,0.07,-0.7,0  
 2VGM,ASP\_294,3.8,0,0,0  
 3EYE,ARG\_87,12.08,-0.42,0,0  
 2WOZ,ARG\_388,10.22,-2.83,0,0.55  
 4DNU,ASP\_51,1.76,0.49,-2.53,0  
 2FZ4,GLU\_74,4.5,0,0,0  
 1DTO,HIS\_136,6.43,0.07,0,-0.14  
 2OKT,HIS\_28,6.31,0.02,0,-0.21  
 3UV9,LYS\_485,10.5,0,0,0  
 2RGY,TYR\_337,13.14,0.35,0.39,2.4  
 3F1X,LYS\_274,10.5,0,0,0  
 2Q12,CYS\_183,9,0,0,0  
 1O17,ARG\_146,12.29,-0.21,0,0  
 1XDZ,LYS\_104,10.5,0,0,0  
 2ZQ5,GLU\_225,3.19,0.49,-1.8,0  
 2R2Y,ASP\_72,4.09,0.42,-0.13,0  
 1WYC,HIS\_375,6.99,1.6,1.89,-3  
 2HP7,GLU\_91,2.95,0.28,-1.83,0  
 3H6Q,ASP\_56,3.59,0.35,-0.56,0  
 2X4L,GLU\_155,3.63,0.28,-1.14,0  
 1XEU,CYS\_258,9.14,0,0,0.14  
 3LJN,TYR\_148,10,0,0,0  
 2NRR,GLU\_345,3.69,0.35,-1.16,0  
 3DB9,ASP\_12,3.62,0.42,-0.6,0  
 2FL4,LYS\_88,10.29,-0.21,0,0  
 2CXV,LYS\_17,10.01,-0.49,0,0  
 4DND,GLU\_87,4.64,0.14,0,0  
 3EST,GLU\_203,4.57,0.07,0,0  
 3EZ7,ARG\_351,11.8,-0.7,0,0  
 1F09,LYS\_401,10.5,0,0,0  
 4E8B,GLU\_187,4.57,0.07,0,0  
 4F3J,CYS\_145,7.93,-1.47,0,0.4  
 2APL,GLU\_89,3.95,0.49,-1.04,0  
 3IVF,LYS\_7,10.43,-0.07,0,0  
 1Y2Q,LYS\_72,10.15,-0.35,0,0  
 2H2W,LYS\_26,10.5,0,0,0  
 3US6,LYS\_120,10.5,0,0,0  
 1YR6,ASP\_75,3.35,0.35,-0.8,0  
 2B0A,ARG\_56,12.08,-0.42,0,0  
 1SIG,ASP\_189,3.32,0.14,-0.63,0  
 1RZ2,GLU\_158,4.69,0.28,-0.09,0  
 3U4K,TYR\_64,10,0,0,0  
 2QK1,GLU\_554,3.94,0.21,-0.77,0  
 3G9G,GLU\_186,4.74,0.63,-0.39,0  
 3GA2,LYS\_109,3.84,0.14,-0.8,0  
 1GVP,ASP\_36,2.97,0.21,-1.04,0  
 2PLQ,ARG\_295,12.5,0,0,0  
 3V55,ASP\_697,3.26,0.07,-0.61,0  
 3JZN,GLU\_392,4.57,0.07,0,0  
 3MIX,GLU\_322,4.71,0.21,0,0  
 1R5Q,TYR\_18,10.38,1.18,-0.8,0  
 3CN5,CYS\_69,9.14,0,0,0.14  
 1L2F,GLU\_268,1.17,1.83,-2.76,-2.4  
 3BQW,ASP\_74,3.77,0,-0.03,0  
 2DFL,TYR\_177,13.17,0.07,0.72,2.38  
 3K8J,LYS\_120,10.5,0,0,0  
 3GFP,ASP\_468,3.38,0.28,-0.69,0  
 1QYI,GLU\_378,3.71,0.77,-1.56,0  
 1LN4,GLU\_69,4.5,0,0,0  
 2VGM,CYS\_155,9.08,-0.98,0,1.05  
 2D7U,TYR\_298,13.46,0.07,0.02,3.37  
 1SNT,HIS\_200,6.43,0,0,-0.07  
 1RLO,ARG\_252,12.08,-0.42,0,0  
 1J8B,ASP\_65,2.93,0.35,-1.22,0  
 3RJK,LYS\_254,10.29,-0.21,0,0  
 2B0J,LYS\_226,10.22,-0.28,0,0  
 1W7B,LYS\_286,10.09,-0.28,0,-0.13  
 1U53,TYR\_170,11.64,1.64,0,0  
 2W0G,LYS\_173,10.29,-0.21,0,0  
 3UV9,ASP\_440,4.01,0.21,0,0  
 3M7G,GLU\_18,4.02,0.42,-1.41,0.51  
 1YLN,HIS\_215,6.43,0,-0.07  
 3A7L,GLU\_126,4.57,0.07,0,0  
 3NR5,LYS\_97,10.5,0,0,0  
 2AZL,ARG\_286,11.31,-1.19,0,0  
 1WXF,GLU\_22,4.06,0.7,-1.14,0  
 3ADO,GLU\_293,4.5,0,0,0  
 3M7D,ARG\_42,12.08,-0.42,0,0  
 2IDC,ARG\_132,12.31,-2.42,0,2.23  
 2BAA,LYS\_26,10.5,0,0,0  
 2E3H,GLU\_240,4.64,0.14,0,0  
 3PBH,ARG\_116,12.15,-0.35,0,0  
 2VGM,GLU\_137,4.57,0.07,0,0  
 2VAN,GLU\_165,4.05,0.35,-0.8,0  
 2Z84,TYR\_178,10.4,0.07,-0.15,0.48  
 350A,LYS\_52,9.8,-0.7,0,0  
 1WXF,ARG\_82,11.66,-0.84,0,0  
 2JEO,GLU\_51,4.5,0,0,0  
 2E3S,LYS\_590,10.29,-0.21,0,0  
 1MTZ,ASP\_224,2.28,0.63,-2.15,0  
 2CYG,ARG\_252,11.94,-0.56,0,0  
 1UAJ,TYR\_86,11.1,1.35,-0.57,0.32  
 3BPP,LYS\_200,9.94,-0.56,0,0  
 1BN6,CYS\_273,9.29,-0.41,-0.17,0.87  
 3PZ9,GLU\_388,2.38,0.28,-2.4,0  
 2Q13,ARG\_72,12.5,0,0,0

2FZPARG\_190,11.8,-0.7,0.0  
 2IF4,GLU\_261,3.71,0.28,-1.07,0  
 2RIK,GLU\_138,3.25,0.7,-1.95,0  
 1GXN,ARG\_625,11.03,-1.47,0.0  
 4ETX,CYS\_236,10.28,-0.18,0,1.46  
 3AU3,CYS\_575,10.06,0,0,1.06  
 2YYO,ASP\_68,2.15,0.35,-2,0  
 2ZCX,ARG\_155,11.87,-0.63,0,0  
 3T5B,HIS\_176,2.12,1.29,0,-5.67  
 1U53,LYS\_14,10.29,-0.21,0,0  
 2Z84,ARG\_128,10.96,-1.54,0,0  
 3CIV,GLU\_231,3.13,4.05,-2.58,-2.84  
 2PGX,ASP\_199,1.13,0.42,-3.09,0  
 3QAV,HIS\_144,6.52,0.09,0,-0.07  
 3JZ9,HIS\_376,4.87,0,0,-1.63  
 2CL3,GLU\_119,4.13,0.21,-0.58,0  
 3IRA,GLU\_32,4.5,0,0,0  
 2OEW,LYS\_234,10.5,0,0,0  
 3M70,ASP\_144,4.01,0.21,0,0  
 2D2S,GLU\_589,4.71,0.21,0,0  
 2ATR,TYR\_126,11.22,0,0,1.22  
 3JRT,TYR\_89,10.83,0.6,0,0.23  
 2X4G,ASP\_323,3.47,0.21,-0.54,0  
 3CO1,TYR\_71,10.12,0.07,0.05,0  
 1KCM,GLU\_28,4.85,0.63,-0.28,0  
 3HOX,LYS\_68,10.08,-0.42,0,0  
 3CSV,LYS\_217,10.22,-0.28,0,0  
 1160,HIS\_79,7.16,0.8,0,-0.14  
 2ZTY,ASP\_66,3.94,0.14,0,0  
 2NSN,ASP\_42,3.26,0.35,-0.89,0  
 3CCY,TYR\_194,10,0,0,0  
 1J33,ARG\_189,11.87,-0.63,0,0  
 1MD6,ASP\_127,3.15,0.56,-1.21,0  
 4FZR,CYS\_9,9.4,-0.38,0,0.78  
 3EVP,HIS\_112,4.35,1.2,-3.35  
 3GW3,GLU\_314,4.71,0.21,0,0  
 2Z84,GLU\_130,3.85,0.28,-0.92,0  
 3CNU,TYR\_42,11.76,0,0,1.76  
 3T8R,ARG\_50,11.87,-0.63,0,0  
 1O9G,GLU\_117,4.5,0,0,0  
 3ZSL,ARG\_169,11.87,-0.63,0,0  
 1SUU,GLU\_709,4.5,0,0,0  
 3TRE,CYS\_113,8.38,-0.65,0,0.03  
 1QVI,HIS\_88,2.44,0.12,0,-4.18  
 3R87,CYS\_74,9.6,-0.06,0,0.66  
 3I0C,LYS\_125,10.5,0,0,0  
 3UAH,HIS\_382,8.48,2.62,2.67,-3.32  
 1MUF,GLU\_138,4.26,0.35,-0.59,0  
 2Q13,ARG\_314,12.29,-0.21,0,0  
 3CS1,GLU\_115,4.02,0.14,-0.62,0  
 1JSX,GLU\_89,3.48,0.84,-1.86,0  
 1WL1,LYS\_294,10.08,-0.42,0,0  
 2CWY,GLU\_7,4.5,0,0,0  
 3COU,ARG\_50,11.89,-0.61,0,0  
 2YLF,TYR\_117,10,0,0,0  
 1ZP2,TYR\_34,11.14,0,0,1.14  
 3ETV,LYS\_161,10.5,0,0,0  
 2X4L,TYR\_130,11.2,1.2,0,0  
 3IRA,LYS\_36,10.5,0,0,0  
 2ZQ5,ARG\_144,12.43,-0.07,0,0  
 2R0S,ASP\_71,3.4,0.21,-0.61,0  
 2CVB,GLU\_104,3.77,0.35,-1.08,0  
 3H9W,GLU\_129,2.45,0.35,-2.4,0  
 2F4Q,LYS\_91,10.58,-0.28,0,0.36  
 3FTT,LYS\_4,10.22,-0.28,0,0  
 1EQ6,ASP\_149,4.08,0.28,0,0  
 2O8I,GLU\_75,4.57,0.07,0,0  
 2NRR,LYS\_357,10.5,0,0,0  
 2A6B,ASP\_156,3.8,0,0,0  
 3GOZ,LYS\_130,10.08,-0.42,0,0  
 3BB7,ARG\_171,11.87,-0.63,0,0  
 4H4J,ASP\_28,3.35,0.42,-0.87,0  
 4FD6,ARG\_10,12.36,-0.14,0,0  
 3UX2,GLU\_68,4.26,0.28,-0.52,0  
 3PZ9,ARG\_364,11.87,-0.63,0,0  
 1RHS,TYR\_107,12.17,2.17,0,0  
 4EVF,TYR\_114,12.56,0.16,0,2.4  
 2RIK,GLU\_135,4.64,0.14,0,0  
 1UCH,TYR\_35,12.77,0.07,0.5,2.19  
 1X8F,GLU\_245,4.5,0,0,0  
 2OPJ,CYS\_93,8.42,-0.5,-0.9,0.81  
 2YWJ,TYR\_58,9.93,0,-0.07,0  
 3CGW,GLU\_25,4.71,0.21,0,0  
 1QQE,LYS\_281,10.36,-0.14,0,0  
 2H01,LYS\_102,10.01,-0.49,0,0  
 2IN0,LYS\_89,10.43,-0.07,0,0  
 2Q5X,ARG\_850,12.01,-0.49,0,0  
 2BAA,ARG\_221,11.67,-1.57,0,0.74  
 1X6J,ARG\_81,11.94,-0.56,0,0  
 2W2S,LYS\_77,10.5,0,0,0  
 1A8Q,ASP\_65,2.95,0.14,-0.99,0  
 1H09,LYS\_288,10.5,0,0,0  
 3LJN,ARG\_25,12.15,-0.35,0,0  
 2OGQ,GLU\_399,4.37,0.07,-0.2,0  
 2FBQ,LYS\_50,10.43,-0.07,0,0  
 3JZ9,GLU\_524,2.15,0.77,-3.13,0  
 2F19,GLU\_70,4.5,0,0,0  
 3QKY,GLU\_68,4.71,0.21,0,0  
 2O0K,CYS\_257,6.11,-3.6,-1.45,2.16  
 3BPV,ARG\_96,12.22,-0.28,0,0  
 1BYI,CYS\_151,6.89,-2.5,0,0.38  
 3K1H,LYS\_76,10.29,-0.21,0,0  
 2D7U,LYS\_142,10.5,0,0,0  
 3GE9,ARG\_172,12.22,-0.28,0,0  
 1XKR,ASP\_97,3.56,0.14,-0.37,0  
 1FQI,GLU\_412,4.64,0.14,0,0  
 2P1W,TYR\_61,12.24,0.82,0,1.42  
 1YG2,HIS\_89,6.5,0,0,0  
 2B0A,LYS\_95,10.36,-0.14,0,0  
 3BWT,ARG\_674,11.8,-0.7,0,0  
 2W0Z,GLU\_321,4.5,0,0,0  
 4DNU,TYR\_194,11.19,0,0,1.19  
 3FFM,GLU\_28,4.85,0.35,0,0  
 1O5T,LYS\_256,10.5,0,0,0  
 2PGX,ARG\_208,12.15,-0.35,0,0  
 2B61,ASP\_10,2.38,0.28,-1.7,0  
 2CWC,ASP\_146,3.89,0.35,-0.26,0  
 2W0Z,LYS\_570,10.08,-0.42,0,0  
 4DNU,LYS\_16,10.5,0,0,0  
 1NJ4,HIS\_151,3.0,0.06,-0.51,-3.06  
 3T5B,GLU\_266,4.5,0,0,0  
 3G59,GLU\_242,4.5,0,0,0  
 3AU3,ARG\_549,12.11,-0.39,0,0  
 3V46,ASP\_372,3.09,0.7,-1.41,0  
 3B4D,HIS\_211,6.5,0,0,0  
 4AM1,ASP\_238,3.05,0.63,-1.38,0  
 1RAJ,ASP\_339,3.94,0.14,0,0  
 3RE9,ARG\_91,12.01,-0.49,0,0  
 1YB2,TYR\_253,11.75,0.21,-0.19,1.73  
 3ANJ,LYS\_89,10.29,-0.21,0,0  
 2E3C,GLU\_271,4.2,0.35,-0.65,0  
 3MIX,GLU\_345,2.97,0.77,-1.26,-1.04  
 1FQI,HIS\_315,6.55,0.12,0,-0.07  
 3JSN,ARG\_301,11.94,-0.56,0,0  
 3JV1,ASP\_214,2.56,0.56,-1.8,0  
 2H01,LYS\_29,10.01,-0.49,0,0  
 3NBI,LYS\_105,10.36,-0.14,0,0  
 1O0X,ARG\_199,12.29,-0.21,0,0  
 3DZ1,GLU\_6,4.28,0.56,-0.78,0  
 1XEU,ARG\_128,12.5,0,0,0  
 2HP7,ASP\_79,3.79,0.28,-0.29,0  
 2FBQ,ASP\_88,2.35,0.28,-1.73,0  
 2XHC,LYS\_219,10.15,-0.35,0,0  
 2YLF,ASP\_198,2.1,0.35,-2.05,0  
 1Y0K,CYS\_34,10.93,-0.24,0,2.17  
 1MJS,GLU\_360,4.47,0.07,-0.1,0  
 3JSN,ASP\_223,2.25,0.35,-1.9,0  
 3AU3,ASP\_605,4.04,0.28,-0.04,0  
 3EGN,TYR\_413,10.66,0.71,-0.05,0  
 3T5B,ARG\_365,11.8,-0.7,0,0  
 1VJG,CYS\_12,10.08,0,0,1.08  
 2GYZ,ARG\_74,12.01,-0.49,0,0  
 2B78,HIS\_164,7.24,1.24,0,-0.49  
 3V55,GLU\_549,4.05,0.21,-0.66,0  
 2ZTY,TYR\_178,10.33,1.17,-1.04,0.21  
 3TIR,ARG\_225,11.8,-0.7,0,0  
 2RGY,ARG\_223,12.95,-4.13,0,4.58  
 3H9W,HIS\_94,5.87,0,0,-0.63  
 1XTD,LYS\_143,10.29,-0.21,0,0  
 2QV2,HIS\_192,6.5,0,0,0  
 3ERF,TYR\_131,10,0,0,0  
 2NRK,GLU\_58,4.5,0,0,0  
 3CS1,TYR\_127,11.17,0.54,-0.54,1.17  
 2B0J,ARG\_268,12.15,-0.35,0,0  
 1PBV,ASP\_131,3.64,0.42,-0.58,0  
 3G9G,LYS\_16,10.22,-0.28,0,0  
 3RZJ,LYS\_200,10.43,-0.07,0,0  
 2EVI,ASP\_199,2.96,0.42,-1.26,0  
 1MTZ,GLU\_4,4.5,0,0,0  
 1DZF,GLU\_34,4.5,0,0,0  
 2Q34,ARG\_252,12.43,-0.07,0,0  
 1WPA,GLU\_452,4.78,0.28,0,0  
 1AKO,ARG\_90,13.64,-2.62,0,3.76  
 2CWY,TYR\_17,10.67,0,0,0.67  
 2OBS,TYR\_118,9.52,0.14,-0.7,0.08  
 3F7M,GLU\_154,4.05,0.35,-0.8,0  
 3GA2,GLU\_55,5.11,0.7,-0.09,0  
 3M70,HIS\_27,5.11,1.64,0,-3.02  
 3EVP,GLU\_300,4.71,0.21,0,0  
 1QQL,ARG\_11,12.5,0,0,0  
 4DNU,TYR\_82,10.15,0.77,-0.62,0  
 2C2Y,ARG\_223,11.66,-0.84,0,0  
 2H2W,ASP\_175,3.78,0,-0.02,0  
 3MTT,ASP\_455,3.67,0.49,-0.62,0  
 3ZXY,GLU\_71,4.57,0.07,0,0  
 2BAA,TYR\_222,11.03,2.91,-1.13,-0.74  
 1XAW,ASP\_518,1.79,0.49,-2.5,0  
 3B87,TYR\_270,10.21,0,-0.17,0.38  
 3M70,ARG\_284,12.08,-0.42,0,0  
 3G6S,LYS\_122,10.36,-0.14,0,0  
 1JSX,HIS\_198,6.55,0.26,0,-0.21  
 1JT9,HIS\_90,3.98,0,0,-2.52  
 2VGM,LYS\_303,10.5,0,0,0  
 3V46,GLU\_261,4.57,0.07,0,0  
 3LD1,LYS\_43,10.5,0,0,0  
 2RGY,GLU\_262,4.85,0.35,0,0  
 1X9G,LYS\_62,10.5,0,0,0  
 2BV9,ARG\_124,12.15,-0.35,0,0  
 1YM5,ASP\_289,3.21,0.28,-0.87,0  
 3B21,GLU\_105,4.57,0.07,0,0  
 2D8N,LYS\_170,10.36,-0.14,0,0  
 2FL7,ASP\_170,3.12,0.49,-1.17,0  
 1FQI,ARG\_403,12.29,-0.21,0,0  
 3CSV,LYS\_358,10.5,0,0,0  
 2V5B,HIS\_123,3.94,0,-0.16,-2.4  
 3N2T,ASP\_230,1.04,0.84,-3.59,0  
 4EKU,CYS\_89,12.3,0,1.55,1.75  
 2XMZ,HIS\_180,6.29,0,0,-0.21  
 1U53,LYS\_32,9.8,-0.7,0,0  
 3C6B,LYS\_5,10.36,-0.14,0,0  
 4HDE,ASP\_46,3.35,0.35,-0.8,0  
 2Q07,ASP\_259,2.2,0.49,-2.09,0  
 2XMZ,HIS\_168,6.5,0,0,0  
 1U7U,ASP\_319,4.01,0.21,0,0  
 2PGE,ARG\_201,10.78,-1.72,0,0  
 2O8P,TYR\_186,8.63,0.18,-0.8,-0.75  
 2D59,ASP\_121,3.87,0.07,0,0  
 1ZBM,GLU\_242,3.57,0.07,-1,0  
 1T3J,GLU\_692,4.64,0.14,0,0  
 1P4X,ARG\_21,11.5,-1,0,0  
 3LH5,GLU\_526,4.5,0,0,0  
 2XJ4,GLU\_12,4.38,0.49,-0.61,0  
 2RGY,ASP\_188,2.88,0.49,-1.41,0  
 3A7L,GLU\_12,4.64,0.14,0,0  
 3HKX,ARG\_274,11.94,-0.56,0,0  
 3HZQ,LYS\_92,10.5,0,0,0  
 2HNG,ASP\_120,3.8,0,0,0  
 1PDB,LYS\_98,10.36,-0.14,0,0  
 1UAJ,GLU\_126,4.86,0.42,-0.06,0  
 2W1R,ASP\_143,3.49,0.49,-0.8,0  
 3CS1,GLU\_151,3.13,0.91,-2.29,0  
 3RLE,ARG\_130,11.94,-0.56,0,0  
 1YB2,TYR\_160,8.75,0.14,-1.39,0  
 3M66,TYR\_377,10.62,1.42,-0.8,0  
 1TLV,TYR\_94,10.95,0.07,0,0.88  
 2E3C,TYR\_272,9.59,0.07,-0.48,0  
 3F1X,ASP\_34,4.01,0.42,-0.22,0  
 1CHD,GLU\_169,4.5,0,0,0  
 1P4X,GLU\_135,5.93,0.5,-0.87,1.81  
 3S0A,ASP\_117,4.01,0.21,0,0  
 1JT9,GLU\_246,4.64,0.14,0,0  
 1MUF,TYR\_98,10.07,0.07,0,0  
 1Y2Q,GLU\_14,4.12,0.42,-0.8,0  
 4ETX,ARG\_199,12.36,-0.14,0,0  
 1YTD,GLU\_315,4.64,0.14,0,0  
 2A6B,HIS\_165,3.64,0,-2.86  
 2B0J,GLU\_328,4.5,0,0,0  
 2OJQ,LYS\_510,10.29,-0.21,0,0  
 1L2F,LYS\_20,10.29,-0.21,0,0  
 3GYW,ARG\_108,11.87,-0.63,0,0  
 1Z9L,ASP\_116,4.02,0.35,-0.13,0  
 3KEY,LYS\_457,10.5,0,0,0  
 3A7L,GLU\_128,4.49,0.35,-0.36,0  
 1NFN,ARG\_145,11.61,-0.89,0,0  
 3BWT,ARG\_879,11.52,-0.98,0,0  
 2Z0M,CYS\_191,9.63,0.56,0,0.07  
 2E3C,LYS\_438,10.36,-0.14,0,0  
 157K,TYR\_161,9.61,0.07,-0.46,0  
 3PM2,GLU\_113,4.64,0.14,0,0  
 2IF4,LYS\_57,10.43,-0.07,0,0  
 2PLQ,LYS\_92,9.87,-0.63,0,0  
 3EGN,ARG\_421,11.59,-0.91,0,0  
 2B0J,GLU\_70,4.64,0.14,0,0  
 2H85,GLU\_170,4.5,0,0,0  
 1KN3,TYR\_176,10.17,0.17,0,0  
 3HWV,GLU\_271,4.54,0.35,-0.31,0  
 1160,HIS\_58,6.91,0.9,0,-0.49  
 2F19,ASP\_99,3.38,0.21,-0.63,0  
 2Z84,TYR\_209,11.27,0.21,-1.23,2.29  
 1R16,LYS\_208,10.5,0,0,0  
 2H85,HIS\_242,6.43,0,-0.07  
 3B21,GLU\_120,3.92,0.21,-0.79,0  
 3JZN,LYS\_332,9.8,-0.7,0,0  
 2PLQ,LYS\_268,10.29,-0.21,0,0  
 1R3D,ARG\_40,12.36,-0.14,0,0  
 3ANJ,CYS\_124,10.48,-1.32,0,2.8



3EVP,ARG\_280,12.15,-0.35,0,0  
1WPA,GLU\_463,4.71,0.21,0,0  
1Y0K,ASP\_28,3.28,0.28,-0.8,0  
2FD4,ASP\_501,4.09,0.7,-0.41,0  
3CGW,ARG\_62,12.29,-0.21,0,0  
1OXZ,LYS\_198,10.5,0,0,0  
3IRA,LYS\_142,10.29,-0.21,0,0  
1C44,GLU\_17,4.57,0.07,0,0  
2A1V,LYS\_117,10.15,-0.35,0,0  
1T3Y,LYS\_118,10.5,0,0,0  
1SIG,ARG\_285,12.5,0,0,0  
2R57,ASP\_324,2.59,0.98,-2.19,0  
2DVK,GLU\_132,4.13,0.21,-0.58,0  
3ZTA,LYS\_117,10.29,-0.21,0,0  
1M5I,TYR\_133,10.64,0,0,0.65  
3MEW,HIS\_203,6.81,0.52,0,-0.21  
3M7D,LYS\_248,9.94,-0.56,0,0  
2BV9,ARG\_244,12.08,-0.42,0,0  
2G9D,ARG\_39,11.1,-1.4,0,0  
2OSA,ARG\_428,11.4,-1.1,0,0  
2BDD,TYR\_138,10,0,0,0  
2RJD,CYS\_403,12.14,0.44,2.4,0.3  
3J5N,CYS\_109,10.83,0,0,1.83  
4E9E,TYR\_523,11.54,0.88,-0.55,1.21  
3HUE,GLU\_7,3.2,0.35,-1.65,0  
1MML,LYS\_257,10.5,0,0,0  
2OJQ,LYS\_541,10.5,0,0,0  
3ONT,ARG\_38,12.15,-0.35,0,0  
1PVT,LYS\_199,10.5,0,0,0  
4DIU,ARG\_174,12.15,-0.35,0,0  
3EJG,ASP\_29,2.67,0.42,-1.54,0  
1MD6,LYS\_95,10.36,-0.14,0,0  
2E3C,GLU\_357,4.5,0,0,0  
1Q42,ARG\_15,11.45,-1.05,0,0  
2AH5,HIS\_150,6.22,0,0,-0.28  
1Q46,GLU\_37,3.59,1.97,-1.89,-1  
3LPZ,ARG\_230,11.73,-0.91,0,0.14  
2VAN,GLU\_129,4.31,0,-0.19,0  
3DZ1,ASP\_186,2.72,0.91,-1.98,0  
2AZP,GLU\_270,4.03,0.21,-0.68,0  
2BLL,HIS\_372,6.5,0,0,0  
3C38,ASP\_241,3.39,0.42,-0.83,0  
4ANN,LYS\_187,10.5,0,0,0  
2B0J,LYS\_300,10.36,-0.14,0,0  
1LTU,ASP\_75,3.94,0.14,0,0  
3K9I,LYS\_133,10.29,-0.21,0,0  
3K8J,GLU\_215,3.64,0.85,-1.71,0  
3AUF,ARG\_46,11.45,-1.05,0,0  
2PIM,ARG\_108,12.22,-0.28,0,0  
2BCF,CYS\_102,6.6,-2.4,0,0  
2C13,CYS\_273,11.81,-2.79,2.39,3.23  
2WB8,LYS\_584,10.5,0,0,0  
3OOP,ARG\_74,12.08,-0.42,0,0  
3T8R,GLU\_125,4.4,0.35,-0.45,0  
1OST,LYS\_450,10.5,0,0,0  
2QHT,ARG\_101,12.22,-0.28,0,0  
2H2Z,GLU\_270,4.31,0.21,-0.4,0  
1EYH,ARG\_139,11.94,-0.56,0,0  
1P6F,GLU\_87,4.78,0.28,0,0  
1UAJ,HIS\_28,6.43,0,0,-0.07  
3L7N,HIS\_179,10.16,5.2,4.57,-6.12  
1XWM,TYR\_123,11.79,2.51,-0.71,0  
3KT9,ARG\_42,12.36,-0.14,0,0  
1T07,TYR\_31,9.56,0.07,-0.51,0  
1CBY,LYS\_79,10.36,-0.14,0,0  
1E5S,HIS\_135,6.35,0.06,0,-0.21  
3F5D,LYS\_146,10.29,-0.21,0,0  
4EZB,LYS\_134,10.08,-0.42,0,0  
1R1S,ARG\_232,12.29,-0.21,0,0  
3I4T,ARG\_153,10.74,-1.76,0,0  
2RGY,HIS\_189,4.96,4.4,-1.07,-4.87  
1JKS,ASP\_10,3.83,0.21,-0.18,0  
2R2Y,GLU\_118,3.84,0.14,-0.8,0  
3N0K,TYR\_56,9.17,0.28,-1.11,0  
1VSM,ARG\_70,11.45,-1.05,0,0  
2H30,ASP\_106,3.15,0.35,-1,0  
2E3C,ARG\_217,12.29,-0.21,0,0  
3O48,ASP\_57,3.81,0.35,-0.34,0  
3UAH,ARG\_448,12.08,-0.42,0,0  
2D0A,TYR\_210,11.81,1.8,0,0.01  
1R9W,CYS\_240,8.26,-0.95,0,0.21  
1J74,ARG\_45,11.87,-0.63,0,0  
1WRU,LYS\_287,10.29,-0.21,0,0  
2RGY,GLU\_346,4.64,0.14,0,0  
3F6F,GLU\_111,4.71,0.21,0,0  
3EUR,LYS\_119,10.5,0,0,0  
2ILR,LYS\_525,10.5,0,0,0  
1LZL,ARG\_314,12.5,0,0,0  
1EDG,ARG\_30,12.06,-0.44,0,0  
2GEN,HIS\_105,6.75,0.32,0,-0.07  
3CBN,GLU\_54,4.5,0,0,0  
2P1W,ARG\_227,12.29,-0.21,0,0  
1DOV,ASP\_143,3.35,0.35,-0.8,0  
2G5X,LYS\_44,10.22,-0.28,0,0  
1HF8,GLU\_232,4.5,0,0,0  
3BA1,ARG\_92,12.08,-0.42,0,0  
3BQW,ARG\_19,12.01,-0.49,0,0  
3U2R,GLU\_102,4.71,0.21,0,0  
3CO1,ASP\_123,3.8,0,0,0  
3FNI,ARG\_123,11.94,-0.56,0,0  
2GYZ,ARG\_8,11.52,-0.98,0,0  
4F8A,LYS\_673,10.43,-0.07,0,0  
1YB2,ARG\_225,12.36,-0.14,0,0  
1OIS,HIS\_196,6.67,0.24,0,-0.07  
1L2H,TYR\_90,13.41,0.21,0.8,2.4  
1NJ4,GLU\_318,4.71,0.21,0,0  
1HF8,GLU\_51,3.79,0.07,-0.78,0  
2IXM,GLU\_270,4.64,0.14,0,0  
1P6F,TYR\_147,9.93,0.28,-0.35,0  
2FXT,CYS\_369,9.57,-1.1,0,1.67  
3RFY,ASP\_284,3.36,0.84,-1.28,0  
2EEY,HIS\_77,7.43,1.14,0,-0.21  
3ANJ,TYR\_266,10.8,0,0,0.8  
1R3F,LYS\_33,10.36,-0.14,0,0  
3DTE,ARG\_242,12.01,-0.49,0,0  
2CWW,ARG\_90,12.22,-0.28,0,0  
1F2V,GLU\_15,4.85,0.35,0,0  
1YR6,TYR\_221,13.17,0.97,0.16,2.04  
2OJQ,TYR\_677,13.6,0.4,0.8,2.4  
3JRT,LYS\_6,10.43,-0.07,0,0  
2F4Q,ASP\_269,3.82,0.14,-0.12,0  
1MTZ,HIS\_255,6.94,0.58,0,-0.14  
3DSH,ARG\_301,11.66,-0.84,0,0  
1WXQ,GLU\_383,4.5,0,0,0  
2CBE,GLU\_236,4.0,49,-0.99,0  
2NMU,ARG\_141,11.31,-1.19,0,0  
1X7F,CYS\_146,12.06,0,-0.27,3.34  
1TJE,ARG\_110,12.15,-0.35,0,0  
2Z14,TYR\_34,10,0,0,0  
1YTQ,ASP\_91,2.77,0.28,-1.31,0  
3LD1,ARG\_228,12.36,-0.14,0,0  
1BN6,GLU\_109,4.5,0,0,0  
2XJ4,ARG\_125,11.73,-0.77,0,0  
3ODJ,GLU\_31,3.91,0.21,-0.8,0  
2G2D,HIS\_150,6.37,0.08,0,-0.21  
2A4D,GLU\_144,4.5,0,0,0  
1RZ2,ASP\_218,3.87,0.07,0,0  
2XWS,GLU\_52,3.32,0.7,-1.88,0  
1YR6,TYR\_28,13.27,0.07,0.8,2.4  
3EIZ,ASP\_15,3.63,0.63,-0.8,0  
1TJE,LYS\_200,10.5,0,0,0  
2A6B,LYS\_19,10.29,-0.21,0,0  
3EUR,LYS\_103,10.43,-0.07,0,0  
3JSN,LYS\_121,10.29,-0.21,0,0  
3BJV,GLU\_139,4.0,14,-0.64,0  
2F9F,ARG\_27,11.59,-0.91,0,0  
1SIG,LYS\_289,10.5,0,0,0  
1NWA,ASP\_143,3.56,0.56,-0.8,0  
2A1V,TYR\_83,10.07,0.07,0,0  
3IL3,ARG\_43,11.8,-0.7,0,0  
2C2Y,ARG\_281,12.29,-0.21,0,0  
3HNX,ARG\_81,12.29,-0.21,0,0  
2FXT,TYR\_338,12.15,0.07,0,2.08  
1LN4,HIS\_16,6.5,0,0,0  
1XIP,HIS\_95,5.62,1,0,-1.88  
3LJC,ASP\_18,3.87,0.07,0,0  
3C38,LYS\_80,10.5,0,0,0  
1VSM,TYR\_194,10.24,0,0,0.24  
1ILW,LYS\_41,10.5,0,0,0  
3V46,LYS\_304,10.43,-0.07,0,0  
3RJZ,ARG\_107,12.22,-0.28,0,0  
1MTZ,ARG\_184,11.73,-0.77,0,0  
2G5X,HIS\_211,6.92,0.56,0,-0.14  
2PIM,ARG\_103,11.94,-0.56,0,0  
4DNU,ASP\_34,4.15,0.35,0,0  
4F8A,ARG\_591,12.08,-0.42,0,0  
3U2R,GLU\_308,4.16,0.35,-0.69,0  
3FFM,ASP\_68,2.54,0.7,-1.96,0  
4EVF,ARG\_132,12.08,-0.42,0,0  
1JT9,GLU\_83,4.64,0.14,0,0  
3VJ8,GLU\_83,6.63,2.82,-0.79,0.1  
3I47,GLU\_83,4.5,0,0,0  
1UXQ,ASP\_168,3.86,0.07,-0.01,0  
3Q6L,GLU\_110,4.78,0.28,0,0  
3GFP,GLU\_471,4.71,0.21,0,0  
4ETX,TYR\_399,11.25,1.56,-0.22,-0.09  
3H8Y,ARG\_62,12.43,-0.07,0,0  
1MHN,ASP\_117,3.05,0.49,-1.24,0  
1R29,GLU\_41,4.71,0.21,0,0  
1OST,ARG\_141,13.93,-0.97,0,2.4  
3GA2,LYS\_235,10.43,-0.07,0,0  
3H04,GLU\_226,3.68,0.14,-0.96,0  
1MTZ,GLU\_27,4.12,0.42,-0.8,0  
2JEO,GLU\_41,4.57,0.07,0,0  
1CHD,LYS\_157,10.08,-0.42,0,0  
1L2F,GLU\_228,3.32,0.42,-1.6,0  
3U2R,ASP\_75,3.03,0.07,-0.84,0  
1R53,LYS\_141,9.94,-0.56,0,0  
1VJG,GLU\_174,2.94,0.91,-2.47,0  
1L2F,LYS\_37,10.43,-0.07,0,0  
3I4T,LYS\_44,10.5,0,0,0  
2QZQ,LYS\_143,10.15,-0.35,0,0  
1MUF,ASP\_194,1.47,0.56,-2.64,-0.25  
2HRZ,TYR\_173,12.8,0.21,0.19,2.4  
1TWU,GLU\_40,3.89,0.14,-0.75,0  
2NRR,HIS\_469,6.36,0,0,-0.14  
2OJQ,GLU\_511,4.5,0,0,0  
2POY,LYS\_79,9.87,-0.63,0,0  
1ILW,GLU\_56,2.48,0.42,-2.44,0  
2QK1,LYS\_360,10.36,-0.14,0,0  
1IDK,TYR\_209,13.82,0.28,0.8,2.74  
2C13,GLU\_22,4.57,0.07,0,0  
3DSH,LYS\_333,10.5,0,0,0  
3FHF,GLU\_76,3.9,0.07,-0.67,0  
2RGY,HIS\_205,4.97,1.4,0,-2.93  
3UOV,GLU\_212,3.58,0.28,-1.2,0  
4F8A,LYS\_574,10.5,0,0,0  
3HQX,GLU\_51,4.5,0,0,0  
1X9G,ARG\_3,12.43,-0.07,0,0  
3UPD,HIS\_-21,6.49,0.2,-0.21  
2ZTY,LYS\_156,10.5,0,0,0  
3GE9,GLU\_115,4.05,0.35,-0.8,0  
2APL,TYR\_75,10.6,0,0,0.6  
1Q46,TYR\_126,12.63,1.87,0,0.76  
3BWT,HIS\_688,4.79,0.05,0,-1.76  
3M7G,ARG\_42,12.5,0,0,0  
3M70,LYS\_94,10.5,0,0,0  
1WYC,ASP\_150,3.09,0.42,-1.13,0  
1YTQ,ASP\_126,3.76,0.14,-0.18,0  
4FCU,TYR\_186,12.61,2.61,0,0  
2H80,TYR\_316,13.41,0.21,0.8,2.4  
1O9G,HIS\_23,1.5,0.41,-2.4,-3  
2GQV,LYS\_32,9.94,-0.56,0,0  
2NRR,GLU\_467,4.64,0.14,0,0  
3LJC,ARG\_8,12.5,0,0,0  
3PU6,GLU\_115,4.61,0.14,-0.03,0  
2CL3,HIS\_164,6.46,0.03,0,-0.07  
3KV0,HIS\_147,6.36,0,0,-0.14  
1WLJ,CYS\_91,11.74,0,0,2.74  
1BKR,TYR\_105,10,0,0,0  
2P4D,TYR\_140,10,0,0,0  
1Y2Q,TYR\_102,9.65,0,-0.35,0  
2W0G,LYS\_276,10.22,-0.28,0,0  
4DNU,HIS\_235,0.24,0.25,0,-6.51  
3GV0,ARG\_146,12.22,-0.28,0,0  
1Q2Y,LYS\_139,10.15,-0.35,0,0  
2EJX,TYR\_74,10.6,1.44,-0.84,0  
2Q07,ARG\_436,11.8,-0.7,0,0  
1UAJ,GLU\_202,3.95,0.35,-0.9,0  
2OB5,LYS\_60,10.5,0,0,0  
1XAW,LYS\_496,10.43,-0.07,0,0  
3GW3,ASP\_327,3.45,0.35,-0.7,0  
3EGN,GLU\_485,2,0.7,-3.2,0  
3CCY,ARG\_105,11.82,-0.68,0,0  
4FZN,HIS\_140,1.64,0,0,-4.86  
2R2Y,ASP\_63,2.07,0.84,-2.56,0  
3Q2C,TYR\_38,10.07,0.07,-0.58,0.57  
1WXQ,ARG\_65,12.22,-0.28,0,0  
3IL3,ASP\_236,2.93,0.56,-1.43,0  
3H6Q,ASP\_61,3.1,0.07,-0.77,0  
2PGE,CYS\_194,9.21,0,0,0.21  
3JSN,ARG\_250,12.8,-1.59,0,1.89  
1EYH,ARG\_72,12.01,-0.49,0,0  
3M66,GLU\_268,4.71,0.21,0,0  
3ERF,TYR\_22,13.34,0.14,0.8,2.4  
3EJG,GLU\_1,2.35,0.63,-2.78,0  
4F85,TYR\_216,9.27,0.07,-0.8,0  
3BWT,ASP\_707,3.42,0.35,-0.73,0  
1MTZ,ASP\_227,3.69,0.21,-0.32,0  
3I47,ASP\_242,3.69,0,-0.11,0  
3C6B,ASP\_239,2.35,0.84,-2.3,0  
2H2W,GLU\_129,3.49,0.42,-1.43,0  
1PDB,LYS\_173,9.66,-0.84,0,0  
2OJQ,ARG\_649,12.76,-1.75,0,2.01  
1XDZ,HIS\_125,6.79,0.57,0,-0.28  
2CL3,LYS\_50,9.73,-0.77,0,0  
3M7D,ARG\_288,12.5,0,0,0  
1PV5,HIS\_193,5.8,0.99,2.09,-3.78  
1AM2,ARG\_26,12.5,0,0,0  
1W24,LYS\_81,10.01,-0.49,0,0  
1ZB5,LYS\_258,10.5,0,0,0  
1W7B,GLU\_156,3.91,0.21,-0.8,0  
3CNU,ASP\_13,3.81,0.07,-0.06,0  
2RFA,HIS\_227,6.54,0.04,0,0  
2G2D,LYS\_86,10.5,0,0,0  
3M7D,GLU\_74,2.91,0.93,-0.8,-1.72

2X5Y,ASP\_834,2.85,0.42,-1.37,0  
 2Z61,GLU\_25,3.99,0.21,-0.72,0  
 1TD6,GLU\_284,1.64,0.34,-0.8,-2.4  
 2B61,GLU\_259,4.71,0.21,0,0  
 1RL0,TYR\_34,8.68,0.21,-1.53,0  
 4F85,HIS\_156,6.42,0.06,0,-0.14  
 2YT4,ASP\_496,4.29,0.49,0,0  
 3GOZ,HIS\_300,6.43,0,0,-0.07  
 1L3K,TYR\_62,10.46,1.13,-0.67,0  
 3RE9,LYS\_108,10.15,-0.35,0,0  
 1OST,LYS\_369,10.36,-0.14,0,0  
 1J33,GLU\_195,4.57,0.07,0,0  
 3GS3,GLU\_47,4.49,0.14,-0.15,0  
 2ILR,ASP\_338,2.57,0.14,-1.36,0  
 1K95,ASP\_102,1.98,0.91,-2.73,0  
 3CAX,TYR\_406,10,0,0,0  
 2EA9,GLU\_67,3.68,0.35,-1.17,0  
 2FBQ,GLU\_71,1.8,0.49,-3.19,0  
 3FRR,ASP\_93,2.89,0.35,-1.26,0  
 3R87,ASP\_114,1.89,1.33,-3.26,0  
 2BLL,ASP\_384,2.96,0.49,-1.33,0  
 1H09,ARG\_172,13.4,-2.0,0,2.94  
 1NAR,TYR\_44,13.06,1.05,-0.18,2.18  
 1J74,GLU\_75,4.71,0.21,0,0  
 2OEW,LYS\_350,10.5,0,0,0  
 3IDW,HIS\_60,6.86,0.36,0,0  
 1SUU,LYS\_577,10.5,0,0,0  
 3VJ8,LYS\_318,10.36,-0.14,0,0  
 3RZE,GLU\_73,3.24,0.21,-1.48,0  
 2QV2,LYS\_45,10.36,-0.14,0,0  
 4GCO,GLU\_246,3.28,0.28,-0.81,-0.69  
 3RNV,GLU\_341,4.5,0,0,0  
 3EVN,GLU\_144,3.98,0.28,-0.8,0  
 3V3T,ARG\_267,12.01,-0.49,0,0  
 2WB8,LYS\_470,10.5,0,0,0  
 3M70,LYS\_277,10.22,-0.28,0,0  
 3NJM,ASP\_81,1.95,0.49,-2.34,0  
 1Q46,ARG\_56,12.5,0,0,0  
 1YR6,GLU\_83,4.12,0.42,-0.8,0  
 1EV8,ARG\_126,12.5,0,0,0  
 3L3P,GLU\_335,4.57,0.07,0,0  
 3ZXY,TYR\_190,10.66,1.85,-1.19,0  
 2O4D,LYS\_23,10.29,-0.21,0,0  
 2P65,ARG\_40,12.08,-0.42,0,0  
 3HKX,LYS\_140,10.36,-0.14,0,0  
 2B61,LYS\_125,10.08,-0.42,0,0  
 2QK1,ARG\_474,11.45,-1.05,0,0  
 4EUG,ASP\_55,4.01,0.21,0,0  
 1MUF,HIS\_192,6.5,0,0,0  
 1NWA,GLU\_70,2.28,0.98,-3.2,0  
 2CL3,HIS\_89,6.51,0.01,0,0  
 3I82,TYR\_185,10.71,1.2,-0.54,0.05  
 3O7K,GLU\_166,4.29,0.21,-0.42,0  
 1GQE,ARG\_159,12.3,-2.58,0.238  
 2EFK,GLU\_142,4.11,0.21,-0.59,0  
 1DUP,GLU\_42,4.51,0.14,-0.13,0  
 3ERF,TYR\_165,9.41,0.21,-0.8,0  
 3ETV,GLU\_148,4.5,0,0,0  
 2Q99,LYS\_184,10.43,-0.07,0,0  
 3EVZ,CYS\_105,8.65,-0.73,0.39  
 1FOI,ARG\_310,13.61,-0.71,0.182  
 3P28,HIS\_217,6.5,0,0,0  
 3H8Y,HIS\_79,6.43,0,0,-0.07  
 2IN0,ARG\_88,11.94,-0.56,0,0  
 2IRM,LYS\_49,10.43,-0.07,0,0  
 1OST,CYS\_309,5.33,-4.41,-1.78,2.52  
 1MUF,TYR\_122,10.11,0.11,0,0  
 1L2F,LYS\_82,10.43,-0.07,0,0  
 2Q12,ARG\_121,11.87,-0.63,0,0  
 3D9H,ASP\_32,3.8,0,0,0  
 1LTU,LYS\_161,10.36,-0.14,0,0  
 1H4U,GLU\_372,4.5,0,0,0  
 1FKM,LYS\_452,10.5,0,0,0  
 1YM5,GLU\_203,4.5,0,0,0  
 2ZCX,TYR\_192,10,0,0,0  
 1YG2,GLU\_43,4.71,0.21,0,0  
 1NRI,ARG\_70,11.59,-0.91,0,0  
 4ECC,GLU\_101,3.06,0.28,-1.72,0  
 3BQW,TYR\_86,9.58,0.97,-1.82,0.42  
 2CVB,ARG\_178,11.1,-1.4,0,0  
 3C6B,CYS\_10,8.84,-0.16,0,0  
 3ONH,GLU\_515,4.49,0.28,-0.29,0  
 1T3Y,GLU\_119,4.64,0.14,0,0  
 1V43,ARG\_21,12.29,-0.21,0,0  
 3B21,ASP\_194,3.66,0,-0.14,0  
 2FZ4,ASP\_96,3.94,0.14,0,0  
 1W24,HIS\_86,6.6,1.6,4.05,-5.55  
 3M70,GLU\_242,4.5,0,0,0  
 3C5V,GLU\_59,4.5,0,0,0  
 3LQE,ARG\_523,12.29,-0.21,0,0  
 1QYI,GLU\_303,4.71,0.21,0,0  
 1TD6,HIS\_46,6.51,0.01,0,0  
 3NBI,LYS\_50,10.5,0,0,0  
 3NBI,GLU\_11,4.5,0,0,0  
 2G7O,GLU\_88,4.5,0,0,0  
 3ELI,HIS\_73,6.43,0.07,0,-0.14  
 1XAW,GLU\_473,3.69,0.28,-1.09,0  
 3AUF,ARG\_183,11.87,-0.63,0,0  
 1Z9L,CYS\_41,9.11,0,0,0.11  
 3FK5,ARG\_28,12.15,-0.35,0,0  
 1FO9,GLU\_222,3.19,0.63,-1.93,0  
 1R5Q,LYS\_33,10.29,-0.21,0,0  
 200K,GLU\_29,4.57,0.07,0,0  
 2CIU,LYS\_164,10.5,0,0,0  
 2R51,HIS\_150,3.35,0,-0.36,-2.79  
 2CL3,ASP\_203,3.8,0,0,0  
 1PDB,GLU\_62,4.5,0,0,0  
 4F3J,LYS\_222,10.5,0,0,0  
 3BA1,CYS\_120,8.83,-0.17,0,0  
 1RZ2,GLU\_80,4.26,0.56,-0.8,0  
 1UXO,ASP\_49,3.89,0.14,-0.05,0  
 1LN4,LYS\_8,10.29,-0.21,0,0  
 1TXD,GLU\_785,1.49,0.87,-1.48,-2.4  
 4E9E,ARG\_497,12.01,-0.49,0,0  
 3Q9P,LYS\_141,10.5,0,0,0  
 1T3Y,ARG\_91,11.66,-0.84,0,0  
 3T57,GLU\_104,4.5,0,0,0  
 2IIA,HIS\_44,6.5,0,0,0  
 1ZP2,CYS\_214,10.43,0,0.143  
 2OPJ,ARG\_259,12.12,-1.28,0.09  
 1BYI,ARG\_60,11.94,-0.56,0,0  
 1T95,GLU\_52,4.5,0,0,0  
 2Q5X,HIS\_776,6.93,0.71,0,-0.28  
 2HNG,ASP\_66,3.76,0,-0.04,0  
 2QDJ,GLU\_53,3.88,0.56,-1.18,0  
 1SNT,ARG\_208,11.74,-0.76,0,0  
 3HNX,GLU\_34,3.84,0.14,-0.8,0  
 1R15,CYS\_56,9.96,-0.05,0.101  
 3CX2,LYS\_246,10.5,0,0,0  
 3CGW,GLU\_157,4.71,0.21,0,0  
 2BLL,ASP\_631,1.89,0.49,-2.4,0  
 1X7F,LYS\_153,10.5,0,0,0  
 3TMO,HIS\_318,6.29,0,0,-0.21  
 1X91,ARG\_148,12.29,-0.21,0,0  
 4HDE,ASP\_121,2.48,0.42,-1.74,0  
 1WNH,ASP\_174,3.87,0.07,0,0  
 2V5B,ASP\_79,3.83,0.07,-0.04,0  
 3SMD,ARG\_11,11.1,-1.4,0,0  
 1SUU,GLU\_599,3.91,0.14,-0.73,0  
 2AH5,HIS\_124,6.96,0.46,0,0  
 4FZR,GLU\_152,4.28,0.49,-0.71,0  
 4FZR,GLU\_332,4.78,0.28,0,0  
 3CAX,GLU\_308,3.93,0.21,-0.78,0  
 4DNU,ARG\_354,11.87,-0.63,0,0  
 1LPL,GLU\_141,4.5,0,0,0  
 2YX0,ARG\_296,11.94,-0.56,0,0  
 1S17,ARG\_321,11.38,-1.12,0,0  
 3JSN,TYR\_18,13.7,0.07,0.31,3.32  
 2AD6,LYS\_427,10.43,-0.07,0,0  
 2P1W,ASP\_139,3.16,0.91,-1.54,0  
 2CN1,HIS\_57,1.82,0.54,-0.86,-4.37  
 2CN1,TYR\_212,11.28,1.28,0,0  
 2POL,GLU\_39,4.54,0.47,-0.8,0.37  
 3MTT,LYS\_503,10.36,-0.14,0,0  
 3HVM,CYS\_278,10.35,0,0.135  
 2P52,TYR\_231,12.66,2.66,0,0  
 2G9D,ARG\_333,12.43,-0.07,0,0  
 3UAH,LYS\_279,10.43,-0.07,0,0  
 3LJC,LYS\_89,10.43,-0.07,0,0  
 2X4L,LYS\_203,10.29,-0.21,0,0  
 1NJJ,ASP\_283,3.36,0.21,-0.65,0  
 3P28,ASP\_69,2.87,0.21,-1.14,0  
 2IXM,HIS\_248,7.09,0.8,0,-0.21  
 1O17,GLU\_64,4.5,0,0,0  
 2R57,LYS\_192,10.5,0,0,0  
 3CNU,GLU\_99,3.76,0.35,-1.1,0  
 2PWQ,ASP\_114,3.87,0.07,0,0  
 3N2T,GLU\_144,4.14,0.42,-0.78,0  
 3JRT,GLU\_9,3.91,0.21,-0.8,0  
 2PWQ,HIS\_76,2.06,0.58,-5.02  
 2GEN,ARG\_6,11.8,-0.7,0,0  
 3KEY,TYR\_407,7.62,0.16,-0.35,-2.19  
 2R4Q,ARG\_257,11.94,-0.56,0,0  
 3HVM,HIS\_319,6.28,0.74,1.45,-2.41  
 1YTD,ARG\_242,12.36,-0.14,0,0  
 2CIU,ARG\_173,12.15,-0.35,0,0  
 3UPD,TYR\_102,9.41,0.21,-0.8,0  
 2P5D,ARG\_30,12.36,-0.14,0,0  
 3A0X,LYS\_673,10.29,-0.21,0,0  
 2H2W,GLU\_51,2.17,2.37,-2.4,-2.3  
 2GZR,CYS\_235,9,0,0,0  
 2PP6,ASP\_37,3.51,0.21,-0.5,0  
 1MIX,LYS\_256,10.36,-0.14,0,0  
 3IBT,ASP\_69,3.87,0.07,0,0  
 2OOK,GLU\_255,2.92,1.67,-0.84,-2.4  
 2CN1,HIS\_203,7.16,0.8,0,-0.14  
 1WP5,TYR\_195,10.31,0.46,-0.15,0  
 3GFP,LYS\_312,10.5,0,0,0  
 3HVV,ASP\_236,3.85,0.14,-0.09,0  
 1UCH,ASP\_109,3.82,0.07,-0.05,0  
 2EEY,ASP\_85,3.38,0.35,-0.77,0  
 1ZBM,HIS\_-1,6.8,0.3,0,0  
 1Q46,HIS\_4,6.36,0,0,-0.14  
 3G9T,GLU\_15,4.64,0.14,0,0  
 1L2F,LYS\_300,10.5,0,0,0  
 3EVN,ASP\_161,1.89,0.49,-2.4,0  
 1XTZ,TYR\_60,13.09,0.14,0.55,2.4  
 3I0C,ARG\_241,11.87,-0.63,0,0  
 4ANN,TYR\_49,10.07,0.07,0,0  
 2JEO,CYS\_199,10.14,-0.87,0.201  
 3GMS,ARG\_81,12.08,-0.42,0,0  
 3K8U,HIS\_5,6.5,0,0,0  
 2V81,ARG\_14,12.29,-0.21,0,0  
 2Q99,LYS\_254,10.5,0,0,0  
 1EQ6,LYS\_101,10.29,-0.21,0,0  
 2BLL,CYS\_536,11.55,0.97,1.58  
 2YYO,GLU\_164,3.63,0.07,-0.94,0  
 1V6T,ASP\_151,3.44,0.07,-0.43,0  
 1DVO,LYS\_168,9.94,-0.56,0,0  
 3UPD,LYS\_35,10.15,-0.35,0,0  
 2AHE,LYS\_85,10.29,-0.21,0,0  
 3EZ7,CYS\_220,9.35,0,0.035  
 2QEV,GLU\_7,3.26,1.72,-0.72,-2.24  
 3DTE,ARG\_226,12.5,0,0,0  
 1QZN,LYS\_42,9.94,-0.56,0,0  
 2CBE,ASP\_72,2.81,0.42,-1.41,0  
 3LJC,ASP\_245,3.8,0,0,0  
 3O7K,CYS\_22,9.53,-0.21,0,0.74  
 2QOP,GLU\_67,3.32,2.04,-0.83,-2.4  
 2AXO,ASP\_205,3.14,0.42,-1.08,0  
 2H14,LYS\_46,10.5,0,0,0  
 2FL7,TYR\_69,12.41,0.78,-0.44,2.08  
 1DTO,ASP\_22,3.8,0,0,0  
 3M7D,ASP\_29,2.05,0.56,-2.16,0  
 2DVK,LYS\_162,10.5,0,0,0  
 1UOH,ASP\_37,0.95,1.19,-4.04,0  
 1DUN,TYR\_4,13.41,0.21,0.8,2.4  
 3ODJ,LYS\_188,10.36,-0.14,0,0  
 2AZL,ASP\_110,4.06,0.28,-0.02,0  
 1WNH,GLU\_177,3.98,0.56,-1.08,0  
 2ZQ5,HIS\_334,7.71,3.4,0,-0.14  
 1RHS,GLU\_222,6.96,2.46,0,0  
 3D9H,TYR\_156,10,0,0,0  
 3OA7,ARG\_462,12.15,-0.35,0,0  
 2QOP,LYS\_188,10.36,-0.14,0,0  
 2QRX,HIS\_173,6.5,0,0,0  
 1RL0,LYS\_129,10.5,0,0,0  
 3QKY,GLU\_266,4.85,0.35,0,0  
 3DHN,LYS\_51,10.15,-0.35,0,0  
 3VJ8,LYS\_241,10.5,0,0,0  
 3EVP,HIS\_183,7.33,0.83,0,0  
 2IIA,CYS\_8,9.07,0,0.007  
 3OOP,GLU\_126,4.18,0.35,-0.67,0  
 3JSN,GLU\_100,4.78,0.28,0,0  
 1R16,TYR\_319,8.96,0.07,-1.11,0  
 1SQH,ARG\_134,11.8,-0.7,0,0  
 1ES9,HIS\_170,6.22,0,0,-0.28  
 3AAC,ARG\_481,12.5,0,0,0  
 1AKO,LYS\_24,10.01,-0.49,0,0  
 1WLJ,LYS\_22,10.22,-0.28,0,0  
 2DVK,GLU\_48,4.71,0.21,0,0  
 3EJC,TYR\_160,11.39,0.9,0.049  
 3TMO,TYR\_329,10,0,0,0  
 2Q34,ARG\_192,11.45,-1.05,0,0  
 2AHE,GLU\_229,1.45,0.42,-3.47,0  
 2FM9,LYS\_68,10.5,0,0,0  
 3V46,HIS\_319,6.5,0,0,0  
 3H13,ARG\_397,12.29,-0.21,0,0  
 2NSN,GLU\_28,4.57,0.07,0,0  
 3PPN,ASP\_37,2.45,0.49,-1.84,0  
 1ZBP,TYR\_64,10.93,0,0.93  
 2EYI,ARG\_76,12.5,0,0,0  
 2G3A,GLU\_70,4.5,0,0,0  
 1D2K,CYS\_189,11.4,-0.22,0.262  
 2G3A,ARG\_42,11.8,-0.7,0,0  
 2I88,ASP\_350,3.8,0.14,-0.14,0  
 2AH5,LYS\_76,10.15,-0.35,0,0  
 2ZQ5,ASP\_240,2.61,0.42,-1.61,0  
 3EZ7,GLU\_382,4.69,0.28,-0.09,0  
 3BB7,ASP\_277,2.78,0.35,-1.37,0  
 3X8F,ASP\_123,3.77,0,-0.03,0  
 1RFY,GLU\_381,5.88,1.38,0,0  
 3F53,TYR\_259,10.07,0.07,0,0  
 1N81,ARG\_131,11.94,-0.56,0,0  
 3GS9,GLU\_15,4.57,0.07,0,0  
 3V3T,LYS\_44,10.43,-0.07,0,0

2WOZ,ASP\_457,3.46,0.07,-0.41,0  
 1R7J,GLU\_15,2.03,0.49,-2.96,0  
 1TXJ,LYS\_100,10.5,0,0,0  
 3L3P,CYS\_337,7.61,-1.6,0,0,21  
 1V43,ARG\_122,11.59,-0.91,0,0  
 2P1W,LYS\_142,9.31,-1.19,0,0  
 3P28,GLU\_226,4.57,0.07,0,0  
 3B7X,GLU\_136,4.15,0.28,-0.63,0  
 3QKY,TYR\_118,7.82,0.06,-0.28,-1.95  
 1WXQ,ARG\_237,12.29,-0.21,0,0  
 2H30,ASP\_151,2.64,0.35,-1.5,0  
 2Q99,ARG\_9,11.33,-3.01,0,1.84  
 2DG7,TYR\_44,10.92,1.11,-0.48,0.29  
 2R57,ASP\_356,3.76,0.77,-0.81,0  
 1YTD,ARG\_37,12.15,-0.35,0,0  
 2E3I,ASP\_93,1.89,0.63,-2.54,0  
 3I47,ASP\_66,2.02,0.49,-2.26,0  
 2AD1,LYS\_9,10.22,-0.28,0,0  
 2E3C,TYR\_242,10.6,0.6,0,0  
 1LFP,LYS\_71,10.22,-0.28,0,0  
 2O8I,HIS\_125,6.5,0,0,0  
 3RNV,ASP\_384,3.45,0.07,-0.42,0  
 1WPA,CYS\_500,9.07,0,0,0,07  
 3PZ9,TYR\_45,11.49,1.7,-0.8,0.59  
 3UPD,TYR\_77,9.81,0,-0.19,0  
 2Z84,ARG\_215,11.73,-0.77,0,0  
 3O48,LYS\_111,10.5,0,0,0  
 3CE7,LYS\_34,10.5,0,0,0  
 3TMO,LYS\_205,10.29,-0.21,0,0  
 2CVB,ARG\_22,11.87,-0.63,0,0  
 2D7U,GLU\_291,4.57,0.07,0,0  
 1S17,ASP\_187,2.6,0.7,-1.9,0  
 1YOY,GLU\_62,3.57,0.21,-1.13,0  
 2NMM,GLU\_135,4.05,0.35,-0.8,0  
 2FGG,GLU\_81,4.71,0.21,0,0  
 1R16,HIS\_18,3.41,0,0,-3.09  
 3PP8,LYS\_244,9.59,-0.91,0,0  
 2AHE,HIS\_111,7.6,1.1,0,0  
 2A1V,GLU\_69,4.42,0,-0.08,0  
 4F8A,CYS\_619,10.31,-1.02,0,2.33  
 2OKT,ASP\_74,3.38,0.42,-0.84,0  
 3LJN,GLU\_170,2.68,0.9,-1.04,-1.68  
 3HQX,LYS\_35,10.36,-0.14,0,0  
 2IF4,GLU\_135,4.64,0.14,0,0  
 3RKV,LYS\_197,10.5,0,0,0  
 1L2F,LYS\_330,10.08,-0.42,0,0  
 3GMS,ARG\_142,12.22,-0.28,0,0  
 2XJ4,GLU\_200,3.86,0.21,-0.84,0  
 3AU3,LYS\_586,10.22,-0.28,0,0  
 2A6B,GLU\_187,1.15,0.65,-4,0  
 2BDV,ARG\_175,11.66,-0.84,0,0  
 2EEY,LYS\_149,9.73,-0.77,0,0  
 3EVN,TYR\_189,9.93,0.73,-0.8,0  
 2R51,TYR\_253,9.75,0,-0.25,0  
 2YWX,TYR\_137,13.54,0.0,25,3.28  
 3B7H,LYS\_46,10.5,0,0,0  
 1NIJ,CYS\_118,9.07,0,0,0,07  
 1KCM,TYR\_58,10.14,0.14,0,0  
 4EKU,TYR\_118,13.22,1.59,0,1.63  
 3ONH,ASP\_518,3.61,0.14,-0.33,0  
 2HRZ,ARG\_307,11.79,-0.99,0,0.28  
 2B3M,CYS\_49,8.89,-0.11,0,0  
 3P28,TYR\_95,6.75,0.59,-1.44,-2.4  
 4EVF,ARG\_151,13.64,-1.12,0,2.26  
 2OKT,TYR\_301,13.8,2.22,-0.64,2.21  
 4DEZ,GLU\_168,4.03,0.28,-0.75,0  
 3M9A,ASP\_85,3.69,0,-0.11,0  
 3SMD,GLU\_131,3.77,0.07,-0.8,0  
 3LQE,ASP\_440,4.08,0.28,0,0  
 3L0D,GLU\_70,4.64,0.14,0,0  
 3B21,HIS\_110,6.29,0,0,-0.21  
 1F2V,ASP\_102,2.46,0.56,-1.9,0  
 3ELI,CYS\_106,8.41,-0.66,0,0.07  
 1WXF,TYR\_206,10.96,0.07,0,0.89  
 2B0J,ASP\_310,2.45,0.84,-2.2,0  
 1X9G,ARG\_126,11.52,-0.98,0,0  
 2Q13,LYS\_152,10.5,0,0,0  
 4H86,LYS\_7,10.08,-0.42,0,0  
 4DBX,ASP\_206,2.49,0.56,-1.87,0  
 1AK1,TYR\_271,10.0,0,0,0  
 3F53,LYS\_199,10.36,-0.14,0,0  
 1J8B,GLU\_32,4.27,0.7,-0.93,0  
 2IXM,GLU\_241,4.5,0,0,0  
 1QYI,LYS\_189,10.5,0,0,0  
 2INO,ARG\_26,12.29,-0.21,0,0  
 2FL4,CYS\_91,10.33,0,0,1.33  
 2O8P,TYR\_39,10.0,0,0,0  
 3GE9,GLU\_202,4.5,0,0,0  
 1L2F,ASP\_176,3.13,0.49,-1.16,0  
 3HUE,ARG\_27,11.8,-0.7,0,0  
 1XIP,ARG\_119,12.5,0,0,0  
 2CVB,ARG\_113,11.66,-0.84,0,0  
 3PP8,GLU\_50,3.77,0.07,-0.8,0  
 1EQ6,GLU\_182,1.11,0.77,-4.16,0  
 4ETX,ARG\_435,12.5,0,0,0  
 1S7K,HIS\_167,7.29,0.79,0,0  
 3K8J,TYR\_225,10.11,0.52,-0.41,0  
 2G3A,TYR\_98,10.0,0,0,0  
 1Y2Q,GLU\_87,4.71,0.21,0,0  
 2P0Y,TYR\_271,10.0,0,0,0  
 2CXA,ARG\_88,11.94,-0.56,0,0  
 2IXM,GLU\_117,4.71,0.21,0,0  
 3BCY,GLU\_26,4.5,0,0,0  
 2F9F,LYS\_147,10.43,-0.07,0,0  
 3ZXY,ASP\_176,3.77,0,-0.03,0  
 1O59,ARG\_56,12.29,-0.21,0,0  
 3M3P,ARG\_216,12.15,-0.35,0,0  
 3HVM,TYR\_191,10.21,0,0,0.21  
 2B0J,LYS\_341,10.43,-0.07,0,0  
 2R57,ASP\_204,4.01,0.21,0,0  
 1S17,GLU\_252,3.47,0.28,-1.31,0  
 1Y0K,ARG\_12,11.94,-0.56,0,0  
 2B6P,HIS\_61,6.97,0.61,0,-0.14  
 3CO1,ASP\_26,3.89,0.14,-0.05,0  
 3CIV,LYS\_89,10.5,0,0,0  
 2VGY,ARG\_146,12.08,-0.42,0,0  
 3UAH,LYS\_287,10.29,-0.21,0,0  
 2Z61,ASP\_238,3.37,0.07,-0.5,0  
 3RLE,ASP\_51,4.01,0.21,0,0  
 2G9D,LYS\_299,10.5,0,0,0  
 2AZL,GLU\_143,4.22,0.66,0,-0.94  
 1ZBS,GLU\_110,2.38,0.28,-2.4,0  
 2AH5,TYR\_130,9.34,0.14,-0.8,0  
 1YTD,LYS\_317,10.29,-0.21,0,0  
 2Z61,LYS\_74,10.5,0,0,0  
 2YXO,GLU\_186,4.71,0.21,0,0  
 2P65,ARG\_150,11.8,-0.7,0,0  
 2O8P,ASP\_101,3.94,0.21,-0.07,0  
 2FZ4,GLU\_158,4.5,0,0,0  
 1X8F,LYS\_91,10.01,-0.49,0,0  
 1O6D,LYS\_142,10.29,-0.21,0,0  
 2D7J,LYS\_63,10.15,-0.35,0,0  
 2F4Q,ASP\_208,1.98,1.05,-2.88,0  
 3C6B,LYS\_200,9.59,-0.91,0,0  
 3RLN,ASP\_709,1.35,1.26,-3.71,0  
 3K8J,LYS\_73,10.5,0,0,0  
 3MIX,GLU\_325,4.5,0,0,0  
 4EKU,CYS\_246,9.91,-0.24,0,1.15  
 1TUL,ARG\_38,12.5,0,0,0  
 2FL7,ARG\_194,12.15,-0.35,0,0  
 3PU6,LYS\_140,10.15,-0.35,0,0  
 3I4T,LYS\_52,10.29,-0.21,0,0  
 3BPV,ARG\_128,12.5,0,0,0  
 2D0A,GLU\_274,3.83,0.21,-0.88,0  
 2CYG,TYR\_218,10.88,0.88,0,0  
 1NAR,GLU\_24,4.64,0.14,0,0  
 3LPZ,HIS\_132,3.63,1.01,0,-3.88  
 1FQI,TYR\_404,10.18,0.98,-0.8,0  
 1WLJ,GLU\_208,4.85,0.35,0,0  
 2GEN,ARG\_164,12.15,-0.35,0,0  
 3BB7,HIS\_176,7.02,0.8,0,-0.28  
 2BQQ,ASP\_135,3.87,0.07,0,0  
 1MN3,ARG\_409,12.08,-0.42,0,0  
 2WB3,GLU\_271,3.66,1.05,-1.89,0  
 1N81,ASP\_111,4.01,0.21,0,0  
 2JHY,TYR\_175,9.92,0.28,-0.36,0  
 3VHJ,ASP\_81,2.06,0.28,-2.02,0  
 2FZ4,HIS\_123,7.09,0.66,0,-0.07  
 2ILR,GLU\_430,4.5,0,0,0  
 3UAH,ASP\_294,3.97,0.21,-0.04,0  
 3A7L,GLU\_130,1.39,0,-1.47,-3.64  
 3LJN,GLU\_228,4.5,0,0,0  
 3PZ9,LYS\_166,10.29,-0.21,0,0  
 2VC8,ARG\_55,12.29,-0.21,0,0  
 1FQI,CYS\_332,10.7,-0.01,0,1.71  
 2CXA,ASP\_54,3.07,0.49,-1.22,0  
 3RAZ,ARG\_57,12.08,-0.42,0,0  
 1J33,GLU\_4,4.57,0.07,0,0  
 3IU5,HIS\_51,7.23,0.87,0,-0.14  
 1VSM,LYS\_184,10.29,-0.21,0,0  
 1OIS,ARG\_279,11.59,-0.91,0,0  
 2Q13,GLU\_125,4.64,0.14,0,0  
 3G59,HIS\_170,7.16,0.8,0,-0.14  
 1GQE,HIS\_214,6.81,0.38,0,-0.07  
 1MIX,HIS\_228,2.59,0,0,-3.91  
 1Q2Y,TYR\_114,11.96,1.96,0,0  
 2EYI,ASP\_117,3.42,0.42,-0.8,0  
 2PGX,ASP\_7,1.74,0.49,-2.55,0  
 3B7X,ASP\_54,4.01,0.21,0,0  
 1O6D,GLU\_108,3.84,0.14,-0.8,0  
 2EYI,LYS\_103,9.73,-0.77,0,0  
 2QRX,GLU\_118,3.34,0.35,-1.51,0  
 2X4J,LYS\_136,10.01,-0.49,0,0  
 3CN5,LYS\_33,10.5,0,0,0  
 2R57,TYR\_286,10.71,0.14,0,0.57  
 1XTD,TYR\_100,10.76,0.07,-0.8,1.5  
 4H89,GLU\_42,3.46,0.21,-1.25,0  
 2AHE,GLU\_20,4.05,0.35,-0.8,0  
 3HYQ,ARG\_124,11.8,-0.7,0,0  
 3DTE,CYS\_175,11.01,0,0,2.01  
 1X8F,CYS\_38,10.44,0,0,1.44  
 1OTM,LYS\_217,10.43,-0.07,0,0  
 1JB3,ASP\_29,1.75,0.91,-2.96,0  
 3U4K,TYR\_29,10.0,0,0,0  
 3EX9,LYS\_69,10.43,-0.07,0,0  
 2AZL,GLU\_182,4.71,0.21,0,0  
 2ZOW,ARG\_16,12.5,0,0,0  
 1RAJ,TYR\_313,11.09,0.14,-1.14,2.08  
 1SBX,CYS\_150,9.29,0,0,0.29  
 1F2V,HIS\_43,6.43,0,0,-0.07  
 2FBQ,LYS\_176,10.36,-0.14,0,0  
 1SUU,GLU\_661,4.17,1.03,-1.36,0  
 1XDZ,LYS\_234,10.29,-0.21,0,0  
 4H4J,TYR\_144,10.07,0.07,0,0  
 2CBE,ARG\_254,11.32,-1.95,0,0.77  
 3L7N,ASP\_44,3.78,0.14,-0.16,0  
 1WXF,GLU\_259,1.48,0.6,-1.36,-2.27  
 2YWJ,HIS\_15,6.97,1.6,2.32,-3.45  
 3O48,HIS\_106,6.43,0,0,-0.07  
 4FZN,ARG\_37,12.5,0,0,0  
 3UAH,LYS\_428,10.43,-0.07,0,0  
 2B6P,ARG\_127,7.96,-4.54,0,0  
 3M7G,GLU\_215,0.53,1.75,-2.23,-3.5  
 2QZQ,ASP\_88,3.28,0.28,-0.8,0  
 2IRM,HIS\_329,6.5,0,0,0  
 4E6S,ARG\_4,12.43,-0.07,0,0  
 3CQ1,LYS\_95,10.5,0,0,0  
 3GE9,GLU\_233,4.57,0.07,0,0  
 1R6Y,ARG\_9,12.29,-0.21,0,0  
 2WB3,LYS\_373,10.5,0,0,0  
 1FKM,CYS\_428,11.72,0,0,2.72  
 4FZR,ASP\_164,3.23,0.28,-0.85,0  
 2X4L,ASP\_193,3.94,0.14,0,0  
 3ZTA,ARG\_136,10.5,0,0,0  
 2F4Q,ASP\_70,1.44,0.98,-3.34,0  
 3RJX,GLU\_93,3.31,0.28,-1.47,0  
 2Q99,GLU\_263,4.5,0,0,0  
 4FH3,TYR\_178,11.13,2.42,-1.29,0  
 2B61,ARG\_350,11.52,-0.98,0,0  
 3A7L,GLU\_19,3.12,0.35,-1.73,0  
 1XIPCYS\_93,11.36,-0.97,1.12,2.2  
 1XKR,ASP\_163,3.73,0.35,-0.42,0  
 2B78,TYR\_143,11.1,1.48,0,-0.38  
 1T95,GLU\_53,4.24,0.49,-0.75,0  
 1YM5,GLU\_30,4.5,0,0,0  
 3EX9,ARG\_159,12.5,0,0,0  
 1NAR,GLU\_46,4.5,0,0,0  
 2FM9,ASP\_64,3.94,0.14,0,0  
 1SQW,GLU\_8,1.13,0.77,-4.14,0  
 2EFK,GLU\_88,4.19,0.49,-0.8,0  
 3Q1C,ASP\_268,3.73,0,-0.07,0  
 1ZBS,TYR\_64,11.35,0.1,0,1.25  
 3UAH,TYR\_499,10.02,0.07,-0.05,0  
 1O5T,ASP\_205,3.8,0,0,0  
 1ZBM,HIS\_58,2.19,0.84,-1.71,-3.44  
 3H04,ASP\_54,3.24,0.28,-0.84,0  
 1NJ4,ARG\_174,12.68,-0.69,0,0.87  
 1ZKZ,LYS\_68,10.5,0,0,0  
 3RLE,HIS\_132,7.23,0.8,0,-0.07  
 2V81,ASP\_19,2.6,0.28,-1.49,0  
 1WYC,GLU\_74,4.64,0.14,0,0  
 1RZ2,ASP\_88,3.79,0.07,-0.08,0  
 2NRR,TYR\_396,7.12,0.5,-0.98,-2.39  
 2W0G,LYS\_224,10.15,-0.35,0,0  
 1J33,ARG\_10,12.43,-0.07,0,0  
 3DB9,GLU\_135,4.6,0.21,-0.11,0  
 2IDC,ASP\_77,3.73,0.07,-0.14,0  
 2C2Y,CYS\_91,7.29,-1.09,-1.75,1.13  
 2V5B,ARG\_221,12.43,-0.07,0,0  
 1O5T,GLU\_385,4.02,0.28,-0.76,0  
 3I47,GLU\_225,4.5,0,0,0  
 2OJQ,GLU\_453,4.64,0.14,0,0  
 3BA1,ARG\_249,11.38,-1.12,0,0  
 1QQH,LYS\_71,10.29,-0.21,0,0  
 2Q99,LYS\_177,10.5,0,0,0  
 2D2S,ARG\_551,12.01,-0.49,0,0  
 1RZ2,ARG\_243,11.37,-1.45,0,0.32  
 2P0Y,CYS\_227,10.96,-0.97,0.7,2.23  
 1UXO,ASP\_147,3.62,0.42,-0.6,0  
 1QQH,ARG\_156,11.87,-0.63,0,0  
 1WXQ,LYS\_375,10.5,0,0,0  
 1XAW,LYS\_462,10.36,-0.14,0,0  
 1MHN,CYS\_98,9.03,-0.12,0,0.15  
 1SJV,ASP\_89,2.67,0.35,-1.49,0  
 3JV1,GLU\_74,4.5,0,0,0  
 3G9B,LYS\_123,10.43,-0.07,0,0

2YWX, GLU\_139, 3.83, 0.35, -1.02, 0  
 2CN1, LYS\_121, 10.5, 0, 0, 0  
 3M7D, HIS\_200, 3.62, 1.6, 0.28, -4.76  
 1FKM, ARG\_310, 11.94, -0.56, 0, 0  
 1RHS, CYS\_63, 10.66, 0, 0, 1.66  
 1TR9, HIS\_212, 6.6, 0.17, 0, -0.07  
 2NSN, GLU\_81, 3.77, 0.28, -1.01, 0  
 2CVB, LYS\_176, 9.94, -0.56, 0, 0  
 3U0V, CYS\_98, 7.14, -0.97, -2.26, 1.38  
 2GKG, GLU\_23, 4.12, 0.42, -0.8, 0  
 1R3D, ARG\_142, 11.59, -0.91, 0, 0  
 4EKU, ARG\_159, 12.54, -3.48, 0.35, 2  
 2B78, LYS\_92, 10.5, 0, 0, 0  
 3CAX, LYS\_298, 10.29, -0.21, 0, 0  
 1MUF, GLU\_254, 4.5, 0, 0, 0  
 2B0A, CYS\_122, 12.09, -0.04, 0.3, 1.3  
 3QAV, ARG\_177, 11.03, -1.47, 0, 0  
 3RFF, GLU\_56, 1.97, 0.56, -3.09, 0  
 1UW7, GLU\_3, 4.64, 0.14, 0, 0  
 2VGM, ASP\_38, 4.01, 0.21, 0, 0  
 1OLR, ARG\_97, 11.59, -0.91, 0, 0  
 2AD1, GLU\_84, 5.24, 3.97, -3.24, 0  
 2R0S, HIS\_265, 3.1, 0.05, 0, -3.45  
 1X7F, TYR\_289, 13.03, 0.14, 0.51, 2.38  
 1OLR, TYR\_132, 10, 0, 0, 0  
 2BT8, CYS\_182, 7.64, -1.36, 0, 0  
 3N2T, ASP\_322, 2.47, 0.35, -1.68, 0  
 3JV1, GLU\_100, 4.71, 0.21, 0, 0  
 1R3F, GLU\_300, 4.32, 0.42, -0.6, 0  
 3E7P, LYS\_142, 10.43, -0.07, 0, 0  
 3F5D, GLU\_30, 4.5, 0, 0, 0  
 3CAX, LYS\_463, 10.5, 0, 0, 0  
 3A4C, GLU\_468, 4.5, 0, 0, 0  
 1TXD, ASP\_914, 3.87, 0.07, 0, 0  
 3TMO, LYS\_219, 9.94, -0.56, 0, 0  
 3IDW, CYS\_12, 9.27, -0.36, 0, 0.63  
 1TP6, LYS\_52, 10.22, -0.28, 0, 0  
 3HVV, ARG\_265, 12.36, -0.14, 0, 0  
 2O8P, GLU\_93, 4.5, 0, 0, 0  
 4H86, GLU\_129, 3.86, 0.42, -1.06, 0  
 2XHC, TYR\_173, 10, 0, 0, 0  
 1ZYL, TYR\_252, 10.12, 2.09, -0.89, -1.09  
 2RIK, LYS\_37, 9.94, -0.56, 0, 0  
 3GE9, LYS\_164, 10.5, 0, 0, 0  
 2IXM, ASP\_250, 3.78, 0.35, -0.36, 0  
 3EJG, GLU\_155, 2.47, 0.73, -2.76, 0  
 1PV5, HIS\_90, 6.43, 0, 0, -0.07  
 3M7D, ASP\_75, 3.35, 0.49, -0.94, 0  
 3ZRI, ARG\_77, 12.5, 0, 0, 0  
 1UOH, TYR\_160, 10, 0, 0, 0  
 1SBX, ARG\_132, 12.43, -0.07, 0, 0  
 3IDW, GLU\_33, 4.64, 0.14, 0, 0  
 3CBN, GLU\_51, 4.05, 0.35, -0.8, 0  
 3A0X, ARG\_627, 11.94, -0.56, 0, 0  
 3DB9, ASP\_218, 2.37, 0.7, -2.13, 0  
 2ZCO, LYS\_13, 10.5, 0, 0, 0  
 4E6S, LYS\_46, 10.5, 0, 0, 0  
 1YB2, ARG\_65, 11.94, -0.56, 0, 0  
 3HVM, LYS\_195, 10.5, 0, 0, 0  
 2Q34, LYS\_235, 10.43, -0.07, 0, 0  
 1Y2Q, LYS\_16, 10.5, 0, 0, 0  
 2CXK, GLU\_73, 2.86, 0.63, -2.26, 0  
 1AK1, GLU\_145, 4.57, 0.07, 0, 0  
 1WJG, HIS\_37, 4.02, 0.89, 0, -3.37  
 2YWJ, LYS\_83, 10.22, -0.28, 0, 0  
 3C5V, GLU\_290, 4.48, 0.14, -0.16, 0  
 2RIK, GLU\_154, 4.27, 0.42, -0.65, 0  
 1W24, LYS\_23, 10.29, -0.21, 0, 0  
 2AD1, GLU\_157, 3.52, 0.42, -1.39, 0  
 2Z0M, GLU\_19, 2.71, 0.77, -2.56, 0  
 4ACJ, ASP\_749, 3.94, 0.14, 0, 0  
 3OBS, LYS\_101, 10.5, 0, 0, 0  
 3MIX, GLU\_574, 4.64, 0.14, 0, 0  
 3MTT, GLU\_555, 4.17, 0.07, -0.4, 0  
 3DZ1, ASP\_294, 3.12, 0.49, -1.16, 0  
 3LJC, TYR\_22, 11.02, 1.22, -0.2, 0  
 3DTE, ASP\_132, 3.49, 0.49, -0.8, 0  
 1GXN, GLU\_624, 0.4, 0.7, -4.8, 0  
 2BDV, LYS\_188, 10.08, -0.42, 0, 0  
 4DNU, HIS\_78, 7.28, 7.31, -0.6, -5.94  
 1JB3, HIS\_53, 6.43, 0, 0, -0.07  
 2ZQ5, GLU\_38, 3.25, 0.35, -1.6, 0  
 3NR5, GLU\_55, 4.48, 0.28, -0.3, 0  
 2OEW, ARG\_70, 11.76, -0.74, 0, 0  
 3Q1C, CYS\_325, 9.46, -0.09, 0.55, 2  
 2D2S, ASP\_677, 2.92, 0.07, -0.95, 0  
 2QOP, ARG\_13, 11.94, -0.56, 0, 0  
 2Z84, HIS\_24, 6.5, 0, 0, 0  
 1DZF, LYS\_171, 10.5, 0, 0, 0  
 1RHS, ARG\_158, 11.87, -0.63, 0, 0  
 3GA2, GLU\_225, 4.14, 0.28, -0.64, 0  
 3P2F, ASP\_182, 1.9, 0.84, -2.74, 0  
 2E3S, ARG\_405, 11.66, -0.84, 0, 0  
 3CS1, GLU\_32, 4.5, 0, 0, 0  
 4GCO, LYS\_171, 10.43, -0.07, 0, 0  
 1ES9, ARG\_198, 11.8, -0.7, 0, 0  
 3IOO, ARG\_148, 11.31, -1.19, 0, 0  
 3CCY, ARG\_26, 11.87, -0.63, 0, 0  
 3RNV, TYR\_390, 10, 0, 0, 0  
 3CGW, GLU\_84, 3.45, 0.42, -1.47, 0  
 2C13, GLU\_265, 2.02, 2.16, -2.4, -2.24  
 3CO1, HIS\_18, 6.5, 0, 0, 0  
 1RHS, ARG\_205, 12.15, -0.35, 0, 0  
 1TXJ, LYS\_2, 10.01, -0.49, 0, 0  
 3US6, TYR\_13, 9.82, 0.07, -0.25, 0  
 1SJV, ARG\_14, 12.22, -0.28, 0, 0  
 1C3K, GLU\_75, 3.68, 0.21, -1.03, 0  
 1PGV, CYS\_227, 8.95, -0.34, 0.29, 2  
 2BDV, GLU\_77, 3.91, 0.21, -0.8, 0  
 1ZBS, GLU\_129, 4.5, 0, 0, 0  
 3N0K, ASP\_26, 3.59, 0, -0.21, 0  
 1NFN, GLU\_49, 4.5, 0, 0, 0  
 1N81, LYS\_200, 10.43, -0.07, 0, 0  
 2QEV, GLU\_114, 4.46, 2.03, -0.8, -1.27  
 3ZRI, ARG\_3, 12.5, 0, 0, 0  
 3IV4, TYR\_53, 10.4, 0.0, 4, 0  
 2AZL, GLU\_237, 4.13, 0.21, -0.58, 0  
 2CWC, ARG\_133, 9.71, -4.81, 0.2, 0.2  
 3M7G, ARG\_172, 12.22, -0.28, 0, 0  
 1RAJ, CYS\_418, 9.07, -0.83, 0.0, 9  
 1RSS, ARG\_78, 12.36, -0.14, 0, 0  
 2Q98, TYR\_96, 9.51, 0, -0.49, 0  
 3Q1C, ASP\_46, 3.73, 0, -0.07, 0  
 4DEZ, TYR\_164, 10, 0, 0, 0  
 1JSX, LYS\_100, 10.5, 0, 0, 0  
 1X9G, LYS\_143, 10.5, 0, 0, 0  
 3EVN, GLU\_123, 3.82, 3.96, -2.24, 2.4  
 2FM9, LYS\_228, 10.29, -0.21, 0, 0  
 3ETU, GLU\_297, 4.57, 0.07, 0, 0  
 3M70, GLU\_247, 4.71, 0.21, 0, 0  
 3GG6, GLU\_56, 4.71, 0.21, 0, 0  
 1SQW, CYS\_153, 8.76, -0.5, 0.0, 26  
 3GV0, ASP\_222, 3.6, 0.07, -0.27, 0  
 1WP5, LYS\_243, 10.5, 0, 0, 0  
 3U0V, HIS\_184, 7.15, 0.79, 0, -0.14  
 2Q07, ARG\_343, 12.08, -0.42, 0, 0  
 1WYC, ARG\_62, 12.43, -0.07, 0, 0  
 3RJX, TYR\_207, 10.26, 0.18, 0, 0.08  
 100X, ARG\_178, 12.29, -0.21, 0, 0  
 1TWU, TYR\_112, 10, 0, 0, 0  
 2EYI, ARG\_232, 12.08, -0.42, 0, 0  
 3JV1, GLU\_216, 3.61, 0.21, -1.1, 0  
 3S0A, ARG\_20, 4.64, 0.14, 0, 0  
 3RRQ, LYS\_131, 10.5, 0, 0, 0  
 1EW4, ARG\_8, 12.5, 0, 0, 0  
 3EAZ, TYR\_145, 10.89, 0.21, -0.8, 1.48  
 4FH3, GLU\_284, 4.15, 0.07, -0.42, 0  
 3QAV, GLU\_79, 1.29, 1.16, -1.96, -2.4  
 1NWA, ASP\_87, 3.4, 0.42, -0.82, 0  
 3BQE, TYR\_296, 10.21, 0.21, 0, 0  
 1LPL, GLU\_228, 4.5, 0, 0, 0  
 3P28, GLU\_224, 4.5, 0, 0, 0  
 3N0K, GLU\_116, 4.5, 0, 0, 0  
 3GA2, ASP\_111, 2.07, 0.77, -2.51, 0  
 1T6L, ARG\_28, 11.73, -0.77, 0, 0  
 1NIJ, ASP\_79, 2.08, 1.26, -2.99, 0  
 1ILW, GLU\_161, 4.37, 0.14, -0.27, 0  
 4EF5, TYR\_274, 10, 0, 0, 0  
 1R53, LYS\_212, 10.5, 0, 0, 0  
 1NFN, ARG\_158, 12.15, -0.35, 0, 0  
 1YTD, LYS\_202, 10.43, -0.07, 0, 0  
 1R16, ASP\_263, 1.25, 0.42, -2.97, 0  
 1W7B, LYS\_233, 10.43, -0.07, 0, 0  
 3CAX, LYS\_437, 10.36, -0.14, 0, 0  
 2P65, GLU\_109, 3.39, 0.91, -2.02, 0  
 2ILR, ARG\_343, 11.94, -0.56, 0, 0  
 1NWA, CYS\_154, 8.48, -0.78, 0.0, 26  
 3IOO, GLU\_145, 3.87, 0.14, -0.77, 0  
 2QVO, LYS\_39, 10.5, 0, 0, 0  
 1H09, LYS\_250, 10.5, 0, 0, 0  
 3M16, GLU\_78, 3.95, 0.07, -0.62, 0  
 1YB2, LYS\_199, 10.43, -0.07, 0, 0  
 3US6, GLU\_54, 4.57, 0.07, 0, 0  
 3LMO, LYS\_91, 10.29, -0.21, 0, 0  
 2YX0, LYS\_259, 10.29, -0.21, 0, 0  
 3LOD, ARG\_102, 11.87, -0.63, 0, 0  
 1SNT, ASP\_131, 0.88, 0.91, -3.83, 0  
 4GA2, ARG\_120, 12.15, -0.35, 0, 0  
 1X91, LYS\_65, 10.29, -0.21, 0, 0  
 1YTO, GLU\_62, 3.58, 0.63, -1.55, 0  
 1QSZ, ASP\_540, 4.01, 0.21, 0, 0  
 2EDM, LYS\_198, 10.43, -0.07, 0, 0  
 1UAJ, ARG\_121, 12.29, -0.21, 0, 0  
 3I4T, LYS\_75, 10.43, -0.07, 0, 0  
 1MUS, CYS\_393, 10.23, -0.64, 0.43, 1.45  
 3EJC, HIS\_164, 6.5, 0, 0, 0  
 2D7J, ASP\_7, 3.13, 0.42, -1.09, 0  
 2H30, LYS\_42, 10.5, 0, 0, 0  
 2GAU, GLU\_24, 4.5, 0, 0, 0  
 1O59, ARG\_240, 12.29, -0.21, 0, 0  
 3BZT, ASP\_344, 4.37, 0.35, 0.22, 0  
 1QQE, TYR\_66, 10.47, 0.14, -0.37, 0.7  
 3O7K, HIS\_42, 6.5, 0, 0, 0  
 2R4Q, LYS\_204, 9.73, -0.77, 0, 0  
 2F8H, ARG\_353, 12.5, 0, 0, 0  
 1JSX, ASP\_18, 3.44, 0, -0.36, 0  
 2B2H, ARG\_111, 8.99, -4, 0, 0.48  
 3VHJ, HIS\_114, 6.62, 0.26, 0, -0.14  
 2VAN, GLU\_329, 4.53, 0.14, -0.11, 0  
 1HF8, ARG\_139, 12.08, -0.42, 0, 0  
 4FH3, TYR\_366, 10, 0, 0, 0  
 3RE9, ARG\_104, 4.5, 0, 0, 0  
 2P65, ARG\_17, 12.15, -0.35, 0, 0  
 3A7L, ASP\_68, 3.8, 0.14, -0.15, 0  
 3JZN, ARG\_169, 11.94, -0.56, 0, 0  
 3RFF, ARG\_121, 12.15, -0.35, 0, 0  
 4ANN, GLU\_43, 3.92, 0.49, -1.07, 0  
 3A4C, HIS\_550, 6.5, 0, 0, 0  
 2E3H, LYS\_277, 10.36, -0.14, 0, 0  
 3H13, HIS\_287, 6.5, 0, 0, 0  
 3CSR, ARG\_147, 13.23, -2.66, 0.3, 38  
 3JZ9, LYS\_385, 10.5, 0, 0, 0  
 2FZP, ARG\_270, 12.29, -0.21, 0, 0  
 2W2S, GLU\_195, 4.57, 0.07, 0, 0  
 2CBE, ARG\_89, 11.31, -1.19, 0, 0  
 4F8A, TYR\_666, 10, 0, 0, 0  
 3G9T, GLU\_23, 4.57, 0.07, 0, 0  
 2P5D, GLU\_139, 4.71, 0.21, 0, 0  
 3HVV, ARG\_268, 12.36, -0.14, 0, 0  
 2VAN, LYS\_220, 10.5, 0, 0, 0  
 2QZQ, HIS\_110, 2.38, 0.31, -1.52, -2.91  
 3UPD, HIS\_-18, 6.5, 0, 0, 0  
 4FCU, ASP\_89, 2.79, 0.28, -1.29, 0  
 1X1A, LYS\_236, 9.59, -0.91, 0, 0  
 2OBI, ASP\_165, 2.62, 0.42, -1.6, 0  
 3U4K, LYS\_106, 10.5, 0, 0, 0  
 3QAV, ASP\_65, 3.85, 0.07, -0.02, 0  
 1R16, GLU\_197, 1.58, 2.03, -1.38, -3.56  
 1X1E, ASP\_56, 3.96, 0.63, -0.48, 0  
 3ASE, LYS\_236, 9.59, -0.91, 0, 0  
 1SQW, ASP\_87, 3.73, 0, -0.07, 0  
 2OBI, LYS\_127, 10.5, 0, 0, 0  
 3RLN, GLU\_739, 4.64, 0.14, 0, 0  
 2OBI, ASP\_30, 3.37, 0.42, -0.85, 0  
 1ZCU, TYR\_186, 13.44, 0.24, 0.8, 2.4  
 3N0K, TYR\_75, 2.22, 1.12, -2.7, 0  
 3H9W, ARG\_63, 10.75, -1.75, 0, 0  
 3EJC, TYR\_8, 9.03, 0, -0.97, 0  
 3GEC, HIS\_493, 1.41, 0, 0, -5.09  
 1S7K, LYS\_133, 10.43, -0.07, 0, 0  
 1R9W, TYR\_329, 10, 0, 0, 0  
 3CS1, LYS\_178, 10.29, -0.21, 0, 0  
 2P4D, LYS\_53, 10.43, -0.07, 0, 0  
 3M7G, HIS\_246, 4.58, 1.39, 0, -3.31  
 3TOW, LYS\_144, 10.01, -0.49, 0, 0  
 1ZYL, GLU\_267, 1.98, 0.9, -1.02, -2.4  
 2AD1, ARG\_289, 12.5, 0, 0, 0  
 1Q5Z, LYS\_586, 10.43, -0.07, 0, 0  
 1XTD, GLU\_144, 4.71, 0.21, 0, 0  
 100X, HIS\_174, 1.59, 0.08, -1.98, -3.01  
 1V43, GLU\_63, 4.84, 0.63, -0.29, 0  
 2GZQ, GLU\_67, 4.57, 0.07, 0, 0  
 1XEU, LYS\_120, 10.22, -0.28, 0, 0  
 2GZR, ARG\_97, 12.01, -0.49, 0, 0  
 3T5B, ARG\_337, 11.66, -0.84, 0, 0  
 2H30, HIS\_36, 6.5, 0, 0, 0  
 1I60, TYR\_100, 12.24, 0.95, 0, 1.29  
 1DZF, ASP\_182, 2.49, 0.49, -1.8, 0  
 2OKT, ASP\_227, 3.39, 0.07, -0.47, 0  
 3BWT, ARG\_666, 11.94, -0.56, 0, 0  
 4F85, GLU\_150, 4.78, 0.28, 0, 0  
 2YX0, GLU\_138, 3.46, 0.49, -1.53, 0  
 4ETX, GLU\_363, 4.76, 0.49, -0.23, 0  
 1TD6, ASP\_59, 2.7, 0.42, -1.52, 0  
 1PGV, ARG\_230, 11.8, -0.7, 0, 0  
 1R29, GLU\_115, 4.57, 0.07, 0, 0  
 3GFP, LYS\_454, 10.5, 0, 0, 0  
 1RSS, LYS\_138, 10.29, -0.21, 0, 0  
 3MTT, ARG\_539, 11.73, -0.77, 0, 0  
 4EKU, LYS\_334, 10.08, -0.42, 0, 0  
 3LQE, LYS\_349, 10.5, 0, 0, 0  
 2QVT, TYR\_42, 10.38, 0, -0.66, 1.04  
 3BZT, LYS\_254, 10.5, 0, 0, 0  
 3PP8, HIS\_267, 7.16, 0.8, 0, -0.14  
 1AM2, ASP\_158, 2.8, 0.49, -1.49, 0  
 3S0A, ASP\_30, 3.45, 0.42, -0.77, 0



3IL3,GLU\_218,4.13,0.28,-0.65,0  
 1XFK,LYS\_60,10.5,0,0,0  
 1T95,GLU\_197,3.19,0.49,-1.8,0  
 3COU,HIS\_133,6.22,0,0,-0.28  
 3C2E,TYR\_46,9.27,0.07,-0.8,0  
 2B61,ARG\_260,9.17,-1.82,0,-1.51  
 1UAJ,ASP\_44,1.68,0.84,-2.96,0  
 1Q46,HIS\_139,4.01,0.3,0,-2.79  
 3BJV,TYR\_44,10,0,0,0  
 1AIL,ARG\_19,11.8,-0.7,0,0  
 1T3J,HIS\_735,6.83,0.46,0,-0.14  
 3VJ8,TYR\_139,13.55,0.35,0.8,2.4  
 3Q6L,GLU\_117,4.22,0.07,-0.35,0  
 1T3J,GLU\_723,4.5,0,0,0  
 1GQE,LYS\_302,10.43,-0.07,0,0  
 3RLE,ARG\_21,12.15,-0.35,0,0  
 3BB7,ASP\_261,2.61,0.35,-1.54,0  
 2RGY,HIS\_167,5.59,1.6,0,-2.51  
 3GFP,LYS\_443,10.5,0,0,0  
 2IRM,HIS\_194,7.28,0.78,0,0  
 1FO9,ARG\_380,12.22,-0.28,0,0  
 3VHJ,LYS\_63,10.15,-0.35,0,0  
 1QYI,CYS\_18,11.55,-1.07,1.48,2.13  
 2OSA,GLU\_365,4.16,0.28,-0.62,0  
 2YWX,GLU\_44,3.84,0.14,-0.8,0  
 1ES9,GLU\_60,4.5,0,0,0  
 2RIK,HIS\_171,6.59,0.16,0,-0.07  
 2C2Y,ASP\_68,3.92,0.49,-0.37,0  
 1SUU,GLU\_590,4.64,0.14,0,0  
 2GEN,GLU\_140,4.85,0.35,0,0  
 3ULX,ARG\_109,12.29,-0.21,0,0  
 4GA2,GLU\_102,4.86,0.36,0,0  
 1OGL,ARG\_267,11.03,-1.47,0,0  
 2Q34,HIS\_240,0.64,0,-2.22,-3.64  
 3RLN,LYS\_762,9.73,-0.77,0,0  
 3I47,ASP\_84,3.42,0.42,-0.8,0  
 2B0J,GLU\_83,4.5,0,0,0  
 3J5N,GLU\_88,3.98,0.28,-0.8,0  
 3CIV,ASP\_271,3.78,0.07,-0.09,0  
 1SJJ,ARG\_75,12.01,-0.49,0,0  
 2RJD,GLU\_429,4.57,0.07,0,0  
 1N81,ASP\_59,3.2,0.56,-1.15,0  
 2XHC,GLU\_16,4.31,0.07,-0.26,0  
 1OOX,LYS\_59,10.36,-0.14,0,0  
 2OJQ,GLU\_547,4.5,0,0,0  
 1MIX,LYS\_295,10.01,-0.49,0,0  
 2AZL,GLU\_12,4.01,0.63,-1.12,0  
 4EVF,ASP\_53,2.69,0.7,-1.81,0  
 2JKF,ARG\_108,11.87,-0.63,0,0  
 1RWZ,ASP\_209,3.12,0.56,-1.23,0  
 2YXO,LYS\_30,10.01,-0.49,0,0  
 3GEC,GLU\_472,4.44,0,-0.06,0  
 2RJD,ASP\_418,3.54,0.28,-0.53,0  
 350A,ASP\_24,3.71,0,-0.09,0  
 1FO9,LYS\_126,10.43,-0.07,0,0  
 1QQE,LYS\_159,10.15,-0.35,0,0  
 2XHC,LYS\_185,10.43,-0.07,0,0  
 2NRK,ASP\_64,0.98,0.49,-3.31,0  
 1WXF,ARG\_123,12.08,-0.42,0,0  
 2ZTY,GLU\_93,4.5,0,0,0  
 1BKB,GLU\_77,3.84,0.14,-0.8,0  
 3FRR,TYR\_173,10.07,0.07,0,0  
 2R2Y,LYS\_62,10.36,-0.14,0,0  
 2CBE,TYR\_191,10.47,0.47,0,0  
 3QAV,LYS\_42,10.36,-0.14,0,0  
 2GZR,ARG\_225,13.26,-0.56,0.1,32  
 2RJD,CYS\_390,9.34,-1.99,0.08,2.24  
 2GEN,ARG\_172,12.5,0,0,0  
 2CXA,ARG\_161,12.15,-0.35,0,0  
 1WRU,GLU\_34,3.84,0.14,-0.8,0  
 1NJ4,ASP\_16,3.36,0.35,-0.79,0  
 3MTT,ARG\_508,11.94,-0.56,0,0  
 3L3P,ARG\_516,11.94,-0.56,0,0  
 1ANU,TYR\_21,10,0,0,0  
 2P52,TYR\_100,9.84,0,-0.16,0  
 1PBV,LYS\_108,9.94,-0.56,0,0  
 1R9W,CYS\_311,8.31,-0.69,0,0  
 3U0V,ARG\_19,12.5,0,0,0  
 1DZF,LYS\_24,10.15,-0.35,0,0  
 1SJJ,GLU\_32,1.06,0.77,-3.29,-0.91  
 4FZR,ARG\_214,11.45,-1.05,0,0  
 2IRM,TYR\_366,9.48,0.07,-0.59,0  
 3LPZ,LYS\_150,10.5,0,0,0  
 1R7J,LYS\_23,10.08,-0.42,0,0  
 3O16,ARG\_59,11.66,-0.84,0,0  
 3MEW,ASP\_160,3.18,0.63,-1.25,0  
 2GAU,ASP\_30,2.52,0.49,-1.77,0  
 3L3P,ASP\_269,3.1,0.35,-1.05,0  
 1DIO,ASP\_31,2.33,0.49,-1.96,0  
 1QYI,GLU\_102,4.71,0.21,0,0  
 2OKT,LYS\_65,10.01,-0.49,0,0  
 3H5T,GLU\_342,4.5,0,0,0  
 1JKS,ARG\_263,11.37,-3.53,0,2.4  
 1IDK,TYR\_305,10.42,0,0,0.42  
 3GE9,GLU\_33,3.72,1.57,-2.36,0  
 3G9T,LYS\_11,10.5,0,0,0  
 2O8P,ASP\_66,4.01,0.21,0,0  
 2X4G,HIS\_37,6.29,0,0,-0.21  
 3FFM,ASP\_128,3.34,0.35,-0.81,0  
 1OXZ,ARG\_258,11.73,-0.77,0,0  
 1QQE,CYS\_140,7.91,-0.03,-2.3,1.24  
 4EZB,GLU\_188,4.5,0,0,0  
 2ZTY,LYS\_19,10.5,0,0,0  
 3TMO,HIS\_334,6.95,0.66,0,-0.21  
 2W2S,CYS\_62,9,0,0,0  
 3CIV,ARG\_320,12.43,-0.07,0,0  
 4FZN,ASP\_235,3.23,0.49,-1.06,0  
 3V75,ASP\_15,3.88,0.21,-0.13,0  
 3C2E,ARG\_194,11.8,-0.7,0,0  
 2G55,ASP\_57,3.59,0.14,-0.35,0  
 2Z0M,ARG\_66,12.43,-0.07,0,0  
 3HVM,TYR\_110,13.27,0.07,0.8,2.4  
 3CIV,GLU\_221,4.71,0.21,0,0  
 1NAR,LYS\_67,9.66,-0.84,0,0  
 1T3J,GLU\_694,4.05,0.35,-0.8,0  
 1R16,ARG\_318,11.87,-0.63,0,0  
 3LJN,GLU\_111,3.65,0,-0.85,0  
 3DSH,ASP\_345,4.29,0.49,0,0  
 1ES9,ARG\_153,11.87,-0.63,0,0  
 1NAR,HIS\_173,7.5,1.28,0,-0.28  
 3CCY,LYS\_93,10.08,-0.42,0,0  
 2OEW,GLU\_119,3.13,3.4,-2.37,-2.4  
 1G5Z,LYS\_115,9.94,-0.56,0,0  
 2POL,LYS\_152,10.36,-0.14,0,0  
 2OJQ,LYS\_699,10.22,-0.28,0,0  
 1YM5,TYR\_278,8.64,1.02,-0.38,-2  
 3ZRI,HIS\_-3,6.36,0,0,-0.14  
 2X4G,GLU\_256,4.19,0.49,-0.8,0  
 2D0A,TYR\_247,11.73,0,0,1.73  
 3CJW,HIS\_306,6.36,0,0,-0.14  
 3LD1,GLU\_267,4.58,0.21,-0.13,0  
 3N0K,ASP\_54,3,0.42,-1.21,0  
 1D2K,HIS\_92,7.96,1.6,0,-0.14  
 4DIU,GLU\_208,4.57,0.07,0,0  
 3RRQ,HIS\_107,6.36,0,0,-0.14  
 3HKX,ARG\_22,11.17,-1.33,0,0  
 2YYO,HIS\_69,6.54,0.32,0,-0.28  
 2Q99,ASP\_220,2.48,0.28,-1.6,0  
 3ZRI,ARG\_126,12.15,-0.35,0,0  
 3ULX,LYS\_102,10.43,-0.07,0,0  
 2H2Z,GLU\_55,4.5,0,0,0  
 2Q99,GLU\_172,3.6,0.65,-1.55,0  
 1BKR,ASP\_81,3.23,0.49,-1.06,0  
 3A0X,LYS\_625,10.29,-0.21,0,0  
 2Q99,ARG\_18,11.79,-3.11,0,2.4  
 1IAP,ASP\_133,3.55,0.35,-0.6,0  
 3P28,ARG\_32,11.87,-0.63,0,0  
 2QDJ,GLU\_97,3.45,0.49,-1.54,0  
 1G8P,ARG\_296,12.26,-0.7,0,0.46  
 1UCH,LYS\_21,10.43,-0.07,0,0  
 2YYO,ASP\_49,2.99,0.35,-1.16,0  
 2WOZ,ARG\_532,12.98,-1.92,0,2.4  
 2R57,ARG\_236,12.08,-0.42,0,0  
 2FZ4,GLU\_30,4.1,0.28,-0.68,0  
 1TXJ,ASP\_64,3.77,0,-0.03,0  
 2X4L,ARG\_174,13.08,-0.81,0,1.39  
 3AUF,GLU\_159,3.84,0.14,-0.8,0  
 2R0S,ASP\_220,3.37,0.28,-0.71,0  
 2B0J,LYS\_109,10.5,0,0,0  
 3I0C,GLU\_322,2.39,2.3,-2.68,-1.73  
 2IXM,TYR\_251,11.27,0.53,-0.12,0.85  
 1MTZ,LYS\_98,10.22,-0.28,0,0  
 3BWT,ARG\_651,11.59,-0.91,0,0  
 1ANU,ARG\_100,12.08,-0.42,0,0  
 3F6M,LYS\_132,9.73,-0.77,0,0  
 2D0A,LYS\_56,10.5,0,0,0  
 1NIJ,GLU\_205,2.17,0.42,-2.75,0  
 3PBH,ARG\_54,12.01,-0.49,0,0  
 3MIX,ARG\_628,12.22,-0.28,0,0  
 2H85,LYS\_64,10.43,-0.07,0,0  
 2H2Z,ASP\_263,3.24,0.28,-0.84,0  
 2CBE,LYS\_257,10.15,-0.35,0,0  
 3DZ1,TYR\_121,10.04,0.45,-0.41,0  
 2FD5,GLU\_81,3.1,0.35,-1.75,0  
 4DIU,HIS\_46,3.01,0.68,0,-4.17  
 2VC8,GLU\_51,3.3,0.21,-1.4,0  
 3ETU,CYS\_80,10.13,-0.03,0,1.16  
 1ZCU,GLU\_51,4.64,0.14,0,0  
 3EGN,LYS\_466,10.36,-0.14,0,0  
 1H09,LYS\_246,10.36,-0.14,0,0  
 2B0J,ARG\_24,12.33,-1.79,0,1.62  
 3IVF,GLU\_20,4.5,0,0,0  
 1PVT,ASP\_190,4.01,0.21,0,0  
 1YOY,LYS\_152,10.36,-0.14,0,0  
 2P5D,ARG\_84,12.5,0,0,0  
 3IBT,ARG\_242,11.87,-0.63,0,0  
 1RAJ,GLU\_247,4.57,0.07,0,0  
 3PM2,LYS\_7,10.29,-0.21,0,0  
 4DBX,ASP\_7,3.75,0,-0.05,0  
 2H85,TYR\_230,10,0,0,0  
 3QKY,ARG\_239,12.08,-0.42,0,0  
 3M70,ASP\_83,3.8,0.07,-0.07,0  
 3RE9,HIS\_92,6.22,0,0,-0.28  
 2P5D,LYS\_20,10.5,0,0,0  
 3RFY,LYS\_202,10.15,-0.35,0,0  
 1TXD,CYS\_784,9.43,0.22,0.21  
 1TP6,ASP\_113,3.5,0.07,-0.37,0  
 3RVC,LYS\_108,10.5,0,0,0  
 1MTZ,HIS\_292,6.22,0,0,-0.28  
 3T5B,ARG\_56,11.02,-1.48,0,0  
 1PVT,GLU\_40,4.71,0.21,0,0  
 3CX,ARG\_116,11.45,-1.05,0,0  
 2EJX,ARG\_134,11.73,-0.77,0,0  
 1ES5,TYR\_23,10.1,0.16,-0.06,0  
 4FZN,LYS\_215,10.01,-0.49,0,0  
 1QQH,CYS\_128,8.21,-0.79,0,0  
 4DNU,ARG\_346,11.94,-0.56,0,0  
 2D7J,CYS\_148,8.07,-5.5,3.37,1.2  
 1ZKZ,LYS\_78,10.5,0,0,0  
 1G8P,ARG\_231,12.01,-0.49,0,0  
 1CHD,HIS\_224,7.32,0.96,0,-0.14  
 1UXO,HIS\_59,6.45,0.09,0,-0.14  
 2VAN,HIS\_135,4.3,0,-0.16,-2.04  
 4DEZ,ARG\_178,12.15,-0.35,0,0  
 2Q98,GLU\_118,3.72,0.42,-1.2,0  
 1RLO,GLU\_177,3.7,2.9,-1.54,-2.16  
 1YW5,LYS\_59,10.5,0,0,0  
 2YLF,HIS\_206,7,0.85,0,-0.35  
 1XEU,ASP\_111,2.26,0.35,-1.89,0  
 3EOD,GLU\_89,4.5,0,0,0  
 4DVD,TYR\_69,9.52,0,-0.48,0  
 3MTT,LYS\_564,10.29,-0.21,0,0  
 2G5X,GLU\_91,0.58,0.88,-2.4,-2.4  
 1YOY,GLU\_148,9.87,-0.63,0,0  
 3GEC,LYS\_390,10.5,0,0,0  
 2JEO,ARG\_155,12.01,-0.49,0,0  
 3CRM,TYR\_270,10.99,0,0.99  
 2PP6,GLU\_92,4.64,0.14,0,0  
 3DZ1,TYR\_295,9.58,0,-0.42,0  
 2AD1,LYS\_148,9.87,-0.63,0,0  
 1CHD,HIS\_248,7.06,0.77,0,-0.21  
 2X4G,HIS\_132,6.36,0,0,-0.14  
 3B4D,CYS\_195,9,0,0,0  
 1SQH,ASP\_19,1.75,0.35,-2.4,0  
 2DG7,GLU\_116,4.57,0.07,0,0  
 3RFY,GLU\_279,4.78,0.28,0,0  
 1RWZ,ASP\_168,3.72,0,-0.08,0  
 4EZB,LYS\_116,10.36,-0.14,0,0  
 1HF8,LYS\_163,10.22,-0.28,0,0  
 3BA1,TYR\_185,9.38,0.14,-0.76,0  
 1PBV,GLU\_222,4.64,0.14,0,0  
 1J8B,LYS\_19,4.85,0.35,0,0  
 1P4X,ASP\_226,3.82,0.07,-0.05,0  
 3GFP,GLU\_353,4.09,0.14,-0.55,0  
 3F5D,LYS\_5,10.5,0,0,0  
 3DSH,GLU\_274,3.09,0.42,-1.83,0  
 3ON1,ARG\_74,12.5,0,0,0  
 1BDK,TYR\_85,10,0,0,0  
 2GZQ,LYS\_14,10.43,-0.07,0,0  
 2AZL,HIS\_80,5.04,0.57,0,-2.03  
 3MIX,GLU\_328,3.55,0.14,-1.09,0  
 1UAJ,HIS\_200,6.43,0,0,-0.07  
 3ODJ,TYR\_43,11.72,0,0,1.72  
 3F5X,ARG\_225,12.43,-0.07,0,0  
 1SJJ,LYS\_33,9.87,-0.63,0,0  
 3P28,LYS\_158,10.5,0,0,0  
 2XWS,LYS\_45,10.5,0,0,0  
 2CWC,HIS\_281,6.22,0,0,-0.28  
 3H5T,ASP\_50,3.84,0.28,-0.24,0  
 2AH5,LYS\_118,10.5,0,0,0  
 1O17,ASP\_66,0.68,0.49,-3.6,0  
 3GOZ,LYS\_246,10.22,-0.28,0,0  
 2WB8,TYR\_739,10.21,0.21,0,0  
 1EW4,TYR\_69,9.56,0,-0.44,0  
 1WLJ,ARG\_34,12.08,-0.42,0,0  
 1PBV,ARG\_212,12.5,0,0,0  
 3A7L,GLU\_34,4.39,0.07,-0.18,0  
 1P6F,LYS\_22,10.5,0,0,0  
 1R2Z,TYR\_104,10.18,0,-0.03,0.21  
 2ZQ5,LYS\_8,10.5,0,0,0  
 2CWC,ARG\_89,12.08,-0.42,0,0  
 3NJM,ASP\_28,2.29,0.91,-2.42,0  
 1LPL,TYR\_207,10.35,0,0,0.35  
 4F3J,ARG\_127,12.36,-0.14,0,0  
 2R0S,TYR\_225,10.69,0.69,0,0  
 2QRX,ARG\_32,12.29,-0.21,0,0

2FM9,ASP\_212,4.08,0.28,0,0  
 3CS1,GLU\_188,4.11,0.28,-0.67,0  
 3HVV,ASP\_329,3.05,0.42,-1.17,0  
 4E9E,CYS\_549,10.64,0,0,1.64  
 3BWT,HIS\_648,6.43,0,0,-0.07  
 3M7D,ARG\_267,11.8,-0.7,0,0  
 3RE9,LYS\_172,10.08,-0.42,0,0  
 2G5X,LYS\_98,10.15,-0.35,0,0  
 4EUG,GLU\_95,2.86,0.82,-2.46,0  
 2X4G,ASP\_78,2.99,0.28,-1.09,0  
 2G3A,ASP\_44,3.8,0,0,0  
 3M9A,GLU\_16,4.02,0.07,-0.55,0  
 3B79,GLU\_90,5.13,0.63,0,0  
 2GAU,GLU\_207,4.05,0.35,-0.8,0  
 4FZR,GLU\_381,4.22,0.42,-0.7,0  
 1ZKZ,ASP\_19,3.79,0.21,-0.22,0  
 1FQJ,GLU\_294,4.71,0.21,0,0  
 4H4J,LYS\_175,10.36,-0.14,0,0  
 2QVT,LYS\_93,10.43,-0.07,0,0  
 2GEN,LYS\_7,10.5,0,0,0  
 2IXM,CYS\_299,10.08,-1.43,0,2.51  
 3E5T,ASP\_151,3.42,0.42,-0.8,0  
 3G9T,ASP\_42,3.8,0,0,0  
 4FZN,GLU\_115,4.44,0.14,-0.2,0  
 1J85,TYR\_150,10.07,0.07,0,0  
 2CWC,ARG\_85,11.94,-0.56,0,0  
 1QSZ,ARG\_656,11.73,-0.77,0,0  
 1OST,TYR\_212,12.47,0.2,0.2,2.27  
 1L3K,HIS\_119,6.29,0,0,-0.21  
 2PGX,TYR\_245,11.54,0.15,-0.52,1.91  
 3O7K,ARG\_97,11.8,-0.7,0,0  
 2BDD,GLU\_59,4.48,0,-0.02,0  
 2Z14,TYR\_44,10.14,0.14,0,0  
 1SQH,GLU\_51,4.5,0,0,0  
 3C6B,ARG\_294,12.08,-0.42,0,0  
 2Z0M,ARG\_10,11.8,-0.7,0,0  
 3F53,GLU\_61,4.71,0.21,0,0  
 1L2F,GLU\_202,3.94,0.35,-0.91,0  
 1V8E,LYS\_19,10.5,0,0,0  
 2CXA,LYS\_79,10.5,0,0,0  
 2POY,HIS\_244,2.66,0.62,0,-4.46  
 3PM2,GLU\_148,4.5,0,0,0  
 1DCF,LYS\_98,10.43,-0.07,0,0  
 2RJD,HIS\_502,3.1,1.14,0.14,-4.68  
 1T95,LYS\_56,10.01,-0.49,0,0  
 1PVT,LYS\_147,10.5,0,0,0  
 1OST,GLU\_455,3.65,0.49,-1.34,0  
 3F53,ASP\_55,3.93,0.42,-0.29,0  
 2WZ9,GLU\_23,4.78,0.28,0,0  
 4AM1,GLU\_147,3.84,0.14,-0.8,0  
 2P5D,LYS\_23,10.36,-0.14,0,0  
 1DOV,ASP\_159,3.73,0.14,-0.21,0  
 2QV2,ARG\_285,11.8,-0.7,0,0  
 2Q98,GLU\_161,2.31,0.21,-2.4,0  
 2CXA,TYR\_87,10.08,0.07,-0.11,0.12  
 3T5B,ASP\_123,3.8,0,0,0  
 1ZCU,LYS\_228,10.5,0,0,0  
 2OJQ,LYS\_614,10.36,-0.14,0,0  
 4E6S,ASP\_76,2.91,0.35,-1.25,0  
 3RE9,HIS\_228,6.38,0.02,0,-0.14  
 2R51,GLU\_169,4.5,0,0,0  
 2JHY,GLU\_109,4.57,0.07,0,0  
 4DNU,LYS\_372,10.36,-0.14,0,0  
 2F8H,LYS\_212,6.5,0,0,0  
 3MIX,ASP\_363,3.58,0.07,-0.29,0  
 1QQE,GLU\_6,4.04,0.28,-0.74,0  
 4E6S,ARG\_39,12.22,-0.28,0,0  
 2AZL,GLU\_121,4.57,0.07,0,0  
 3IBT,LYS\_84,10.15,-0.35,0,0  
 1X6J,ASP\_21,3.04,0.77,-1.53,0  
 3M7G,GLU\_194,3.94,0.21,-0.77,0  
 1RZ2,LYS\_129,10.29,-0.21,0,0  
 2O0K,LYS\_70,10.15,-0.35,0,0  
 1BKR,LYS\_93,10.5,0,0,0  
 2D2S,GLU\_541,3.92,0.42,-1,0  
 2CBE,ARG\_182,11.94,-0.56,0,0  
 2HNG,TYR\_112,11.96,0,-0.45,2.41  
 3JRT,TYR\_71,13.48,0.28,0.8,2.4  
 2FBI,ASP\_108,3.19,0.07,-0.69,0  
 3ELI,LYS\_138,10.08,-0.42,0,0  
 2GEN,ASP\_161,3.87,0.07,0,0  
 2IQT,GLU\_93,4.5,0,0,0  
 2E3S,GLU\_589,4.5,0,0,0  
 2POY,ASP\_237,3.4,0.35,-0.74,0  
 3H13,ARG\_432,11.73,-0.77,0,0  
 3ASA,ASP\_87,4.08,0.28,0,0  
 2RFA,GLU\_249,4.64,0.14,0,0  
 1UAJ,GLU\_129,3.18,0.28,-1.6,0  
 2CIU,LYS\_190,10.5,0,0,0  
 1AM2,HIS\_52,6.22,0,0,-0.28  
 3B21,LYS\_207,10.29,-0.21,0,0  
 4FLE,GLU\_135,3.81,0.63,-1.32,0  
 3FFM,GLU\_144,4.12,0.42,-0.8,0  
 1R53,ARG\_191,10.73,-1.94,0,0.16  
 1Q46,LYS\_145,10.43,-0.07,0,0  
 2HP7,GLU\_225,4.56,0.07,-0.01,0  
 4ANN,HIS\_73,6.43,0,0,-0.07  
 1H4U,ARG\_580,12.43,-0.07,0,0  
 1TXD,GLU\_878,4.64,0.14,0,0  
 3LJC,GLU\_118,4.64,0.14,0,0  
 3GMS,HIS\_268,6.36,0,0,-0.14  
 3UAH,LYS\_229,10.08,-0.42,0,0  
 1JB3,GLU\_13,4.15,0.42,-0.77,0  
 1S17,ARG\_141,11.8,-0.7,0,0  
 3ZTA,GLU\_49,4.92,0.42,0,0  
 2Q12,GLU\_80,4.5,0,0,0  
 3N2T,TYR\_59,13.54,2.08,0,1.46  
 1UOH,GLU\_127,4.49,0.42,-0.43,0  
 2W2S,GLU\_149,4.06,0.35,-0.79,0  
 3KT9,LYS\_75,10.5,0,0,0  
 3IU5,ASP\_83,3.81,0.07,-0.06,0  
 1RZ2,TYR\_94,10.73,1.84,-1.23,0.11  
 1NRI,LYS\_239,10.36,-0.14,0,0  
 3RFY,ARG\_108,12.64,-2.46,0,2.6  
 1Q2Y,LYS\_88,10.5,0,0,0  
 1FQI,GLU\_330,2.29,0.41,-0.8,-1.82  
 3MIX,TYR\_418,10,0,0,0  
 3VJ8,LYS\_358,10.5,0,0,0  
 1MHN,ASP\_140,3.46,0.35,-0.69,0  
 2R57,ASP\_178,3.71,0,-0.09,0  
 1Q8B,TYR\_54,10,0,0,0  
 1GPP,LYS\_53,10.29,-0.21,0,0  
 1XTZ,ARG\_101,12.36,-0.14,0,0  
 2A4D,LYS\_184,10.5,0,0,0  
 1WYC,GLU\_143,3.62,0.77,-1.65,0  
 4AM1,LYS\_255,10.29,-0.21,0,0  
 1PGV,LYS\_388,10.5,0,0,0  
 3F53,LYS\_70,10.29,-0.21,0,0  
 2YLF,CYS\_203,10.56,-0.62,0,2.18  
 3COU,GLU\_173,3.91,0.21,-0.8,0  
 2B0J,ASP\_77,3.49,0.07,-0.38,0  
 3ONH,ASP\_532,4.11,0.42,-0.11,0  
 3C5V,GLU\_75,4.5,0,0,0  
 2GQV,GLU\_58,3.5,0.14,-1.14,0  
 2B0A,TYR\_90,11.07,0,-0.01,1.08  
 1RLO,ASP\_228,3.45,0.35,-0.7,0  
 3DSH,HIS\_233,6.36,0,0,-0.14  
 2E3C,ASP\_433,3.87,0.07,0,0  
 1LTU,ASP\_252,4.15,0.42,-0.07,0  
 3CGW,LYS\_291,10.01,-0.49,0,0  
 2V4X,GLU\_94,4.71,0.21,0,0  
 1S17,ASP\_32,3.55,0.42,-0.67,0  
 3BCY,LYS\_110,10.15,-0.35,0,0  
 2FBQ,LYS\_34,10.22,-0.28,0,0  
 1PSW,GLU\_337,4.21,0.14,-0.43,0  
 1OGL,ASP\_223,2.52,0.28,-1.56,0  
 1V43,GLU\_12,3.84,0.14,-0.8,0  
 3CCY,CYS\_74,9.84,0,0,0.84  
 1BGF,ARG\_87,12.01,-0.49,0,0  
 1GSZ,LYS\_122,10.36,-0.14,0,0  
 1AKO,GLU\_137,4.02,0.28,-0.76,0  
 3M9A,ASP\_71,4.08,0.28,0,0  
 1R3F,TYR\_68,9.54,0.23,-0.69,0  
 1ANU,GLU\_115,4.5,0,0,0  
 2H14,TYR\_252,10.92,0.92,0,0  
 1YDL,HIS\_42,6.29,0,0,-0.21  
 2POY,CYS\_296,9.51,-0.28,0,0.79  
 1PVT,ARG\_68,12.15,-0.35,0,0  
 2AZL,TYR\_11,10.98,0.07,0,0.9  
 2V1L,HIS\_10,6.43,0,0,-0.07  
 2FZP,TYR\_275,12.2,1.38,0,0.82  
 4FZR,LYS\_247,10.22,-0.28,0,0  
 1WP5,GLU\_227,4.5,0,0,0  
 2AH5,TYR\_74,12.99,0.42,0.17,2.4  
 3AU3,TYR\_622,13.05,0.28,0.37,2.4  
 2APL,LYS\_2,10.5,0,0,0  
 1OOX,LYS\_69,10.43,-0.07,0,0  
 1FKM,TYR\_412,10.7,0.7,0,0  
 3ULX,TYR\_94,9.23,0,-0.77,0  
 2POY,TYR\_131,9.8,0.07,-0.27,0  
 3HNX,ASP\_91,3.81,0.21,-0.2,0  
 2C13,ARG\_44,12.01,-0.49,0,0  
 1TLV,LYS\_143,9.94,-0.56,0,0  
 2R0S,HIS\_89,6.15,0,0,-0.35  
 4DNU,HIS\_183,4.43,4.13,0,-6.2  
 3ONH,LYS\_440,10.43,-0.07,0,0  
 1A8Q,TYR\_67,9.83,1.07,-1.24,0  
 3EVZ,LYS\_215,10.22,-0.28,0,0  
 3ASA,GLU\_323,0.07,0.02,-0.37,-4.08  
 3ASA,TYR\_301,12.14,0.6,0,1.54  
 4DIU,LYS\_7,10.08,-0.42,0,0  
 4HDE,ASP\_135,2.04,0.28,-2.04,0  
 3H5T,HIS\_307,6.56,0.06,0,0  
 3LH5,ARG\_690,12.22,-0.28,0,0  
 2VGM,LYS\_77,10.5,0,0,0  
 1SQH,GLU\_108,3.98,0.28,-0.8,0  
 3BCH,ARG\_63,12.08,-0.42,0,0  
 1R53,GLU\_182,4.5,0,0,0  
 1YTD,GLU\_370,4.5,0,0,0  
 3OIP,HIS\_208,4.92,1.16,0,-2.74  
 1HF8,LYS\_227,10.29,-0.21,0,0  
 1QQE,GLU\_101,3.97,0.38,-0.68,-0.24  
 3N2T,ASP\_168,2.96,0.42,-1.26,0  
 3OIP,LYS\_215,10.5,0,0,0  
 2VGM,ASP\_180,2.93,0.35,-1.22,0  
 2F4Q,GLU\_257,4.71,0.21,0,0  
 1T95,TYR\_32,13.34,0.14,0.8,2.4  
 3LMF,TYR\_22,10.07,0.07,0,0  
 3IL3,ASP\_260,2.16,0.35,-1.99,0  
 3U2R,GLU\_118,3.91,0.21,-0.8,0  
 1XFK,ARG\_14,12.22,-0.28,0,0  
 2RFA,HIS\_185,7.39,0.96,0,-0.07  
 4AM1,HIS\_227,1.7,0.95,0,-5.75  
 1ZCE,LYS\_45,10.36,-0.14,0,0  
 2EFK,GLU\_283,4.5,0,0,0  
 1QQE,GLU\_262,4.5,0,0,0  
 2NRR,LYS\_397,10.43,-0.07,0,0  
 1T07,CYS\_7,1.32,-7.97,0,0.28  
 2D7U,LYS\_111,9.94,-0.56,0,0  
 4H89,ASP\_13,3.56,0.07,-0.31,0  
 2POY,ARG\_65,11.87,-0.63,0,0  
 2OEW,ASP\_328,4.01,0.21,0,0  
 1UW7,ASP\_26,3.65,0.56,-0.7,0  
 3RVC,GLU\_152,4.33,0.21,-0.38,0  
 1WPA,ARG\_429,11.59,-0.91,0,0  
 4H4J,HIS\_111,2.16,1.01,-1.17,-4.18  
 2GEN,GLU\_69,3.98,0.28,-0.8,0  
 1R3F,GLU\_157,3.97,0.21,-0.74,0  
 2Q13,LYS\_270,10.43,-0.07,0,0  
 1E5S,LYS\_25,9.94,-0.56,0,0  
 2V81,CYS\_81,8.29,-2.38,0,1.67  
 2G5X,ARG\_56,12.22,-0.28,0,0  
 3BQW,GLU\_152,3.93,0.21,-0.78,0  
 2H2Z,ASP\_153,3.41,0.7,-1.09,0  
 3E7P,GLU\_33,3.24,0.77,-2.04,0  
 2FL7,ASP\_60,1.48,0.63,-2.95,0  
 1J74,TYR\_113,10,0,0,0  
 2F4Q,CYS\_270,10.12,0,0,1.12  
 2RIS,HIS\_145,10.18,3.2,4.19,-3.72  
 1W7B,LYS\_313,10.36,-0.14,0,0  
 3M7G,GLU\_74,3.13,0.99,-0.86,-1.5  
 1TD6,LYS\_254,10.08,-0.42,0,0  
 2B61,CYS\_91,8.86,-2.65,0.78,1.74  
 3O48,ASP\_5,2.6,0,-1.2,0  
 4EVF,TYR\_173,9.89,0.33,-0.3,-0.13  
 3TIR,LYS\_196,9.87,-0.63,0,0  
 2QV2,CYS\_212,9.05,-0.74,0,0.79  
 1T3Y,ASP\_20,2.82,0.28,-1.26,0  
 3V55,HIS\_681,6.5,0,0,0  
 3IV4,GLU\_59,4.92,0.42,0,0  
 3G9T,GLU\_34,3.39,0.49,-1.6,0  
 3LJC,LYS\_147,10.5,0,0,0  
 1JKS,CYS\_30,8.36,-1.04,0,0.4  
 1T07,GLU\_69,3.25,0.35,-1.6,0  
 3RUX,TYR\_69,10.82,0.52,-0.28,0.59  
 1RHS,TYR\_164,10.14,0.14,0,0  
 1KCM,LYS\_135,10.22,-0.28,0,0  
 1YLN,HIS\_214,6.5,0,0,0  
 2Z61,ASP\_81,4.01,0.21,0,0  
 3EVP,HIS\_94,1.23,0.55,-1.08,-4.74  
 3FRR,ASP\_42,4.04,0.42,-0.18,0  
 3PP8,GLU\_256,0.48,1.03,-2.65,-2.4  
 2G9D,LYS\_171,10.36,-0.14,0,0  
 2FL7,LYS\_42,10.5,0,0,0  
 3UPD,TYR\_255,11.6,0.07,0,1.53  
 2X5Y,HIS\_734,6.36,0,0,-0.14  
 1DTO,GLU\_142,3.35,0,-1.15,0  
 3TIR,HIS\_90,6.36,0,0,-0.14  
 1JKS,LYS\_86,10.5,0,0,0  
 3BA1,GLU\_263,4.17,0.07,-0.4,0  
 3ERF,GLU\_91,3.61,0.28,-1.17,0  
 4D8L,ARG\_242,10.86,-1.64,0,0  
 2WOZ,ASP\_415,2.63,0.56,-1.72,0  
 3DB9,ARG\_163,11.59,-0.91,0,0  
 1R3F,ARG\_201,13.98,-0.92,0,2.4  
 2AHE,TYR\_104,13.34,0.14,0.8,2.4  
 1BKR,ASP\_47,1.38,0.7,-3.12,0  
 4FD6,TYR\_196,13.61,0.41,0.8,2.4  
 3ONH,ASP\_493,3.54,0.28,-0.54,0  
 1ZKZ,LYS\_53,10.5,0,0,0  
 2W1R,ASP\_92,3.9,0.28,-0.18,0  
 1ZCE,ARG\_38,11.38,-1.12,0,0  
 2G2D,GLU\_152,4.64,0.14,0,0  
 3HQX,GLU\_95,4.57,0.07,0,0  
 1WXQ,ASP\_202,2.39,0.7,-2.1,0  
 3GYW,LYS\_81,10.5,0,0,0

2G9D,ASP\_243,4.03,0.63,-0.4,0  
 1MN3,GLU\_440,4.5,0,0,0  
 2WOZ,GLU\_559,4.57,0.07,0,0  
 1CBY,TYR\_169,11.98,2.04,-0.06,0  
 1P6F,GLU\_36,3.17,0.63,-1.96,0  
 2OSA,TYR\_346,11.92,1.92,0,0  
 1SJY,GLU\_56,3.39,0.77,-1.87,0  
 3ZTA,HIS\_75,6.5,0,0,0  
 2IF4,TYR\_221,13.34,0.14,0.8,2.4  
 1O6D,ASP\_94,2.93,0.35,-1.22,0  
 3G59,GLU\_282,4.57,0.07,0,0  
 3CO1,TYR\_124,13.89,0.71,0.78,2.4  
 1W24,GLU\_71,3.23,0.21,-1.48,0  
 1WYC,ARG\_182,10.89,-1.61,0,0  
 4EZB,GLU\_11,4.5,0,0,0  
 1OXZ,GLU\_275,4.5,0,0,0  
 3HVM,LYS\_133,10.01,-0.49,0,0  
 2RIK,LYS\_131,9.8,-0.7,0,0  
 2Z61,LYS\_80,9.94,-0.56,0,0  
 1ZBP,CYS\_42,10.87,0,1.87  
 2POL,ASP\_249,3.78,0.07,-0.09,0  
 2OJQ,GLU\_527,4.5,0,0,0  
 1RI6,ARG\_250,11.32,-3.36,0.2,18  
 4FLE,GLU\_35,3.78,0.28,-1,0  
 1WXF,TYR\_174,10,0,0,0  
 3M7D,ARG\_187,12.01,-0.49,0,0  
 2QZQ,CYS\_122,9.99,-0.44,-0.41,1.84  
 2AHS,ASP\_109,2.95,0.07,-0.92,0  
 2Z84,ARG\_185,12.01,-0.49,0,0  
 2O4D,GLU\_119,3.14,0.63,-1.99,0  
 2R2Y,TYR\_22,10.08,0,-0.14,0.23  
 3B7X,ASP\_69,3.23,0.07,-0.64,0  
 3GFP,LYS\_341,10.43,-0.07,0,0  
 1QQE,GLU\_146,4.92,0.42,0,0  
 2BLL,GLU\_579,4.56,0.35,-0.29,0  
 1PGV,GLU\_259,4.5,0,0,0  
 1J33,GLU\_43,4.71,0.21,0,0  
 3KB5,GLU\_407,4.06,0.14,-0.59,0  
 3AU3,LYS\_455,10.43,-0.07,0,0  
 1T95,ARG\_106,12.08,-0.42,0,0  
 3K9I,LYS\_148,10.36,-0.14,0,0  
 1RHS,ARG\_175,11.38,-1.12,0,0  
 2G2D,ARG\_91,11.31,-1.19,0,0  
 3TIR,CYS\_192,8.59,-0.48,0,0.07  
 1X04,LYS\_34,10.43,-0.07,0,0  
 2QZQ,LYS\_40,10.29,-0.21,0,0  
 1JB3,ARG\_43,12.43,-0.07,0,0  
 1SBX,ARG\_96,12.29,-0.21,0,0  
 3EJG,LYS\_54,10.5,0,0,0  
 3LQE,GLU\_338,4.63,0.28,-0.15,0  
 3RKV,HIS\_260,6.43,0,0,-0.07  
 2P0Y,GLU\_218,4.57,0.07,0,0  
 1NRI,GLU\_120,4.86,0.36,0,0  
 4H89,GLU\_129,3.49,0.14,-1.15,0  
 3M7G,ARG\_37,11.66,-0.84,0,0  
 1WPS,HIS\_320,6.5,0,0,0  
 4E5S,GLU\_102,4.99,0.49,0,0  
 3ERF,ASP\_157,3.32,0.28,-0.77,0  
 1V43,ARG\_182,11.17,-1.33,0,0  
 4F3J,GLU\_112,3.67,0.14,-0.97,0  
 3F5D,LYS\_80,10.01,-0.49,0,0  
 3IOO,GLU\_197,3.92,4.18,-2.93,-1.83  
 1HUFL,LYS\_53,10.43,-0.07,0,0  
 2OJQ,LYS\_640,10.5,0,0,0  
 1ZHV,GLU\_43,4.57,0.07,0,0  
 2H8O,ARG\_227,9.77,-1.39,0,-1.34  
 3CSV,ASP\_65,3.06,0.91,-1.86,0.21  
 1OGL,LYS\_109,9.94,-0.56,0,0  
 2RIK,LYS\_226,10.5,0,0,0  
 3AU3,GLU\_538,2.69,0.98,-2.8,0  
 1MD6,CYS\_69,8.57,-1.6,0.1,1.7  
 2HRZ,LYS\_127,10.36,-0.14,0,0  
 3V46,ARG\_310,11.45,-1.05,0,0  
 2YT4,CYS\_657,7.75,-1.6,0.0,35  
 1XIPLY,LYS\_48,10.22,-0.28,0,0  
 1GPP,TYR\_179,9.84,0,-0.16,0  
 1YIB,ASP\_209,3.87,0.14,-0.07,0  
 3M7G,TYR\_5,9.29,0.21,-0.92,0  
 3CBN,GLU\_74,4.64,0.14,0,0  
 3COU,GLU\_79,4.17,0.35,-0.68,0  
 1X91,ASP\_9,3.14,0.42,-1.08,0  
 2R51,GLU\_157,4.64,0.14,0,0  
 1OTM,HIS\_151,6.22,0,0,-0.28  
 3G9T,ARG\_14,11.87,-0.63,0,0  
 2P5D,ARG\_93,11.03,-1.47,0,0  
 1WRU,TYR\_150,10.95,0.95,0,0  
 2QDJ,TYR\_321,12.6,1.99,-1.37,1.99  
 3QAV,LYS\_159,10.36,-0.14,0,0  
 3JRT,LYS\_2,10.36,-0.14,0,0  
 2OKT,LYS\_140,10.43,-0.07,0,0  
 2B61,LYS\_293,9.94,-0.56,0,0  
 2Z84,TYR\_55,10.36,1.17,-0.81,0  
 3RJZ,TYR\_150,10,0,0,0  
 1RSS,GLU\_146,4.71,0.21,0,0  
 2AZP,HIS\_217,6.36,0,0,-0.14  
 2D7J,ARG\_180,12.43,-0.07,0,0  
 3MIX,LYS\_579,10.5,0,0,0  
 2IRN,ARG\_104,12.15,-0.35,0,0  
 3KVO,GLU\_176,4.5,0,0,0  
 1ZBM,TYR\_152,10.21,0,-0.04,0.25  
 2GZQ,LYS\_60,10.36,-0.14,0,0  
 4HDE,GLU\_195,2.59,0.49,-2.4,0  
 1Y0K,ARG\_166,12.08,-0.42,0,0  
 3E5T,LYS\_136,10.22,-0.28,0,0  
 3N2T,LYS\_75,10.29,-0.21,0,0  
 3LJC,ARG\_214,12.15,-0.35,0,0  
 1R5Q,HIS\_57,3.94,0,0,-2.56  
 2Q13,GLU\_10,4.5,0,0,0  
 3QAV,TYR\_118,13.41,0.21,0.8,2.4  
 2XWS,LYS\_100,10.22,-0.28,0,0  
 2ZQ5,HIS\_117,2,1,-1.49,-4.01  
 3I4T,GLU\_12,3.95,0.42,-0.97,0  
 3ERF,ARG\_154,12.5,0,0,0  
 3G59,LYS\_182,10.5,0,0,0  
 1UXO,HIS\_128,6.43,0,0,-0.07  
 3PZ9,TYR\_332,9.4,2.54,-1.2,-1.94  
 2W0G,CYS\_194,8.56,-1.88,0,1.44  
 1YM5,LYS\_16,10.5,0,0,0  
 3AUF,ARG\_48,11.94,-0.56,0,0  
 1O0X,LYS\_23,10.36,-0.14,0,0  
 3HYQ,ARG\_83,13.76,-0.87,0.2,13  
 3V75,HIS\_57,6.22,0,0,-0.28  
 1LPL,LYS\_175,10.5,0,0,0  
 2NRR,ARG\_395,11.31,-1.19,0,0  
 2PGE,ARG\_36,11.94,-0.56,0,0  
 3QKY,ARG\_65,11.59,-0.91,0,0  
 2OEW,ASP\_59,3.69,0.7,-0.81,0  
 2V1L,GLU\_27,4.57,0.07,0,0  
 2C13,LYS\_99,10.5,0,0,0  
 1AD6,TYR\_446,11.75,1.78,-0.03,0  
 1NWA,TYR\_144,9.49,0,-0.51,0  
 3G9G,LYS\_227,10.29,-0.21,0,0  
 3EZ7,LYS\_375,10.15,-0.35,0,0  
 2JHY,LYS\_105,10.5,0,0,0  
 3H6Q,GLU\_14,4.71,0.21,0,0  
 1M5I,LYS\_167,10.43,-0.07,0,0  
 3AUF,GLU\_74,4.5,0,0,0  
 2YXO,ARG\_56,12.29,-0.21,0,0  
 1YTQ,GLU\_105,4.64,0.14,0,0  
 2HZZ,GLU\_166,4.06,0.21,-0.65,0  
 2A6B,LYS\_35,10.29,-0.21,0,0  
 2B61,ARG\_295,11.66,-0.84,0,0  
 4FZ2,ARG\_2,11.8,-0.7,0,0  
 1WLY,LYS\_188,10.43,-0.07,0,0  
 1MIX,CYS\_336,8.36,-1.3,0,0.66  
 3UOV,CYS\_174,7.19,-3.88,0.1,1.97  
 1MJS,TYR\_296,13.34,0.14,0.8,2.4  
 4DIU,ASP\_236,3.15,0.56,-1.21,0  
 2RGY,ARG\_238,11.94,-0.56,0,0  
 1RHS,GLU\_285,3.87,0.35,-0.98,0  
 3M9A,LYS\_79,10.08,-0.42,0,0  
 2GZQ,GLU\_8,4.62,0.14,-0.02,0  
 1ZBM,GLU\_135,4.09,0.35,-0.76,0  
 2ZOW,ASP\_53,2.08,0.28,-2,0  
 1UCH,ASP\_198,3.25,0.14,-0.69,0  
 1JSX,GLU\_126,4.5,0,0,0  
 1X04,GLU\_97,4.15,0.07,-0.42,0  
 1Z9L,LYS\_17,10.01,-0.49,0,0  
 1MTZ,LYS\_157,10.08,-0.42,0,0  
 2R57,ARG\_238,11.8,-0.7,0,0  
 4EKU,HIS\_122,6.22,0,0,-0.28  
 1U7U,LYS\_303,10.5,0,0,0  
 2V5B,ARG\_193,11.87,-0.63,0,0  
 2Q13,GLU\_69,3.84,0.14,-0.8,0  
 2OGQ,ASP\_371,2.1,0.14,-1.84,0  
 2FBI,ARG\_89,12.29,-0.21,0,0  
 3CE7,GLU\_68,3.79,0.49,-1.2,0  
 1X7F,ASP\_291,3.94,0.14,0,0  
 3JSN,GLU\_238,3.4,0.98,-2.08,0  
 2A0J,GLU\_141,2.53,0.7,-2.67,0  
 3BPV,HIS\_58,6.36,0,0,-0.14  
 2PPN,TYR\_82,10.32,0.32,0,0  
 1FQI,TYR\_401,10.63,0.63,0,0  
 3BPP,GLU\_134,4.64,0.14,0,0  
 1L2F,GLU\_124,4.5,0,0,0  
 3F6M,HIS\_125,6.41,0.12,0,-0.21  
 2H2W,GLU\_206,4.26,0.56,-0.8,0  
 4AM1,GLU\_335,3.88,2.13,-2.28,-0.47  
 1OST,TYR\_316,10,0,0,0  
 3C5V,GLU\_124,3.76,0.35,-1.09,0  
 2EA9,LYS\_46,10.5,0,0,0  
 3IVF,GLU\_182,2.9,0.56,-2.16,0  
 3BA1,LYS\_25,10.43,-0.07,0,0  
 2PLQ,HIS\_3,7.15,0.93,0,-0.28  
 2D2S,ASP\_736,2.77,0.28,-1.31,0  
 1SFE,HIS\_147,4.67,1.6,1.44,-4.88  
 1TR9,GLU\_19,4.5,0,0,0  
 1R6Y,HIS\_80,6.37,0.15,0,-0.28  
 2EDM,LYS\_119,9.59,-0.91,0,0  
 2ZOM,ASP\_260,3.33,0.21,-0.67,0  
 2FD5,GLU\_57,2.45,0.35,-2.4,0  
 3ETU,LYS\_331,10.29,-0.21,0,0  
 1OST,LYS\_277,10.22,-0.28,0,0  
 2ZCO,TYR\_131,12.67,0.52,-0.25,2.4  
 3H04,GLU\_241,4.53,0.28,-0.25,0  
 2E3H,LYS\_238,10.5,0,0,0  
 1ZBM,GLU\_211,4.15,0.21,-0.56,0  
 3H04,GLU\_80,4.57,0.07,0,0  
 3LH5,ARG\_762,12.22,-0.28,0,0  
 3EOH,LYS\_96,10.43,-0.07,0,0  
 1O0X,CYS\_73,11.49,-1.57,1.47,2.59  
 2RJD,ARG\_478,12.18,-0.56,0.24  
 1TWU,GLU\_62,4.37,0.49,-0.62,0  
 1ZP2,CYS\_87,9.93,0,0,0.93  
 1LN4,LYS\_48,9.73,-0.77,0,0  
 2HRZ,LYS\_30,10.5,0,0,0  
 2QV2,GLU\_153,4.64,0.14,0,0  
 3US6,ASP\_35,2.77,0.63,-1.65,0  
 1SIG,ARG\_436,12.22,-0.28,0,0  
 3NBI,TYR\_151,10,0,0,0  
 2OEW,LYS\_239,10.5,0,0,0  
 3LPZ,LYS\_157,10.36,-0.14,0,0  
 2Q07,TYR\_398,9.75,0.14,-0.39,0  
 2AHE,GLU\_183,4.84,0.35,-0.01,0  
 2HRZ,GLU\_320,2.94,0.42,-1.97,0  
 2EFK,ASP\_144,3.03,0.56,-1.33,0  
 3G53,ARG\_174,11.24,-1.26,0,0  
 2BDV,GLU\_53,3.79,0.42,-1.13,0  
 1SQH,ASP\_169,3.8,0,0,0  
 3DTE,LYS\_190,10.36,-0.14,0,0  
 2RGY,GLU\_251,3.34,0.35,-1.51,0  
 1OST,ARG\_448,12.08,-0.42,0,0  
 1LN4,GLU\_45,1.53,1.19,-4.16,0  
 3DB9,ARG\_65,10.53,0,0,1.53  
 3GYW,CYS\_133,8.68,-0.06,-1.49,1.23  
 3N0K,ARG\_135,12.01,-0.49,0,0  
 2F9F,ARG\_60,12.29,-0.21,0,0  
 3PBH,TYR\_177,10,0,0,0  
 2G9D,LYS\_35,10.29,-0.21,0,0  
 3K8S,GLU\_315,5.34,0.84,0,0  
 3V55,LYS\_648,10.29,-0.21,0,0  
 3UPD,LYS\_43,10.29,-0.21,0,0  
 1DZF,ASP\_84,3.6,0,-0.19,0  
 1YM5,GLU\_142,3.19,0.63,-1.94,0  
 2CVB,ARG\_116,12.47,-0.07,0,0.04  
 1A8Q,ARG\_151,12.22,-0.28,0,0  
 1EV8,HIS\_32,6.36,0,0,-0.14  
 2AHE,LYS\_212,10.5,0,0,0  
 2FG1,LYS\_7,10.5,0,0,0  
 1YG2,ARG\_161,12.22,-0.28,0,0  
 1JTR,ARG\_2,11.73,-0.77,0,0  
 3ETU,GLU\_146,4.57,0.07,0,0  
 3G9G,ASP\_145,3.99,0.28,-0.09,0  
 3R2E,GLU\_77,2.38,0.28,-2.4,0  
 2QV2,ARG\_274,11.66,-0.84,0,0  
 2ZCO,ARG\_158,11.8,-0.7,0,0  
 3IVF,LYS\_256,10.5,0,0,0  
 1O9G,ARG\_158,12.5,0,0,0  
 3PBH,LYS\_62,10.5,0,0,0  
 2B0J,HIS\_88,9.18,4.34,2.36,-4.01  
 2YYO,CYS\_109,12,0,0,3  
 2AZL,CYS\_267,9.03,-0.93,0,0.96  
 2QEV,GLU\_31,3.98,0.28,-0.8,0  
 1YLN,GLU\_87,3.85,0.28,-0.93,0  
 2X4L,GLU\_188,4.64,0.14,0,0  
 4HDE,ASP\_54,2.85,0.56,-1.51,0  
 3COU,ASP\_132,4.09,0.35,-0.06,0  
 4H89,ASP\_64,1.97,1.05,-2.89,0  
 3EVZ,GLU\_118,3.45,0.49,-1.54,0  
 2OB5,ARG\_114,12.29,-0.21,0,0  
 2CL3,LYS\_73,10.08,-0.42,0,0  
 3DHN,ASP\_54,2.51,0.42,-1.71,0  
 1BKR,HIS\_89,6.36,0,0,-0.14  
 3CS1,ARG\_154,11.94,-0.56,0,0  
 1ZKZ,LYS\_30,10.5,0,0,0  
 1E5S,ARG\_230,11.45,-1.05,0,0  
 4FH3,LYS\_144,10.22,-0.28,0,0  
 2RGY,LYS\_207,10.5,0,0,0  
 3FFM,GLU\_109,4.64,0.14,0,0  
 2ZCX,ASP\_99,3.94,0.35,-0.22,0  
 1TD6,LYS\_187,10.36,-0.14,0,0  
 1DVO,ARG\_165,12.15,-0.35,0,0  
 1XKR,GLU\_175,4.64,0.14,0,0  
 3GEC,ASP\_529,3.94,0.14,0,0  
 1SQW,HIS\_112,6.36,0,0,-0.14  
 2BDD,LYS\_118,10.43,-0.07,0,0

1Y0K,GLU\_3,4.57,0.07,0,0  
1VJG,GLU\_190,3.36,0.49,-1.63,0  
2BLL,GLU\_576,3.74,0.21,-0.97,0  
1UXO,ARG\_87,12.43,-0.07,0,0  
3H13,LYS\_462,10.36,-0.14,0,0  
1U3Y,ARG\_332,11.73,-0.77,0,0  
3DHN,HIS\_191,7.15,0.72,0,-0.07  
3L7N,LYS\_168,9.87,-0.63,0,0  
1QQE,LYS\_168,10.08,-0.42,0,0  
3LH5,GLU\_541,1.52,1.33,-1.97,-2.35  
2AZP,CYS\_88,7.36,-5.56,0.04,3.88  
2OKT,GLU\_84,4.57,0.07,0,0  
1XEU,LYS\_206,10.5,0,0,0  
3GYW,LYS\_93,10.5,0,0,0  
1WXQ,GLU\_135,1.17,1.13,-2.29,-2.18  
2DVK,LYS\_87,10.01,-0.49,0,0  
1FHL,ASP\_125,3.79,0,-0.01,0  
3ELI,ARG\_64,12.29,-0.21,0,0  
1TR9,LYS\_226,10.43,-0.07,0,0  
1WP5,ARG\_130,12.43,-0.07,0,0  
3A2Z,TYR\_52,11.78,0.38,0,1.4  
3LH5,GLU\_581,4.71,0.21,0,0  
3LMO,TYR\_74,13.22,0.14,0.68,2.4  
1AT0,HIS\_329,0.6,0.91,-2.34,-4.47  
2HRZ,ASP\_172,3.43,0.42,-0.79,0  
4E6S,GLU\_79,4.71,0.21,0,0  
1H09,TYR\_93,11.71,1.15,-1.1,1.65  
3V3T,TYR\_73,10.48,0.48,0,0  
2PWQ,TYR\_129,10.0,0,0,0  
1UW7,LYS\_84,10.15,-0.35,0,0  
1WRU,ARG\_269,12.01,-0.49,0,0  
2V4X,ASP\_65,3.68,0.07,-0.2,0  
1AKO,TYR\_215,8.53,0.86,-1.44,-0.89  
2JEO,GLU\_147,4.57,0.07,0,0  
1R3D,GLU\_82,4.5,0,0,0  
1Y0K,HIS\_186,6.57,0.07,0,0  
2I6I,GLU\_27,3.11,0.21,-1.6,0  
3JRT,LYS\_95,10.43,-0.07,0,0  
1GVP,TYR\_34,10.0,0,0,0  
3RJX,HIS\_45,7.37,1.6,2,-2.73  
3IPZ,LYS\_159,10.43,-0.07,0,0  
2A1V,ARG\_72,12.01,-0.49,0,0  
1ZCE,ASP\_93,2.54,0.49,-1.75,0  
1R3F,GLU\_120,4.5,0,0,0  
2CXC,LYS\_134,10.22,-0.28,0,0  
2FZP,ARG\_279,11.66,-0.84,0,0  
3EZ7,GLU\_393,4.5,0,0,0  
1X1E,TYR\_91,10.0,0,0,0  
1J74,GLU\_20,4.45,0.28,-0.33,0  
1ES9,LYS\_95,10.5,0,0,0  
3G9G,GLU\_158,4.64,0.14,0,0  
3IVF,ARG\_35,12.01,-0.49,0,0  
3VJ8,GLU\_343,3.98,0.28,-0.8,0  
2GZQ,ARG\_57,12.5,0,0,0  
4EZB,ASP\_66,2.72,0.56,-1.64,0  
2X5Y,TYR\_740,10.07,0.07,0,0  
2ZTY,TYR\_113,10.14,0.14,0,0  
1J74,GLU\_68,4.48,0.07,-0.09,0  
3I0C,GLU\_203,3.38,0.28,-1.4,0  
1HF8,ASP\_61,3.49,0.07,-0.38,0  
3CGW,ARG\_281,11.59,-0.91,0,0  
2RIK,ASP\_165,3.79,0.07,-0.08,0  
1CHD,LYS\_232,10.22,-0.28,0,0  
2BT8,ARG\_299,11.87,-0.63,0,0  
4DBX,ARG\_66,11.8,-0.7,0,0  
3TOW,ASP\_121,3.06,0.42,-1.16,0  
1LTU,ARG\_231,12.29,-0.21,0,0  
3TOW,HIS\_194,6.5,0,0,0  
3BA1,CYS\_86,9.51,-0.03,0,0.54  
2Q13,TYR\_203,10.0,0,0,0  
1YG2,ARG\_123,12.08,-0.42,0,0  
2C2Y,HIS\_254,6.26,0.04,0,-0.28  
2IXM,ARG\_106,11.87,-0.63,0,0  
3JZN,ARG\_269,11.94,-0.56,0,0  
2X4L,TYR\_282,12.97,0.28,0.29,2.4  
2F4Q,HIS\_80,7.34,0.98,0,-0.14  
1ZBM,LYS\_258,10.15,-0.35,0,0  
1YTD,TYR\_105,10.19,0.19,0,0  
3V46,TYR\_307,9.95,0,-0.05,0  
3IL3,TYR\_11,13.67,0.07,0.49,3.11  
2GKG,LYS\_76,10.29,-0.21,0,0  
3LH5,ASP\_678,3.87,0.07,0,0  
1FO9,TYR\_223,13.36,3.67,-0.31,0  
3CIV,ARG\_185,13.85,-0.89,0.224  
3MEW,TYR\_190,9.19,0.35,-1.16,0  
2CIU,TYR\_141,13.27,0.07,0.8,2.4  
2O0K,ASP\_296,3.94,0.14,0,0  
3BZT,GLU\_307,3.68,0.28,-1.1,0  
2FL4,ARG\_64,12.15,-0.35,0,0  
2B3M,ASP\_71,3.79,0,-0.01,0  
3JSN,HIS\_150,1.63,0,-1.21,-3.66  
1U3Y,GLU\_265,4.64,0.14,0,0  
1MUF,ASP\_101,3.51,0.14,-0.43,0  
3QKY,GLU\_126,4.43,0,-0.07,0  
3M66,LYS\_211,10.5,0,0,0  
2ZQ5,TYR\_307,13.41,0.21,0.8,2.4  
2OJQ,GLU\_672,4.5,0,0,0  
3OA7,GLU\_7,3.98,0.63,-1.15,0  
2CWY,ARG\_91,12.22,-0.28,0,0  
2INO,HIS\_17,6.36,0,0,-0.14  
2V81,ASP\_58,3.8,0,0,0  
2WZ9,LYS\_67,10.22,-0.28,0,0  
3CSR,LYS\_7,10.43,-0.07,0,0  
3ODJ,TYR\_23,8.99,0.35,-1.36,0  
2Q12,ARG\_237,12.5,0,0,0  
2B6P,ARG\_196,12.43,-0.07,0,0  
2FC3,LYS\_34,10.5,0,0,0  
2H14,TYR\_75,11.69,0.21,-0.71,2.2  
4EKU,GLU\_325,3.85,0.14,-0.79,0  
3EZ7,ASP\_383,3.83,0.28,-0.25,0  
2FD5,CYS\_104,7.46,-3.07,-1.04,2.57  
3I4T,GLU\_46,3.26,0.63,-1.87,0  
1T95,LYS\_225,10.43,-0.07,0,0  
1DTO,ASP\_124,3.23,0.42,-0.99,0  
3H9W,GLU\_37,4.35,0.28,-0.43,0  
3ELI,ASP\_41,3.92,0.21,-0.09,0  
2F8H,ASP\_134,2.72,0.42,-1.49,0  
2A6B,HIS\_71,6.88,0.59,0,-0.21  
1AD6,GLU\_440,4.22,0.7,-0.98,0  
2RIS,GLU\_19,4.78,0.28,0,0  
1X04,GLU\_184,4.5,0,0,0  
3M3P,HIS\_140,10.09,2.6,6.05,-5.06  
3BA1,GLU\_259,3.34,0.42,-1.58,0  
1XAW,GLU\_470,3.19,0.42,-1.73,0  
3UPD,ARG\_6,12.36,-0.14,0,0  
3DZ1,HIS\_240,7.19,0.83,0,-0.14  
3IVF,GLU\_189,3.29,0.77,-1.98,0  
2X4G,GLU\_58,3.6,0.42,-1.32,0  
2B78,ASP\_261,2.9,0.28,-1.18,0  
2Q34,ARG\_38,12.01,-0.49,0,0  
1BGF,LYS\_13,10.5,0,0,0  
2OYZ,GLU\_74,4.71,0.21,0,0  
2C13,LYS\_246,10.29,-0.21,0,0  
3B21,GLU\_154,4.5,0,0,0  
3ZRI,ARG\_31,12.22,-0.28,0,0  
1T95,HIS\_141,6.36,0,0,-0.14  
1ZBS,GLU\_93,4.21,0.27,-0.1,-0.45  
2EJB,ASP\_68,2.36,0.7,-2.13,0  
2O8PLYS\_208,10.5,0,0,0  
1G8P,ARG\_126,12.08,-0.42,0,0  
1AT0,LYS\_372,10.36,-0.14,0,0  
2B6P,GLU\_257,4.5,0,0,0  
1X04,ARG\_45,11.73,-0.77,0,0  
3DHN,ASP\_86,3.96,0.21,-0.05,0  
1WYC,CYS\_332,9.63,-1.52,0.2,1.6  
2Q34,GLU\_90,4.47,0.77,-0.8,0  
3V55,LYS\_404,10.43,-0.07,0,0  
3JZ9,TYR\_396,10.22,-0.28,0,0  
1W7B,CYS\_335,7.39,-1.95,-1.45,1.79  
1WJG,ARG\_124,11.8,-0.7,0,0  
4DVD,ASP\_148,3.72,0,-0.08,0  
1ZBM,HIS\_1,6.7,0.2,0,0  
2B3M,TYR\_44,9.42,0.39,-0.15,-0.82  
2VGM,GLU\_149,4.47,0,-0.03,0  
3VHJ,LYS\_159,10.29,-0.21,0,0  
2Z61,TYR\_224,12.05,2.05,0,0  
3KVO,ARG\_75,12.01,-0.49,0,0  
2O8I,GLU\_6,3.75,0.21,-0.96,0  
1OXZ,GLU\_230,4.5,0,0,0  
2NRK,ASP\_147,3.68,0,-0.12,0  
2VGM,HIS\_235,6.42,0.13,0,-0.21  
3Q9P,ASP\_115,4.08,0.28,0,0  
2YX0,GLU\_249,4.71,0.21,0,0  
3PZ9,ASP\_135,3.14,0.21,-0.87,0  
3GW3,ARG\_41,12.29,-0.21,0,0  
1TR9,HIS\_207,7.34,1.6,1.91,-2.67  
3F6F,GLU\_195,4.64,0.14,0,0  
3ASA,LYS\_331,10.36,-0.14,0,0  
3M7G,ASP\_49,3.69,0.28,-0.38,0  
2PP6,ARG\_81,11.94,-0.56,0,0  
2G55,GLU\_151,4.71,0.21,0,0  
1Z3X,ARG\_169,12.15,-0.35,0,0  
1AIL,ARG\_46,11.87,-0.63,0,0  
2AD1,HIS\_268,7.1,0.68,0,-0.07  
4H86,GLU\_82,4.5,0,0,0  
2Q34,LYS\_143,10.29,-0.21,0,0  
1GXN,CYS\_510,3.86,-7.77,0.2,63  
2CE6,ARG\_43,12.5,0,0,0  
3EOD,ASP\_104,2.87,0.35,-1.28,0  
1XDZ,LYS\_228,10.5,0,0,0  
1O17,ASP\_223,3.92,0.14,-0.02,0  
3JZ9,ASP\_354,3.28,0.28,-0.8,0  
3EVN,ARG\_232,12.29,-0.21,0,0  
2HYO,CYS\_29,10.05,-0.51,0,1.56  
1HU,ARG\_41,12.22,-0.28,0,0  
2QK0,GLU\_85,4.12,0.28,-0.66,0  
2G5X,LYS\_30,10.22,-0.28,0,0  
2EYI,ARG\_86,11.66,-0.84,0,0  
3AUF,TYR\_62,10.0,0,0,0  
2HRZ,GLU\_310,4.71,0.21,0,0  
3DSH,ASP\_294,3.93,0.14,-0.01,0  
2HNG,GLU\_29,4.5,0,0,0  
1Q2Y,LYS\_2,10.29,-0.21,0,0  
1OIS,GLU\_268,4.64,0.14,0,0  
4DBX,GLU\_243,4.5,0,0,0  
1E59,ASP\_36,4.31,0.56,-0.05,0  
2CXA,ARG\_227,11.73,-0.77,0,0  
2R57,GLU\_256,3.15,0.63,-0.43,-1.55  
3CAX,GLU\_278,2.2,2.12,-1.19,-3.22  
1Z9L,LYS\_107,10.5,0,0,0  
3CCY,LYS\_55,9.66,-0.84,0,0  
2ZQ5,ARG\_179,10.65,-3.62,0.1,77  
1WRU,LYS\_328,10.22,-0.28,0,0  
2FBI,GLU\_110,4.63,0.21,-0.08,0  
1QYI,GLU\_15,7.32,1.51,0.1,31  
2INO,ARG\_410,12.15,-0.35,0,0  
3A2Z,GLU\_170,4.57,0.07,0,0  
1PBV,HIS\_133,2.08,0,0,-4.42  
2Q12,TYR\_68,10.47,0,0,0.47  
3ZSL,HIS\_208,7.09,0.8,0,-0.21  
2X4J,ARG\_100,11.94,-0.56,0,0  
2EFK,LYS\_110,10.01,-0.49,0,0  
1IAP,GLU\_71,4.64,0.14,0,0  
3ANJ,TYR\_51,11.1,2.27,-1.17,0  
3VJ8,ARG\_185,11.49,-1.01,0,0  
1V6T,ARG\_195,11.46,-1.04,0,0  
1EV8,TYR\_71,9.51,0.07,-0.56,0  
3ULX,GLU\_29,4.81,0.35,-0.04,0  
2Z0M,TYR\_185,11.9,0.14,0,1.76  
1PVT,TYR\_205,13.75,0.83,0.57,2.35  
4FZR,GLU\_61,4.04,0.28,-0.74,0  
3EVP,ASP\_275,3.87,0.07,0,0  
2O0K,CYS\_158,11.09,0,0.2,09  
3M7G,ARG\_131,13.24,-1.83,0.2,57  
3ZSL,LYS\_226,10.36,-0.14,0,0  
3RHE,CYS\_120,9.07,0,0,0.07  
3DSH,ASP\_429,4.16,0.42,-0.06,0  
1RWZ,GLU\_178,4.5,0,0,0  
1EDG,LYS\_64,10.08,-0.42,0,0  
1EJG,HIS\_14,6.5,0,0,0  
3ADO,GLU\_83,4.78,0.28,0,0  
4EUG,ARG\_195,12.5,0,0,0  
3K8J,GLU\_122,4.85,0.35,0,0  
4DVD,ASP\_164,2.71,0.56,-1.65,0  
2WB8,LYS\_575,10.43,-0.07,0,0  
1RHS,HIS\_2,6.08,0,-0.42  
2FD4,ASP\_465,2.18,0.98,-2.61,0  
3QAV,CYS\_223,9,0,0,0  
3IL3,LYS\_200,10.22,-0.28,0,0  
3M3P,HIS\_250,7.02,0.8,0,-0.28  
2IXM,GLU\_202,4.78,0.28,0,0  
1FHL,ASP\_322,4.08,0.28,0,0  
2G70,TYR\_102,10.0,0,0,0  
3U2R,GLU\_144,4.57,0.07,0,0  
2IF4,ASP\_185,3.87,0.07,0,0  
1RZ2,TYR\_175,13.96,0.76,0.8,2.4  
2GAU,GLU\_94,4.57,0.07,0,0  
3EVP,ASP\_194,3.81,0.21,-0.2,0  
3FRR,LYS\_118,10.29,-0.21,0,0  
2HXB,ARG\_160,11.8,-0.7,0,0  
1OXZ,ARG\_191,12.22,-0.28,0,0  
3F53,LYS\_40,9.94,-0.56,0,0  
3MIX,HIS\_496,6.5,0,0,0  
3IU5,ARG\_146,11.94,-0.56,0,0  
1XWM,ASP\_156,3.87,0.07,0,0  
2F8H,ARG\_91,12.15,-0.35,0,0  
3FHF,GLU\_107,4.05,0.35,-0.8,0  
2P65,LYS\_108,10.5,0,0,0  
2CBE,ASP\_180,1.01,0.7,-3.49,0  
4HDE,TYR\_163,10.0,0.78,-0.78,0  
1NIJ,ARG\_172,10.78,-1.72,0,0  
2P5D,LYS\_77,10.36,-0.14,0,0  
2Q13,LYS\_173,10.5,0,0,0  
3BB7,GLU\_123,4.64,0.14,0,0  
3EJG,LYS\_70,10.5,0,0,0  
1RHS,TYR\_261,9.32,0.76,-0.29,-1.15  
1ZHV,HIS\_133,6.22,0,0,-0.28  
1GXN,ARG\_483,12.22,-0.28,0,0  
2ZQ5,HIS\_183,3.24,1.02,0,-4.28  
2RJD,HIS\_447,4.98,1.48,0,-3  
2HRZ,LYS\_123,10.5,0,0,0  
4FD6,LYS\_110,10.22,-0.28,0,0  
4GCO,TYR\_234,10.49,0.49,0,0  
1P1L,GLU\_51,2.66,0.56,-2.4,0  
3M70,LYS\_162,10.08,-0.42,0,0  
1XFK,LYS\_66,10.15,-0.35,0,0



1T95,ARG\_201,12.5,0,0,0  
3UOV,TYR\_210,10,0,0,0  
2CYG,TYR\_116,11.61,1.85,0.25,-0.49  
2WOG,GLU\_184,4.62,0.35,-0.23,0  
2HP7,GLU\_193,3.33,0.63,-1.8,0  
3I82,ARG\_67,12.36,-0.14,0,0  
2CYG,TYR\_284,12.38,3.18,-0.8,0  
2BDD,LYS\_49,10.5,0,0,0  
1MML,GLU\_35,1.9,0.7,-3.3,0  
2P52,CYS\_235,4.71,-4.89,-0.42,1.01  
3R87,LYS\_87,10.22,-0.28,0,0  
1BKB,ASP\_26,3.94,0.14,0,0  
1Q46,ARG\_135,11.8,-0.7,0,0  
1SIG,LYS\_264,10.01,-0.49,0,0  
1EV8,ASP\_205,3.66,0.28,-0.41,0  
3ETV,LYS\_242,10.5,0,0,0  
3EX9,GLU\_47,3.11,0.35,-1.73,0  
2GZR,ARG\_68,11.59,-0.91,0,0  
1EV8,LYS\_233,10.29,-0.21,0,0  
3HZQ,LYS\_54,10.5,0,0,0  
2BDV,TYR\_119,10,0,0,0  
3H5T,GLU\_285,4.45,0.49,-0.54,0  
1FKM,CYS\_579,8.57,-3.6,0.3,17  
2E35,HIS\_365,6.43,0,0,-0.07  
2IF4,LYS\_79,10.43,-0.07,0,0  
2V4X,CYS\_77,10.6,-0.02,0,1.62  
4FH3,GLU\_257,3.89,0.42,-1.03,0  
2DFL,LYS\_289,10.22,-0.28,0,0  
1KCM,GLU\_257,4.57,0.07,0,0  
3P2F,ARG\_136,12.22,-0.28,0,0  
1NFN,TYR\_118,9.69,0.18,-0.49,0  
3CAN,GLU\_59,1.75,0.77,-3.52,0  
2R2Y,GLU\_25,4.64,0.14,0,0  
2EJB,GLU\_112,3.33,0.35,-1.52,0  
1P6F,LYS\_7,10.15,-0.35,0,0  
3M7D,GLU\_266,4.69,0.14,0.05,0  
1UOH,LYS\_203,10.5,0,0,0  
3VHJ,HIS\_108,5.55,0.8,0,-1.75  
1SUU,LYS\_708,10.43,-0.07,0,0  
2XMZ,ASP\_76,3.41,0.28,-0.67,0  
3JZ9,ASP\_415,3.81,0.07,-0.06,0  
1V43,ASP\_73,3.86,0.07,-0.01,0  
4DND,LYS\_103,10.22,-0.28,0,0  
2ILR,ASP\_432,3.65,0,-0.15,0  
3VHJ,LYS\_162,10.29,-0.21,0,0  
1XTZ,HIS\_182,6.57,0.14,0,-0.07  
3LMO,LYS\_54,10.5,0,0,0  
3I4T,HIS\_158,3.17,0.8,0,-4.13  
1W24,TYR\_163,10.3,0.07,-0.18,0.41  
1LZL,HIS\_290,5.12,1.6,2.4,-5.38  
3KEY,LYS\_370,10.29,-0.21,0,0  
1TP6,HIS\_10,7.3,1.15,0,-0.35  
1EV8,CYS\_161,11.18,0,0,2.18  
3I0C,ASP\_183,4.021,-0.01,0  
1Q5Z,ASP\_578,2.26,0.49,-2.02,0  
3GW3,ASP\_29,3.8,0,0,0  
2H30,LYS\_105,10.5,0,0,0  
1UAJ,ARG\_154,12.5,0,0,0  
4AM1,ASP\_62,1.21,0.42,-3.01,0  
1XDZ,GLU\_4,4.21,0.28,-0.57,0  
1NAR,GLU\_150,4.5,0,0,0  
1H4U,TYR\_531,10.53,0.07,0,0.46  
2VGY,GLU\_152,4.64,0.14,0,0  
3RFY,ASP\_292,2.72,0.35,-1.43,0  
1XDZ,HIS\_93,7.37,1.07,0,-0.21  
2NYC,HIS\_293,6.5,0,0,0  
1DCF,ARG\_71,12.36,-0.14,0,0  
2J8A,ASP\_257,2.76,0.14,-1.18,0  
1Q2Y,ARG\_120,12.5,0,0,0  
1BKB,GLU\_110,1.44,0.26,-0.92,-2.4  
1RWZ,TYR\_106,10.14,0.14,0,0  
1T07,GLU\_12,4.64,0.14,0,0  
3A0X,LYS\_701,10.15,-0.35,0,0  
3BB7,TYR\_168,8.85,0.21,-1.36,0  
2EYI,ASP\_217,3.4,0.21,-0.61,0  
1MD6,ARG\_131,12.43,-0.07,0,0  
2OB5,ARG\_40,12.08,-0.42,0,0  
2YWX,GLU\_128,4.5,0,0,0  
3O16,ARG\_222,11.87,-0.63,0,0  
3C38,TYR\_187,10.1,0.92,-0.82,0  
3AU3,CYS\_661,10.06,0,0,1.06  
2PLQ,TYR\_194,9.27,0.07,-0.8,0  
2V4U,GLU\_408,1.91,2.05,-2.24,-2.4  
4GA2,GLU\_142,4.64,0.14,0,0  
3OIP,TYR\_139,10.17,0,0,0  
3GMS,GLU\_252,3.98,0.28,-0.8,0  
1AK1,TYR\_248,12.31,0.07,0.2,2.4  
2PGE,ARG\_137,12.01,-0.49,0,0  
2E3C,ASP\_279,2.07,0.49,-2.22,0  
4H4J,LYS\_234,10.43,-0.07,0,0  
2YXO,GLU\_183,3.72,1.17,-1.8,-0.16  
1YR6,CYS\_207,9.14,0,0,0.14  
1TD6,GLU\_230,5.26,0.76,0,0  
3GYW,LYS\_51,10.43,-0.07,0,0  
1SIG,ARG\_441,12.22,-0.28,0,0  
3LJN,GLU\_37,4.21,0.28,-0.57,0  
1PGV,CYS\_262,9.6,-0.15,0,0.75  
1XDZ,LYS\_38,9.94,-0.56,0,0  
3LJC,LYS\_82,10.5,0,0,0  
2XHC,LYS\_150,10.29,-0.21,0,0  
1X1E,ARG\_168,11.45,-1.05,0,0  
2BLL,GLU\_446,6.76,2.43,-2.35,2.18  
1C3K,CYS\_40,9.45,0,0,0.45  
3V55,GLU\_704,4.5,0,0,0  
3GW3,ARG\_365,10.87,-1.63,0,0  
4H86,LYS\_102,10.29,-0.21,0,0  
3ETU,LYS\_286,10.36,-0.14,0,0  
2YXO,LYS\_304,10.08,-0.42,0,0  
3EGN,LYS\_481,10.36,-0.14,0,0  
3ZRI,HIS\_33,7.08,0.79,0,-0.21  
1PVT,HIS\_87,6.5,0.14,0,-0.14  
2P1W,HIS\_81,6.5,0,0,0  
2G3A,ARG\_28,12.15,-0.35,0,0  
3RNV,LYS\_412,10.5,0,0,0  
3EJG,HIS\_97,6.5,0,0,0  
1EQ6,LYS\_119,10.5,0,0,0  
4E8B,ARG\_146,11.87,-0.63,0,0  
3JSN,ASP\_13,3.86,0.07,-0.01,0  
3CCY,GLU\_18,4.5,0,0,0  
1D2K,TYR\_93,12.8,0.49,-0.09,2.4  
2P65,LYS\_20,10.43,-0.07,0,0  
1J33,ARG\_334,12.29,-0.21,0,0  
4D8L,GLU\_109,4.5,0,0,0  
2WOZ,LYS\_426,10.5,0,0,0  
4EKU,LYS\_223,10.5,0,0,0  
1Q42,GLU\_161,3.58,0.28,-1.19,0  
2R2Y,ASP\_41,0.77,0.56,-3.59,0  
4E9E,GLU\_483,4.49,0.28,-0.29,0  
3GFP,ASP\_319,3.64,0.21,-0.37,0  
2CBE,HIS\_4,6.22,0,0,-0.28  
2D0A,ARG\_164,12.15,-0.35,0,0  
3IVF,GLU\_38,3.87,0.28,-0.91,0  
3B21,LYS\_117,10.29,-0.21,0,0  
3UC9,TYR\_57,11.36,0.24,0,1.12  
3TMO,LYS\_210,10.5,0,0,0  
1BKR,LYS\_55,10.43,-0.07,0,0  
2CBE,HIS\_107,3.71,1.6,1.8,-6.19  
2IIA,GLU\_46,4.71,0.21,0,0  
1Y0K,HIS\_136,7.68,1.31,0,-0.14  
2PGX,GLU\_26,4.71,0.21,0,0  
3GMS,ASP\_307,3.87,0.07,0,0  
4AF2,LYS\_48,9.73,-0.77,0,0  
3HUE,ASP\_91,3.04,0.49,-1.25,0  
2HP7,GLU\_180,4.71,0.21,0,0  
3V55,GLU\_534,4.5,0,0,0  
3BA1,ARG\_215,12.01,-0.49,0,0  
1RWZ,LYS\_98,10.15,-0.35,0,0  
3BCY,HIS\_122,6.85,0.7,0,-0.35  
4FD6,LYS\_92,10.43,-0.07,0,0  
1XIP,ASP\_238,3.55,0.21,-0.46,0  
4FCU,HIS\_176,7.4,0.9,0,0  
3V46,GLU\_386,3.62,0.75,-0.42,-1.21  
3A2Z,ASP\_96,3.28,0.21,-0.73,0  
3C6B,LYS\_148,10.36,-0.14,0,0  
3V46,TYR\_378,13.34,0.14,0.8,2.4  
3PZ9,HIS\_151,6.36,0,0,-0.14  
2FD5,LYS\_51,9.8,-0.7,0,0  
1WYC,GLU\_297,4.05,0.35,-0.8,0  
3ASA,ARG\_186,11.87,-0.63,0,0  
1ILW,ARG\_38,11.87,-0.63,0,0  
3OBS,GLU\_24,3.77,1.43,-2.16,0  
4AE7,LYS\_78,10.5,0,0,0  
2QHT,GLU\_40,2.96,0.58,-1.2,-0.93  
2IXM,ARG\_293,12.01,-0.49,0,0  
3MTT,GLU\_499,4.5,0,0,0  
3FNI,HIS\_155,6.39,0.1,0,-0.21  
1R3F,TYR\_156,10.55,0,0.55  
2NRK,ARG\_90,12.15,-0.35,0,0  
2VGM,LYS\_337,10.5,0,0,0  
1ZBP,ASP\_225,3.69,0.07,-0.18,0  
3HVM,CYS\_324,10.9,-4.49,2.85,3.55  
3I4T,GLU\_32,2.29,1.89,-2.02,-2.08  
1UJ8,ASP\_42,3.34,0.35,-0.81,0  
2IXM,HIS\_230,6.08,0,0,-0.42  
1QYI,GLU\_100,3.74,0.77,-1.53,0  
3F6M,GLU\_137,4.34,0.07,-0.23,0  
3RLN,GLU\_729,4.04,0.21,-0.67,0  
2X4G,ARG\_131,12.08,-0.42,0,0  
1SUU,GLU\_525,4.5,0,0,0  
1WLY,GLU\_101,3.9,0.14,-0.74,0  
1DZF,ARG\_7,12.22,-0.28,0,0  
3CSV,GLU\_129,3.6,0.28,-1.18,0  
4DND,ARG\_11,12.15,-0.35,0,0  
3G9T,LYS\_8,10.36,-0.14,0,0  
2BDD,HIS\_126,7.02,0.8,0,-0.28  
1O6D,ASP\_87,3.28,0.28,-0.8,0  
2OEW,LYS\_312,10.22,-0.28,0,0  
1DVO,ASP\_107,2.64,0.42,-1.58,0  
3ZTA,HIS\_99,6.71,0.28,0,-0.07  
4FZR,ARG\_106,12.43,-0.07,0,0  
3EVP,TYR\_95,10,0,0,0  
1CBY,GLU\_78,4.5,0,0,0  
4EKU,GLU\_113,3.27,0.49,-1.72,0  
1SIG,ARG\_150,12.08,-0.42,0,0  
1ZCU,LYS\_96,10.01,-0.49,0,0  
3Q6L,LYS\_38,10.43,-0.07,0,0  
1WXQ,ASP\_327,4.01,0.21,0,0  
3P2F,ASP\_59,2.31,1.05,-2.54,0  
1R7J,LYS\_55,10.5,0,0,0  
3GMS,LYS\_10,10.5,0,0,0  
2O4D,GLU\_6,4.57,0.07,0,0  
2YXO,GLU\_26,3.92,0.21,-0.79,0  
1QYI,LYS\_62,10.43,-0.07,0,0  
1ANU,TYR\_88,11.49,0,0,1.49  
3LH5,GLU\_788,3.84,0.14,-0.8,0  
2QOP,ARG\_209,11.8,-0.7,0,0  
3BB7,GLU\_214,4.35,0.14,-0.29,0  
3RLN,GLU\_692,4.57,0.07,0,0  
15JY,GLU\_115,4.64,0.14,0,0  
3BQE,GLU\_323,1.9,1.27,-1.56,-2.3  
2ZCO,HIS\_116,6.5,0.07,0,-0.07  
1P2F,LYS\_140,10.5,0,0,0  
3CE7,ARG\_48,11.94,-0.56,0,0  
3G9B,CYS\_58,5.98,-3.34,0,0.33  
3EZ7,LYS\_29,10.15,-0.35,0,0  
2WB8,ASP\_597,3.05,0.21,-0.96,0  
2D0A,ARG\_27,12.5,0,0,0  
1A8Q,ASP\_157,3.33,0.35,-0.81,0  
3AU3,ARG\_623,12.5,0,0,0  
4ECC,LYS\_188,10.5,0,0,0  
2OJQ,LYS\_486,10.5,0,0,0  
1BN6,GLU\_287,0.61,2.44,-3.86,-2.47  
4EVF,ASP\_167,3.8,0,0,0  
3ZXV,LYS\_58,6.74,1.6,2.4,-3.76  
2ATR,TYR\_115,10.57,0.57,0,0  
1R3F,ARG\_306,11.59,-0.91,0,0  
1AKO,CYS\_177,10.8,0.33,0.56,0.91  
2OGQ,GLU\_555,3.4,0.42,-1.53,0  
2GAU,LYS\_132,10.5,0,0,0  
2O4D,ASP\_117,3.2,0.21,-0.81,0  
4EKU,CYS\_120,9,0,0,0  
3MIX,GLU\_557,3.69,2.19,-0.39,-2.6  
3DB9,ASP\_210,2.69,0.42,-1.53,0  
2BCF,TYR\_223,12.81,0.41,0.2,4  
2PGX,ARG\_188,12.15,-0.35,0,0  
2O4D,ASP\_117,3.2,0.21,-0.81,0  
1LN4,LYS\_19,10.5,0,0,0  
1S17,LYS\_67,10.5,0,0,0  
1RZZ,ASP\_38,3.44,0.56,-0.91,0  
1TR9,LYS\_141,10.29,-0.21,0,0  
3Q9P,HIS\_124,6.36,0,0,-0.14  
3L7N,TYR\_36,9.97,0,-0.03,0  
3CAX,ARG\_211,13.43,-1.47,0,2.4  
1RAJ,LYS\_395,10.43,-0.07,0,0  
1K95,TYR\_167,12.3,0.87,0,1.43  
2CL3,LYS\_189,10.5,0,0,0  
2HRZ,LYS\_41,10.15,-0.35,0,0  
1WYC,ASP\_357,3.28,0.28,-0.8,0  
1C3K,ASP\_52,3.87,0.07,0,0  
2RGY,CYS\_336,9.78,0,0,0.78  
3N2T,TYR\_246,8.07,0.41,0,-2.34  
1SQH,CYS\_164,9.07,0,0,0.07  
1GVP,ARG\_16,12.43,-0.07,0,0  
1R3F,ARG\_116,11.73,-0.77,0,0  
2E3C,ARG\_275,11.8,-0.7,0,0  
1YTD,ARG\_251,12.08,-0.42,0,0  
1XTZ,LYS\_40,10.5,0,0,0  
3CBN,HIS\_165,6.29,0,0,-0.21  
1O5J,CYS\_29,8.18,-0.89,0,0.07  
2RJD,TYR\_396,11.87,0.87,0.38,0.62  
2H2Z,LYS\_100,10.43,-0.07,0,0  
1WYC,HIS\_309,6.43,0,0,-0.07  
1V43,HIS\_328,7.23,0.8,0,-0.07  
3RUX,ARG\_295,11.48,-2.86,0,1.84  
1YQT,ARG\_187,12.29,-0.21,0,0  
2OHT,ARG\_97,12.5,0,0,0  
1R15,TYR\_91,10.06,0.06,0,0  
2X5Y,LYS\_829,10.43,-0.07,0,0  
2XHC,LYS\_191,10.29,-0.21,0,0  
1NFN,ARG\_61,12.29,-0.21,0,0  
2OKT,LYS\_78,10.01,-0.49,0,0  
3T5B,LYS\_235,10.43,-0.07,0,0  
3DHN,LYS\_3,10.5,0,0,0  
2G3A,GLU\_14,3.74,0.07,-0.83,0  
1R16,TYR\_246,11.52,1.52,0,0  
2E0T,ARG\_196,12.15,-0.35,0,0

1J33,ARG\_138,11.94,-0.56,0,0  
1WP5,ASP\_143,2.63,0.21,-1.39,0  
2FM9,LYS\_129,10.5,0,0,0  
12LF,GLU\_214,3.33,0.77,-1.94,0  
3JSN,TYR\_22,10.33,0,0,33  
3IRA,GLU\_151,4.5,0,0,0  
3OOP,ARG\_87,12.5,0,0,0  
2XHC,ARG\_338,11.24,-1.26,0,0  
1CHD,HIS\_190,6.26,1.6,1.69,-3.53  
4DNU,HIS\_131,0.7,0.4,0,-6.2  
1YR6,GLU\_19,3.56,0.49,-1.43,0  
2CN1,LYS\_141,10.15,-0.35,0,0  
3ANJ,LYS\_142,10.01,-0.49,0,0  
2AD1,LYS\_122,10.36,-0.14,0,0  
1SI7,GLU\_275,0.84,2.57,-3.83,-2.4  
1YM5,TYR\_141,9.58,1.18,-1.6,0  
1T3Y,TYR\_14,7.8,0.21,-2.4,0  
3EX9,ARG\_160,12.29,-0.21,0,0  
2WB3,ASP\_300,3.65,0.21,-0.36,0  
3F5D,TYR\_131,9.19,0.07,-0.88,0  
1A8Q,TYR\_103,10.7,1.06,-0.36,0  
1RHS,LYS\_23,10.5,0,0,0  
3RXX,GLU\_130,3.65,0.14,-0.99,0  
2GAU,GLU\_25,3.22,0.63,-1.91,0  
3CE7,LYS\_37,10.5,0,0,0  
2VGM,TYR\_374,10.07,0.07,0,0  
2H2W,LYS\_99,10.5,0,0,0  
3BPV,LYS\_129,10.5,0,0,0  
3K9I,LYS\_92,10.22,-0.28,0,0  
2V5B,ASP\_202,2.59,0.63,-1.84,0  
2I88,GLU\_468,4.71,0.21,0,0  
3OAT,LYS\_491,10.29,-0.21,0,0  
1W24,GLU\_120,2.97,0.64,-0.19,-1.98  
3T5B,HIS\_170,6.22,0,0,-0.28  
2CVB,HIS\_148,7.16,0.8,0,-0.14  
1YG2,ASP\_20,2.19,0.49,-2.1,0  
3EZ7,TYR\_109,10.07,0.07,0,0  
3FFM,ARG\_94,11.94,-0.56,0,0  
2X4G,TYR\_127,7.65,1.05,-1,-2.4  
2VAN,CYS\_178,9.1,-1.88,-0.16,2.13  
1GXN,GLU\_402,4.05,0.35,-0.8,0  
2B78,LYS\_3,9.59,-0.91,0,0  
1MD6,ARG\_102,12.29,-0.21,0,0  
3B21,ASP\_59,3.6,0.07,-0.27,0  
2ZOM,TYR\_300,11.08,1.21,-0.13,0  
2PGE,CYS\_255,10.58,0.14,0,1.52  
3M66,LYS\_321,10.3,0,0,0  
1V6T,LYS\_77,10.43,-0.07,0,0  
1ZBM,LYS\_2,10.5,0,0,0  
2B0A,HIS\_44,7.43,4.57,2.01,-5.66  
3QKY,HIS\_31,6.42,0.06,0,-0.14  
3V75,ASP\_213,3.58,0,-0.22,0  
1SUU,ASP\_660,3.4,0.28,-0.68,0  
1ZCU,TYR\_223,11.57,0.14,0,1.43  
3EJC,ASP\_135,2.55,0.77,-2.02,0  
2ZTY,GLU\_24,2.64,0.7,-2.56,0  
2O4D,ASP\_13,3.73,0,-0.07,0  
3ADO,GLU\_93,2.11,2.85,-3.17,-2.07  
2PIM,GLU\_34,4.5,0,0,0  
3H6Q,CYS\_105,8.49,-1.6,0,1.09  
2ZQ5,TYR\_36,8.65,0.56,-0.95,-0.97  
1IDK,ARG\_176,11.9,-2.4,0,1.8  
1XDZ,GLU\_5,3.72,0.42,-1.2,0  
3TOW,LYS\_120,10.5,0,0,0  
2IIA,ARG\_61,12.5,0,0,0  
1YR6,GLU\_120,4.64,0.14,0,0  
1OXZ,ARG\_260,12.22,-0.28,0,0  
1W7B,HIS\_94,6.34,0.05,0,-0.21  
2Q13,LYS\_192,10.01,-0.49,0,0  
3FRR,ARG\_53,11.52,-0.98,0,0  
2ZQ5,ASP\_32,3.78,0.7,-1.3,0.58  
1OST,GLU\_151,4.14,0.42,-0.78,0  
4DVD,ARG\_52,12.5,0,0,0  
3BCH,LYS\_52,10.5,0,0,0  
2E3C,ASP\_414,3.87,0.07,0,0  
1SUU,ASP\_543,4.01,0.21,0,0  
3JSN,LYS\_207,9.8,-0.7,0,0  
2BAA,ASP\_235,2.84,0.42,-1.38,0  
1SIG,LYS\_236,10.5,0,0,0  
3GS9,CYS\_95,10.1,-0.4,0,1.5  
1ZBS,LYS\_21,10.43,-0.07,0,0  
1SIG,GLU\_219,4.5,0,0,0  
1RIS,ARG\_165,12.22,-0.28,0,0  
1IDK,ARG\_127,12.29,-0.21,0,0  
3K1H,GLU\_134,4.45,0.28,-0.33,0  
2ZQ5,TYR\_82,10.0,0,0,0  
3GMS,GLU\_99,3.52,0.49,-1.47,0  
2D7U,ASP\_95,3.94,0.14,0,0  
1ZBP,LYS\_76,10.43,-0.07,0,0  
3M3P,TYR\_141,13.58,0.38,0.8,2.4  
3PZ9,ASP\_360,2.9,0.7,-1.6,0  
2RIS,GLU\_166,4.61,0.87,-2.18,1.42  
1DUN,HIS\_108,6.36,0,0,-0.14  
2P0L,HIS\_69,6.36,0,0,-0.14  
2JEO,HIS\_120,6.6,0.24,0,-0.14  
2D7J,HIS\_171,6.5,0,0,0  
2W0G,GLU\_257,3.84,0.14,-0.8,0  
4DEZ,CYS\_140,9.58,-0.03,-0.81,1.43  
4EFS,TYR\_164,10.07,0.07,0,0  
2IDC,GLU\_121,4.5,0,0,0  
1A8Q,ARG\_233,12.22,-0.28,0,0  
3BPV,HIS\_28,6.78,0.49,0,-0.21  
2V4U,GLU\_438,3.33,0.84,-2.01,0  
1KCM,GLU\_132,3.91,0.21,-0.8,0  
3KB5,ARG\_404,12.5,0,0,0  
3RXX,LYS\_266,10.43,-0.07,0,0  
3FXH,GLU\_39,4.85,0.35,0,0  
1V43,LYS\_366,10.29,-0.21,0,0  
3N0K,TYR\_59,10.34,0,0.34  
2YXO,HIS\_83,1.83,0,0,-4.67  
2WOZ,ASP\_304,3.59,0.14,-0.35,0  
3PZ9,HIS\_283,5.98,0,-0.52  
2H8O,CYS\_119,11.52,-0.66,0.75,2.44  
2R57,ARG\_364,12.64,-2.26,0,2.4  
1WXF,GLU\_124,4.24,0.14,-0.4,0  
2EA9,GLU\_30,4.41,0.21,-0.3,0  
1VSM,GLU\_133,4.5,0,0,0  
1YR6,ARG\_146,10.7,-1.8,0,0  
2P52,HIS\_165,6.87,0.72,0,-0.35  
4H4J,GLU\_169,2.75,0.93,-2.68,0  
2GEN,HIS\_53,3.58,0,0,-2.92  
3K1H,GLU\_123,4.71,0.21,0,0  
1OI7,GLU\_83,3.98,0.64,-1.16,0  
3PBH,TYR\_94,11.25,0,0,1.25  
1PSW,ASP\_211,3.87,0.07,0,0  
2RFA,GLU\_93,2.98,0.35,-1.87,0  
1GVV,HIS\_64,6.36,0,0,-0.14  
2DFL,ARG\_223,12.5,0,0,0  
4DIU,LYS\_143,9.87,-0.63,0,0  
1C3K,TYR\_56,13.27,0.07,0.8,2.4  
3L3P,ARG\_292,12.36,-0.14,0,0  
2W0G,ASP\_169,3.04,0.14,-0.9,0  
2CN1,ARG\_253,13.52,-0.76,0,1.78  
4FCU,CYS\_128,10.14,0,0,1.14  
2FXT,LYS\_239,10.5,0,0,0  
3LMO,ASP\_6,2.74,0.21,-1.27,0  
1Q5Z,GLU\_628,4.05,0.35,-0.8,0  
1V43,GLU\_118,4.06,0,-0.44,0  
3GW3,GLU\_48,4.5,0,0,0  
1OIS,GLU\_264,4.2,0.28,-0.58,0  
1UAJ,GLU\_185,4.57,0.07,0,0  
1XEU,LYS\_296,10.5,0,0,0  
3M7D,ARG\_283,12.15,-0.35,0,0  
3CJW,GLU\_347,4.66,0.49,-0.33,0  
2QEV,TYR\_58,10.48,0,0,0.48  
3I82,TYR\_160,11.27,0,0,1.27  
3GA2,LYS\_75,10.29,-0.21,0,0  
2OPJ,ARG\_15,12.15,-0.35,0,0  
3NZL,LYS\_78,10.5,0,0,0  
3COU,ASP\_31,2.78,0.49,-1.51,0  
1FQI,ASP\_306,0.03,0.98,-4.75,0  
2VGM,GLU\_232,4.78,0.28,0,0  
3GE9,ARG\_41,11.66,-0.84,0,0  
2EFK,ARG\_139,11.94,-0.56,0,0  
1X7F,HIS\_58,6.35,0.06,0,-0.21  
3DSH,TYR\_266,10.0,0,0,0  
3HVW,ASP\_298,2.23,0.56,-2.13,0  
1GQE,CYS\_274,6.63,-3.58,0,1.21  
2D0A,ARG\_246,11.64,-0.86,0,0  
1MTZ,ARG\_252,11.8,-0.7,0,0  
1Q46,GLU\_123,4.19,0.07,-0.38,0  
1WNH,ARG\_115,12.5,0,0,0  
1LZL,GLU\_187,7.61,3.11,0,0  
3BA1,CYS\_122,9.07,-0.07,0,0.14  
1WXF,LYS\_41,10.43,-0.07,0,0  
1SBX,ARG\_100,11.8,-0.7,0,0  
2Q07,LYS\_449,9.66,-0.84,0,0  
3FS3,HIS\_72,6.43,0,0,-0.07  
3IL3,ASP\_184,2.08,1.05,-2.77,0  
3O7K,GLU\_59,3.01,0.28,-1.78,0  
3ETV,LYS\_213,10.43,-0.07,0,0  
4DIU,TYR\_238,12.96,0.07,0.49,2.4  
1LZL,ASP\_231,1.8,0.77,-2.78,0  
3T5B,GLU\_243,3.57,0.49,-1.42,0  
2H2W,TYR\_151,13.33,0.21,0.72,2.4  
3Q1C,GLU\_316,4.5,0,0,0  
3S0A,LYS\_99,10.01,-0.49,0,0  
2B2H,LYS\_243,10.5,0,0,0  
1U7U,TYR\_207,10.0,0,0,0  
3N0K,CYS\_60,7.56,-2.1,-1.31,1.97  
3T57,GLU\_300,4.5,0,0,0  
2VAN,ASP\_318,2.46,0.21,-1.55,0  
1XIP,ASP\_6,3.7,0.07,-0.17,0  
1PVT,TYR\_57,10.39,0.35,-1.21,1.25  
1MD6,ASP\_103,2.75,0.49,-1.54,0  
1TLV,ASP\_261,2.36,0.42,-1.86,0  
4FH3,LYS\_288,10.22,-0.28,0,0  
2X4G,CYS\_157,7.87,0,-1.13,0  
1CHD,GLU\_218,3.41,0.8,-1.89,0  
2XJ4,ARG\_185,10.22,-1.18,0,-1.1  
3A0X,ARG\_616,12.29,-0.21,0,0  
2A4D,GLU\_151,4.19,0.28,-0.59,0  
2R2Y,GLU\_126,4.57,0.07,0,0  
2Q13,GLU\_223,4.5,0,0,0  
3RKV,ARG\_333,12.43,-0.07,0,0  
3VHJ,ARG\_69,12.08,-0.42,0,0  
3MTT,ARG\_571,11.87,-0.63,0,0  
2GZQ,ASP\_26,3.21,0.21,-0.8,0  
3C6B,TYR\_78,12.31,0.21,0,2.1  
1J33,ARG\_316,11.19,-1.31,0,0  
1Z9L,TYR\_52,12.87,0.55,-0.08,2.4  
1WP5,GLU\_174,3.73,0.42,-1.19,0  
3N0K,LYS\_51,10.29,-0.21,0,0  
3V55,LYS\_661,10.5,0,0,0  
3IBT,ARG\_146,11.62,-0.88,0,0  
2G9D,ASP\_272,3.8,0,0,0  
4E9E,HIS\_561,6.5,0,0,0  
2H14,LYS\_78,10.5,0,0,0  
3N2T,ASP\_4,2.98,0.63,-1.45,0  
2B6P,GLU\_3,4.57,0.07,0,0  
2Q13,GLU\_53,4.5,0,0,0  
2P1W,LYS\_99,10.5,0,0,0  
2QOP,LYS\_6,10.01,-0.49,0,0  
3G9G,ARG\_5,11.94,-0.56,0,0  
1JYH,GLU\_61,4.5,0,0,0  
2BQQ,LYS\_112,10.29,-0.21,0,0  
4DEZ,GLU\_102,3.32,0.42,-1.6,0  
3CAX,TYR\_145,10.0,0,0,0  
2Q12,LYS\_130,10.22,-0.28,0,0  
3U56,CYS\_115,9.19,-0.08,0,0.27  
1S17,CYS\_109,8.93,-1.01,0,0.94  
1XEU,LYS\_57,10.36,-0.14,0,0  
1PV5,GLU\_179,4.85,0.35,0,0  
1UOH,HIS\_144,4.87,1.6,1.42,-4.64  
3V4G,ARG\_110,12.43,-0.07,0,0  
2H2W,GLU\_122,4.5,0,0,0  
1WPA,GLU\_472,4.5,0,0,0  
2RIK,GLU\_93,4.03,0.14,-0.61,0  
3BQW,GLU\_137,4.73,4.01,-3.78,0  
3C5V,GLU\_209,4.64,0.14,0,0  
2IXM,LYS\_63,10.15,-0.35,0,0  
3AUF,GLU\_174,6.88,2.38,0,0  
3M3P,GLU\_126,4.05,0.35,-0.8,0  
2XMZ,GLU\_35,4.5,0,0,0  
2ZTY,LYS\_176,9.8,-0.7,0,0  
1GVO,HIS\_186,10.36,-0.14,0,0  
2PLQ,ARG\_176,11.53,-0.97,0,0  
1RIS,LYS\_75,10.36,-0.14,0,0  
3KEY,ASP\_397,3.36,0.56,-1.0  
1NFN,LYS\_146,10.5,0,0,0  
3G9G,GLU\_117,4.43,0.21,-0.28,0  
1DVO,ASP\_89,3.83,0.14,-0.11,0  
3ILC,GLU\_179,3.7,0.56,-1.36,0  
1G5Z,LYS\_136,9.94,-0.56,0,0  
4HDE,ARG\_30,12.5,0,0,0  
3K1H,GLU\_81,4.43,0.21,-0.28,0  
1D2K,HIS\_54,2.96,0,0,-3.54  
2OSA,ARG\_445,12.08,-0.42,0,0  
1DOV,TYR\_222,10.0,0,0,0  
2IF4,TYR\_67,10.42,0.79,0,-0.37  
4AE7,TYR\_215,13.18,0.07,0.27,2.85  
2D2S,LYS\_740,9.59,-0.91,0,0  
2YT4,GLU\_502,4.5,0,0,0  
4ECC,ARG\_149,11.73,-0.77,0,0  
1NAR,ASP\_203,3.28,0.28,-0.8,0  
1RHS,LYS\_223,10.29,-0.21,0,0  
2EYI,LYS\_121,10.5,0,0,0  
3HVW,GLU\_257,4.5,0,0,0  
3PAC,ARG\_94,12.15,-0.35,0,0  
1FQI,ASP\_386,3.68,0.42,-0.54,0  
2GZR,GLU\_305,4.29,0.42,-0.63,0  
3AU3,GLU\_468,4.64,0.14,0,0  
2B61,TYR\_171,12.29,0.29,-0.4,2.4  
3LH5,GLU\_756,4.44,0.21,-0.27,0  
2Q12,LYS\_173,10.43,-0.07,0,0  
3L7N,GLU\_122,4.57,0.07,0,0  
2RIK,ARG\_105,11.66,-0.84,0,0  
1ZBP,ASP\_115,2.94,0.63,-1.49,0  
2IQT,GLU\_83,4.64,0.14,0,0  
1WXQ,ARG\_136,12.15,-0.35,0,0  
3CO1,GLU\_13,3.32,0,-1.18,0  
2DFL,ARG\_284,13.77,-1.91,0,3.18  
2QDJ,HIS\_281,4.8,0.62,0,-2.32  
2BAA,ASP\_135,2.79,0.49,-1.49,0  
1YLN,LYS\_75,10.5,0,0,0  
1RAJ,LYS\_220,10.5,0,0,0

3HVM,HIS\_202,13.05,5.2,7.22,-5.87  
 3DSH,ARG\_432,12.36,-0.14,0,0  
 3G9T,GLU\_279,3.76,0.21,-0.95,0  
 2HP7,ARG\_119,13.03,-0.47,0,1  
 2OEW,ASP\_143,3.75,0.07,-0.12,0  
 1UXO,GLU\_124,4.1,0.28,-0.68,0  
 2FBQ,ARG\_179,12.22,-0.28,0,0  
 1K95,ASP\_104,3.86,0.07,-0.01,0  
 1QYI,CYS\_34,11.55,0.32,2.2,0.02  
 3V4G,ARG\_48,12.01,-0.49,0,0  
 2POL,GLU\_4,4.29,0,-0.21,0  
 2RIS,ARG\_169,11.87,-0.63,0,0  
 3N2T,ASP\_223,3.54,0.35,-0.61,0  
 3EJG,ASP\_50,3,0.63,-1.43,0  
 1T95,LYS\_105,9.8,-0.7,0,0  
 3EVN,ASP\_274,3.87,0.07,0,0  
 3LMF,GLU\_89,4.53,0.28,-0.25,0  
 2P65,LYS\_104,10.5,0,0,0  
 3HST,ASP\_101,3.79,0.07,-0.08,0  
 2X4G,ARG\_237,11.21,-2.48,0,1.19  
 2X4J,TYR\_123,10.52,0,-0.08,0.61  
 2ZOM,LYS\_97,10.36,-0.14,0,0  
 1LFP,LYS\_220,9.94,-0.56,0,0  
 3CBN,HIS\_40,6.62,0.19,0,-0.07  
 1V8E,ARG\_114,12.36,-0.14,0,0  
 1X6J,LYS\_40,10.15,-0.35,0,0  
 3IL3,ASP\_72,3.21,0.21,-0.8,0  
 3UC9,HIS\_176,2.33,0.15,0,-4.32  
 2OSA,ASP\_433,3.21,0.28,-0.87,0  
 1WYC,TYR\_81,10,0,0,0  
 1L2F,GLU\_46,4.5,0,0,0  
 1OIS,ASP\_276,2.37,0.77,-2.19,0  
 3NOK,LYS\_32,9.38,-1.12,0,0  
 1J74,ASP\_40,2.94,0.28,-1.14,0  
 1SNT,CYS\_125,11.89,-0.1,1.87,1.12  
 3BQW,ASP\_175,4.08,0.28,0,0  
 4ETX,ARG\_256,12.5,0,0,0  
 2XMZ,ARG\_187,11.73,-0.77,0,0  
 1KW4,ASP\_38,3.71,0,-0.09,0  
 3TIR,ARG\_141,11.63,-0.87,0,0  
 2Q98,GLU\_131,4.03,0.21,-0.68,0  
 1OTM,LYS\_89,10.5,0,0,0  
 2BT8,ASP\_259,2.46,0.35,-1.69,0  
 1FKM,TYR\_629,9.63,0,-0.37,0  
 2D7J,HIS\_82,0.69,0.29,0,-6.1  
 2G7O,GLU\_118,4.03,0.42,-0.89,0  
 1WPS,HIS\_323,6.43,0,0,-0.07  
 2ZOM,HIS\_203,6.92,0.49,0,-0.07  
 4FZR,CYS\_286,11.52,-0.45,1.2,1.76  
 4E8B,ARG\_220,12.29,-0.21,0,0  
 1WNH,TYR\_23,9.77,0.9,-1.13,0  
 3BPV,ASP\_118,3.87,0.07,0,0  
 1P4X,HIS\_45,4.14,0,0,-2.36  
 3RFY,LYS\_138,10.5,0,0,0  
 3CIV,GLU\_159,4.12,0.42,-0.8,0  
 2EDM,ASP\_86,2.39,0.14,-1.56,0  
 1XFK,TYR\_88,10.38,0.35,-0.18,0.21  
 1P4X,GLU\_250,4.78,0.28,0,0  
 1SQW,GLU\_14,4.1,0.28,-0.67,0  
 2RIK,LYS\_32,10.36,-0.14,0,0  
 2PPN,LYS\_44,10.5,0,0,0  
 1YLN,ARG\_136,12.08,-0.42,0,0  
 1TD6,LYS\_110,10.5,0,0,0  
 1GPP,TYR\_101,10,0,0,0  
 1QYI,TYR\_361,11.22,0.07,0,1.15  
 2X4G,ARG\_33,12.01,-0.49,0,0  
 2IIA,LYS\_70,10.43,-0.07,0,0  
 1JB3,ASP\_70,3.27,0.56,-1.09,0  
 2BCF,LYS\_262,10.5,0,0,0  
 2JHY,LYS\_135,10.29,-0.21,0,0  
 1XFK,ARG\_25,11.8,-0.7,0,0  
 2G55,ASP\_104,3.68,0,-0.12,0  
 2OEW,ASP\_321,3.01,0.42,-1.21,0  
 2ZCX,GLU\_127,4.11,0.28,-0.67,0  
 2H2Z,ASP\_48,2.18,0.49,-2.11,0  
 1WOU,GLU\_109,3.6,0.28,-1.18,0  
 2BDD,TYR\_83,13.46,0.71,-0.26,3.01  
 1LPL,ASP\_215,4.19,0.42,-0.03,0  
 3FHF,TYR\_199,10.07,0.07,0,0  
 1SNT,GLU\_323,4.5,0,0,0  
 3EGN,ARG\_391,12.22,-0.28,0,0  
 2NSN,ARG\_69,11.94,-0.56,0,0  
 3QAV,CYS\_75,9.9,-0.21,-1.33,2.44  
 4DEZ,ASP\_24,2.87,0.84,-1.77,0  
 1ESS,TYR\_63,13.58,1.2,-0.02,2.4  
 4FZR,GLU\_269,4.5,0,0,0  
 3DHN,ARG\_123,11.87,-0.63,0,0  
 3ANJ,ASP\_45,3.93,0.14,-0.01,0  
 3IRA,ASP\_63,2.09,0.56,-2.26,0  
 2EFK,CYS\_248,8.03,-1.11,0,0.14  
 1XFK,LYS\_290,10.43,-0.07,0,0  
 1SNT,CYS\_164,12.48,-0.46,0,3.94  
 1MUF,CYS\_318,9.6,-0.96,-0.18,1.74  
 1X8F,LYS\_154,9.87,-0.63,0,0  
 3GW3,ASP\_54,3.07,0.35,-1.08,0  
 1D2K,ASP\_301,3.28,0.07,-0.59,0  
 2QRX,ARG\_28,12.22,-0.28,0,0  
 3IOC,HIS\_301,6.36,0,0,-0.14  
 1U53,LYS\_63,10.08,-0.42,0,0  
 3BWT,ASP\_750,3.32,0.07,-0.55,0  
 2B6P,CYS\_144,10.01,-0.15,0,1.16  
 3E5T,LYS\_44,10.5,0,0,0  
 3ANJ,LYS\_287,10.29,-0.21,0,0  
 2FC3,GLU\_44,4.64,0.14,0,0  
 1YTD,LYS\_389,10.5,0,0,0  
 3NJM,ASP\_70,1.5,0.7,-3,0  
 4EZB,ARG\_225,12.08,-0.42,0,0  
 3CGW,GLU\_263,4.71,0.21,0,0  
 2IF4,LYS\_50,10.22,-0.28,0,0  
 1T6L,HIS\_131,6.5,0,0,0  
 3ADO,ASP\_170,3.16,0.21,-0.86,0  
 1GXN,TYR\_494,11.1,1.62,-0.52,0  
 3C2E,ARG\_166,11.1,-1.4,0,0  
 1HUF,ARG\_14,11.94,-0.56,0,0  
 3G9G,ARG\_90,12.29,-0.21,0,0  
 3FK5,ARG\_319,11.87,-0.63,0,0  
 3V75,LYS\_81,9.87,-0.63,0,0  
 1PSW,TYR\_169,9.55,0.07,-0.52,0  
 1YTD,ASP\_101,3.4,0.42,-0.82,0  
 3BQW,LYS\_88,10.15,-0.35,0,0  
 3R87,HIS\_6,7.23,0.8,0,-0.07  
 1X1E,GLU\_88,4.64,0.14,0,0  
 3FNI,TYR\_17,9.68,0.07,-0.39,0  
 3RFY,LYS\_315,10.43,-0.07,0,0  
 3FHF,ARG\_136,12.31,-3.72,0,3.52  
 1S17,ARG\_136,12.01,-0.49,0,0  
 3T57,LYS\_327,10.15,-0.35,0,0  
 1WPA,LYS\_496,10.22,-0.28,0,0  
 3LPZ,GLU\_18,4.71,0.21,0,0  
 2FBI,ARG\_5,12.5,0,0,0  
 2EYI,LYS\_214,10.36,-0.14,0,0  
 3IVF,CYS\_286,9.81,0,0,0.81  
 2R4Q,ASP\_190,3.8,0.14,-0.14,0  
 2YLF,GLU\_145,3.94,0.28,-0.84,0  
 3F53,LYS\_59,10.29,-0.21,0,0  
 1H09,TYR\_176,11.59,1.59,0,0  
 3RLN,HIS\_601,2.34,1.23,-0.65,-4.74  
 3P2F,GLU\_29,4.5,0.49,-0.49,0  
 3LH5,ARG\_544,12.01,-0.49,0,0  
 2OOK,GLU\_351,4.57,0.07,0,0  
 3T8R,ASP\_109,3.12,0.63,-1.32,0  
 3CAX,ARG\_469,12.43,-0.07,0,0  
 1R3F,ASP\_238,1.9,0.63,-2.53,0  
 3K8J,LYS\_74,10.22,-0.28,0,0  
 1MD6,GLU\_111,3.62,0.28,-1.16,0  
 3DSH,GLU\_222,4.31,0.28,-0.47,0  
 3FHF,TYR\_128,10.47,0.21,-0.8,1.06  
 3G65,CYS\_31,9.33,-0.44,0,0.78  
 1SQW,LYS\_78,10.5,0,0,0  
 2R51,ARG\_294,12.95,-1.95,0,2.4  
 3RFY,ASP\_242,3.42,0.42,-0.8,0  
 3ERF,ARG\_171,12.43,-0.07,0,0  
 3CGW,LYS\_212,10.15,-0.35,0,0  
 2AHE,GLU\_83,4.5,0,0,0  
 3C6B,GLU\_255,4.64,0.14,0,0  
 1WXF,GLU\_119,3.92,0.35,-0.93,0  
 3IU5,LYS\_102,10.5,0,0,0  
 2XHC,LYS\_300,10.5,0,0,0  
 2FXT,GLU\_334,4.71,0.21,0,0  
 2EYI,GLU\_142,2.45,0.35,-2.4,0  
 1F09,LYS\_284,9.94,-0.56,0,0  
 1PVT,LYS\_96,10.22,-0.28,0,0  
 1P2F,CYS\_62,10.17,0,-0.29,1.46  
 3V3T,TYR\_72,10,0,0,0  
 2CIU,ASP\_130,1.35,1.05,-3.5,0  
 2ATR,ARG\_80,12.36,-0.14,0,0  
 3EX9,ASP\_88,3.66,0.07,-0.21,0  
 2FB6,TYR\_26,9.55,0.07,-0.52,0  
 4FH3,ASP\_59,3.66,0,-0.14,0  
 2RGY,ASP\_229,3.63,0.14,-0.31,0  
 1G8PLYS\_130,10.5,0,0,0  
 3IOC,ARG\_161,12.43,-0.07,0,0  
 1Y2Q,GLU\_12,3.81,0.14,-0.83,0  
 3IVF,CYS\_243,10.36,0,0,1.36  
 1FKM,LYS\_257,10.43,-0.07,0,0  
 2CE6,TYR\_69,13.04,0.14,0.5,2.4  
 1O9G,ARG\_229,11.8,-0.7,0,0  
 2I88,ASP\_408,2.34,0.28,-1.74,0  
 2AXO,ASP\_139,3.98,0.21,-0.03,0  
 1Q42,TYR\_172,9.62,0,-0.41,0.03  
 2B61,LYS\_314,10.36,-0.14,0,0  
 3MTT,GLU\_512,4.54,0.35,-0.31,0  
 1NUJ,ARG\_317,12.15,-0.35,0,0  
 3ETV,LYS\_163,10.5,0,0,0  
 2YT4,HIS\_517,6.5,0,0,0  
 2NSN,GLU\_84,4.71,0.21,0,0  
 1R29,TYR\_91,8.81,0.92,-1.05,-1.06  
 2POY,ASP\_146,3.47,0.21,-0.54,0  
 3CNU,CYS\_51,8.77,-0.33,0,0.1  
 3ON1,LYS\_50,9.94,-0.56,0,0  
 1PV5,GLU\_185,4.99,0.49,0,0  
 1BN6,GLU\_154,4.5,0,0,0  
 4DND,LYS\_77,10.43,-0.07,0,0  
 2AXO,LYS\_127,10.5,0,0,0  
 2ILR,GLU\_279,4.57,0.07,0,0  
 2H85,ASP\_267,2.8,0.77,-1.77,0  
 3ON1,ASP\_54,3.87,0.07,0,0  
 2QEV,LYS\_99,10.5,0,0,0  
 3GT0,LYS\_62,10.5,0,0,0  
 1TR9,ARG\_34,11.45,-1.05,0,0  
 2WOZ,GLU\_572,3.95,0.14,-0.69,0  
 2GYZ,HIS\_43,6.66,0.16,0,0  
 2G9D,GLU\_71,4.19,0.93,-1.24,0  
 1Q8B,LYS\_89,10.43,-0.07,0,0  
 1ZBM,HIS\_33,2.05,0,-1.57,-2.88  
 3OKQ,ASP\_662,3.85,0.14,-0.09,0  
 3QKY,ARG\_168,11.94,-0.56,0,0  
 1QYI,GLU\_28,4.26,2.52,-1.29,-1.47  
 1Q8B,LYS\_36,9.87,-0.63,0,0  
 4F8A,LYS\_650,10.36,-0.14,0,0  
 2QV2,LYS\_156,10.36,-0.14,0,0  
 1TXJ,LYS\_84,10.36,-0.14,0,0  
 2WZ9,GLU\_14,4.5,0,0,0  
 2PIM,ARG\_93,12.15,-0.35,0,0  
 100X,GLU\_123,4.09,0.28,-0.69,0  
 1R7J,LYS\_72,10.5,0,0,0  
 2JHY,ARG\_180,11.51,-0.99,0,0  
 2D8N,CYS\_39,0,0,0,0  
 3GV0,ASP\_157,3.8,0,0,0  
 3QKY,GLU\_255,4.5,0,0,0  
 1J74,ARG\_124,11.94,-0.56,0,0  
 3TOW,ARG\_142,12.22,-0.28,0,0  
 3E7P,ASP\_117,3.3,0.63,-1.14,0  
 3E7M,LYS\_59,10.43,-0.07,0,0  
 1EQ6,ASP\_213,2.29,0.42,-1.93,0  
 2CWC,ARG\_10,11.71,-0.79,0,0  
 1ZBS,TYR\_231,10.28,1.09,-1.57,0.77  
 3K9I,TYR\_77,10.07,0.07,0,0  
 1NWA,HIS\_155,2.51,1.01,0,-5.01  
 1R3F,ASP\_126,165.455,0.14,-0.09,0  
 2XWS,ARG\_18,11.8,-0.7,0,0  
 4GA2,GLU\_88,3.85,0.35,-1,0  
 1SQW,HIS\_82,9.65,3.6,1.96,-2.41  
 1XTD,ASP\_122,3.12,0.07,-0.75,0  
 2B78,HIS\_311,7.26,1.11,0,-0.35  
 2DFL,LYS\_81,10.36,-0.14,0,0  
 1X04,ASP\_110,4.15,0.35,0,0  
 1Q46,LYS\_77,10.5,0,0,0  
 1H09,CYS\_45,8.54,-0.46,0,0  
 2YX0,ARG\_233,12.01,-0.49,0,0  
 1FKM,LYS\_608,10.5,0,0,0  
 2VGM,ASP\_380,3.62,0.42,-0.6,0  
 1MJS,HIS\_288,7.51,1.01,0,0  
 2H2Z,CYS\_117,10,-0.39,0,1.39  
 1AKO,ARG\_267,12.5,0,0,0  
 3L3P,ASP\_339,4.12,0.35,-0.03,0  
 3M7G,HIS\_260,5.92,0.73,0,-1.31  
 2APL,TYR\_127,11.87,0.31,-0.3,1.86  
 1UOH,GLU\_204,4.64,0.14,0,0  
 2YYO,TYR\_65,8.51,0.99,-2.8,0.33  
 3GA2,HIS\_237,6.45,0.02,0,-0.07  
 2QDJ,LYS\_80,10.5,0,0,0  
 3MEW,CYS\_243,8.5,-0.65,0,0.15  
 1WNH,LYS\_55,10.29,-0.21,0,0  
 1YTQ,ARG\_88,12.5,0,0,0  
 4GCO,GLU\_226,4.5,0,0,0  
 1FHL,TYR\_111,13.41,0.21,0.8,2.4  
 2OKT,LYS\_200,10.29,-0.21,0,0  
 3BZT,GLU\_327,4.5,0,0,0  
 2E3I,GLU\_79,4.5,0,0,0  
 1PBV,LYS\_78,10.29,-0.21,0,0  
 1SNT,LYS\_262,10.43,-0.07,0,0  
 1WLY,HIS\_299,6.44,0.15,0,-0.21  
 1YIB,ARG\_222,12.29,-0.21,0,0  
 3C5V,GLU\_140,4.5,0,0,0  
 3F7M,HIS\_176,2.92,1.4,-4.98  
 1WJG,TYR\_45,10,0,0,0  
 1HUF,HIS\_62,7.01,0.51,0,0  
 1T95,ASP\_67,3.5,0,-0.31,0  
 1X9G,ASP\_141,3.84,0.14,-0.1,0  
 2ZCO,TYR\_192,10.07,0.07,0,0  
 3M7G,ARG\_14,11.94,-0.56,0,0  
 3AU3,GLU\_418,4.57,0.07,0,0  
 3NR5,TYR\_144,12.64,0.43,0,1.2,1  
 2E3I,LYS\_98,10.43,-0.07,0,0  
 1WLY,GLU\_184,2.31,0.28,-2.47,0

1RSS,LYS\_36,10.5,0,0,0  
2YWX,LYS\_85,10.5,0,0,0  
1ZBM,GLU\_121,3.95,0.35,-0.9,0  
2OJQ,ASP\_579,3.21,0.21,-0.8,0  
1QQ,ARG\_88,12.08,-0.42,0,0  
3ETV,ASP\_12,3.73,0,-0.07,0  
1MIX,CYS\_243,10.38,0,0,1.38  
3ERF,LYS\_59,10.29,-0.21,0,0  
1PBV,GLU\_211,4.11,0.07,-0.46,0  
1RWZ,TYR\_59,10.26,0.68,-0.42,0  
2IIA,GLU\_31,3.15,0.7,-2.06,0  
3DZ1,HIS\_254,4.37,0,0,-2.13  
3T5B,ASP\_333,3.94,0.14,0,0  
1UAJ,ASP\_69,3.51,0.56,-0.85,0  
1L3K,LYS\_144,10.5,0,0,0  
1YOK,HIS\_127,6.43,0,0,-0.07  
1ILW,LYS\_28,10.43,-0.07,0,0  
3RAZ,ASP\_150,3.18,0.28,-0.9,0  
4EKU,ASP\_211,3.28,0.14,-0.65,0  
3AOX,HIS\_729,3.94,0.84,-0.3,4  
2YLF,ARG\_79,11.66,-0.84,0,0  
1EV8,HIS\_51,6.5,0,0,0  
1PNE,ASP\_75,1.12,0.63,-3.31,0  
3LPZ,ARG\_204,11.87,-0.63,0,0  
2XJ4,ARG\_46,13.44,-0.87,0,1.81  
1TP6,LYS\_62,10.15,-0.35,0,0  
4ETX,TYR\_327,6.9,1.51,-0.8,-3.81  
3DTE,ASP\_152,3.8,0,0,0  
3R87,TYR\_23,10.0,0,0,0  
3US6,TYR\_123,11.89,0.77,-0.1,1.22  
2O8I,GLU\_53,4.27,0.42,-0.65,0  
4H4J,TYR\_98,11.71,0.95,0.49,0.26  
2JKF,LYS\_73,10.29,-0.21,0,0  
2E3I,LYS\_127,10.5,0,0,0  
2Y2T,CYS\_31,8.66,-0.34,0,0  
1XDZ,GLU\_12,4.64,0.14,0,0  
1P1L,GLU\_24,4.57,0.07,0,0  
3DB9,ASP\_261,3.49,0.49,-0.8,0  
2G9D,ARG\_159,11.46,-1.04,0,0  
3PBH,ASP\_159,2.29,0.77,-2.28,0  
3Q1C,GLU\_258,4.44,0.14,-0.2,0  
3BJV,ASP\_78,2.52,0.7,-1.98,0  
3G65,LYS\_1,10.22,-0.28,0,0  
3KEY,GLU\_409,4.77,0.34,0,-0.07  
1OST,GLU\_451,4.64,0.14,0,0  
2PWQ,GLU\_10,3.93,2.07,-2.64,0  
3BQW,GLU\_320,4.39,0.21,-0.32,0  
1WP5,GLU\_192,4.5,0,0,0  
4EKU,GLU\_263,3.04,2.42,-1.48,-2.4  
1R2Z,HIS\_140,9.97,2.92,4.35,-3.8  
3LJI,ASP\_132,3.8,0,0,0  
3GFP,ASP\_374,3.85,0.14,-0.09,0  
2E0T,HIS\_171,6.08,0,0,-0.42  
1V6T,ARG\_15,12.5,0,0,0  
4F8A,HIS\_570,6.36,0,0,-0.14  
3Q6L,ARG\_31,11.38,-1.12,0,0  
1UJ8,GLU\_21,3.29,0.91,-2.11,0  
3Q9P,GLU\_160,4.16,0.49,-0.84,0  
1SJ8,ASP\_537,3.93,0.14,-0.01,0  
3LE4,CYS\_352,9.54,0.54,0,0  
2B78,LYS\_214,10.5,0,0,0  
3OBS,TYR\_110,13.34,0.14,0.8,2.4  
3OIP,ASP\_104,3.9,0.14,-0.04,0  
3IVF,TYR\_26,12.79,0.039,2,4  
1JB3,TYR\_94,10.07,0.07,0,0  
2O8P,GLU\_204,4.64,0.14,0,0  
2D7U,ASP\_137,3.63,0.21,-0.38,0  
3DB9,ARG\_24,12.08,-0.42,0,0  
2BAA,GLU\_89,3.0,49,-1.99,0  
1QQE,CYS\_260,9.81,-0.03,0,0.84  
3GV0,ARG\_212,11.87,-0.63,0,0  
3G65,TYR\_207,13.14,0.21,0.54,2.4  
2XMX,ARG\_128,11.87,-0.63,0,0  
3UV9,TYR\_448,10.21,0.21,0,0  
1RKA,GLU\_147,3.6,0.28,-1.17,0  
3BWT,LYS\_655,10.29,-0.21,0,0  
2DG7,ARG\_119,11.94,-0.56,0,0  
2R57,ARG\_352,12.5,0,0,0  
3EYE,HIS\_111,6.72,0.22,0,0  
3B79,LYS\_35,10.43,-0.07,0,0  
1YOY,GLU\_147,4.92,0.42,0,0  
2W0G,GLU\_255,4.5,0,0,0  
4FZR,GLU\_244,3.84,0.14,-0.8,0  
3U4K,LYS\_74,10.29,-0.21,0,0  
2O0K,GLU\_198,4.64,0.14,0,0  
3EGN,GLU\_414,4.5,0,0,0  
3MIX,GLU\_475,4.47,0.21,-0.24,0  
2D0A,ARG\_207,11.94,-0.56,0,0  
1D2K,LYS\_229,10.29,-0.21,0,0  
1SQW,GLU\_171,3.88,0.28,-0.9,0  
2IXM,GLU\_29,4.87,0.42,-0.05,0  
1AKO,LYS\_141,10.43,-0.07,0,0  
3ULX,TYR\_165,10.04,0.04,0,0  
1SJY,TYR\_83,7.86,1.06,-0.8,-2.4  
3RUX,TYR\_209,10.0,0,0,0  
1EDG,ARG\_333,10.66,-1.84,0,0  
3MTT,GLU\_534,4.39,0.35,-0.46,0  
3DZ1,ARG\_270,13.47,-1.43,0,2.4  
2AD1,LYS\_198,10.43,-0.07,0,0  
3Q1C,ARG\_94,11.66,-0.84,0,0  
1QQE,LYS\_23,10.5,0,0,0  
2W0Z,CYS\_324,9.36,0,0,0.36  
3CX2,ARG\_160,12.08,-0.42,0,0  
1X8F,HIS\_246,6.5,0,0,0  
2CN1,TYR\_81,13.41,0.21,0.8,2.4  
3A7L,TYR\_121,8.92,0.76,-1.87,0.03  
3CAN,ARG\_90,11.87,-0.63,0,0  
2VAN,LYS\_131,10.43,-0.07,0,0  
1RWZ,GLU\_94,4.5,0,0,0  
3HNX,GLU\_68,2.59,0.49,-2.4,0  
1OIS,GLU\_228,3.98,0.28,-0.8,0  
3CAN,HIS\_73,6.49,0.2,0,-0.21  
1SBX,LYS\_179,10.08,-0.42,0,0  
1JT9,LYS\_64,10.5,0,0,0  
3C5V,LYS\_121,10.43,-0.07,0,0  
3ETV,CYS\_92,10.45,0,0,1.45  
4ANN,ARG\_67,12.5,0,0,0  
3H9W,ASP\_125,2.35,0.49,-1.94,0  
1AKO,GLU\_182,3.12,0.42,-1.8,0  
2P4D,ARG\_160,11.8,-0.7,0,0  
1YR6,LYS\_138,10.15,-0.35,0,0  
1KCM,HIS\_64,7.09,0.8,0,-0.21  
2WB3,HIS\_281,6.29,0,0,-0.21  
3M70,LYS\_41,10.5,0,0,0  
1PNE,TYR\_139,10.0,0,0,0  
1DTO,HIS\_187,6.36,0,0,-0.14  
2F8H,ASP\_50,3.2,0.35,-0.95,0  
2VAN,HIS\_197,7.16,0.8,0,-0.14  
3COU,ARG\_149,12.29,-0.21,0,0  
2R4Q,LYS\_197,10.5,0,0,0  
1TJE,LYS\_213,10.43,-0.07,0,0  
3G9T,TYR\_216,13.2,0.21,0.59,2.4  
2WB8,ARG\_644,12.08,-0.42,0,0  
3MTT,ARG\_554,12.36,-0.14,0,0  
1BKR,HIS\_25,6.31,0.02,0,-0.21  
1L2F,LYS\_94,10.29,-0.21,0,0  
3ANJ,ASP\_192,3.0,35,-1.15,0  
2OBS,GLU\_132,0.6,0.91,-4.81,0  
1RSS,LYS\_48,10.43,-0.07,0,0  
1CBY,GLU\_214,4.3,0.56,-0.77,0  
2OBI,LYS\_31,10.29,-0.21,0,0  
1R53,GLU\_150,4.05,0.14,-0.59,0  
3P29,ARG\_391,10.5,0,0,0  
3GW3,ARG\_292,10.58,-1.92,0,0  
1RI6,GLU\_79,3.91,0.21,-0.8,0  
1NIJ,TYR\_183,10.07,0.07,0,0  
1YOK,GLU\_68,2.29,1.79,-1.6,-2.4  
1XWM,ARG\_78,12.08,-0.42,0,0  
3F6F,GLU\_203,3.91,0.21,-0.8,0  
3L3P,ASP\_365,3.73,0.14,-0.21,0  
3F6F,ASP\_173,3.0,28,-1.08,0  
2QVQ,TYR\_35,13.0,07,0.53,2.4  
1MML,TYR\_109,10.23,0.28,-1.07,1.02  
3GYW,LYS\_47,10.36,-0.14,0,0  
2AD1,ARG\_73,11.59,-0.91,0,0  
4GA2,LYS\_133,10.29,-0.21,0,0  
1MIX,ASP\_201,3.32,0.42,-0.9,0  
1L3K,ARG\_82,12.5,0,0,0  
1A8Q,ASP\_7,4.02,0.42,-0.19,0  
2JEO,LYS\_192,10.29,-0.21,0,0  
1O17,CYS\_123,9.93,-1.67,0.2,61  
1UAJ,LYS\_235,10.43,-0.07,0,0  
1FQI,LYS\_406,10.5,0,0,0  
4EF5,TYR\_240,10.0,0,0,0  
1VJG,TYR\_158,12.33,2.15,-0.95,1.13  
1XTZ,TYR\_52,13.34,0.14,0.8,2.4  
1RI5,ARG\_108,12.08,-0.42,0,0  
2W0Z,ARG\_586,12.22,-0.28,0,0  
3C5V,GLU\_54,4.64,0.14,0,0  
3C6B,HIS\_19,4.69,0.04,1.28,-3.13  
2CYG,GLU\_45,3.98,0.28,-0.8,0  
3H6Q,LYS\_31,10.43,-0.07,0,0  
1RI6,GLU\_171,4.41,0.28,-0.38,0  
1V6T,LYS\_17,10.22,-0.28,0,0  
2ZCX,GLU\_77,2.0,7,-0.8,-2.4  
1BN6,LYS\_274,10.5,0,0,0  
3V4G,LYS\_52,10.43,-0.07,0,0  
2OSA,ARG\_295,11.1,-1.4,0,0  
2P1W,GLU\_128,4.64,0.14,0,0  
4EKU,CYS\_352,11.01,0.69,1.32  
2ILR,ARG\_524,12.43,-0.07,0,0  
2R2Y,LYS\_123,10.43,-0.07,0,0  
2HRZ,ARG\_111,12.36,-0.14,0,0  
2YWM,TYR\_146,10.34,0,0,0.34  
1ZBM,ARG\_193,12.01,-0.49,0,0  
3F6M,LYS\_71,10.29,-0.21,0,0  
1YB2,HIS\_32,6.43,0,0,-0.07  
1K95,LYS\_165,10.43,-0.07,0,0  
2EFK,ASP\_161,3.09,0.56,-1.27,0  
3U4K,LYS\_78,10.5,0,0,0  
1T6L,ASP\_134,3.84,0.07,-0.03,0  
2CW4,ASP\_7,3.44,0.07,-0.43,0  
1UAJ,ASP\_40,3.99,0.21,-0.02,0  
1AK1,TYR\_267,10.39,0.14,-0.42,0.67  
2QK0,ARG\_93,11.38,-1.12,0,0  
3QKY,ARG\_163,12.1,-0.46,0,0.06  
1T6L,LYS\_78,9.66,-0.84,0,0  
3K9I,CYS\_76,9.05,-0.02,0,0.07  
2CL3,TYR\_40,11.08,0,0,1.08  
2AHE,LYS\_106,10.5,0,0,0  
2PIM,ARG\_29,12.29,-0.21,0,0  
3IL3,GLU\_285,1.87,1.27,-1.5,-2.4  
3EVP,LYS\_298,10.08,-0.42,0,0  
2I88,GLU\_361,4.5,0,0,0  
2BCF,ARG\_247,11.94,-0.56,0,0  
1YTQ,GLU\_69,4.19,0.28,-0.59,0  
4FZR,GLU\_115,2.77,3.46,-2.78,-2.4  
2Z0W,TYR\_61,7.58,0.21,-2.62,0  
4FH3,HIS\_170,4.33,0,0,-2.17  
1DOV,LYS\_99,10.5,0,0,0  
1FKM,HIS\_575,5.63,4.46,0,-5.33  
3P29,ARG\_116,13.77,-1.83,0,3.1  
4FLE,LYS\_133,10.5,0,0,0  
2D2S,LYS\_587,10.08,-0.42,0,0  
2PLQ,HIS\_26,6.29,0,0,-0.21  
3CGW,LYS\_293,10.36,-0.14,0,0  
1BYI,TYR\_187,10,0,0,0  
3IDW,GLU\_51,2.45,0.35,-2.4,0  
1VSM,CYS\_125,9.6,-0.41,0.19,0.82  
2QK1,TYR\_492,10,0,0,0  
1R5Q,ASP\_17,3.8,0.14,-0.14,0  
4DVD,ARG\_187,12.08,-0.42,0,0  
3UV9,ASP\_295,3.68,0.14,-0.26,0  
3UPD,GLU\_304,4.57,0.07,0,0  
2G9D,ARG\_114,10.71,-1.79,0,0  
2B78,LYS\_384,10.15,-0.35,0,0  
3CIV,TYR\_65,10.76,0.12,0.0,64  
2H85,ASP\_39,3.16,0.28,-0.92,0  
1AM2,TYR\_59,11.09,0,0,1.09  
3ANJ,TYR\_128,10.07,0.07,0,0  
1R3F,CYS\_174,8.3,-2.01,0,1.31  
1ESS,ARG\_117,11.52,-0.98,0,0  
3CBN,LYS\_134,10.22,-0.28,0,0  
3BCY,HIS\_48,7.0,71,0,-0.21  
3GV0,ARG\_239,12.29,-0.21,0,0  
2OBS,CYS\_138,10.91,-2.15,2.4,1.66  
2EJX,LYS\_6,10.29,-0.21,0,0  
4EKU,ARG\_287,11.94,-0.56,0,0  
1ILW,GLU\_164,5.32,0.77,0.05,0  
2CWC,ASP\_75,2.6,0.56,-1.76,0  
3HQX,LYS\_14,10.08,-0.42,0,0  
2RH3,GLU\_94,4.5,0,0,0  
4ETX,GLU\_186,4.5,0,0,0  
2EDM,GLU\_182,4.66,0.42,-0.26,0  
2V5B,GLU\_112,4.57,0.07,0,0  
1KCM,HIS\_127,5.12,1.34,1.83,-4.56  
1IAP,ARG\_189,12.01,-0.49,0,0  
3HVV,ASP\_295,3.75,0.42,-0.47,0  
3H8Y,GLU\_32,4.64,0.14,0,0  
1R29,ASP\_33,3.07,0.84,-1.56,0  
3V55,CYS\_539,4.04,-5.02,0,0.07  
3K1H,TYR\_141,12.19,0.32,1.87  
2PGE,ARG\_276,11.37,-1.13,0,0  
1L2F,ARG\_326,11.66,-0.84,0,0  
1RLO,LYS\_201,10.15,-0.35,0,0  
1VSM,HIS\_198,6.5,0,0,0  
2F8H,TYR\_59,9.62,0.42,-0.8,0  
1R3F,GLU\_164,3.9,0.14,-0.74,0  
3F7M,ASP\_148,2.77,0.35,-1.38,0  
3E2Z,ARG\_74,12.43,-0.07,0,0  
1F09,ARG\_300,12.66,-2.57,0,2.73  
2CYG,TYR\_204,9.45,0.01,-0.56,0  
2H2W,ARG\_239,12.08,-0.42,0,0  
2IRM,ARG\_47,11.75,-0.75,0,0  
2FBQ,GLU\_69,4.5,0,0,0  
1YB6,GLU\_176,4.71,0.21,0,0  
3NR5,ARG\_43,12.36,-0.14,0,0  
1ZBS,HIS\_279,6.37,0.15,0,-0.28  
2B2H,ASP\_86,3.82,0.07,-0.05,0  
3EUR,ASP\_107,0.86,0.56,-3.5,0  
4FCU,CYS\_46,10.3,0,-0.21,1.52  
2QEV,LYS\_9,10.29,-0.21,0,0  
2P5D,LYS\_54,10.5,0,0,0  
1XFK,ARG\_285,11.87,-0.63,0,0  
2ZCO,GLU\_269,4.5,0,0,0  
3P2F,ARG\_123,11.73,-0.77,0,0



2APL,GLU\_26,3.61,0.8,-1.11,-0.58  
 3T5B,ASP\_339,3.18,0.14,-0.76,0  
 1DOV,ASP\_146,3.8,0.07,-0.07,0  
 2QEV,ARG\_41,11.87,-0.63,0,0  
 1MD6,ASP\_147,4.01,0.21,0,0  
 3CAN,CYS\_58,8.61,-1.6,0,1.21  
 3T5B,LYS\_321,9.8,-0.7,0,0  
 3BZT,ASP\_288,3.24,0.35,-0.91,0  
 3GFP,CYS\_311,9.32,-0.46,0,0.78  
 2H2W,GLU\_25,4.57,0.07,0,0  
 1X04,LYS\_151,10.5,0,0,0  
 4E9E,HIS\_574,7.55,1.12,0,-0.07  
 3V55,GLU\_453,4.64,0.14,0,0  
 4EKU,LYS\_303,10.5,0,0,0  
 2YWJ,LYS\_113,10.29,-0.21,0,0  
 4FZN,HIS\_241,3.47,0.24,0,-3.27  
 1QQE,ASP\_133,3.49,0.35,-0.66,0  
 2BLL,TYR\_463,13.64,2.89,-0.66,1.41  
 2PLQ,ASP\_5,2.37,0.21,-1.64,0  
 1N81,TYR\_179,10.31,0.31,0,0  
 3LJC,TYR\_195,12.79,0.14,0.25,2.4  
 3Q1C,ASP\_353,3.51,0.07,-0.36,0  
 2C13,GLU\_36,3.51,0.35,-1.34,0  
 2F8H,HIS\_11,3.35,0.0,-3.15  
 2Y2T,GLU\_51,4.78,0.28,0,0  
 1X1E,ARG\_203,12.15,-0.35,0,0  
 1YB2,TYR\_139,9.06,0.21,-1.15,0  
 3EYE,HIS\_17,7.92,1.6,1.98,-2.16  
 3OOP,GLU\_140,4.85,0.35,0,0  
 1X7F,ARG\_297,13.72,-1.18,0,2.4  
 3V75,GLU\_160,3.27,0.49,-1.73,0  
 1NUJ,GLU\_267,4.71,0.21,0,0  
 4F85,ASP\_71,2.92,0.28,-1.16,0  
 3ETV,LYS\_15,10.5,0,0,0  
 4HDE,LYS\_48,10.5,0,0,0  
 3RFY,ASP\_130,3.62,0,-0.18,0  
 2VAN,ARG\_102,12.01,-0.49,0,0  
 3CCY,TYR\_171,10.42,0.42,0,0  
 3JZN,TYR\_138,11.39,0,-0.46,1.85  
 2O8I,GLU\_34,4.5,0,0,0  
 2HNG,ARG\_22,11.52,-0.98,0,0  
 2A0J,ARG\_143,12.36,-0.14,0,0  
 3JV1,GLU\_108,4.36,0.49,-0.62,0  
 1WXQ,LYS\_197,10.36,-0.14,0,0  
 3L3P,ARG\_534,12.15,-0.35,0,0  
 2DVK,GLU\_125,4.5,0,0,0  
 2RS1,ARG\_137,12.5,0,0,0  
 3CAN,TYR\_137,11.7,0.07,0,1.63  
 3U56,LYS\_15,10.5,0,0,0  
 1Q8B,LYS\_81,10.43,-0.07,0,0  
 3GG6,GLU\_66,4.03,0.28,-0.75,0  
 3CX5,TYR\_177,11.97,0,0,1.97  
 1AKO,GLU\_243,4.29,0.14,-0.35,0  
 2YLF,GLU\_56,3.39,0.49,-1.6,0  
 3MEW,LYS\_230,10.43,-0.07,0,0  
 3RLE,GLU\_147,4.5,0,0,0  
 3M66,LYS\_361,10.08,-0.42,0,0  
 1QY1,LYS\_94,10.36,-0.14,0,0  
 3CSV,ARG\_199,12.08,-0.42,0,0  
 3DTE,ASP\_93,3.79,0.14,-0.15,0  
 4FZN,GLU\_102,3.87,0.49,-1.11,0  
 4EF5,HIS\_185,7.23,0.73,0,0  
 2RJD,ASP\_227,3.59,0,-0.21,0  
 2ATR,ASP\_14,3.98,0.35,-0.17,0  
 3EGN,LYS\_429,10.43,-0.07,0,0  
 1P4X,ASP\_222,3.21,0.21,-0.8,0  
 3B21,TYR\_90,9.5,0.3,-0.8,0  
 2RCY,HIS\_318,8.86,1.6,2.39,-1.64  
 1YB2,ASP\_44,2.41,0.63,-2.02,0  
 1Z3X,ARG\_133,12.43,-0.07,0,0  
 3B79,LYS\_53,10.43,-0.07,0,0  
 1LTU,ASP\_275,3.01,0.42,-1.21,0  
 1T95,GLU\_136,4.57,0.07,0,0  
 3S0A,CYS\_47,10.8,-0.13,0,1.93  
 3AU3,ARG\_401,12.5,0,0,0  
 3Q1C,GLU\_91,1.7,0.84,-3.64,0  
 1G5Z,GLU\_71,3.88,0.14,-0.76,0  
 3M70,GLU\_253,4.56,0.07,-0.01,0  
 2G3A,ASP\_100,3.41,0.42,-0.81,0  
 3M7G,ARG\_83,12.08,-0.42,0,0  
 2W8B,LYS\_595,10.43,-0.07,0,0  
 1T95,GLU\_230,4.9,0.14,0.26,0  
 2FM9,LYS\_173,10.29,-0.21,0,0  
 1H09,ASP\_169,3.26,0.21,-0.75,0  
 3DTE,ARG\_136,12.29,-0.21,0,0  
 2QZQ,TYR\_82,9.58,0,-0.42,0  
 1FHL,GLU\_276,4.64,0.14,0,0  
 1PGV,LYS\_269,10.5,0,0,0  
 2AZP,TYR\_273,10.21,0.21,0,0  
 3HUE,TYR\_167,11.53,0.21,0,1.32  
 3U2R,TYR\_46,9.47,0.22,-0.75,0  
 1O6D,HIS\_126,5.59,0.95,0,-1.86  
 2Z61,GLU\_27,3.91,0.21,-0.8,0  
 3CE7,ASP\_16,2.74,0.42,-1.47,0  
 3C2E,ARG\_107,12.15,-0.35,0,0  
 3BCY,LYS\_90,10.43,-0.07,0,0  
 2FD4,TYR\_506,10.2,0.14,-1.19,1.25  
 2RIK,LYS\_7,10.43,-0.07,0,0  
 3Q1C,GLU\_368,4.71,0.21,0,0  
 3IRA,CYS\_95,9.58,-0.13,0,0.71  
 3H04,ASP\_193,2.43,0.56,-1.93,0  
 2B78,TYR\_166,10.95,0.95,0,0  
 2FXT,GLU\_245,3.56,0.21,-1.15,0  
 1EQ6,HIS\_196,6.51,0.08,0,-0.07  
 1RHS,ARG\_116,11.17,-2.48,0,1.15  
 3G53,ARG\_258,10.43,-2.07,0,0  
 1PVS,ARG\_12,12.08,-0.42,0,0  
 3EIZ,LYS\_10,10.5,0,0,0  
 3PP8,HIS\_7,3.29,0.0,-3.21  
 1XFK,HIS\_310,6.43,0.0,-0.07  
 1GPP,ARG\_414,11.87,-0.63,0,0  
 4EVF,GLU\_124,4.57,0.07,0,0  
 2YT4,GLU\_701,2.89,1.07,-0.7,-1.98  
 2JEO,ARG\_175,12.15,-0.35,0,0  
 2CE6,TYR\_89,13.27,0.07,0.8,2.4  
 3GA2,GLU\_173,4.49,0,-0.01,0  
 3RRQ,ARG\_112,12.22,-0.28,0,0  
 2WOZ,LYS\_476,10.29,-0.21,0,0  
 2PP6,LYS\_9,10.5,0,0,0  
 3T5B,GLU\_305,4.3,1.91,-1.85,-0.26  
 2J8A,TYR\_275,10.48,0.19,-0.28,0.57  
 3LJC,TYR\_229,9.83,0,-0.17,0  
 3P28,LYS\_237,10.01,-0.49,0,0  
 3E5T,LYS\_120,10.5,0,0,0  
 1P2F,LYS\_112,10.43,-0.07,0,0  
 1WXQ,HIS\_48,4.34,1.07,0,-3.23  
 2FZ4,TYR\_29,10.37,1.23,-0.86,0  
 1OIS,HIS\_165,6.5,0,0,0  
 3ANJ,LYS\_62,10.5,0,0,0  
 2WOZ,TYR\_348,10.41,0.41,0,0  
 1P1L,GLU\_87,4.5,0,0,0  
 3IDW,LYS\_64,10.5,0,0,0  
 3PBH,LYS\_141,10.08,-0.42,0,0  
 3CQ1,ARG\_97,11.73,-0.77,0,0  
 2ZOW,TYR\_41,10,0,0,0  
 1NAR,ASP\_202,2.98,0.28,-1.1,0  
 1ES9,ASP\_16,1.31,0.91,-3.39,0  
 4ETX,GLU\_409,4.5,0,0,0  
 1G5Z,ASP\_152,2.69,0.49,-1.6,0  
 2EFK,GLU\_64,4.5,0,0,0  
 4H86,GLU\_76,4.64,0.14,0,0  
 3F1X,TYR\_23,10,0,0,0  
 2D2S,LYS\_680,10.36,-0.14,0,0  
 3MEW,ARG\_207,11.8,-0.7,0,0  
 3G9T,ARG\_87,13.94,-0.96,0,2.4  
 2FXT,ASP\_281,3.17,0.7,-1.33,0  
 1AM2,ARG\_62,12.01,-0.49,0,0  
 3TIR,ARG\_206,12.43,-0.07,0,0  
 3OA7,GLU\_24,4.85,0.35,0,0  
 3P2F,HIS\_98,7.17,0.67,0,0  
 2EFK,LYS\_262,10.5,0,0,0  
 2FD4,ASP\_489,3.87,0.07,0,0  
 2H2W,TYR\_290,9.03,0.14,-1.11,0  
 1CHD,ARG\_257,11.66,-0.84,0,0  
 1Q8B,LYS\_44,10.22,-0.28,0,0  
 1R16,ASP\_221,0.96,0.7,-3.54,0  
 1WOU,TYR\_99,10.21,0,0,0.21  
 3ONT,TYR\_142,10,0,0,0  
 2EJB,HIS\_181,7.57,1.21,0,-0.14  
 1FO9,ARG\_122,11.8,-0.7,0,0  
 2RJD,LYS\_405,10.43,-0.07,0,0  
 2V1L,GLU\_127,3.06,1.32,-2.76,0  
 4EKU,LYS\_145,10.5,0,0,0  
 1YR6,TYR\_187,10.24,0.07,0,0.17  
 2BAA,TYR\_237,9.89,0,-1.14,1.02  
 1EW4,LYS\_74,10.5,0,0,0  
 2F8H,ARG\_90,11.59,-0.91,0,0  
 1SIG,CYS\_295,9.21,0,0,0.21  
 3JSN,GLU\_234,3.73,0.42,-1.19,0  
 3FRR,ARG\_16,12.29,-0.21,0,0  
 1FO9,GLU\_382,3.11,0.49,-1.88,0  
 3ELI,LYS\_66,10.08,-0.42,0,0  
 3JZN,LYS\_342,10.5,0,0,0  
 2C2Y,ASP\_220,2.75,0.28,-1.33,0  
 1EW4,HIS\_70,6.15,0,0,-0.35  
 1V43,ARG\_310,12.08,-0.42,0,0  
 1ZCE,GLU\_28,2.42,0.56,-2.64,0  
 2AD1,GLU\_182,4.64,0.14,0,0  
 3ULX,TYR\_31,10.12,0.24,-0.12,0  
 3F6M,HIS\_44,6.21,1.6,2.05,-3.94  
 4FH3,LYS\_60,10.5,0,0,0  
 2QZQ,ARG\_149,10.82,-1.68,0,0  
 4FH3,GLU\_353,3.56,0.58,0,-1.52  
 1KW4,GLU\_54,4.85,0.35,0,0  
 2O4D,ARG\_137,11.59,-0.91,0,0  
 3U4K,TYR\_92,9.98,0.14,-0.16,0  
 3IL3,GLU\_225,3.45,0.42,-1.47,0  
 2OPJ,ARG\_45,12.5,0,0,0  
 3M7D,HIS\_360,6.5,0,0,0  
 1ZCU,ARG\_47,11.87,-0.63,0,0  
 2D59,GLU\_35,4.14,0.7,-1.06,0  
 2JEO,ARG\_55,12.08,-0.42,0,0  
 3R87,LYS\_115,10.43,-0.07,0,0  
 2CW4,GLU\_42,4.5,0,0,0  
 4F3J,LYS\_187,10.5,0,0,0  
 1U3Y,LYS\_323,10.5,0,0,0  
 3NOK,GLU\_25,2.73,0.63,-2.4,0  
 2IQT,TYR\_40,10.07,0.07,0,0  
 2XJ4,GLU\_165,4.71,0.21,0,0  
 3GA2,LYS\_12,10.22,-0.28,0,0  
 2ILR,ASP\_325,3.87,0.07,0,0  
 2CXC,LYS\_67,10.08,-0.42,0,0  
 2IDC,GLU\_124,4.5,0,0,0  
 1J8B,GLU\_85,4.71,0.21,0,0  
 1XDZ,ARG\_134,12.01,-0.49,0,0  
 3E5T,GLU\_204,3.99,0.28,-0.79,0  
 2X5Y,TYR\_857,10,0,0,0  
 2FG1,HIS\_23,5.64,4.4,0,-5.26  
 2O8I,ASP\_126,2.95,0.49,-1.35,0  
 3BWT,LYS\_692,10.01,-0.49,0,0  
 2A6B,TYR\_6,10.24,0.24,0,0  
 1EV8,HIS\_147,12.92,0.17,0,-3.75  
 3HZQ,ASP\_16,3.8,0,0,0  
 1JYH,ARG\_64,12.08,-0.42,0,0  
 3MIX,HIS\_417,6.5,0,0,0  
 1WPA,LYS\_497,10.43,-0.07,0,0  
 1PGV,HIS\_368,6.43,0,0,-0.07  
 1WRU,HIS\_145,6.5,0,0,0  
 2G3A,CYS\_94,9.03,-0.04,0,0.07  
 1X7F,LYS\_261,10.5,0,0,0  
 3A4C,ASP\_496,3.98,0.21,-0.03,0  
 2O0K,HIS\_129,6.5,0,0,0  
 1BKR,HIS\_42,7.15,0.86,0,-0.21  
 3Q1C,GLU\_83,2.2,3.05,-1.92,-3.43  
 2O0K,ASP\_327,4.01,0.21,0,0  
 2ZOW,HIS\_49,6.43,0,0,-0.07  
 1A8Q,GLU\_138,4.5,0,0,0  
 2WOZ,TYR\_420,10.07,0.07,0,0  
 1ZBP,ARG\_81,12.18,-3.65,0,3.33  
 1WOU,GLU\_14,3.8,0.35,-1.05,0  
 2HXB,GLU\_76,4.5,0,0,0  
 1UJ8,GLU\_66,4.64,0.14,0,0  
 1N81,LYS\_58,10.5,0,0,0  
 1UW7,ASP\_47,2.47,0.42,-1.75,0  
 3JV1,ASP\_109,3.12,0.35,-1.03,0  
 1R15,LYS\_291,10.22,-0.28,0,0  
 2O4D,ARG\_60,11.94,-0.56,0,0  
 3HVW,ARG\_177,12.22,-0.28,0,0  
 2B0J,GLU\_49,0.79,3.54,-3.09,-4.16  
 3HYQ,ASP\_138,3.28,0.28,-0.8,0  
 2OQG,ASP\_558,3.83,0.21,-0.18,0  
 1IDK,ASP\_88,3.44,0.42,-0.78,0  
 1YW5,LYS\_52,10.36,-0.14,0,0  
 1TJE,HIS\_194,6.88,0.59,0,-0.21  
 2OEW,HIS\_152,3.04,0,-0.18,-3.28  
 1PDB,LYS\_122,9.66,-0.84,0,0  
 1TLV,GLU\_167,4.96,0.56,-0.1,0  
 2ZTY,HIS\_167,6.46,0.03,0,-0.07  
 2IXM,GLU\_255,3.85,1.17,-0.8,-1.02  
 1EV8,ASP\_198,3.69,0.35,-0.46,0  
 1TR9,ARG\_230,13.15,-1.23,0,1.88  
 3BA1,ARG\_288,11.03,-1.47,0,0  
 3IU5,ASP\_45,3.17,0.35,-0.97,0  
 3H6Q,ARG\_137,11.59,-0.91,0,0  
 3IV4,TYR\_20,10.07,0.07,0,0  
 3GA2,LYS\_70,10.08,-0.42,0,0  
 4EKU,TYR\_351,10.95,1.96,-1.01,0.01  
 3H13,GLU\_445,3.71,0.56,-1.35,0  
 1A8Q,LYS\_127,10.43,-0.07,0,0  
 3VHU,LYS\_14,10.5,0,0,0  
 3PBH,HIS\_97,6.35,0.06,0,-0.21  
 4D8L,ARG\_20,12.5,0,0,0  
 3GE9,GLU\_30,4.5,0,0,0  
 1Z9L,ARG\_120,12.29,-0.21,0,0  
 3TIR,ASP\_111,3.59,0,-0.21,0  
 1N81,ASP\_117,3.8,0,0,0  
 2Q34,LYS\_226,10.5,0,0,0  
 1J33,ASP\_109,3.0,0.14,-0.94,0  
 3G59,ARG\_257,11.41,-1.09,0,0  
 1WXQ,GLU\_254,3.64,2.06,-0.52,-2.4  
 1ZBP,TYR\_155,11.24,1.24,0,0  
 2F9F,CYS\_93,11.35,-0.89,0.51,2.73  
 2APL,LYS\_114,10.29,-0.21,0,0  
 3CIV,ASP\_174,3.01,0.28,-1.07,0  
 2EYI,CYS\_154,10.87,-0.25,0.2,1.2  
 1Z3X,TYR\_197,12.37,0.07,-0.01,2.3

3CIV,CYS\_234,11.42,0.0,71,1.71  
1RAJ,GLU\_399,4.78,0.28,0,0  
3IRA,LYS\_33,10.22,-0.28,0,0  
2H85,ASP\_36,3.94,0.14,0,0  
3N2T,ARG\_101,12.01,-0.49,0,0  
1KN3,GLU\_35,4.54,0.14,-0.1,0  
3UOV,HIS\_211,7.21,1.6,2.38,-3.27  
2OJQ,LYS\_501,10.43,-0.07,0,0  
3TMO,LYS\_245,10.29,-0.21,0,0  
1EDG,LYS\_143,10.22,-0.28,0,0  
1TLV,GLU\_193,4.42,0.21,-0.29,0  
4E6S,ARG\_2,12.08,-0.42,0,0  
2FM9,GLU\_156,3.61,2.09,-0.8,-2.18  
3JZ9,LYS\_503,10.5,0,0,0  
2R51,ARG\_212,11.87,-0.63,0,0  
1AM2,LYS\_36,10.22,-0.28,0,0  
1NJ4,ARG\_302,11.87,-0.63,0,0  
3V4G,LYS\_45,10.22,-0.28,0,0  
3IPZ,LYS\_72,10.5,0,0,0  
1SOH,ASP\_218,2.56,0.84,-2.09,0  
2CBE,LYS\_133,10.29,-0.21,0,0  
2GEN,TYR\_89,11.12,1.12,0,0  
3ULX,GLU\_168,10.5,0,0,0  
3A2Z,LYS\_122,10.5,0,0,0  
4ETX,ARG\_402,11.8,-0.7,0,0  
3ONT,HIS\_130,6.36,0.0,-0.14  
3VJ8,TYR\_44,13.32,1.3,0.01,2.01  
3LJN,TYR\_67,10.54,0.07,-0.2,0.67  
4EVF,GLU\_29,4.71,0.21,0,0  
3FXH,ARG\_40,12.29,-0.21,0,0  
2DG7,GLU\_118,1.05,1.03,-1.01,-3.47  
1ZCU,ARG\_231,12.29,-0.21,0,0  
2WOZ,TYR\_325,13.34,0.14,0.8,2.4  
2AZP,ARG\_233,12.08,-1.27,0.0,85  
1VJG,GLU\_75,4.64,0.14,0,0  
1PGV,ASP\_279,2.44,0.7,-2.06,0  
1UOH,GLU\_24,4.5,0,0,0  
3H13,GLU\_265,3.46,0.56,-1.6,0  
3RJZ,LYS\_83,10.15,-0.35,0,0  
2V4U,GLU\_343,3.97,0.63,-1.15,0  
1EQ6,ASP\_79,3.33,0.49,-0.95,0  
1OST,GLU\_459,4.64,0.14,0,0  
3RVC,ASP\_120,1.53,1.19,-3.46,0  
2Z61,LYS\_341,10.29,-0.21,0,0  
2CYG,ARG\_290,12.36,-0.14,0,0  
3BWT,TYR\_854,9.29,0.07,-0.78,0  
2Z61,ASP\_49,4.07,0.42,-0.15,0  
3GMS,GLU\_26,4.5,0,0,0  
3P2F,CYS\_132,10.58,0.58,0,1  
1YLN,LYS\_148,10.29,-0.21,0,0  
2OGQ,ARG\_557,12.01,-0.49,0,0  
1R3F,LYS\_290,10.43,-0.07,0,0  
2ILR,LYS\_475,9.52,-0.98,0,0  
1X8F,GLU\_261,3.29,0.28,-1.49,0  
2CBE,LYS\_80,10.36,-0.14,0,0  
2IXM,TYR\_199,10.46,0.55,-0.09,0  
2P5D,LYS\_97,10.15,-0.35,0,0  
3AUF,GLU\_24,3.53,0.42,-1.39,0  
1GQE,ARG\_240,1.2,0.29,-0.21,0,0  
1V8E,CYS\_161,9,0,0,0  
3IPZ,GLU\_123,3.32,0.42,-1.6,0  
3M7G,LYS\_244,10.36,-0.14,0,0  
2P0L,ASP\_226,3.8,0,0,0  
1O3X,ARG\_265,12.5,0,0,0  
2E3C,ARG\_248,11.8,-0.7,0,0  
2Q13,GLU\_198,4.57,0.07,0,0  
3TRE,ASP\_20,2.76,0.56,-1.6,0  
1V43,ARG\_155,9.85,-0.86,-1.79  
2YXO,ASP\_234,4.15,0.35,0,0  
3FK5,HIS\_265,5.38,3.6,0,-4.72  
1YW5,TYR\_58,10,0,0,0  
2P0L,CYS\_183,7.3,-1.69,0,0  
2R51,TYR\_155,10,0,0,0  
4GA2,GLU\_71,3.46,0.56,-1.6,0  
2IDC,GLU\_56,4.11,0.07,-0.46,0  
2EYI,LYS\_174,9.94,-0.56,0,0  
1QQH,HIS\_155,5.78,1.13,0,-1.85  
2D7J,GLU\_157,4.64,0.14,0,0  
1KW4,HIS\_56,6.7,0.27,0,-0.07  
1X04,GLU\_73,4.44,0.21,-0.27,0  
3LMO,LYS\_59,10.5,0,0,0  
3DSH,GLU\_285,3.92,0.14,-0.72,0  
1ZBM,GLU\_166,4.57,0.07,0,0  
2FZP,ARG\_269,12.29,-0.21,0,0  
2VAN,GLU\_153,4.5,0,0,0  
2E3C,LYS\_286,10.5,0,0,0  
2IRM,GLU\_75,4.71,0.21,0,0  
3D9H,GLU\_176,4.71,0.21,0,0  
3GOZ,GLU\_310,4.4,0.21,-0.31,0  
2R51,TYR\_77,13.41,1,-1.91E-17,2.4  
1ZCU,HIS\_211,6.37,2.03,2.64,-4.8  
1JYH,HIS\_17,6.36,0.0,-0.14  
1WXF,TYR\_33,10.32,0.0,0.32  
2BT8,TYR\_292,10,0,0,0  
3HYQ,GLU\_134,4.5,0,0,0  
3CSR,LYS\_32,10.01,-0.49,0,0  
3T57,TYR\_274,10.68,0.7,-0.06,0.04  
3ERF,GLU\_76,3.36,0.35,-1.49,0  
1WXF,ARG\_186,10.5,-2,0,0  
3DSH,CYS\_262,10.39,-0.62,0,2.01  
2BLL,HIS\_588,6.95,0.8,-0.35  
1NJ4,ASP\_307,3.32,0.35,-0.83,0  
2XMX,ASP\_132,3.97,0.21,-0.04,0  
3GW3,ASP\_326,3.32,0.35,-0.83,0  
3BCY,CYS\_49,10.44,0,1.44  
3IL3,GLU\_210,4.56,0.07,-0.01,0  
1XFK,HIS\_159,11.06,3.2,4.9,-3.54  
3NR5,GLU\_94,4.5,0,0,0  
3EVN,GLU\_168,4.57,0.07,0,0  
2VGM,ASP\_378,4.13,0.42,-0.09,0  
1ZCE,ASP\_74,1.28,1.19,-3.7,0  
3ADO,ARG\_231,12.08,-0.42,0,0  
2D8N,LYS\_154,9.94,-0.56,0,0  
2CXC,GLU\_92,4.4,0.7,-0.8,0  
3MTT,HIS\_536,6.54,0.11,0,-0.07  
4H86,CYS\_62,1.76,-6.08,-2.32,1.16  
2BLL,ARG\_337,11.87,-0.63,0,0  
1GXN,LYS\_369,10.5,0,0,0  
1OTM,CYS\_242,7.47,-1.6,0,0.07  
1RIS,GLU\_263,3.81,0.21,-0.9,0  
2G55,CYS\_70,9.07,0,0,0.07  
4AE7,LYS\_76,10.43,-0.07,0,0  
2Q07,ASP\_438,1.83,0.91,-2.87,0  
1SIG,LYS\_296,10.43,-0.07,0,0  
2YWK,LYS\_58,10.5,0,0,0  
4ACJ,ARG\_772,11.73,-0.77,0,0  
2C2Y,ASP\_43,1.74,0.49,-2.55,0  
4DND,GLU\_72,4.1,0.21,-0.61,0  
2YXO,GLU\_112,2.45,0.35,-2.4,0  
3LJN,GLU\_116,2.04,0.28,-0.35,-2.4  
2BDV,ARG\_136,10.77,-1.73,0,0  
4H89,TYR\_35,11.02,1.02,0,0  
1X7F,GLU\_54,4.31,0.28,-0.47,0  
2Q98,GLU\_128,3.58,0.28,-1.2,0  
1YB2,LYS\_51,9.59,-0.91,0,0  
3V75,GLU\_141,4.62,0.21,-0.09,0  
1H09,TYR\_88,10.81,1.17,-0.36,0.01  
1R6Y,ASP\_22,3.28,0.35,-0.87,0  
2CE6,LYS\_6,10.29,-0.21,0,0  
3JV1,GLU\_77,4.5,0,0,0  
4FCU,GLU\_228,4.05,0.35,-0.8,0  
2IRM,LYS\_248,10.22,-0.28,0,0  
3GJZ,LYS\_113,10.5,0,0,0  
1RIS,TYR\_254,9.31,0.33,-1.02,0  
3U2R,ARG\_93,12.36,-0.14,0,0  
3IL3,ASP\_48,3.33,0.21,-0.68,0  
3BQW,ASP\_270,3.79,0,-0.01,0  
3AUF,HIS\_109,5.86,0.87,2.32,-3.83  
1E59,HIS\_27,7.41,2.37,1.85,-3.31  
1SQW,ASP\_61,3.79,0.21,-0.22,0  
1OST,GLU\_429,3.58,0.28,-1.2,0  
3RLE,ARG\_201,11.59,-0.91,0,0  
1KCM,LYS\_165,10.15,-0.35,0,0  
2QRX,TYR\_88,12.33,0.14,-0.21,2.4  
1ZYL,ARG\_51,12.22,-0.28,0,0  
2G9D,ASP\_13,3.79,0.91,-0.92,0  
3IRA,GLU\_83,4.85,0.35,0,0  
3FXH,ARG\_19,12.08,-0.42,0,0  
1PVT,LYS\_10,10.36,-0.14,0,0  
1LTU,TYR\_210,9.86,0,-0.14,0  
3C2E,LYS\_41,10.5,0,0,0  
3BA1,GLU\_191,4.64,0.14,0,0  
2RIK,TYR\_270,10,0,0,0  
3T5B,GLU\_385,4.5,0,0,0  
3LPZ,LYS\_250,10.5,0,0,0  
2BDD,LYS\_135,10.5,0,0,0  
3GMS,GLU\_73,4.21,0.28,-0.57,0  
1UOH,ASP\_39,3.94,0.14,0,0  
3EUR,TYR\_30,11.76,0,0,1.76  
2ZOM,LYS\_15,10.15,-0.35,0,0  
2Q07,LYS\_386,10.36,-0.14,0,0  
1XWM,GLU\_191,4.73,0.28,-0.05,0  
2IQT,LYS\_105,10.01,-0.49,0,0  
3ZXY,GLU\_128,1.77,0.91,-3.65,0  
3I82,ARG\_97,12.29,-0.21,0,0  
1KCM,CYS\_95,10.2,-0.64,0,1.84  
1AD6,GLU\_398,4.5,0,0,0  
3EGN,ASP\_456,4.05,0.35,-0.1,0  
1Q46,ASP\_166,3.7,0.35,-0.45,0  
2PGX,ARG\_22,12.01,-0.49,0,0  
1YTD,ARG\_367,11.94,-0.56,0,0  
1RSS,HIS\_153,6.5,0,0,0  
4F85,ARG\_237,12.46,-0.56,0,0.52  
1JKS,GLU\_197,4.52,1.07,-1.05,0  
3IVF,ASP\_175,3.03,0.56,-1.33,0  
1F2V,GLU\_95,4.26,0.07,-0.31,0  
3VHJ,ASP\_79,3.59,0.28,-0.49,0  
1CBY,ASP\_235,3.9,0.28,-0.18,0  
1MUF,GLU\_326,4.57,0.07,0,0  
2YT4,ARG\_700,12.43,-0.07,0,0  
3A2Z,ASP\_128,3.94,0.14,0,0  
2WB8,GLU\_492,3.86,1.05,-2.79,1.1  
2E3S,ASP\_460,3.72,0,-0.08,0  
3L3P,ARG\_387,12.43,-0.07,0,0  
2QK1,ARG\_550,11.59,-0.91,0,0  
3UAH,LYS\_169,10.43,-0.07,0,0  
3KB5,ASP\_324,3.12,0.56,-1.24,0  
4ESS,GLU\_161,4.68,0.35,-0.17,0  
3ULX,GLU\_48,3.77,0.07,-0.8,0  
2PGX,HIS\_240,2.75,0.23,-1.85,-2.12  
2FBQ,LYS\_101,10.5,0,0,0  
1R2Z,LYS\_208,10.5,0,0,0  
3GAD,TYR\_86,10,0,0,0  
3FNI,ARG\_51,12.15,-0.35,0,0  
2ZCO,HIS\_96,6.43,0,-0.07  
2AZL,ARG\_161,11.87,-0.63,0,0  
2QHT,GLU\_192,4.14,0.56,-0.92,0  
3FTT,HIS\_37,7.07,0.85,0,-0.28  
2FBQ,GLU\_5,4.64,0.14,0,0  
2Z61,TYR\_345,9.27,0.07,-0.8,0  
4EF5,ARG\_293,12.43,-0.07,0,0  
3GW3,GLU\_348,4.36,0,-0.14,0  
3G9G,GLU\_63,4.5,0,0,0  
3CZC,ASP\_81,3.64,0.35,-0.51,0  
3GMS,ASP\_16,3.67,0.28,-0.41,0  
2RIS,ASP\_172,2.55,0.84,-2.09,0  
1OLR,ARG\_108,12.5,0,0,0  
3LQE,CYS\_489,11.48,-0.24,0,2.72  
2AZP,LYS\_229,10.36,-0.14,0,0  
1L2H,HIS\_30,7.74,1.45,0,-0.21  
1R3F,ARG\_282,12.54,-1.45,0,1.49  
1K95,LYS\_194,10.5,0,0,0  
3IOC,GLU\_197,3.94,0.21,-0.77,0  
3M70,HIS\_66,6.5,0,0,0  
1SUU,TYR\_721,10.07,0.07,0,0  
2APL,GLU\_133,3.25,0.35,-1.6,0  
1X04,HIS\_134,6.5,0,0,0  
3P28,HIS\_33,2.95,0,-0.5,-3.05  
1JT9,ASP\_195,3.34,0.35,-0.81,0  
2WB8,ASP\_716,2.21,0.56,-2.14,0  
3CXS,LYS\_108,10.36,-0.14,0,0  
2VC8,GLU\_66,4.57,0.07,0,0  
3M3P,ASP\_63,4.19,0.42,-0.03,0  
2BLL,ARG\_619,10.36,-3.3,0,1.16  
2YWW,ASP\_119,4.15,0.35,0,0  
1O59,HIS\_164,3.5,0.03,0,-3.03  
1V43,ARG\_218,12.43,-0.07,0,0  
3BQW,GLU\_327,4.39,1.01,-1.12,0  
1WNH,GLU\_102,4.39,0.42,-0.53,0  
1R53,ARG\_368,12.29,-0.21,0,0  
2RJD,ARG\_324,12.5,0,0,0  
3HUE,LYS\_58,10.5,0,0,0  
3N2T,GLU\_111,2.82,2.55,-1.9,-2.33  
3M7G,ARG\_109,12.22,-0.28,0,0  
3V55,TYR\_615,9.68,0,-0.32,0  
1TR9,ASP\_135,2.14,0.49,-2.14,0  
2OEW,TYR\_319,11.41,0,0,1.41  
1TP6,CYS\_3,3.45,-5.62,0,0.07  
1TR9,GLU\_281,4.71,0.21,0,0  
1I60,LYS\_25,10.22,-0.28,0,0  
2FBI,LYS\_124,10.5,0,0,0  
2AD1,LYS\_199,10.5,0,0,0  
1O5J,HIS\_2,6.5,0,0,0  
3LJC,TYR\_141,13.38,0.21,0.8,2.37  
2P65,TYR\_164,11.76,0.38,-0.79,2.18  
2FB6,LYS\_110,10.15,-0.35,0,0  
2Q99,ARG\_130,12.5,0,0,0  
3TIR,TYR\_221,9.59,0,-0.41,0  
2CXC,ARG\_99,12.36,-0.14,0,0  
2Z14,ARG\_72,11.45,-1.05,0,0  
1Q46,GLU\_49,1.8,0.77,-3.47,0  
3IVF,ARG\_207,11.94,-0.56,0,0  
3DZ1,ASP\_30,3.64,0.84,-1,0  
3P28,ASP\_28,3.68,0.07,-0.19,0  
2BLL,ARG\_510,11.42,-2.74,0,1.66  
1R53,ARG\_47,12.43,-0.07,0,0  
1JT9,HIS\_65,6.29,0.07,0,-0.28  
3RLN,LYS\_732,10.5,0,0,0  
3P28,ARG\_167,12.08,-0.42,0,0  
2H2W,ARG\_243,11.87,-0.63,0,0  
4DVD,GLU\_31,4.55,0.21,-0.16,0  
2AD1,LYS\_215,10.5,0,0,0  
1AD6,GLU\_551,4.5,0.14,-0.14,0  
1AD6,GLU\_545,4.5,0,0,0  
1PBV,ARG\_232,12.5,0,0,0  
1OST,GLU\_217,3.71,0.21,-1,0

1ZBS,ARG\_25,12.29,-0.21,0,0  
3BJV,GLU\_52,4.13,0.21,-0.58,0  
3DTE,LYS\_204,10.22,-0.28,0,0  
3CSR,ASP\_91,3.29,0.35,-0.86,0  
3B7H,HIS\_11,7.02,0.8,0,-0.28  
3CGW,LYS\_78,10.5,0,0,0  
3V55,GLU\_585,4.21,0.49,-0.78,0  
3BPP,ARG\_121,12.01,-0.49,0,0  
1DOV,ASP\_200,3.39,0.28,-0.69,0  
3BWT,GLU\_623,4.2,0.14,-0.44,0  
1VSM,ARG\_168,11.94,-0.56,0,0  
1RL0,ASP\_120,2.46,0.35,-1.69,0  
1SI7,LYS\_127,10.36,-0.14,0,0  
3BB7,ASP\_116,2.4,0.63,-2.02,0  
1FQI,ARG\_361,11.94,-0.56,0,0  
1X6J,LYS\_6,10.29,-0.21,0,0  
2OKT,ASP\_163,3.74,0.07,-0.13,0  
1ZHV,ARG\_108,12.01,-0.49,0,0  
2Z61,ARG\_131,12.29,-0.21,0,0  
2VGM,ASP\_73,3.55,0.35,-0.6,0  
1X6J,GLU\_29,4.02,0.21,-0.69,0  
4EVF,LYS\_267,10.43,-0.07,0,0  
4FLE,GLU\_149,4.5,0,0,0  
2F4Q,ARG\_216,11.38,-1.12,0,0  
3GV0,HIS\_162,4.06,0.72,0,-3.16  
3A4C,TYR\_532,11.76,0,0,1.76  
1YTQ,TYR\_111,9.64,0.14,-0.52,0,0.22  
1PZC,LYS\_38,10.5,0,0,0  
2OSA,CYS\_288,11.54,-0.04,0,2.58  
4F8A,ARG\_693,12.08,-0.42,0,0  
3TMO,GLU\_309,3.98,0.28,-0.8,0  
2E3C,HIS\_369,6.43,0,0,-0.07  
3EIZ,LYS\_152,10.5,0,0,0  
4FZR,ASP\_353,2.32,0.49,-1.97,0  
1HF8,TYR\_96,10.85,0,-0.39,1.24  
1HF8,LYS\_39,10.29,-0.21,0,0  
3ODJ,GLU\_192,4.57,0.07,0,0  
2X4J,TYR\_130,8.44,0.48,-2.05,0  
3CCY,CYS\_43,7.38,-1.76,0,0.14  
1ILW,ARG\_64,11.73,-0.77,0,0  
1TXJ,ARG\_30,11.59,-0.91,0,0  
3G9G,ARG\_28,12.08,-0.42,0,0  
1RI5,ARG\_112,11.87,-0.63,0,0  
2GEN,ASP\_188,2.68,0.42,-1.54,0  
1GPP,LYS\_124,10.36,-0.14,0,0  
1QQH,CYS\_196,6.75,-2.61,0,0.35  
1R9W,ARG\_231,11.59,-0.91,0,0  
2D7U,HIS\_26,6.83,0.4,0,-0.07  
1WNH,CYS\_70,9.79,-0.02,0,0.81  
2EFK,LYS\_171,10.5,0,0,0  
3EVP,GLU\_85,4.92,0.42,0,0  
1SUU,LYS\_696,10.5,0,0,0  
1PSW,GLU\_190,3.62,1.32,-2.2,0  
4D8L,LYS\_46,10.5,0,0,0  
1W7B,GLU\_125,3.92,0.35,-0.93,0  
3CCY,ASP\_68,3.39,0.42,-0.83,0  
1JKS,LYS\_262,10.29,-0.21,0,0  
2DVK,GLU\_22,4.57,0.07,0,0  
2D2S,ASP\_692,4.15,0.49,-0.14,0  
200K,ARG\_279,12.22,-0.28,0,0  
1ZCU,GLU\_115,4.38,0.21,-0.33,0  
2BV9,LYS\_100,10.43,-0.07,0,0  
2CYG,ARG\_84,12.29,-0.21,0,0  
2H2W,GLU\_126,4.64,0.14,0,0  
2EEY,ASP\_23,3.17,0.21,-0.84,0  
4FH3,ASP\_70,3.65,0.14,-0.29,0  
1KCM,LYS\_200,10.36,-0.14,0,0  
2Z84,ARG\_96,12.5,0,0,0  
3BJV,LYS\_27,10.36,-0.14,0,0  
2B2H,ASP\_288,3.65,0.49,-0.63,0  
3PAC,ARG\_172,12.36,-0.14,0,0  
3MTT,GLU\_517,4.38,0.14,-0.26,0  
3GFP,LYS\_349,10.29,-0.21,0,0  
3I4T,ARG\_126,11.03,-1.47,0,0  
1J85,LYS\_73,10.5,0,0,0  
3OIP,LYS\_73,10.08,-0.42,0,0  
1CHD,ARG\_316,12.15,-0.35,0,0  
2O0K,LYS\_182,10.5,0,0,0  
1XFK,TYR\_221,13.4,0.07,0.78,2.55  
4FCU,LYS\_86,11.55,-0.21,0,1.26  
1E55,ASP\_28,1.96,0.56,-2.4,0  
1SUU,ASP\_611,3.67,0,-0.13,0  
3C6B,GLU\_99,4.6,0.14,-0.04,0  
3F7M,LYS\_191,10.5,0,0,0  
1EV8,HIS\_108,6.55,0.05,0,0  
4ANN,GLU\_149,4.14,0.42,-0.78,0  
2NRR,LYS\_352,10.22,-0.28,0,0  
2GZQ,LYS\_110,10.5,0,0,0  
2XHC,CYS\_145,6.9,-2.24,0,0.14  
2R2Y,LYS\_30,10.15,-0.35,0,0  
1UAJ,GLU\_80,4.5,0,0,0  
1T3Y,ARG\_63,11.17,-1.33,0,0  
3KV0,GLU\_202,4.57,0.07,0,0  
3C38,ASP\_65,3.23,0.42,-0.99,0  
2H2W,TYR\_153,11.02,1.02,0,0  
1K95,TYR\_207,10.07,0.07,0,0  
1EYH,ASP\_136,3.28,0.42,-0.93,0  
2CBE,LYS\_111,10.43,-0.07,0,0  
1XWM,LYS\_209,10.43,-0.07,0,0  
1LTU,ARG\_76,12.36,-0.14,0,0  
1XIP,GLU\_63,4.28,0.35,-0.57,0  
3BCY,LYS\_135,10.01,-0.49,0,0  
3IBT,HIS\_174,6.29,0,0,-0.21  
3MEW,HIS\_185,6.36,0,0,-0.14  
1R3F,LYS\_64,10.15,-0.35,0,0  
1UOH,GLU\_139,4.64,0.14,0,0  
3RFY,ASP\_90,4.08,0.42,-0.14,0  
3NZL,CYS\_42,6.57,-2.77,0,0.34  
1QYI,ASP\_49,3.47,0.21,-0.54,0  
4DND,ARG\_22,12.29,-0.21,0,0  
3FXH,ARG\_29,12.15,-0.35,0,0  
3DZ1,CYS\_41,9.81,-0.3,0,1.11  
1WRU,ASP\_92,3.81,0.07,-0.06,0  
3A2Z,ARG\_88,11.8,-0.7,0,0  
3OIP,LYS\_161,10.5,0,0,0  
3CAX,ARG\_326,12.5,0,0,0  
1W7B,GLU\_149,4.08,0.35,-0.77,0  
2F8H,HIS\_81,6.43,0,0,-0.07  
3Q1C,ARG\_138,11.66,-0.84,0,0  
1S7K,LYS\_30,10.08,-0.42,0,0  
1AD6,ARG\_552,12.08,-0.42,0,0  
3VJ8,GLU\_64,3.91,0.21,-0.8,0  
2FD4,HIS\_532,3.76,0,-2.74  
2YWJ,ASP\_140,2.3,0.42,-1.91,0  
1L2F,GLU\_63,4.57,0.07,0,0  
2IF4,GLU\_129,4.53,0.56,-0.53,0  
1T07,HIS\_45,6.36,0,0,-0.14  
2R51,GLU\_144,2.11,0.74,-1.38,-1.76  
1NRI,TYR\_159,9.27,0.07,-0.8,0  
2AD1,GLU\_60,3.25,0.35,-1.6,0  
4E9E,LYS\_484,10.43,-0.07,0,0  
1SIG,TYR\_268,10,0,0,0  
1KN3,LYS\_129,10.29,-0.21,0,0  
3TR8,TYR\_122,10,0,0,0  
1EDG,ASP\_21,3.72,0,-0.08,0  
1DVO,GLU\_131,3.5,0.42,-1.42,0  
1RAJ,LYS\_255,10.36,-0.14,0,0  
1X91,ASP\_73,3.8,0.14,-0.14,0  
3FHF,LYS\_189,10.5,0,0,0  
1X7F,LYS\_18,10.36,-0.14,0,0  
3UW9,ARG\_297,12.15,-0.35,0,0  
3R2E,ASP\_49,3.37,0.63,-1.06,0  
3UZA,GLU\_80,4.5,0,0,0  
3N2T,LYS\_110,10.29,-0.21,0,0  
3V75,GLU\_271,4.57,0.07,0,0  
3CX2,TYR\_237,10.65,0.65,0,0  
2R0S,LYS\_276,10.22,-0.28,0,0  
1H09,TYR\_124,12.2,-1.46,1.26  
1WPA,LYS\_455,10.5,0,0,0  
1LTU,ASP\_61,3.7,0,-0.1,0  
1RSS,GLU\_139,4.71,0.21,0,0  
2YX0,CYS\_71,11.84,-0.12,0.56,2.39  
2QDJ,GLU\_313,3.59,0.77,-1.68,0  
3VHJ,ASP\_92,3,0.42,-1.22,0  
3G9T,CYS\_54,11.98,-0.11,2.53,0.56  
2RIK,ASP\_38,2.44,0.63,-1.99,0  
2E3C,ASP\_365,2.85,0.21,-1.16,0  
2PPN,GLU\_61,3.99,0.49,-1,0  
3N2T,LYS\_95,10.5,0,0,0  
3C38,TYR\_133,13.16,0.56,0.2,2.4  
2V4U,LYS\_363,10.36,-0.14,0,0  
4ETX,GLU\_222,4.16,0.07,-0.41,0  
2ZCO,TYR\_112,10.14,0.14,0,0  
1XTZ,ASP\_88,3.94,0.14,0,0  
1WLJ,LYS\_213,10.5,0,0,0  
2GEN,ARG\_191,12.15,-0.35,0,0  
1Y2Q,GLU\_46,3.06,0.56,-2,0  
2GAU,ARG\_156,11.31,-1.19,0,0  
3IPZ,CYS\_172,9.07,0,0,0.07  
3E27,LYS\_386,10.29,-0.21,0,0  
3FTT,LYS\_47,9.8,-0.7,0,0  
3TIR,GLU\_142,2.52,0.42,-2.4,0  
1WRU,ASP\_10,3.48,0.21,-0.53,0  
3CNU,ASP\_37,4.08,0.28,0,0  
2R51,LYS\_295,10.43,-0.07,0,0  
1RHS,GLU\_233,4.5,0,0,0  
3CX5,HIS\_111,6.43,0,0,-0.07  
1T95,GLU\_100,3.91,0.21,-0.8,0  
1XEU,GLU\_151,4.57,0.07,0,0  
3H6Q,ASP\_117,3.81,0.07,-0.06,0  
2DFL,ASP\_192,4.39,0.63,-0.04,0  
2W88,HIS\_579,6.5,0,0,0  
2CIU,GLU\_177,4.05,0.35,-0.8,0  
2E3C,LYS\_321,10.29,-0.21,0,0  
3TOW,ARG\_61,12.5,0,0,0  
3FHF,LYS\_171,10.36,-0.14,0,0  
2ILR,LYS\_532,10.5,0,0,0  
2F8H,ARG\_144,11.8,-0.7,0,0  
1PVT,GLU\_69,3.91,0.21,-0.8,0  
1O59,LYS\_303,10.29,-0.21,0,0  
3PM2,TYR\_81,12.02,2.11,-0.09,0  
1XWM,HIS\_13,5.12,0.96,0,-2.34  
1X1E,GLU\_2,4.47,0.21,-0.24,0  
1GPP,GLU\_134,4.5,0,0,0  
2OJQ,GLU\_483,4.5,0,0,0  
2V5B,CYS\_15,9,0,0,0  
1PGV,GLU\_365,3.93,0.21,-0.78,0  
3F1X,GLU\_16,4.34,0.07,-0.23,0  
3ERF,HIS\_161,6.43,0,0,-0.07  
3KEY,ARG\_379,12.22,-0.28,0,0  
1ZBM,TYR\_60,10.76,0.68,-1.08,1.16  
3HUE,GLU\_295,3.92,0.21,-0.79,0  
2OKT,ARG\_279,11.14,-3.57,0,2.21  
4EVF,LYS\_199,10.29,-0.21,0,0  
1ZBS,GLU\_165,4.75,0.21,0.04,0  
1TD6,GLU\_175,4.5,0,0,0  
1MIX,LYS\_254,10.5,0,0,0  
4FLE,ARG\_82,12.36,-0.14,0,0  
1UAJ,ARG\_-3,12.5,0,0,0  
2EA9,GLU\_93,3.28,0.21,-1.42,0  
2OJQ,LYS\_120,10.5,0,0,0  
1BN6,GLU\_151,4.57,0.07,0,0  
1T95,ARG\_133,12.43,-0.07,0,0  
3H04,HIS\_248,8.69,1.6,5.54,-4.95  
2DFL,ARG\_229,11.38,-1.12,0,0  
2P65,LYS\_145,10.01,-0.49,0,0  
1YDL,ASP\_24,2.37,0.77,-2.2,0  
1S7K,TYR\_98,10.23,0.5,-0.27,0  
3MIX,LYS\_478,10.22,-0.28,0,0  
2RJD,ASP\_383,3.06,0.21,-0.96,0  
1NWA,ARG\_45,12.5,0,0,0  
1S7K,LYS\_157,10.43,-0.07,0,0  
4H4J,TYR\_218,9.02,0.26,-1.24,0  
2Q07,LYS\_392,10.5,0,0,0  
3A7L,ASP\_82,3.8,0.21,-0.21,0  
2Q34,GLU\_167,1.72,0.42,-3.2,0  
3GS3,TYR\_137,10.41,0,0,0.41  
3RE9,GLU\_140,2.66,0.92,-2.76,0  
2RFA,CYS\_172,11.41,0,0,2.41  
1D0T,LYS\_14,10.01,-0.49,0,0  
1XIP,GLU\_329,4.57,0.07,0,0  
4EVF,LYS\_3,10.43,-0.07,0,0  
2B2H,ARG\_32,12.89,-1.27,0,1.66  
1W7B,TYR\_30,10.04,0,0,0.04  
2R0S,LYS\_45,10.29,-0.21,0,0  
3COU,ARG\_96,12.3,-0.85,0,0.65  
3B7H,ARG\_44,12.5,0,0,0  
1PBV,CYS\_174,4.89,-4.26,0,0.14  
1X7F,ASP\_160,3.77,0,-0.03,0  
2Q13,ARG\_279,11.94,-0.56,0,0  
3A7L,TYR\_24,10.49,0,0,0.49  
1WJG,GLU\_40,4.64,0.14,0,0  
3LD1,LYS\_107,10.29,-0.21,0,0  
1X04,GLU\_140,2.52,0.42,-2.4,0  
1DCF,GLU\_33,4.57,0.07,0,0  
1U53,TYR\_158,11.58,3.18,-1.6,0  
2IQT,LYS\_293,9.94,-0.56,0,0  
2AZL,LYS\_15,10.29,-0.21,0,0  
2FD5,GLU\_68,4.57,0.07,0,0  
3B21,LYS\_34,10.29,-0.21,0,0  
1RKA,ARG\_198,12.29,-0.21,0,0  
2HRZ,ASP\_329,1.79,0.42,-2.43,0  
4E5S,ARG\_127,12.15,-0.35,0,0  
1XFK,GLU\_18,4,0.56,-1.06,0  
1V43,GLU\_103,4.57,0.07,0,0  
4ETX,GLU\_241,4.45,0.07,-0.12,0  
3ETU,GLU\_275,4.5,0,0,0  
3PAC,HIS\_127,4.14,0,-1.05,-1.31  
2Q98,LYS\_53,10.29,-0.21,0,0  
3CS1,GLU\_167,4.5,0,0,0  
3IVF,LYS\_316,10.5,0,0,0  
3GA2,ARG\_94,11.59,-0.91,0,0  
4E9E,HIS\_535,6.42,0.2,-0.28  
2JKF,GLU\_30,3.64,0.35,-1.21,0  
3BQW,ARG\_218,11.8,-0.7,0,0  
3CBN,GLU\_106,4.57,0.07,0,0  
1OIS,LYS\_301,10.36,-0.14,0,0  
2FXT,ARG\_342,12.29,-0.21,0,0  
3K8U,LYS\_59,10.22,-0.28,0,0  
3ADO,GLU\_211,4.13,0.07,-0.44,0  
3ASA,ARG\_362,12.5,0,0,0  
3CBN,GLU\_106,4.57,0.07,0,0  
3CAN,ASP\_78,3.87,0.07,0,0  
1UOH,HIS\_156,6.36,0,0,-0.14  
2OB5,GLU\_89,4,0.21,-0.71,0  
1MJS,LYS\_377,10.36,-0.14,0,0

3GEC,HIS\_279,6.29,0,0,-0.21  
1O5J,LYS\_49,10.36,-0.14,0,0  
1R2Z,ASP\_114,3.51,0,-0.29,0  
3A2Z,TYR\_18,10,0,0,0  
1XIP,ASP\_333,3.24,0.21,-0.77,0  
3F6F,LYS\_90,10.5,0,0,0  
3ONT,GLU\_144,4.52,0.14,-0.12,0  
2FZ4,ARG\_167,11.87,-0.63,0,0  
2PGX,LYS\_184,9.94,-0.56,0,0  
1S18,ARG\_532,10.82,-1.68,0,0  
2R4Q,LYS\_214,10.22,-0.28,0,0  
1JB3,GLU\_102,4.49,1.51,-1.52,0  
1YW5,GLU\_150,4.08,0.14,-0.56,0  
1WRU,ARG\_336,11.66,-0.84,0,0  
2A6B,LYS\_104,10.43,-0.07,0,0  
1W24,GLU\_175,4.56,0.14,-0.08,0  
1R15,CYS\_272,8.91,-0.09,0,0  
1PDB,GLU\_44,4.5,0,0,0  
3CO1,CYS\_39,9.34,-0.36,0,0.69  
2OGQ,LYS\_574,10.29,-0.21,0,0  
3ULX,ASP\_101,2.04,0.63,-2.39,0  
3M66,ASP\_409,3.47,0.07,-0.4,0  
1T6L,LYS\_101,10.5,0,0,0  
2EFK,TYR\_105,10.28,0.28,0,0  
3JZN,ARG\_420,12.08,-0.42,0,0  
2P52,ARG\_178,12.43,-0.07,0,0  
3E5T,LYS\_138,10.43,-0.07,0,0  
1TLV,GLU\_69,4.71,0.21,0,0  
4FZN,ASP\_214,4.11,0.35,-0.04,0  
3R1X,GLU\_58,0.41,1.8,-3.49,-2.4  
3JV1,ASP\_197,4.12,0.42,-0.1,0  
3GMS,ARG\_169,12.15,-0.35,0,0  
1SQH,CYS\_152,7.39,-0.8,-1.78,0.98  
2G9D,ASP\_280,3.12,0.14,-0.82,0  
2ZQ5,ASP\_27,3.8,0.14,-0.14,0  
3COU,TYR\_43,9.92,0,-0.08,0  
3ETV,ARG\_21,12.01,-0.49,0,0  
1MUF,ASP\_99,2.71,0.84,-1.94,0  
1JB3,ARG\_111,12.08,-0.42,0,0  
1MS1,LYS\_226,9.8,-0.7,0,0  
1PBV,ARG\_61,12.22,-0.28,0,0  
3V3T,TYR\_50,10.14,0.14,0,0  
3B7H,ASP\_4,3.12,0.21,-0.89,0  
3OA7,ARG\_555,12.5,0,0,0  
2P4D,ASP\_84,2.16,0.98,-2.62,0  
4DND,ARG\_27,12.5,0,0,0  
1WLY,GLU\_19,4.19,0.49,-0.8,0  
3IOC,ARG\_146,12.08,-0.42,0,0  
1WLY,CYS\_191,10.45,-0.05,0,1.5  
1PZC,LYS\_57,10.36,-0.14,0,0  
1YTQ,HIS\_31,6.23,0.01,0,-0.28  
3RHE,ASP\_27,3.94,0.14,0,0  
2A6B,ASP\_91,3.76,0.35,-0.39,0  
3RFY,TYR\_209,13.41,0.21,0.8,2.4  
1YTD,TYR\_72,12.24,0.27,-0.04,2.01  
3ON1,ASP\_100,3.39,0.42,-0.83,0  
2GQV,GLU\_53,2.56,0.84,-2.78,0  
2Q07,TYR\_460,9.84,0.65,0,-0.8  
2VAN,LYS\_127,10.43,-0.07,0,0  
4DVD,GLU\_128,4.57,0.07,0,0  
1U3Y,LYS\_317,10.29,-0.21,0,0  
3C6B,CYS\_169,10.49,-0.44,-0.8,2.72  
3L3P,GLU\_529,4.5,0,0,0  
1QQH,CYS\_109,8.94,-0.81,-0.71,1.47  
1VJG,LYS\_105,10.5,0,0,0  
2HRZ,ARG\_286,12.08,-0.42,0,0  
2EEY,ASP\_93,3.27,0.21,-0.74,0  
1OGL,ASP\_40,3.21,0.21,-0.8,0  
4AF2,ASP\_158,3.35,0.21,-0.66,0  
3H5T,GLU\_230,4.76,0.63,-0.37,0  
1XWM,ARG\_154,12.01,-0.49,0,0  
2XWS,GLU\_56,3.91,0.21,-0.8,0  
3Q1C,ARG\_382,12.01,-0.49,0,0  
3P2F,TYR\_54,11.98,1.26,0.24,0.49  
3DSH,HIS\_344,6.29,0,0,-0.21  
2IRM,HIS\_172,6.37,0.01,0,-0.14  
1AK1,HIS\_101,7.41,0.98,0,-0.07  
3ETV,ARG\_205,11.66,-0.84,0,0  
3TIR,ASP\_191,3.63,0.28,-0.45,0  
2BQQ,GLU\_121,4.07,0.56,-0.99,0  
2O0K,GLU\_320,2.1,1.61,-1.67,-2.34  
2ZQ5,ARG\_299,12.15,-0.35,0,0  
2QV2,LYS\_289,10.29,-0.21,0,0  
2G5X,ASP\_179,3.85,0.07,-0.02,0  
2QVO,TYR\_32,13.48,0,0,1.338  
3BWT,ARG\_555,12.5,0,0,0  
3EX9,HIS\_123,7.16,0.8,0,-0.14  
2BLL,HIS\_359,6.36,0,0,-0.14  
2CVB,LYS\_110,10.29,-0.21,0,0  
3LQE,ARG\_396,12.29,-0.21,0,0  
4EF5,GLU\_249,4.21,0.42,-0.71,0  
2RIK,LYS\_66,10.22,-0.28,0,0  
2W0Z,LYS\_521,10.5,0,0,0  
1ZYL,ARG\_157,11.73,-0.77,0,0  
2JEO,ASP\_163,3.13,0.14,-0.81,0  
2RIK,LYS\_100,10.5,0,0,0  
3F53,TYR\_127,10,0,0,0  
1S7K,GLU\_12,3.98,0.28,-0.8,0  
2YT4,LYS\_669,10.5,0,0,0  
1WYC,TYR\_97,12.82,0.04,0,2.78  
1GXN,TYR\_437,10.07,0.07,0,0  
2V5B,ASP\_37,3.35,0.35,-0.8,0  
1V8E,HIS\_13,6.8,1.6,2.5,-3.8  
2EFK,LYS\_187,10.29,-0.21,0,0  
1C3K,TYR\_48,10,0,0,0  
1O9G,GLU\_228,2.88,0.7,-2.32,0  
3KT9,LYS\_34,10.5,0,0,0  
2HXB,TYR\_43,11.59,0.28,-1.02,2.33  
1SQH,GLU\_173,3.23,0.42,-1.69,0  
2PLQ,ARG\_267,10.55,-2.62,0,0.67  
1DUN,LYS\_88,10.5,0,0,0  
3T8R,ARG\_8,12.5,0,0,0  
2H2Z,CYS\_300,9.38,-0.13,0,0.51  
3TRE,LYS\_57,10.43,-0.07,0,0  
3RVC,LYS\_110,10.5,0,0,0  
2ZTY,LYS\_65,10.29,-0.21,0,0  
4EUG,ARG\_31,11.24,-1.26,0,0  
1WP5,GLU\_207,3.01,1.06,-2.32,-0.23  
1Q8B,GLU\_96,4.44,0.21,-0.27,0  
2EEY,GLU\_50,4.5,0,0,0  
3AU3,HIS\_427,6.48,0.33,0,-0.35  
4FCU,ASP\_92,2.52,0.98,-2.26,0  
1XTZ,ASP\_103,1.79,0.63,-2.63,0  
2EYI,GLU\_213,4.5,0.28,-0.28,0  
2PP6,ASP\_65,3.28,0.7,-1.23,0  
1YLN,ARG\_99,12.15,-0.35,0,0  
2Q07,LYS\_255,10.15,-0.35,0,0  
2FC3,LYS\_33,10.43,-0.07,0,0  
2VGM,LYS\_226,10.01,-0.49,0,0  
1DZF,GLU\_133,2.15,2.45,-2.4,-2.4  
1EV8,ASP\_105,2.07,0.63,-2.37,0  
2XMX,LYS\_184,9.8,-0.7,0,0  
2J8A,GLU\_363,4.67,0.49,-0.31,0  
1W24,ASP\_170,3.8,0,0,0  
3RRQ,ARG\_143,12.08,-0.42,0,0  
2IXM,CYS\_256,9.82,-1.36,-1.18,3.35  
2BV9,TYR\_131,13.84,3.84,0,0  
3C2E,LYS\_100,10.29,-0.21,0,0  
2OEW,GLU\_240,3.83,0.35,-1.01,0  
1F09,LYS\_287,10.29,-0.21,0,0  
2Q5X,TYR\_831,13.39,0.83,0,2.57  
2B0J,LYS\_154,10.5,0,0,0  
2B2H,GLU\_386,4.5,0,0,0  
3ON1,GLU\_80,3.96,0.28,-0.82,0  
3PZ9,ARG\_361,12.36,-0.14,0,0  
1XTZ,TYR\_27,12.61,0.21,0,2.4  
2AH5,GLU\_52,3.44,0,-1.06,0  
1ZP2,LYS\_204,10.5,0,0,0  
1EQ6,ARG\_162,11.73,-0.77,0,0  
2G9D,LYS\_75,10.43,-0.07,0,0  
2YT4,HIS\_491,6.36,0,0,-0.14  
2CBE,LYS\_168,10.36,-0.14,0,0  
3DB9,ASP\_53,2.84,0.56,-1.52,0  
4FZN,ASP\_194,3.13,0.98,-1.65,0  
3O16,GLU\_84,4.5,0,0,0  
1RL0,TYR\_229,13.34,0.14,0.8,2.4  
1P6F,HIS\_142,6.77,0.27,0,0  
3HYQ,GLU\_74,1.79,0.84,-3.55,0  
3RLN,CYS\_727,9.3,0,0,0.3  
2H2Z,TYR\_182,12.14,1.61,-0.98,1.51  
3HVM,LYS\_300,10.29,-0.21,0,0  
1YB2,GLU\_216,4.64,0.14,0,0  
3ONT,HIS\_120,6.43,0,0,-0.07  
4DVD,ARG\_115,12.08,-0.42,0,0  
2FPN,HIS\_134,7.16,0.8,0,-0.14  
3OKQ,LYS\_601,10.08,-0.42,0,0  
3E27,ARG\_16,12.5,0,0,0  
3OA7,TYR\_36,10,0,0,0  
1MIX,HIS\_283,2.94,0,0,-3.56  
4AF2,TYR\_159,13.95,0.75,0.8,2.4  
1J8B,LYS\_23,10.29,-0.21,0,0  
2EDM,LYS\_165,9.94,-0.56,0,0  
1T95,GLU\_88,4.71,0.21,0,0  
1OST,TYR\_201,10,0,0,0  
3EX9,HIS\_42,6.91,0.55,0,-0.14  
3LOD,ASP\_22,3.27,0.35,-0.88,0  
1DZF,ARG\_200,12.5,0,0,0  
1R3F,TYR\_179,10,0,0,0  
3G9T,GLU\_238,2.27,3.44,-3.67,-2  
3IVF,TYR\_270,12.99,0.88,0.17,1.94  
1XTD,GLU\_125,4.5,0,0,0  
1U3Y,TYR\_283,10.07,0.07,0,0  
3QKY,ARG\_40,12.01,-0.49,0,0  
2B78,ARG\_85,12.46,-2.82,0,2.78  
1XTZ,LYS\_220,10.29,-0.21,0,0  
3C38,ASP\_92,3.19,0.21,-0.83,0  
1NAF,TYR\_294,10.05,0.07,-0.02,0  
2CXA,ASP\_206,3.98,0.28,-0.1,0  
2QK1,CYS\_477,7.84,-1.16,-1.65,1.65  
2QK1,LYS\_327,10.08,-0.42,0,0  
2P65,TYR\_8,9.8,0,-0.2,0  
1R15,ARG\_213,12.22,-0.28,0,0  
3TOW,LYS\_82,10.5,0,0,0  
2JKF,ARG\_152,12.15,-0.35,0,0  
2GAU,ARG\_216,12.22,-0.28,0,0  
3R1X,GLU\_68,4.64,0.14,0,0  
3M66,LYS\_171,10.43,-0.07,0,0  
2QEV,LYS\_76,10.36,-0.14,0,0  
2ZCO,GLU\_254,4.12,0.42,-0.8,0  
1OST,ARG\_122,11.73,-0.77,0,0  
2PIM,LYS\_125,10.5,0,0,0  
2D7U,GLU\_107,3.11,0.21,-1.6,0  
4FZR,GLU\_105,4.71,0.21,0,0  
2H2Z,GLU\_14,4.05,0.35,-0.8,0  
1YTQ,CYS\_37,7.08,-1.99,0,0.07  
3G9G,TYR\_160,11.37,0,0,1.37  
1NAF,GLU\_173,4.5,0,0,0  
1ZBS,LYS\_56,10.43,-0.07,0,0  
2YLF,GLU\_227,4.18,0.21,-0.53,0  
1KCM,LYS\_252,10.5,0,0,0  
2OKT,HIS\_337,6.5,0,0,0  
3IUS,LYS\_77,10.36,-0.14,0,0  
4GA2,ARG\_23,12.15,-0.35,0,0  
3IOC,GLU\_97,0.49,0.78,-0.8,-3.99  
2EJX,LYS\_60,10.29,-0.21,0,0  
1XFK,HIS\_235,6.55,0.12,0,-0.07  
2FZP,GLU\_198,4.05,0.35,-0.8,0  
3HUE,LYS\_96,10.08,-0.42,0,0  
3O16,LYS\_50,10.29,-0.21,0,0  
1L2H,CYS\_8,9.64,-0.36,0,1  
1WPA,LYS\_521,10.08,-0.42,0,0  
3COU,ARG\_168,11.94,-0.56,0,0  
3C5V,ARG\_303,12.29,-0.21,0,0  
3F6M,GLU\_30,4.35,0.42,-0.57,0  
1AK1,ASP\_159,3.91,0.21,-0.1,0  
1YOY,LYS\_110,10.5,0,0,0  
1TD6,TYR\_283,10,0,0,0  
1PBV,TYR\_101,9.99,0,-0.01,0  
1S18,CYS\_719,11.16,-0.13,0,2.29  
2H30,TYR\_52,11.42,0,-0.2,1.63  
1T3J,GLU\_701,4.39,0.35,-0.46,0  
3PZ9,LYS\_245,10.5,0,0,0  
1U7U,ASP\_401,3.93,0.21,-0.08,0  
3LJC,LYS\_235,10.22,-0.28,0,0  
3M3P,GLU\_193,3.58,0.28,-1.2,0  
3EYE,ASP\_101,3.56,0.28,-0.52,0  
2P0L,ASP\_203,3.94,0.14,0,0  
3Q6L,GLU\_23,4.57,0.07,0,0  
2B61,LYS\_39,10.43,-0.07,0,0  
2YX0,HIS\_144,1.69,0.05,-0.54,-4.32  
3F1X,LYS\_40,10.5,0,0,0  
2OBI,ARG\_12,12.5,0,0,0  
3JRT,ARG\_46,11.8,-0.7,0,0  
3V75,ARG\_45,11.8,-0.7,0,0  
1OIS,GLU\_182,3.67,1.11,-1.94,0  
1NRI,ARG\_200,12.43,-0.07,0,0  
4AM1,TYR\_30,13.41,0.21,0.8,2.4  
3E7P,CYS\_18,9.03,-0.26,0.29  
3UV9,LYS\_413,10.29,-0.21,0,0  
3G59,ASP\_167,3.21,0.21,-0.8,0  
3OA7,GLU\_42,4.64,0.14,0,0  
4EKU,LYS\_206,10.5,0,0,0  
1OLR,TYR\_66,13.1,1.76,-0.25,1.59  
2EER,LYS\_95,4.5,0,0,0  
4GCO,LYS\_156,10.5,0,0,0  
2F8H,ARG\_294,12.43,-0.07,0,0  
1V43,HIS\_201,6.47,0.11,0,-0.14  
1KCM,GLU\_218,5.92,1.42,0,0  
1TLV,GLU\_150,3.91,0.21,-0.8,0  
2BCF,GLU\_218,4.05,0.35,-0.8,0  
3BA1,GLU\_161,4.78,0.28,0,0  
1TXD,HIS\_842,5.45,1.6,2.02,-4.67  
2Q07,ASP\_482,1.97,0.49,-2.32,0  
1T3Y,TYR\_31,13.2,0.55,0.25,2.4  
3CAN,GLU\_49,4.09,0.21,-0.62,0  
1NFN,LYS\_72,10.08,-0.42,0,0  
3GA2,GLU\_71,4.38,0.14,-0.26,0  
3ETV,ARG\_281,11.19,-1.31,0,0  
4DND,GLU\_93,4.55,0.07,-0.02,0  
1MS1,ARG\_217,11.59,-0.91,0,0  
1WYC,ARG\_189,11.8,-0.7,0,0  
2CYC,ARG\_102,12.08,-0.42,0,0  
3F1X,ASP\_257,4.15,0.35,0,0  
3G9G,GLU\_142,3.98,0.28,-0.8,0  
2G9D,GLU\_89,3.98,2.08,-0.5,-2.09  
2FBQ,GLU\_132,3.98,0.28,-0.8,0



3EVN,LYS\_260,10.36,-0.14,0,0  
15J8,GLU\_694,4.66,0.28,-0.12,0  
3CJW,GLU\_225,4.33,0.63,-0.8,0  
1O6D,ARG\_72,12.08,-0.42,0,0  
3QYB,LYS\_875,10.5,0,0,0  
2FD5,ARG\_160,11.21,-1.29,0,0  
3C6B,CYS\_219,11.91,-0.09,1.5,1.5  
1FKM,ASP\_264,3.8,0,0,0  
3U56,GLU\_106,4.5,0,0,0  
2B78,ARG\_154,12.77,-1.8,0,2.07  
3GT0,ARG\_117,11.52,-0.98,0,0  
4EZB,GLU\_259,4.5,0,0,0  
3GV0,HIS\_295,6.56,1.06,1.42,-2.42  
1WYC,GLU\_20,3.92,0.35,-0.93,0  
2W2S,HIS\_163,6.5,0,0,0  
1X04,GLU\_101,4.71,0.21,0,0  
3H13,ASP\_306,2.14,1.05,-2.71,0  
2GAU,LYS\_107,10.29,-0.21,0,0  
3MIX,ARG\_586,12.22,-0.28,0,0  
3HQX,GLU\_45,4.5,0,0,0  
2D7J,CYS\_61,10.02,-1.73,0.78,1.97  
3EJG,ASP\_161,3.84,0.14,-0.1,0  
15UJ,ASP\_747,1.79,0.98,-2.99,0  
3IRA,LYS\_115,10.29,-0.21,0,0  
3T57,ARG\_258,12.01,-0.49,0,0  
2FPN,ASP\_51,3.94,0.14,0,0  
3A0X,LYS\_710,10.5,0,0,0  
3CSR,ARG\_126,11.8,-0.7,0,0  
1ZBS,ASP\_42,3.64,0.28,-0.44,0  
2B0J,GLU\_69,4.57,0.07,0,0  
3EVP,GLU\_273,4.05,0.35,-0.8,0  
3NZL,TYR\_57,10,0,0,0  
1NWA,ASP\_109,3.91,0.14,-0.03,0  
3EVN,LYS\_5,10.5,0,0,0  
3LQE,ARG\_478,12.01,-0.49,0,0  
1K95,CYS\_181,10.74,0,0,1.74  
3CGW,GLU\_75,4.57,0.07,0,0  
2D7J,LYS\_116,10.5,0,0,0  
1LZL,ARG\_153,11.52,-0.98,0,0  
1O5J,GLU\_68,3.97,0.35,-0.88,0  
1XFK,HIS\_140,3.87,0,0,-2.63  
2DFL,ASP\_321,1.36,0.91,-3.35,0  
3Q2C,HIS\_80,6.5,0,0,0  
3UC9,HIS\_16,6.22,0,0,-0.28  
1WPA,ASP\_492,3.58,0.35,-0.57,0  
3CS1,GLU\_69,4.64,0.14,0,0  
3MTT,LYS\_489,10.5,0,0,0  
1Q46,GLU\_42,4.73,0.49,-0.26,0  
3IV4,ASP\_38,3.37,0.28,-0.71,0  
2YYO,HIS\_151,6.64,0.21,0,-0.07  
3BPV,ASP\_122,3.74,0,-0.06,0  
1XDZ,ARG\_216,11.94,-0.56,0,0  
3R2E,ARG\_86,12.36,-0.14,0,0  
2W2S,GLU\_37,4.64,0.14,0,0  
2YX0,LYS\_11,10.5,0,0,0  
3PZ9,ARG\_83,12.29,-0.21,0,0  
3EUR,LYS\_51,10.22,-0.28,0,0  
2B6P,GLU\_16,4.65,3.26,-3.11,0  
2RJD,GLU\_430,4.26,0.56,-0.8,0  
1Q46,TYR\_171,10,0,0,0  
2O0K,GLU\_108,4.64,0.14,0,0  
2R51,CYS\_171,9,0,0,0  
1O9G,GLU\_180,4.78,0.28,0,0  
1O9G,GLU\_91,4.5,0,0,0  
1WRU,ASP\_323,3.9,0.14,-0.04,0  
2O8I,LYS\_110,10.08,-0.42,0,0  
2OSA,GLU\_324,4.5,0,0,0  
2BCF,LYS\_145,9.94,-0.56,0,0  
2H14,HIS\_86,4.73,1.66,1.34,-4.77  
2AH5,ARG\_72,11.7,-0.8,0,0  
1SIG,GLU\_378,3.91,0.21,-0.8,0  
1YTQ,GLU\_46,4.03,0.28,-0.75,0  
3A2Z,TYR\_71,10.23,0.23,0,0  
3EYE,ASP\_104,3.35,0.35,-0.8,0  
1HF8,GLU\_33,4.04,0.21,-0.67,0  
2CXC,ARG\_127,12.23,-2,0,1.73  
2C2Y,ARG\_66,11.8,-0.7,0,0  
1O0X,ARG\_30,11.94,-0.56,0,0  
2EDM,LYS\_79,10.43,-0.07,0,0  
2P4D,ARG\_116,13.39,-0.79,0,1.68  
1RZ2,HIS\_163,7.03,1.03,0,-0.49  
1NJ4,ARG\_261,12.15,-0.35,0,0  
1YTD,TYR\_99,11.82,0.6,0,1.22  
1QYI,GLU\_179,1.52,0.79,-1.78,-1.99  
2G3A,LYS\_117,10.29,-0.21,0,0  
2IRM,ASP\_96,3.21,0.21,-0.8,0  
1X7F,GLU\_236,4.5,0,0,0  
2WZ9,HIS\_115,7.16,0.8,0,-0.14  
4ESS,HIS\_162,7.13,0.7,0,-0.07  
2BCF,GLU\_210,4.5,0,0,0  
2B0J,GLU\_338,4.15,0.14,-0.49,0  
1SFE,GLU\_73,4.71,0.21,0,0  
3F6F,LYS\_175,10.5,0,0,0  
3KEY,GLU\_371,4.56,0.07,-0.01,0  
1MIX,LYS\_268,10.5,0,0,0  
1N81,ASP\_195,3.84,0.28,-0.24,0  
3ANJ,TYR\_364,13.87,1.81,0,2.06  
2G2D,ARG\_174,11.73,-0.77,0,0  
3U4K,ARG\_125,12.36,-0.14,0,0  
2Q34,GLU\_179,3.11,0.35,-1.74,0  
2WB3,GLU\_378,4.85,0.35,0,0  
2CL3,ASP\_116,2.55,0.49,-1.73,0  
3K9I,ASP\_159,3.79,0.07,-0.08,0  
1N81,TYR\_21,10,0,0,0  
2QK0,LYS\_100,9.8,-0.7,0,0  
3RFF,HIS\_70,6.29,0,0,-0.21  
3OA7,ARG\_441,12.36,-0.14,0,0  
2O8P,LYS\_80,10.15,-0.35,0,0  
2FBI,GLU\_130,4.5,0,0,0  
3ONT,CYS\_12,4.39,-4.67,0,0.07  
2V5B,LYS\_154,10.08,-0.42,0,0  
2RIK,LYS\_22,10.5,0,0,0  
2R51,ARG\_136,12.15,-0.35,0,0  
3PAC,LYS\_15,10.15,-0.35,0,0  
1R3F,ASP\_87,3.83,0.28,-0.24,0  
2VGY,HIS\_56,6.4,0.04,0,-0.14  
3KEY,LYS\_449,10.43,-0.07,0,0  
4EZB,GLU\_-7,4.78,0.28,0,0  
4HDE,LYS\_150,10.15,-0.35,0,0  
1UAJ,GLU\_34,3.94,0.28,-0.83,0  
3O7K,GLU\_14,4.5,0,0,0  
4E8B,ASP\_214,3.16,0.49,-1.12,0  
1LZL,ASP\_62,3.31,0.35,-0.84,0  
1TXJ,GLU\_169,3.8,0.21,-0.91,0  
1KN3,HIS\_159,6.36,0,0,-0.14  
3RVC,HIS\_169,6.44,0.01,0,-0.07  
2GAU,LYS\_165,10.43,-0.07,0,0  
3LJC,ASP\_179,2.62,0.28,-1.46,0  
1ANU,GLU\_81,1.33,1.26,-4.43,0  
4ESS,GLU\_59,4.54,0.28,-0.24,0  
2O0K,GLU\_220,4.26,0.35,-0.58,0  
2B02,GLU\_398,3.82,0.49,-1.17,0  
3M9A,TYR\_81,13.27,0.07,0.8,2.4  
2Q13,GLU\_155,4.5,0,0,0  
4HDE,ARG\_192,11.94,-0.56,0,0  
4E9E,GLU\_501,3.91,0.21,-0.8,0  
2A6B,ASP\_197,0.85,0.49,-3.43,0  
1RKA,ARG\_171,12.08,-0.42,0,0  
3D9H,HIS\_204,5.58,1.51,0.8,-3.24  
3CSV,ARG\_102,11.73,-0.77,0,0  
2JKF,TYR\_10,12.75,0.07,0.58,2.11  
1O5J,ASP\_48,2.51,0.35,-1.64,0  
1EV8,LYS\_18,10.43,-0.07,0,0  
3ZTA,ARG\_38,12.22,-0.28,0,0  
2D7U,TYR\_187,10.65,0,0,0.65  
3V3T,GLU\_176,4.58,0.73,-0.65,0  
2BV9,ARG\_234,12.29,-0.21,0,0  
4DIU,GLU\_141,4.19,0.49,-0.8,0  
2IF4,ASP\_211,2.97,0.21,-1.04,0  
2CI3,HIS\_231,6.43,0,0,-0.07  
1YB2,TYR\_107,10,0,0,0  
3AUF,HIS\_-1,6.39,0.1,0,-0.21  
4DEZ,GLU\_54,4.5,0,0,0  
3IV4,HIS\_74,2.33,0,-2.4,-1.77  
1YLN,LYS\_243,10.29,-0.21,0,0  
2YWX,GLU\_150,3.92,0.07,-0.65,0  
1R53,LYS\_203,10.43,-0.07,0,0  
2EVI,LYS\_220,10.15,-0.35,0,0  
3P51,GLU\_67,3.92,0.21,-0.79,0  
1PNE,LYS\_37,10.08,-0.42,0,0  
2CVB,GLU\_161,3.94,0.07,-0.63,0  
2YX0,LYS\_193,10.08,-0.42,0,0  
4H4J,ASP\_248,4.14,0.35,-0.01,0  
2F9F,LYS\_123,10.36,-0.14,0,0  
3K8U,TYR\_101,11.34,1.34,0,0  
2GZQ,TYR\_71,11.62,0.38,-0.31,1.55  
3I4T,ASP\_14,2.48,0.56,-1.88,0  
1WRU,ASP\_116,2.83,0.42,-1.39,0  
2Q12,HIS\_175,6.5,0,0,0  
1ILW,ARG\_165,12.22,-0.28,0,0  
1UAJ,ARG\_52,12.36,-0.14,0,0  
1BN6,GLU\_110,4.71,0.21,0,0  
2Q12,LYS\_66,10.08,-0.42,0,0  
2YT4,LYS\_667,10.29,-0.21,0,0  
1ILW,TYR\_124,10.66,0,0,0.66  
1J7G,GLU\_36,4.5,0,0,0  
2R2Y,LYS\_99,10.5,0,0,0  
3LXF,ARG\_27,12.15,-0.35,0,0  
2XMZ,HIS\_42,7.07,0.77,0,-0.21  
1P1L,GLU\_65,3.99,0.28,-0.79,0  
3D9H,LYS\_163,10.15,-0.35,0,0  
3G9E,HIS\_194,6.5,0,0,0  
1MJS,ARG\_267,11.73,-0.77,0,0  
1BRK,GLU\_71,3.99,0.49,-1,0  
1AD6,HIS\_483,0.25,0.74,-2.26,-4.72  
1F2V,GLU\_147,4.5,0,0,0  
3R87,ARG\_101,12.08,-0.42,0,0  
1RL0,GLU\_164,1.47,1.77,-2.4,-2.4  
3DHN,ARG\_174,12.29,-0.21,0,0  
3V55,GLU\_355,3.6,0.28,-1.18,0  
1MUF,LYS\_143,10.5,0,0,0  
3RRQ,ASP\_77,3.96,0.28,-0.12,0  
1TWU,GLU\_107,4.39,0,-0.11,0  
3PBH,HIS\_111,6.28,0.13,0,-0.35  
1NRI,GLU\_193,2.36,1.5,-2.19,-1.45  
1V43,TYR\_102,13.48,0.28,0.8,2.4  
1PSW,ASP\_124,3.1,0.42,-1.12,0  
1BN6,GLU\_27,4.64,0.14,0,0  
1P4X,ARG\_193,11.87,-0.63,0,0  
1YIB,CYS\_228,8.95,-0.12,0,0.07  
1NFN,ARG\_38,12.15,-0.35,0,0  
1DTC,CYS\_109,8.87,0,-1.35,1.22  
1ZBM,ARG\_227,12.22,-0.28,0,0  
4H4J,HIS\_227,1.52,0.03,-1.57,-3.44  
1R3F,ASP\_299,3.06,0.14,-0.88,0  
3ANJ,GLU\_395,3.7,0.34,0,-1.14  
1YLN,HIS\_38,6.5,0,0,0  
1N81,TYR\_86,10.09,0.14,-0.8,0.75  
2R51,LYS\_36,10.5,0,0,0  
4AM1,GLU\_149,4.72,1.14,-0.92,0  
1EQ6,LYS\_189,10.5,0,0,0  
3M7D,LYS\_47,10.01,-0.49,0,0  
3QYB,LYS\_897,10.36,-0.14,0,0  
3VJ8,GLU\_191,4.5,0,0,0  
1MUF,HIS\_297,6.29,0,0,-0.21  
3GS9,ASP\_97,3.7,0.07,-0.17,0  
3G9T,GLU\_189,4.5,0,0,0  
1X7F,TYR\_317,10.14,0,0,0.14  
3BCV,LYS\_102,10.15,-0.35,0,0  
2FC3,TYR\_79,9.44,1.11,-1.67,0  
3ANJ,GLU\_28,0.37,0.77,-4.9,0  
2R05,LYS\_106,10.22,-0.28,0,0  
1UAJ,ARG\_208,12.36,-0.14,0,0  
3V55,GLU\_388,4.4,0.7,-0.8,0  
3DSH,ARG\_443,12.29,-0.21,0,0  
3IOO,ARG\_203,12.43,-0.07,0,0  
2VGM,LYS\_103,10.43,-0.07,0,0  
2HRZ,HIS\_-3,6.36,0.07,0,-0.21  
3HKX,ARG\_89,12.29,-0.21,0,0  
3HEY,LYS\_103,10.29,-0.21,0,0  
1R3F,ARG\_40,12.43,-0.07,0,0  
3GFP,GLU\_473,4.64,0.14,0,0  
1R29,ASP\_119,3.28,0.28,-0.79,0  
2D0A,TYR\_114,12.13,0.07,-0.34,2.4  
2FI9,ASP\_58,2.51,0.49,-1.78,0  
1WPS,TYR\_262,10,0,0,0  
4ACJ,HIS\_770,7.16,0.8,0,-0.14  
2A6B,LYS\_78,10.36,-0.14,0,0  
2X5Y,LYS\_779,10.43,-0.07,0,0  
1X04,LYS\_39,10.5,0,0,0  
2PLQ,CYS\_189,13.6,0,0,4.6  
3GFP,ARG\_426,11.66,-0.84,0,0  
2I6I,TYR\_16,10,0,0,0  
2YT4,LYS\_679,10.15,-0.35,0,0  
3B7X,GLU\_96,4.78,0.28,0,0  
2OGQ,LYS\_388,10.5,0,0,0  
1CBY,GLU\_136,4.43,0.14,-0.21,0  
2B0J,GLU\_110,4.71,0.21,0,0  
3F6M,LYS\_89,10.36,-0.14,0,0  
3ANJ,LYS\_264,10.5,0,0,0  
3ASA,ASP\_74,3.43,0.07,-0.44,0  
3GW3,GLU\_250,4.48,0.14,-0.16,0  
3G6S,LYS\_87,12.62,-0.28,0.2,4  
3DB9,ARG\_115,11.94,-0.2,0.56,0,0  
3ETV,GLU\_23,4.57,0.07,0,0  
3LMO,LYS\_78,10.5,0,0,0  
2YLF,TYR\_63,10.14,0.14,0,0  
2CL3,ASP\_142,4.01,0.21,0,0  
2HNG,GLU\_87,2.99,0.35,-1.86,0  
3ASA,LYS\_12,10.15,-0.35,0,0  
2JKF,GLU\_29,4.27,0.42,-0.65,0  
2H01,LYS\_73,10.08,-0.42,0,0  
1FQI,ARG\_360,12.29,-0.21,0,0  
3G9G,LYS\_200,10.5,0,0,0  
3LPZ,CYS\_96,8.56,-2.23,0,1.8  
3V55,ASP\_535,3.13,0.42,-1.1,0  
2FPN,ASP\_108,3.08,0.21,-0.93,0  
3C2E,LYS\_202,10.43,-0.07,0,0  
1WXQ,GLU\_267,4.42,0.21,-0.29,0  
3LJN,GLU\_311,4.17,0.14,-0.47,0  
1J7G,ARG\_7,11.8,-0.7,0,0  
1G5Z,GLU\_87,4.64,0.14,0,0  
1R15,LYS\_238,10.29,-0.21,0,0  
3HVM,LYS\_242,9.66,-0.84,0,0  
1Q2Y,GLU\_37,4.5,0,0,0  
2BLL,GLU\_479,3.84,0.14,-0.8,0

3V55,LYS\_341,10.08,-0.42,0,0  
1U53,LYS\_172,10.29,-0.21,0,0  
3RKV,GLU\_298,4.57,0.07,0,0  
3CJW,CYS\_213,9,0,0,0  
1X04,LYS\_172,10.01,-0.49,0,0  
4EVF,ASP\_135,3.01,0.49,-1.29,0  
3E7P,ASP\_107,3.29,0.14,-0.65,0  
1O59,ARG\_153,11.52,-0.98,0,0  
3PZ9,TYR\_179,12.86,0.07,0.39,2.4  
2VC8,GLU\_61,4.71,0.21,0,0  
3LH5,ARG\_658,12.78,-2.68,0,2.96  
2RGY,ARG\_345,11.45,-1.05,0,0  
1OOX,GLU\_254,4.47,0.49,-0.52,0  
1AT0,LYS\_340,10.43,-0.07,0,0  
1X1E,ARG\_156,12.08,-0.42,0,0  
2XMZ,GLU\_53,4.37,0.21,-0.34,0  
1PZ2,HIS\_137,2.69,0.06,-0.387  
2OGQ,TYR\_552,12.07,0.57,-0.68,2.17  
2EJB,HIS\_64,7.12,1.63,1.9,-2.91  
3PP8,LYS\_21,10.43,-0.07,0,0  
1WRU,GLU\_206,4.64,0.14,0,0  
3V4G,LYS\_34,10.43,-0.07,0,0  
2EHG,LYS\_107,10.36,-0.14,0,0  
3CSV,ARG\_39,12.22,-0.28,0,0  
3BB7,TYR\_138,10.135,-1.35,0  
1P4X,GLU\_98,4.5,0,0,0  
2G9D,ASP\_117,2.27,1.12,-2.65,0  
3ETU,GLU\_254,6.07,0.45,-0.8,1.92  
3IVF,TYR\_81,11.52,0.44,-0.24,1.32  
1RAJ,TYR\_73,10,0,0,0  
4ETX,ARG\_210,11.87,-0.63,0,0  
2HZZ,LYS\_180,10.5,0,0,0  
3F1X,ARG\_128,11.87,-0.63,0,0  
2F4Q,GLU\_312,4.71,0.21,0,0  
2QV2,ARG\_325,12.08,-0.42,0,0  
4ESS,GLU\_149,4.09,0.35,-0.76,0  
2WB8,CYS\_679,9.08,-0.31,0,0.39  
4E6S,CYS\_14,9.07,0,0,0.07  
2Z61,LYS\_213,9.94,-0.56,0,0  
3H6Q,GLU\_142,4.71,0.21,0,0  
2GEN,ARG\_138,11.52,-0.98,0,0  
3K8J,ARG\_161,11.2,-2.05,0,0.75  
2ZCO,GLU\_175,5.4,0.21,-0.8,1.49  
3F1X,ASP\_256,2.82,0.42,-1.4,0  
3CSV,ARG\_228,11.59,-0.91,0,0  
1H09,ARG\_73,11.87,-0.63,0,0  
2O8I,ARG\_56,11.52,-0.98,0,0  
2QZQ,ASP\_60,2.23,0.91,-2.48,0  
1W7B,LYS\_329,10.08,-0.42,0,0  
2EFK,GLU\_238,4.05,0.35,-0.8,0  
3EYE,GLU\_114,4.5,0,0,0  
3LJN,GLU\_105,4.5,0,0,0  
3M66,CYS\_399,9.07,0,0,0.07  
3GS9,GLU\_67,4.23,1.01,-1.28,0  
3A7L,GLU\_30,4.11,0.28,-0.67,0  
3ZXY,ASP\_37,3.84,0.28,-0.24,0  
2B6P,GLU\_151,3.55,0.35,-1.3,0  
1FQI,GLU\_333,3.41,0.7,-1.79,0  
3C01,ARG\_130,11.87,-0.63,0,0  
1P6F,TYR\_167,10.5,0.5,0,0  
3CJW,LYS\_303,9.73,-0.77,0,0  
1SOH,TYR\_69,10.49,0.49,0,0  
3JV1,HIS\_150,6.43,0,0,-0.07  
1OIS,TYR\_169,9.29,0.07,-0.78,0  
3VHJ,GLU\_94,4.5,0,0,0  
3F7M,TYR\_340,11.09,0.83,-1.13,1.39  
1PDB,LYS\_184,9.31,-1.19,0,0  
3H9W,HIS\_86,10.29,4.73,1.87,-2.81  
2CBE,GLU\_239,4.69,0.21,-0.02,0

3CQ1,ASP\_35,3.09,0.28,-0.98,0  
2Q07,CYS\_253,5.36,-1.71,-2.4,0.47  
2CL3,GLU\_115,1.68,0.77,-3.59,0  
1AK1,LYS\_306,10.43,-0.07,0,0  
2XJ4,ARG\_254,12.08,-0.42,0,0  
1GQE,ASP\_329,2.95,0.42,-1.27,0  
1O5J,GLU\_34,4.5,0,0,0  
3UC9,ASP\_129,3.26,0.35,-0.89,0  
3H5T,ASP\_116,1.87,0.49,-2.42,0  
2B61,ASP\_197,2.42,0.56,-1.94,0  
3V3T,CYS\_243,9.69,-0.49,0,1.18  
1T95,ASP\_36,3.23,0.35,-0.92,0  
3ERF,LYS\_118,10.29,-0.21,0,0  
1CHD,GLU\_326,4.26,0.56,-0.8,0  
2YWK,TYR\_76,10,0,0,0  
2FG1,LYS\_90,10.08,-0.42,0,0  
3V55,HIS\_718,6.5,0,0,0  
3I0C,ARG\_198,12.15,-0.35,0,0  
3H5T,LYS\_322,10.15,-0.35,0,0  
2WB8,ASP\_696,3.87,0.07,0,0  
1T6L,ARG\_243,11.73,-0.77,0,0  
1TP6,ARG\_111,12.01,-0.49,0,0  
2A4D,LYS\_84,10.5,0,0,0  
1LN4,ASP\_2,3.5,0.14,-0.44,0  
3ZSL,TYR\_247,10.07,0.07,0,0  
3PP8,LYS\_127,10.5,0,0,0  
2G9D,GLU\_308,1.02,0.98,-4.46,0  
1X8F,LYS\_47,10.29,-0.21,0,0  
1O5J,ARG\_25,11.87,-0.63,0,0  
3I4T,CYS\_134,10.84,0,1.82,0.03  
1XWM,LYS\_171,10.43,-0.07,0,0  
2YX0,GLU\_208,3.87,0.35,-0.98,0  
1D2K,LYS\_205,10.5,0,0,0  
1X04,ARG\_152,12.22,-0.28,0,0  
3Q6L,LYS\_59,10.5,0,0,0  
3R87,TYR\_86,10.07,0.07,0,0  
3F53,GLU\_41,4.5,0,0,0  
3CIV,CYS\_300,7.83,-3.11,-0.32,2.26  
4DNU,ASP\_159,2.43,0.77,-2.14,0  
2DVK,ASP\_157,3.3,0.35,-0.85,0  
1G8P,ARG\_183,11.94,-0.56,0,0  
3M70,LYS\_286,10.43,-0.07,0,0  
3LQE,ARG\_392,13.39,-1.0,1.89  
1K9S,CYS\_182,11.84,-0.58,1.09,2.32  
3OKQ,GLU\_627,3.76,0.28,-1.02,0  
3IVF,TYR\_308,9.76,0,-0.24,0  
2P0L,TYR\_148,9.9,2.31,-1.59,-0.83  
1EV8,ASP\_241,3.2,0.21,-0.81,0  
2PGE,LYS\_229,10.5,0,0,0  
2E0T,ARG\_186,12.29,-0.21,0,0  
1Ri6,ASP\_123,2.39,0.42,-1.83,0  
2V4U,ASP\_312,3.59,0,-0.21,0  
3CRM,TYR\_201,9.67,0.21,-0.54,0  
3BQE,LYS\_234,10.5,0,0,0  
3JSN,GLU\_183,4.71,0.21,0,0  
3AU3,ARG\_640,12.01,-0.49,0,0  
2P5D,ASP\_55,3.94,0.14,0,0  
2X4J,TYR\_44,10,0,0,0  
3IRA,HIS\_16,0.67,0.07,-1.68,-4.22  
3ZTA,LYS\_8,10.29,-0.21,0,0  
2WB3,CYS\_350,9,0,0,0  
3P2F,ASP\_51,1.09,0.42,-3.13,0  
3C6B,ARG\_13,12.01,-0.49,0,0  
1Q5Z,LYS\_635,10.43,-0.07,0,0  
3IBT,LYS\_205,9.66,-0.84,0,0  
3HKX,ARG\_275,12.36,-0.14,0,0  
3A2Z,ASP\_40,4.14,0.35,-0.01,0  
1XWM,ARG\_124,12.29,-0.21,0,0  
3O7K,ARG\_36,11.24,-1.26,0,0

3ETV,LYS\_316,10.01,-0.49,0,0  
3VHJ,CYS\_86,8.75,-1.55,0,1.29  
2NSN,ASP\_95,3.8,0,0,0  
1YDL,ASP\_62,3.8,0,0,0  
2ZOM,CYS\_235,10.43,-0.07,0,0  
1ZBM,GLU\_115,3.85,0.07,-0.72,0  
3GYW,GLU\_41,4.5,0,0,0  
2Q12,ARG\_146,12.22,-0.28,0,0  
4ESS,LYS\_94,10.43,-0.07,0,0  
4ETX,ASP\_337,1.86,0.49,-2.43,0  
1X9G,LYS\_131,10.43,-0.07,0,0  
3ADO,GLU\_239,4.71,0.21,0,0  
1OOX,GLU\_14,3.25,0.49,-1.75,0  
3IV4,ASP\_64,3.8,0,0,0  
3N0K,ARG\_35,11.88,-0.62,0,0  
2IF4,GLU\_196,4.5,0,0,0  
1XTD,GLU\_151,4.14,0.21,-0.57,0  
2P52,ARG\_245,12.5,0,0,0  
1C44,LYS\_98,10.15,-0.35,0,0  
3IBT,GLU\_176,4.5,0,0,0  
3LPZ,ARG\_7,11.94,-0.56,0,0  
3EVP,ARG\_231,12.01,-0.49,0,0  
1DOV,LYS\_163,10.43,-0.07,0,0  
1EDG,LYS\_27,10.43,-0.07,0,0  
2RJD,LYS\_509,10.5,0,0,0  
1ZHV,HIS\_132,6.56,0.06,0,0  
3PBH,LYS\_19,10.5,0,0,0  
3EX9,GLU\_103,3.86,0.21,-0.85,0  
1QYI,GLU\_273,3.59,0.28,-1.19,0  
2YLF,GLU\_230,4.57,0.07,0,0  
2A1V,LYS\_43,9.94,-0.56,0,0  
2CIU,ARG\_167,11.8,-0.7,0,0  
2FXT,LYS\_311,10.5,0,0,0  
4E8B,GLU\_63,4.01,0.21,-0.7,0  
4F8A,GLU\_627,4.19,0.49,-0.8,0  
3BQE,LYS\_302,10.5,0,0,0  
2P52,ASP\_278,2.43,0.35,-1.72,0  
3COU,ARG\_78,11.73,-0.77,0,0  
2XMZ,HIS\_246,3.19,1.6,1.42,-6.33  
2H8S,ASP\_219,3.32,0.07,-0.55,0  
1J74,ARG\_14,12.22,-0.28,0,0  
3KEY,LYS\_433,10.5,0,0,0  
4EKU,GLU\_66,4.05,0.35,-0.8,0  
4F85,HIS\_58,1.38,0.87,-0.92,-5.07  
2OEW,GLU\_165,4.71,0.21,0,0  
3IBT,ASP\_158,2.93,0.07,-0.94,0  
1NFN,ARG\_147,12.08,-0.42,0,0  
1O5J,LYS\_84,10.43,-0.07,0,0  
1ILW,GLU\_87,4.5,0,0,0  
3EVN,GLU\_97,4.64,3.03,-1.44,-1.45  
3MUF,GLU\_330,3.27,0.77,-2,0  
1CAN,HIS\_128,7.22,0.79,0,-0.07  
1OIS,ARG\_296,12.5,0,0,0  
3DSH,GLU\_241,2.38,0.28,-2.4,0  
1EDG,LYS\_129,10.5,0,0,0  
2G3A,ARG\_112,11.8,-0.7,0,0  
2YLF,GLU\_44,3.26,0.35,-1.59,0  
1V6T,TYR\_89,10,0,0,0  
3NR5,ASP\_128,3.64,0.56,-0.72,0  
2FPN,ASP\_15,3.87,0.07,0,0  
3HUE,CYS\_105,5.93,-3.27,0,0.2  
3HUE,CYS\_204,8.53,-2.12,1.64,0.01  
2HRZ,TYR\_145,8.89,0.21,-1.32,0  
2Q13,TYR\_41,10.29,0,0,0.29  
3OIP,CYS\_51,9.82,0,0,0.82  
1R6Y,LYS\_33,10.5,0,0,0  
3CIV,GLU\_75,1.73,1.05,-3.82,0  
1R7J,GLU\_85,4.5,0,0,0  
3FRR,ARG\_55,12.22,-0.28,0,0

1R6Y,HIS\_75,3.17,0.05,0,-3.38  
3KB5,ARG\_369,11.66,-0.84,0,0  
3JSN,GLU\_180,4.5,0,0,0  
2QVT,LYS\_149,10.43,-0.07,0,0  
3ADO,CYS\_125,7.81,-1.26,0,0.07  
3B79,GLU\_126,4.65,0.21,-0.06,0  
4EUG,ASP\_9,2.07,0.35,-2.09,0  
1ZBS,GLU\_169,3.71,0.42,-1.21,0  
3QKY,LYS\_49,10.29,-0.21,0,0  
1Y2Q,HIS\_7,6.22,0,0,-0.28  
3G53,ARG\_122,12.76,-1.59,0,1.85  
3F7M,TYR\_375,10,0,0,0  
3GT0,GLU\_162,3.3,0.7,-1.9,0  
2B0A,GLU\_1,4.13,0.07,-0.44,0  
2R0S,LYS\_74,10.08,-0.42,0,0  
3ULX,GLU\_136,4.248,-1.78,-1.2  
3M7G,GLU\_19,2.02,2.33,-2.78,-2.02  
1HF8,LYS\_239,10.29,-0.21,0,0  
3JV1,HIS\_96,6.43,0,0,-0.07  
3F6F,TYR\_113,11.16,1.16,0,0  
1SIG,LYS\_251,10.5,0,0,0  
1ZBP,GLU\_177,4.35,0.07,-0.22,0  
1FHL,ARG\_5,11.8,-0.7,0,0  
2O8I,GLU\_55,2.59,0.56,-2.46,0  
3GE9,GLU\_145,4.5,0,0,0  
2D0A,LYS\_129,10.5,0,0,0  
2WB8,HIS\_794,3.03,0,0,-3.47  
4DIU,GLU\_39,4.71,0.49,-0.28,0  
3IVF,GLU\_80,4.64,0.14,0,0  
3BCY,LYS\_154,10.43,-0.07,0,0  
4H4J,LYS\_194,10.29,-0.21,0,0  
1YOY,ASP\_112,2.48,0.35,-1.67,0  
3U0V,HIS\_28,2.46,0.96,0,-5  
3H04,TYR\_67,13.08,3.39,-0.31,0  
1J85,GLU\_33,4.27,0,-0.23,0  
3CJW,GLU\_335,3.98,0.28,-0.8,0  
3OKQ,ARG\_588,12.29,-0.21,0,0  
2XHC,ARG\_156,12.08,-0.42,0,0  
2EYI,ASP\_200,3.11,0.35,-1.04,0  
3DTE,TYR\_25,10.4,0.76,-0.36,0  
1OIS,LYS\_173,10.29,-0.21,0,0  
1TXJ,GLU\_31,3.77,0.07,-0.8,0  
1PSW,LYS\_167,10.08,-0.42,0,0  
2NSN,HIS\_17,6.43,0,0,-0.07  
1MJS,ARG\_367,12.5,0,0,0  
2X4J,ASP\_107,3.24,0.42,-0.98,0  
3CXJ,LYS\_42,10.5,0,0,0  
3EVZ,LYS\_135,9.73,-0.77,0,0  
2IRM,CYS\_189,10.61,0,1,1.61  
2HRZ,ARG\_253,12.5,0,0,0  
2FZ4,ASP\_108,4.08,0.28,0,0  
3CBN,ASP\_146,1.41,0.91,-3.3,0  
3GOZ,TYR\_3,9.46,0,-0.54,0  
4DVD,ARG\_36,12.08,-0.42,0,0  
2P5D,GLU\_103,4.78,0.28,0,0  
1ANU,GLU\_4,3.98,0.28,-0.8,0  
3PBH,TYR\_146,10,0,0,0  
2Z14,CYS\_107,9.18,-0.11,0,0.29  
3ASA,ARG\_61,11.87,-0.63,0,0  
3H5T,LYS\_288,10.5,0,0,0  
3HVW,GLU\_260,2.95,0.28,-1.83,0  
3FTT,LYS\_165,10.5,0,0,0  
1OXZ,ARG\_180,12.22,-0.28,0,0  
2IRM,GLU\_312,4.11,0.07,-0.46,0  
3GMS,CYS\_151,10.72,-0.68,0,2.4  
1IAP,GLU\_155,4.5,0,0,0  
3CIV,ARG\_260,11.8,-0.7,0,0  
1RHS,CYS\_254,11.47,-0.04,-1.09,3.6  
3EVZ,GLU\_181,4.34,0.28,-0.43,0

1V6T,ARG\_237,11.64,-0.86,0,0  
1XIP,ASP\_180,2.21,0.42,-2.01,0  
1NAR,ASP\_156,3.25,0.14,-0.69,0  
2Z14,GLU\_56,4.46,0,-0.04,0  
2AZL,ARG\_243,12.22,-0.28,0,0  
3UX2,GLU\_75,4.5,0,0,0  
3I82,TYR\_135,11.34,1.34,0,0  
2EA9,TYR\_36,10.07,0,07,0,0  
2QDJ,LYS\_96,10.43,-0.07,0,0  
2FD5,GLU\_60,4.92,0.42,0,0  
2H2W,TYR\_120,11.77,1.51,0,0.26  
1MIX,LYS\_234,10.43,-0.07,0,0  
3GMS,LYS\_15,10.5,0,0,0  
1MIX,LYS\_278,10.36,-0.14,0,0  
1QSZ,LYS\_594,10.5,0,0,0  
2FXT,GLU\_319,4.57,0,07,0,0  
3V3T,ASP\_156,2.9,0.7,-1.6,0  
1EV8,GLU\_86,3.77,0.28,-1.01,0  
3ASA,GLU\_253,3.49,0.77,-1.78,0  
1RIS,GLU\_151,4.57,0,07,0,0  
3I4T,ASP\_11,3.18,0.77,-1.39,0  
2XJ4,ARG\_55,13.9,-2.44,0,3.84  
3SMD,GLU\_108,3.98,0.28,-0.8,0  
4EKU,LYS\_197,10.5,0,0,0  
4D8L,HIS\_279,6.5,0.07,0,-0.07  
1ZBM,LYS\_250,10.5,0,0,0  
3UC9,LYS\_163,10.15,-0.35,0,0  
2B0A,GLU\_24,4.57,0,07,0,0  
3L7N,GLU\_84,4.5,0,0,0  
2QDJ,GLU\_282,4.5,0,0,0  
2QZQ,LYS\_114,10.5,0,0,0  
1RAJ,ARG\_443,11.66,-0.84,0,0  
3HVV,ASP\_221,3.28,0.28,-0.8,0  
3ADO,ARG\_308,12.29,-0.21,0,0  
2G9D,ARG\_27,12.5,0,0,0  
3F5D,ASP\_145,2.31,0.7,-2.19,0  
1YM5,ARG\_260,12.36,-0.54,0,0.4  
1GQE,HIS\_199,0.97,1.06,-1.2,-5.39  
2CIU,LYS\_181,10.22,-0.28,0,0  
1JB3,GLU\_125,4.05,0.35,-0.8,0  
1EV8,ASP\_81,4.11,0.42,-0.11,0  
2D0A,ARG\_117,11.87,-0.63,0,0  
3I4T,TYR\_145,11.15,1.15,0,0  
1GQE,GLU\_172,2.91,0.14,-1.73,0  
1LTU,GLU\_157,3.86,0.42,-1.06,0  
3OKQ,ASP\_616,3.32,0.21,-0.69,0  
3BOE,GLU\_212,4.36,1.73,-1.87,0  
3BB7,GLU\_83,3.89,0.35,-0.96,0  
3CSV,TYR\_49,13.68,0.48,0.8,2.4  
3EZ7,ARG\_396,12.5,0,0,0  
1X04,HIS\_60,6.5,0,0,0  
2H30,ASP\_84,2.2,0.42,-2.02,0  
1XAW,ARG\_418,12.5,0,0,0  
1NAR,GLU\_77,4.5,0,0,0  
2CWC,ARG\_88,12.01,-0.49,0,0  
1YTD,TYR\_233,10.59,0.29,0,0.3  
3KT9,ARG\_3,11.94,-0.56,0,0  
1R3D,ARG\_132,13.04,-1.86,0,2.4  
3OAT,ARG\_33,12.36,-0.14,0,0  
1NAF,ARG\_258,11.94,-0.56,0,0  
3N2T,GLU\_65,3.18,2.93,-2.4,-1.85  
1L2F,LYS\_303,10.5,0,0,0  
3CRM,ARG\_225,12.29,-0.21,0,0  
3MIX,LYS\_589,10.22,-0.28,0,0  
3I4T,LYS\_150,10.29,-0.21,0,0  
1YR6,ARG\_218,12.5,0,0,0  
1RHS,LYS\_241,10.15,-0.35,0,0  
1PNE,CYS\_16,8.65,-0.77,0,0.42  
2NYC,LYS\_200,10.43,-0.07,0,0  
1I60,TYR\_253,10.91,1,-1.01,0.92  
2P65,GLU\_123,4.5,0,0,0  
3QKY,TYR\_257,9.73,0.07,-0.34,0  
1IDK,TYR\_268,11.23,0,0,1.23  
2FD4,LYS\_529,10.36,-0.14,0,0  
3R2E,ASP\_2,2.46,0.35,-1.7,0  
2EFK,ASP\_159,3.62,0.14,-0.32,0  
1L2F,GLU\_13,3.76,0.7,-1.44,0  
3BB7,LYS\_94,10.43,-0.07,0,0  
4EVF,LYS\_55,10.5,0,0,0  
2QEV,ASP\_71,3.21,0.21,-0.8,0  
1Ri6,HIS\_244,3.9,0.13,0,-2.74  
2P4D,LYS\_98,10.22,-0.28,0,0  
1ILW,HIS\_144,6.5,0,0,0  
1Sj8,GLU\_517,4.03,0.14,-0.61,0  
1BN6,GLU\_211,2.44,0.57,-2.4,-0.23  
4F8A,GLU\_613,3.06,0.35,-1.79,0  
2OJQ,ARG\_698,11.45,-1.05,0,0  
157K,ASP\_168,2.92,0.35,-1.23,0  
3GEC,LYS\_374,10.15,-0.35,0,0  
3RLN,GLU\_728,4.16,0.35,-0.69,0  
2ZQ5,ASP\_198,3.28,0.27,-0.8,0  
2YyO,ARG\_131,11.73,-0.78,0,0  
3GG6,ARG\_68,12.08,-0.42,0,0  
1L2F,LYS\_190,10.5,0,0,0  
4H89,ASP\_10,3.18,0.28,-0.9,0  
1RSS,ARG\_119,11.8,-0.7,0,0  
1RKA,GLU\_190,4.74,1.94,-1.19,-0.51  
1YM5,LYS\_291,10.22,-0.28,0,0  
2CBE,LYS\_172,10.08,-0.42,0,0  
3IVF,ARG\_131,11.73,-0.77,0,0  
1LFP,LYS\_189,10.36,-0.14,0,0  
3GYW,ASP\_189,3.79,0.42,-0.43,0  
1JSX,GLU\_125,4.78,0.28,0,0  
2BDV,ASP\_124,3.87,0.07,0,0  
3Q2C,ARG\_39,11.24,-1.26,0,0  
15J8,ASP\_659,3.42,0.35,-0.72,0  
3RLE,GLU\_34,2.94,1.08,-0.8,-1.84  
3D9H,LYS\_233,10.5,0,0,0  
2DVK,ARG\_75,12.01,-0.49,0,0  
2G9D,LYS\_3,10.36,-0.14,0,0  
2DVK,ASP\_18,2.67,1.05,-2.18,0  
3CZC,ASP\_76,4.03,0.28,-0.05,0  
4H4J,GLU\_73,4.29,0.59,-0.8,0  
2Z61,LYS\_23,10.5,0,0,0  
2B0J,HIS\_14,1.75,0,0,-4.75  
3GE9,ARG\_168,12.36,-0.14,0,0  
3CS1,GLU\_118,3.45,0.87,-1.92,0  
1J33,ASP\_299,3.45,0.42,-0.77,0  
3A4C,ARG\_462,12.15,-0.35,0,0  
3E7P,ASP\_108,3.8,0,0,0  
2Z84,LYS\_200,10.5,0,0,0  
3VJ8,ARG\_281,12.29,-0.21,0,0  
3H5T,TYR\_218,9.61,1.87,-1.59,-0.68  
1LFP,GLU\_179,4.5,0,0,0  
3GT0,CYS\_134,8.51,-0.56,0,0.07  
2YT4,CYS\_666,6.55,-2.52,0,0.07  
4GA2,ARG\_85,12.22,-0.28,0,0  
2QOP,LYS\_152,10.5,0,0,0  
1V43,ARG\_84,10.75,-1.75,0,0  
2NSN,LYS\_67,9.73,-0.77,0,0  
2X5Y,LYS\_752,10.08,-0.42,0,0  
1JSX,ARG\_68,11.8,-0.7,0,0  
3RFF,HIS\_107,6.5,0,0,0  
3RKV,ARG\_325,11.87,-0.63,0,0  
1D2K,LYS\_91,10.5,0,0,0  
1MIX,ARG\_328,12.01,-0.49,0,0  
3PAC,ASP\_49,3.72,0.14,-0.22,0  
3GFP,ARG\_377,12.5,0,0,0  
4DNU,ASP\_190,2.7,0.28,-1.38,0  
2D25,GLU\_546,3.94,0.7,-1.26,0  
3FHF,ASP\_17,3.77,0,-0.03,0  
3MIX,LYS\_476,10.15,-0.35,0,0  
2RGY,ARG\_330,11.59,-0.91,0,0  
3ANJ,TYR\_321,12.35,0.5,0.42,1.43  
2ZQ5,ASP\_87,3.99,0.21,-0.02,0  
2X4G,GLU\_186,3.08,0.27,0,-1.69  
4ACJ,TYR\_680,12.42,1.17,-0.38,1.64  
1TR9,GLU\_92,4.57,0.07,0,0  
3JZ9,ARG\_342,12.36,-0.14,0,0  
4DEZ,ARG\_53,13.76,-0.98,0,2.24  
2O8P,GLU\_110,3.09,0.71,-1.33,-0.79  
1WYC,TYR\_215,12.21,3.01,-0.8,0  
3SMD,TYR\_39,10,0,0,0  
2Q07,HIS\_278,1.53,1.14,-2,-4.11  
1NWA,ARG\_88,12.5,0,0,0  
2POL,LYS\_74,10.08,-0.42,0,0  
1O59,ARG\_317,12.08,-0.42,0,0  
3CX2,ARG\_177,12.22,-0.28,0,0  
2D0A,LYS\_122,10.01,-0.49,0,0  
3JZN,ARG\_414,13,-1.9,0.2,4  
1OIS,HIS\_331,7.16,0.8,0,-0.14  
1WRU,ARG\_262,12.22,-0.28,0,0  
2PLQ,ASP\_148,3.04,0.21,-0.97,0  
1IAP,GLU\_171,3.2,0.63,-1.93,0  
3I47,ARG\_157,12.5,0,0,0  
3BQW,GLU\_92,4.64,0.14,0,0  
1T95,GLU\_90,3.82,0.21,-0.89,0  
1SNT,GLU\_225,3.67,0.21,-1.04,0  
1TJE,ARG\_39,11.8,-0.7,0,0  
4EKU,ASP\_278,1.96,0.56,-2.4,0  
1SNT,ARG\_230,12.08,-0.42,0,0  
3V75,ASP\_101,3.15,0.35,-1,0  
1RIS,TYR\_284,12.77,2.5,0,0.27  
1R3F,ARG\_9,11.59,-0.91,0,0  
3CAN,ASP\_26,3.35,0.35,-0.8,0  
4EKU,GLU\_245,3.85,0.49,-1.14,0  
2Q34,TYR\_62,13.41,0.21,0.8,2.4  
1NIJ,GLU\_165,3.91,0.21,-0.8,0  
3CO1,LYS\_66,10.5,0,0,0  
1Q8B,HIS\_78,3.91,0.8,0,-3.39  
1NJ4,TYR\_159,9.76,0.07,-0.31,0  
2EOT,GLU\_82,4.05,0.35,-0.8,0  
2EJX,LYS\_133,10.08,-0.42,0,0  
3I82,ARG\_26,12.08,-0.42,0,0  
1QQE,HIS\_259,6.61,0.46,0,-0.35  
1XTZ,HIS\_39,4.13,0.28,0,-2.65  
3R87,ASP\_107,3.37,0.35,-0.78,0  
3P29,LYS\_322,10.5,0,0,0  
2P4D,LYS\_8,10.5,0,0,0  
2AXO,ARG\_110,11.87,-0.63,0,0  
3V55,LYS\_360,10.29,-0.21,0,0  
1WNH,GLU\_101,4.5,0,0,0  
2IXM,GLU\_190,2.85,0.82,-0.77,-1.7  
1PDB,LYS\_18,10.29,-0.21,0,0  
1RKA,HIS\_279,3.25,0.27,0,-3.52  
3IBT,ARG\_112,12.01,-0.49,0,0  
2A4D,TYR\_139,10.32,0.65,-0.33,0  
2YLF,GLU\_146,4.5,0,0,0  
3G65,ASP\_70,4.22,0.42,0,0  
3KB5,HIS\_345,9.5,2.73,2.34,-2.07  
3BPP,GLU\_175,3.27,0.35,-1.57,0  
2XTZ,HIS\_123,8.16,1.17,0.76,-0.28  
1CYT,GLU\_97,3.43,0.14,-1.21,0  
3V75,ASP\_16,3.96,0.21,-0.05,0  
3C6B,TYR\_216,9.45,1.21,-1.15,-0.62  
2NSN,TYR\_49,10,0,0,0  
2X5Y,LYS\_822,10.29,-0.21,0,0  
2X5Y,HIS\_746,4.54,0.07,0,-2.03  
1O6D,TYR\_103,10,0,0,0  
2QOP,LYS\_146,10.29,-0.21,0,0  
2IXM,HIS\_271,6.15,0,0,-0.35  
3ZXY,ASP\_287,3.27,0.28,-0.81,0  
3C6B,ARG\_45,12.5,0,0,0  
1FKM,LYS\_630,10.36,-0.14,0,0  
2Q07,ARG\_335,12.08,-0.42,0,0  
2G2D,ASP\_98,3.28,0.42,-0.94,0  
3CQ1,ARG\_42,12.36,-0.14,0,0  
2OYZ,TYR\_35,10.07,0,07,0,0  
1F2V,ARG\_65,11.68,-1.39,0,0.57  
1RWZ,LYS\_166,10.5,0,0,0  
1SBX,HIS\_147,6.5,0,0,0  
3JV1,GLU\_211,4.5,0,0,0  
2B2H,LYS\_241,10.15,-0.35,0,0  
2B78,CYS\_14,12.85,-2.45,0,2.3  
1RHS,ARG\_64,11.52,-0.98,0,0  
2VGM,ASP\_90,2.24,1.05,-2.61,0  
3JV1,TYR\_170,9.96,0,-0.04,0  
4FZN,CYS\_59,10.69,0,0,1.69  
2X4G,HIS\_243,5.15,0.32,0,-1.67  
2V5B,ARG\_208,10.63,-1.87,0,0  
2XJ4,GLU\_68,4.04,0.56,-0.8,-0.22  
2YWJ,LYS\_150,10.29,-0.21,0,0  
2POL,GLU\_261,4.19,0.49,-0.8,0  
3GS3,CYS\_247,9.06,-0.84,0,0.9  
3C2E,GLU\_210,4.5,0,0,0  
3BJV,ARG\_14,12.01,-0.49,0,0  
2OBI,ASP\_58,1.75,0.35,-2.4,0  
4DBX,LYS\_253,10.29,-0.21,0,0  
1C44,LYS\_87,10.5,0,0,0  
3G9T,GLU\_119,4.25,0.35,-0.6,0  
1V43,ARG\_290,13.35,-2.2,0,3.04  
3L3P,ARG\_436,11.8,-0.7,0,0  
1X91,LYS\_116,10.43,-0.07,0,0  
2AD1,HIS\_187,6.93,0.64,0,-0.21  
3D9H,GLU\_148,4.08,0.21,-0.63,0  
3GS9,GLU\_58,3.98,0.28,-0.8,0  
1CBY,LYS\_116,10.5,0,0,0  
3DTE,ARG\_142,12.36,-0.14,0,0  
1YG2,ASP\_169,3.51,0.49,-0.78,0  
2F4Q,ARG\_310,12.5,0,0,0  
2QV2,ARG\_133,11.94,-0.56,0,0  
3TIR,GLU\_162,1.73,0.77,-3.54,0  
3OKQ,LYS\_674,10.29,-0.21,0,0  
2A0J,GLU\_140,3.51,0.35,-1.35,0  
2E3C,TYR\_329,13.18,0.07,0.73,2.39  
1JKS,ARG\_156,11.94,-0.56,0,0  
1Q42,HIS\_83,5.88,1.6,2.25,-4.47  
1E55,TYR\_102,10.55,0.07,0,0.48  
3ETV,TYR\_215,10.29,1.09,-0.8,0  
2HXB,ARG\_117,12.08,-0.42,0,0  
3RNV,GLU\_358,4.5,0,0,0  
2AZP,ARG\_3,12.5,0,0,0  
3GEC,GLU\_518,4.5,0,0,0  
2EYI,GLU\_148,3.9,0.42,-1.02,0  
2X4J,LYS\_80,10.5,0,0,0  
1RIS,GLU\_199,4.1,0.21,-0.61,0  
2AZP,ARG\_35,11.29,-1.21,0,0  
2GEN,ARG\_118,12.01,-0.49,0,0  
2R05,TYR\_284,11.48,0.36,0,1.12  
1JKS,GLU\_115,2.56,0.49,-2.43,0  
2AH5,TYR\_28,12.54,0,0,14.24  
2EJB,TYR\_16,10.39,0.39,0,0  
2VC8,TYR\_21,10.07,0.07,0,0  
3C2E,GLU\_42,4.5,0,0,0  
3ETV,TYR\_109,10.46,0.81,-0.36,0  
2G7O,LYS\_99,10.43,-0.07,0,0

3R87,LYS\_3,10.43,-0.07,0,0  
2FD5,GLU\_27,4.44,0,-0.06,0  
3HYQ,ARG\_82,11.45,-1.05,0,0  
2CXA,GLU\_125,4.42,0.14,-0.22,0  
1H4U,HIS\_573,6.92,0.56,0,-0.14  
3ERF,TYR\_175,9.73,0,-0.27,0  
4ANN,ASP\_195,3.76,0,-0.04,0  
1T3Y,CYS\_52,10.29,0,0,1.29  
3EUR,TYR\_136,10.43,0,0,0.43  
3V4G,CYS\_149,7.83,-1.7,0,0.53  
1YR6,ASP\_141,1.98,0.84,-2.66,0  
2FL7,TYR\_66,11.01,0.45,0.3,0.25  
2FM9,LYS\_59,10.29,-0.21,0,0  
3T57,CYS\_326,7.61,-2.6,0,1.21  
2ZCO,ASP\_225,3.2,0.28,-0.88,0  
1KCM,LYS\_216,10.5,0,0,0  
1BYI,GLU\_78,4.68,0.07,-0.1,0  
2BAA,ASP\_182,1.65,0.49,-2.65,0  
1JB3,LYS\_129,10.29,-0.21,0,0  
2QK1,LYS\_540,10.5,0,0,0  
1BYI,LYS\_27,10.5,0,0,0  
3FHF,ASP\_181,3.83,0.21,-0.18,0  
1BN6,HIS\_34,4.65,1.6,0.14,-3.59  
3ETU,LYS\_340,10.22,-0.28,0,0  
2X4J,CYS\_23,9.04,-0.03,0,0.07  
4H4J,LYS\_261,10.29,-0.21,0,0  
4ANN,HIS\_80,4.46,0,-0.2,0  
3B79,GLU\_54,4.59,0.28,-0.19,0  
1IAP,GLU\_91,3.98,0.07,-0.59,0  
2WB3,LYS\_303,10.29,-0.21,0,0  
1OIS,LYS\_257,10.36,-0.14,0,0  
3VHJ,LYS\_103,10.08,-0.42,0,0  
1ZBM,TYR\_216,9.95,0,-0.05,0  
2HRZ,GLU\_328,4.5,0,0,0  
4FLE,LYS\_127,10.36,-0.14,0,0  
2WOZ,ASP\_573,3.09,0.63,-1.34,0  
3IL3,GLU\_31,4.5,0,0,0  
3HUE,TYR\_93,12.29,0.07,-0.09,2.31  
2JEO,ARG\_212,12.01,-0.49,0,0  
2ZOW,TYR\_68,10.07,0.07,0,0  
1FQJ,GLU\_324,4.19,0.49,-0.8,0  
3GV0,HIS\_106,3.84,0.01,0,-2.67  
1QQE,ARG\_48,12.15,-0.35,0,0  
2WB8,LYS\_754,10.29,-0.21,0,0  
3OA7,ARG\_506,12.15,-0.35,0,0  
1HU,ASP\_89,3.23,0.77,-1.34,0  
3GG5,LYS\_126,10.08,-0.42,0,0  
2P1W,LYS\_34,10.43,-0.07,0,0  
2FXT,GLU\_384,4.5,0,0,0  
2VGM,TYR\_335,13.84,0.63,0.59,2.63  
1OXZ,LYS\_226,10.5,0,0,0  
3OIP,ARG\_60,12.5,0,0,0  
1WYC,HIS\_165,3.87,0.07,0,0  
2OPJ,HIS\_262,6.43,0,0,-0.07  
1PDB,GLU\_81,4.78,0.28,0,0  
1GPP,ARG\_162,11.8,-0.7,0,0  
3J5N,TYR\_126,11.8,0,0,1.8  
3CO1,ARG\_17,12.36,-0.14,0,0  
2PGX,ASP\_13,2.03,0.49,-2.26,0  
2FC3,ARG\_45,12.01,-0.49,0,0  
3Q1C,ASP\_232,3.87,0.07,0,0  
3ETV,ASP\_169,3.65,0,-0.15,0  
2YYO,ASP\_142,3.87,0.07,0,0  
3J5N,TYR\_262,12.15,1.52,-0.09,0.71  
3M7D,CYS\_297,10.32,0,0,1.32  
2QOP,ARG\_161,12.15,-0.35,0,0  
1U7U,ASP\_365,3.6,0.07,-0.27,0  
1WPA,LYS\_511,10.5,0,0,0  
3GA2,TYR\_202,10.07,0.07,0,0  
1UOH,ASP\_86,4.18,0.49,-0.11,0  
2IDC,ARG\_123,11.45,-1.05,0,0  
3C6B,ARG\_179,13.16,-1.74,0,2.4  
1O59,LYS\_310,10.36,-0.14,0,0  
1R2Z,ASP\_188,3.27,0.49,-1.02,0  
3ANJ,ASP\_213,3.64,0.07,-0.23,0  
1R53,LYS\_253,10.5,0,0,0  
1PZC,GLU\_62,4.1,0.77,-1.17,0  
1O59,HIS\_268,6.4,0.25,0,-0.35  
1J7G,ARG\_90,12.5,0,0,0  
2HRZ,LYS\_195,10.5,0,0,0  
3EVP,ASP\_103,3.59,0.07,-0.28,0  
2CBE,ASP\_75,3.41,0.42,-0.81,0  
1MJS,GLU\_245,4.5,0,0,0  
3O7K,GLU\_161,4.64,0.14,0,0  
3L7N,LYS\_32,10.5,0,0,0  
4DIU,TYR\_181,11.65,0,0,1.65  
3B79,LYS\_122,10.5,0,0,0  
3B4D,ARG\_200,12.5,0,0,0  
3ADO,ARG\_299,11.94,-0.56,0,0  
1ZKZ,HIS\_7,6.87,0.65,0,-0.28  
2W2S,ARG\_156,11.94,-0.56,0,0  
3RKV,LYS\_271,10.29,-0.21,0,0  
3LJN,ARG\_249,13.79,-0.8,0,2.09  
2DG7,ARG\_159,11.94,-0.56,0,0  
2QDJ,LYS\_327,10.5,0,0,0  
3G9B,ARG\_32,11.94,-0.56,0,0  
3NBI,ARG\_62,11.8,-0.7,0,0  
2QK0,ARG\_99,11.52,-0.98,0,0  
1U53,LYS\_56,10.5,0,0,0  
3BJV,HIS\_68,1.07,0,-1.74,-3.69  
1DVO,ARG\_174,12.08,-0.42,0,0  
2F4Q,TYR\_250,11.75,0.07,0,1.68  
1YR6,LYS\_193,10.5,0,0,0  
2OJQ,LYS\_675,10.5,0,0,0  
2X4G,GLU\_140,2.61,1.87,-2.27,-1.49  
1MTZ,GLU\_262,4.57,0.07,0,0  
3K8J,GLU\_177,2.69,0.77,-2.58,0  
2OEW,ASP\_330,3.55,0.07,-0.32,0  
2FC3,LYS\_124,10.5,0,0,0  
3CRM,LYS\_108,10.22,-0.28,0,0  
1DZF,LYS\_45,10.5,0,0,0  
1OIS,HIS\_150,3.21,1.26,0,-4.55  
1E5S,ASP\_54,3.28,0.28,-0.8,0  
3FK5,LYS\_205,10.01,-0.49,0,0  
3L7N,TYR\_226,9.93,0,-0.07,0  
3U4K,GLU\_30,4.14,0.14,-0.5,0  
2H01,GLU\_158,4.19,0.49,-0.8,0  
4EZB,GLU\_245,4.12,0.35,-0.73,0  
2EJX,GLU\_130,3.42,0.49,-1.57,0  
3LJN,GLU\_73,4.23,0.35,-0.62,0  
1QQL,ASP\_9,2.93,0.14,-1.01,0  
3OOP,ASP\_96,3.74,0,-0.06,0  
2I6I,LYS\_7,10.01,-0.49,0,0  
3LJN,CYS\_132,5.8,-3.27,-0.37,0.44  
2Z0M,GLU\_264,4.5,0,0,0  
1FQI,TYR\_351,10.0,0,0,0  
2HRZ,LYS\_37,10.5,0,0,0  
2APL,TYR\_19,10.07,0.07,0,0  
3LD1,CYS\_331,9.45,-1.68,0,2.12  
2B61,TYR\_29,10.07,0.07,0,0  
1WP5,GLU\_312,4.63,0.14,-0.01,0  
2AZP,ARG\_141,11.94,-0.56,0,0  
1W7B,TYR\_151,10.32,0.32,0,0  
1EV8,CYS\_167,8.35,0,-1.39,0.74  
3FK5,LYS\_315,10.43,-0.07,0,0  
2H85,ASP\_106,2.37,1.05,-2.48,0  
1PSW,GLU\_238,3.95,0.42,-0.97,0  
1V43,LYS\_337,10.43,-0.07,0,0  
2HXB,CYS\_68,9.38,0,0,0.38  
1KW4,ASP\_45,2.34,0.35,-1.81,0  
3BQE,HIS\_245,7.08,0.72,0,-0.14  
4GA2,LYS\_135,10.36,-0.14,0,0  
1YG2,TYR\_31,9.79,0,-0.57,0.35  
1L2F,LYS\_280,10.43,-0.07,0,0  
4DIU,GLU\_85,4.71,0.21,0,0  
2FPN,GLU\_57,4.5,0,0,0  
3U56,GLU\_2,4.5,0,0,0  
1VJG,TYR\_128,11.09,0.04,0.01,1.04  
2DFL,LYS\_60,10.5,0,0,0  
2WB8,ASP\_720,3.14,0.07,-0.73,0  
2YYO,TYR\_64,10,0,0,0  
1VJG,LYS\_62,10.5,0,0,0  
1MIX,LYS\_318,10.5,0,0,0  
1YM5,GLU\_171,4.57,0.07,0,0  
1YTD,GLU\_32,4.71,0.21,0,0  
3ANJ,LYS\_38,10.5,0,0,0  
1PSW,GLU\_166,1,0.35,-3.85,0  
3I47,ARG\_239,12.43,-0.07,0,0  
2XWS,GLU\_109,4.5,0,0,0  
1JSX,GLU\_178,4.71,0.21,0,0  
1XTD,ASP\_121,2.33,0.84,-2.32,0  
1DUP,ARG\_34,12.01,-0.49,0,0  
3GFP,ASP\_316,3.47,0.21,-0.54,0  
3GS3,CYS\_211,5.55,-3.52,0,0.07  
1WLY,ASP\_201,2.21,0.84,-2.44,0  
2FXT,ASP\_340,3.94,0.56,-0.42,0  
1PSW,TYR\_323,8.82,0.5,-1.95,0.26  
1TUL,LYS\_46,10.43,-0.07,0,0  
2O8I,GLU\_109,4.5,0,0,0  
1Q46,TYR\_81,10,0,0,0  
3BCH,LYS\_57,10.36,-0.14,0,0  
1N4J,LYS\_59,10.36,-0.14,0,0  
1R5S,GLU\_67,3.98,0.28,-0.8,0  
1S17,GLU\_319,4.05,0.35,-0.8,0  
1O9G,GLU\_9,4.5,0,0,0  
1DVO,CYS\_142,8.8,-0.2,0,0  
1NRI,LYS\_224,10.36,-0.14,0,0  
2W0G,ARG\_262,11.87,-0.63,0,0  
4FZR,ARG\_87,11.94,-0.56,0,0  
3ETU,ASP\_349,3.8,0,0,0  
1SIG,ASP\_445,3.67,0.28,-0.41,0  
2H2W,HIS\_79,6.56,0.06,0,0  
1BN6,GLU\_141,1.72,3.83,-5.01,-1.6  
4EZB,TYR\_131,10,0,0,0  
3H04,LYS\_184,10.29,-0.21,0,0  
2PWQ,HIS\_25,7.17,0.74,0,-0.07  
2EJB,TYR\_86,11.04,1.67,-0.63,0  
2QOP,LYS\_116,10.08,-0.42,0,0  
3U56,ASP\_75,1.82,0.42,-2.4,0  
3F7M,LYS\_158,10.5,0,0,0  
1F2V,ARG\_207,12.08,-0.42,0,0  
3B21,LYS\_26,10.43,-0.07,0,0  
3ELI,ARG\_117,11.73,-0.77,0,0  
2RFA,GLU\_232,2.86,1.12,-0.8,-1.96  
1V8E,HIS\_155,6.5,0,0,0  
3CBN,ARG\_29,12.22,-0.28,0,0  
3BA1,GLU\_121,4.86,0.42,-0.06,0  
2EFK,TYR\_190,10.07,0.07,0,0  
1E59,ARG\_132,11.8,-0.7,0,0  
3G6S,ARG\_148,12.36,-0.14,0,0  
3G9G,ARG\_239,10.89,-1.61,0,0  
1ILW,GLU\_163,3.92,0.49,-1.07,0  
2CIU,ASP\_148,3.94,0.14,0,0  
4DBX,LYS\_139,10.5,0,0,0  
1L3K,LYS\_166,10.5,0,0,0  
2QDJ,GLU\_352,4.71,0.21,0,0  
3RJX,LYS\_137,10.29,-0.21,0,0  
2F4Q,ARG\_286,12.15,-0.35,0,0  
2OKT,ASP\_326,2.65,0.49,-1.63,0  
3QKY,LYS\_134,10.43,-0.07,0,0  
1LTU,GLU\_71,3.85,0.07,-0.72,0  
3ADO,GLU\_163,4.64,0.14,0,0  
2FL4,TYR\_59,9.34,0.14,-0.8,0  
1O0X,LYS\_144,10.5,0,0,0  
1Z3X,LYS\_103,10.22,-0.28,0,0  
1SQH,HIS\_86,1.48,0.56,-1.3,-4.27  
1WRU,GLU\_189,4.64,0.14,0,0  
1RHS,ARG\_50,12.22,-0.28,0,0  
1MD6,GLU\_72,4.5,0,0,0  
2HXB,TYR\_86,9.72,0,-0.28,0  
4E88,ASP\_241,3.93,0.63,-0.5,0  
2P52,ARG\_279,11.59,-0.91,0,0  
1MUF,HIS\_283,6.29,0,0,-0.21  
3CNU,GLU\_80,4.71,0.21,0,0  
2QVT,ARG\_98,11.45,-1.05,0,0  
2PLQ,ASP\_265,3.25,0.14,-0.69,0  
2EDM,ARG\_136,12.36,-0.14,0,0  
3EUR,LYS\_1,10.43,-0.07,0,0  
1S18,LYS\_529,10.08,-0.42,0,0  
2A0J,GLU\_28,4.64,0.14,0,0  
1WYC,CYS\_271,11.57,-0.12,0.17,2.52  
3DHN,GLU\_143,4.64,0.14,0,0  
4ANN,HIS\_44,6.5,0,0,0  
3BA1,ARG\_128,11.87,-0.63,0,0  
3ELI,ASP\_90,3.94,0.14,0,0  
2A0J,GLU\_28,4.64,0.14,0,0  
3O7K,GLU\_128,4.1,0.42,-0.83,0  
1SBX,ASP\_181,3.39,0.35,-0.76,0  
2AD1,LYS\_266,10.5,0,0,0  
3EIZ,ARG\_51,11.87,-0.63,0,0  
1R3F,HIS\_163,7.19,0.9,0,-0.21  
2FBQ,HIS\_45,6.36,0.0,-0.14  
1WOU,LYS\_58,10.29,-0.21,0,0  
1Y0K,ASP\_19,3.85,0.14,-0.09,0  
1RAJ,LYS\_75,10.43,-0.07,0,0  
3LD1,GLU\_314,4.06,0.07,-0.51,0  
2B0A,LYS\_26,10.5,0,0,0  
3M70,LYS\_246,10.5,0,0,0  
3GEC,ARG\_319,11.94,-0.56,0,0  
1QZN,ASP\_44,3.06,0.49,-1.23,0  
1S17,ASP\_38,2.85,0.7,-1.66,0  
3RKV,ARG\_283,13.47,-1.43,0,2.4  
1DOV,ARG\_204,12.01,-0.49,0,0  
1FOV,GLU\_148,4.59,0.21,-0.12,0  
3GV0,GLU\_218,0.56,0.86,-2.4,-2.4  
3EGN,GLU\_476,4.71,0.21,0,0  
3GS3,ASP\_192,2.2,0.7,-2.29,0  
3KV0,GLU\_31,4.5,0,0,0  
2IRM,ARG\_39,12.5,0,0,0  
2CBE,GLU\_205,3.45,0.91,-1.96,0  
3V55,HIS\_584,5.29,1.03,-0.85,-1.39  
4FZR,GLU\_208,3.5,0.14,-1.14,0  
1PSW,GLU\_204,4.57,0.07,0,0  
2V5B,GLU\_27,4.53,0.07,-0.04,0  
2AH5,GLU\_66,4.26,0.14,-0.38,0  
1ZCE,LYS\_22,10.01,-0.49,0,0  
3LD1,ARG\_122,12.01,-0.49,0,0  
2FBQ,HIS\_83,6.5,0,0,0  
3ILC,GLU\_158,4.5,0,0,0  
2H2Z,ARG\_88,12.01,-0.49,0,0  
3JZN,LYS\_83,10.5,0,0,0  
4E5S,GLU\_48,3.86,0.56,-1.2,0  
4H89,GLU\_38,4.5,0,0,0  
2I88,ASP\_450,2.64,0.28,-1.44,0  
3R2E,LYS\_98,10.29,-0.21,0,0  
1AKO,TYR\_56,10.88,0,0,0.88



2B6P,HIS\_66,1.09,0,0,-5.41  
 2Y2T,ARG\_76,12.5,0,0,0  
 3Q1C,HIS\_280,6.91,0.62,0,-0.21  
 2WB8,CYS\_564,10.1,-0.15,0,1.25  
 3HXK,CYS\_165,10.96,-2.58,1.52,3.03  
 3Q9P,ASP\_107,3.87,0.07,0,0  
 3ANJ,TYR\_41,13.5,0.35,0.75,2.4  
 1S17,CYS\_53,9.14,-0.21,0,0.35  
 3U2A,ARG\_92,11.8,-0.7,0,0  
 3GV0,LYS\_232,10.5,0,0,0  
 3V3T,GLU\_189,4.92,0.42,0,0  
 3FRR,LYS\_28,10.5,0,0,0  
 1YLN,LYS\_137,10.5,0,0,0  
 3H13,CYS\_298,9.07,0,0,0.07  
 2V4X,TYR\_10,10,0,0,0  
 1L2F,GLU\_67,4.71,0.21,0,0  
 2RJD,ASP\_491,2.97,0.98,-1.81,0  
 1P4X,ASP\_243,3.99,0.28,-0.09,0  
 3PP8,GLU\_30,4.25,0.21,-0.46,0  
 1YR6,CYS\_143,11.54,0,1.87,0.67  
 1PBV,LYS\_207,9.59,-0.91,0,0  
 2P1W,ASP\_129,3.01,0.42,-1.2,0  
 2CL3,GLU\_88,4.63,0.14,-0.01,0  
 2HRZ,ARG\_233,11.94,-0.56,0,0  
 1P2F,LYS\_206,9.94,-0.56,0,0  
 2IF4,LYS\_134,10.08,-0.42,0,0  
 2OJQ,GLU\_449,4.57,0.07,0,0  
 1XFK,ARG\_272,12.08,-0.42,0,0  
 1V6T,ARG\_148,12.08,-0.42,0,0  
 2GZR,ARG\_152,11.8,-0.7,0,0  
 3H6Q,ASP\_32,4.06,0.28,-0.02,0  
 1Z3X,ARG\_219,11.94,-0.56,0,0  
 1YTD,TYR\_156,8.66,0.22,0,-1.56  
 3DZ1,LYS\_23,10.36,-0.14,0,0  
 2YWX,LYS\_133,10.15,-0.35,0,0  
 3V55,GLU\_652,3.28,0.14,-1.36,0  
 3TOW,HIS\_193,6.43,0,0,-0.07  
 1HF8,CYS\_27,8.97,-0.1,0,0.07  
 2FD5,GLU\_166,4.5,0,0,0  
 1YTQ,GLU\_74,4.5,0,0,0  
 3EVZ,ARG\_79,11.73,-0.77,0,0  
 2HP7,ASP\_85,3.21,0.14,-0.73,0  
 4F3J,HIS\_156,6.36,0,0,-0.14  
 3CAN,ASP\_69,2.58,0.49,-1.71,0  
 4E5S,ARG\_156,11.66,-0.84,0,0  
 3FTT,LYS\_45,10.29,-0.21,0,0  
 1WNH,ASP\_124,1.82,0.91,-2.89,0  
 1G5Z,ASP\_147,3.7,0,-0.1,0  
 3H9W,ASP\_112,3.71,0,-0.09,0  
 3H5T,ASP\_145,3.68,0.14,-0.26,0  
 2EDM,LYS\_174,10.5,0,0,0  
 4ACJ,LYS\_745,10.29,-0.21,0,0  
 2OEW,LYS\_110,10.5,0,0,0  
 2AZL,TYR\_100,13.27,0.07,0.8,2.4  
 3F1X,ASP\_15,3.78,0.14,-0.16,0  
 4DEZ,ARG\_21,12.22,-0.28,0,0  
 2B0J,ASP\_319,3.66,0.63,-0.78,0  
 3FK5,GLU\_24,4.04,0.21,-0.67,0  
 1DZF,LYS\_103,10.5,0,0,0  
 3P51,ASP\_135,2.48,0.7,-2.02,0  
 1TUL,ASP\_10,3.73,0.14,-0.21,0  
 3CRM,ARG\_287,11.87,-0.63,0,0  
 3CBN,TYR\_102,9.78,0,-0.22,0  
 1PV5,GLU\_151,2.19,2.08,-1.99,-2.4  
 1MIX,GLU\_384,4.57,0.07,0,0  
 2B61,TYR\_219,13.62,2.55,0.07,1  
 1G5Z,LYS\_174,10.5,0,0,0  
 3G9T,HIS\_137,6.5,0,0,0  
 3H04,ARG\_242,11.87,-0.63,0,0  
 2IQT,GLU\_196,4.76,0.49,-0.23,0  
 3H9W,GLU\_87,4.47,0.07,-0.1,0  
 3OAA,ARG\_25,12.15,-0.35,0,0  
 2CE6,ARG\_1,12.01,-0.49,0,0  
 2HRZ,LYS\_101,10.36,-0.14,0,0  
 3C6B,ASP\_97,2.08,1.05,-2.78,0  
 3UPD,LYS\_293,10.15,-0.35,0,0  
 1YDL,ASP\_13,3.24,0.35,-0.91,0  
 2YWX,GLU\_113,4.39,0.14,-0.25,0  
 1PV7,GLU\_3,4.5,0,0,0  
 1U53,LYS\_167,10.43,-0.07,0,0  
 4DBX,LYS\_275,9.8,-0.7,0,0  
 3FRR,TYR\_132,13.04,0.83,-0.19,2.4  
 2Z0M,GLU\_329,4.5,0,0,0  
 3BWT,ARG\_579,12.43,-0.07,0,0  
 3AAZ,GLU\_83,3.18,0.28,-1.6,0  
 2J8A,TYR\_296,12.46,1.01,0,1.45  
 2AHE,LYS\_150,10.43,-0.07,0,0  
 2A4D,GLU\_94,2.58,2.04,-2.57,-1.39  
 2Q13,GLU\_358,6.04,0.07,0,1.47  
 2E3C,ARG\_439,12.7,-1.38,0,1.58  
 2AD1,ASP\_287,3.83,0.21,-0.18,0  
 2F4Q,ARG\_129,11.24,-1.26,0,0  
 2QVT,HIS\_88,6.15,0,0,-0.35  
 1LTU,ARG\_15,11.94,-0.56,0,0  
 2GZQ,TYR\_158,10,0,0,0  
 3RNV,GLU\_363,3.77,0.07,-0.8,0  
 2QVT,GLU\_62,4.5,0,0,0  
 1D7O,GLU\_176,4.78,0.28,0,0  
 2FZ4,LYS\_169,10.08,-0.42,0,0  
 3OIP,HIS\_119,2.7,0,0,-3.8  
 2BDV,ASP\_142,2.51,0.77,-2.05,0  
 3NR5,GLU\_30,2.46,1.95,-2.38,-1.6  
 1AD6,CYS\_553,9.3,-0.41,-0.45,1.16  
 1LFP,ARG\_21,12.08,-0.42,0,0  
 1XKR,LYS\_173,9.87,-0.63,0,0  
 3GOZ,LYS\_314,10.5,0,0,0  
 2GZR,ARG\_182,12.13,-0.37,0,0  
 4DIU,LYS\_41,10.5,0,0,0  
 2E3S,GLU\_397,4.71,0.21,0,0  
 1R29,LYS\_126,10.5,0,0,0  
 2F9F,GLU\_106,5.03,1.33,-0.8,0  
 1WXQ,ASP\_77,3.49,0.49,-0.8,0  
 2FZP,ASP\_299,3.64,0.21,-0.37,0  
 2Q07,ASP\_379,3.65,0,-0.15,0  
 1S17,ASP\_314,2.41,0.7,-2.09,0  
 2RH3,ASP\_171,2.76,0.91,-1.95,0  
 2J8A,CYS\_326,7.62,-2.1,0.0,72  
 3GEC,GLU\_336,4.24,0.35,-0.61,0  
 3UPD,CYS\_227,7.75,-0.73,-2.12,1.6  
 4FZN,GLU\_15,3.23,0.21,-1.49,0  
 3IBT,GLU\_155,2.61,0.77,-2.66,0  
 2E3C,TYR\_447,10,0,0,0  
 1WLY,CYS\_288,3.8,-3.6,-2.4,0.8  
 1L2F,GLU\_14,4.71,0.21,0,0  
 1AK1,HIS\_65,6.5,0,0,0  
 2Q5X,CYS\_743,7.86,-1.14,0,0  
 4FZN,ASP\_28,3.94,0.14,0,0  
 2V1L,GLU\_89,4.5,0,0,0  
 1DOV,GLU\_89,4.0,28,-0.78,0  
 3V55,ARG\_392,11.7,-0.8,0,0  
 2HXB,ASP\_109,2.2,0.56,-2.16,0  
 2Q13,LYS\_360,10.5,0,0,0  
 1QYI,TYR\_191,12.77,0.62,-0.09,2.23  
 4E8B,ASP\_23,3.37,0.21,-0.64,0  
 3CNU,LYS\_90,10.43,-0.07,0,0  
 3AU3,GLU\_574,4.57,0.07,0,0  
 3IV4,ARG\_91,12.15,-0.35,0,0  
 3IVF,GLU\_187,2.36,0.2,-0.07,-2.27  
 3EZ7,GLU\_107,4.57,0.07,0,0  
 3AU3,GLU\_650,4.14,0.35,-0.71,0  
 2FL7,ARG\_210,11.59,-0.91,0,0  
 4FZR,CYS\_301,11.16,-0.27,0.2,43  
 3I0C,GLU\_297,4.26,0.56,-0.8,0  
 3BCY,ARG\_82,12.5,0,0,0  
 2Q07,LYS\_457,10.5,0,0,0  
 3I0O,LYS\_301,10.5,0,0,0  
 3I0C,HIS\_313,7.03,0.6,0,-0.07  
 3TOW,ASP\_48,3.87,0.07,0,0  
 4ANN,TYR\_57,11.72,0.07,0,1.65  
 2IF4,ARG\_269,11.23,-1.94,0,0.67  
 3LD1,ARG\_103,12.22,-0.28,0,0  
 1ZYL,CYS\_202,13.29,0.15,2.79  
 3D9H,HIS\_48,6.36,0,0,-0.14  
 2ZCX,GLU\_206,4.64,0.14,0,0  
 1H09,ASP\_133,4.03,0.28,-0.05,0  
 1R3D,HIS\_7,4.15,0.05,0,-2.4  
 1PV5,LYS\_24,10.43,-0.07,0,0  
 2QHT,TYR\_117,13.19,0.14,0.65,2.4  
 1TXJ,ASP\_22,3.29,0.35,-0.86,0  
 1S17,LYS\_64,10.29,-0.21,0,0  
 1TLV,LYS\_88,9.94,-0.56,0,0  
 1IDK,ASP\_37,2.69,0.98,-2.1,0  
 1SJ8,GLU\_738,3.98,0.28,-0.8,0  
 1J74,TYR\_58,10.93,1.02,-0.19,0.09  
 2POY,ARG\_297,12.29,-0.21,0,0  
 2QOP,GLU\_176,4.3,0.28,-0.48,0  
 3RKV,ASP\_222,3.8,0,0,0  
 2EVI,TYR\_161,9.48,0.28,-0.8,0  
 3EYE,LYS\_68,10.29,-0.21,0,0  
 3DHN,LYS\_6,10.5,0,0,0  
 3Q1C,GLU\_113,4.05,0.35,-0.8,0  
 2FD5,GLU\_140,3.3,0.49,-1.69,0  
 3L3P,HIS\_279,6.5,0,0,0  
 3MTT,LYS\_456,10.29,-0.21,0,0  
 2CL3,GLU\_154,4.71,0.21,0,0  
 1NR1,GLU\_117,4.57,0.14,-0.07,0  
 4E9E,LYS\_472,10.5,0,0,0  
 3BPV,GLU\_45,3.83,0.42,-1.09,0  
 3L7H,HIS\_26,6.55,0.05,0,0  
 2F8H,GLU\_10,4.57,0.07,0,0  
 3GOZ,GLU\_215,3.39,0.49,-1.61,0  
 2EJX,ASP\_13,2.18,0.42,-2.04,0  
 1O17,ASP\_180,3.17,0.21,-0.84,0  
 2PLQ,ARG\_188,10.02,-3.66,0.1,18  
 3MTT,ARG\_531,12.43,-0.07,0,0  
 2CYG,TYR\_33,11.25,1.25,0,0  
 4F85,TYR\_55,10.44,0.65,-0.21,0  
 3LJ1,ASP\_170,2.5,0.42,-1.72,0  
 1R3F,ASP\_71,4.07,0.28,-0.01,0  
 1CHD,CYS\_309,9.26,-0.04,0,0.3  
 2PPN,HIS\_94,6.43,0,0,-0.07  
 3EYE,GLU\_154,3.91,0.21,-0.8,0  
 3VHJ,LYS\_111,10.5,0,0,0  
 2NYC,ASP\_300,3.59,0,-0.21,0  
 3CAX,TYR\_190,11.6,1.3,-0.04,0.35  
 2OBS,TYR\_136,10.45,0,0,0.45  
 1R6Y,ARG\_11,12.29,-0.21,0,0  
 3LOD,ARG\_53,11.87,-0.63,0,0  
 3NJM,LYS\_92,10.43,-0.07,0,0  
 3V55,ASP\_634,3.81,0.28,-0.27,0  
 2CN1,GLU\_162,3.41,0.42,-1.51,0  
 2Q12,ASP\_141,3.88,0.14,-0.06,0  
 2R2Y,ASP\_117,1.96,0.7,-2.54,0  
 1XKR,GLU\_57,4.5,0,0,0  
 2FC3,LYS\_49,10.22,-0.28,0,0  
 1TXJ,ASP\_108,3.41,0.21,-0.6,0  
 3L3P,GLU\_477,4.57,0.07,0,0  
 1O5J,GLU\_59,4.64,0.14,0,0  
 2D7U,ARG\_315,12.22,-0.28,0,0  
 1BKR,LYS\_56,10.36,-0.14,0,0  
 3CAX,ARG\_224,11.87,-0.63,0,0  
 3R0E,LYS\_162,10.22,-0.28,0,0  
 3Q9P,HIS\_103,6.5,0,0,0  
 1EW4,LYS\_48,10.5,0,0,0  
 2O4D,HIS\_105,6.5,0,0,0  
 1Q46,CYS\_114,9.38,-0.23,0.61  
 1WOU,TYR\_76,9.51,0,-1.93,1.44  
 1WJG,ASP\_101,2.09,0.56,-2.27,0  
 3PM2,ASP\_2,3.71,0,-0.09,0  
 2G2D,ASP\_30,2.46,0.56,-1.88,0  
 3RFF,LYS\_41,10.43,-0.07,0,0  
 3RFY,LYS\_329,10.22,-0.28,0,0  
 1RI6,ASP\_160,3.08,0.21,-0.93,0  
 2D59,ASP\_93,12.03,0.56,-0.34,0  
 3CGW,ARG\_93,11.94,-0.56,0,0  
 2F4Q,ARG\_44,12.08,-0.42,0,0  
 2FG1,ARG\_51,11.73,-0.77,0,0  
 3NR5,ASP\_98,3.87,0.07,0,0  
 3ILC,HIS\_177,7.09,0.8,0,-0.21  
 2B9V,TYR\_59,10.88,2.06,-1.18,0  
 2Q99,ARG\_270,10.73,-1.77,0,0  
 3F1X,TYR\_43,13.49,0.05,3.44  
 2POL,GLU\_98,3.83,0.35,-1.02,0  
 2PLQ,HIS\_275,4.08,0.2,0,-2.62  
 3IVF,ASP\_375,3.87,0.07,0,0  
 2A6B,LYS\_120,10.29,-0.21,0,0  
 1J7G,ASP\_84,2.79,0.28,-1.29,0  
 3F7M,ARG\_355,12.08,-0.42,0,0  
 2X4G,ARG\_213,13.32,-1.58,0.2,4  
 2OEW,LYS\_81,9.73,-0.77,0,0  
 2EFK,GLU\_79,3.54,0.42,-1.38,0  
 2B78,LYS\_120,10.15,-0.35,0,0  
 3ON1,ARG\_93,12.15,-0.35,0,0  
 3BB7,GLU\_348,2.04,0.61,-1.6,-1.47  
 1A8Q,CYS\_3,9.27,0.1,0.0,17  
 3CS1,ARG\_35,11.8,-0.7,0,0  
 3H04,LYS\_198,10.22,-0.28,0,0  
 3K1H,LYS\_55,10.22,-0.28,0,0  
 2Q34,LYS\_208,10.5,0,0,0  
 3GV0,ARG\_306,11.66,-0.84,0,0  
 1G8P,GLU\_214,4.71,0.21,0,0  
 3NBI,LYS\_21,10.5,0,0,0  
 4EVF,TYR\_46,9.34,0.14,-0.8,0  
 3NR5,CYS\_86,9.07,0,0.07  
 3R2E,ASP\_55,3.38,0.14,-0.55,0  
 3BJV,ASP\_126,3.87,0.07,0,0  
 3M66,HIS\_366,3.23,0,0,-3.27  
 3M66,ASP\_219,2.95,0.63,-1.48,0  
 2CWC,ARG\_283,11.8,-0.7,0,0  
 4FZN,LYS\_240,4.05,0.35,-0.8,0  
 3V3T,ARG\_62,13.07,-1.54,0.2,12  
 3BPP,LYS\_227,10.5,0,0,0  
 3JZN,ARG\_302,12.15,-0.35,0,0  
 1NFN,GLU\_27,4.85,0.35,0,0  
 1MML,TYR\_268,11.59,1.38,-0.17,0.38  
 2E3C,GLU\_240,4.05,0.35,-0.8,0  
 2RJD,LYS\_426,10.36,-0.14,0,0  
 1NKD,ARG\_13,11.94,-0.56,0,0  
 3HQX,GLU\_76,4.64,0.14,0,0  
 3O7K,GLU\_127,4.12,0.42,-0.8,0  
 2QV2,GLU\_178,2.48,2.15,-1.77,-2.4  
 2RFA,CYS\_213,8.74,-0.4,0.0,14  
 1PVT,GLU\_89,4.71,0.21,0,0  
 3JRT,LYS\_128,10.36,-0.14,0,0  
 1XKR,LYS\_2,10.5,0,0,0  
 1O5J,GLU\_67,4.64,0.14,0,0

2FXT,GLU\_350,4.5,0,0,0  
 3OBS,LYS\_9,9.87,-0.63,0,0  
 1RAJ,LYS\_314,10.5,0,0,0  
 3ERF,LYS\_158,10.36,-0.14,0,0  
 1J8B,ARG\_83,12.08,-0.42,0,0  
 3ADO,LYS\_188,10.5,0,0,0  
 1YG2,TYR\_69,10,0,0,0  
 4D8L,ASP\_138,2.79,0.21,-1.22,0  
 2F8H,HIS\_165,0.76,0.43,0,-6.17  
 3M9A,CYS\_66,9,0,0,0  
 1D2K,LYS\_384,9.94,-0.56,0,0  
 1AD6,TYR\_424,9.78,0.07,-0.29,0  
 1JT9,LYS\_14,10.5,0,0,0  
 4EKU,GLU\_207,4.57,0.07,0,0  
 1UXO,ASP\_35,2.62,0.42,-1.6,0  
 3LPZ,ASP\_174,2.44,0.49,-1.85,0  
 1RHS,LYS\_235,10.7,0,0.18,1.4,0  
 2P4D,ASP\_17,4.08,0.28,0,0  
 3GMS,LYS\_178,10.43,-0.07,0,0  
 3RLN,CYS\_637,9,0,0,0  
 3LJC,GLU\_108,4.66,0.21,-0.05,0  
 3M3P,ASP\_77,3.88,0.14,-0.06,0  
 4E8B,CYS\_139,10.7,0,0.18,1.53  
 3EVN,GLU\_322,4.41,0.07,-0.16,0  
 3CSV,GLU\_61,4.5,0,0,0  
 3HVM,TYR\_330,12.54,2.49,-0.93,0.98  
 3CAN,ASP\_95,3.22,0.14,-0.72,0  
 3FRR,LYS\_35,10.5,0,0,0  
 1GPP,ARG\_87,11.45,-1.05,0,0  
 2FD5,ARG\_93,12.5,0,0,0  
 1XIP,ASP\_318,3.87,0.28,-0.21,0  
 1XTZ,LYS\_174,10.36,-0.14,0,0  
 1L3K,LYS\_145,10.01,-0.49,0,0  
 1KCM,HIS\_215,3.67,0.87,0,-3.7  
 3ASA,GLU\_318,3.91,0.21,-0.8,0  
 1GVPL,LYS\_7,10.22,-0.28,0,0  
 2FI9,ARG\_88,11.66,-0.84,0,0  
 3ZRI,HIS\_147,6.36,0,0,-0.14  
 3HYQ,LYS\_145,10.36,-0.14,0,0  
 1WRU,TYR\_32,13.43,0.23,0.8,2.4  
 2D7U,GLU\_314,4.64,0.14,0,0  
 3M7G,ASP\_201,2.94,0.35,-1.21,0  
 2AD1,TYR\_227,12.31,0,0.39,1.92  
 3HVM,GLU\_62,4.71,0.21,0,0  
 3IRA,GLU\_146,3.98,0.28,-0.8,0  
 1YR6,ASP\_96,0.98,0.77,-3.6,0  
 3BJV,LYS\_95,10.15,-0.35,0,0  
 3EVN,ARG\_269,12.08,-0.42,0,0  
 1JB3,ARG\_9,12.29,-0.21,0,0  
 3IL3,LYS\_133,10.29,-0.21,0,0  
 3ADO,GLU\_69,2.61,0.42,-2.31,0  
 1D2K,LYS\_148,10.08,-0.42,0,0  
 3R2E,LYS\_27,10.43,-0.07,0,0  
 3BPV,HIS\_43,6.5,0,0,0  
 1WLY,LYS\_287,10.29,-0.21,0,0  
 1WRU,ARG\_201,12.29,-0.21,0,0  
 3GMS,ARG\_185,12.29,-0.21,0,0  
 2RFA,HIS\_264,6.68,0.18,0,0  
 2QRX,LYS\_39,10.5,0,0,0  
 3P28,GLU\_47,4.22,0.14,-0.42,0  
 1TJE,ASP\_133,3.07,0.07,-0.8,0  
 2CWC,ARG\_111,11.8,-0.7,0,0  
 1YLN,ARG\_169,12.22,-0.28,0,0  
 1Q5Z,ASP\_652,2.042,-2.22,0  
 2CVG,TYR\_182,9.99,0,-0.01,0  
 1WNH,TYR\_107,12.06,0.21,0,1.85  
 1RHS,GLU\_62,4.78,0.28,0,0  
 1UOH,ASP\_71,3.92,0.42,-0.3,0  
 3PAC,ARG\_179,12.43,-0.07,0,0  
 4GCO,TYR\_153,10,0,0,0  
 3I47,GLU\_80,3.27,0.42,-1.65,0  
 2RIK,ARG\_43,12.01,-0.49,0,0  
 3AU3,ARG\_399,12.36,-0.14,0,0  
 3FK5,HIS\_18,7.16,0.8,0,-0.14  
 2Z84,GLU\_187,4.5,0,0,0  
 3NR5,TYR\_141,12.3,0.51,0,1.79  
 3MEW,GLU\_265,4.17,0.42,-0.75,0  
 2OBI,CYS\_148,9,0,0,0  
 2B61,TYR\_329,12.01,0,-0.23,2.25  
 1PGV,GLU\_352,4.25,0.07,-0.32,0  
 2NRK,HIS\_98,3.9,0.14,-2.74  
 2CXC,TYR\_27,9.67,0,-0.32,0  
 3ETU,GLU\_118,4.64,0.14,0,0  
 2V81,GLU\_160,4.34,0.42,-0.58,0  
 4EF5,TYR\_199,12.19,1.33,-0.33,1.2  
 2FBI,TYR\_52,10,0,0,0  
 2B0J,ARG\_136,11.66,-0.84,0,0  
 1Y0K,LYS\_26,10.08,-0.42,0,0  
 3JRT,LYS\_118,10.5,0,0,0  
 3ZXY,HIS\_177,6.5,0,0,0  
 1OTM,ASP\_68,2.79,0.63,-1.64,0  
 2OJQ,ARG\_566,11.36,-1.14,0,0  
 3R87,TYR\_13,10,0,0,0  
 3N2T,TYR\_197,12.82,0.42,0.2,4  
 3GOZ,LYS\_182,9.87,-0.63,0,0  
 1ANU,ASP\_53,3.37,0.14,-0.57,0  
 1Q2Y,GLU\_20,3.97,0.14,-0.67,0  
 1X04,ASP\_30,2.12,0.63,-2.31,0  
 3CJW,GLU\_346,2.59,0.49,-2.4,0  
 2WB3,TYR\_375,10,0,0,0  
 1PGV,GLU\_252,4.5,0,0,0  
 2OGQ,ASP\_554,1.41,1.33,-3.72,0  
 1QYI,HIS\_98,6.76,0.33,0,-0.07  
 2IF4,LYS\_292,10.5,0,0,0  
 4EUG,GLU\_112,3.84,0.14,-0.8,0  
 2OSA,GLU\_410,4.5,0,0,0  
 3FTT,ARG\_121,11.94,-0.56,0,0  
 1SUU,GLU\_506,4.5,0,0,0  
 3EVP,LYS\_210,10.5,0,0,0  
 4FH3,LYS\_227,10.43,-0.07,0,0  
 1YMS,LYS\_96,10.5,0,0,0  
 1YB2,ARG\_148,12.22,-0.28,0,0  
 1XWM,GLU\_32,4.57,0.07,0,0  
 3RFY,ARG\_119,12.91,-1.73,0.2,15  
 3U4K,ARG\_105,12.5,-1.45,0.1,45  
 4DIU,ASP\_245,3.74,0,-0.06,0  
 3F5D,TYR\_180,10,0,0,0  
 2RH3,TYR\_139,10.63,1.28,-0.65,0  
 4EZB,ASP\_57,3.87,0.14,-0.07,0  
 2E0T,ARG\_98,12.43,-0.07,0,0  
 1KN3,HIS\_145,6.36,0,0,-0.14  
 2AZP,TYR\_231,9.91,0.14,-0.23,0  
 1FO9,TYR\_204,10.07,0.07,0,0  
 1J7G,LYS\_25,10.22,-0.28,0,0  
 2CXC,LYS\_120,10.5,0,0,0  
 4FH3,ARG\_184,13.86,-1.04,0.2,4  
 2IF4,GLU\_49,4.44,0,-0.06,0  
 3GA2,GLU\_51,4.5,0,0,0  
 2YT4,HIS\_687,6.37,0.01,0,-0.14  
 2E3C,LYS\_375,10.5,0,0,0  
 3CAN,ARG\_56,11.87,-0.63,0,0  
 3BWT,GLU\_627,3.68,0.21,-1.03,0  
 3TIR,ARG\_185,11.66,-0.84,0,0  
 2V4X,ARG\_79,12.01,-0.49,0,0  
 1T3Y,ARG\_57,11.45,-1.05,0,0  
 3DSH,ARG\_399,12.08,-0.42,0,0  
 2YWJ,ARG\_129,12.36,-0.21,0,0.07  
 3HUE,ASP\_200,3.33,0.42,-0.89,0  
 4HDE,GLU\_89,4.5,0,0,0  
 1YDL,GLU\_48,3.56,0.28,-1.22,0  
 1ILW,GLU\_97,4.57,0.07,0,0  
 1ZHV,HIS\_130,6.99,0.49,0,0  
 2D59,LYS\_99,10.5,0,0,0  
 1XTD,ASP\_110,3.12,0.49,-1.17,0  
 2IIA,TYR\_50,10,0,0,0  
 3Q6L,ARG\_131,11.94,-0.56,0,0  
 2QK1,LYS\_437,10.36,-0.14,0,0  
 2H01,GLU\_9,3.99,0.14,-0.65,0  
 3DSH,ASP\_395,2.17,0.77,-2.39,0  
 2RIS,GLU\_171,3.63,0.28,-1.16,0  
 2PGX,ARG\_146,11.45,-1.05,0,0  
 2IF4,ARG\_181,12.15,-1.69,0,1.34  
 3CCY,GLU\_130,4.61,0.14,-0.03,0  
 2VGM,GLU\_280,3.82,1.8,-1.3,-1.17  
 1ZBS,ARG\_61,11.8,-0.7,0,0  
 1C44,LYS\_110,10.43,-0.07,0,0  
 2WOZ,CYS\_593,10.64,-0.98,0.2,62  
 4H86,LYS\_124,10.36,-0.14,0,0  
 1O17,ARG\_106,12.29,-0.21,0,0  
 3DSH,GLU\_391,4.21,0.88,-1.17,0  
 2V5B,GLU\_245,4.57,0.07,0,0  
 3M66,ASP\_259,3.21,0.21,-0.8,0  
 1YB2,GLU\_14,4.5,0,0,0  
 2EJX,ARG\_71,12.15,-0.35,0,0  
 2B2H,TYR\_59,12.11,0.59,0.1,52  
 3LH5,ASP\_517,3.55,0,-0.25,0  
 2NSN,ARG\_101,12.5,0,0,0  
 3ZRI,HIS\_-7,6.29,0,0,-0.21  
 1WLY,GLU\_281,3.08,0.56,-1.98,0  
 2HNG,ASP\_81,3.21,0.21,-0.8,0  
 3CX2,TYR\_220,10,0,0,0  
 2IF4,GLU\_58,4.2,0.14,-0.44,0  
 3Q1C,GLU\_118,4.74,0.42,-0.18,0  
 4ECC,LYS\_132,10.36,-0.14,0,0  
 3M66,ASP\_187,2.64,0.84,-2,0  
 3ZSL,ARG\_144,12.04,-0.46,0,0  
 3LD1,LYS\_32,10.36,-0.14,0,0  
 2CBE,HIS\_94,0.75,0.8,-1.27,-5.28  
 1MHN,LYS\_119,10.5,0,0,0  
 2OSA,GLU\_392,1.77,0.35,-3.08,0  
 3LQE,GLU\_336,3.86,0.28,-0.92,0  
 2QEV,LYS\_56,10.08,-0.42,0,0  
 3GA2,HIS\_7,3.7,0,0,-2.8  
 1NIJ,GLU\_250,4.5,0,0,0  
 3ADO,LYS\_286,10.5,0,0,0  
 3P51,TYR\_89,11.62,0,0,1.62  
 1ZHV,HIS\_104,9.56,3.65,1.85,-2.44  
 1Q8B,GLU\_40,4.48,0,-0.02,0  
 1WXF,ARG\_249,12.36,-0.14,0,0  
 2AZL,HIS\_118,6.36,0,0,-0.14  
 1TO7,GLU\_28,4.5,0,0,0  
 3C2E,TYR\_275,8.42,0.21,-2.65,0.86  
 1YMS,LYS\_269,10.5,0,0,0  
 3IRA,ASP\_154,3.35,0.35,-0.8,0  
 1Q42,ASP\_153,3.24,0.42,-0.98,0  
 1MUF,GLU\_90,4.88,0.35,0.03,0  
 2PLQ,TYR\_214,10.71,1.62,-0.92,0  
 1G8PLYS\_248,10.36,-0.14,0,0  
 3E7P,ARG\_132,11.94,-0.56,0,0  
 1YDL,ASP\_37,2.86,0.35,-1.29,0  
 3F7M,ARG\_293,11.8,-0.7,0,0  
 2OKT,ARG\_317,11.66,-0.84,0,0  
 3M7D,ARG\_252,11.94,-0.56,0,0  
 4FCU,ASP\_25,3.8,0,0,0  
 2R57,ASP\_176,3.03,0.28,-1.05,0  
 2V1L,CYS\_93,6.18,-3.45,0.25,0.38  
 3GV0,HIS\_200,4.61,0.84,-0.21,-2.52  
 2H30,LYS\_57,10.36,-0.14,0,0  
 3FRR,HIS\_150,6.5,0,0,0  
 2J8A,LYS\_356,10.5,0,0,0  
 1EYH,HIS\_73,7.41,1.12,0,-0.21  
 3F1X,ARG\_109,12.15,-0.35,0,0  
 2DG7,ARG\_182,12.01,-0.49,0,0  
 2QHT,HIS\_151,2.05,0,-0.13,-4.32  
 3ZSL,GLU\_165,1.75,0.42,-3.17,0  
 3HUE,ASP\_261,3.94,0.14,0,0  
 3EAZ,GLU\_127,4.64,0.14,0,0  
 2RIS,ARG\_142,11.94,-0.56,0,0  
 1J7G,TYR\_52,10,0,0,0  
 3V4G,GLU\_39,4.5,0,0,0  
 2B78,GLU\_11,4.02,0.21,-0.69,0  
 3JRT,HIS\_109,6.29,0,0,-0.21  
 2POL,ASP\_185,3.12,0.35,-1.02,0  
 2D2S,ASP\_699,4.11,0.42,-0.18,0  
 2P5D,LYS\_121,9.59,-0.91,0,0  
 2Q12,TYR\_203,9.98,0,-0.02,0  
 2CN1,GLU\_94,3.06,0.56,-2,0  
 2FPN,TYR\_67,12.06,0,0.2,06  
 1R1S,GLU\_89,3.84,0.14,-0.8,0  
 4DIU,GLU\_145,4.5,0,0,0  
 1L2H,TYR\_121,13.23,0,0.3,23  
 1SJ8,GLU\_632,4.48,0.7,-0.73,0  
 4F85,LYS\_221,10.43,-0.07,0,0  
 1WNH,ASP\_173,2.54,0.84,-2.09,0  
 2VAN,TYR\_327,9.63,0.26,-0.14,-0.5  
 3G9G,LYS\_33,10.08,-0.42,0,0  
 1DVO,ASP\_74,3.6,0.21,-0.41,0  
 3CO1,LYS\_100,10.01,-0.49,0,0  
 1P2F,ASP\_185,2.8,0.49,-1.49,0  
 3CXS,GLU\_69,3.73,0.56,-1.33,0  
 3M66,GLU\_174,4.5,0,0,0  
 3RLE,HIS\_114,4.62,0.7,-2.58  
 3OOP,ARG\_25,12.01,-0.49,0,0  
 3F1X,ARG\_297,12.5,0,0,0  
 2JEO,TYR\_187,8.32,0.01,-0.22,-1.47  
 2B6P,LYS\_259,10.5,0,0,0  
 1OIS,GLU\_350,1.67,1.05,-3.87,0  
 1E59,ARG\_59,12.29,-0.21,0,0  
 2WB8,TYR\_464,11.9,0.09,0.1,81  
 2P52,TYR\_217,10.09,0.09,0,0  
 2AZP,ARG\_260,12.5,0,0,0  
 1YLN,GLU\_159,4.05,0.35,-0.8,0  
 1PNE,HIS\_133,6.5,0,0,0  
 2V4U,ARG\_508,12.83,-1.27,0,1.61  
 1ZP2,GLU\_102,4.2,0.35,-0.65,0  
 3VJ8,LYS\_242,10.22,-0.28,0,0  
 1KN3,HIS\_118,7.38,2.49,2.9,-4.5  
 1ZBS,ARG\_46,12.15,-0.35,0,0  
 3IVF,TYR\_395,9.97,0,-0.03,0  
 2B3M,GLU\_50,3.55,0.07,-1.02,0  
 1WOU,GLU\_117,4.78,0.28,0,0  
 2OKT,HIS\_341,6.37,0.01,0,-0.14  
 4FH3,ARG\_359,12.01,-0.49,0,0  
 2F4Q,ARG\_323,12.29,-0.21,0,0  
 3L0D,TYR\_2,10.14,0.14,0,0  
 3K8J,ASP\_77,3.87,0.14,-0.07,0  
 2QV2,TYR\_257,10,0,0,0  
 1NJ4,ASP\_218,3.75,0,-0.05,0  
 3H5T,TYR\_9,10,0,0,0  
 3T8R,LYS\_19,10.29,-0.21,0,0  
 2DG7,ARG\_41,12.22,-0.28,0,0  
 1IDK,HIS\_259,6.79,1.61,93,-3.24  
 3M16,LYS\_151,10.5,0,0,0  
 1SUU,ASP\_545,2.18,1.12,-2.75,0  
 2RJD,GLU\_297,4.5,0,0,0  
 3BA1,ARG\_47,11.87,-0.63,0,0

3MTT,ARG\_547,12.08,-0.42,0,0  
1OST,ARG\_417,11.94,-0.56,0,0  
2E3C,ASP\_281,3.94,0.14,0,0  
2X4L,TYR\_248,10.74,0.56,0,0.18  
2Q07,LYS\_270,10.43,-0.07,0,0  
1P6F,ASP\_49,3.98,0.21,-0.03,0  
3CJW,GLU\_214,4.5,0,0,0  
1RHS,GLU\_226,4.5,0,0,0  
2OEW,LYS\_23,10.5,0,0,0  
2A4D,GLU\_215,4.85,0.35,0,0  
2FM9,HIS\_193,6.41,0.05,0,-0.14  
1XDZ,TYR\_29,10.2,0.14,-0.22,0.28  
2OSA,GLU\_416,4.5,0,0,0  
3G53,HIS\_238,6.5,0,0,0  
2ROS,LYS\_87,10.36,-0.14,0,0  
3CGW,ARG\_76,12.01,-0.49,0,0  
3PU6,ASP\_55,3.4,0.63,-1.02,0  
3HVM,GLU\_226,3.73,0.35,-1.12,0  
2D7U,TYR\_250,10,0,0,0  
2B0J,LYS\_298,10.43,-0.07,0,0  
3F6F,TYR\_177,13.13,0.21,-0.46,3.38  
2HRZ,ARG\_118,11.94,-0.56,0,0  
2Q99,GLU\_81,4.57,0.07,0,0  
3AU3,GLU\_565,4.85,0.35,0,0  
1C44,CYS\_71,9.39,-0.15,0,0.54  
3ETV,GLU\_214,3.51,0.49,-1.48,0  
1LPL,ASP\_220,3.94,0.14,0,0  
3GE9,ARG\_163,12.29,-0.21,0,0  
1V6T,LYS\_159,10.43,-0.07,0,0  
1QQ,GLU\_70,4.5,0,0,0  
3CQ1,GLU\_62,3.74,0.35,-1.11,0  
3ELI,GLU\_118,4.5,0,0,0  
2B6P,ARG\_226,13.46,-1.26,0,2.22  
3K1H,CYS\_86,9.61,-0.05,0,0.66  
1MUF,ASP\_112,3.98,0.21,-0.03,0  
3PZ9,ASP\_204,0.75,0.84,-3.9,0  
2FPN,GLU\_176,4.13,0.21,-0.58,0  
3B7X,GLU\_138,3.98,0.28,-0.8,0  
1MML,TYR\_64,10,0,0,0  
3GA2,LYS\_151,10.43,-0.07,0,0  
2BT8,ASP\_178,2.89,0.91,-1.83,0  
2B78,LYS\_84,10.29,-0.21,0,0  
1J33,ARG\_21,12.5,0,0,0  
1D2K,LYS\_348,10.36,-0.14,0,0  
3ELI,HIS\_128,2.23,0,-1.37,-2.9  
2C13,CYS\_73,6.2,-2.58,-1.28,1.07  
1FKM,TYR\_440,12.4,2.13,0,0.27  
1EV8,ARG\_127,12.5,0,0,0  
2CW4,TYR\_98,10,0,0,0  
3M7D,ARG\_270,12.5,0,0,0  
3FXH,CYS\_18,9.06,-0.01,0,0.07  
1P4X,GLU\_89,4.5,0,0,0  
4EKU,LYS\_169,10.43,-0.07,0,0  
1AK1,ASP\_237,3.82,0.14,-0.12,0  
3LJN,LYS\_92,10.5,0,0,0  
1WYC,GLU\_78,4.71,0.21,0,0  
1P4X,ASP\_31,3.86,0.07,-0.01,0  
3HZQ,LYS\_11,10.5,0,0,0  
1GPP,ARG\_91,11.87,-0.63,0,0  
3HVM,LYS\_10,10.5,0,0,0  
3N2T,TYR\_208,11.12,1.12,0,0  
1OST,ARG\_119,11.59,-0.91,0,0  
3RLE,ARG\_174,11.59,-0.91,0,0  
1ZBS,HIS\_282,6.67,0.24,0,-0.07  
2H2W,ARG\_171,12.01,-0.49,0,0  
4FLE,HIS\_30,6.22,0,0,-0.28  
3CAN,HIS\_20,6.44,0.01,0,-0.07  
2FL7,LYS\_183,10.5,0,0,0  
3PAC,LYS\_41,10.29,-0.21,0,0  
2PP6,LYS\_85,10.01,-0.49,0,0  
1MUF,ARG\_320,12.86,-1.17,0,1.53  
1U53,LYS\_94,10.36,-0.14,0,0  
2I88,ASP\_423,3.18,0.49,-1.11,0  
2F8H,HIS\_272,7.23,0.8,0,-0.07  
2JEO,GLU\_138,3.07,2.51,-1.54,-2.4  
3LH5,HIS\_766,5.96,0.86,0,-1.4  
2AZL,ARG\_130,11.87,-0.63,0,0  
1PZC,LYS\_109,10.43,-0.07,0,0  
2I6I,LYS\_48,10.29,-0.21,0,0  
3UX2,GLU\_60,4.5,0,0,0  
1WRU,GLU\_337,4.52,0.07,-0.05,0  
2D7U,GLU\_176,3.31,4.42,-3.24,-2.37  
1NIJ,GLU\_74,4.64,0.28,-0.14,0  
1ILW,TYR\_132,10.75,0,0,0.75  
1UJ8,HIS\_9,7.16,0.8,0,-0.14  
3HYQ,TYR\_104,10,0,0,0  
2RH3,CYS\_192,8.37,-0.87,0,0.24  
1HF8,ASP\_276,4.14,0.49,-0.15,0  
1X91,LYS\_51,10.43,-0.07,0,0  
4DIU,ARG\_36,11.94,-0.56,0,0  
4DBX,TYR\_240,12.13,1.92,0,0.21  
3O48,CYS\_87,10.48,0.18,0,1.29  
2AH5,GLU\_172,4.78,0.28,0,0  
3G9G,ASP\_238,3.41,0.35,-0.74,0  
2BLL,HIS\_363,4.51,0.34,0,-2.33  
1V43,LYS\_330,10.43,-0.07,0,0  
2QHT,TYR\_71,11.82,0,-0.58,2.4  
3F7M,GLU\_278,4.03,0.63,-1.1,0  
3OKQ,GLU\_645,3.98,0.28,-0.8,0  
1RHS,TYR\_83,11.94,1.5,-1.19,1.63  
2FPN,HIS\_161,6.36,0,0,-0.14  
2OEW,ARG\_173,12.5,0,0,0  
1TWU,ARG\_17,12.51,-1.36,0,1.37  
3I0C,ASP\_326,2.92,0.77,-1.65,0  
3C38,ASP\_233,3.67,0.21,-0.34,0  
1O5J,LYS\_24,9.87,-0.63,0,0  
1WYC,ASP\_252,3.71,0,-0.09,0  
2HXB,TYR\_11,11.47,0.21,-0.56,1.82  
3EVZ,LYS\_45,10.29,-0.21,0,0  
4H89,CYS\_107,10.44,0,1.44  
3OA7,GLU\_27,4.57,0.07,0,0  
3BWT,TYR\_775,9.76,0,-0.24,0  
2E3C,ASP\_230,3.28,0.35,-0.87,0  
1AKO,LYS\_218,10.43,-0.07,0,0  
3KB5,LYS\_460,10.5,0,0,0  
1LZL,ASP\_175,2.6,0.49,-1.7,0  
3U2A,LYS\_119,10.36,-0.14,0,0  
3TRE,ARG\_44,12.29,-0.21,0,0  
4H4J,ASP\_232,3.62,0.14,-0.32,0  
2HNG,GLU\_95,3.14,0.63,-1.99,0  
1RAJ,ARG\_306,9.14,-3.71,0,0.35  
1L2F,GLU\_141,4.5,0,0,0  
1AT0,GLU\_361,4.5,0,0,0  
3LE4,ARG\_325,12.43,-0.07,0,0  
1WP5,GLU\_319,4.5,0,0,0  
3CGW,LYS\_154,10.36,-0.14,0,0  
1NIJ,ASP\_47,3.07,0.14,-0.87,0  
1D2K,TYR\_133,9.68,0.05,-0.37,0  
2RIK,LYS\_233,10.5,0,0,0  
1YM5,HIS\_82,5.52,2.18,2.34,-5.51  
2CBE,LYS\_24,10.22,-0.28,0,0  
1NAR,ASP\_119,3.31,0.21,-0.7,0  
4EZB,LYS\_78,10.43,-0.07,0,0  
2O8P,ASP\_214,3.79,0,-0.01,0  
4FCU,TYR\_196,13.35,1.21,-0.12,2.26  
3ASA,LYS\_310,10.22,-0.28,0,0  
1J74,ARG\_11,11.57,-0.98,0,0.05  
3M7G,HIS\_200,4.89,1.6,0.52,-3.73  
3FWU,LYS\_33,10.43,-0.07,0,0  
2P65,GLU\_114,4.5,0,0,0  
4GCO,CYS\_203,9.32,-0.42,0,0.74  
4DVD,ARG\_127,12.5,0,0,0  
2H2Z,ASP\_33,3.85,0.28,-0.22,0  
3CQ1,TYR\_44,11.6,0.07,-0.8,2.33  
1XDZ,ARG\_138,12.53,-1.37,0,1.4  
3H9W,GLU\_115,4.5,0,0,0  
1WLY,GLU\_74,3.32,0.42,-1.6,0  
1RI5,ARG\_259,12.01,-0.49,0,0  
2HXB,GLU\_93,2.37,0.63,-2.76,0  
4H86,ASP\_134,3.94,0.14,0,0  
1XIP,ARG\_274,10.68,-3.84,0,2.02  
3RE9,HIS\_182,4.93,0.73,0,-2.3  
2BQQ,GLU\_120,4.64,0.14,0,0  
1T07,ARG\_36,12.22,-0.28,0,0  
1VAN,HIS\_252,5.28,0.51,0.49,-2.22  
2Q5X,ARG\_825,12.01,-0.49,0,0  
3GA2,CYS\_153,9,0,0,0  
3HUE,ASP\_59,2.16,0.49,-2.14,0  
1YTD,GLU\_309,4.35,0.49,-0.64,0  
4FCU,ARG\_78,10.7,-1.8,0,0  
1X8F,HIS\_67,6.5,0,0,0  
4FLE,TYR\_44,9.8,0.07,-0.83,0.56  
2P1W,ARG\_177,13.14,-1.33,0,1.97  
2H80,HIS\_56,6.5,0,0,0  
2RGY,ARG\_359,11.87,-0.63,0,0  
1U7U,TYR\_280,11.18,0,0,1.18  
1K95,ASP\_132,3.77,1.12,-1.15,0  
2CVB,LYS\_86,10.5,0,0,0  
1ILW,LYS\_159,10.43,-0.07,0,0  
1MTZ,TYR\_44,12.37,4.12,-1.75,0  
1PV5,GLU\_188,4.71,0.21,0,0  
3CNU,TYR\_91,9.96,0.14,-0.18,0  
3BCY,LYS\_97,10.29,-0.21,0,0  
2E3C,LYS\_205,10.5,0,0,0  
1OGL,LYS\_210,10.5,0,0,0  
2I6I,ASP\_124,3.81,0.14,-0.13,0  
3UAH,ARG\_404,12.01,-0.49,0,0  
3G53,LYS\_256,10.5,0,0,0  
4H89,CYS\_107,10.44,0,1.44  
3G53,CYS\_139,8.96,-0.67,0,0.63  
1ZBM,LYS\_169,10.29,-0.21,0,0  
3C01,GLU\_68,4.64,0.14,0,0  
1TLV,TYR\_254,9.7,0.13,-0.43,0  
3MIX,TYR\_558,10,0,0,0  
1XIPL,LYS\_58,10.22,-0.28,0,0  
2OGQ,GLU\_568,4.19,0.49,-0.8,0  
1O6D,HIS\_41,7.17,0.81,0,-0.14  
3JV1,GLU\_99,4.33,0.63,-0.8,0  
3CX5,LYS\_135,10.08,-0.42,0,0  
2RGY,HIS\_203,6.36,0,0,-0.14  
1XAW,LYS\_485,10.36,-0.14,0,0  
1MUF,TYR\_86,10,0,0,0  
3V3T,TYR\_273,10.09,0.14,-0.05,0  
2E3C,LYS\_214,10.5,0,0,0  
1O6D,GLU\_80,3.33,0.28,-1.46,0  
1YW5,GLU\_32,4.64,0.14,0,0  
2B0A,GLU\_108,4.5,0,0,0  
1DUN,CYS\_22,8.94,-0.06,0,0  
1XEU,GLU\_276,4.57,0.07,0,0  
1RI6,ARG\_181,5.78,-4.41,0,-2.32  
3C2E,GLU\_24,4.5,0,0,0  
1ZP2,ASP\_226,3.87,0.07,0,0  
2O8P,ASP\_214,3.79,0,0,0  
2WOZ,ARG\_485,11.48,-2.84,0,1.82  
3M3P,HIS\_88,3.2,0.181,-5.11  
1FHL,ASP\_17,3.87,0.07,0,0  
3FHF,GLU\_8,4.17,0.28,-0.61,0  
4ECC,LYS\_126,10.5,0,0,0  
3H9W,TYR\_99,10.01,0.07,-0.06,0  
3G59,GLU\_234,4.57,0.07,0,0  
3E7Z,ARG\_13,12.29,-0.21,0,0  
3LH5,GLU\_640,4.57,0.07,0,0  
1X7F,LYS\_237,10.29,-0.21,0,0  
3LH5,GLU\_659,4.57,0.07,0,0  
4FZR,ARG\_351,11.73,-0.77,0,0  
3CS1,LYS\_108,10.5,0,0,0  
4FH3,GLU\_54,4.5,0,0,0  
3I47,ARG\_50,11.59,-0.91,0,0  
1TXJ,GLU\_21,4.02,0.21,-0.69,0  
2RIK,GLU\_17,4.57,0.07,0,0  
1CBY,TYR\_48,10.17,0.07,-0.8,0.9  
1TD6,GLU\_156,1.44,2.32,-2.53,-2.85  
3ONT,ARG\_19,12.43,-0.07,0,0  
1O6D,TYR\_22,13.34,0.14,0.8,2.4  
3MTT,LYS\_590,10.22,-0.28,0,0  
2C2Y,GLU\_80,4.71,0.21,0,0  
3EJG,GLU\_63,4.08,0.35,-0.77,0  
3D9H,ASP\_68,3.87,0.07,0,0  
2B0A,GLU\_34,4.5,0,0,0  
2R51,LYS\_49,10.36,-0.14,0,0  
3ULX,ASP\_55,2.83,0.84,-1.81,0  
2H2W,GLU\_226,4.43,0.9,-0.97,0  
2YYO,ARG\_95,12.5,0,0,0  
1H09,TYR\_238,13.53,0.35,0.78,2.4  
1YM5,GLU\_223,3.07,1.74,-0.77,-2.4  
2R51,LYS\_49,10.36,-0.14,0,0  
4EKU,GLU\_202,4.57,0.07,0,0  
2IQT,TYR\_133,11.35,0,1.35  
2BAA,GLU\_56,5.19,2.66,-1.97,0  
3GA2,ARG\_27,12.29,-0.21,0,0  
2X4G,ASP\_145,3.77,0,-0.03,0  
1OLR,ARG\_3,12.36,-0.14,0,0  
1L3K,ARG\_14,11.17,-1.33,0,0  
3RLN,ASP\_656,3.87,0.07,0,0  
1O17,LYS\_284,10.29,-0.21,0,0  
2QV2,ASP\_195,4.08,0.28,0,0  
3A0X,ARG\_738,12.15,-0.35,0,0  
2BV9,TYR\_74,10,0,0,0  
2OSA,ARG\_304,12.22,-0.28,0,0  
3Q6L,LYS\_32,10.29,-0.21,0,0  
1U53,LYS\_184,10.36,-0.14,0,0  
2YWK,GLU\_23,3.61,0.21,-1.1,0  
4F85,LYS\_171,10.5,0,0,0  
1NAB,GLU\_275,4.5,0,0,0  
3DHN,GLU\_44,4.5,0,0,0  
2Q07,LYS\_344,10.01,-0.49,0,0  
3CS1,ARG\_120,12.63,-2.27,0,2.4  
1QQE,ARG\_192,12.5,0,0,0  
1ZKZ,HIS\_98,6.36,0,0,-0.14  
1T95,CYS\_207,8.61,-0.76,0,0.37  
1XKR,TYR\_28,10,0,0,0  
3G9G,TYR\_53,13.27,0.07,0.8,2.4  
1AIL,HIS\_59,6.36,0,0,-0.14  
2NSN,ASP\_66,2.22,0.14,-1.72,0  
3V55,GLU\_390,0.86,1.88,-3.11,-2.4  
2IRM,LYS\_190,10.43,-0.07,0,0  
2QDJ,GLU\_72,4.57,0.07,0,0  
2ZOM,GLU\_315,4.18,0.35,-0.67,0  
3BQW,GLU\_234,4.57,0.07,0,0  
1FKM,ARG\_286,12.12,-2.78,0,2.4  
1SNT,ARG\_189,12.5,0,0,0  
2C2Y,ASP\_153,3.87,0.07,0,0  
1R3F,HIS\_196,3.58,0.45,0,-3.38  
3RKV,LYS\_241,10.5,0,0,0  
2CWC,ARG\_203,11.8,-0.7,0,0  
3C6B,LYS\_249,10.15,-0.35,0,0

3RLN,LYS\_598,10.5,0,0,0  
1DUN,HIS\_107,6.29,0,-0.21  
3EZ7,LYS\_234,10.22,-0.28,0,0  
1T3Y,GLU\_128,4.1,0.21,-0.61,0  
2OPJ,ARG\_13,11.73,-0.77,0,0  
2Q34,GLU\_35,4.57,0.07,0,0  
2D8N,LYS\_180,10.15,-0.35,0,0  
3GW3,GLU\_119,4.64,0.14,0,0  
1QQE,ASP\_179,3.74,0.42,-0.48,0  
1NFN,ARG\_150,11.94,-0.56,0,0  
1RAJ,TYR\_384,10,0,0,0  
2A6B,HIS\_172,1.63,1.14,0,-6.01  
3CCY,ASP\_14,3.8,0.56,-0.56,0  
2X4G,GLU\_236,3.63,0.35,-1.22,0  
2X5Y,GLU\_745,4.64,0.14,0,0  
4D8L,LYS\_137,10.22,-0.28,0,0  
1ZKZ,ASP\_88,4.0,4.2,-0.22,0  
2CXA,GLU\_163,4.57,0.07,0,0  
1GPP,GLU\_100,4.57,0.07,0,0  
1SOH,ASP\_101,3.87,0.07,0,0  
3CGW,HIS\_146,4.35,0,-2.15  
1R53,LYS\_6,10.5,0,0,0  
2HRZ,GLU\_40,4.53,0.28,-0.25,0  
3AUF,GLU\_127,4.13,0.42,-0.79,0  
2B0J,CYS\_253,7.99,-1.08,0,0.07  
1AD6,LYS\_432,10.43,-0.07,0,0  
1EV8,ASP\_139,3.65,0,-0.15,0  
3IOC,ARG\_248,11.17,-1.33,0,0  
1MML,LYS\_103,10.15,-0.35,0,0  
3KB5,HIS\_299,3.89,0.27,0,-2.88  
3RHE,ARG\_117,13.53,-2.35,0,3.38  
2QRX,GLU\_25,4.78,0.28,0,0  
1RHS,LYS\_153,9.87,-0.63,0,0  
3DZ1,ARG\_91,12.5,0,0,0  
4DBX,GLU\_77,4.64,0.14,0,0  
2QO7,ASP\_466,3.04,0.28,-1.04,0  
1R29,TYR\_58,10,0,0,0  
1GXN,LYS\_411,10.08,-0.42,0,0  
3UC9,ASP\_177,3.8,0,0,0  
1W7B,GLU\_242,4.25,0.28,-0.53,0  
2OYZ,LYS\_49,10.5,0,0,0  
2FZ4,GLU\_99,4.86,0.77,-0.41,0  
3GV0,CYS\_183,8.42,-0.65,0,0.07  
3JV1,ARG\_110,12.5,0,0,0  
2IIA,HIS\_85,6.91,0.55,0,-0.14  
2F4Q,LYS\_22,10.22,-0.28,0,0  
3LPZ,TYR\_124,10,0,0,0  
1SI7,ARG\_164,10.28,-2.22,0,0  
2VGM,GLU\_72,1.53,0.61,-1.18,-2.4  
2H85,TYR\_32,12.46,0.07,0.33,2.06  
1A8Q,HIS\_57,5.18,5.25,-0.94,-5.63  
1R3D,HIS\_37,6.36,0,0,-0.14  
1YIB,LYS\_204,10.43,-0.07,0,0  
3CRM,TYR\_42,10.33,0.46,-0.13,0  
2CXC,GLU\_139,4.26,0.56,-0.8,0  
1ZBP,LYS\_82,10.29,-0.21,0,0  
4D8L,ASP\_256,3.87,0.07,0,0  
1YB2,ARG\_123,12.08,-0.42,0,0  
3PAC,GLU\_156,4.57,0.07,0,0  
4H89,ARG\_100,12.29,-0.21,0,0  
2H85,HIS\_337,6.99,0.56,0,-0.07  
1YB2,GLU\_125,4.5,0,0,0  
3LP3,GLU\_439,3.91,0.21,-0.8,0  
4GA2,GLU\_81,4.09,0.35,-0.76,0  
3LP3,ARG\_323,11.24,-1.26,0,0  
3O16,LYS\_102,10.5,0,0,0  
3H6Q,GLU\_85,4.5,0,0,0  
2HRZ,GLU\_51,4.5,0,0,0  
2P5D,TYR\_60,10.14,0.14,0,0  
3BWT,ASP\_602,3.92,0.14,-0.02,0  
2Q34,GLU\_173,4.5,0,0,0  
2Z0M,ASP\_207,2.35,0.56,-3.55,1.54  
3HVW,ARG\_179,12.36,-0.14,0,0  
2VGM,LYS\_297,9.94,-0.56,0,0  
3UV9,CYS\_471,9.52,-0.32,0,0.84  
3DHN,LYS\_101,10.5,0,0,0  
1R6Y,GLU\_86,3.91,0.21,-0.8,0  
1ZBS,GLU\_174,4.33,0.35,-0.52,0  
3HXK,ARG\_85,12.08,-0.42,0,0  
1GXN,GLU\_529,2.84,0.28,-1.94,0  
2EA9,ARG\_78,12.43,-0.07,0,0  
1PVT,GLU\_137,4.92,0.42,0,0  
2C2Y,ASP\_238,3.75,0.21,-0.26,0  
3M7G,GLU\_50,4.66,0.21,-0.05,0  
4FLE,HIS\_180,6.5,0,0,0  
1XEU,HIS\_106,6.5,0,0,0  
2G7O,LYS\_83,10.15,-0.35,0,0  
3PAC,GLU\_18,4.26,0.14,-0.38,0  
3PU6,ASP\_15,2.62,0.7,-1.87,0  
2ZTY,GLU\_21,3.81,0,-0.69,0  
1GPP,LYS\_26,10.15,-0.35,0,0  
3ANJ,TYR\_347,11.48,1,0.48,0  
2XJ4,ARG\_5,12.01,-0.49,0,0  
4DIU,CYS\_45,10.9,-0.1,0.2,0.1  
1WXQ,LYS\_74,10.15,-0.35,0,0  
1XFK,ARG\_213,11.97,-0.53,0,0  
1O0X,ASP\_44,2.28,0.42,-1.95,0  
3PP8,GLU\_284,4.56,0.07,-0.01,0  
1NAF,GLU\_251,4.78,0.28,0,0  
3H5T,ARG\_201,11.99,-0.84,0,0.33  
2G3A,ARG\_73,11.66,-0.84,0,0  
3TMO,HIS\_330,5.3,0.74,0,-1.94  
3U2A,GLU\_54,4.7,0.35,-0.15,0  
2G2D,ASP\_181,3.12,0.56,-1.25,0  
3CNU,LYS\_23,10.22,-0.28,0,0  
3GEC,ARG\_317,11.8,-0.7,0,0  
3U2R,CYS\_123,9,0,0,0  
2B6P,ARG\_113,11.24,-1.26,0,0  
2Q13,HIS\_45,6.43,0,0,-0.07  
1J8B,LYS\_91,10.43,-0.07,0,0  
1HF8,LYS\_112,10.29,-0.21,0,0  
2RGY,GLU\_162,4.38,0,-0.12,0  
3EST,ASP\_165,4.19,0.49,-0.1,0  
1EQ6,TYR\_39,12.46,1.34,-0.43,1.55  
3C2E,GLU\_215,3.49,0.7,-1.72,0  
2OKT,TYR\_273,11.35,1.35,0,0  
2AD1,ARG\_188,12.01,-0.49,0,0  
3EX9,GLU\_12,4.5,0,0,0  
2CXA,ARG\_84,12.36,-0.14,0,0  
2WZ9,GLU\_24,4.05,0.35,-0.8,0  
2WZO,ASP\_398,4.15,0.35,0,0  
3RJZ,LYS\_198,9.8,-0.7,0,0  
1WXQ,TYR\_43,11.32,0,0,1.32  
3H04,GLU\_247,4.85,0.35,0,0  
1D2K,ARG\_407,12.46,-1.24,0,1.21  
3ZRI,LYS\_12,10.29,-0.21,0,0  
3M3P,ARG\_76,11.8,-0.7,0,0  
1SQH,ARG\_258,11.94,-0.56,0,0  
1LZL,HIS\_86,2.29,0.97,0,-5.19  
1X6J,TYR\_32,10.42,0.42,0,0  
3UPD,LYS\_42,10.5,0,0,0  
3P2F,GLU\_150,2.46,0.56,-2.6,0  
3HXK,CYS\_73,9,0,0,0  
3R87,ARG\_15,24.62,9,0,-0.21  
3U2R,ARG\_98,12.29,-0.21,0,0  
1OIS,ARG\_349,11.8,-0.7,0,0  
1ANU,LYS\_73,10.5,0,0,0  
3PM2,GLU\_48,4.5,0,0,0  
2GKG,ASP\_73,3.33,0.07,-0.55,0  
1RAJ,ASP\_319,3.3,0.21,-0.71,0  
3ELI,ASP\_46,1.68,0.49,-2.61,0  
2Q98,ARG\_176,12.08,-0.42,0,0  
2B3M,ARG\_135,12.08,-0.42,0,0  
2CXC,GLU\_44,3.98,0.21,-0.73,0  
2AH5,LYS\_31,10.5,0,0,0  
2JKF,LYS\_126,10.29,-0.21,0,0  
1W7B,ASP\_209,3.45,0.35,-0.69,0  
1ILW,LYS\_143,10.15,-0.35,0,0  
2XHC,ARG\_222,13.82,-0.86,0,2.18  
2X4G,GLU\_220,1.42,1.06,-4.2,0.06  
1TJE,ARG\_207,11.38,-1.12,0,0  
1V43,ASP\_316,3.94,0.14,0,0  
3M7O,LYS\_102,10.08,-0.42,0,0  
4F8A,CYS\_667,5.25,-3.83,0,0.07  
3COU,LYS\_131,10.5,0,0,0  
3GOZ,GLU\_128,3.14,0.28,-1.65,0  
4DBX,HIS\_68,6.36,0,0,-0.14  
3QAV,GLU\_48,4.37,0.21,-0.34,0  
1XIP,TYR\_248,13.67,0.6,0.67,2.4  
1X1E,ARG\_83,11.56,-0.94,0,0  
3BPP,LYS\_21,10.08,-0.42,0,0  
2B3M,GLU\_43,4.57,0.07,0,0  
1UJ8,CYS\_48,9.03,-0.04,0,0.07  
3L7N,LYS\_85,10.29,-0.21,0,0  
4H86,HIS\_111,7.31,0.95,0,-0.14  
3RKV,GLU\_228,4.5,0,0,0  
1UAJ,TYR\_115,11.97,0.07,0,1.9  
2O8P,GLU\_86,4.06,0.14,-0.58,0  
1AK1,LYS\_4,10.5,0,0,0  
3JZ9,GLU\_392,4.5,0,0,0  
2JEO,ARG\_99,12.29,-0.21,0,0  
1LFP,CYS\_129,8.03,-1.04,0,0.07  
1KCM,CYS\_188,8.31,0,-1.3,0.61  
1RSS,ASP\_20,1.98,0.56,-2.38,0  
3GV0,GLU\_285,4.41,0.35,-0.45,0  
3IVF,TYR\_127,10.75,0,0,0.75  
3V3T,ASP\_172,3.57,0.28,-0.51,0  
1YR6,ASP\_232,3.72,0.07,-0.15,0  
2H01,LYS\_59,10.36,-0.14,0,0  
3RHE,HIS\_83,6.29,0,0,-0.21  
2H14,LYS\_109,10.43,-0.07,0,0  
3AU3,GLU\_411,4.45,0.35,-0.4,0  
3ETV,ASP\_186,3.62,0.42,-0.6,0  
3A0X,ASP\_632,3.21,0.21,-0.8,0  
2CBE,GLU\_187,4.5,0,0,0  
2B3M,GLU\_14,4.5,0,0,0  
3HQX,ASP\_101,4.03,0.28,-0.05,0  
2QZQ,CYS\_49,9.51,-0.07,-0.12,0.7  
2EFK,ARG\_122,12.01,-0.49,0,0  
1NFN,ARG\_103,11.73,-0.77,0,0  
2EJB,CYS\_97,8.86,-0.28,0,0.14  
2RIS,GLU\_9,3.91,0.21,-0.8,0  
3V55,ARG\_671,12.42,-2.48,0,2.4  
2IXM,ASP\_176,2.36,0.63,-2.08,0  
1AM2,ARG\_107,11.73,-0.77,0,0  
2VOC,LYS\_63,10.5,0,0,0  
1Y0Y,LYS\_63,10.15,-0.35,0,0  
3PU6,LYS\_147,10.22,-0.28,0,0  
3FK5,CYS\_185,5.85,-5.01,0,1.86  
1NWA,ARG\_165,12.5,0,0,0  
2DFL,ARG\_154,11.8,-0.7,0,0  
1T95,GLU\_169,4.12,0.35,-0.73,0  
1L2F,GLU\_28,3.4,0.42,-1.52,0  
3A7L,LYS\_64,10.36,-0.14,0,0  
1T6L,LYS\_97,10.5,0,0,0  
2INO,ARG\_60,11.73,-0.77,0,0  
3F6F,ASP\_152,3.94,0.14,0,0  
3M7G,GLU\_17,4.55,0.14,-0.09,0  
3KEY,LYS\_389,10.36,-0.14,0,0  
1NJ4,GLU\_264,3.69,0.21,-1.02,0  
3H6Q,GLU\_41,3.29,0.77,-1.98,0  
1C3K,LYS\_36,10.22,-0.28,0,0  
2P52,GLU\_168,3.91,0.21,-0.8,0  
2EFK,GLU\_149,4.5,0,0,0  
3LPZ,LYS\_262,10.5,0,0,0  
1P2F,TYR\_56,10.57,0,0,0.56  
1Q46,GLU\_14,4.5,0,0,0  
2P4D,ASP\_90,3.08,0.14,-0.86,0  
3JRT,CYS\_53,9.25,-0.19,0,0.44  
4DEZ,ASP\_79,3.56,0.28,-0.52,0  
1TR9,GLU\_277,4.5,0,0,0  
3M7O,ARG\_201,11.94,-0.56,0,0  
3OIF,CYS\_128,11.14,0,0,2.14  
1UJ8,LYS\_181,8.85,0.21,-1.36,0  
2H2W,TYR\_262,10.03,1.15,-1.22,0.11  
3CAN,TYR\_177,13.27,0.07,0.8,2.4  
3RLN,ARG\_699,11.87,-0.63,0,0  
3O7K,ARG\_159,12.22,-0.28,0,0  
1R5Q,GLU\_34,4.64,0.14,0,0  
2NYC,ARG\_303,12.22,-0.28,0,0  
3PP8,ARG\_112,12.5,0,0,0  
3IU5,LYS\_135,10.29,-0.21,0,0  
3GS9,ARG\_87,12.15,-0.35,0,0  
2EJB,ASP\_164,1.79,0.35,-2.36,0  
1QQE,CYS\_40,9.55,-0.43,0,0.98  
1O9G,CYS\_18,9.28,-0.06,0,0.34  
2PGX,TYR\_88,10.23,0.27,0,-0.04  
2X4G,HIS\_27,2.74,1.03,-0.82,-3.98  
2C13,LYS\_143,10.5,0,0,0  
1NAR,ASP\_240,3.87,0.07,0,0  
3RNV,LYS\_442,10.01,-0.49,0,0  
2D8N,HIS\_91,4.51,0,0,-1.99  
3OA7,GLU\_537,4.18,0.07,-0.39,0  
2QZQ,TYR\_111,9.8,0.07,-0.27,0  
1ZBS,TYR\_175,12.56,0.14,0.08,2.35  
3NZL,LYS\_40,10.5,0,0,0  
2E3I,LYS\_70,10.01,-0.49,0,0  
3C51,LYS\_28,10.5,0,0,0  
1WLY,LYS\_108,9.66,-0.84,0,0  
1NAR,ASP\_274,3.19,0.84,-1.46,0  
2C2Y,ARG\_172,12.5,0,0,0  
2EFK,GLU\_147,4.5,0.14,-0.14,0  
2FZ4,LYS\_172,10.22,-0.28,0,0  
1R15,LYS\_200,10.43,-0.07,0,0  
2CW4,LYS\_21,10.29,-0.21,0,0  
1WYC,TYR\_242,11.81,0,-0.38,2.19  
2XJ4,ARG\_221,11.94,-0.56,0,0  
3CE7,GLU\_78,3.69,0.35,-1.16,0  
2WZ9,GLU\_51,4.5,0,0,0  
3G5X,TYR\_176,11.42,0,0,1.42  
1WNH,LYS\_51,10.29,-0.21,0,0  
3JZ9,GLU\_374,3.86,0.14,-0.78,0  
1S17,ARG\_298,11.69,-3.21,0,2.4  
2QV2,GLU\_247,3.62,0.28,-1.17,0  
3GS9,GLU\_28,4.12,1.22,-1.6,0  
3HXK,ARG\_175,11.8,-0.7,0,0  
2WZ9,ASP\_130,3.8,0,0,0  
3P51,ARG\_70,12.29,-0.21,0,0  
4DEZ,ASP\_234,4.02,0.35,-0.13,0  
3LJC,ASP\_47,3.8,0,0,0  
1JT9,GLU\_217,2.76,1.05,-2.79,0  
1PVT,LYS\_184,9.87,-0.63,0,0  
3C6B,GLU\_117,4.34,0.7,-0.86,0  
2QK1,ASP\_401,2.97,0.42,-1.25,0  
3US6,GLU\_20,4.71,0.21,0,0  
1MJS,GLU\_301,3.02,0.63,-2.11,0



204D,GLU\_110,4.5,0,0,0  
 2F8H,ASP\_254,2.85,0.42,-1.36,0  
 3ADO,LYS\_313,10.29,-0.21,0,0  
 3PP8,GLU\_176,3.48,0.21,-1.22,0  
 2FC3,LYS\_119,9.73,-0.77,0,0  
 2V4X,ASP\_106,3.73,0,-0.07,0  
 2Q98,ARG\_164,11.66,-0.84,0,0  
 2Z14,ASP\_47,1.95,0.7,-2.54,0  
 3BCY,LYS\_23,10.29,-0.21,0,0  
 1ZCE,TYR\_4,10.02,0.14,-1.36,1.24  
 3RFY,CYS\_256,8.58,-0.49,0,0.07  
 3CX5,GLU\_62,4.5,0,0,0  
 4ECC,ARG\_35,12.01,-0.49,0,0  
 2WOZ,LYS\_482,10.01,-0.49,0,0  
 1SNT,ARG\_140,11.94,-0.56,0,0  
 2J8A,LYS\_349,10.36,-0.14,0,0  
 3CIV,ASP\_129,3.2,0.28,-0.88,0  
 2C13,GLU\_43,4.71,0.21,0,0  
 2X4L,TYR\_85,10.4,1.55,-1.15,0  
 2FBI,GLU\_134,4.64,0.14,0,0  
 1WXQ,HIS\_359,6.47,0.04,0,-0.07  
 1P6F,GLU\_98,4.78,0.28,0,0  
 1YB2,GLU\_12,4.78,0.28,0,0  
 2B3M,TYR\_143,12.12,0,0,2.12  
 3ZRI,LYS\_131,10.5,0,0,0  
 3V55,GLU\_500,4.92,0.42,0,0  
 1WRU,LYS\_81,10.29,-0.21,0,0  
 3L3P,ASP\_470,3.62,0,-0.18,0  
 4FCU,ARG\_221,12.22,-0.28,0,0  
 3EJG,ASP\_20,3.81,0.07,-0.06,0  
 2D59,GLU\_61,4.5,0,0,0  
 3P29,GLU\_270,4.5,0,0,0  
 1SUU,LYS\_534,10.29,-0.21,0,0  
 1WXQ,TYR\_62,10.05,0.56,-0.51,0  
 1LTU,ARG\_177,11.14,-1.36,0,0  
 2QDJ,CYS\_61,9.57,-0.08,0,0.65  
 3E7P,GLU\_214,3.81,0.91,-1.6,0  
 2FXT,ASP\_411,1.82,0.7,-2.68,0  
 1EYH,ASP\_45,3.43,0.21,-0.58,0  
 3GV0,GLU\_266,4.05,0.35,-0.8,0  
 2FG1,LYS\_115,10.5,0,0,0  
 2P65,GLU\_175,3.67,0.35,-1.18,0  
 1AD6,ASP\_479,3.02,0.42,-1.21,0  
 2CN1,LYS\_190,10.43,-0.07,0,0  
 1R3D,LYS\_195,9.94,-0.56,0,0  
 2B6P,CYS\_14,8.94,-0.13,0,0.07  
 1YOY,GLU\_150,4.6,0.14,-0.04,0  
 2XMZ,ARG\_127,11.92,-2.24,0,1.66  
 3A2Z,GLU\_51,4.05,0.35,-0.8,0  
 3ANJ,ASP\_87,2.28,0.56,-2.09,0  
 3ZTA,GLU\_59,4.3,0.56,-0.76,0  
 2OJQ,ARG\_489,11.59,-0.91,0,0  
 3DHN,ASP\_69,1.94,0.42,-2.28,0  
 1DZF,TYR\_211,10.01,0.07,-0.06,0  
 1GPP,GLU\_160,4.74,0.71,-0.9,0.43  
 2H2W,LYS\_270,10.43,-0.07,0,0  
 3OBS,ASP\_19,3.78,0,-0.02,0  
 3JZ9,HIS\_488,7.29,0.86,0,-0.07  
 2F9F,CYS\_160,10.59,0,1.59  
 3UOV,LYS\_115,10.01,-0.49,0,0  
 1R3D,ASP\_154,3.37,0.35,-0.78,0  
 1SFE,GLU\_175,4.35,0.35,-0.5,0  
 4F8A,HIS\_610,7.16,0.73,0,-0.07  
 3O48,GLU\_121,4.12,0.42,-0.8,0  
 1BKB,ARG\_31,12.36,-0.14,0,0  
 1ZYL,TYR\_277,10.72,0.72,0,0  
 3MIX,ASP\_342,3.04,0.49,-1.25,0  
 3P51,LYS\_35,10.15,-0.35,0,0  
 3T5B,LYS\_172,10.62,-0.14,0,0.26  
 3Q1C,GLU\_125,4.5,0,0,0  
 3A0X,ASP\_641,3.72,0.28,-0.36,0  
 1DZF,ASP\_48,0.84,1.19,-4.14,0  
 3ERF,LYS\_214,10.22,-0.28,0,0  
 1P4X,LYS\_215,10.5,0,0,0  
 2PLQ,HIS\_110,6.9,0.68,0,-0.28  
 3CQ1,ASP\_26,1.9,1.05,-2.95,0  
 1C44,LYS\_19,9.52,-0.98,0,0  
 2D7J,ASP\_110,3.0,0.63,-1.43,0  
 2CXC,GLU\_10,4.05,0.35,-0.8,0  
 3LJC,GLU\_115,4.79,0.35,-0.06,0  
 1TXJ,LYS\_37,9.66,-0.84,0,0  
 2QRX,LYS\_127,10.43,-0.07,0,0  
 2QK0,LYS\_96,10.5,0,0,0  
 3BPP,GLU\_163,3.98,0.28,-0.8,0  
 3P28,ASP\_142,3.87,0.07,0,0  
 4ACJ,GLU\_648,4.5,0,0,0  
 4FD6,ARG\_162,11.94,-0.56,0,0  
 3EJC,ASP\_41,3.85,0.07,-0.02,0  
 3BJV,GLU\_146,4.01,0.14,-0.63,0  
 3UAH,LYS\_167,10.5,0,0,0  
 2IN0,GLU\_427,3.98,0.28,-0.8,0  
 1Z3X,HIS\_230,3.47,0.03,0,-3.06  
 3NR5,TYR\_119,11.82,0.25,-0.47,2.03  
 2QDJ,ASP\_68,3.34,0.07,-0.52,0  
 3G9T,LYS\_250,10.15,-0.35,0,0  
 3B4D,TYR\_175,9.6,0,-0.4,0  
 3GA2,ARG\_177,10.9,-1.6,0,0  
 2O0K,GLU\_309,4.78,0.28,0,0  
 2XWS,CYS\_104,9.02,-0.74,0,0.75  
 3I47,GLU\_79,4.71,0.21,0,0  
 1TD6,TYR\_206,10.07,0.77,-0.7,0  
 3KV0,ASP\_175,3.52,0.35,-0.63,0  
 3DZ1,LYS\_280,10.5,0,0,0  
 3KEY,LYS\_453,10.29,-0.21,0,0  
 3UAH,ASP\_283,4.0,21,-0.01,0  
 1OIS,ARG\_360,12.5,0,0,0  
 1D2K,HIS\_200,7.05,0.76,0,-0.21  
 1O0X,TYR\_116,11.04,1.2,-0.16,0  
 2O0K,TYR\_119,13.18,0.14,0.64,2.4  
 3V55,ASP\_403,3.85,0.21,-0.16,0  
 3HYQ,ARG\_85,12.15,-0.35,0,0  
 1YOY,HIS\_42,8.44,1.6,4.07,-3.72  
 1UOH,CYS\_180,9.96,-0.11,0,1.07  
 3RFY,TYR\_229,10.08,0,0.08  
 3L7N,GLU\_181,3.42,3.94,-2.62,-2.4  
 3LD1,LYS\_55,10.43,-0.07,0,0  
 3BQW,TYR\_196,12.9,0.96,0,1.94  
 2FM9,CYS\_225,9.1,0,0,0.1  
 4DND,GLU\_62,4.59,0.21,-0.12,0  
 2EDM,GLU\_200,4.5,0,0,0  
 1DOV,ASP\_102,3.4,0.14,-0.54,0  
 2PWQ,LYS\_138,10.5,0,0,0  
 2Q98,GLU\_140,3.95,0.63,-1.18,0  
 3K9I,TYR\_147,10,0,0,0  
 1XIPL,LYS\_179,10.43,-0.07,0,0  
 3GV0,HIS\_202,1.46,0,-2.33,-2.71  
 3DHN,GLU\_87,4.57,0.07,0,0  
 1L2F,LYS\_263,10.59,0,0,0  
 3FWU,TYR\_23,11.04,1.84,-0.8,0  
 4EVF,ASP\_157,3.16,0.07,-0.71,0  
 3FHF,ARG\_170,12.08,-0.42,0,0  
 2YT4,GLU\_593,4.26,0.56,-0.8,0  
 3UOV,ASP\_79,1.6,0.84,-3.04,0  
 2F9F,GLU\_141,3.23,0.56,-1.83,0  
 1YOK,ARG\_149,11.87,-0.63,0,0  
 2APL,HIS\_129,6.59,0.09,0,0  
 3C2E,LYS\_89,10.15,-0.35,0,0  
 3C5V,TYR\_143,11.13,1.13,0,0  
 2JHY,GLU\_95,4.05,0.35,-0.8,0  
 2B0A,CYS\_84,9.65,-0.32,0,0.98  
 3ZXY,ARG\_94,12.01,-0.49,0,0  
 1J33,GLU\_153,3.47,0.49,-1.52,0  
 2EFK,GLU\_236,4.92,0.42,0,0  
 3IOC,HIS\_148,3.71,0,0,-2.79  
 3N2T,ARG\_117,11.94,-0.56,0,0  
 3CIV,LYS\_139,10.29,-0.21,0,0  
 1NJ4,GLU\_185,0.38,0.68,-2.4,-2.4  
 1X7F,GLU\_90,4.5,0,0,0  
 3LJI,GLU\_57,3.45,0.65,-0.8,-0.9  
 3C2E,GLU\_218,4.34,0.14,-0.3,0  
 3FRR,LYS\_90,10.5,0,0,0  
 1OSJ,HIS\_1,7.16,0.8,0,-0.14  
 3SMD,TYR\_44,10,0,0,0  
 1NWA,ASP\_82,4.01,0.21,0,0  
 3IOC,GLU\_303,4.84,2.33,-1.99,0  
 2B0A,TYR\_69,10.07,0.07,0,0  
 2G5X,LYS\_132,10.43,-0.07,0,0  
 2W8B,TYR\_580,12.01,0.12,0,1.89  
 3T5B,LYS\_395,10.43,-0.07,0,0  
 2W0G,HIS\_161,6.36,0,0,-0.14  
 1BKB,TYR\_22,10.5,0.5,0,0  
 1W7B,TYR\_333,9.7,0,-0.3,0  
 3ONT,ASP\_51,3.71,0.07,-0.16,0  
 3Q9P,TYR\_142,9.72,0.07,-0.35,0  
 3B21,LYS\_165,10.29,-0.21,0,0  
 2POY,ASP\_243,2.23,0.35,-1.92,0  
 2Q07,HIS\_494,4.52,0.46,0,-2.43  
 3HKX,ARG\_158,12.01,-0.49,0,0  
 1L2H,LYS\_63,10.22,-0.28,0,0  
 3M9A,ASP\_21,3.32,0.35,-0.83,0  
 2RJD,TYR\_266,9.75,0.55,-0.8,0  
 2I6I,GLU\_40,1.5,0.56,-3.56,0  
 1YLN,LYS\_53,10.29,-0.21,0,0  
 2G9D,ARG\_149,11.17,-1.33,0,0  
 1BN6,HIS\_241,7.12,0.76,0,-0.14  
 3VJ8,TYR\_346,10,0,0,0  
 1WXF,ASP\_28,3.49,0.35,-0.66,0  
 3ELI,GLU\_34,3.57,0.56,-1.49,0  
 1UAJ,ASP\_50,3.45,0.14,-0.49,0  
 2A6B,ASP\_124,3.22,0.35,-0.93,0  
 1OIS,ARG\_260,12.43,-0.07,0,0  
 3LH5,ARG\_639,12.29,-0.21,0,0  
 1YTD,GLU\_386,4.5,0,0,0  
 4DNU,ASP\_65,3.44,0.56,-0.92,0  
 4DND,TYR\_34,10,0,0,0  
 3ASA,HIS\_6.643,0,0,-0.07  
 4GA2,CYS\_50,9.46,0,0,0.46  
 3GG6,GLU\_134,4.71,0.21,0,0  
 2AXO,HIS\_201,2.23,1.05,-1.4,-3.93  
 3FTT,TYR\_110,10,0,0,0  
 3HYQ,TYR\_139,9.82,0,-0.18,0  
 2AZP,CYS\_65,9.17,-0.2,-1.19,1.56  
 4EUG,LYS\_42,10.08,-0.42,0,0  
 3TIR,TYR\_66,10,0,0,0  
 1L3K,HIS\_173,6.45,0.16,0,-0.21  
 3CCY,GLU\_118,4.48,0.42,-0.44,0  
 2YX0,GLU\_255,3.9,0.56,-1.17,0  
 3Q2C,LYS\_56,10.5,0,0,0  
 4FH3,LYS\_77,10.22,-0.28,0,0  
 1W7B,ARG\_205,11.59,-0.91,0,0  
 1R2Z,LYS\_153,10.36,-0.14,0,0  
 2H2Z,GLU\_47,4.5,0,0,0  
 2EFK,ASP\_281,3.72,0,-0.08,0  
 3HKX,ARG\_87,11.8,-0.7,0,0  
 3A4C,ASP\_530,3.94,0.14,0,0  
 3RE9,HIS\_106,6.43,0,0,-0.07  
 2Q12,LYS\_192,10.43,-0.07,0,0  
 2PP6,ASP\_13,3.32,0.21,-0.69,0  
 3COU,TYR\_28,9.6,0.06,0,-0.46  
 1KCM,GLU\_106,4.64,0.14,0,0  
 4HDE,ASP\_36,3.11,0.14,-0.83,0  
 2B02,HIS\_378,6.43,0,0,-0.07  
 4EKU,GLU\_244,4.02,0.35,-0.83,0  
 2Q5X,GLU\_742,4.01,0.28,-0.77,0  
 2EJX,ASP\_89,2.23,0.56,-2.13,0  
 1FHL,TYR\_238,11.34,0.32,-0.12,1.14  
 2P65,LYS\_170,10.01,-0.49,0,0  
 3TIR,LYS\_173,10.43,-0.07,0,0  
 2NRR,GLU\_440,4.57,0.07,0,0  
 3V46,TYR\_326,11.07,1.87,-0.8,0  
 3JRT,ASP\_140,3.93,0.14,-0.01,0  
 1G5Z,ASP\_70,3.74,0.28,-0.34,0  
 1RWZ,ASP\_170,3.91,0.28,-0.17,0  
 2WB3,LYS\_154,10.22,-0.28,0,0  
 1LN4,LYS\_12,10.5,0,0,0  
 2JKF,TYR\_144,10.68,0.24,-0.8,1.24  
 2Z0M,LYS\_313,10.5,0,0,0  
 1X04,ASP\_85,3.12,0.07,-0.74,0  
 3COU,HIS\_24,2.1,0.01,0,-4.41  
 2W0G,LYS\_260,10.01,-0.49,0,0  
 3GFP,ASP\_302,3.94,0.14,0,0  
 2EA9,GLU\_51,3.24,0.28,-1.53,0  
 3DZ1,HIS\_246,4.04,0,0,-2.46  
 2CXA,ARG\_122,11.73,-0.77,0,0  
 1PZC,GLU\_19,3.77,0.35,-1.08,0  
 2WB3,ASP\_363,3.02,0.14,-0.92,0  
 1UOH,HIS\_111,1.94,1.15,-0.94,-4.78  
 3IOC,ARG\_110,12.22,-0.28,0,0  
 3GV0,GLU\_77,4.29,0.56,-0.77,0  
 2H14,GLU\_80,4.64,0.14,0,0  
 1UW7,TYR\_87,10.14,0.14,0,0  
 3GE9,ASP\_237,2.5,0.35,-1.65,0  
 2BLL,ARG\_400,12.15,-0.35,0,0  
 2BV9,HIS\_257,3.41,0.87,0,-3.97  
 4D8L,ARG\_52,11.59,-0.91,0,0  
 1UAJ,LYS\_47,10.5,0,0,0  
 3GYW,TYR\_191,10.07,0.07,0,0  
 4DIU,GLU\_66,4.5,0,0,0  
 1TD6,HIS\_18,4.18,0.64,0,-2.96  
 1HF8,GLU\_133,5.19,0.69,0,0  
 3LPZ,LYS\_40,10.5,0,0,0  
 1GPP,GLU\_137,3.73,0.35,-1.12,0  
 3UPD,HIS\_19,7.04,1.6,1.55,-2.61  
 1X7F,ARG\_304,11.73,-0.77,0,0  
 3CQ1,ASP\_58,3.05,0.35,-1.1,0  
 3F53,LYS\_137,10.5,0,0,0  
 2OEW,LYS\_229,10.15,-0.35,0,0  
 3HUE,GLU\_245,4.57,0.07,0,0  
 2IRM,GLU\_305,4.5,0,0,0  
 1LZL,TYR\_226,13.86,0.82,0.61,2.43  
 1EV8,GLU\_6,4.57,0.07,0,0  
 3A0X,LYS\_671,10.36,-0.14,0,0  
 3GYW,LYS\_44,10.43,-0.07,0,0  
 3LQE,TYR\_295,10.54,0.68,-0.14,0  
 3U2R,HIS\_137,6.47,0.04,0,-0.07  
 3F7M,ARG\_301,12.5,0,0,0  
 1ZCU,ARG\_179,12.22,-0.28,0,0  
 3V46,ARG\_286,12.5,0,0,0  
 2C13,GLU\_136,3.57,0.67,-1.6,0  
 3GS9,TYR\_249,8.5,0.94,-1.04,-1.4  
 3CX2,ASP\_248,2.01,0.42,-2.21,0  
 1M3P,GLU\_15,5.13,1.67,0,-1.04  
 2EJX,LYS\_88,10.01,-0.49,0,0  
 2FZ4,ASP\_81,3.93,0.28,-0.15,0  
 3V3T,TYR\_116,10,0,0,0  
 1YTQ,ARG\_188,11.31,-1.19,0,0

2YWJ, TYR\_159, 10.28, 0.28, 0.0  
 15UU, LYS\_515, 10.43, -0.07, 0.0  
 1C44, GLU\_47, 3.97, 0.21, -0.74, 0  
 2ZCX, HIS\_56, 6.5, 0.0, 0.0  
 2YX0, GLU\_34, 4.45, 0.75, -0.8, 0  
 2H2Z, CYS\_128, 11.24, -0.1, 0.5, 1.83  
 1WXQ, ASP\_229, 2.99, 0.21, -1.02, 0  
 1WNH, HIS\_53, 7.12, 0.69, 0, -0.07  
 1NWA, HIS\_141, 3.73, 0, -0.277  
 1SI7, GLU\_270, 4.71, 0.21, 0, 0  
 1P6F, TYR\_100, 10.0, 0, 0, 0  
 2G55, GLU\_30, 4.5, 0, 0, 0  
 3M7D, ARG\_205, 11.94, -0.56, 0, 0  
 1H4U, GLU\_398, 4.85, 0.35, 0, 0  
 1GQE, ARG\_245, 11.8, -0.7, 0, 0  
 2ZQ5, GLU\_274, 4.38, 0.14, -0.26, 0  
 2BLL, TYR\_419, 11.09, 0.08, -0.25, 1.26  
 2CYG, ARG\_299, 11.6, -0.9, 0, 0  
 2A1V, LYS\_87, 9.94, -0.56, 0, 0  
 1KCM, GLU\_130, 4.5, 0, 0, 0  
 2Z14, LYS\_13, 10.5, 0, 0, 0  
 2QOP, CYS\_148, 9.64, 0.0, 0.64  
 3L0D, GLU\_74, 2.98, 1.49, -0.8, -2.21  
 1NIJ, ASP\_92, 3.78, 0.28, -0.3, 0  
 3CXS, GLU\_174, 4.5, 0, 0, 0  
 3IV4, HIS\_93, 7.16, 0.8, 0, -0.14  
 1XEU, GLU\_262, 4.12, 0.42, -0.8, 0  
 3BZT, ASP\_328, 3.69, 0, -0.11, 0  
 3JRT, HIS\_82, 6.5, 0, 0, 0  
 3TIR, GLU\_41, 4.05, 0.35, -0.8, 0  
 1YM5, LYS\_151, 10.43, -0.07, 0, 0  
 1G8P, ARG\_246, 12.9, -0.72, 0, 1.12  
 2WZ9, GLU\_15, 3.91, 0.35, -0.94, 0  
 1A8Q, ASP\_197, 2.51, 0.35, -1.64, 0  
 1NAF, ARG\_265, 12.15, -0.35, 0, 0  
 3OA7, GLU\_6, 4.5, 0, 0, 0  
 1XAW, LYS\_506, 10.43, -0.07, 0, 0  
 1JSX, HIS\_32, 6.5, 0, 0, 0  
 2XHC, LYS\_201, 10.43, -0.07, 0, 0  
 2BT8, ARG\_205, 12.15, -0.35, 0, 0  
 1Q8B, GLU\_60, 4.5, 0, 0, 0  
 1O6D, LYS\_31, 10.22, -0.28, 0, 0  
 3F5D, CYS\_190, 9.16, -0.05, 0.0, 0.21  
 3LH5, GLU\_802, 4.65, 0.28, -0.13, 0  
 2R51, TYR\_37, 12.94, 0.07, 0.35, 2.52  
 1R3F, GLU\_169, 3.39, 0.49, -1.6, 0  
 3G0Z, GLU\_271, 3.63, 0.49, -1.36, 0  
 2EFK, LYS\_104, 10.5, 0, 0, 0  
 3CRM, GLU\_235, 3.53, 1.97, -4.17, 1.22  
 1GSZ, GLU\_118, 4.57, 0.07, 0, 0  
 2D59, LYS\_66, 10.36, -0.14, 0, 0  
 1H09, TYR\_314, 10.07, 0.07, 0, 0  
 3PP8, ARG\_113, 11.38, -1.12, 0, 0  
 3N2T, ARG\_285, 12.29, -0.21, 0, 0  
 2DFL, ASP\_185, 3.12, 0.07, -0.75, 0  
 1UXO, LYS\_3, 10.5, 0, 0, 0  
 3IBT, ARG\_35, 13.8, -0.63, 0, 1.93  
 2ATR, TYR\_19, 11.85, 0.85, 0.3, 0.7  
 2JF, LYS\_148, 10.43, -0.07, 0, 0  
 1T07, LYS\_26, 10.5, 0, 0, 0  
 3EVN, ASP\_57, 3.67, 0.14, -0.27, 0  
 3PU6, GLU\_141, 4.51, 0.56, -0.55, 0  
 2D7U, CYS\_103, 11.19, -1.78, 1.6, 2.37  
 1D7O, GLU\_100, 4.57, 0.07, 0, 0  
 3L0D, ASP\_38, 3.94, 0.14, 0, 0  
 1SFE, ASP\_44, 3.37, 0.63, -1.06, 0  
 3H5T, ARG\_43, 12.5, 0, 0, 0  
 3D9H, LYS\_197, 10.29, -0.21, 0, 0  
 3M66, ASP\_148, 2.26, 0.07, -1.61, 0  
 3RFY, HIS\_281, 6.57, 0.14, 0, -0.07  
 3I0C, TYR\_264, 13.87, 1.47, 0, 2.4  
 2J8A, LYS\_274, 10.5, 0, 0, 0  
 3CS1, LYS\_158, 10.5, 0, 0, 0  
 1NJ4, TYR\_136, 10.07, 0.07, 0, 0  
 2P65, GLU\_6, 4.32, 0.07, -0.25, 0  
 1DVO, GLU\_152, 3.32, 0.84, -2.02, 0  
 2X4G, ARG\_334, 12.15, -0.35, 0, 0  
 2IF4, GLU\_91, 4.5, 0, 0, 0  
 1Q8B, ASP\_27, 1.96, 0.56, -2.4, 0  
 3ODJ, GLU\_44, 4.5, 0, 0, 0  
 1KCM, ARG\_227, 11.03, -1.48, 0.0, 0.01  
 4ANN, ASP\_78, 2.75, 0.07, -1.12, 0  
 1P6F, GLU\_42, 3.45, 0.14, -1.19, 0  
 2EYI, GLU\_56, 3.98, 0.28, -0.8, 0  
 3E0H, GLU\_110, 4.71, 0.21, 0, 0  
 1YTQ, TYR\_153, 9.41, 0.21, -0.8, 0  
 1TR9, GLU\_231, 4.78, 0.28, 0, 0  
 1U7U, ARG\_281, 11.66, -0.84, 0, 0  
 2D7U, ARG\_303, 12.5, 0, 0, 0  
 2JEO, LYS\_203, 10.29, -0.21, 0, 0  
 1RAJ, GLU\_428, 4.64, 0.14, 0, 0  
 3P28, ASP\_107, 2.82, 0.49, -1.47, 0  
 4E65, GLU\_55, 2.07, 0.77, -3.2, 0  
 1RIG, HIS\_163, 6.43, 0, -0.07  
 1YTQ, GLU\_112, 3.61, 0.28, -1.17, 0  
 3E7P, TYR\_248, 11.42, 1.42, 0, 0  
 1XWM, TYR\_189, 10.14, 0.14, 0, 0  
 2YT4, LYS\_561, 10.5, 0, 0, 0  
 1IAP, HIS\_65, 4.5, 0.8, 0, -2.8  
 4EKU, TYR\_46, 11.3, 1.96, -0.8, 0.14  
 3DB9, ASP\_116, 3.73, 0, -0.07, 0  
 1J33, ASP\_270, 3.9, 0.21, -0.11, 0  
 2FGG, GLU\_19, 4.89, 0.21, 0.18, 0  
 3OA7, LYS\_456, 10.5, 0, 0, 0  
 3BWT, TYR\_856, 11.32, 0.35, -0.32, 1.29  
 3B4D, ARG\_240, 12.08, -0.42, 0, 0  
 1SUU, LYS\_644, 10.5, 0, 0, 0  
 3GG6, ASP\_136, 1.71, 0.77, -2.86, 0  
 3FWU, LYS\_86, 10.43, -0.07, 0, 0  
 3UC9, GLU\_122, 4.5, 0, 0, 0  
 3C6B, ARG\_48, 12.22, -0.28, 0, 0  
 1WYC, TYR\_170, 12.89, 0.22, 0.27, 2.4  
 3B7H, GLU\_75, 4.64, 0.14, 0, 0  
 1AKO, ARG\_89, 11.87, -0.63, 0, 0  
 1XAW, CYS\_500, 9.07, 0.0, 0.07  
 3GA2, ARG\_214, 11.4, -1.0, 0, 0  
 1V43, TYR\_280, 13.27, 0.07, 0.8, 2.4  
 2D7U, ARG\_256, 12.29, -0.21, 0, 0  
 2RGY, CYS\_258, 8.18, -0.9, 0.0, 0.07  
 2QDJ, LYS\_289, 10.5, 0, 0, 0  
 1FKM, LYS\_459, 10.5, 0, 0, 0  
 1TWU, LYS\_3, 9.8, -0.7, 0, 0  
 1ZP2, GLU\_122, 4.04, 0.3, -0.76, 0  
 3RVC, ASP\_125, 4.15, 0.35, 0, 0  
 1ZBM, HIS\_7, 5.86, 1.6, 2.35, -4.59  
 3CIV, GLU\_110, 4.5, 0, 0, 0  
 3LJI, ARG\_179, 12.15, -0.35, 0, 0  
 2Z84, GLU\_163, 3.37, 0.56, -1.69, 0  
 3GW3, ASP\_344, 2.77, 0.28, -1.31, 0  
 3L0D, GLU\_112, 4.5, 0.84, -0.84, 0  
 3F6M, GLU\_120, 4.15, 0.07, -0.42, 0  
 3GG6, ARG\_170, 11.94, -0.56, 0, 0  
 3CSR, TYR\_8, 9.53, 0, -0.48, 0  
 2Q99, ASP\_83, 4.21, 0.42, -0.01, 0  
 3HUE, ASP\_32, 1.92, 0.77, -2.66, 0  
 1VJG, ASP\_155, 3.94, 0.14, 0, 0  
 1T95, GLU\_137, 4.5, 0, 0, 0  
 2OSA, ASP\_358, 3.8, 0, 0, 0  
 2D7U, ARG\_67, 13.86, -1.04, 0, 2.4  
 1YG2, TYR\_19, 10.0, 0, 0, 0  
 2RIK, HIS\_207, 7.16, 0.8, 0, -0.14  
 4EKU, GLU\_126, 4.09, 0.56, -0.97, 0  
 2YT4, LYS\_650, 10.36, -0.14, 0, 0  
 3TMO, HIS\_201, 6.5, 0, 0, 0  
 1LFP, LYS\_155, 10.08, -0.42, 0, 0  
 1MML, LYS\_75, 10.15, -0.35, 0, 0  
 3UX2, LYS\_36, 10.01, -0.49, 0, 0  
 3OOP, ASP\_70, 3.43, 0.21, -0.59, 0  
 2IQT, GLU\_223, 2.92, 0.35, -1.93, 0  
 1ZYL, ARG\_273, 12.47, -2.02, 0, 1.99  
 3RJX, GLU\_334, 3.5, 1.19, -2.19, 0  
 1YW5, HIS\_171, 0.2, 0.02, -1.44, -4.89  
 1RKA, GLU\_71, 4.5, 0, 0, 0  
 1YTD, LYS\_360, 10.08, -0.42, 0, 0  
 3CZC, ASP\_65, 3.87, 0.07, 0, 0  
 1LTU, GLU\_68, 4.5, 0, 0, 0  
 1IDK, TYR\_231, 11.29, 0, -0.04, 1.32  
 2GZR, GLU\_173, 1.32, 1.45, -2.23, -2.4  
 2QDJ, ASP\_139, 3.78, 0, -0.02, 0  
 1ZB5, ARG\_188, 12.08, -0.42, 0, 0  
 2AH5, GLU\_121, 4.5, 0, 0, 0  
 2NRK, GLU\_29, 3.54, 0.14, -1.1, 0  
 4EZB, ARG\_27, 12.43, -0.07, 0, 0  
 1EDG, ASP\_191, 2.5, 0.56, -1.86, 0  
 3GS3, GLU\_149, 4.57, 0.07, 0, 0  
 3FS3, TYR\_151, 8.15, 0.27, -0.89, -1.22  
 2G55, ARG\_55, 12.08, -0.42, 0, 0  
 2X5Y, LYS\_726, 10.29, -0.21, 0, 0  
 3HKX, HIS\_279, 6.29, 0, -0.21  
 2RIK, ARG\_192, 12.22, -0.28, 0, 0  
 1IAP, ARG\_227, 12.08, -0.42, 0, 0  
 3CX2, LYS\_202, 10.5, 0, 0, 0  
 3C01, ASP\_88, 3.23, 0.56, -1.13, 0  
 1BN6, HIS\_95, 1.2, 0, 0, -5.3  
 3M3P, HIS\_158, 6.5, 0, 0, 0  
 3LJI, HIS\_19, 6.5, 0, 0, 0  
 3Q1C, GLU\_305, 4.5, 0, 0, 0  
 2GAU, ARG\_224, 11.8, -0.7, 0, 0  
 3M66, LYS\_412, 10.43, -0.07, 0, 0  
 1X91, LYS\_19, 10.5, 0, 0, 0  
 2JHY, LYS\_138, 9.45, -1.05, 0, 0  
 3JSN, GLU\_34, 3.77, 0.07, -0.8, 0  
 2Z84, GLU\_83, 2.81, 0.7, -2.39, 0  
 2P1W, ARG\_213, 12.08, -0.42, 0, 0  
 3FS3, ASP\_189, 3.95, 0.28, -0.13, 0  
 2FXT, TYR\_325, 10.69, 1.11, -0.42, 0  
 3PZ9, HIS\_278, 7.46, 3.43, 4.81, -7.28  
 3RJX, ARG\_211, 12.29, -0.21, 0, 0  
 2NRK, HIS\_101, 4.37, 1.6, 0.76, -4.49  
 1NAF, GLU\_199, 4.57, 0.07, 0, 0  
 3M7D, GLU\_255, 3.84, 0.14, -0.8, 0  
 2G5X, ASP\_90, 1.98, 0.77, -2.59, 0  
 1GSZ, LYS\_79, 10.29, -0.21, 0, 0  
 3GYW, ASP\_55, 4.09, 0.35, -0.06, 0  
 3MTT, GLU\_459, 4.5, 0, 0, 0  
 3ANJ, ASP\_297, 2.71, 0.63, -1.71, 0  
 4H89, ASP\_41, 3.14, 0.28, -0.94, 0  
 1NAR, ARG\_73, 12.22, -0.28, 0, 0  
 2D59, GLU\_95, 3.91, 0.21, -0.8, 0  
 1NAR, ASP\_118, 2.56, 0.63, -1.86, 0  
 1PDB, ASP\_95, 2.34, 0.77, -2.24, 0  
 2P1W, GLU\_141, 4.55, 0.28, -0.23, 0  
 2XMZ, GLU\_12, 4.5, 0, 0, 0  
 1YG2, CYS\_103, 9, 0, 0, 0  
 1UCH, ARG\_136, 12.5, 0, 0, 0  
 2B2H, TYR\_180, 12.06, 0.0, 11.1, 9.5  
 2Q99, ARG\_192, 12.5, 0, 0, 0  
 1TR9, LYS\_54, 10.29, -0.21, 0, 0  
 1PDB, GLU\_180, 1.58, 0.99, -1.6, -2.31  
 1AM2, ASP\_154, 3.8, 0, 0, 0  
 2CL3, TYR\_160, 10.0, 0, 0, 0  
 1XIP, GLU\_125, 4.5, 0, 0, 0  
 2E3S, GLU\_372, 4.5, 0, 0, 0  
 1OLR, GLU\_53, 4.57, 0.07, 0, 0  
 2OJQ, ARG\_448, 12.43, -0.07, 0, 0  
 2R05, LYS\_189, 10.22, -0.28, 0, 0  
 2HRZ, LYS\_274, 10.29, -0.21, 0, 0  
 1H4U, GLU\_587, 3.33, 0.49, -1.65, 0  
 3IRA, GLU\_28, 4.5, 0, 0, 0  
 1PVT, ASP\_74, 3.41, 0.21, -0.6, 0  
 2G2D, ASP\_105, 3.78, 0.07, -0.09, 0  
 2F9F, ASP\_97, 2.87, 0.49, -1.43, 0  
 3O48, ASP\_122, 4.1, 0.42, -0.12, 0  
 2QOP, LYS\_189, 10.43, -0.07, 0, 0  
 1O5J, GLU\_12, 3.64, 0.35, -1.21, 0  
 1ZBS, TYR\_139, 10.14, 0.14, 0, 0  
 3KB5, GLU\_312, 2.52, 0.42, -2.4, 0  
 1XTZ, GLU\_19, 2.51, 0.28, -2.27, 0  
 3L3P, LYS\_389, 10.5, 0, 0, 0  
 2QOP, GLU\_132, 4.68, 0.49, -0.31, 0  
 2VGM, GLU\_79, 3.85, 0.14, -0.79, 0  
 2R4Q, LYS\_244, 9.66, -0.84, 0, 0  
 1NIJ, HIS\_29, 8.67, 2.38, 0, -0.21  
 3P2F, ASP\_192, 3.57, 0.56, -0.79, 0  
 3EAZ, ARG\_107, 12.24, -1.05, 0.0, 0.79  
 3M70, LYS\_250, 10.36, -0.14, 0, 0  
 2V1L, ARG\_46, 12.08, -0.42, 0, 0  
 1WJG, GLU\_20, 4.5, 0, 0, 0  
 3BA1, LYS\_289, 10.15, -0.35, 0, 0  
 2EHG, ARG\_30, 12.29, -0.21, 0, 0  
 2EFK, GLU\_39, 3.53, 0.63, -1.6, 0  
 3A7L, ASP\_43, 3.99, 0.21, -0.02, 0  
 2FZ4, GLU\_91, 4.5, 0, 0, 0  
 2P1W, TYR\_209, 10.32, 0.21, -0.16, 0.26  
 1O0X, TYR\_189, 10.0, 0, 0, 0  
 1VJG, ARG\_138, 12.36, -0.14, 0, 0  
 4D8L, LYS\_139, 10.5, 0, 0, 0  
 1HU6, GLU\_71, 3.77, 0.21, -0.94, 0  
 2CXA, ASP\_62, 2.41, 0.49, -1.88, 0  
 1IAP, TYR\_225, 12.68, 1.04, 0, 1.64  
 1J74, ARG\_61, 11.66, -0.84, 0, 0  
 2DVK, ASP\_126, 2.54, 0.49, -1.75, 0  
 1E5S, ARG\_114, 12.01, -0.49, 0, 0  
 1H09, LYS\_222, 9.94, -0.56, 0, 0  
 3LE4, ASP\_344, 3.87, 0.07, 0, 0  
 2O8P, GLU\_51, 3.77, 0.07, -0.8, 0  
 2I6I, LYS\_83, 10.5, 0, 0, 0  
 1IDK, ARG\_41, 11.66, -0.84, 0, 0  
 1YB2, ASP\_19, 3.16, 0.49, -1.13, 0  
 1XKR, TYR\_184, 11.21, 0.21, 0, 1  
 3IVF, LYS\_357, 10.5, 0, 0, 0  
 2R4Q, ASP\_233, 3.29, 0.63, -1.14, 0  
 3KB5, ARG\_412, 11.94, -0.56, 0, 0  
 2G2D, CYS\_104, 9.91, -0.08, 0.47, 0.53  
 3U4K, LYS\_53, 10.43, -0.07, 0, 0  
 2G7O, ASP\_125, 3.05, 0.07, -0.82, 0  
 2CXA, ARG\_215, 11.8, -0.7, 0, 0  
 2Q13, GLU\_245, 4.5, 0, 0, 0  
 3BQE, GLU\_334, 2.17, 0.77, -3.1, 0  
 3A0X, ARG\_650, 12.22, -0.28, 0, 0  
 2OKT, GLU\_81, 3.83, 0.28, -0.94, 0  
 2IXM, ASP\_85, 2.77, 0.35, -1.38, 0  
 2D7U, LYS\_50, 10.08, -0.42, 0, 0  
 2V1L, GLU\_53, 4.5, 0, 0, 0  
 2ZTY, ARG\_134, 11.87, -0.63, 0, 0  
 1GPP, LYS\_72, 10.5, 0, 0, 0

3LD1,LYS\_85,10.43,-0.07,0,0  
2OBI,LYS\_80,10.5,0,0,0  
1YLN,GLU\_101,4.85,0.35,0,0  
3GV0,GLU\_161,4.13,0.07,-0.44,0  
2FPN,ARG\_48,12.5,0,0,0  
3UPD,HIS\_322,3.77,1.6,-0.31,-4.02  
1TXJ,LYS\_151,10.36,-0.14,0,0  
1YTQ,ARG\_80,12.29,-0.21,0,0  
1Z3X,GLU\_43,4.11,0.28,-0.67,0  
1OXZ,LYS\_176,10.29,-0.21,0,0  
1XFK,HIS\_82,6.5,0,0,0  
2YWK,CYS\_42,8.6,-0.4,0,0  
1P4X,ASP\_179,4.08,0.28,0,0  
1NRI,LYS\_161,10.29,-0.21,0,0  
1X8F,GLU\_39,4.06,0.14,-0.58,0  
1OGL,LYS\_247,10.5,0,0,0  
2GEN,GLU\_114,4.5,0,0,0  
4DBX,LYS\_166,10.5,0,0,0  
3ZXY,ASP\_91,2.17,0.91,-2.54,0  
3BZT,LYS\_273,10.5,0,0,0  
3KV0,ASP\_25,4.07,0.28,-0.01,0  
1TP6,ARG\_6,12.01,-0.49,0,0  
2OKT,ARG\_178,12.22,-0.28,0,0  
3JV1,ASP\_49,2.85,0.21,-1.16,0  
1XDZ,ASP\_126,1.99,0.98,-2.79,0  
3GE9,HIS\_203,6.5,0,0,0  
2F4Q,LYS\_302,10.08,-0.42,0,0  
1YOY,GLU\_165,4.6,0.14,-0.04,0  
1UAJ,ARG\_219,12.08,-0.42,0,0  
1YLN,GLU\_37,4.64,0.14,0,0  
3QAV,GLU\_141,4.37,1.05,-1.6,0.42  
2CN1,GLU\_242,3.84,0.14,-0.8,0  
1NKD,GLU\_35,4.5,0,0,0  
3P51,HIS\_96,7.03,0.95,0,-0.42  
4EUG,TYR\_38,10.14,0.14,0,0  
3T5B,CYS\_68,11.61,-0.48,0.3,0.9  
2OPJ,TYR\_251,10.47,0.15,0,0.32  
1DZF,TYR\_28,10.69,1.21,-0.4,-0.12  
1RL0,ARG\_68,11.8,-0.7,0,0  
2B2H,LYS\_270,10.5,0,0,0  
2OYZ,LYS\_4,10.29,-0.21,0,0  
2EHG,LYS\_139,10.5,0,0,0  
4FZR,GLU\_11,4.15,0.07,-0.42,0  
2YWX,GLU\_121,4.22,0.14,-0.42,0  
3NOK,GLU\_95,4.5,0,0,0  
3F6F,LYS\_130,10.43,-0.07,0,0  
2DOA,LYS\_140,10.29,-0.21,0,0  
1X6J,LYS\_63,10.29,-0.21,0,0  
2IF4,ARG\_270,11.85,-0.7,0,0.05  
2XHC,LYS\_330,10.29,-0.21,0,0  
1H4U,ARG\_393,12.36,-0.14,0,0  
1RL0,ASP\_241,3.97,0.21,-0.04,0  
2XJ4,GLU\_103,3.78,0.42,-1.14,0  
1WLY,ARG\_237,12.5,0,0,0  
1ZBM,GLU\_89,4.61,0.28,-0.17,0  
2H01,TYR\_30,13.3,0.21,0.69,2.4  
1IAP,GLU\_202,4.5,0,0,0  
1TP6,HIS\_13,1.99,0,0,-4.51  
2DBN,LYS\_11,10.29,-0.21,0,0  
3G9G,ASP\_10,3.93,0.42,-0.29,0  
1TXJ,TYR\_149,13.34,0.73,0.17,2.44  
2EHG,LYS\_74,10.43,-0.07,0,0  
3BA1,CYS\_168,7.23,-2.09,0,0.32  
1X1E,GLU\_37,4.54,0.28,-0.24,0  
1VJG,ASP\_199,3.28,0.21,-0.73,0  
4FD6,LYS\_129,10.22,-0.28,0,0  
3F6F,ARG\_182,11.73,-0.77,0,0  
2POY,ASP\_287,3.55,0.63,-0.87,0  
2IF4,LYS\_242,10.36,-0.14,0,0  
3NJM,TYR\_26,10.63,1.08,-0.45,0  
1XKR,GLU\_178,4.48,0,-0.02,0  
3JRT,ASP\_136,2.99,0,-0.81,0  
3DB9,CYS\_233,9.46,-1.34,-0.04,1.84  
2I88,LYS\_453,10.43,-0.07,0,0  
1VSM,LYS\_178,10.5,0,0,0  
1XDZ,LYS\_185,10.43,-0.07,0,0  
2F19,HIS\_11,6.29,0,-0.21  
2W1R,LYS\_91,10.5,0,0,0  
3EGN,ASP\_435,3.13,0.56,-1.22,0  
2B6P,ARG\_33,11.45,-1.05,0,0  
1BGF,ASP\_24,3.8,0,0,0  
2Q99,TYR\_292,12.84,1.11,-0.67,2.4  
2BLL,HIS\_592,7.03,0.6,-0.07  
3V75,HIS\_27,4.73,0,0.38,-2.15  
3LJC,LYS\_56,10.15,-0.35,0,0  
1EV8,GLU\_237,4.5,0,0,0  
3RE9,TYR\_180,10.07,0.07,0,0  
1T95,ARG\_99,11.8,-0.7,0,0  
2AD1,LYS\_267,10.43,-0.07,0,0  
3AUF,ARG\_195,12.22,-0.28,0,0  
2IRM,ASP\_298,3.2,0.07,-0.67,0  
4E8B,LYS\_98,10.29,-0.21,0,0  
2CVB,HIS\_32,6.74,0.38,0,-0.14  
3GEC,LYS\_437,10.29,-0.21,0,0  
1RWZ,ARG\_190,11.94,-0.56,0,0  
1XDZ,ARG\_127,11.87,-0.63,0,0  
3T5H,HIS\_208,4.28,0.06,0,-2.28  
3LJN,ARG\_314,12.08,-0.42,0,0  
1BYI,ARG\_183,12.36,-0.14,0,0  
2RJD,TYR\_309,10.07,0.07,0,0  
2ILR,ASP\_354,3.34,0.21,-0.68,0  
1PSW,GLU\_179,4.56,0.07,-0.01,0  
1J8B,GLU\_70,4.26,0.56,-0.8,0  
4DBX,GLU\_148,4.57,0.07,0,0  
2P1W,LYS\_46,9.87,-0.63,0,0  
2EA9,ASP\_39,3.95,0.42,-0.27,0  
3RKV,TYR\_246,11.5,0.41,0,1.09  
1X1E,GLU\_66,4.71,0.21,0,0  
1XKR,ASP\_159,4.22,0.42,0,0  
2ZCX,ARG\_89,12.36,-0.14,0,0  
2RIS,GLU\_40,3.95,0.63,-1.18,0  
3M70,GLU\_256,3.66,0.14,-0.98,0  
2Z84,HIS\_16,3.89,0,0.59,-3.2  
2QHT,GLU\_2,4.14,0.14,-0.5,0  
3C2E,CYS\_197,8.44,-0.77,0,0.21  
3IVF,LYS\_234,10.29,-0.21,0,0  
2CN1,LYS\_105,10.43,-0.07,0,0  
2EHG,TYR\_99,10,0,0,0  
1WPA,TYR\_443,9.99,0,-0.01,0  
1DTO,HIS\_161,6.78,0.42,0,-0.14  
2AHE,HIS\_74,6.81,0.31,0,0  
2PWQ,TYR\_63,10,0,0,0  
1LTU,ASP\_213,3.73,0.35,-0.42,0  
3M70,ARG\_133,10.66,-1.84,0,0  
1RHS,TYR\_47,9.15,0.57,-1.42,0  
2O4D,HIS\_114,7.17,0.74,0,-0.07  
3M3P,ASP\_132,3.23,0.07,-0.64,0  
1FQL,LYS\_411,10.15,-0.35,0,0  
2CIU,ARG\_154,12.15,-0.35,0,0  
2B0A,CYS\_128,6.34,-1.25,-2.39,0.98  
2XWS,ASP\_51,3.15,0.42,-1.06,0  
4F3J,ARG\_114,12.5,0,0,0  
4AM1,TYR\_323,10,0,0,0  
3B7H,ARG\_54,12.15,-0.35,0,0  
3P28,GLU\_198,4.57,0.07,0,0  
4DVD,ARG\_156,11.94,-0.56,0,0  
3JZN,LYS\_211,10.43,-0.07,0,0  
2R51,ARG\_24,11.52,-0.98,0,0  
2B0A,GLU\_152,3.5,0.07,-1.07,0  
3H5T,GLU\_214,4.5,0,0,0  
4EF5,LYS\_224,9.73,-0.77,0,0  
1Y2Q,GLU\_134,4.5,0,0,0  
1P1L,GLU\_14,3.36,0.7,-1.84,0  
3BWT,LYS\_878,10.36,-0.14,0,0  
3UX2,GLU\_150,4.57,0.07,0,0  
2Q07,ARG\_279,11.73,-0.77,0,0  
2AXO,GLU\_40,3.86,0.14,-0.78,0  
1OTM,LYS\_58,10.29,-0.21,0,0  
2YX0,CYS\_45,9.68,-1.64,0.2,3.2  
3G9B,TYR\_37,10,0,0,0  
2BLL,ASP\_441,2.71,0.28,-1.37,0  
2RIS,HIS\_128,7.09,0.8,0,-0.21  
1NAR,GLU\_7,12.04,3.54,1.6,2.4  
1UAJ,ARG\_234,12.5,0,0,0  
2I88,LYS\_402,10.29,-0.21,0,0  
2PLQ,ARG\_282,11.94,-0.56,0,0  
3IRA,TYR\_122,13.24,0.21,0.63,2.4  
3BPV,ASP\_60,1.98,0.56,-2.38,0  
1Q46,GLU\_92,4.08,0.14,-0.56,0  
2Q98,HIS\_27,6.43,0,-0.07  
2RGY,ARG\_354,11.66,-0.84,0,0  
3P28,ASP\_54,3.46,0.42,-0.76,0  
1SUU,LYS\_519,10.15,-0.35,0,0  
2OBI,GLU\_91,4.57,0.07,0,0  
3R87,TYR\_5,11.16,0.07,0,1.09  
3M7D,ARG\_14,12.43,-0.07,0,0  
3KT9,LYS\_48,10.43,-0.07,0,0  
1PSW,GLU\_50,4.61,1.12,-1.01,0  
4FZR,ARG\_361,12.43,-0.07,0,0  
3TMO,TYR\_335,10,0,0,0  
4ETX,ARG\_336,12.22,-0.28,0,0  
2F9F,GLU\_25,3.84,0.49,-1.15,0  
3BPV,ARG\_110,12.08,-0.42,0,0  
2R51,TYR\_271,11.75,0,-0.12,1.87  
1T95,GLU\_132,4.52,0.07,-0.05,0  
2QZQ,GLU\_79,4.71,0.21,0,0  
1YOY,LYS\_21,10.5,0,0,0  
3K1H,LYS\_56,10.43,-0.07,0,0  
2DOA,LYS\_301,10.43,-0.07,0,0  
3NJM,ASP\_52,1.72,0.98,-3.06,0  
2G5X,LYS\_79,10.5,0,0,0  
2RIK,ARG\_114,12.08,-0.42,0,0  
2PLQ,CYS\_139,9.28,-0.09,0,0.37  
2B61,ASP\_78,3.94,0.14,0,0  
3U56,ASP\_24,2.79,0.7,-1.71,0  
4DBX,LYS\_159,10.5,0,0,0  
3BJV,GLU\_140,3.28,0.49,-1.71,0  
1PBV,ARG\_118,12.5,0,0,0  
1NKD,ARG\_57,12.5,0,0,0  
1SJ8,LYS\_685,9.87,-0.63,0,0  
3PM2,LYS\_105,10.5,0,0,0  
2CXC,GLU\_98,4.71,0.21,0,0  
1RWZ,ARG\_73,12.43,-0.07,0,0  
3GEC,LYS\_387,10.5,0,0,0  
3CBN,TYR\_161,11.7,0.07,0,1.63  
3CBN,ASP\_110,3.28,0.63,-1.15,0  
1SUU,ARG\_724,10.96,-1.54,0,0  
2D59,HIS\_137,4.25,0.02,0,-2.27  
1T95,LYS\_60,10.43,-0.07,0,0  
1T95,LYS\_175,10.43,-0.07,0,0  
1FKM,HIS\_468,6.84,0.48,0,-0.14  
1X7F,GLU\_107,2.51,1.48,-3.47,0  
3AU3,TYR\_493,8.78,0.28,-1.51,0  
1WLY,ARG\_207,11.58,-0.98,0,0.66  
3MIX,HIS\_472,6.43,0,0,-0.07  
2H2W,GLU\_111,4.87,1.54,-1.17,0  
2BDD,GLU\_116,4.12,0.42,-0.8,0  
1NJ4,HIS\_320,6.46,0.03,0,-0.07  
3C5V,ARG\_113,13.3,-1.6,0.2,4  
3CIV,ARG\_208,12.29,-0.21,0,0  
2D8N,CYS\_29,8.94,-0.13,0,0.07  
1J7G,GLU\_22,10.5,0,0,0  
1H09,ARG\_213,11.45,-1.05,0,0  
3RVC,LYS\_131,10.22,-0.28,0,0  
2RGY,GLU\_126,4.5,0,0,0  
2Z14,ASP\_28,3.87,0.14,-0.07,0  
2X4L,GLU\_272,3.6,0.7,-1.6,0  
2XWS,GLU\_77,4.52,0.21,-0.19,0  
3AUF,GLU\_173,4.05,0.35,-0.8,0  
3EAZ,ARG\_166,12.36,-0.14,0,0  
1BKB,LYS\_100,9.87,-0.63,0,0  
3ULX,HIS\_21,6.5,0,0,0  
1ZBM,GLU\_39,4.51,2.14,-2.13,0  
3ASA,ARG\_285,12.29,-0.21,0,0  
3AU3,ARG\_564,11.94,-0.56,0,0  
1RZ2,ASP\_176,3.56,0.56,-0.8,0  
3OKQ,ARG\_595,12.5,0,0,0  
2ZQ5,ASP\_204,2.41,0.49,-1.88,0  
2WZ9,LYS\_29,10.43,-0.07,0,0  
3TRE,LYS\_42,10.43,-0.07,0,0  
3CXS,LYS\_79,10.29,-0.21,0,0  
3VHJ,LYS\_160,10.36,-0.14,0,0  
2EJX,ARG\_131,11.87,-0.63,0,0  
1V43,GLU\_184,3.65,0.36,-0.02,-1.19  
1I60,LYS\_77,10.43,-0.07,0,0  
3ASA,ARG\_285,12.29,-0.21,0,0  
2HRZ,GLU\_96,3.45,0.42,-1.47,0  
2P1W,ARG\_45,12.01,-0.49,0,0  
1DCF,HIS\_73,6.85,0.56,0,-0.21  
4E6S,ARG\_68,12.15,-0.35,0,0  
2ZQ5,ASP\_202,11.66,-0.84,0,0  
3BQW,LYS\_221,10.29,-0.21,0,0  
3GS9,ASP\_85,3.99,0.21,-0.02,0  
1ZHV,ASP\_103,3.49,0.49,-0.8,0  
3AUF,ARG\_38,12.08,-0.42,0,0  
2OBI,ASP\_112,3.87,0.07,0,0  
3LE4,ASP\_305,3.63,0,-0.17,0  
1H4U,HIS\_575,6.36,0,0,-0.14  
3BPP,ASP\_42,2.95,0.35,-1.2,0  
2FB6,GLU\_60,4.71,0.21,0,0  
2FXT,LYS\_315,9.87,-0.63,0,0  
2NRR,TYR\_494,10.15,0.14,-0.22,0.23  
4DVD,LYS\_136,10.5,0,0,0  
3U56,CYS\_694,10.13,-0.26,0,1.39  
3FFM,ASP\_53,3.26,0.35,-0.89,0  
1YTQ,ASP\_125,2.64,0.7,-1.86,0  
3EZZ,HIS\_33,7.17,0.75,0,-0.07  
1DOV,ARG\_165,11.94,-0.56,0,0  
3R2E,TYR\_53,10,0,0,0  
2E0T,ARG\_85,12.08,-0.42,0,0  
3A2Z,TYR\_26,9.1,0.25,0,-1.15  
3ZTA,LYS\_85,10.29,-0.21,0,0  
3M70,TYR\_257,11.54,0.14,-1,2.4  
1V43,ASP\_257,3.18,0.07,-0.68,0  
2POY,GLU\_164,3.56,0.14,-1.08,0  
1DOV,GLU\_178,4.5,0,0,0  
2PLQ,LYS\_37,10.5,0,0,0  
3B79,CYS\_79,10.23,-0.33,0.02,1.54  
3ASA,ASP\_94,2.86,0.42,-1.36,0  
3U2R,GLU\_33,4.57,0.07,0,0  
2YX0,TYR\_315,9.92,0,-0.08,0  
2B0J,LYS\_339,10.5,0,0,0  
2POL,GLU\_34,1.56,1.11,-1.36,-2.69  
3M7G,ARG\_205,11.87,-0.63,0,0  
3M66,ASP\_183,2.31,0.49,-1.98,0  
3CQ1,GLU\_84,4.5,0,0,0

1J7G,ASP\_43,3.3,0.42,-0.92,0  
3M7D,ASP\_49,1.91,0.63,-2.52,0  
1L3K,TYR\_128,11.23,0.5,0.73,0  
1V43,LYS\_339,10.22,-0.28,0,0  
2ZCO,ARG\_84,12.08,-0.42,0,0  
1RKA,GLU\_105,4.57,0.07,0,0  
1OLR,TYR\_9,10.07,0.07,0,0  
2JEO,ASP\_234,3.94,0.14,0,0  
4F85,GLU\_283,4.36,0,-0.14,0  
3BQW,ARG\_135,11.46,-1.04,0,0  
3UPD,ARG\_108,10.56,-1.94,0,0  
4EF5,ARG\_169,12.43,-0.07,0,0  
2CE6,ASP\_11,2.46,0.63,-1.97,0  
2B0A,GLU\_135,3.1,0.35,-1.75,0  
2BDD,HIS\_23,6.87,0.51,0,-0.14  
2D7J,TYR\_12,10.07,0.07,0,0  
3IPZ,LYS\_83,10.08,-0.42,0,0  
3UC9,TYR\_160,10,0,0,0  
1LPL,ASP\_185,2.13,0.77,-2.44,0  
3G9G,GLU\_165,4.5,0,0,0  
3TIR,ARG\_32,12.22,-0.28,0,0  
3QKY,TYR\_237,11.88,0.21,0,1.67  
2AZL,GLU\_158,3.39,0.49,-1.61,0  
1SQH,ARG\_87,11.87,-0.63,0,0  
3O48,LYS\_11,10.43,-0.07,0,0  
2G9D,HIS\_289,7.33,0.9,0,-0.07  
1Ri6,HIS\_299,6.15,0,0,-0.35  
1R3D,ASP\_263,3.8,0,0,0  
2CIU,ASP\_199,3.66,0.28,-0.43,0  
1QSZ,GLU\_637,4.57,0.07,0,0  
1PVT,GLU\_37,4.5,0,0,0  
1Z3X,GLU\_72,4.21,0.35,-0.64,0  
1JB3,CYS\_37,8.15,-1.61,0,0.76  
1AKO,CYS\_240,9,0,0,0  
3LPZ,LYS\_108,10.5,0,0,0  
1AIL,ASP\_12,3.28,0.28,-0.8,0  
3LJI,GLU\_34,4.64,0.14,0,0  
1YR6,GLU\_107,4.5,0,0,0  
1W7B,LYS\_281,10.5,0,0,0  
1PNE,GLU\_116,4.64,0.14,0,0  
1P4X,ARG\_107,11.87,-0.63,0,0  
1P4X,GLU\_36,3.04,0.5,-1.96,0  
2CN1,GLU\_256,4.09,0.35,-0.76,0  
2QV2,ARG\_260,12.29,-0.21,0,0  
2CN1,GLU\_195,4.68,0.28,-0.1,0  
3CSV,LYS\_328,10.5,0,0,0  
2QW2,ASP\_82,3.94,0.14,0,0  
1TLV,HIS\_100,6.41,1.6,2.4,-4.09  
3EX9,ARG\_14,12.01,-0.49,0,0  
3ERF,ARG\_32,13.51,-3.16,0.4,1.7  
2W0G,GLU\_153,4.78,0.28,0,0  
3G59,ASP\_297,4.22,0.42,0,0  
3MTT,ARG\_520,12.43,-0.07,0,0  
2GEN,GLU\_117,3.79,0.07,-0.78,0  
2YWJ,GLU\_116,4.12,0.42,-0.8,0  
1PVT,GLU\_34,4.79,0.07,0.22,0  
2OKT,GLU\_334,3.91,0.21,-0.8,0  
1RAJ,GLU\_72,4.46,0.14,-0.18,0  
1WPA,LYS\_433,10.5,0,0,0  
2YWJ,GLU\_13,3.92,0.42,-1,0  
3BPV,ARG\_69,12.5,0,0,0  
3M7G,HIS\_56,2.35,0.54,-1,-3.69  
3BQE,GLU\_239,3.73,0.35,-1.12,0  
2YWX,LYS\_153,10.08,-0.42,0,0  
3ERF,LYS\_224,10.29,-0.21,0,0  
4E9E,LYS\_526,10.29,-0.21,0,0  
1Q46,LYS\_162,10.29,-0.21,0,0  
1JB3,TYR\_35,8.29,0.21,-1.92,0  
2OEW,CYS\_122,7.74,-1.62,-1.96,2.33  
1DCF,GLU\_134,4.64,0.14,0,0  
1NAR,LYS\_214,10.5,0,0,0  
3L7N,GLU\_194,4.05,0.48,-0.93,0  
3CIV,GLU\_272,3.4,0.42,-1.52,0  
1XKR,GLU\_13,4.71,0.21,0,0  
2V81,LYS\_6,10.5,0,0,0  
2EEY,LYS\_133,10.43,-0.07,0,0  
3M3P,GLU\_186,4.85,0.35,0,0  
3H5T,HIS\_352,7.44,0.94,0,0  
1D2K,LYS\_247,10.5,0,0,0  
4ANN,LYS\_102,10.43,-0.07,0,0  
1WXQ,LYS\_293,9.8,-0.7,0,0  
1JYH,GLU\_57,4.71,0.21,0,0  
3M70,ARG\_77,11.87,-0.63,0,0  
2RGY,ARG\_165,12.43,-0.07,0,0  
3L0D,ARG\_126,11.8,-0.7,0,0  
3HZQ,GLU\_94,4.5,0,0,0  
1O0X,LYS\_141,10.5,0,0,0  
3ETU,ASP\_157,3.17,0.14,-0.77,0  
1ZP2,GLU\_69,4.3,0.56,-0.76,0  
2OEW,GLU\_197,4.72,3.42,-0.8,-2.4  
3O7K,GLU\_143,3.16,0.42,-1.76,0  
2Q12,TYR\_161,10.83,0.0,0.83  
3HQX,GLU\_107,4.25,0.14,-0.39,0  
1WP5,LYS\_133,10.5,0,0,0  
2R57,TYR\_180,13.87,0.28,1.19,2.4  
2R4Q,GLU\_194,4.5,0,0,0  
1UCH,ASP\_204,2.67,0.63,-1.76,0  
3R87,LYS\_85,10.01,-0.49,0,0  
2X4G,GLU\_167,4.57,0.07,0,0  
3L3P,ASP\_505,3.46,0.07,-0.41,0  
3E5T,CYS\_114,9,0,0,0  
1W7B,TYR\_199,10,0,0,0  
3LPZ,TYR\_38,10.07,0.07,0,0  
3ERF,HIS\_133,7.49,1.6,2.4,-3.01  
2F4Q,LYS\_272,10.5,0,0,0  
2AZL,HIS\_74,0.72,0.01,-2.4,-3.39  
1Q8B,GLU\_34,3.45,0.28,-1.33,0  
4ANN,GLU\_62,5.27,0.77,0,0  
2QVO,CYS\_62,8.85,-0.32,0,0.17  
1YM5,LYS\_63,10.43,-0.07,0,0  
3EAZ,GLU\_174,4.5,0,0,0  
3GS9,TYR\_266,13.83,0.0,15.3,6.8  
3FS3,HIS\_168,7.02,0.8,0,-0.28  
2B02,GLU\_370,3.77,0.07,-0.8,0  
3ETV,ASP\_162,3.94,0.14,0,0  
1RWZ,ASP\_93,0.9,0.63,-3.52,0  
1YM5,GLU\_106,3.49,0.91,-1.92,0  
3FS3,LYS\_194,10.36,-0.14,0,0  
2QHT,HIS\_24,5.07,1.22,0,-2.65  
1X7F,GLU\_2,4.69,0.14,0,0.05  
2IDC,HIS\_134,7.23,0.8,0,-0.07  
3M70,TYR\_174,8.81,0.25,-1.45,0  
1JKS,GLU\_114,4.5,0,0,0  
1N81,ASP\_181,3.34,0.14,-0.03,-0.57  
1DZF,GLU\_137,1.32,1.62,-2.4,-2.4  
3MIX,GLU\_499,4.57,0.07,0,0  
2EFK,LYS\_33,10.29,-0.21,0,0  
2OBP,GLU\_162,4.64,0.14,0,0  
3GW3,GLU\_271,3.83,0.28,-0.95,0  
1W7B,LYS\_88,10.5,0,0,0  
2X4L,LYS\_129,10.43,-0.07,0,0  
1SUU,LYS\_729,10.29,-0.21,0,0  
2PGX,CYS\_4,8.83,-0.17,0,0  
2BQX,ARG\_89,12.5,0,0,0  
1SBX,GLU\_102,3.84,0.14,-0.8,0  
1MHN,CYS\_123,8.01,-0.99,0,0  
1EYH,LYS\_128,10.5,0,0,0  
1J7G,ASP\_60,3.8,0,0,0  
3GG6,ARG\_174,12.5,0,0,0  
3ADQ,CYS\_285,7.58,-1.49,0,0.07  
2BV9,TYR\_171,13.8,0.76,0.64,2.4  
1J7G,TYR\_106,10.79,0.96,-1.61,1.44  
2HRZ,TYR\_126,11.55,1.55,0,0  
3IL3,LYS\_235,10.5,0,0,0  
3VHJ,LYS\_157,10.43,-0.07,0,0  
1R9W,LYS\_277,10.36,-0.14,0,0  
1Ri6,ARG\_61,11.66,-0.84,0,0  
2AXO,ASP\_164,3.41,0.35,-0.74,0  
3UX2,GLU\_71,3.58,0.49,-1.41,0  
1GPP,ASP\_439,3.84,0.07,-0.03,0  
3P51,LYS\_3,10.5,0,0,0  
3M3PLY,4.10,15,-0.35,0,0  
1X1E,GLU\_221,3.07,0.42,-1.85,0  
3B7H,ARG\_25,12.22,-0.28,0,0  
1RSQ,ASP\_75,3.5,0.49,-0.79,0  
3RLN,GLU\_749,4.07,0.51,-0.94,0  
1EYH,GLU\_98,4.71,0.21,0,0  
1KN3,LYS\_78,10.5,0,0,0  
2DG7,ASP\_179,3.2,0.21,-0.81,0  
3CAN,GLU\_16,4.71,0.21,0,0  
1SUU,GLU\_764,4.06,0.35,-0.79,0  
2C2Y,ARG\_51,12.15,-0.35,0,0  
3F6M,GLU\_146,4.57,0.63,-0.56,0  
2BCF,TYR\_268,11.12,1.68,-0.56,0  
3O16,LYS\_38,10.5,0,0,0  
3G65,ARG\_29,11.45,-1.05,0,0  
2E3S,ARG\_478,11.8,-0.7,0,0  
3G9B,GLU\_113,4.5,0,0,0  
1SI7,HIS\_43,7.09,0.86,0,-0.28  
2HNG,ARG\_9,11.52,-0.98,0,0  
2EYI,ASP\_223,2.89,0.56,-1.47,0  
1P4X,GLU\_99,4.5,0,0,0  
1WJG,TYR\_39,13.14,0.07,0.67,2.4  
2H2Z,HIS\_134,6.29,0,0,-0.21  
2RIK,ASP\_132,2.51,0.63,-1.92,0  
1O59,TYR\_343,10.74,0,0.74  
2D7U,LYS\_150,10.43,-0.07,0,0  
1JYH,LYS\_27,10.43,-0.07,0,0  
1GPP,HIS\_442,7.5,1.15,0,-0.14  
1WJG,ARG\_56,12.01,-0.49,0,0  
3FHF,GLU\_36,4.5,0,0,0  
2XHC,ARG\_98,11.45,-1.05,0,0  
1TWU,ASP\_48,3.04,0.63,-1.39,0  
3AU3,CYS\_599,5.22,-4,0,0.21  
1QZN,LYS\_13,10.01,-0.49,0,0  
2X4L,ASP\_144,1.97,0.98,-2.82,0  
3HVM,GLU\_34,4.57,0.07,0,0  
3CQ1,GLU\_39,3.87,0.28,-0.91,0  
2ROS,TYR\_112,9.46,0.07,-0.8,0.19  
2R4Q,GLU\_239,3.54,0.21,-1.17,0  
3HVV,ARG\_212,12.22,-0.28,0,0  
2W1R,ASP\_57,2.96,0.35,-1.19,0  
3QAV,TYR\_77,13.34,0.14,0.8,2.4  
3PBH,TYR\_31,9.92,0.14,-0.22,0  
2V1L,ASP\_97,3.2,0.56,-1.16,0  
1O3X,ARG\_214,11.59,-0.91,0,0  
2FC3,LYS\_41,10.22,-0.28,0,0  
1PVT,GLU\_136,4.5,0,0,0  
3EAZ,LYS\_86,10.5,0,0,0  
4AF2,LYS\_67,10.43,-0.07,0,0  
1X7F,ASP\_191,2.79,0.14,-1.14,0  
2O8I,GLU\_96,3.58,0.56,-1.47,0  
1GPP,ASP\_441,2.29,0.63,-2.14,0  
2B0A,GLU\_101,3.15,0.28,-1.62,0  
1LTU,ASP\_280,1.19,0.91,-3.52,0  
1Ri6,HIS\_286,4.93,0.82,0,-2.39  
1N81,ASP\_177,3.8,0,0,0  
3LQE,LYS\_345,10.36,-0.14,0,0  
1WP5,LYS\_313,10.01,-0.49,0,0  
2Q98,GLU\_110,4.57,0.07,0,0  
1WP5,LYS\_267,10.01,-0.49,0,0  
2JHY,LYS\_167,10.5,0,0,0  
3IV4,LYS\_69,10.15,-0.35,0,0  
3GT0,LYS\_84,10.29,-0.21,0,0  
1DOV,ASP\_233,3.94,0.14,0,0  
4H86,ASP\_75,3.8,0.07,-0.07,0  
3M7D,ARG\_293,11.11,-2.55,0,1.15  
4AE7,CYS\_119,8.63,-0.51,0,0.14  
3QAV,HIS\_209,6.31,0.02,0,-0.21  
3CAX,LYS\_235,10.22,-0.28,0,0  
2OKT,CYS\_48,8,-3.87,0.2,87  
3O7K,GLU\_96,3.84,0.14,-0.8,0  
1L2F,LYS\_320,10.36,-0.14,0,0  
3EOD,ARG\_74,11.29,-1.21,0,0  
1P2F,ARG\_192,11.98,-1.05,0,0.53  
3TMO,ASP\_249,4.08,0.28,0,0  
3EVN,GLU\_41,4.16,0.21,-0.55,0  
3ODJ,ASP\_33,3.87,0.07,0,0  
1UCH,ARG\_145,12.15,-0.35,0,0  
1L2F,LYS\_111,10.43,-0.07,0,0  
1AKO,GLU\_86,2.86,0.39,-0.53,-1.49  
4FD6,LYS\_96,10.29,-0.21,0,0  
2H85,ASP\_212,3.07,-1.5,0  
4DNU,ASP\_327,3.85,0.14,-0.09,0  
3M16,LYS\_29,10.43,-0.07,0,0  
2R57,ARG\_217,11.8,-0.7,0,0  
1X04,LYS\_106,10.15,-0.35,0,0  
3S0A,HIS\_97,6.5,0,0,0  
2P0Y,GLU\_265,3.46,0.21,-1.25,0  
3BQW,LYS\_274,10.43,-0.07,0,0  
3JSN,LYS\_72,10.36,-0.14,0,0  
2AZL,GLU\_58,4.5,0,0,0  
2AHE,LYS\_110,10.5,0,0,0  
2FBI,ARG\_88,12.5,0,0,0  
3B79,TYR\_11,10.14,0.14,0,0  
2WZ9,LYS\_128,10.5,0,0,0  
1VJG,LYS\_176,9.94,-0.56,0,0  
3P2F,ASP\_190,3.36,0.35,-0.79,0  
1SQH,ARG\_285,12.5,0,0,0  
2AHE,ARG\_133,12.22,-0.28,0,0  
1ZCE,LYS\_111,10.5,0,0,0  
1NAR,LYS\_110,10.08,-0.42,0,0  
1G8P,ARG\_101,11.8,-0.7,0,0  
2AHE,GLU\_135,1.45,0.42,-3.47,0  
1OGL,ARG\_75,11.87,-0.63,0,0  
1Z9L,LYS\_43,10.01,-0.49,0,0  
4FZR,ASP\_66,2.29,0.98,-2.49,0  
1BKR,ASP\_50,3.45,0.49,-0.84,0  
1NAF,LYS\_213,10.5,0,0,0  
3RE9,LYS\_174,10.5,0,0,0  
2D59,LYS\_100,9.94,-0.56,0,0  
1YG2,ARG\_156,12.15,-0.35,0,0  
1YTD,GLU\_10,4.48,0,-0.02,0  
1FKM,LYS\_585,10.5,0,0,0  
2NRK,HIS\_36,2.5,0.06,0,-4.06  
3P51,ARG\_146,12.43,-0.07,0,0  
1GXN,ARG\_329,12.15,-0.35,0,0  
3M70,ASP\_17,3.84,0.07,-0.03,0  
2CL3,LYS\_192,10.43,-0.07,0,0  
4FH3,ARG\_364,12.43,-0.07,0,0  
1MML,ARG\_211,11.14,-1.36,0,0  
2CWY,ARG\_16,12.08,-0.42,0,0  
3KB5,HIS\_373,6.6,0,1,0,0  
3N2T,LYS\_135,10.5,0,0,0  
1JT9,ASP\_32,3.87,0.07,0,0  
3TMO,CYS\_224,6.24,-2.83,0,0.07



3F5D, TYR\_55, 10.29, 0, 0, 0, 29  
3TMO, GLU\_321, 4.5, 0, 0, 0  
1E59, ARG\_168, 12.08, -0.42, 0, 0  
1DTO, TYR\_159, 11.11, 0, -0.1, 1.2  
1TD6, GLU\_178, 3.51, 0.42, -1.41, 0  
3ZXY, LYS\_12, 10.5, 0, 0, 0  
1AK1, LYS\_18, 10.29, -0.21, 0, 0  
1J74, ARG\_55, 12.5, 0, 0, 0  
3JRT, ARG\_164, 11.94, -0.56, 0, 0  
1V43, ASP\_367, 3.93, 0.14, -0.01, 0  
3JZN, ASP\_109, 3.94, 0.14, 0, 0  
3ELI, HIS\_116, 0.8, 0, -1.41, -4.29  
3ADO, GLU\_86, 4.5, 0, 0, 0  
2H30, LYS\_86, 10.22, -0.28, 0, 0  
3OOP, CYS\_113, 9, 0, 0, 0  
1YTD, GLU\_256, 3.63, 0.42, -1.28, 0  
3ODJ, ASP\_130, 4.01, 0.21, 0, 0  
1YTD, ARG\_380, 11.92, -2.37, 0, 1.79  
3ZXY, ARG\_238, 11.8, -0.7, 0, 0  
1NIJ, ASP\_290, 3.23, 0.07, -0.64, 0  
4FD6, LYS\_154, 10.29, -0.21, 0, 0  
2ZCO, HIS\_18, 1.66, 0, -2.4, 2.44  
1DUN, LYS\_98, 10.29, -0.21, 0, 0  
1R3F, ARG\_34, 12.5, 0, 0, 0  
3JRT, LYS\_70, 10.36, -0.14, 0, 0  
1ILW, GLU\_35, 3.7, 0.21, -1.01, 0  
1DTO, HIS\_35, 7.58, 1.22, 0, -0.14  
3HQX, TYR\_85, 10.45, 0.07, -0.21, 0.6  
3HST, GLU\_84, 4.52, 0.07, -0.05, 0  
3HUE, GLU\_95, 4.26, 0.21, -0.45, 0  
1PBV, ASP\_75, 3.17, 0.35, -0.98, 0  
2NYC, GLU\_259, 2.99, 0.42, -1.93, 0  
2O4D, GLU\_113, 4.57, 0.07, 0, 0  
1OGL, HIS\_269, 6.5, 0, 0, 0  
3NOK, ARG\_21, 12.12, -1.38, 0, 1  
2ZOM, TYR\_82, 12.94, 0.21, 0.33, 2.4  
2QZQ, LYS\_100, 10.5, 0, 0, 0  
1WXF, ARG\_68, 11.66, -0.84, 0, 0  
3LH5, ASP\_682, 3.41, 0.07, -0.46, 0  
1PVT, HIS\_17, 0.04, 0.54, 0, 0  
3CN5, ASP\_184, 2.36, 0.84, -2.28, 0  
2E3C, GLU\_341, 4.05, 0.28, -0.73, 0  
2VGM, LYS\_373, 10.08, -0.42, 0, 0  
3EJC, ASP\_163, 3.87, 0.63, -0.56, 0  
2Q12, ARG\_20, 12.5, 0, 0, 0  
3F1X, CYS\_108, 3.74, -5.32, 0, 0.07  
1XDZ, LYS\_111, 10.15, -0.35, 0, 0  
3UOV, TYR\_66, 9.77, 1, -0.07, -1.17  
2GZR, GLU\_243, 5.96, 1.56, -0.1, 0  
1P1L, GLU\_47, 4.24, 0.49, -0.75, 0  
1O9G, LYS\_218, 10.29, -0.21, 0, 0  
2DG7, ARG\_160, 12.29, -0.21, 0, 0  
3BWT, ASP\_558, 3.94, 0.14, 0, 0  
3ETV, ASP\_274, 4.08, 0.28, 0, 0  
3VHJ, ASP\_117, 3.73, 0, -0.07, 0  
1MJS, TYR\_363, 10, 0, 0, 0  
2GZQ, HIS\_43, 7.09, 0.8, 0, -0.21  
1XIP, GLU\_328, 4.5, 0, 0, 0  
1SIG, ARG\_225, 12.08, -0.42, 0, 0  
3UV9, TYR\_414, 10.98, 0.35, 0.63, 0  
1G8P, HIS\_184, 3.05, 0.66, 0, -4.11  
3JZN, LYS\_284, 10.5, 0, 0, 0  
2JKF, GLU\_43, 4.5, 0, 0, 0  
1AKO, ARG\_268, 12.5, 0, 0, 0  
3M70, HIS\_212, 7.23, 1.02, 0, -0.28  
2F4Q, GLU\_319, 4.57, 0.07, 0, 0  
3P29, GLU\_382, 0.95, 0.83, -2.11, -2.28  
2CVB, ARG\_130, 11.94, -0.56, 0, 0  
3H04, ARG\_117, 12.34, -0.63, 0, 0.47  
2RJD, GLU\_277, 4.43, 0, -0.07, 0  
3ASA, GLU\_230, 5.37, 3.83, -2.96, 0  
2C13, LYS\_210, 10.29, -0.21, 0, 0  
3V4G, HIS\_99, 4.46, 0, 0, -2.04  
2D59, LYS\_24, 9.73, -0.77, 0, 0  
1X6J, GLU\_82, 4.64, 0.14, 0, 0  
3FRR, ARG\_82, 12.22, -0.28, 0, 0  
2FB6, ASP\_5, 4.15, 0.35, 0, 0  
1O59, ARG\_321, 12.22, -0.28, 0, 0  
1WLW, GLU\_181, 4.5, 0, 0, 0  
4EUG, ASP\_176, 2.43, 0.98, -2.34, 0  
2NRR, TYR\_393, 12.69, 0.28, 0.01, 2.4  
3ERF, LYS\_105, 10.5, 0, 0, 0  
2ZQ5, LYS\_59, 10.5, 0, 0, 0  
2Z84, HIS\_40, 3.8, 1.46, 0, -4.17  
2GZQ, GLU\_142, 4.57, 0.07, 0, 0  
1X7F, ARG\_286, 11.8, -0.7, 0, 0  
1T07, ARG\_8, 11.87, -0.63, 0, 0  
4F8A, ARG\_702, 11.73, -0.77, 0, 0  
2DFL, ARG\_217, 10.99, -1.51, 0, 0  
3CX2, ARG\_215, 12.5, 0, 0, 0  
3EJG, LYS\_144, 9.52, -0.98, 0, 0  
1R53, TYR\_276, 10.23, 0.21, 0, 0.02  
3G9T, LYS\_35, 10.43, -0.07, 0, 0  
3CBN, ARG\_81, 11.31, -1.19, 0, 0  
3UPD, GLU\_300, 2.27, 3.04, -3.74, -1.53  
4AE7, ARG\_114, 12.01, -0.49, 0, 0  
3UC9, ASP\_159, 3.02, 0.07, -0.85, 0  
2HXB, LYS\_24, 10.36, -0.14, 0, 0  
1ZP2, LYS\_154, 10.5, 0, 0, 0  
2EJB, LYS\_3, 10.5, 0, 0, 0  
2PGE, ASP\_108, 3.31, 0.35, -0.84, 0  
1SIG, GLU\_254, 4.07, 0.21, -0.64, 0  
3CS1, GLU\_41, 1.92, 0.66, -1.81, -1.43  
1QQL, LYS\_27, 10.29, -0.21, 0, 0  
1AT0, ARG\_348, 12.22, -0.28, 0, 0  
2PGE, ARG\_82, 11.87, -0.63, 0, 0  
1OXZ, ASP\_189, 2.89, 0.42, -1.32, 0  
3BCH, LYS\_11, 10.15, -0.35, 0, 0  
2BDD, ASP\_151, 3.97, 0.28, -0.11, 0  
4DEZ, LYS\_192, 10.5, 0, 0, 0  
2AD1, LYS\_167, 10.5, 0, 0, 0  
3RLE, TYR\_196, 11.0, 0.14, -0.18, 1.04  
2EYI, TYR\_241, 11.78, 2.18, -0.4, 0  
1J7G, LYS\_116, 10.5, 0, 0, 0  
2C2Y, ARG\_181, 12.5, 0, 0, 0  
1ZCE, GLU\_110, 4.57, 0.07, 0, 0  
3ANJ, ASP\_393, 3.87, 0.07, 0, 0  
2FL4, TYR\_62, 13.56, 0.36, 0.8, 2.4  
1R6Y, GLU\_73, 4.71, 0.21, 0, 0  
3A2Z, ARG\_110, 12.15, -0.35, 0, 0  
3V3T, LYS\_276, 10.43, -0.07, 0, 0  
2P0L, ARG\_169, 12.29, -0.21, 0, 0  
3RAZ, GLU\_24, 4.37, 0.28, -0.41, 0  
4FH3, LYS\_255, 10.5, 0, 0, 0  
2IF4, CYS\_232, 9.14, -0.35, -1.01, 1.5  
2R57, TYR\_361, 12.52, 0.21, -0.42, 2.73  
3CRM, ARG\_282, 12.15, -0.35, 0, 0  
2HNG, LYS\_36, 10.5, 0, 0, 0  
2X4G, ARG\_72, 12.5, 0, 0, 0  
1TD6, GLU\_27, 4.64, 0.14, 0, 0  
2RH3, HIS\_143, 6.29, 0, -0.21  
3IOC, TYR\_149, 11.85, 1.56, 0.29, 0  
3UPD, HIS\_22, 6.5, 0, 0, 0  
2OGQ, LYS\_420, 10.5, 0, 0, 0  
2JKF, LYS\_100, 10.5, 0, 0, 0  
3UPD, ARG\_61, 11.8, -0.7, 0, 0  
2H2Z, HIS\_41, 6.17, 3.6, 0, -3.93  
2EDM, GLU\_66, 4.64, 0.14, 0, 0  
3JSN, ARG\_230, 12.43, -0.07, 0, 0  
3G53, CYS\_252, 8.98, -0.09, 0, 0.07  
1O5J, GLU\_86, 4.5, 0.07, -0.07, 0  
1H4U, GLU\_512, 4.5, 0, 0, 0  
3C2E, CYS\_269, 8.88, -0.12, 0, 0  
1Q8B, GLU\_73, 4.18, 0.35, -0.67, 0  
1TR9, ARG\_86, 11.8, -0.7, 0, 0  
1HF8, LYS\_238, 10.5, 0, 0, 0  
1WRU, ARG\_71, 11.66, -0.84, 0, 0  
3UAH, ASP\_465, 2.95, 0.35, -1.2, 0  
2D0A, ASP\_208, 3.87, 0.07, 0, 0  
2IDC, TYR\_44, 12.79, 1.89, -0.74, 1.64  
4DND, LYS\_89, 10.22, -0.28, 0, 0  
3UX2, GLU\_115, 3.77, 0.07, -0.8, 0  
2IXM, ASP\_240, 2.97, 0.56, -1.39, 0  
2ZOW, GLU\_46, 4.57, 0.07, 0, 0  
3G59, TYR\_191, 10, 0, 0, 0  
4ETX, ARG\_410, 11.94, -0.56, 0, 0  
3GOZ, LYS\_4, 10.5, 0, 0, 0  
2BAA, HIS\_169, 4.23, 0.3, 0, -2.57  
2PGE, GLU\_149, 4.41, 0.28, -0.37, 0  
1WRU, ARG\_286, 13.9, -1, 0, 2.4  
3ILC, GLU\_7, 4.35, 0, -0.15, 0  
1NAR, ARG\_135, 12.08, -0.42, 0, 0  
2BAA, HIS\_66, 6.85, 1.6, 2.39, -3.64  
3L7N, ASP\_27, 3.87, 0.07, 0, 0  
3BCY, GLU\_89, 4.12, 0.42, -0.8, 0  
2CL3, ARG\_78, 11.94, -0.56, 0, 0  
3G59, LYS\_84, 10.22, -0.28, 0, 0  
2P5D, TYR\_92, 13.3, 0.14, 0.76, 2.4  
3M3P, ASP\_168, 3.31, 0.21, -0.7, 0  
1BN6, LYS\_206, 10.5, 0, 0, 0  
1G8P, GLU\_152, 4.64, 0.14, 0, 0  
2IDC, ARG\_171, 12.5, 0, 0, 0  
1EYH, LYS\_97, 10.22, -0.28, 0, 0  
1BN6, ARG\_71, 11.87, -0.63, 0, 0  
1EV8, HIS\_217, 6.66, 0.16, 0, 0  
1RAJ, LYS\_435, 10.15, -0.35, 0, 0  
1JYH, GLU\_88, 3.98, 0.28, -0.8, 0  
3IRZ, ASP\_161, 3.02, 0.7, -1.47, 0  
4FNA, GLU\_169, 4.57, 0.07, 0, 0  
1YTD, LYS\_266, 10.29, -0.21, 0, 0  
2E0T, ARG\_100, 12.43, -0.07, 0, 0  
2FB1, ARG\_74, 11.87, -0.63, 0, 0  
3V46, ARG\_292, 12.36, -0.14, 0, 0  
2ILR, GLU\_418, 4.36, 0.21, -0.35, 0  
4ANN, LYS\_94, 9.8, -0.7, 0, 0  
1R7J, ASP\_69, 3.92, 0.14, -0.02, 0  
4F85, ARG\_126, 11.31, -1.19, 0, 0  
1SUU, ASP\_647, 3.87, 0.07, 0, 0  
4AE7, GLU\_151, 3.81, 0.49, -1.18, 0  
3TOW, ARG\_59, 12.5, 0, 0, 0  
3RLN, ARG\_657, 11.73, -0.77, 0, 0  
2BLL, ARG\_460, 13.08, -1.09, 0, 1.67  
3K1H, GLU\_137, 4.18, 0, -0.32, 0  
2FL7, LYS\_111, 10.08, -0.42, 0, 0  
3K8U, LYS\_46, 10.5, 0, 0, 0  
3JSN, ASP\_205, 2.56, 0.56, -1.79, 0  
1WXF, LYS\_112, 10.5, 0, 0, 0  
3F53, GLU\_63, 4.5, 0, 0, 0  
1QQE, LYS\_68, 10.22, -0.28, 0, 0  
3IBT, HIS\_244, 4.73, 1.65, 2.06, -5.48  
1AKO, LYS\_2, 9.8, -0.7, 0, 0  
1XTZ, GLU\_179, 4.85, 0.35, 0, 0  
3E0H, TYR\_132, 11.08, 1.08, 0, 0  
3EJG, HIS\_41, 3.03, 0.01, 0, -3.48  
2XJ4, ARG\_170, 11.45, -1.05, 0, 0  
1JKS, GLU\_143, 1.83, 0.53, -0.8, -2.4  
3P28, HIS\_191, 6.36, 0, -0.14  
3LQE, GLU\_471, 2.43, 0.42, -2.49, 0  
3H13, HIS\_283, 7.14, 0.78, 0, -0.14  
3TMO, ARG\_220, 4.5, 0, 0, 0  
1JT9, ARG\_253, 12.5, 0, 0, 0  
3O16, LYS\_116, 10.5, 0, 0, 0  
1E55, LYS\_233, 10.36, -0.14, 0, 0  
4GA2, TYR\_36, 11.41, 0, 0, 1.41  
1U7U, GLU\_383, 4.92, 0.42, 0, 0  
2WB8, CYS\_550, 8.71, -0.29, 0, 0  
2F8H, ASP\_94, 3.71, 0.28, -0.37, 0  
2VAN, GLU\_232, 4.78, 0.28, 0, 0  
2FL4, ASP\_52, 3.28, 0.28, -0.8, 0  
3GW3, ARG\_21, 12.08, -0.42, 0, 0  
1QZN, GLU\_124, 4.64, 0.14, 0, 0  
1UAJ, TYR\_54, 10, 0, 0, 0  
1RZ2, CYS\_233, 9.37, -0.3, -1.38, 2.05  
3PBH, LYS\_31, 10.22, -0.28, 0, 0  
3GE9, LYS\_153, 10.5, 0, 0, 0  
2GAU, LYS\_218, 10.43, -0.07, 0, 0  
1RLO, ARG\_24, 7.91, -2.43, 0, -2.16  
3P28, ASP\_149, 1.8, 0.42, -2.42, 0  
2AH5, ARG\_171, 12.5, 0, 0, 0  
1MJS, ARG\_322, 10.5, 0, 0, 0  
2FG1, LYS\_41, 10.5, 0, 0, 0  
3BB7, TYR\_256, 10.2, 0.14, 0, 0.06  
2JEO, GLU\_181, 4.5, 0, 0, 0  
3RKV, TYR\_214, 10.67, 0.65, -1.32, 1.34  
4DND, GLU\_42, 4.57, 0.07, 0, 0  
2D7U, ASP\_299, 3.64, 0, -0.16, 0  
3EZ7, CYS\_352, 9.06, -0.01, 0, 0.07  
1WLW, CYS\_240, 11.41, 0.65, 1.76  
3RE9, ARG\_165, 12.08, -0.42, 0, 0  
2DVK, ARG\_149, 11.8, -0.7, 0, 0  
1O6D, GLU\_36, 2.99, 0.42, -1.93, 0  
3FNI, LYS\_31, 10.22, -0.28, 0, 0  
1NJ4, GLU\_187, 4.2, 0.42, -0.72, 0  
2PGX, ARG\_47, 12.08, -0.42, 0, 0  
1Z3X, GLU\_13, 3.98, 0.28, -0.8, 0  
3UOV, GLU\_107, 4.12, 0.42, -0.8, 0  
4DEZ, LYS\_3, 10.43, -0.07, 0, 0  
3QO1, TYR\_6, 13.3, 0.21, 0.69, 2.4  
2OGQ, ARG\_579, 11.52, -0.98, 0, 0  
2CYG, ARG\_57, 12.68, -1.55, 0, 1.73  
2Z61, ARG\_318, 12.08, -0.42, 0, 0  
2JKF, GLU\_87, 4.63, 0.14, -0.01, 0  
3KB5, TYR\_450, 9.55, 0.07, -0.52, 0  
2RIK, ASP\_12, 3.85, 0.21, -0.16, 0  
4H86, TYR\_18, 10.82, 0.86, -0.04, 0  
2H01, CYS\_164, 8.93, -0.07, 0, 0  
3FK5, LYS\_23, 10.5, 0, 0, 0  
1YTQ, TYR\_158, 12.13, 0.07, 0, 2.06  
4FD6, LYS\_149, 10.43, -0.07, 0, 0  
2Z14, ASP\_108, 1.27, 0.63, -3.17, 0  
1Y2Q, LYS\_128, 9.87, -0.63, 0, 0  
1UXO, ARG\_26, 11.8, -0.7, 0, 0  
3T57, LYS\_55, 10.5, 0, 0, 0  
4EVF, ASP\_52, 3.82, 0.07, -0.05, 0  
3O16, ASP\_64, 3.8, 0, 0, 0  
2P52, ARG\_206, 12.08, -0.42, 0, 0  
3HYQ, ASP\_94, 2.73, 0.35, -1.43, 0  
2GZQ, LYS\_192, 10.43, -0.07, 0, 0  
3V46, GLU\_333, 4.73, 0.28, -0.05, 0  
1QQH, TYR\_87, 13.08, 0.28, -0.22, 3.04  
1X1E, ARG\_123, 10.27, -2.23, 0, 0  
1Z9L, ASP\_79, 3.25, 0.84, -1.39, 0  
1JT9, HIS\_232, 5.1, 1.78, 0, -3.18  
1YM5, TYR\_130, 10.73, 0.16, 0, 0.57  
1XEU, TYR\_225, 10.49, 0.49, 0, 0  
1T6L, GLU\_140, 4.76, 0.98, -0.72, 0

2WB8,GLU\_708,4.5,0,0,0  
3COU,GLU\_136,4.5,0,0,0  
3MTT,GLU\_440,4.44,0.28,-0.34,0  
3RLN,HIS\_757,6.89,1.62,17,-3.38  
1TJE,ARG\_151,10.54,-1.65,0,-0.31  
1X9G,ASP\_98,2.83,0.35,-1.32,0  
3PAC,GLU\_160,4.78,0.28,0,0  
1OST,ARG\_326,12.15,-0.35,0,0  
1XKR,GLU\_162,3.7,0.35,-1.15,0  
3NZL,TYR\_58,10,0,0,0  
2X5Y,GLU\_892,2.79,0.69,-2.4,0  
1QQH,TYR\_120,10.26,0.07,0.19,0  
2PGE,LYS\_184,10.5,0,0,0  
2P4D,LYS\_22,10.22,-0.28,0,0  
1YOY,LYS\_12,10.5,0,0,0  
3EIZ,ASP\_34,2.8,0.49,-1.49,0  
2BLI,ARG\_651,11.94,-0.56,0,0  
3N2T,LYS\_153,10.22,-0.28,0,0  
3KEY,ARG\_343,11.94,-0.56,0,0  
3ETV,ASP\_312,4.15,0.35,0,0  
1WXQ,GLU\_170,4.5,0,0,0  
1X1E,TYR\_176,11.2,1.2,0,0  
2OOK,ASP\_10,3.06,0.35,-1.09,0  
1AM2,ARG\_160,12.01,-0.49,0,0  
2OBI,LYS\_145,10.5,0,0,0  
2BOJ,ASP\_189,3.45,0.42,-0.77,0  
4E9E,LYS\_504,9.8,-0.7,0,0  
2R0S,TYR\_136,12.37,0.08,0.229  
1YM5,LYS\_62,10.36,-0.14,0,0  
3FHF,HIS\_149,7.69,0.126,-0.07  
1P6F,HIS\_163,6.63,0.27,0,-0.14  
1TXJ,LYS\_97,10.36,-0.14,0,0  
3C5V,GLU\_184,2.63,0.7,-2.57,0  
2H85,HIS\_234,4.01,0,-0.2,-2.29  
1NKD,LYS\_6,10.29,-0.21,0,0  
3ULX,LYS\_96,10.36,-0.14,0,0  
2NYC,CYS\_274,9.96,0,0,0.96  
3GMS,GLU\_21,2.73,0.63,-2.4,0  
1RL0,ARG\_137,13.88,-2.01,0,3.39  
1R53,ASP\_213,3.04,0.21,-0.97,0  
2D59,ARG\_114,12.29,-0.21,0,0  
1OXZ,HIS\_235,6.82,0.39,0,-0.07  
2V1L,HIS\_18,4.39,0.1,0,-2.21  
3B79,ARG\_43,12.08,-0.42,0,0  
1M5I,GLU\_151,3.73,0.56,-1.33,0  
3OA7,LYS\_514,10.36,-0.14,0,0  
2GEN,GLU\_29,3.36,0.14,-1.29,0  
2YYO,HIS\_10,6.63,0.34,0,-0.21  
3RNV,HIS\_417,6.43,0,0,-0.07  
2G2D,HIS\_54,6.65,0.15,0,0  
2GKG,ASP\_48,2.72,0.35,-1.43,0  
3IVF,ASP\_77,2.96,0.35,-1.18,0  
1T3Y,ASP\_54,2.99,0.07,-0.88,0  
2PPN,LYS\_17,10.5,0,0,0  
3NBI,ASP\_94,2.64,0.91,-2.07,0  
2XJ4,ARG\_99,12.22,-0.28,0,0  
1X9G,ASP\_100,3.28,0.28,-0.8,0  
2R57,ASP\_342,3.31,0.28,-0.77,0  
3A7L,GLU\_109,4.5,0,0,0  
2ZCX,ARG\_39,12.22,-0.28,0,0  
3F6F,LYS\_107,10.5,0,0,0  
3D5H,CYS\_332,11.95,0.133,1.62  
2VGM,GLU\_233,4.82,0.7,-0.38,0  
3G65,ARG\_165,11.87,-0.63,0,0  
1QQH,LYS\_148,9.66,-0.84,0,0  
3AUF,ARG\_198,12.01,-0.49,0,0  
4E9E,TYR\_545,11.08,0.36,0.72  
2H14,TYR\_284,13.34,0.14,0.8,2.4  
1GQE,LYS\_362,10.15,-0.35,0,0  
1YW5,LYS\_22,10.5,0,0,0  
1UUA,GLU\_232,2.38,0.28,-2.4,0  
1P2F,LYS\_119,10.29,-0.21,0,0  
2Z61,LYS\_200,10.5,0,0,0  
2I88,LYS\_512,10.22,-0.28,0,0  
4FCU,ARG\_31,11.52,-0.98,0,0  
3B79,GLU\_112,4.08,0.07,-0.49,0  
3M3P,ASP\_22,3.24,0.28,-0.84,0  
3PP8,ARG\_163,11.59,-0.91,0,0  
2EHG,LYS\_106,10.36,-0.14,0,0  
3FK5,LYS\_82,10.5,0,0,0  
2JHY,ASP\_89,2.43,0.56,-1.93,0  
1T3J,GLU\_706,4.44,0.21,-0.27,0  
3Q1C,ARG\_262,11.87,-0.63,0,0  
1H09,TYR\_273,12.1,1.27,-0.66,1.49  
3OKQ,CYS\_677,9.07,0,0,0.07  
3LJC,ARG\_226,12.36,-0.14,0,0  
3NJM,LYS\_59,10.5,0,0,0  
3ZXY,CYS\_32,8.16,-1.78,0,0.94  
3JV1,ASP\_138,3.8,0,0,0  
3LD1,ARG\_183,11.94,-0.56,0,0  
1QZN,ASP\_81,3.87,0.07,0,0  
2W1R,ARG\_104,12.15,-0.35,0,0  
1SQW,TYR\_35,13.27,0.07,0.8,2.4  
1FO9,GLU\_385,1.31,0.87,-2.4,-1.66  
1G5Z,ASP\_166,2.73,0.42,-1.49,0  
2H2Z,ARG\_222,12.29,-0.21,0,0  
3OA7,GLU\_469,4.43,0.35,-0.42,0  
2QK1,LYS\_467,10.5,0,0,0  
3ILC,GLU\_96,4.19,0.49,-0.8,0  
1SJB,LYS\_535,10.36,-0.14,0,0  
1ZYL,ARG\_131,11.73,-0.77,0,0  
3RNV,ARG\_406,11.38,-1.12,0,0  
1JKS,ASP\_149,3.2,0.56,-1.16,0  
1AM2,LYS\_165,10.08,-0.42,0,0  
2X4G,ARG\_311,12.01,-0.49,0,0  
1X1E,TYR\_99,10,0,0,0  
3GA2,CYS\_61,10.02,0,0,1.02  
2FM9,ASP\_72,3,0.49,-1.29,0  
1TWU,ASP\_58,3.79,0.14,-0.15,0  
3P2F,TYR\_77,10.87,0.75,-0.05,0.17  
2B0A,GLU\_104,4.64,0.14,0,0  
1MTZ,LYS\_123,10.29,-0.21,0,0  
2G9D,ASP\_296,4.15,0.35,0,0  
3V4G,GLU\_31,3.91,0.21,-0.8,0  
2CI3,GLU\_68,2.76,0.91,-2.65,0  
1V6T,TYR\_16,10,0,0,0  
4EKU,ARG\_85,12.29,-0.21,0,0  
2BAA,ARG\_90,12.36,-0.14,0,0  
2F8H,ARG\_62,11.1,-1.4,0,0  
2WOZ,TYR\_367,10,0,0,0  
3JZ9,LYS\_438,10.36,-0.14,0,0  
3CBN,LYS\_154,10.29,-0.21,0,0  
3V46,ARG\_268,12.5,0,0,0  
3HVM,LYS\_65,10.43,-0.07,0,0  
1FQI,GLU\_320,4.2,0.42,-0.72,0  
2FXT,GLU\_303,4.57,0.07,0,0  
2QHT,ARG\_104,11.87,-0.63,0,0  
3FTT,TYR\_82,9.73,0.07,-0.34,0  
2HXB,LYS\_151,10.5,0,0,0  
2P4D,LYS\_165,10.29,-0.21,0,0  
2RJD,GLU\_262,3.99,0.28,-0.79,0  
1XFK,ASP\_234,3.68,0.07,-0.19,0  
3MIX,GLU\_333,4.14,0.42,-0.79,0  
3RFY,ARG\_152,12.5,0,0,0  
3Q1C,ARG\_208,12.15,-0.35,0,0  
1AK1,CYS\_273,10.88,0.14,1.74  
3RLE,HIS\_156,7.33,0.97,0,-0.14  
3IBT,ARG\_198,11.43,-2.22,0,1.15  
1BN6,ARG\_299,12.43,-0.07,0,0  
1H09,TYR\_252,11.13,0,0,1.12  
2PIM,ARG\_111,12.5,0,0,0  
3H8Y,HIS\_85,6.5,0,0,0  
1Q5Z,ARG\_565,12.36,-0.14,0,0  
1SQH,ASP\_189,3.87,0.07,0,0  
1EV8,ASP\_156,3.87,0.07,0,0  
2CE6,GLU\_30,3.32,0.42,-1.6,0  
1XTZ,LYS\_226,10.36,-0.14,0,0  
2D7U,LYS\_304,10.29,-0.21,0,0  
3CS1,GLU\_150,4.5,0,0,0  
2H2Z,CYS\_145,7.4,-3.77,0,2.17  
4ECC,TYR\_7,10.31,1.84,-1.77,0.25  
4EVF,ARG\_229,12.24,-0.26,0,0  
2CIU,ARG\_111,11.66,-0.84,0,0  
2AXO,LYS\_95,10.22,-0.28,0,0  
1NJ4,ARG\_194,11.45,-1.05,0,0  
4ECC,LYS\_77,10.43,-0.07,0,0  
2Z61,LYS\_84,10.5,0,0,0  
2CI3,ARG\_135,12.15,-0.35,0,0  
3IRA,HIS\_149,7.24,0.74,0,0  
2RQY,ASP\_295,2.4,0.35,-1.76,0  
2OJG,GLU\_529,5.06,0.56,0,0  
1I60,CYS\_93,10.1,-0.12,0,1.22  
3H8Y,ASP\_25,3.56,0.35,-0.59,0  
4DBL,ASP\_64,3.25,0.35,-0.9,0  
1TJE,ARG\_145,12.15,-0.35,0,0  
2CN1,CYS\_53,9.14,0,0,0.14  
3ETU,LYS\_90,10.43,-0.07,0,0  
2JKF,LYS\_156,10.22,-0.28,0,0  
2IXM,LYS\_286,10.43,-0.07,0,0  
1RSQ,GLU\_4,3.52,0.07,-1.05,0  
3M16,LYS\_32,10.5,0,0,0  
3MIX,TYR\_545,10.62,0,0,0.62  
1UOH,GLU\_183,4.64,0.14,0,0  
3IL3,ARG\_196,12.5,0,0,0  
1X91,TYR\_68,10.02,0.07,-1.02,0.97  
4EVF,GLU\_185,3.24,0.7,-1.96,0  
2NSN,TYR\_88,11.24,0,0,1.24  
2W2S,ASP\_146,3.87,0.07,0,0  
3WPD,LYS\_297,10.36,-0.14,0,0  
1YDL,ASP\_39,2.81,0.14,-1.12,0  
1JYH,ASP\_141,3.23,0.28,-0.85,0  
1WLY,TYR\_135,11.83,1.15,0,0.68  
2B78,TYR\_26,11.32,1.32,0,0  
1R29,GLU\_77,4.5,0,0,0  
1BYI,ARG\_91,12.5,0,0,0  
3PM2,GLU\_58,4.33,0.82,-0.99,0  
1AKQ,TYR\_63,11.18,0,-0.1,1.28  
1ZCU,ARG\_33,12.15,-0.35,0,0  
1P6F,GLU\_153,4.57,0.07,0,0  
2P1W,GLU\_181,2.63,0.84,-0.74,-1.97  
2OBP,HIS\_153,2.95,0.79,-0.51,-3.83  
3M7D,GLU\_309,4.57,0.07,0,0  
1TLV,LYS\_82,10.15,-0.35,0,0  
3UPD,HIS\_310,7.44,1.08,0,-0.14  
2B6P,ARG\_11,12.36,-0.14,0,0  
3GA2,HIS\_125,3.75,0,0,-2.75  
3UAH,GLU\_272,4.62,0.14,-0.02,0  
2P65,LYS\_172,10.43,-0.07,0,0  
1TUL,TYR\_33,9.34,0.14,-0.8,0  
2EHG,GLU\_119,3.64,0.21,-1.06,0  
1ES9,HIS\_108,7.16,0.8,0,-0.14  
4AF2,ASP\_142,3.28,0.28,-0.8,0  
2E3H,GLU\_211,4.5,0,0,0  
3ONH,ASP\_460,3.93,0.14,-0.01,0  
1YTD,TYR\_387,10,0,0,0  
1YW5,LYS\_76,9.87,-0.63,0,0  
3MIX,ASP\_464,2.39,0.28,-1.7,0  
3HUE,GLU\_57,4.5,0,0,0  
3T57,ARG\_323,11.8,-0.7,0,0  
3ETU,LYS\_320,10.22,-0.28,0,0  
1ILW,GLU\_147,3.78,0.35,-1.07,0  
1WLY,GLU\_67,5.72,3.8,-2.04,-0.54  
3HQX,HIS\_26,6.99,0.63,0,-0.14  
2CXV,ARG\_30,12.15,-0.35,0,0  
3MTT,LYS\_516,10.5,0,0,0  
2EJB,ASP\_175,3.27,0.35,-0.88,0  
1MUF,ASP\_88,3.87,0.07,0,0  
1JSX,GLU\_183,4.19,0.49,-0.8,0  
2HRZ,TYR\_159,12.3,2.3,0,0  
4FLE,GLU\_98,4.1,0.35,-0.75,0  
1DZF,GLU\_203,4.38,0.07,-0.19,0  
3LMO,ASP\_48,3.23,0.77,-1.33,0  
1SUU,GLU\_718,3.08,0.29,-1.7,0  
1JYH,CYS\_65,8.12,-1.74,0,0.85  
1Y2Q,TYR\_120,10,0,0,0  
1WP5,GLU\_46,4.33,0.63,-0.8,0  
3G9G,LYS\_109,10.22,-0.28,0,0  
2W2S,ARG\_70,12.29,-0.21,0,0  
3G6S,TYR\_62,10.88,0.83,-0.05,0.09  
1UW7,GLU\_70,3.87,0.35,-0.98,0  
3DZ1,ARG\_31,11.73,-0.77,0,0  
2E0T,LYS\_180,10.29,-0.21,0,0  
1OLR,ARG\_193,12.5,0,0,0  
2B6P,HIS\_40,6.75,0.46,0,-0.21  
1NIJ,LYS\_211,10.15,-0.35,0,0  
1UXO,TYR\_57,10,0,0,0  
3K8U,ARG\_15,11.94,-0.56,0,0  
1G8P,GLU\_346,3.84,0.14,-0.8,0  
2R51,LYS\_203,10.43,-0.07,0,0  
3B7H,GLU\_10,3.98,0.28,-0.8,0  
1WOU,GLU\_62,4.5,0,0,0  
4E9E,LYS\_576,10.15,-0.35,0,0  
2VGM,LYS\_190,10.5,0,0,0  
1Y0K,GLU\_163,2.52,0.42,-2.4,0  
2V4X,LYS\_20,10.5,0,0,0  
3H5T,LYS\_260,10.36,-0.14,0,0  
2FPN,LYS\_185,10.5,0,0,0  
2O8P,ASP\_62,6.74,-2.33,0,0.07  
2OB5,LYS\_46,10.29,-0.21,0,0  
2H14,ASP\_76,2.54,0.35,-1.61,0  
1ZHV,LYS\_67,9.8,-0.7,0,0  
1SQW,ASP\_138,3.07,0.07,-0.8,0  
2QOP,HIS\_115,6.9,0.61,0,-0.21  
3QV0,ASP\_111,3.62,0.42,-0.61,0  
2FM9,LYS\_71,10.5,0,0,0  
2E3H,LYS\_268,10.36,-0.14,0,0  
2XMZ,ASP\_65,3.94,0.14,0,0  
3F6F,LYS\_206,10.29,-0.21,0,0  
1SNT,TYR\_310,10.83,1.6,-0.77,0  
2OBP,HIS\_153,2.95,0.79,-0.51,-3.83  
3L3P,GLU\_380,5.49,0.89,-0.13,0.22  
3M66,LYS\_224,10.29,-0.21,0,0  
1U7U,ARG\_226,12.22,-0.28,0,0  
1SBX,ARG\_184,12.43,-0.07,0,0  
3HKX,ASP\_273,3.91,0.14,-0.03,0  
3BZT,GLU\_284,3.07,0.7,-2.13,0  
3EJG,ARG\_59,11.94,-0.56,0,0  
2GAU,ARG\_88,11.91,-2.04,0,1.45  
2B0J,GLU\_193,4.64,0.14,0,0  
2RIS,ARG\_133,11.1,-1.4,0,0  
2GEN,GLU\_79,4.71,0.21,0,0  
2PGX,LYS\_69,10.5,0,0,0  
1PZC,LYS\_107,9.31,-1.19,0,0  
1ZBS,ASP\_235,2.91,0.84,-1.73,0  
1SQW,TYR\_172,10.99,0,0,0.99  
2R4Q,LYS\_195,10.15,-0.35,0,0

3M9A,GLU\_89,4.64,0.14,0,0  
2O4D,LYS\_27,10.36,-0.14,0,0  
1E5S,GLU\_219,4.71,0.21,0,0  
1YOY,LYS\_66,9.73,-0.77,0,0  
3Q6L,TYR\_129,9.6,1.82,-0.33,-1.89  
4ETX,GLU\_281,4.78,0.28,0,0  
1LN4,LYS\_6,10.29,-0.21,0,0  
1QSZ,LYS\_551,10.5,0,0,0  
3D9H,LYS\_185,10.29,-0.21,0,0  
1QYI,GLU\_158,3.98,0.28,-0.8,0  
3EGN,ARG\_401,12.43,-0.07,0,0  
1O6D,LYS\_51,10.15,-0.35,0,0  
2R4Q,GLU\_198,3.91,0.21,-0.8,0  
3G6S,LYS\_124,10.36,-0.14,0,0  
3AUF,HIS\_56,6.74,0.59,0,-0.35  
1UXQ,TYR\_6,9.83,0.07,-0.8,0.56  
3I47,LYS\_138,10.22,-0.28,0,0  
3UC9,TYR\_49,10,0,0,0  
2PPN,HIS\_25,6.47,0.04,0,-0.07  
1R3F,TYR\_263,10,0,0,0  
2OGQ,HIS\_468,6.5,0,0,0  
4DIU,TYR\_76,10.38,0.38,0,0  
1XKR,GLU\_112,4.31,0.28,-0.47,0  
3FHF,GLU\_53,3.91,0.21,-0.8,0  
3UV9,CYS\_438,8.04,-0.96,0,0  
1NFN,GLU\_121,3.82,0.21,-0.89,0  
2NRR,TYR\_361,13.66,0.02,3.64  
4EKU,HIS\_96,6.58,0.43,0,-0.35  
1PDB,LYS\_55,9.8,-0.7,0,0  
2AXO,GLU\_182,4.31,0.21,-0.4,0  
3HUE,ASP\_146,3.81,0.07,-0.06,0  
1ZBP,GLU\_186,2.99,0.49,-2,0  
3B4D,GLU\_187,2.95,0.63,-2.18,0  
1OST,TYR\_240,10.32,1.61,-1.29,0  
3JSN,ASP\_90,2.04,0.49,-2.25,0  
2X4L,GLU\_121,4.07,0.28,-0.71,0  
3G6S,GLU\_144,4.44,0,-0.06,0  
3GE9,GLU\_214,4.56,0.38,-0.32,0  
3FRR,HIS\_58,6.43,0,0,-0.07  
1GQE,CYS\_128,11.17,-0.43,0.2,6  
3CIV,HIS\_188,7.37,1.01,0,-0.14  
3ADO,HIS\_161,6.29,0,0,-0.21  
2O8P,GLU\_168,2.45,0.35,-2.4,0  
4ETX,ARG\_312,11.87,-0.63,0,0  
1O3X,GLU\_275,4.09,0.28,-0.69,0  
3HUE,ARG\_143,12.22,-0.28,0,0  
2HNG,GLU\_94,4.5,0,0,0  
4ESS,GLU\_87,4.64,0.14,0,0  
2V1L,CYS\_73,8.82,-0.18,0,0  
1BN6,GLU\_104,3.98,0.28,-0.8,0  
3EJG,GLU\_131,3.86,0.42,-1.06,0  
3IBT,GLU\_226,4.71,0.21,0,0  
4E9E,ASP\_521,3.78,0.42,-0.44,0  
2QOP,GLU\_72,4.5,0,0,0  
1UOH,GLU\_182,4.57,0.07,0,0  
1UOH,TYR\_161,12.5,0.07,0.43,2  
4FCU,ARG\_9,11.1,-1.4,0,0  
1PVT,ARG\_220,12.5,0,0,0  
3LJC,GLU\_34,4.25,0,-0.25,0  
1HUF,GLU\_124,4.57,0.07,0,0  
2QZQ,LYS\_97,10.01,-0.49,0,0  
2Z84,ASP\_204,2.49,0.35,-1.66,0  
1RWZ,HIS\_28,7.71,1.6,2.13,-2.52  
1PDB,ARG\_36,12.22,-0.28,0,0  
1ILW,LYS\_156,10.36,-0.14,0,0  
3GVO,HIS\_100,6.5,0,0,0  
2CW4,GLU\_81,4.5,0,0,0  
4EVF,LYS\_282,10.5,0,0,0  
2R2Y,ARG\_64,12.15,-0.35,0,0  
1X8F,GLU\_126,4.5,0,0,0  
1SIG,ASP\_118,3.79,0.07,-0.08,0  
3M3P,ARG\_38,12.5,0,0,0  
2OJQ,ARG\_478,11.38,-1.12,0,0  
3TIR,LYS\_220,10.29,-0.21,0,0  
3GFP,GLU\_323,4.5,0,0,0  
1R53,LYS\_366,10.01,-0.49,0,0  
3RRQ,ASP\_48,3.62,0.21,-0.39,0  
2Z84,CYS\_53,0.64,-7.9,-2.08,1.62  
1TUL,GLU\_80,3.86,0.49,-1.13,0  
3UOV,ASP\_48,1.96,0.56,-2.4,0  
1T95,GLU\_46,4.5,0,0,0  
3GOZ,CYS\_233,11.36,-0.63,2.02,0.96  
1CHD,ARG\_197,12.5,0,0,0  
1UJ8,GLU\_24,4.12,0.42,-0.8,0  
2FBQ,ARG\_140,11.52,-0.98,0,0  
2CE6,LYS\_33,10.29,-0.21,0,0  
2V5B,LYS\_251,10.22,-0.28,0,0  
1DUN,LYS\_56,10.29,-0.21,0,0  
3ANJ,LYS\_146,9.8,-0.7,0,0  
2HP7,ASP\_128,4.1,0.35,-0.05,0  
2P0L,ARG\_87,12.26,-1.67,0,1.43  
1JKS,GLU\_32,3.51,0.42,-1.41,0  
3G59,ARG\_188,12.08,-0.42,0,0  
3OIP,ARG\_79,12.5,0,0,0  
3ANJ,ARG\_247,10.03,-4.54,0,2.07  
1RAJ,GLU\_369,4.5,0,0,0  
2B0A,LYS\_137,10.43,-0.07,0,0  
3HUE,GLU\_313,4.08,0.28,-0.7,0  
1SQH,ARG\_178,12.15,-0.35,0,0  
2P1W,GLU\_164,4.57,0.07,0,0  
1WYC,ASP\_169,4.03,0.35,-0.12,0  
2P5D,LYS\_57,9.24,-1.26,0,0  
3F5D,LYS\_132,10.36,-0.14,0,0  
3O48,CYS\_79,9.75,-0.18,0.22,0.72  
3D9H,ARG\_234,12.08,-0.42,0,0  
1DZF,ARG\_26,11.77,-3.25,0.2,5.2  
1OGL,TYR\_209,11.11,0,-0.51,1.63  
1A8Q,ASP\_267,2.75,0.49,-1.54,0  
1NAF,CYS\_256,9.11,-0.03,0,0.14  
3KVO,GLU\_115,4.72,0.22,0,0  
2CN1,ARG\_233,12.29,-0.21,0,0  
1SNT,ARG\_182,12.08,-0.42,0,0  
1U3Y,ASP\_336,0.66,0.77,-3.91,0  
3M70,TYR\_185,11.27,0.24,-0.87,1.9  
2JEO,GLU\_45,3.91,0.21,-0.8,0  
3RFF,GLU\_96,3.71,0.07,-0.86,0  
3VJ8,GLU\_199,4.85,0.35,0,0  
1DTO,TYR\_167,12.61,0.21,0.2,4  
2QOP,ARG\_162,12.29,-0.21,0,0  
1Z9L,CYS\_53,9,0,0,0  
2E3S,TYR\_466,12.69,0.35,-0.06,2.4  
1RAJ,ARG\_376,11.02,-1.48,0,0  
1WRU,ASP\_251,3.27,0.56,-1.09,0  
2P4D,ARG\_19,12.5,0,0,0  
3N2T,GLU\_92,4.25,0.14,-0.39,0  
3GG6,CYS\_67,7.92,-1.08,0,0  
1MSI,ARG\_194,12.15,-0.35,0,0  
2WB8,LYS\_456,10.15,-0.35,0,0  
2HRZ,GLU\_321,3.38,0.56,-1.68,0  
1WRU,LYS\_308,9.45,-1.05,0,0  
2Z61,LYS\_29,10.22,-0.28,0,0  
1FO9,GLU\_373,4.5,0,0,0  
2B61,TYR\_32,10.56,1.31,-1.52,0.77  
2CXA,GLU\_133,3.01,2.7,-4.19,0  
3DHN,LYS\_100,10.15,-0.35,0,0  
2D7U,GLU\_108,4.58,0.21,-0.13,0  
2F8H,ASP\_78,2.37,0.28,-1.71,0  
1YIB,LYS\_212,10.5,0,0,0  
2CE6,HIS\_84,7.16,0.8,0,-0.14  
3PM2,LYS\_111,10.43,-0.07,0,0  
3EST,GLU\_141,3.51,0.42,-1.41,0  
2F8H,TYR\_36,8.78,0.14,-1.36,0  
1A8Q,HIS\_252,4.47,1.6,2.4,-6.03  
3GW3,TYR\_342,10.76,0.19,0.57  
2EJB,GLU\_25,4.24,0.84,-1.1,0  
2GEN,ASP\_148,3.26,0.35,-0.9,0  
3M7G,ARG\_93,12.5,0,0,0  
1XKR,GLU\_72,3.12,0.56,-1.94,0  
3JZN,LYS\_275,10.36,-0.14,0,0  
1L2F,GLU\_216,4.71,0.21,0,0  
1ZBM,TYR\_252,11.87,1.59,-0.1,0.38  
2E3S,HIS\_469,3.27,0.27,0,-3.5  
3FS3,TYR\_75,10,0,0,0  
3O7K,ARG\_103,11.94,-0.56,0,0  
4ESS,GLU\_47,4.85,0.35,0,0  
1XDZ,CYS\_124,9.49,0,0,0.49  
3RKV,GLU\_263,3.35,0.42,-1.57,0  
2WB8,ASP\_459,3.92,0.63,-0.51,0  
3FHF,ARG\_71,11.87,-0.63,0,0  
4FZR,HIS\_291,1.12,0.78,-0.7,-5.46  
1X7F,TYR\_244,9.47,0.07,-1.2,0.6  
2FXT,ARG\_404,11.54,-0.96,0,0  
3KEY,GLU\_369,3.46,0.42,-1.46,0  
3ETU,TYR\_111,9.38,0.14,-0.8,0.04  
3ERF,TYR\_213,11.08,1.08,0,0  
1OIS,LYS\_249,10.43,-0.07,0,0  
3G6S,TYR\_25,10,0,0,0  
1AD6,LYS\_420,10.43,-0.07,0,0  
2PGX,ARG\_214,11.55,-0.99,0,0.04  
3M70,ASP\_186,2.34,0.42,-1.88,0  
3I47,ARG\_152,12.22,-0.28,0,0  
1TUL,GLU\_22,4.5,0,0,0  
2CBE,HIS\_36,6.43,0,0,-0.07  
2FXT,ARG\_378,12.15,-0.35,0,0  
1O59,ARG\_254,12.08,-0.42,0,0  
3P28,ARG\_120,12.22,-0.28,0,0  
1V43,HIS\_304,6.43,0,0,-0.07  
3F7M,ASP\_201,0.49,0.84,-4.15,0  
3M66,GLU\_364,4.85,0.35,0,0  
3NBI,ARG\_107,12.5,0,0,0  
3HNX,HIS\_65,6.22,0,0,-0.28  
1FKM,HIS\_321,6.43,0,0,-0.07  
3GT0,LYS\_3,10.15,-0.35,0,0  
1TUL,GLU\_32,4.64,0.14,0,0  
3V1Q,TYR\_586,9.16,0.07,-0.95,0.04  
4FLE,HIS\_197,6.46,0.17,0,-0.21  
3NOK,ASP\_53,3.86,0.14,-0.08,0  
1DCF,ARG\_20,11.45,-1.05,0,0  
1SBX,CYS\_186,9.33,-0.07,0,0.4  
4ETX,ARG\_311,12.22,-0.28,0,0  
2EJB,ARG\_78,12.29,-0.21,0,0  
3M7G,GLU\_183,4.5,0,0,0  
2YYO,GLU\_112,4.05,0.35,-0.8,0  
1F2V,ARG\_116,12.29,-0.21,0,0  
2OBS,ASP\_86,3.87,0.07,0,0  
1NIJ,HIS\_23,6.43,0,0,-0.07  
3P28,HIS\_151,3.68,1.18,0,-4  
1O17,ARG\_6,11.94,-0.56,0,0  
1R9W,TYR\_327,10.87,1.07,-0.2,0  
4HDE,GLU\_152,4.5,0,0,0  
3ZXY,ARG\_18,11.94,-0.56,0,0  
3H6Q,ASP\_4,3.1,0.56,-1.26,0  
2H85,GLU\_304,3.91,0.21,-0.8,0  
2EFK,HIS\_272,6.74,0.31,0,-0.07  
1YR6,GLU\_25,3.92,0.21,-0.79,0  
2BLL,GLU\_434,2.56,2.43,-1.54,-2.83  
1RSS,ASP\_15,1.23,1.4,-3.96,0  
2YWJ,LYS\_177,10.36,-0.14,0,0  
3O47,GLU\_451,4.64,0.14,0,0  
3NBI,ARG\_9,12.22,-0.28,0,0  
2A4D,CYS\_218,8.49,-0.59,0,0.07  
1XFK,ARG\_119,10.47,-2.03,0,0  
2AZL,ARG\_91,10.81,-0.25,0,-1.45  
2O8I,ARG\_10,12.15,-0.35,0,0  
2R0S,ASP\_52,4.01,0.21,0,0  
2GAU,TYR\_129,13.19,1.25,0,1.94  
1KN3,GLU\_31,4.64,0.14,0,0  
1R3F,ARG\_181,13.39,-1.38,0,2.27  
1J8B,ARG\_54,11.94,-0.56,0,0  
1ZYL,GLU\_312,4.64,0.14,0,0  
2HNG,HIS\_46,7.09,0.66,0,-0.07  
2AZP,HIS\_90,6.26,3.6,1.87,-5.71  
3GVO,HIS\_165,2.58,0.03,0,-3.95  
1X8F,ARG\_63,11.31,-1.19,0,0  
2B61,GLU\_247,2.66,0.49,-2.33,0  
2JEO,GLU\_125,4.5,0,0,0  
2P52,ARG\_277,12.29,-0.21,0,0  
2YYO,ARG\_53,12.29,-0.21,0,0  
1YLN,GLU\_153,4.5,0,0,0  
3O16,GLU\_136,3.32,0.77,-1.95,0  
1G5Z,LYS\_195,10.22,-0.28,0,0  
2ILR,GLU\_299,3.43,0.35,-1.42,0  
1NRI,GLU\_59,4.6,0.14,-0.04,0  
4EZB,ARG\_47,12.36,-0.14,0,0  
2D2S,ASP\_728,4.01,0.28,-0.08,0  
3IBT,ASP\_47,12.08,-0.42,0,0  
2V4X,GLU\_99,3.98,0.28,-0.8,0  
3HVW,GLU\_233,4.5,0,0,0  
1SNT,GLU\_10,3.84,0.14,-0.8,0  
1S7K,HIS\_120,6.43,0,0,-0.07  
3UX2,ARG\_31,11.94,-0.56,0,0  
4DVD,ARG\_47,12.08,-0.42,0,0  
3T5B,GLU\_348,4.5,0,0,0  
4AE7,HIS\_94,6.33,0.11,0,-0.28  
1WXF,LYS\_14,10.29,-0.21,0,0  
3EVP,ASP\_86,2.77,0.35,-1.38,0  
3QAV,LYS\_132,10.29,-0.21,0,0  
3US6,ARG\_113,11.73,-0.77,0,0  
3LD1,LYS\_161,10.22,-0.28,0,0  
2ZCX,CYS\_87,8.56,-0.91,0,0.47  
3UC9,CYS\_181,8.64,-0.71,0,0.35  
3TRE,ARG\_10,12.22,-0.28,0,0  
3CIV,GLU\_187,0.86,0.71,-1.95,-2.4  
2CBE,LYS\_261,10.43,-0.07,0,0  
3AU3,LYS\_560,10.43,-0.07,0,0  
3OKQ,GLU\_661,4.5,0,0,0  
3A2Z,ASP\_9,3.96,0.35,-0.19,0  
3CSR,TYR\_24,11.59,0,0,1.59  
3G53,GLU\_69,4.5,0,0,0  
2Q12,LYS\_193,10.5,0,0,0  
3HQX,GLU\_74,4.5,0,0,0  
2H85,LYS\_344,10.5,0,0,0  
3FHF,GLU\_40,2.83,2.33,-1.6,-2.4  
3LJN,LYS\_58,10.29,-0.21,0,0  
1X8F,CYS\_249,8.67,-0.54,0,0.21  
3CGW,LYS\_215,10.5,0,0,0  
2FZ4,GLU\_151,4.5,0,0,0  
2E0T,HIS\_90,3.76,0,0,-2.74  
3H13,CYS\_345,8.05,-1.59,-0.07,0.71  
1BGF,ASP\_65,3.23,0.21,-0.78,0  
2B2H,GLU\_179,4.5,0,0,0  
2RFA,TYR\_89,10,0,0,0  
1YTD,ARG\_235,12.4,-2.5,0,2.4  
2HXB,ARG\_122,12.08,-0.42,0,0  
1DTO,HIS\_18,7.16,0.8,0,-0.14  
1SNT,CYS\_196,12.74,-0.02,0.99,2.77

1T95,ARG\_19,12.08,-0.42,0,0  
 15QW,LYS\_53,10.43,-0.07,0,0  
 2G55,TYR\_45,10.98,0,0,0.98  
 1OIS,LYS\_245,10.22,-0.28,0,0  
 2OEW,ASP\_16,3.22,0.56,-1.14,0  
 3MTT,LYS\_584,10.08,-0.42,0,0  
 1WYC,GLU\_212,3.84,0.14,-0.8,0  
 1XIP,HIS\_381,6.7,0.2,0,0  
 1BGF,ARG\_113,11.87,-0.63,0,0  
 1JKS,GLU\_118,4.21,0.07,-0.36,0  
 3O48,ARG\_98,12.08,-0.42,0,0  
 2PPN,TYR\_26,12.91,0.52,-0.01,2.4  
 3HVW,ARG\_253,12.15,-0.35,0,0  
 3I4T,GLU\_199,4.39,0.35,-0.47,0  
 3EUR,GLU\_134,4.05,0.35,-0.8,0  
 3TIR,LYS\_5,10.43,-0.07,0,0  
 2D7U,ASP\_337,3.8,0,0,0  
 2RIK,ASP\_5,3.79,0.56,-0.57,0  
 3E0H,ARG\_150,11.7,-0.8,0,0  
 3TRE,LYS\_14,10.22,-0.28,0,0  
 3EVZ,ARG\_217,12.22,-0.28,0,0  
 3H04,LYS\_24,10.15,-0.35,0,0  
 2PIM,ARG\_101,11.8,-0.7,0,0  
 2H2W,TYR\_247,10.07,0.07,0,0  
 2HNG,HIS\_18,6.29,0,0,-0.21  
 2RIK,LYS\_262,10.5,0,0,0  
 3CRM,GLU\_32,3.8,0.42,-1.12,0  
 3CZC,ARG\_67,12.08,-0.42,0,0  
 3ADO,GLU\_38,4.47,0.28,-0.31,0  
 3CCY,ASP\_61,3.65,0.42,-0.57,0  
 2R51,TYR\_231,8.86,0,-1.14,0  
 3NJM,ASP\_37,3.68,0.56,-0.68,0  
 2B0A,LYS\_155,10.5,0,0,0  
 2WB8,LYS\_726,10.22,-0.28,0,0  
 2C2Y,HIS\_54,6.69,3.68,0,-3.49  
 3GE9,ARG\_209,11.52,-0.98,0,0  
 2RIS,GLU\_64,4.78,0.28,0,0  
 1R16,HIS\_300,6.08,0,0,-0.42  
 1VJG,TYR\_76,9.91,0,-0.22,0.14  
 3G9G,LYS\_7,10.5,0,0,0  
 1OGL,GLU\_49,4.64,0.14,0,0  
 3ZXY,GLU\_134,4.56,0.07,-0.01,0  
 1DUN,ASP\_20,3.42,0.42,-0.8,0  
 4H4J,LYS\_102,10.5,0,0,0  
 3EVP,HIS\_130,7.39,1.17,0,-0.28  
 1CBY,HIS\_158,4.27,0,0,-2.23  
 3IU5,LYS\_124,10.43,-0.07,0,0  
 2IDC,GLU\_29,4.64,0.14,0,0  
 3GE9,TYR\_81,9.73,0,-0.27,0  
 4EVF,TYR\_42,13.67,0.23,0.82,6.4  
 3BWT,GLU\_861,4.71,0.21,0,0  
 3LPZ,LYS\_172,10.36,-0.14,0,0  
 3LD1,LYS\_211,9.8,-0.7,0,0  
 1DTO,GLU\_80,4.13,0.35,-0.72,0  
 3ONT,HIS\_72,7.46,1.03,0,-0.07  
 2B2H,LYS\_293,10.43,-0.07,0,0  
 1HF8,ASP\_180,2.66,0.49,-1.63,0  
 1U7U,LYS\_215,10.08,-0.42,0,0  
 2QZQ,GLU\_107,2.54,1.51,-0.8,-2.67  
 1MTZ,TYR\_165,10,0,0,0  
 4FH3,TYR\_122,9.6,0.07,-0.47,0  
 2IXM,ASP\_89,3.05,0.21,-0.96,0  
 2Z14,ARG\_116,11.94,-0.56,0,0  
 2FC3,LYS\_18,10.15,-0.35,0,0  
 3TRE,TYR\_90,10,0,0,0  
 1YR6,LYS\_175,9.87,-0.63,0,0  
 3UAH,LYS\_456,10.5,0,0,0  
 1ZCE,ASP\_84,1.86,0.56,-2.5,0  
 4EVF,LYS\_142,10.15,-0.35,0,0  
 2B2H,CYS\_283,11.46,0,0,2.46  
 3MIX,GLU\_649,4.5,0,0,0  
 3FRR,LYS\_159,10.5,0,0,0  
 2EJB,LYS\_104,10.43,-0.07,0,0  
 1ILW,ASP\_162,3.94,0.14,0,0  
 4DVD,GLU\_26,3.43,0.77,-1.84,0  
 1Z3X,ARG\_65,11.89,-2.72,0.2,1.1  
 3P28,LYS\_195,10.36,-0.14,0,0  
 3BWT,LYS\_601,10.29,-0.21,0,0  
 3P28,HIS\_100,3.68,0.14,0,-2.96  
 3IL3,LYS\_185,10.5,0,0,0  
 1H4U,LYS\_409,10.5,0,0,0  
 1ES9,GLU\_5,3.94,0.21,-0.77,0  
 2HP7,TYR\_124,11.71,0.35,-0.66,2.01  
 3FXH,GLU\_16,2.8,1.05,-2.75,0  
 2OB5,ARG\_57,12.15,-0.35,0,0  
 3CS1,ARG\_33,11.45,-1.05,0,0  
 2IIA,ARG\_67,12.15,-0.35,0,0  
 3LJC,GLU\_7,4.64,0.14,0,0  
 1TLV,GLU\_152,2.38,1.88,-1.6,-2.4  
 3RLE,ARG\_205,12.22,-0.28,0,0  
 2IDC,GLU\_119,4.85,0.35,0,0  
 3H13,CYS\_254,11.34,0.02,3.4  
 3IRA,HIS\_51,6.5,0,0,0  
 2Z0M,ASP\_149,3.89,0.14,-0.05,0  
 1PNE,LYS\_126,10.15,-0.35,0,0  
 4H86,TYR\_14,9.83,0.07,-0.24,0  
 3EYE,ASP\_43,3.35,0.35,-0.8,0  
 1TJE,ASP\_15,2.73,0.14,-1.21,0  
 1ZCE,LYS\_108,10.15,-0.35,0,0  
 1R16,ASP\_35,3.87,0.07,0,0  
 1TP6,ARG\_100,12.01,-0.49,0,0  
 1A8Q,ARG\_55,12.86,-1.96,0,2.32  
 3CRM,ASP\_265,4.13,0.42,-0.09,0  
 2FM9,ARG\_204,12.22,-0.28,0,0  
 2GEN,ARG\_144,12.5,0,0,0  
 3LE4,ARG\_331,11.66,-0.84,0,0  
 1Q5Z,LYS\_520,10.36,-0.14,0,0  
 3GG6,TYR\_44,8.42,0.14,-1.73,0  
 1R7J,TYR\_34,10,0,0,0  
 1SJB,ARG\_624,12.15,-0.35,0,0  
 3OKQ,GLU\_636,4.71,0.21,0,0  
 2BT8,ASP\_212,1.7,0.77,-2.87,0  
 2XJ4,GLU\_226,4.64,0.14,0,0  
 2EJX,ARG\_62,12.15,-0.35,0,0  
 2QHT,GLU\_69,4.38,0.14,-0.26,0  
 3U2R,LYS\_29,10.36,-0.14,0,0  
 1CBY,ASP\_69,2.23,0.49,-2.07,0  
 2O8P,LYS\_103,10.36,-0.14,0,0  
 2W0G,ASP\_245,3.04,0.35,-1.11,0  
 1YM5,GLU\_254,7.61,3.65,-1.24,0.7  
 1WNH,LYS\_210,10.43,-0.07,0,0  
 1JYH,GLU\_79,4.5,0,0,0  
 1X91,LYS\_50,10.5,0,0,0  
 3ZTA,GLU\_23,4.36,0.28,-0.42,0  
 1PNE,LYS\_107,10.5,0,0,0  
 3BWT,ARG\_858,11.8,-0.7,0,0  
 2PGE,ASP\_102,3.33,0.42,-0.89,0  
 2WB8,HIS\_737,6.68,1.46,0.9,-2.17  
 1R53,GLU\_128,2.6,0.29,-0.69,-1.49  
 2FM9,TYR\_186,13.93,1.27,0.33,2.33  
 1WXQ,LYS\_161,10.43,-0.07,0,0  
 3ON1,LYS\_55,10.43,-0.07,0,0  
 2VAN,GLU\_295,4.63,0.28,-0.15,0  
 3K85,GLU\_387,4.49,0,-0.01,0  
 2F9F,ASP\_14,2.61,0.28,-1.47,0  
 3N2T,LYS\_286,10.43,-0.07,0,0  
 4H86,TYR\_73,12.12,0,0,2.12  
 2BLI,ASP\_529,4.01,0.21,0,0  
 2V5B,LYS\_177,10.15,-0.35,0,0  
 1ZCU,LYS\_26,10.43,-0.07,0,0  
 3Q1C,ARG\_72,11.87,-0.63,0,0  
 1RLO,ASP\_197,3.76,0.07,-0.11,0  
 1ILW,ASP\_162,3.94,0.14,0,0  
 3HVM,LYS\_243,9.87,-0.63,0,0  
 1MUF,ARG\_115,11.88,-0.98,0,0.36  
 3O16,GLU\_76,4.23,0.35,-0.62,0  
 2O8P,ASP\_111,3.35,0.28,-0.73,0  
 3RKV,LYS\_205,10.5,0,0,0  
 1R15,TYR\_169,9.68,0.21,-0.53,0  
 2QZQ,ASP\_71,3.49,0.49,-0.8,0  
 2F4Q,ARG\_4,9.46,-3.13,0,0.09  
 1NFN,LYS\_157,10.43,-0.07,0,0  
 4FLE,GLU\_50,4.78,0.28,0,0  
 2E3C,CYS\_354,8.64,-1.04,0,0.68  
 3I47,ARG\_229,11.87,-0.63,0,0  
 1P4X,LYS\_27,10.5,0,0,0  
 1AD6,LYS\_524,10.29,-0.21,0,0  
 3TIR,ASP\_224,3.35,0.42,-0.87,0  
 3CS1,GLU\_61,4.5,0,0,0  
 1L3K,LYS\_15,10.36,-0.14,0,0  
 3CAX,ARG\_374,12.15,-0.35,0,0  
 3EVP,GLU\_175,4.12,0.42,-0.8,0  
 2XMZ,ARG\_134,12.7,-1.31,0,1.51  
 3B79,TYR\_16,9.43,0,-0.57,0  
 2Q5X,ASP\_732,3.14,0.14,-0.8,0  
 2I88,LYS\_436,10.5,0,0,0  
 3RNV,TYR\_429,10.07,0.07,0,0  
 1YOY,LYS\_157,10.36,-0.14,0,0  
 1ZKZ,TYR\_99,10.14,0.14,0,0  
 3BCY,GLU\_40,3.77,0.07,-0.8,0  
 3HVW,ASP\_183,3.44,0.56,-0.92,0  
 3HYQ,ARG\_51,12.7,-1.51,0,1.71  
 3A2Z,ARG\_144,11.45,-1.05,0,0  
 1OGL,ARG\_161,12.36,-0.14,0,0  
 3BWT,GLU\_791,4.1,0.35,-0.75,0  
 2H2W,LYS\_174,10.22,-0.28,0,0  
 1XDZ,GLU\_110,4.64,0.14,0,0  
 3M7D,ASP\_178,3.8,0,0,0  
 3CWC,ARG\_7,12.43,-0.07,0,0  
 1NAR,HIS\_217,6.36,0,0,-0.14  
 2BAA,ASP\_224,3.2,0.35,-0.95,0  
 1YIB,ARG\_214,12.08,-0.42,0,0  
 4FLE,LYS\_59,10.29,-0.21,0,0  
 1TXJ,LYS\_5,10.08,-0.42,0,0  
 2EFK,ARG\_47,11.66,-0.84,0,0  
 3LPZ,ARG\_37,12.22,-0.28,0,0  
 4EUG,ASP\_219,3.24,0.35,-0.91,0  
 1MML,HIS\_204,2.43,0.01,-2.38,-1.7  
 3H04,GLU\_205,4.64,0.14,0,0  
 3I4T,LYS\_100,10.43,-0.07,0,0  
 1ILW,HIS\_58,3.76,0.95,0,-3.69  
 2QV2,TYR\_249,10.25,0.1,-0.73,0.88  
 4GA2,ASP\_95,2.98,0.56,-1.38,0  
 3HUE,ARG\_307,11.8,-0.7,0,0  
 1R3F,LYS\_176,10.43,-0.07,0,0  
 1L2H,LYS\_109,9.38,-1.12,0,0  
 1NIJ,CYS\_98,11.11,-0.29,0.2,4  
 1Q8B,GLU\_91,4.5,0,0,0  
 1X7F,HIS\_269,3.14,0.92,0,-4.27  
 2NYC,ASP\_278,2.73,0.35,-1.42,0  
 3IDW,ASP\_27,3.97,0.21,-0.04,0  
 3DSH,GLU\_450,4.5,0,0,0  
 3UC9,ARG\_110,11.59,-0.91,0,0  
 2PWQ,ASP\_23,3.24,0.28,-0.84,0  
 3H6Q,ARG\_50,12.36,-0.14,0,0  
 2QRX,GLU\_20,2.72,0.42,-2.2,0  
 2H85,LYS\_34,10.22,-0.28,0,0  
 2H2Z,LYS\_12,10.36,-0.14,0,0  
 3T8R,ARG\_68,12.22,-0.28,0,0  
 3F6M,ARG\_26,12.08,-0.42,0,0  
 2PGX,HIS\_41,6.66,0.72,0,-0.56  
 1X04,ARG\_130,11.94,-0.56,0,0  
 3LMO,CYS\_16,9,0,0,0  
 1AD6,TYR\_498,12.23,0,-0.17,2.4  
 2XMZ,GLU\_252,4.57,0.07,0,0  
 2R05,LYS\_291,10.5,0,0,0  
 2V5B,LYS\_240,10.43,-0.07,0,0  
 2EJB,TYR\_82,13.22,0.56,0.26,2.4  
 3ELI,GLU\_129,4.57,0.07,0,0  
 3HUE,GLU\_303,4.57,0.07,0,0  
 1OXZ,GLU\_209,3.96,0.07,-0.61,0  
 3CQ1,TYR\_19,11,0,0,1  
 1OIS,GLU\_193,4.71,0.21,0,0  
 3H6Q,GLU\_68,3.52,1,-1.98,0  
 1X1E,ARG\_28,12.15,-0.35,0,0  
 1R16,GLU\_315,4.5,0,0,0  
 1MIX,ARG\_358,12.08,-0.42,0,0  
 2FBI,ARG\_71,12.22,-0.28,0,0  
 2AZL,GLU\_122,4.64,0.14,0,0  
 3EIZ,ARG\_87,11.94,-0.56,0,0  
 1QYI,HIS\_380,6.94,0.44,0,0  
 2G9D,ASP\_79,3.67,0.7,-0.83,0  
 1AD6,ARG\_451,11.38,-1.12,0,0  
 3RFF,TYR\_97,10,0,0,0  
 1TXJ,GLU\_154,2.07,0.77,-3.2,0  
 4DIU,GLU\_151,2.91,0.49,-2.08,0  
 1DVO,GLU\_147,4.64,0.14,0,0  
 1UAJ,LYS\_210,9.94,-0.56,0,0  
 1H4U,ARG\_438,11.31,-1.19,0,0  
 2APL,HIS\_23,7.23,0.8,0,-0.07  
 1TJE,ASP\_99,3.71,0,-0.09,0  
 4DIU,GLU\_151,2.91,0.49,-2.08,0  
 1DVO,GLU\_147,4.64,0.14,0,0  
 1UAJ,LYS\_210,9.94,-0.56,0,0  
 1H4U,ARG\_438,11.31,-1.19,0,0  
 2APL,HIS\_23,7.23,0.8,0,-0.07  
 1TJE,ASP\_99,3.71,0,-0.09,0  
 4DIU,GLU\_151,2.91,0.49,-2.08,0  
 1DVO,GLU\_147,4.64,0.14,0,0  
 3NJM,GLU\_18,4.64,0.14,0,0  
 1XWM,GLU\_24,5.19,1.41,-0.72,0  
 3SMD,GLU\_106,4.52,0.35,-0.33,0  
 3RLE,GLU\_175,4.01,0.28,-0.77,0  
 3ERF,TYR\_146,9.34,0.14,-0.8,0  
 1ZP2,TYR\_223,11.36,0,0,1.36  
 4GCO,ASP\_207,3.37,0.56,-0.98,0  
 1WXY,ASP\_298,2.91,0.49,-1.38,0  
 2CCY,LYS\_90,10.15,-0.35,0,0  
 3SMD,GLU\_68,4.23,0.35,-0.62,0  
 1MML,ARG\_110,12.29,-0.21,0,0  
 2CBE,ARG\_27,10.27,-2.23,0,0  
 3LMF,GLU\_79,4.5,0,0,0  
 2NRK,GLU\_35,2.45,0.81,-0.8,-2.06  
 2VGM,LYS\_183,10.5,0,0,0  
 1XWM,GLU\_57,4.5,0,0,0  
 1ATO,ARG\_358,11.94,-0.56,0,0  
 2YLF,GLU\_143,3.21,0.21,-1.49,0  
 1PDB,GLU\_101,4.5,0.21,-0.21,0  
 1GQE,TYR\_123,12.82,0.21,0.46,2.15  
 1ES9,ARG\_149,10.82,-1.68,0,0  
 3DB9,ARG\_159,12.22,-0.28,0,0  
 3T58,ARG\_259,12.77,-1.69,0,1.96  
 4DVD,LYS\_180,10.43,-0.07,0,0  
 3QKY,LYS\_169,10.01,-0.49,0,0  
 1TXJ,GLU\_168,4.5,0.28,-0.28,0  
 3ON1,LYS\_94,10.5,0,0,0  
 1NIJ,TYR\_151,13.67,1.8,-0.07,1.94  
 3FRR,TYR\_43,10.01,0.14,-1.51,1.37  
 3GT0,GLU\_137,3.77,0.35,-1.08,0  
 3ETV,CYS\_269,11.29,-0.22,0.02,2.5



3O48,ARG\_42,11.24,-1.26,0,0  
 3A7L,ASP\_117,2.42,0.42,-1.8,0  
 2EDM,LYS\_157,10.36,-0.14,0,0  
 2RH3,ARG\_118,12.29,-0.21,0,0  
 3OAF,CYS\_470,9,0,0,0  
 3BCY,GLU\_113,4.5,0,0,0  
 3GS3,GLU\_217,4.5,0,0,0  
 3JZN,CYS\_361,8.54,-0.06,-1.84,1.44  
 1XAW,LYS\_455,10.5,0,0,0  
 2PGE,ASP\_67,3.3,0.35,-0.85,0  
 2X4L,LYS\_99,10.5,0,0,0  
 2IN0,ARG\_92,12.15,-0.35,0,0  
 3KB5,LYS\_398,10.5,0,0,0  
 3B7H,ASP\_66,3.5,0.07,-0.37,0  
 1WL,ARG\_87,13.18,-1.16,0,1.84  
 2FC3,ARG\_112,12.08,-0.42,0,0  
 2F9F,GLU\_41,1.48,0.57,-1.19,-2.4  
 1QSZ,HIS\_538,6.43,0,0,-0.07  
 3V55,LYS\_679,10.29,-0.21,0,0  
 1RAJ,LYS\_375,10.29,-0.21,0,0  
 2X5Y,TYR\_833,10.37,0,0.37,0  
 1EV8,ASP\_66,2.54,0.14,-1.39,0  
 1JB3,ARG\_115,12.43,-0.07,0,0  
 2JEO,LYS\_108,10.5,0,0,0  
 2CXY,CYS\_101,7.32,-1.82,0,0.14  
 2V5B,ARG\_100,9.82,-2.68,0,0  
 3L3P,HIS\_275,6.29,0,0,-0.21  
 3ETU,TYR\_203,11.77,0.69,0,1.08  
 1ZP2,LYS\_37,10.5,0,0,0  
 1HF8,ASP\_260,2.98,0.35,-1.17,0  
 4GCO,GLU\_141,4.2,0.07,-0.37,0  
 2GQV,TYR\_46,9.87,0.07,-0.2,0  
 1J33,ASP\_93,3.21,0.21,-0.8,0  
 1T95,LYS\_234,10.5,0,0,0  
 4H89,ARG\_98,11.9,-0.6,0,0  
 1XEU,ARG\_241,12.5,0,0,0  
 1BKB,ASP\_89,3.94,0.14,0,0  
 2Q99,ASP\_127,3.18,0.28,-0.9,0  
 1MJS,ASP\_261,3.89,0.14,-0.05,0  
 2EEY,GLU\_22,4.5,0,0,-1.5  
 3V55,ASP\_629,3.85,0.21,-0.16,0  
 1RZ2,ARG\_164,11.8,-0.7,0,0  
 1DTO,CYS\_11,9.93,-0.18,0.74,0.37  
 2P65,TYR\_95,9.6,0.07,-0.47,0  
 2QK1,LYS\_425,10.5,0,0,0  
 3CSV,CYS\_312,9.35,-0.25,-0.38,0.98  
 3BCH,LYS\_42,10.36,-0.14,0,0  
 1LZL,ARG\_52,12.22,-0.28,0,0  
 2QOP,HIS\_147,6.64,0.21,0,-0.07  
 2AD1,TYR\_281,10.43,0.94,-0.51,0  
 4DVD,GLU\_41,4.5,0,0,0  
 3IRA,GLU\_1,4.64,0.14,0,0  
 2QK1,ARG\_423,11.15,-1.35,0,0  
 1JKS,LYS\_167,10.29,-0.21,0,0  
 1MUF,GLU\_272,4.5,0,0,0  
 2FBQ,LYS\_49,9.87,-0.63,0,0  
 1OGL,HIS\_38,7.1,0.74,0,-0.14  
 2E3S,GLU\_398,4.64,0.14,0,0  
 4AM1,ARG\_229,13.28,-3.07,0,3.85  
 2Q99,ASP\_238,3.66,0,-0.14,0  
 1GXN,TYR\_428,11.96,0.13,0,1.83  
 2R2Y,ARG\_122,11.87,-0.63,0,0  
 3MTT,TYR\_449,9.13,0.07,-0.94,0  
 1IAP,HIS\_192,6.5,0,0,0  
 3G9T,GLU\_92,4.46,0.76,-0.8,0  
 2Q13,TYR\_340,9.13,0.14,-1.01,0  
 1PSW,TYR\_140,9.81,0,-0.19,0  
 1ILW,GLU\_3,4.12,0.42,-0.8,0  
 2OKT,LYS\_137,10.29,-0.21,0,0  
 1EDG,HIS\_87,3.59,1.19,0,-4.1  
 4GA2,ASP\_7,1.42,0.28,-2.65,0  
 3RE9,GLU\_98,1.18,0.49,-3.81,0  
 3K8U,GLU\_125,4.5,0,0,0  
 1J33,GLU\_106,3.69,0.14,-0.95,0  
 3ODJ,TYR\_36,11.29,0,-0.09,1.38  
 1PSW,GLU\_321,4.5,0,0,0  
 1XKR,LYS\_190,10.15,-0.35,0,0  
 3EJG,ASP\_153,2.95,0.07,-0.92,0  
 1MUF,ASP\_136,3.94,0.14,0,0  
 1L3K,LYS\_106,10.36,-0.14,0,0  
 1BKB,LYS\_138,10.43,-0.07,0,0  
 3NR5,ARG\_28,13.62,-0.48,0,1.6  
 2ZTY,LYS\_133,10.43,-0.07,0,0  
 2PLQ,CYS\_91,10.66,-0.08,0,1.74  
 1RAJ,TYR\_454,13.18,0.21,-0.3,3.26  
 3P28,HIS\_192,8.12,1.9,0,-0.28  
 3MIX,GLU\_607,3.49,0.07,-1.08,0  
 1LPL,LYS\_190,10.43,-0.07,0,0  
 1WRU,ASP\_44,2.29,0.49,-2,0  
 3IPZ,LYS\_169,10.43,-0.07,0,0  
 1U53,GLU\_171,4.12,0.42,-0.8,0  
 3FRR,ARG\_51,12.08,-0.42,0,0  
 2F4Q,GLU\_317,4.78,0.28,0,0  
 3E7P,TYR\_247,10,0,0,0  
 1P4X,ASP\_241,3.82,0.07,-0.05,0  
 1Q5Z,ARG\_633,12.36,-0.14,0,0  
 1RHS,HIS\_138,6.72,0.29,0,-0.07  
 3ZTA,GLU\_32,4.92,0.42,0,0  
 2Z0W,ARG\_79,12.43,-0.07,0,0  
 2V4U,ARG\_465,11.59,-0.91,0,0  
 2FL4,GLU\_46,3.91,0.21,-0.8,0  
 4DND,HIS\_105,6.43,0,0,-0.07  
 2IRM,ASP\_17,3.87,0.07,0,0  
 2H14,TYR\_260,11.37,0.14,0,1.23  
 3EVN,LYS\_206,10.5,0,0,0  
 1LZL,ARG\_174,11.38,-1.12,0,0  
 3V55,ASP\_517,3.87,0.07,0,0  
 2IQT,GLU\_149,3.95,0.07,-0.62,0  
 1AK1,HIS\_201,5,0,0,-1.5  
 1O59,LYS\_284,10.43,-0.07,0,0  
 1X6J,HIS\_61,6.81,0.31,0,0  
 2BV9,ASP\_56,3.28,0.35,-0.87,0  
 2X4J,GLU\_41,4.4,0.7,-0.8,0  
 1LPL,GLU\_165,4.64,0.14,0,0  
 1UCH,CYS\_50,9.6,-0.17,-1.05,1.82  
 2H85,GLU\_201,4.5,0,0,0  
 2B78,TYR\_73,10.94,0.94,0,0  
 2B2H,TYR\_390,9.27,0.07,-0.8,0  
 2JKF,ASP\_65,2.22,0.98,-2.55,0  
 3RNV,GLU\_403,4.5,0,0,0  
 1MUF,TYR\_211,9.65,1.55,-0.64,-1.26  
 3ZTA,GLU\_96,4.5,0,0,0  
 3GE9,GLU\_66,4.5,0,0,0  
 3EIZ,LYS\_174,10.43,-0.07,0,0  
 3BB7,LYS\_147,10.5,0,0,0  
 3GA2,ARG\_230,12.01,-0.49,0,0  
 1BN6,HIS\_125,1.67,0,-2.27,-2.56  
 2O8P,ARG\_17,12.08,-0.42,0,0  
 2AH5,LYS\_201,10.5,0,0,0  
 2G3A,ARG\_136,12.15,-0.35,0,0  
 4EZB,LYS\_269,10.43,-0.07,0,0  
 2IXM,GLU\_246,3.98,0.28,-0.8,0  
 3T5B,HIS\_346,6.62,0.4,0,-0.28  
 2APL,LYS\_6,10.5,0,0,0  
 3EGN,ARG\_458,12.43,-0.07,0,0  
 3F5D,HIS\_35,6.36,0,0,-0.14  
 2HRZ,GLU\_74,3.57,0.28,-1.21,0  
 2ZCO,ASP\_228,3.93,0.14,-0.01,0  
 1L2F,GLU\_69,4.57,0.07,0,0  
 2Q12,LYS\_91,10.5,0,0,0  
 1ZBM,ARG\_96,12.08,-0.42,0,0  
 3H8Y,ARG\_51,11.59,-0.91,0,0  
 1P4X,TYR\_62,11.96,1.96,0,0  
 1SJ8,GLU\_586,4.85,0.35,0,0  
 2FB6,TYR\_104,12.99,0.21,0,2.78  
 2X4L,LYS\_197,10.5,0,0,0  
 3C6B,ASP\_138,3.28,0.28,-0.8,0  
 2H8O,HIS\_118,0.79,0.75,-2.4,-4.06  
 1JKS,ARG\_53,12.01,-0.49,0,0  
 3T57,GLU\_203,5.15,0.65,0,0  
 4DIU,HIS\_222,8.4,1.6,4.53,-4.22  
 3EVZ,HIS\_91,2.82,0.22,0,-3.9  
 1JB3,HIS\_33,6.5,0,0,0  
 1RI6,GLU\_309,4.5,0,0,0  
 1SIG,GLU\_155,4.99,0.49,0,0  
 1TLV,LYS\_123,10.15,-0.35,0,0  
 2EYI,ARG\_60,11.8,-0.7,0,0  
 2OJQ,ASP\_518,3.78,0,-0.02,0  
 1WP5,GLU\_241,2.52,0.42,-2.4,0  
 2G7O,LYS\_76,10.5,0,0,0  
 2Q13,ARG\_146,12.43,-0.07,0,0  
 1R53,ARG\_224,10.73,-1.77,0,0  
 3EJC,CYS\_114,9.46,0,0,0.46  
 3JV1,ARG\_64,12.22,-0.28,0,0  
 1FHL,LYS\_23,10.08,-0.42,0,0  
 4ECC,HIS\_228,6.65,0.29,0,-0.14  
 3NJM,LYS\_98,10.5,0,0,0  
 3JSN,GLU\_163,0.73,1.34,-2.57,-2.55  
 1QQL,ARG\_14,11.73,-0.77,0,0  
 1OXZ,GLU\_188,4.1,0.35,-0.75,0  
 3KV0,GLU\_43,4.5,0,0,0  
 3NBI,ASP\_63,3.8,0.14,-0.14,0  
 2A4D,LYS\_209,10.5,0,0,0  
 3FK5,HIS\_293,1.42,0,-1.94,-3.14  
 1V43,LYS\_191,10.36,-0.14,0,0  
 2GAU,ARG\_208,12.43,-0.07,0,0  
 2PPN,HIS\_87,6.5,0,0,0  
 3CRM,GLU\_112,4.71,0.21,0,0  
 3PZ9,GLU\_300,4.71,0.21,0,0  
 2P65,GLU\_163,3.34,0.56,-1.72,0  
 3O16,ASP\_192,3.94,0.14,0,0  
 2YX0,ARG\_338,13.04,-1.75,0,2.29  
 1JT9,HIS\_143,5.1,3.3,0,-2.83  
 3EVN,TYR\_50,13.03,0.14,0.49,2.4  
 2JHY,TYR\_110,12.27,1.48,0,0.79  
 3ZRI,HIS\_-4,7.36,0.93,0,-0.07  
 4EZB,CYS\_258,6.88,-2.26,0,0.14  
 2CIU,ASP\_105,2.75,0.56,-1.61,0  
 2NMU,CYS\_105,7.7,-2.37,0.06,1.01  
 1RAJ,GLU\_449,4.38,0,-0.12,0  
 3I4T,GLU\_203,4.74,0.21,0.03,0  
 4F8A,ASP\_606,2.94,0.35,-1.21,0  
 3Q6L,LYS\_113,10.29,-0.21,0,0  
 3HKX,ARG\_31,12.15,-0.35,0,0  
 4DBX,LYS\_11,10.36,-0.14,0,0  
 1RKA,ARG\_244,12.5,0,0,0  
 2INO,ARG\_416,11.66,-0.84,0,0  
 1TLV,LYS\_58,10.5,0,0,0  
 3K8J,HIS\_253,6.5,0,0,0  
 2HRZ,ARG\_185,12.22,-2.68,0,2.4  
 2FPN,GLU\_179,3.95,0.35,-0.9,0  
 2V81,ARG\_78,12.5,0,0,0  
 1AT0,ASP\_359,2.23,0.63,-2.2,0  
 1SFE,ASP\_153,1.67,0.7,-2.84,0  
 2FXT,ASP\_309,3.68,0.14,-0.26,0  
 2H2Z,ARG\_188,11.94,-0.56,0,0  
 1XTD,HIS\_62,6.5,0,0,0  
 2FBQ,LYS\_70,10.5,0,0,0  
 3O7K,HIS\_139,7.19,0.69,0,0  
 2D7J,CYS\_79,5.43,-4.29,-1.58,2.3  
 3BWT,ASP\_834,2.28,0.91,-2.43,0  
 1PVT,LYS\_18,10.15,-0.35,0,0  
 1M5I,ARG\_230,12.43,-0.07,0,0  
 3BWT,ASP\_586,3.26,0.14,-0.68,0  
 2D59,LYS\_43,10.5,0,0,0  
 4GA2,GLU\_144,4.5,0,0,0  
 2IQT,ASP\_218,3.51,0.21,-0.5,0  
 2BV9,LYS\_260,10.43,-0.07,0,0  
 1S17,ARG\_119,12.36,-0.14,0,0  
 3ILC,GLU\_129,4.05,0.35,-0.8,0  
 4ANN,GLU\_203,4.78,0.28,0,0  
 2P4D,ARG\_149,10.59,-1.91,0,0  
 3AU3,TYR\_500,10.14,0.14,0,0  
 1NJ4,LYS\_270,10.43,-0.07,0,0  
 3NBI,ASP\_160,4.01,0.21,0,0  
 2Q07,LYS\_374,10.5,0,0,0  
 1KN3,TYR\_181,11.09,1.09,0,0  
 1O3X,TYR\_294,10,0,0,0  
 2OJQ,TYR\_513,11.2,-0.07,1.27  
 2H14,GLU\_313,3.93,0.14,-0.71,0  
 3CAX,LYS\_416,10.22,-0.28,0,0  
 2A1V,LYS\_88,10.29,-0.21,0,0  
 1WNH,GLU\_118,4.5,0,0,0  
 1S17,LYS\_154,10.5,0,0,0  
 1G5Z,TYR\_101,11.86,0.07,0,1.79  
 3GT0,CYS\_270,10.9,15,0,0.15  
 1PNE,LYS\_25,10.36,-0.14,0,0  
 2QV2,ARG\_171,12.5,0,0,0  
 3GG6,GLU\_103,2.52,0.42,-2.4,0  
 2PGX,TYR\_222,10.68,0,0,0.68  
 1MML,ARG\_241,12.15,-0.35,0,0  
 2G3A,GLU\_87,4.08,0.07,-0.49,0  
 2H85,LYS\_316,10.43,-0.07,0,0  
 2OJQ,GLU\_665,3.91,0.21,-0.8,0  
 3CSV,GLU\_213,4.05,0.35,-0.8,0  
 1J85,ARG\_45,11.73,-0.77,0,0  
 3IVF,ARG\_91,12.22,-0.28,0,0  
 1YM5,LYS\_93,2.45,0.67,-1.6,-1.12  
 3LH5,ASP\_731,1.39,0.56,-2.96,0  
 3RLN,GLU\_715,4.65,0.35,-0.2,0  
 1OGL,ASP\_140,3.87,0.07,0,0  
 3CSV,CYS\_238,8.57,-0.5,0,0.07  
 1K95,LYS\_108,10.5,0,0,0  
 1SQH,ARG\_32,12.01,-0.49,0,0  
 3UC9,LYS\_96,10.36,-0.14,0,0  
 2H2W,ASP\_244,3.31,0.42,-0.91,0  
 3M3P,ARG\_221,11.66,-0.84,0,0  
 1PZC,TYR\_22,10.81,0.07,0,0.74  
 4GCO,GLU\_146,4.05,0.35,-0.8,0  
 2OJP,CYS\_220,6.6,-2.54,0.14  
 1X7F,TYR\_278,11.18,0,0,1.18  
 1ZBP,LYS\_133,10.36,-0.14,0,0  
 1UW7,ARG\_99,12.15,-0.35,0,0  
 1X7F,ARG\_3,11.31,-1.19,0,0  
 2H2Z,ASP\_229,3.31,0.07,-0.56,0  
 3GV0,ARG\_315,12.01,-0.49,0,0  
 4DBX,GLU\_274,4.03,2.11,-0.8,-1.77  
 1DTO,TYR\_19,9.51,0.31,-0.8,0  
 1L2F,LYS\_209,10.43,-0.07,0,0  
 3E7P,GLU\_151,3.42,2.9,-2.01,-1.97  
 2Z0M,TYR\_324,10.07,0.07,0,0  
 1T95,ARG\_83,12.22,-0.28,0,0  
 2Z84,LYS\_183,10.5,0,0,0  
 3T8R,ARG\_108,11.8,-0.7,0,0  
 1MN3,LYS\_436,10.5,0,0,0  
 3H13,ARG\_315,12.1,-0.4,0,0

2R4Q, TYR\_273, 13.71, 0.07, 0.8, 2.84  
 3P2F, ASP\_180, 3.63, 0.63, -0.8, 0  
 3L7N, GLU\_64, 3.93, 0.49, -1.06, 0  
 1T95, ARG\_35, 11.88, -0.62, 0, 0  
 3I4T, TYR\_239, 9.71, 0.07, -0.36, 0  
 2GAU, LYS\_215, 10.36, -0.14, 0, 0  
 1JT9, LYS\_234, 10.43, -0.07, 0, 0  
 3M70, LYS\_36, 10.43, -0.07, 0, 0  
 2B0J, GLU\_140, 4.57, 0.07, 0, 0  
 3K8U, LYS\_92, 10.5, 0, 0, 0  
 2RGY, GLU\_342, 4.5, 0, 0, 0  
 200K, HIS\_37, 7.24, 0.95, 0, -0.21  
 2I88, LYS\_382, 10.36, -0.14, 0, 0  
 3N2T, GLU\_113, 3.98, 0.28, -0.8, 0  
 3G59, GLU\_16, 4.92, 0.42, 0, 0  
 2Q07, LYS\_417, 10.5, 0, 0, 0  
 2Z0M, GLU\_173, 3.67, 0.21, -1.04, 0  
 1RAJ, ASP\_459, 3.82, 0.07, -0.05, 0  
 3F1X, TYR\_138, 10, 0, 0, 0  
 1EV8, ARG\_21, 12.36, -0.14, 0, 0  
 1JT9, HIS\_222, 6.43, 0, 0, -0.07  
 3A7L, GLU\_14, 6.02, 2.64, -1.12, 0  
 1WYC, ARG\_229, 11.87, -0.63, 0, 0  
 1YB2, ASP\_13, 2.97, 0.42, -1.25, 0  
 3F53, TYR\_53, 12.44, 0, 0.33, 2.11  
 3H9W, LYS\_28, 10.36, -0.14, 0, 0  
 3LJC, ASP\_45, 3.57, 0.07, -0.3, 0  
 3HUE, LYS\_99, 10.5, 0, 0, 0  
 2FXT, TYR\_377, 10.17, 0.24, 0, -0.07  
 1UAJ, GLU\_11, 4.5, 0, 0, 0  
 3PU6, TYR\_84, 10, 0, 0, 0  
 4EKU, LYS\_42, 10.29, -0.21, 0, 0  
 3FHF, LYS\_165, 10.5, 0, 0, 0  
 2G9D, LYS\_304, 9.94, -0.56, 0, 0  
 1G8P, GLU\_86, 3.68, 0.35, -1.17, 0  
 1Z3X, ARG\_162, 11.52, -0.98, 0, 0  
 3F5D, GLU\_18, 5.19, 2.07, -1.38, 0  
 1MUF, CYS\_288, 9.07, 0, 0, 0.07  
 3EZ7, ARG\_217, 12.22, -0.28, 0, 0  
 4FD6, GLU\_212, 4.5, 0, 0, 0  
 1LTU, GLU\_124, 2.34, 0.35, -2.51, 0  
 1UCH, CYS\_209, 11.22, -0.19, 0.2, 41  
 1L2H, ARG\_98, 11.87, -0.63, 0, 0  
 1OIS, GLU\_262, 4.64, 0.14, 0, 0  
 1R53, GLU\_204, 3.77, 0.42, -1.15, 0  
 3ADO, GLU\_300, 4.5, 0, 0, 0  
 1S17, ARG\_191, 12.08, -0.42, 0, 0  
 1XDZ, GLU\_194, 4.57, 0.07, 0, 0  
 3LJI, CYS\_109, 8.72, -0.28, 0, 0  
 1Z3X, GLU\_111, 4.61, 0.35, -0.24, 0  
 3E5T, GLU\_86, 4.06, 0.7, -1.14, 0  
 2F4Q, TYR\_12, 11.38, 1.35, -1.31, 1.34  
 1DTO, CYS\_5, 8.55, -0.51, 0, 0.07  
 2EEY, LYS\_67, 10.5, 0, 0, 0  
 1JYH, GLU\_147, 4.55, 0.6, -0.8, 0.25  
 1O6D, GLU\_23, 4.54, 0.34, -0.3, 0  
 3IL3, ARG\_288, 13.87, -1.03, 0.2, 4  
 2ZCX, ASP\_30, 3.45, 0.21, -0.56, 0  
 2YWK, GLU\_24, 4.5, 0, 0, 0  
 2BDV, ARG\_94, 10.69, -1.81, 0, 0  
 1MUF, TYR\_156, 10.14, 0.14, 0, 0  
 2DOA, HIS\_119, 6.51, 0.01, 0, 0  
 1P1L, ASP\_98, 3.53, 0.7, -0.97, 0  
 2I88, GLU\_388, 3.92, 0.21, -0.79, 0  
 3UX2, LYS\_131, 10.5, 0, 0, 0  
 2B2H, HIS\_385, 4.96, 0.76, 0.31, -2.61  
 1ZBS, ASP\_181, 3.52, 0.21, -0.49, 0  
 1MD6, LYS\_16, 9.59, -0.91, 0, 0  
 1PDB, ARG\_77, 12.29, -0.21, 0, 0  
 2AHE, ASP\_58, 3.26, 0.84, -1.38, 0  
 3N2T, GLU\_172, 4.5, 0, 0, 0  
 3BQW, GLU\_160, 5.99, 0.8, -0.77, 1.46  
 4AM1, HIS\_261, 4.19, 0, 0, -2.31  
 3RFF, ASP\_48, 3.72, 0, -0.08, 0  
 2GZR, ASP\_281, 4.09, 0.63, -0.34, 0  
 2E0T, HIS\_96, 6.77, 0.48, 0, -0.21  
 1N81, HIS\_25, 6.29, 0, 0, -0.21  
 1YLN, GLU\_225, 4.61, 0.14, -0.03, 0  
 1BN6, ASP\_87, 3.87, 0.07, 0, 0  
 1LTU, TYR\_48, 13.1, 0.25, 0.45, 2.4  
 3CSR, TYR\_20, 13.41, 0.21, 0.8, 2.4  
 1KW4, CYS\_32, 9, 0, 0, 0  
 3UC9, ASP\_42, 3.41, 0.28, -0.67, 0  
 1N81, TYR\_84, 12.04, 0.42, -0.1, 1.72  
 2OJQ, ARG\_517, 12.5, 0, 0, 0  
 1F09, ASP\_125, 3.37, 0.42, -0.85, 0  
 2FZP, GLU\_273, 4.05, 0.35, -0.8, 0  
 1O5T, LYS\_220, 10.29, -0.21, 0, 0  
 2D7J, HIS\_14, 6.5, 0, 0, 0  
 2GAU, ASP\_16, 3.13, 0.21, -0.88, 0  
 2OJQ, LYS\_564, 10.5, 0, 0, 0  
 1WLY, LYS\_111, 9.94, -0.56, 0, 0  
 1X7F, TYR\_159, 9.76, 0.56, -0.8, 0  
 2FD5, ARG\_82, 11.8, -0.7, 0, 0  
 3K8J, ASP\_45, 2.74, 0.28, -1.34, 0  
 1LZL, GLU\_230, 4.31, 0, -0.19, 0  
 4F3J, ARG\_161, 12.15, -0.35, 0, 0  
 1RAJ, ASP\_79, 3.17, 0.21, -0.84, 0  
 3ZXY, ARG\_95, 11.87, -0.63, 0, 0  
 3EJG, CYS\_81, 9.14, 0, 0, 0.14  
 3R2E, GLU\_58, 4.71, 0.21, 0, 0  
 3N2T, GLU\_48, 4.71, 0.21, 0, 0  
 1DCF, GLU\_74, 4.56, 0.07, -0.01, 0  
 1WPS, ARG\_283, 12.15, -0.35, 0, 0  
 2YX0, HIS\_67, 5.19, 0, 0, -1.31  
 1PVT, LYS\_213, 10.5, 0, 0, 0  
 3COU, ARG\_142, 12.01, -0.49, 0, 0  
 1DVO, HIS\_153, 6.5, 0, 0, 0  
 1WNH, LYS\_162, 10.08, -0.42, 0, 0  
 2PGE, ARG\_88, 12.01, -0.49, 0, 0  
 1J7G, LYS\_12, 10.22, -0.28, 0, 0  
 1WPS, TYR\_284, 10, 0, 0, 0  
 3IVF, GLU\_291, 3.98, 0.21, -0.73, 0  
 1BKR, HIS\_104, 6.36, 0, 0, -0.14  
 2CN1, GLU\_273, 1.51, 0.94, -2.24, -1.69  
 1TWU, HIS\_100, 6.36, 0, 0, -0.14  
 3B4D, LYS\_247, 9.94, -0.56, 0, 0  
 3PZ9, LYS\_215, 10.43, -0.07, 0, 0  
 1H4U, ARG\_631, 12.22, -0.28, 0, 0  
 3LD1, TYR\_26, 11.74, 0.51, -0.32, 1.55  
 1AKO, GLU\_19, 4.57, 0.07, 0, 0  
 2RGY, LYS\_105, 10.5, 0, 0, 0  
 2Q98, ASP\_68, 1.2, 0.63, -3.22, 0  
 1RKA, LYS\_207, 10.15, -0.35, 0, 0  
 2OEW, ASP\_314, 3.91, 0.14, -0.03, 0  
 2ZCO, ARG\_265, 11.51, -0.96, 0, -0.03  
 1JKS, ARG\_48, 12.15, -0.35, 0, 0  
 2ZCX, GLU\_25, 4.21, 0.07, -0.36, 0  
 2IQT, GLU\_178, 4.49, 1.87, -0.8, -1.08  
 1LZL, GLU\_145, 4.5, 0, 0, 0  
 1H4U, TYR\_546, 11.72, 0.07, -0.75, 2.4  
 3ETU, LYS\_237, 10.5, 0, 0, 0  
 1ZBS, HIS\_278, 2.16, 0, -0.74, -3.6  
 3CGW, GLU\_67, 4.71, 0.21, 0, 0  
 3V55, ASP\_640, 3.8, 0, 0, 0  
 1NWA, ASP\_100, 2.81, 0.56, -1.55, 0  
 3F53, TYR\_56, 11.17, 0, 0, 1.17  
 1CHD, GLU\_215, 3.77, 0.07, -0.8, 0  
 1EDG, LYS\_71, 10.15, -0.35, 0, 0  
 2FGG, ARG\_23, 11.94, -0.56, 0, 0  
 1MTZ, ARG\_49, 12.08, -0.42, 0, 0  
 1W7B, LYS\_28, 9.8, -0.7, 0, 0  
 3T8R, GLU\_94, 3.9, 0.49, -1.09, 0  
 3FTT, LYS\_11, 10.5, 0, 0, 0  
 2B2H, HIS\_185, 5.2, 1.56, 0, -2.86  
 1ZBM, ARG\_180, 11.52, -0.98, 0, 0  
 3OKQ, LYS\_600, 10.15, -0.35, 0, 0  
 3ADO, ARG\_171, 12.08, -0.42, 0, 0  
 3EZ7, TYR\_287, 10.95, 1.75, -0.8, 0  
 1I60, LYS\_235, 10.43, -0.07, 0, 0  
 2CN1, LYS\_64, 10.08, -0.42, 0, 0  
 3ANJ, GLU\_385, 3.78, 4.9, -3.7, -1.92  
 3JZ9, ASP\_477, 3.32, 0.35, -0.83, 0  
 1RIS, ARG\_104, 12.15, -0.35, 0, 0  
 4GA2, ASP\_140, 3.89, 0.14, -0.05, 0  
 1RIS, LYS\_63, 10.22, -0.28, 0, 0  
 3G59, ASP\_194, 3.79, 0, -0.01, 0  
 3BCH, ARG\_191, 12.08, -0.42, 0, 0  
 1RWZ, LYS\_140, 10.5, 0, 0, 0  
 2CYG, ARG\_298, 12.23, -0.7, 0.0, 43  
 1T95, ASP\_119, 3.44, 0.56, -0.92, 0  
 3FWU, GLU\_17, 3.91, 0.21, -0.8, 0  
 3ILC, TYR\_195, 10.09, 0.09, 0, 0  
 3N2T, HIS\_316, 7.23, 0.8, 0, -0.07  
 2B0J, LYS\_82, 10.5, 0, 0, 0  
 3MEW, ASP\_271, 2.88, 0.35, -1.27, 0  
 1XDZ, GLU\_23, 4.57, 0.07, 0, 0  
 1T6L, TYR\_69, 10, 0, 0, 0  
 1IAP, LYS\_160, 10.15, -0.35, 0, 0  
 2Z61, HIS\_61, 6.5, 0, 0, 0  
 3MIX, LYS\_410, 10.43, -0.07, 0, 0  
 3LD1, LYS\_178, 10.43, -0.07, 0, 0  
 2CXY, ARG\_70, 11.87, -0.63, 0, 0  
 2I6I, TYR\_158, 10, 0, 0, 0  
 1DUPLYS\_3, 10.29, -0.21, 0, 0  
 3B21, ARG\_97, 12.01, -0.49, 0, 0  
 3V75, GLU\_4, 2.52, 0.42, -2.4, 0  
 4FLE, GLU\_196, 4.78, 0.28, 0, 0  
 2G3A, TYR\_62, 13.41, 0.21, 0.8, 2.4  
 3L3P, ARG\_443, 12.15, -0.35, 0, 0  
 4FCU, LYS\_203, 10.5, 0, 0, 0  
 3HVW, ARG\_190, 12.36, -0.14, 0, 0  
 1O9G, CYS\_147, 9.85, 0, 0, 0.85  
 3AUF, TYR\_79, 13.27, 0.07, 0.8, 2.4  
 3U4K, ASP\_115, 3.34, 0.28, -0.74, 0  
 2IF4, LYS\_84, 10.22, -0.28, 0, 0  
 1TR9, GLU\_134, 4.64, 0.14, 0, 0  
 2JEO, ASP\_93, 2.7, 0.49, -1.59, 0  
 2Z61, CYS\_140, 9.92, 0, 0, 0.92  
 2QK1, LYS\_402, 10.36, -0.14, 0, 0  
 2IDC, CYS\_30, 7.4, -1.67, 0, 0.07  
 3HVM, LYS\_223, 10.5, 0, 0, 0  
 3FK5, GLU\_97, 4.5, 0, 0, 0  
 2VGM, HIS\_356, 4.96, 0.05, 0, -1.59  
 3NR5, ARG\_58, 12.36, -0.14, 0, 0  
 2FD5, GLU\_32, 3.03, 0.7, -2.17, 0  
 2EYI, LYS\_64, 10.08, -0.42, 0, 0  
 3ILC, ASP\_107, 3.58, 0.07, -0.29, 0  
 2CXA, CYS\_154, 12.72, -0.42, 1.39, 2.75  
 1R3D, LYS\_10, 10.5, 0, 0, 0  
 1NAR, ARG\_248, 11.73, -0.77, 0, 0  
 1WNH, HIS\_29, 6.98, 1.6, 1.54, -2.66  
 3HVM, LYS\_162, 10.5, 0, 0, 0  
 1QYI, GLU\_250, 4.57, 0.07, 0, 0  
 3GFP, LYS\_351, 10.29, -0.21, 0, 0  
 3IO0, ASP\_149, 1.55, 0.77, -3.02, 0  
 2RH3, GLU\_147, 4.78, 0.28, 0, 0  
 1R53, CYS\_192, 9.06, -1.21, 0.1, 2.7  
 2D2S, TYR\_656, 10, 0, 0, 0  
 3F6F, ARG\_205, 12.5, 0, 0, 0  
 1Q42, GLU\_10, 3.18, 0.28, -1.6, 0  
 1T6L, TYR\_227, 10, 0, 0, 0  
 1EQ6, ARG\_207, 12.08, -0.42, 0, 0  
 1C44, LYS\_55, 10.5, 0, 0, 0  
 3MIX, GLU\_540, 4.64, 0.14, 0, 0  
 3IOC, ASP\_83, 1.04, 0.56, -3.32, 0  
 1H4U, HIS\_515, 6.52, 0.09, 0, -0.07  
 1ZYL, TYR\_102, 9.39, 0.07, -0.68, 0  
 1TLV, ASP\_128, 3.68, 0, -0.12, 0  
 3RVC, LYS\_126, 10.22, -0.28, 0, 0  
 1QQE, LYS\_9, 10.43, -0.07, 0, 0  
 1XEU, TYR\_272, 8.25, 1.19, -2.95, 0  
 2HRZ, ARG\_129, 11.86, -1.68, 0.1, 0.4  
 2BLL, GLU\_569, 4.5, 0, 0, 0  
 1XTD, LYS\_66, 10.29, -0.21, 0, 0  
 4EKU, ARG\_353, 13.94, -2.43, 0.3, 86  
 2B3M, GLU\_107, 4.71, 0.21, 0, 0  
 1EDG, TYR\_296, 11.29, 1.29, 0, 0  
 3AU3, LYS\_580, 10.5, 0, 0, 0  
 2GAU, ARG\_66, 12.08, -0.42, 0, 0  
 3GFP, GLU\_378, 4.2, 0.35, -0.65, 0  
 1XIP, LYS\_158, 10.22, -0.28, 0, 0  
 3AUF, HIS\_138, 5.09, 2.28, 1.15, -4.84  
 1GPP, GLU\_45, 3.1, 0.63, -2.03, 0  
 1LN4, ARG\_56, 12.29, -0.21, 0, 0  
 3RRQ, LYS\_135, 10.29, -0.21, 0, 0  
 2RFA, HIS\_165, 3.94, 0.85, -3.41  
 2DFL, TYR\_278, 12.44, 1.84, -1.01, 1.62  
 3OKQ, LYS\_633, 10.29, -0.21, 0, 0  
 3LPZ, ARG\_79, 11.38, -1.12, 0, 0  
 3QKY, HIS\_149, 6.36, 0, 0, -0.14  
 2CVB, LYS\_140, 10.01, -0.49, 0, 0  
 1Q5Z, LYS\_606, 10.29, -0.21, 0, 0  
 2DFL, CYS\_124, 13.26, -1.19, 1.98, 3.47  
 3H6Q, GLU\_3, 4.5, 0, 0, 0  
 3BQW, GLU\_154, 4.38, 0.14, -0.26, 0  
 4AM1, ARG\_264, 11.8, -0.7, 0, 0  
 2C2Y, GLU\_111, 4.13, 0.07, -0.44, 0  
 3MTT, TYR\_453, 9.91, 0, -0.09, 0  
 1MSI, LYS\_155, 10.36, -0.14, 0, 0  
 3US6, GLU\_137, 5.21, 1.51, -0.8, 0  
 3EJC, TYR\_88, 9.68, 0, -0.32, 0  
 2FBI, ARG\_80, 11.8, -0.7, 0, 0  
 2C2Y, GLU\_111, 4.13, 0.07, -0.44, 0  
 2HXB, ASP\_174, 3.81, 0.07, -0.06, 0  
 4DBX, TYR\_4, 10.81, 0.43, 0.38, 0  
 1UCH, GLU\_114, 4.78, 0.28, 0, 0  
 3BWT, TYR\_836, 10.21, 0.21, 0, 0  
 4EF5, ARG\_334, 11.87, -0.63, 0, 0  
 2DOA, HIS\_86, 6.57, 0.07, 0, 0  
 2FB6, HIS\_38, 6.64, 0.28, 0, -0.14  
 1VJG, GLU\_67, 4.12, 0.42, -0.8, 0  
 2NMU, HIS\_84, 6.5, 0, 0, 0  
 1P4X, LYS\_172, 10.15, -0.35, 0, 0  
 2B0J, TYR\_261, 10, 0, 0, 0  
 3RUX, TYR\_138, 10.88, 0.07, 0.8, 1  
 1KN3, GLU\_83, 4.31, 2.7, -2.48, -0.41  
 1U53, LYS\_46, 10.29, -0.21, 0, 0  
 3LJI, ASP\_161, 3.21, 0.21, -0.8, 0  
 2E0T, ASP\_120, 3.14, 0.14, -0.8, 0  
 2RH3, ASP\_129, 2.13, 0.63, -2.3, 0  
 1EYH, ARG\_144, 11.22, -1.28, 0, 0  
 1VJG, ARG\_33, 11.1, -1.4, 0, 0  
 3M7G, TYR\_66, 13.22, 1.2, 0.8, 1.22  
 3NBI, ARG\_176, 12.08, -0.42, 0, 0  
 4EZB, ASP\_103, 2.03, 0.63, -2.39, 0

2Z14,ASP\_48,3.61,0.28,-0.47,0  
 1MUF,TYR\_337,12.58,0.07,0.12,2.39  
 3EX9,GLU\_107,3.95,0.28,-0.83,0  
 1JKS,ARG\_253,12.08,-0.42,0,0  
 1ZHV,HIS\_131,6.5,0,0,0  
 1TWU,HIS\_60,7.32,0.96,0,-0.14  
 2A6B,GLU\_146,7.62,3.53,-0.8,0.39  
 3KV0,GLU\_84,4.21,0.14,-0.43,0  
 1GQE,ARG\_154,11.73,-0.77,0,0  
 2H85,LYS\_226,10.5,0,0,0  
 3I4T,ASP\_212,3.54,0.28,-0.55,0  
 1DOV,LYS\_186,10.22,-0.28,0,0  
 1PDB,GLU\_172,3.88,1.19,-1.81,0  
 2IN0,ARG\_7,12.22,-0.28,0,0  
 4DND,ARG\_88,11.87,-0.63,0,0  
 1DCF,ARG\_80,12.5,0,0,0  
 1WYC,GLU\_92,4.57,0.07,0,0  
 2XHC,LYS\_186,10.29,-0.21,0,0  
 4GA2,LYS\_94,10.5,0,0,0  
 3M66,LYS\_158,10.5,0,0,0  
 2CW4,ARG\_69,12.15,-0.35,0,0  
 2G5X,ARG\_173,11.72,-3.65,0,2.87  
 2ZQ5,ARG\_211,8.38,-3.24,0,-0.88  
 3V75,ASP\_171,2.2,0.7,-2.29,0  
 3EVZ,LYS\_49,10.5,0,0,0  
 3CO1,LYS\_113,10.22,-0.28,0,0  
 1AT0,ASP\_282,2.95,0.42,-1.26,0  
 3LJN,ARG\_180,12.22,-0.28,0,0  
 2O8P,CYS\_91,8.81,-0.19,0,0  
 3BQW,GLU\_55,4.5,0,0,0  
 1WYC,ARG\_107,12.01,-0.49,0,0  
 3C2E,LYS\_125,10.36,-0.14,0,0  
 1RL0,ARG\_87,12.08,-0.42,0,0  
 2R57,GLU\_264,4.5,0,0,0  
 1N81,LYS\_68,10.36,-0.14,0,0  
 1PVT,GLU\_182,4.5,0,0,0  
 2Q99,LYS\_348,10.5,0,0,0  
 3Q6L,ARG\_79,13.9,-2.07,0,3.47  
 2CE6,ASP\_55,4.08,0.28,0,0  
 2GEN,ARG\_51,11.94,-0.56,0,0  
 2B61,TYR\_344,11.0,0.07,-1.43,2.36  
 3F6M,TYR\_29,12.67,0.0,0.39,2.29  
 1X91,GLU\_83,4.64,0.14,0,0  
 1WRU,GLU\_147,3.64,0.91,-1.77,0  
 2WOZ,ASP\_318,2.98,0.63,-1.45,0  
 3ANJ,ARG\_236,10.83,-1.67,0,0  
 3V75,ASP\_211,3.09,0.35,-1.06,0  
 2Q13,GLU\_365,2.19,0.84,-3.15,0  
 2FD5,GLU\_112,3.63,0.77,-1.64,0  
 3EVN,LYS\_49,10.5,0,0,0  
 3F53,ASP\_73,3.83,0.07,-0.04,0  
 4DNU,ASP\_208,1.01,0.77,-3.56,0  
 2GZQ,ASP\_109,2.34,0.63,-2.09,0  
 3EJC,GLU\_42,3.21,0.7,-1.99,0  
 3IO0,ARG\_171,11.94,-0.56,0,0  
 3HNX,ASP\_38,2.57,0.77,-2,0  
 3KV0,CYS\_118,9.02,-1.08,0,1.1  
 1TJE,TYR\_205,10,0,0,0  
 2BDV,GLU\_208,4.68,0.21,-0.03,0  
 1AK1,ARG\_173,11.73,-0.77,0,0  
 3K9I,GLU\_61,4.64,0.14,0,0  
 2B0A,LYS\_121,10.5,0,0,0  
 3IVF,LYS\_300,10.15,-0.35,0,0  
 2B02,TYR\_450,10,0,0,0  
 1WPA,TYR\_493,9.81,0.07,-0.26,0  
 3MIX,ARG\_616,12.43,-0.07,0,0  
 2CN1,GLU\_101,3.91,0.21,-0.8,0  
 2OGQ,ASP\_376,3.81,0.07,-0.06,0  
 3A2Z,LYS\_56,10.29,-0.21,0,0  
 1MTZ,ASP\_50,3.22,0.42,-1,0  
 3FHF,GLU\_75,4.19,0.28,-0.59,0  
 3GS3,ASP\_228,4.06,0.42,-0.16,0  
 1BGF,ASP\_23,2.22,0.63,-2.2,0  
 2AHE,LYS\_146,10.5,0,0,0  
 1RZ2,LYS\_143,10.5,0,0,0  
 2QV2,LYS\_27,10.29,-0.21,0,0  
 1T6L,ASP\_155,3.27,0.35,-0.88,0  
 1L3K,HIS\_77,4.22,0.86,0,-3.14  
 2D2S,GLU\_567,4.5,0,0,0  
 3FWU,ASP\_29,3.47,0.56,-0.89,0  
 1OIS,LYS\_357,10.15,-0.35,0,0  
 3N0K,GLU\_148,4.64,0.14,0,0  
 3RLN,GLU\_579,4.12,0.42,-0.8,0  
 3V4G,LYS\_6,10.43,-0.07,0,0  
 2CWY,TYR\_27,10,0,0,0  
 3L0D,CYS\_106,7.88,-1.53,0,0.41  
 1SFE,ARG\_15,11.8,-0.7,0,0  
 2ILR,CYS\_399,10.47,-0.33,0,1.8  
 3GFP,ARG\_432,12.08,-0.42,0,0  
 2Z0M,ASP\_107,2.57,0.28,-1.51,0  
 3F6M,LYS\_92,10.5,0,0,0  
 2HRZ,LYS\_249,10.5,0,0,0  
 2X4L,LYS\_114,10.43,-0.07,0,0  
 2A4D,LYS\_161,10.36,-0.14,0,0  
 3P28,HIS\_187,6.5,0,0,0  
 2V4U,TYR\_307,9.62,0.07,-0.45,0  
 2ILR,LYS\_393,10.08,-0.42,0,0  
 3UC9,GLU\_121,4.64,0.14,0,0  
 1XDZ,ASP\_66,2.79,0.7,-1.71,0  
 1ILW,GLU\_101,4.57,0.07,0,0  
 1WRU,LYS\_52,10.22,-0.28,0,0  
 3I4T,LYS\_232,10.36,-0.14,0,0  
 2H2W,GLU\_199,4.34,0.07,-0.23,0  
 2OBI,CYS\_10,9,0,0,0  
 3BPV,LYS\_8,10.36,-0.14,0,0  
 3JRT,GLU\_32,1.31,0.7,-3.89,0  
 3UAH,TYR\_230,12.73,0.21,0.12,2.4  
 4FH3,ASP\_115,3.06,0.21,-0.94,0  
 4F85,ARG\_160,11.8,-0.7,0,0  
 1R15,CYS\_73,11.98,-1.08,2.54,1.52  
 1LTU,CYS\_211,11.63,-0.11,0.77,1.97  
 1PBV,ARG\_170,11.8,-0.7,0,0  
 2EFK,ASP\_260,3.2,0.35,-0.95,0  
 3ZTA,GLU\_10,3.91,0.14,-0.73,0  
 2AXO,ASP\_130,2.87,0.14,-1.07,0  
 3BQW,LYS\_222,10.15,-0.35,0,0  
 4E9E,LYS\_437,10.5,0,0,0  
 2F8H,ARG\_289,12.15,-0.35,0,0  
 1XKR,LYS\_12,10.36,-0.14,0,0  
 3FK5,LYS\_285,10.29,-0.21,0,0  
 4EVF,GLU\_134,3.84,0.14,-0.8,0  
 3G9G,ARG\_51,11.73,-0.77,0,0  
 1PV5,GLU\_161,3.97,0.62,-1.15,0  
 1XKR,ASP\_9,3.87,0.07,0,0  
 2IQT,HIS\_51,4.49,0.06,0,-2.07  
 2CBE,LYS\_228,10.5,0,0,0  
 1EDG,LYS\_331,10.36,-0.14,0,0  
 1JSX,ARG\_103,11.94,-0.56,0,0  
 1U53,LYS\_110,10.22,-0.28,0,0  
 3LJN,HIS\_212,2.7,0.11,0,-3.91  
 3A0X,ARG\_684,12.01,-0.49,0,0  
 1T07,GLU\_77,4.77,0.28,-0.01,0  
 4E5S,LYS\_99,10.36,-0.14,0,0  
 2JEG,GLU\_74,4.5,0,0,0  
 1TR9,GLU\_196,4.37,0.21,-0.34,0  
 3RJX,GLU\_38,4.44,0.28,-0.34,0  
 2XMZ,LYS\_234,10.5,0,0,0  
 2IQT,GLU\_226,4.24,0.35,-0.61,0  
 2CWC,ASP\_237,2.89,0.49,-1.4,0  
 2Z84,TYR\_39,11.42,1.03,0,0.39  
 3GE9,ARG\_217,11.94,-0.56,0,0  
 3T57,GLU\_88,4.85,0.35,0,0  
 3G59,GLU\_92,3.57,0.42,-1.35,0  
 2CN1,ARG\_165,12.01,-0.49,0,0  
 2GZQ,CYS\_112,9.01,-0.63,0,0.63  
 2FL7,ARG\_106,11.94,-0.56,0,0  
 3ANJ,GLU\_149,3.98,0.28,-0.8,0  
 1RKA,GLU\_299,4.5,0,0,0  
 1WPA,ASP\_426,3.32,0.49,-0.97,0  
 3TIR,ASP\_71,3.86,0.14,-0.08,0  
 3C5V,GLU\_117,1.51,0.34,-0.35,-2.98  
 4E2B,ARG\_255,11.73,-0.77,0,0  
 1RKA,TYR\_36,9.34,0.14,-0.8,0  
 2JKF,TYR\_59,13.05,0.35,0.3,2.4  
 1ZBP,ARG\_34,12.15,-0.35,0,0  
 2F8H,ARG\_198,12.5,0,0,0  
 3CAX,LYS\_133,10.5,0,0,0  
 2OJQ,GLU\_701,3.9,0.56,-1.16,0  
 1JKS,GLU\_224,3.96,0.42,-0.96,0  
 3MEW,GLU\_225,4.05,0.63,-1.08,0  
 3O7K,ASP\_142,3.65,0,-0.15,0  
 1UJ8,ASP\_28,3.8,0,0,0  
 2FG1,ASP\_98,2.93,0.07,-0.94,0  
 2RIS,ARG\_111,11.61,-0.89,0,0  
 3PZ9,HIS\_175,7.23,1.7,2.4,-3.37  
 1MSI,GLU\_154,4.71,0.21,0,0  
 4H86,ASP\_84,2.7,0.35,-1.46,0  
 3H04,LYS\_22,9.94,-0.56,0,0  
 4EUG,HIS\_155,6.5,0,0,0  
 2H2W,LYS\_198,10.5,0,0,0  
 1MSI,ARG\_186,12.08,-0.42,0,0  
 2ZCX,LYS\_57,10.29,-0.21,0,0  
 2CVB,GLU\_151,4.43,0,-0.07,0  
 4DBX,ASP\_236,3.94,0.14,0,0  
 3GMS,ASP\_144,3.23,0.63,-1.2,0  
 2ZOM,GLU\_172,4.24,0.28,-0.54,0  
 1EDG,LYS\_295,10.08,-0.42,0,0  
 3V3T,TYR\_265,10.43,0.07,-0.31,0.67  
 2Q5X,ARG\_752,11.66,-0.84,0,0  
 1X6J,ARG\_79,12.01,-0.49,0,0  
 3JRT,ARG\_51,12.08,-0.42,0,0  
 2D7J,GLU\_66,4.12,0.42,-0.8,0  
 3RAZ,HIS\_156,7.09,0.73,0,-0.14  
 3GEC,CYS\_369,7.94,-1.13,0,0.07  
 3EVN,GLU\_109,3.46,0.28,-1.32,0  
 2QHT,GLU\_146,4.64,0.14,0,0  
 2GZQ,ASP\_178,3.94,0.14,0,0  
 2FL7,LYS\_144,10.08,-0.42,0,0  
 2CN1,ARG\_208,11.73,-0.77,0,0  
 1MD6,ASP\_142,3.29,0.14,-0.65,0  
 2P52,GLU\_218,4.57,0.07,0,0  
 2BOJ,ASP\_80,3.21,0.84,-1.42,0  
 3DZ1,ARG\_279,11.66,-0.84,0,0  
 3FXH,ARG\_79,11.59,-0.91,0,0  
 3VHJ,ASP\_102,2.31,0.77,-2.26,0  
 3N2T,ASP\_139,3.04,0.07,-0.83,0  
 2OJQ,CYS\_512,9,0,0,0  
 2IRM,GLU\_212,4.5,0,0,0  
 3A7L,LYS\_18,10.5,0,0,0  
 3EVZ,LYS\_177,10.29,-0.21,0,0  
 2D2S,GLU\_697,2.39,1.44,-1.72,-1.83  
 2RFA,GLU\_100,3.91,0.21,-0.8,0  
 2HRZ,GLU\_94,4.15,0.14,-0.49,0  
 2EFK,TYR\_42,10.23,0.07,0.16  
 1Z9L,LYS\_39,10.43,-0.07,0,0  
 2BDD,ASP\_30,3.64,0.7,-0.86,0  
 3JZN,GLU\_276,4.38,0,-0.12,0  
 3HUE,GLU\_5,4.17,0.42,-0.75,0  
 15JY,LYS\_41,10.36,-0.14,0,0  
 1KW4,ARG\_11,12.15,-0.35,0,0  
 1J85,GLU\_113,4.57,0.07,0,0  
 1F09,TYR\_157,13.24,0.28,0.56,2.4  
 3AUF,ASP\_165,2.88,0.21,-1.14,0  
 3GYW,LYS\_40,10.29,-0.21,0,0  
 1BKB,LYS\_4,10.5,0,0,0  
 3TMO,GLU\_200,4.11,0.35,-0.74,0  
 2GEN,LYS\_49,9.87,-0.63,0,0  
 3I82,LYS\_29,10.5,0,0,0  
 2BLL,HIS\_448,6.42,0.06,0,-0.14  
 1JKS,HIS\_131,2.81,1.21,0,-4.9  
 1ZCE,LYS\_104,10.43,-0.07,0,0  
 1HF8,TYR\_211,10.53,1.43,0,-0.9  
 3I4T,GLU\_195,4.5,0,0,0  
 2QDJ,LYS\_151,10.5,0,0,0  
 1Y2Q,GLU\_54,4.5,0,0,0  
 2D2S,ASP\_642,3.71,0.07,-0.16,0  
 3CIV,ASP\_9,3.3,0.14,-0.65,0  
 3N0K,LYS\_61,10.04,-0.77,0,0.31  
 2R0S,LYS\_181,10.22,-0.28,0,0  
 2W2S,ARG\_51,11.59,-0.91,0,0  
 2XHC,GLU\_141,4.42,0.14,-0.22,0  
 1TXJ,LYS\_85,10.5,0,0,0  
 1QZN,GLU\_108,3.21,0.75,-2.04,0  
 3DSH,ASP\_312,2.96,0.35,-1.19,0  
 2OBI,ARG\_9,12.15,-0.35,0,0  
 2YWX,HIS\_37,6.43,0,-0.07  
 2X4L,LYS\_64,10.43,-0.07,0,0  
 1BYI,ARG\_193,11.94,-0.56,0,0  
 2IF4,GLU\_154,4.64,0.14,0,0  
 2B78,ASP\_32,3.61,0.7,-0.9,0  
 2FG1,GLU\_2,4.5,0,0,0  
 3U2A,GLU\_33,4.5,0,0,0  
 1Y0K,ARG\_199,12.29,-0.21,0,0  
 3DSH,LYS\_374,10.22,-0.28,0,0  
 3ODJ,CYS\_19,10.38,-0.17,0,1.55  
 3BA1,ASP\_123,1.82,0.42,-2.4,0  
 4DIU,LYS\_82,10.36,-0.14,0,0  
 3ON1,HIS\_47,6.5,0,0,0  
 1V6T,LYS\_53,10.29,-0.21,0,0  
 3V75,TYR\_-3,10.14,0.14,0,0  
 2YT4,GLU\_610,4.85,0.35,0,0  
 1EV8,LYS\_2,10.5,0,0,0  
 2QVO,GLU\_63,3.84,0.14,-0.8,0  
 2INO,TYR\_406,10,0,0,0  
 2O8P,GLU\_209,4.71,0.21,0,0  
 2HP7,HIS\_59,1.75,0,0,-4.75  
 1EYH,ARG\_91,12.01,-0.49,0,0  
 3PP8,ARG\_291,11.73,-0.77,0,0  
 3V75,ARG\_254,12.15,-0.35,0,0  
 2D59,CYS\_67,9.02,-0.4,0,0.42  
 3A2Z,HIS\_131,9.21,5.2,2.84,-5.33  
 2G5X,ARG\_84,13.55,-1.35,0,2.4  
 2EFK,GLU\_221,4.64,0.14,0,0  
 1UJ8,GLU\_75,3.98,0.28,-0.8,0  
 2IXM,LYS\_60,10.5,0,0,0  
 1OTM,LYS\_63,10.22,-0.28,0,0  
 3IPZ,ARG\_92,11.66,-0.84,0,0  
 3OBS,ASP\_137,3.8,0,0,0  
 2D7U,GLU\_241,4.46,0.42,-0.46,0  
 3QYB,ASP\_911,3.86,0.07,-0.01,0  
 3E27,GLU\_185,3.63,0.63,-1.5,0  
 1FEZ,GLU\_111,4.57,0.07,0,0  
 1XTD,GLU\_123,4.5,0,0,0  
 4EVF,LYS\_56,10.5,0,0,0  
 1TXJ,TYR\_18,12.45,0.15,-0.1,2.4  
 2QDJ,GLU\_204,4.71,0.21,0,0

3EVN,LYS\_214,10.5,0,0,0  
1ZYL,ARG\_137,12.92,-0.88,0,1.3  
3P28,ARG\_61,12.08,-0.42,0,0  
2DG7,ASP\_131,3.2,0.42,-1.02,0  
3LMO,ARG\_83,11.66,-0.84,0,0  
2AHE,LYS\_249,10.29,-0.21,0,0  
2ZTY,ARG\_87,11.66,-0.84,0,0  
1JT9,LYS\_264,10.22,-0.28,0,0  
2YWY,GLU\_30,4.64,0.14,0,0  
1R15,GLU\_83,3.96,0.84,-1.38,0  
1WXQ,LYS\_148,10.5,0,0,0  
4ACJ,GLU\_759,4.25,0.07,-0.32,0  
3M7G,ARG\_250,10.95,-3.3,0,1.74  
1OGL,ASP\_41,2.63,0.77,-1.95,0  
2FL4,ASP\_113,3.61,0.28,-0.46,0  
3ULX,LYS\_115,9.86,-0.77,0,0.13  
2D7U,GLU\_151,3.69,0.42,-1.23,0  
3V55,HIS\_666,6.5,0,0,0  
2HP7,ARG\_64,11.87,-0.63,0,0  
3IV4,GLU\_86,4.5,0,0,0  
2QRX,TYR\_13,10,0,0,0  
4FH3,GLU\_61,3.28,0.7,-1.92,0  
3IU5,CYS\_138,8.8,-0.21,0,0  
3BJV,HIS\_127,6.5,0,0,0  
2CL3,ARG\_131,11.87,-0.63,0,0  
2JEO,ASP\_133,3.32,0.14,-0.62,0  
3FFM,GLU\_127,4.5,0,0,0  
3A2Z,CYS\_59,3.72,-6.05,-1.89,2.65  
3FRR,ASP\_49,3.91,0.21,-0.1,0  
2QO7,HIS\_320,6.5,0,0,0  
1X1E,GLU\_223,3.46,0.21,-1.25,0  
2G55,ASP\_172,2.26,0.56,-2.1,0  
2B61,LYS\_106,10.29,-0.21,0,0  
1OST,CYS\_305,12.21,-0.66,0,3.86  
2OPJ,TYR\_42,11.77,0.33,0,1.44  
1XDZ,LYS\_165,10.43,-0.07,0,0  
4DEZ,GLU\_51,3.36,0.56,-1.7,0  
3K8U,ARG\_121,11.94,-0.56,0,0  
4EF5,GLU\_174,4.56,0.07,-0.01,0  
1Y2Q,TYR\_119,9.78,0.07,-0.29,0  
2NVC,TYR\_236,11.33,0.14,0,1.19  
1NRI,ARG\_243,12.29,-0.21,0,0  
3T8R,GLU\_96,3.87,0.56,-1.19,0  
1GXN,GLU\_571,4.71,0.21,0,0  
2EFK,GLU\_128,4.64,0.14,0,0  
3O48,ARG\_59,12.15,-0.35,0,0  
3OKQ,LYS\_628,10.5,0,0,0  
1J33,GLU\_69,4.41,0.14,-0.23,0  
3JRT,LYS\_113,10.36,-0.14,0,0  
1WOU,GLU\_55,3.92,0.21,-0.79,0  
3MEW,ASP\_193,3.7,0.7,-0.8,0  
2D8N,ARG\_151,10.61,-2.35,0,0.46  
1MML,ASP\_114,3.01,0.21,-1,0  
2W1R,ARG\_109,12.01,-0.49,0,0  
3LPZ,ARG\_109,12.22,-0.28,0,0  
3Q1C,LYS\_126,10.43,-0.07,0,0  
3UV9,TYR\_299,11.56,0,0,1.56  
2X5Y,ARG\_742,11.87,-0.63,0,0  
3EJG,LYS\_72,10.5,0,0,0  
3RLN,LYS\_759,10.43,-0.07,0,0  
2IRM,CYS\_184,7.71,-5.2,0.46,3.46  
2NRK,HIS\_142,6.3,0.01,0,-0.21  
2OSA,ASP\_314,3.14,0.14,-0.8,0  
3A4C,GLU\_480,2.65,0.49,-2.35,0  
1ILW,LYS\_113,10.5,0,0,0  
3E5T,LYS\_74,10.5,0,0,0  
3C2E,ASP\_177,2.98,0.49,-1.31,0  
3GT0,GLU\_85,4.5,0,0,0  
1SQW,HIS\_175,6.43,0,0,-0.07  
3M3P,ARG\_185,12.22,-0.28,0,0  
2OJQ,TYR\_608,10.14,0.14,0,0  
2YWJ,LYS\_185,10.36,-0.14,0,0  
4DNU,ARG\_55,11.94,-0.56,0,0  
3MIX,GLU\_506,4.5,0,0,0  
2C2Y,ARG\_235,12.08,-0.42,0,0  
3H6Q,TYR\_166,10.87,0,0,0.87  
1A8Q,LYS\_144,10.22,-0.28,0,0  
2YT4,TYR\_653,9.34,0.19,-0.85,0  
1FKM,TYR\_395,12.78,1.2,0,1.58  
4AM1,LYS\_296,10.29,-0.21,0,0  
2Z0M,ASP\_268,3.6,0.42,-0.62,0  
4DND,LYS\_79,10.5,0,0,0  
1WRU,ARG\_8,12.01,-0.49,0,0  
3V75,CYS\_21,10.36,-1.6,-0.41,3.37  
1T95,LYS\_146,10.43,-0.07,0,0  
1R3F,ARG\_99,11.45,-1.05,0,0  
3P28,TYR\_152,9.98,0,-0.02,0  
2P4D,TYR\_137,10,0,0,0  
3GOZ,LYS\_291,10.43,-0.07,0,0  
3EX9,ASP\_83,2.65,0.42,-1.57,0  
1X8F,LYS\_248,10.43,-0.07,0,0  
1Q8B,LYS\_37,10.29,-0.21,0,0  
2CXC,LYS\_140,10.5,0,0,0  
3RHE,ASP\_112,3.94,0.14,0,0  
3EVZ,LYS\_142,10.01,-0.49,0,0  
2RH3,LYS\_97,10.29,-0.21,0,0  
1WRU,GLU\_57,4.12,0.35,-0.73,0  
1UJ8,HIS\_6,7.09,0.8,0,-0.21  
3BCH,ARG\_117,11.87,-0.63,0,0  
3RJZ,TYR\_176,9.27,0.07,-0.8,0  
1XIP,ASP\_290,3.8,0,0,0  
1X6J,ARG\_14,12.22,-0.28,0,0  
3IDW,ASP\_62,3.91,0.42,-0.3,0  
2P4D,GLU\_49,4.5,0,0,0  
2C2Y,ARG\_280,12.25,-1.47,0,1.22  
2OEW,LYS\_357,10.5,0,0,0  
2FBQ,LYS\_136,10.43,-0.07,0,0  
4GA2,ARG\_3,12.22,-0.28,0,0  
1UXO,TYR\_66,10.2,0,0,0.2  
3Q1C,ASP\_378,3.69,0,-0.11,0  
2OBI,GLU\_157,3.68,0.35,-1.17,0  
3CNU,LYS\_10,10.29,-0.21,0,0  
1XWM,ARG\_192,11.31,-1.19,0,0  
2P0L,GLU\_71,4.32,0.21,-0.39,0  
2RIS,GLU\_30,4.5,0,0,0  
1SQH,HIS\_71,7.16,0.8,0,-0.14  
4DBX,LYS\_172,10.5,0,0,0  
1HUF,LYS\_35,10.36,-0.14,0,0  
3B21,GLU\_141,3.77,0.07,-0.8,0  
3H9W,HIS\_130,6.08,0,0,-0.42  
1YTD,ASP\_35,3.92,0.14,-0.02,0  
4F85,ARG\_299,11.73,-0.77,0,0  
2YXO,GLU\_93,4.57,0.07,0,0  
2IDC,GLU\_23,3.84,0.14,-0.8,0  
1WOU,GLU\_6,4.13,0.35,-0.72,0  
1EYH,TYR\_111,10.67,0,-0.36,1.03  
3GEC,GLU\_438,4.5,0,0,0  
1LTU,ARG\_195,11.52,-0.98,0,0  
3M16,LYS\_45,10.5,0,0,0  
1U3Y,TYR\_347,11.02,1.02,0,0  
1NAR,LYS\_2,10.29,-0.21,0,0  
1NIJ,GLU\_245,4.5,0,0,0  
3LH5,TYR\_533,10,0,0,0  
1QOE,LYS\_32,9.31,-1.19,0,0  
2B6P,ARG\_233,11.73,-0.77,0,0  
3EUR,LYS\_88,10.5,0,0,0  
1MUF,ARG\_179,12.5,0,0,0  
3ADO,LYS\_260,10.5,0,0,0  
1JSX,GLU\_111,4.5,0,0,0  
1WNH,ASP\_179,3.42,0.42,-0.8,0  
3QAV,LYS\_97,10.43,-0.07,0,0  
4ETX,ARG\_252,12.22,-0.28,0,0  
1OLR,TYR\_17,10.8,0.98,-1.11,0.93  
1I60,LYS\_111,10.5,0,0,0  
2EA9,ASP\_49,3.65,0,-0.15,0  
4E9E,LYS\_554,10.36,-0.14,0,0  
3Q1C,TYR\_339,9.35,1.73,-0.17,-2.21  
1O5J,GLU\_11,4.64,0.14,0,0  
3UX2,GLU\_35,4.19,0.49,-0.8,0  
1WNH,HIS\_202,6.36,0,0,-0.14  
1YOK,ASP\_5,3.27,0.28,-0.81,0  
1N81,LYS\_157,10.36,-0.14,0,0  
1O59,CYS\_202,9.08,-0.75,0,0.83  
2E3S,TYR\_482,10.16,2.48,-0.58,-1.74  
2AD1,ASP\_67,2.91,0.84,-1.73,0  
1L2F,ASP\_245,2.63,0.84,-2.01,0  
2CVB,ARG\_126,12.29,-0.21,0,0  
2O8I,ARG\_91,12.5,0,0,0  
3FK5,CYS\_331,9.25,-1.6,0,1.85  
3M66,ARG\_358,12.43,-0.07,0,0  
2BQO,TYR\_105,10.49,0.35,0,0.14  
3QAV,HIS\_139,8.48,2.55,1.73,-2.31  
1ZCU,LYS\_226,10.5,0,0,0  
3GW3,GLU\_26,4.54,0.28,-0.24,0  
3UAH,ARG\_383,12.56,-2.08,0,2.14  
3Q6L,LYS\_106,10.5,0,0,0  
2CN1,LYS\_49,10.5,0,0,0  
4H89,ARG\_104,12.15,-0.35,0,0  
2B78,LYS\_76,10.5,0,0,0  
1PNE,ASP\_26,4.01,0.21,0,0  
2NRK,HIS\_99,4.44,0.92,-2.98  
1WOU,LYS\_25,10.08,-0.42,0,0  
1O17,GLU\_46,4.71,0.21,0,0  
2Z14,LYS\_117,10.5,0,0,0  
2F9F,LYS\_151,10.5,0,0,0  
2WB3,GLU\_282,4.5,0,0,0  
2QEV,ARG\_51,12.15,-0.35,0,0  
1U7U,GLU\_200,4.42,1.33,-1.41,0  
2HRZ,ASP\_100,3.74,0,-0.06,0  
1MUF,HIS\_293,0.56,0,-1.4,-4.54  
2AH5,ASP\_115,3.84,0.14,-0.1,0  
3UOV,ASP\_86,3.94,0.14,0,0  
3Q2C,GLU\_53,3.81,0.28,-0.97,0  
3ZTA,TYR\_98,10,0,0,0  
3MEW,LYS\_167,10.5,0,0,0  
3IVF,TYR\_199,13.41,0.21,0.8,2.4  
1O0X,HIS\_239,3.55,0.32,0,-3.27  
3N2T,LYS\_306,10.36,-0.14,0,0  
1A8Q,GLU\_10,4.57,0.07,0,0  
1L2F,LYS\_163,10.15,-0.35,0,0  
3I47,ASP\_170,2.52,0.42,-1.7,0  
3C6B,TYR\_265,11.35,0,0,1.35  
3BWT,LYS\_774,10.5,0,0,0  
3LPZ,LYS\_120,10.29,-0.21,0,0  
3BA1,GLU\_17,4.12,0.42,-0.8,0  
3V46,GLU\_384,3.79,0.63,-1.34,0  
3U56,LYS\_94,10.5,0,0,0  
1YB2,LYS\_247,10.29,-0.21,0,0  
2VGM,HIS\_153,3.94,0.47,0,-3.03  
3CIV,GLU\_151,6.11,3.04,-1.9,0.47  
1R3D,CYS\_214,9.43,-0.09,0,0.52  
2D25,ASP\_750,3.35,0.07,-0.52,0  
2H85,GLU\_210,0.48,1.46,-3.08,-2.4  
2RFA,HIS\_84,1.67,0.53,-0.52,-4.84  
4E8B,LYS\_59,10.5,0,0,0  
3RJZ,LYS\_68,10.01,-0.49,0,0  
1FKM,HIS\_347,5.14,0,0,-1.36  
3N2T,GLU\_140,4.57,0.07,0,0  
2JHY,ASP\_184,3.22,0.56,-1.14,0  
2Z0M,ASP\_206,1.38,0.84,-3.26,0  
3H9W,ASP\_59,1.87,0.49,-2.42,0  
3U2A,GLU\_95,5.06,0.56,0,0  
3FTT,ASP\_185,3.81,0.07,-0.06,0  
3IBT,ARG\_180,11.18,-1.32,0,0  
2V1L,GLU\_91,4.71,0.21,0,0  
2FB6,ASP\_54,1.9,0.63,-2.52,0  
1J85,LYS\_71,10.5,0,0,0  
4D8L,ARG\_270,11.87,-0.63,0,0  
3ANJ,ARG\_282,13.22,-1.68,0,2.4  
3V1Q,GLU\_645,4.51,0.21,-0.2,0  
1LFLPL,LYS\_11,9.87,-0.63,0,0  
2OB5,ARG\_78,11.8,-0.7,0,0  
2D8N,LYS\_192,10.43,-0.07,0,0  
4FD6,ARG\_27,11.8,-0.7,0,0  
1JYH,GLU\_8,4.19,0.49,-0.8,0  
3UX2,ARG\_45,12.01,-0.49,0,0  
1K95,HIS\_197,6.36,0,0,-0.14  
1U3Y,TYR\_316,13.41,0.21,0.8,2.4  
3PZ9,GLU\_92,4.85,0.35,0,0  
3QDJ,LYS\_185,10.29,-0.21,0,0  
1QQL,LYS\_101,10.36,-0.14,0,0  
2I6I,GLU\_42,4.78,0.42,-0.14,0  
2G7O,GLU\_101,4.71,0.21,0,0  
3B7H,CYS\_57,9.28,-0.03,0,0.31  
3AU3,GLU\_658,4.13,0.28,-0.65,0  
4ZB5,LYS\_131,10.5,0,0,0  
3T5B,ARG\_197,12.36,-0.14,0,0  
1T6L,LYS\_21,10.01,-0.49,0,0  
1T3Y,ASP\_68,3.23,0.07,-0.64,0  
1MUF,LYS\_168,10.5,0,0,0  
2CE6,ASP\_22,3.25,0.7,-1.24,0  
2GAU,LYS\_151,9.87,-0.63,0,0  
1L3K,GLU\_85,4.39,0.14,-0.25,0  
1SJ8,ARG\_606,11.94,-0.56,0,0  
1Q46,LYS\_174,10.15,-0.35,0,0  
1N81,ARG\_160,11.45,-1.05,0,0  
1N81,LYS\_79,10.5,0,0,0  
1QQE,ASP\_29,2.15,0.56,-2.21,0  
3CIV,HIS\_158,4.93,0.66,0,-2.23  
3Q1C,ASP\_101,0.98,0.98,-3.8,0  
1MIX,LYS\_357,10.5,0,0,0  
3HQX,LYS\_93,10.15,-0.35,0,0  
2D7U,LYS\_94,10.5,0,0,0  
3DZ1,TYR\_36,12.51,2.51,0,0  
1TR9,HIS\_23,6.37,0.08,0,-0.21  
1TXJ,LYS\_40,10.5,0,0,0  
2CWC,ARG\_236,12.29,-0.21,0,0  
4AM1,LYS\_16,9.94,-0.56,0,0  
1R9W,LYS\_210,10.29,-0.21,0,0  
3GW3,GLU\_278,1.11,1.62,-2.6,-2.4  
4FH3,GLU\_375,4.71,0.21,0,0  
1TXD,GLU\_776,4.35,0.14,-0.28,0  
2AHE,LYS\_238,10.5,0,0,0  
1AK1,ASP\_45,3.9,0.21,-0.11,0  
1AK1,TYR\_156,12.62,1.27,-0.26,1.6  
2F4A,ASP\_67,3.87,0.07,0,0  
2CN1,ASP\_204,3.75,0.07,-0.12,0  
2ZCO,CYS\_44,13.08,-0.09,0,7.347  
2DVK,ARG\_171,11.08,-1.42,0,0  
2Z14,TYR\_42,10,0,0,0  
3HNX,ARG\_79,12.08,-0.42,0,0  
4FLE,ASP\_179,3.5,0.35,-0.64,0  
2VAN,LYS\_230,10.5,0,0,0  
3I4T,GLU\_259,1.61,1.05,-3.94,0  
2BDD,TYR\_122,9.76,0.07,-0.31,0  
1PSW,LYS\_71,10.5,0,0,0



3EZ7, TYR\_93, 9.99, 0.23, -0.23, 0  
1BN6, ARG\_41, 11.31, -1.19, 0, 0  
2CX, HIS\_19, 6.59, 0.09, 0, 0  
3TMO, TYR\_292, 10.0, 0, 0  
1US3, ASP\_183, 2.7, 0.49, -1.59, 0  
3RJZ, LYS\_26, 10.43, -0.07, 0, 0  
1UCH, HIS\_193, 4.41, 1.6, 0.35, -4.03  
3US6, LYS\_127, 10.36, -0.14, 0, 0  
1NIJ, GLU\_137, 4.92, 0.42, 0, 0  
1FHL, TYR\_218, 11.32, 1.32, 0, 0  
2F19, ARG\_82, 12.22, -0.28, 0, 0  
3P28, ASP\_211, 3.21, 0.21, -0.8, 0  
2H8O, LYS\_301, 10.29, -0.21, 0, 0  
3CO1, LYS\_62, 10.5, 0, 0, 0  
4FCU, ASP\_166, 3.8, 0, 0, 0  
3IVF, LYS\_278, 10.15, -0.35, 0, 0  
3OOP, TYR\_30, 11.6, 0.07, 0, 1.53  
2FPN, TYR\_110, 11.17, 0.05, -1.22  
1VJG, TYR\_47, 10.23, 1.34, -1.75, 0.63  
3O16, LYS\_73, 10.29, -0.21, 0, 0  
2VGM, GLU\_169, 4.78, 0.28, 0, 0  
2EJX, LYS\_65, 10.22, -0.28, 0, 0  
3BZT, ASP\_308, 3.21, 0.42, -1.01, 0  
3RFY, ASP\_414, 2.43, 1.26, -2.63, 0  
3IVF, LYS\_324, 10.5, 0, 0, 0  
2CX, GLU\_104, 4.4, 0.7, -0.8, 0  
3CO1, ASP\_103, 3.73, 0.28, -0.35, 0  
3IU5, LYS\_100, 10.15, -0.35, 0, 0  
1WXF, GLU\_91, 3.98, 0.28, -0.8, 0  
3F6F, ARG\_13, 11.13, -3.77, 0, 2.4  
2C13, LYS\_33, 10.22, -0.28, 0, 0  
3FHF, TYR\_140, 11.95, 0.53, 0, 1.42  
1HU, ARG\_91, 12.22, -0.28, 0, 0  
1MHN, CYS\_146, 8.5, -0.51, 0, 0  
3FK5, ARG\_175, 12.5, 0, 0, 0  
3LMO, GLU\_72, 2.54, 0.07, -2.03, 0  
3AU3, ASP\_700, 3.8, 0, 0, 0  
1L3K, ASP\_27, 2.86, 0.35, -1.29, 0  
1NWA, ARG\_158, 11.15, -1.89, 0, 0.54  
2ZQ5, HIS\_108, 1.23, 0.14, -0.89, -4.52  
1PSW, LYS\_2, 10.36, -0.14, 0, 0  
1UAJ, ARG\_24, 12.01, -0.49, 0, 0  
3RKV, TYR\_207, 9.6, 0.07, -0.47, 0  
4H4J, LYS\_239, 10.43, -0.07, 0, 0  
2OGQ, HIS\_489, 6.91, 0.76, 0, -0.35  
2WB8, CYS\_702, 9.94, -0.65, 1.59  
1XFK, LYS\_292, 10.08, -0.42, 0, 0  
1XWM, GLU\_58, 4.04, 0.07, -0.53, 0  
1IAP, ASP\_128, 3.51, 0.07, -0.36, 0  
3BQW, ASP\_50, 2.9, 0.7, -1.61, 0  
1AKO, LYS\_169, 10.43, -0.07, 0, 0  
3A4C, ARG\_452, 12.15, -0.35, 0, 0  
1IDK, TYR\_202, 10.98, 0, 0, 0.98  
3VJ8, GLU\_91, 4.5, 0, 0, 0  
2OOK, ARG\_57, 12.43, -0.07, 0, 0  
3HKX, GLU\_117, 4.5, 1.66, -1.66, 0  
2P0Y, ASP\_273, 4.01, 0.21, 0, 0  
2HRZ, ARG\_254, 12.18, -1.14, 0, 0.82  
4EZB, GLU\_133, 4.12, 0.56, -0.93, 0  
3GEC, LYS\_514, 9.8, -0.7, 0, 0  
2POL, HIS\_141, 6.77, 0.27, 0, 0  
1FQI, ASP\_339, 1.59, 0.63, -2.84, 0  
1U7U, CYS\_351, 11.6, 0, 0, 2.6  
2YXO, TYR\_125, 10.21, 0.21, 0, 0  
3ANJ, TYR\_290, 10.77, 0.14, -1.4, 2.03  
3BCY, LYS\_79, 10.29, -0.21, 0, 0  
2OEW, LYS\_209, 10.5, 0, 0, 0  
2ILR, GLU\_300, 4.05, 0.35, -0.8, 0  
4E6S, ASP\_20, 3.94, 0.56, -0.42, 0  
3ANJ, ASP\_265, 2.68, 0.77, -1.89, 0  
1ZBP, GLU\_263, 4.5, 0, 0, 0  
2B61, LYS\_227, 10.22, -0.28, 0, 0  
1RAJ, LYS\_405, 10.5, 0, 0, 0  
1YOY, TYR\_135, 10.58, 0.21, -0.85, 1.22  
2Q12, HIS\_59, 6.5, 0, 0, 0  
2CN1, LYS\_80, 10.36, -0.14, 0, 0  
2OKT, HIS\_154, 6.43, 0, 0, -0.07  
3V46, LYS\_256, 10.43, -0.07, 0, 0  
1OGL, GLU\_152, 4.54, 0.14, -0.1, 0  
3DSH, CYS\_347, 7.26, -1.74, 0, 0  
1L2H, GLU\_113, 2.41, 0.56, -2.65, 0  
1FHL, ASP\_84, 2.44, 0.84, -2.2, 0  
2G9D, LYS\_119, 10.15, -0.35, 0, 0  
1DOV, ARG\_121, 12.5, 0, 0, 0  
3M16, ARG\_327, 11.87, -0.63, 0, 0  
1Z3X, TYR\_83, 8.08, 0.1, -0.46, -1.56  
1NRI, LYS\_256, 10.5, 0, 0, 0  
1DOV, TYR\_177, 10.07, 0.07, 0, 0  
3H5T, ASP\_268, 3.07, 0.49, -1.23, 0  
2JEO, TYR\_130, 10, 0, 0, 0  
3DSH, CYS\_330, 7.63, -2.12, -1.22, 1.98  
1ZKZ, LYS\_10, 9.94, -0.56, 0, 0  
2BV9, LYS\_83, 10.5, 0, 0, 0  
1WNH, ASP\_100, 3.95, 0.28, -0.13, 0  
3AUF, LYS\_131, 10.22, -0.28, 0, 0  
1YM5, LYS\_67, 10.22, -0.28, 0, 0  
3PBH, ARG\_20, 12.15, -0.35, 0, 0  
2ILR, GLU\_312, 3.84, 0.21, -0.87, 0  
4F3J, ASP\_224, 4.08, 0.28, 0, 0  
1JB3, GLU\_54, 4.71, 0.21, 0, 0  
1PSW, HIS\_324, 6.36, 0, 0, -0.14  
4DBX, GLU\_10, 4.57, 0.07, 0, 0  
2G5X, LYS\_205, 10.5, 0, 0, 0  
3NZL, HIS\_7, 6.36, 0, 0, -0.14  
3JZ9, HIS\_338, 6.5, 0, 0, 0  
3COU, GLU\_118, 4.5, 0, 0, 0  
3EJG, ASP\_18, 1.78, 0.42, -2.44, 0  
2Q5X, LYS\_735, 10.43, -0.07, 0, 0  
3LH5, ARG\_757, 12.03, -0.47, 0, 0  
2CWY, GLU\_87, 3.25, 0.35, -1.6, 0  
3JV1, ASP\_184, 3.99, 0.28, -0.09, 0  
4ETX, CYS\_264, 12.52, -0.24, 1.85, 1.91  
2ZQ5, GLU\_126, 3.71, 2.06, -1.07, -1.77  
2OEW, LYS\_339, 10.5, 0, 0, 0  
2JHY, ASP\_188, 3.58, 0.63, -0.85, 0  
3HUE, ARG\_155, 12.01, -0.49, 0, 0  
3O48, TYR\_45, 10.87, 0.14, 0, 0.72  
3ZXY, ARG\_268, 12.5, 0, 0, 0  
3UC9, GLU\_130, 4.5, 0, 0, 0  
3V46, GLU\_285, 4.5, 0, 0, 0  
3V55, ARG\_435, 12.01, -0.49, 0, 0  
1KN3, ARG\_146, 9.96, -2.54, 0, 0  
3P2F, ARG\_75, 12.22, -0.28, 0, 0  
3CIV, ARG\_14, 11.24, -1.26, 0, 0  
2C2Y, ASP\_205, 2.21, 0.42, -2.01, 0  
1JT9, GLU\_80, 3.78, 0.14, -0.86, 0  
2AH5, TYR\_208, 11.55, 0.07, 0, 1.48  
2X4J, ARG\_79, 12.5, 0, 0, 0  
3ETU, GLU\_229, 4.5, 0, 0, 0  
2GZQ, LYS\_36, 10.29, -0.21, 0, 0  
3BPP, ARG\_208, 12.5, 0, 0, 0  
1N81, LYS\_150, 10.5, 0, 0, 0  
2YXO, LYS\_168, 9.87, -0.63, 0, 0  
1V6T, ASP\_138, 3.94, 0.14, 0, 0  
1RSS, GLU\_52, 4.5, 0, 0, 0  
3QKY, ARG\_223, 12.08, -0.42, 0, 0  
3ONH, LYS\_455, 10.08, -0.42, 0, 0  
2BLL, GLU\_545, 3.71, 0.77, -1.56, 0  
2RFA, HIS\_73, 6.46, 0.1, 0, -0.14  
2QVO, TYR\_22, 9.94, 0.07, -0.13, 0  
2XMX, GLU\_120, 4.71, 0.21, 0, 0  
3L3P, GLU\_449, 4.44, 0.84, -0.9, 0  
2CVB, ARG\_25, 11.52, -0.98, 0, 0  
1J33, HIS\_283, 2.68, 2.13, -0.89, -5.06  
3M66, GLU\_401, 4.5, 0, 0, 0  
2B78, ASP\_310, 3.74, 0.35, -0.41, 0  
2NYC, TYR\_231, 10.09, 0, 0, 0.09  
1T3J, LYS\_718, 10.5, 0, 0, 0  
3M7T, CYS\_501, 9, 0, 0, 0  
2CIU, LYS\_160, 10.5, 0, 0, 0  
3I82, ARG\_131, 12.29, -0.21, 0, 0  
3V55, ASP\_642, 3.27, 0.42, -0.95, 0  
2FZ4, TYR\_54, 10.14, 0.14, 0, 0  
2ZCO, ARG\_159, 12.01, -0.49, 0, 0  
4F85, ARG\_158, 12.01, -0.49, 0, 0  
1T3J, LYS\_689, 10.43, -0.07, 0, 0  
1ZP2, ARG\_45, 11.38, -1.12, 0, 0  
3EVP, GLU\_248, 3.74, 0.35, -1.11, 0  
3KB5, HIS\_394, 3.43, 0.25, 0, -3.32  
3NOK, LYS\_84, 10.01, -0.49, 0, 0  
3RLN, LYS\_628, 9.66, -0.84, 0, 0  
2W2S, GLU\_137, 4.85, 0.35, 0, 0  
3GYW, ASP\_134, 3.94, 0.14, 0, 0  
3LJC, GLU\_128, 4.32, 0.14, -0.32, 0  
2DG7, ASP\_109, 3.58, 0.56, -0.78, 0  
3F1X, ARG\_118, 12.29, -0.21, 0, 0  
4EKU, ASP\_293, 3.23, 0.63, -1.21, 0  
2OB5, GLU\_94, 2.38, 0.28, -2.4, 0  
1Q2Y, ARG\_19, 10.17, -2.64, 0, 0.32  
3F7M, HIS\_150, 5.28, 0.73, 0.73, -2.68  
1G5Z, GLU\_121, 4.5, 0, 0, 0  
1T6L, ASP\_249, 2.72, 0.07, -1.15, 0  
3IVF, ARG\_178, 11.73, -0.77, 0, 0  
4FZR, GLU\_143, 4.5, 0, 0, 0  
2WB8, GLU\_482, 4.34, 0.07, -0.23, 0  
1HF8, GLU\_162, 4.5, 0, 0, 0  
2OKT, ARG\_143, 13.8, -2.57, 0, 3.87  
4GCO, LYS\_147, 10.22, -0.28, 0, 0  
1RZ2, TYR\_138, 12.94, 1.56, 0.36, 1.01  
3M7D, GLU\_21, 4.57, 0.07, 0, 0  
2W0G, ARG\_246, 12.5, 0, 0, 0  
1SUU, ASP\_540, 3.54, 0.28, -0.54, 0  
3J5N, ASP\_291, 3.85, 0.07, -0.02, 0  
4E8B, LYS\_133, 10.43, -0.07, 0, 0  
1DZF, GLU\_163, 4.5, 0, 0, 0  
1ZCE, ASP\_48, 3.74, 0.7, -0.76, 0  
2V4U, LYS\_392, 10.29, -0.21, 0, 0  
2PLQ, CYS\_300, 6.74, -2.26, 0, 0  
1EDG, ASP\_112, 3.89, 0.14, -0.05, 0  
1SI7, LYS\_96, 10.36, -0.14, 0, 0  
2QVT, GLU\_75, 4.5, 0, 0, 0  
1KCM, ARG\_246, 12.36, -0.14, 0, 0  
2BLL, CYS\_558, 8.87, -0.47, -0.74, 1.07  
2BLL, GLU\_644, 3.56, 0.63, -0.58, -0.99  
3ZSL, ARG\_183, 12.5, 0, 0, 0  
4DND, ARG\_94, 12.36, -0.14, 0, 0  
1Q46, LYS\_103, 10.15, -0.35, 0, 0  
2E3C, LYS\_429, 10.36, -0.14, 0, 0  
3F7M, TYR\_241, 10, 0, 0, 0  
2EJX, LYS\_109, 10.5, 0, 0, 0  
3TOW, CYS\_95, 8.96, -0.89, 0, 0.85  
1RS3, LYS\_207, 10.29, -0.21, 0, 0  
1WRU, LYS\_253, 10.5, 0, 0, 0  
1JT9, GLU\_54, 4.78, 0.28, 0, 0  
3FK5, LYS\_217, 10.5, 0, 0, 0  
3EIZ, TYR\_31, 10, 0, 0, 0  
1EV8, ASP\_85, 1.98, 1.12, -2.96, 0  
2Q13, LYS\_130, 10.43, -0.07, 0, 0  
1Q46, ARG\_112, 12.15, -0.35, 0, 0  
2ZCO, LYS\_17, 10.5, 0, 0, 0  
1XEU, ARG\_144, 12.29, -0.21, 0, 0  
2CXA, ARG\_37, 11.24, -1.26, 0, 0  
3GOZ, LYS\_253, 10.43, -0.07, 0, 0  
1VJG, LYS\_41, 10.43, -0.07, 0, 0  
2D2S, ARG\_591, 11.52, -0.98, 0, 0  
1LTU, ARG\_35, 12.01, -0.49, 0, 0  
1ZCU, ARG\_32, 11.66, -0.84, 0, 0  
2ZOM, ARG\_115, 12.01, -0.49, 0, 0  
1D2K, LYS\_159, 10.15, -0.35, 0, 0  
3V4G, HIS\_91, 6.63, 0.13, 0, 0  
4DIU, HIS\_191, 6.43, 0, 0, -0.07  
2OJQ, HIS\_516, 6.4, 0.04, 0, -0.14  
3I4T, LYS\_267, 10.22, -0.28, 0, 0  
1OGL, LYS\_275, 10.15, -0.35, 0, 0  
2CIU, LYS\_219, 10.5, 0, 0, 0  
1RKA, ARG\_227, 11.31, -1.19, 0, 0  
2OBI, HIS\_168, 6.5, 0, 0, 0  
1P6F, HIS\_40, 7.3, 0.8, 0, 0  
2A4D, ARG\_131, 12.5, 0, 0, 0  
1YTD, CYS\_114, 8.14, -2.15, 0, 1.29  
3LD1, ASP\_338, 3.7, 0.07, -0.17, 0  
3M16, GLU\_254, 3.95, 0.07, -0.62, 0  
1FHL, TYR\_209, 10.66, 0.73, -0.8, 0.73  
2OJQ, ASP\_465, 1.74, 0.7, -2.76, 0  
1RZ2, ASP\_195, 3.41, 0.35, -0.74, 0  
3ADO, ARG\_208, 10.96, -1.54, 0, 0  
3NJM, TYR\_48, 11.72, 1.72, 0, 0  
2CVB, TYR\_112, 11.05, 1.92, -0.87, 0  
3LQE, TYR\_328, 13.16, 3.16, 0, 0  
3LD1, TYR\_332, 9.84, 0.42, -0.58, 0  
3IVF, ARG\_82, 11.86, -0.53, 0, -0.11  
1DVO, ASP\_102, 3.74, 0, -0.06, 0  
2C13, ARG\_41, 12.29, -0.21, 0, 0  
3M7O, LYS\_9, 10.5, 0, 0, 0  
2X4G, ARG\_253, 12.15, -0.35, 0, 0  
3DSH, GLU\_446, 4.08, 0.21, -0.63, 0  
1BN6, ARG\_170, 11.94, -0.56, 0, 0  
2H85, ARG\_138, 11.94, -0.56, 0, 0  
4E8B, ASP\_73, 2.48, 0.56, -1.88, 0  
2B78, TYR\_124, 8.07, 2.77, -0.97, -3.73  
1TD6, GLU\_97, 4.19, 0.49, -0.8, 0  
3BA1, HIS\_302, 5.21, 0.8, 0, -2.09  
1IAP, LYS\_214, 10.01, -0.49, 0, 0  
3M3P, ARG\_242, 12.29, -0.21, 0, 0  
2ZCX, ARG\_112, 11.53, -0.97, 0, 0  
4DND, ARG\_51, 12.36, -0.14, 0, 0  
1KW4, TYR\_35, 10.08, 0.07, 0, 0.01  
3F1X, LYS\_44, 10.5, 0, 0, 0  
2AD1, ARG\_104, 13.45, -1.45, 0, 2.4  
4D8L, ARG\_146, 11.94, -0.56, 0, 0  
3LPZ, TYR\_263, 10.07, 0.07, 0, 0  
2NYC, ASP\_285, 3.08, 0.14, -0.86, 0  
3F6M, TYR\_91, 9.14, 0.14, -1, 0  
2G9D, ARG\_106, 12.95, -2.42, 0, 2.87  
2ZCO, GLU\_125, 3.28, 0.56, -1.78, 0  
3QKY, LYS\_158, 10.22, -0.28, 0, 0  
4E9E, ASP\_498, 3.99, 0.21, -0.02, 0  
2OKT, TYR\_235, 10.64, 0, 0, 0.64  
2CIU, ASP\_206, 2.1, 0.7, -2.4, 0  
1JSX, ARG\_139, 12.13, -0.37, 0, 0  
3GDG, GLU\_293, 4.24, 0.35, -0.61, 0  
1E9T, ARG\_237, 12.5, 0, 0, 0  
2Q98, ARG\_21, 12.5, 0, 0, 0  
1KCM, GLU\_79, 4.5, 0, 0, 0  
4DNU, GLU\_182, 2.44, 1.23, -1.04, -2.24  
1KCM, TYR\_103, 10, 0, 0, 0

2CYG, TYR\_108, 10.05, 0.07, -0.02, 0  
 3I4T, HIS\_246, 2.94, 0.66, 0, -4.22  
 2BAA, ARG\_187, 11.17, -1.33, 0, 0  
 1O6D, GLU\_79, 3.23, 0.28, -1.55, 0  
 3GYW, TYR\_54, 10.3, 0.0, -0.23  
 3U0V, ARG\_136, 13.6, -0.95, 0, 2.05  
 1PBV, ARG\_69, 11.59, -0.91, 0, 0  
 2BV9, ASP\_94, 3.96, 0.21, -0.05, 0  
 1V8E, ARG\_113, 12.01, -0.49, 0, 0  
 4DIU, LYS\_138, 9.8, -0.7, 0, 0  
 3Q9P, LYS\_112, 10.36, -0.14, 0, 0  
 1XAW, HIS\_499, 6.36, 0.0, -0.14  
 1O6D, HIS\_145, 6.81, 0.38, 0, -0.07  
 2V4U, GLU\_460, 4.5, 0.0, 0, 0  
 2RFA, GLU\_55, 4.78, 0.28, 0, 0  
 2D25, GLU\_743, 4.92, 0.42, 0, 0  
 3DZ1, HIS\_19, 6.29, 0.0, -0.21  
 2WB8, HIS\_666, 6.47, 0.04, 0, -0.07  
 1W7B, LYS\_152, 10.22, -0.28, 0, 0  
 1U7U, GLU\_386, 3.86, 0.7, -1.34, 0  
 2H85, TYR\_342, 10, 0, 0, 0  
 2FG1, LYS\_131, 10.29, -0.21, 0, 0  
 3V46, ARG\_289, 11.94, -0.56, 0, 0  
 2YWX, LYS\_157, 10.36, -0.14, 0, 0  
 1LPL, ASP\_136, 3.11, 0.42, -1.11, 0  
 2FD5, ASP\_101, 3.8, 0.0, 0, 0  
 1RWZ, ASP\_40, 1.42, 1.4, -3.78, 0  
 2ZQ5, LYS\_378, 10.5, 0.0, 0, 0  
 3GFP, ARG\_392, 12.43, -0.07, 0, 0  
 2D59, GLU\_13, 3.91, 0.07, -0.66, 0  
 3ETU, LYS\_66, 10.5, 0.0, 0, 0  
 2R0S, TYR\_287, 12.51, 0.07, 0.43, 2.01  
 1ZP2, LYS\_71, 10.08, -0.42, 0, 0  
 1V6T, ARG\_46, 12.01, -0.49, 0, 0  
 2R57, GLU\_311, 4.57, 0.07, 0, 0  
 4FLE, TYR\_159, 10.2, 0.86, -0.66, 0  
 4ACJ, ASP\_698, 3.87, 0.07, 0, 0  
 2A0J, GLU\_34, 4.61, 0.49, -0.38, 0  
 1XEU, ASP\_117, 3.48, 0.49, -0.81, 0  
 2QK1, CYS\_400, 10.34, 0.1, 1.34  
 1AK1, LYS\_246, 10.5, 0.0, 0, 0  
 2A1V, ARG\_125, 11.38, -1.12, 0, 0  
 1RSS, LYS\_29, 10.29, -0.21, 0, 0  
 3ETU, GLU\_45, 4.15, 0.14, -0.49, 0  
 3CRM, TYR\_106, 11.32, 1.26, 0.06  
 1ZBS, ARG\_91, 12.22, -0.28, 0, 0  
 2RIK, ARG\_96, 12.29, -0.21, 0, 0  
 1UAJ, HIS\_180, 6.97, 0.54, 0, -0.07  
 2QOP, ARG\_192, 12.15, -0.35, 0, 0  
 2GZQ, LYS\_144, 10.01, -0.49, 0, 0  
 3BB7, ASP\_67, 2.71, 0.28, -1.38, 0  
 3ERF, LYS\_55, 10.5, 0.0, 0, 0  
 1OST, CYS\_225, 5.95, -3.86, -1.53, 2.34  
 2QK1, TYR\_445, 13.9, 0.21, 0.8, 2.89  
 1NUJ, ARG\_154, 11.57, -1.09, 0.16  
 3DTE, CYS\_116, 8.71, -0.11, -1.46, 1.27  
 1GXN, LYS\_522, 10.22, -0.28, 0, 0  
 1UCH, ASP\_33, 3.42, 0.21, -0.59, 0  
 1CHD, ARG\_172, 12.22, -0.28, 0, 0  
 3V3T, HIS\_48, 6.71, 0.49, 0, -0.28  
 3GW3, HIS\_223, 4.92, 0.43, 0, -2.01  
 3TRE, ARG\_50, 12.5, 0.0, 0, 0  
 2H2Z, HIS\_80, 7.34, 0.91, 0, -0.07  
 2QDJ, HIS\_339, 7.23, 0.8, 0, -0.07  
 2FC3, ASP\_14, 3.3, 0.07, -0.58, 0  
 2POL, GLU\_140, 4.57, 0.07, 0, 0  
 1LPL, TYR\_184, 10.75, 1.08, -0.33, 0  
 2Q12, TYR\_36, 10, 0, 0, 0  
 2GEN, GLU\_20, 4.05, 0.35, -0.8, 0  
 4FCU, LYS\_37, 10.43, -0.07, 0, 0  
 2ZCX, ARG\_148, 11.94, -0.56, 0, 0  
 2YXO, GLU\_187, 4.25, 0.42, -0.67, 0  
 2OSA, ARG\_281, 11.52, -0.98, 0, 0  
 1PSW, GLU\_230, 4.85, 0.35, 0, 0  
 1JT9, GLU\_123, 4.85, 0.35, 0, 0  
 1WPS, GLU\_294, 4.5, 0.0, 0, 0  
 3M70, LYS\_43, 10.5, 0.0, 0, 0  
 1I60, GLU\_91, 3.98, 0.28, -0.8, 0  
 3UAH, ASP\_194, 3.21, 0.28, -0.87, 0  
 2IRM, GLU\_313, 3.82, 0.28, -0.96, 0  
 2XMZ, GLU\_121, 4.57, 0.07, 0, 0  
 1DUP, LYS\_4, 10.5, 0.0, 0, 0  
 2E35, LYS\_573, 10.29, -0.21, 0, 0  
 2Q13, ARG\_299, 11.8, -0.7, 0, 0  
 2E3H, HIS\_276, 6.36, 0.0, -0.14  
 2FGG, ARG\_29, 12.29, -0.21, 0, 0  
 3BPV, ARG\_16, 11.94, -0.56, 0, 0  
 3I82, CYS\_197, 9.04, -0.14, 0.18  
 2H85, GLU\_68, 5.09, 2.46, -1.21, -0.66  
 1DTP, HIS\_29, 3.89, 1.15, 0.3, -3.77  
 2NRK, TYR\_131, 11.8, 1.79, -0.57, 0.57  
 2V4X, ARG\_124, 11.73, -0.77, 0, 0  
 2PPN, ARG\_57, 11.87, -0.63, 0, 0  
 3JRT, GLU\_161, 3.61, 0.28, -1.17, 0  
 1MTZ, GLU\_85, 6.37, 2.87, -1, 0  
 2J8A, LYS\_360, 10.36, -0.14, 0, 0  
 3GW3, ARG\_249, 12.01, -0.49, 0, 0  
 1JKS, TYR\_39, 11.67, 0.07, 0.16  
 2X5Y, ASP\_769, 3.86, 0.14, -0.08, 0  
 3FS3, ARG\_108, 11.59, -0.91, 0, 0  
 2Z61, CYS\_125, 9.49, -0.79, 0.1, 2.8  
 2EHG, TYR\_5, 10.09, 0, -0.01, 0.09  
 1ANU, LYS\_92, 10.36, -0.14, 0, 0  
 2W1R, GLU\_128, 3.52, 0.62, -1.6, 0  
 2YXO, GLU\_314, 3.92, 0.56, -1.14, 0  
 2EDM, LYS\_85, 10.43, -0.07, 0, 0  
 2BT8, ASP\_277, 3.78, 0.07, -0.09, 0  
 3OBS, LYS\_98, 10.5, 0.0, 0, 0  
 3EGN, HIS\_430, 6.5, 0.0, 0, 0  
 3RE9, GLU\_205, 3.98, 0.28, -0.8, 0  
 3UX2, ARG\_138, 12.01, -0.49, 0, 0  
 3CAN, GLU\_106, 4.49, 0.07, -0.08, 0  
 3RFY, LYS\_195, 10.43, -0.07, 0, 0  
 2WB8, GLU\_488, 4.5, 0.0, 0, 0  
 3K8J, LYS\_31, 10.5, 0.0, 0, 0  
 3CCZ, LYS\_85, 10.43, -0.07, 0, 0  
 3U0V, ASP\_219, 4.04, 0.28, -0.04, 0  
 2AD1, ASP\_40, 3.44, 0.42, -0.77, 0  
 3K8J, TYR\_103, 9.9, 0, -0.1, 0  
 3RJX, GLU\_75, 4.5, 0.0, 0, 0  
 3H13, HIS\_469, 6.5, 0.0, 0, 0  
 4ETX, ASP\_430, 3.43, 0.21, -0.57, 0  
 3CCY, ARG\_19, 12.15, -0.35, 0, 0  
 2VGM, GLU\_334, 4.77, 0.07, 0.2, 0  
 2ZTY, ARG\_84, 11.66, -0.84, 0, 0  
 2A1V, TYR\_112, 10.67, 0.67, 0, 0  
 2PGX, GLU\_138, 3.95, 0.14, -0.69, 0  
 1X1E, ARG\_186, 11.1, -1.4, 0, 0  
 2WOZ, LYS\_605, 10.5, 0.0, 0, 0  
 3KEY, GLU\_488, 4.12, 0.42, -0.8, 0  
 3GW3, ARG\_120, 11.8, -0.7, 0, 0  
 2G55, ASP\_121, 3.14, 0.56, -1.22, 0  
 1EYH, ASP\_118, 2.75, 0.91, -1.96, 0  
 2D25, LYS\_707, 10.5, 0.0, 0, 0  
 1TXJ, LYS\_43, 10.5, 0.0, 0, 0  
 1YG2, ASP\_84, 3.96, 0.21, -0.05, 0  
 4DNU, GLU\_262, 4.64, 0.14, 0, 0  
 3JZ9, LYS\_351, 10.43, -0.07, 0, 0  
 1Y0K, GLU\_30, 7.19, 1.09, -0.8, 2.4  
 3EVP, TYR\_64, 9.34, 0.14, -0.8, 0  
 3BA1, ARG\_162, 11.59, -0.91, 0, 0  
 1WXQ, ARG\_376, 12.43, -0.07, 0, 0  
 2ILR, GLU\_517, 4.71, 0.21, 0, 0  
 3K9I, GLU\_75, 4.78, 0.28, 0, 0  
 2G2D, TYR\_36, 11.31, 0.0, 1.31  
 1KN3, HIS\_23, 6.39, 0.1, 0, -0.21  
 2OEW, TYR\_291, 10.07, 0.07, 0, 0  
 1PDB, LYS\_68, 10.08, -0.42, 0, 0  
 1PZC, LYS\_10, 10.01, -0.49, 0, 0  
 3IRA, LYS\_114, 10.36, -0.14, 0, 0  
 2G55, GLU\_44, 4.57, 0.07, 0, 0  
 1YTD, ASP\_31, 3.45, 0.14, -0.49, 0  
 3EVZ, GLU\_111, 3.56, 1.34, -2.27, 0  
 1DUN, ASP\_16, 3.11, 0.42, -1.11, 0  
 2E3C, ARG\_197, 11.94, -0.56, 0, 0  
 2XJ4, ARG\_202, 12.15, -0.35, 0, 0  
 3RKV, LYS\_208, 10.5, 0.0, 0, 0  
 1X6J, CYS\_13, 10.12, 0.0, 1.12  
 1RIS, LYS\_111, 10.5, 0.0, 0, 0  
 1E5S, TYR\_179, 11.37, 0.39, 0.0, 98  
 2B61, HIS\_181, 6.5, 0.0, 0, 0  
 2CXV, LYS\_102, 10.5, 0.0, 0, 0  
 4DNU, HIS\_264, 4.63, 0.0, -1.87  
 4AF2, GLU\_160, 3.53, 0.28, -1.25, 0  
 3DTE, ASP\_92, 2.21, 0.42, -2, 0  
 2CYG, ASP\_128, 3.77, 0, -0.03, 0  
 3BB7, ARG\_267, 12.23, -3.86, 0.3, 59  
 3RFY, ARG\_148, 12.08, -0.42, 0, 0  
 2XHC, LYS\_320, 10.43, -0.07, 0, 0  
 2G55, GLU\_140, 4.71, 0.21, 0, 0  
 1O9G, ARG\_235, 13.47, -1.19, 0.2, 15  
 2A1V, GLU\_106, 2.59, 0.49, -2.4, 0  
 2HNG, TYR\_17, 9.74, 0.54, -0.8, 0  
 3F1X, TYR\_6, 10.14, 0.14, 0, 0  
 3Q1C, TYR\_67, 10.46, 0.71, -0.25, 0  
 1OGL, GLU\_219, 4.5, 0.0, 0, 0  
 3G9G, ASP\_38, 4.02, 0.28, -0.06, 0  
 2PGX, GLU\_40, 4.64, 0.14, 0, 0  
 2EYI, ASP\_58, 2.52, 0.84, -2.12, 0  
 1J85, ASP\_40, 3.8, 0.0, 0, 0  
 3EST, LYS\_6, 10.5, 0.0, 0, 0  
 2QK1, LYS\_330, 10.5, 0.0, 0, 0  
 3N2T, ASP\_303, 3.74, 0, -0.06, 0  
 1RSS, ASP\_33, 3.84, 0.07, -0.03, 0  
 4EF5, TYR\_261, 10.45, 0.96, -0.75, 0.24  
 1PVT, HIS\_149, 6.43, 0.07, 0, -0.14  
 2C13, ARG\_207, 12.5, 0.0, 0, 0  
 3ETU, LYS\_151, 10.5, 0.0, 0, 0  
 2WB8, GLU\_606, 4.71, 0.26, -0.05, 0  
 3ELI, TYR\_65, 10, 0.0, 0, 0  
 1MTZ, TYR\_18, 12.61, 0.62, 0.8, 1.19  
 1TXJ, LYS\_114, 10.5, 0.0, 0, 0  
 2CXV, GLU\_2, 4.64, 0.14, 0, 0  
 4FD6, HIS\_25, 2.53, 0.02, 0.65, -4.64  
 2RIK, GLU\_116, 3.84, 0.14, -0.8, 0  
 1RHS, HIS\_203, 4.06, 0.85, 0, -3.29  
 3OKQ, ASP\_582, 3.94, 0.14, 0, 0  
 1PVT, GLU\_117, 4.5, 0.0, 0, 0  
 1VJG, GLU\_196, 5.23, 0.73, 0, 0  
 3BPP, ASP\_51, 2.9, 0.56, -1.47, 0  
 2QZQ, HIS\_94, 7.34, 0.98, 0, -0.14  
 2E3H, GLU\_245, 3.9, 0.14, -0.74, 0  
 3OKQ, ASP\_658, 3.87, 0.14, -0.07, 0  
 2I88, GLU\_365, 4.5, 0.0, 0, 0  
 3NOK, LYS\_4, 10.43, -0.07, 0, 0  
 1MTZ, GLU\_140, 3.71, 0.56, -1.35, 0  
 1R3D, HIS\_120, 2.83, 0.06, -0.65, -3.08  
 3FRR, ASP\_146, 3.92, 0.14, -0.02, 0  
 3HNX, ARG\_90, 11.59, -0.91, 0, 0  
 2Q13, GLU\_364, 3.91, 0.21, -0.8, 0  
 2P65, LYS\_43, 10.01, -0.49, 0, 0  
 1NFN, TYR\_162, 12.32, 0.07, 0.25, 1.99  
 2PLQ, LYS\_28, 10.29, -0.21, 0, 0  
 2B78, LYS\_353, 10.5, 0.0, 0, 0  
 1UAJ, LYS\_107, 10.36, -0.14, 0, 0  
 1L2F, LYS\_43, 10.5, 0.0, 0, 0  
 2Q99, ARG\_131, 10.95, -2.33, 0.0, 78  
 4F85, LYS\_130, 10.36, -0.14, 0, 0  
 2BLL, ARG\_624, 12.15, -0.35, 0, 0  
 3FWU, GLU\_87, 4.05, 0.35, -0.8, 0  
 1TUL, TYR\_34, 10.55, 0.21, -0.8, 1.14  
 1YTD, LYS\_139, 10.15, -0.35, 0, 0  
 3M7D, ARG\_317, 12.15, -0.35, 0, 0  
 2FD7, ASP\_513, 3.87, 0.07, 0, 0  
 2B0J, LYS\_130, 10.22, -0.28, 0, 0  
 3GYW, ASP\_119, 3.51, 0, -0.29, 0  
 3BCY, TYR\_54, 11.06, 0.0, 1.06  
 3B7H, ARG\_47, 12.15, -0.35, 0, 0  
 3EJC, GLU\_55, 4.57, 0.07, 0, 0  
 2PGX, GLU\_29, 3.84, 0.14, -0.8, 0  
 2IQT, GLU\_157, 3.21, 0.28, -1.57, 0  
 3GMS, TYR\_303, 9.83, 0, -0.17, 0  
 2CBE, LYS\_170, 10.22, -0.28, 0, 0  
 3RFY, LYS\_344, 10.36, -0.14, 0, 0  
 2B78, ASP\_133, 3.75, 0, -0.05, 0  
 2D7J, ASP\_69, 3.64, 0.49, -0.65, 0  
 2NRR, GLU\_348, 4.64, 0.14, 0, 0  
 3MTT, ASP\_437, 3.87, 0.07, 0, 0  
 3CSR, LYS\_123, 10.43, -0.07, 0, 0  
 1WOU, HIS\_22, 7.78, 1.49, 0, -0.21  
 3T57, HIS\_215, 6.95, 0.66, 0, -0.21  
 2E3C, GLU\_283, 3.18, 0.28, -1.61, 0  
 3ETU, GLU\_76, 4.57, 0.07, 0, 0  
 1JKS, GLU\_7, 3.18, 0.28, -1.6, 0  
 3G9T, HIS\_214, 6.36, 0.0, -0.14  
 1R5Q, CYS\_93, 8.86, -0.21, 0.0, 0.07  
 1O6D, LYS\_86, 10.5, 0.0, 0, 0  
 2CYG, TYR\_207, 11.2, 0.0, 1.2  
 1X7F, ARG\_203, 12.94, -1.67, 0.2, 11  
 1HUF, GLU\_19, 4.5, 0.0, 0, 0  
 2ZQ5, ARG\_227, 11.22, -1.28, 0, 0  
 3K9I, TYR\_114, 12.28, 0.07, -0.09, 2.3  
 2H2Z, ARG\_4, 12.15, 0.0, 0, 0  
 3CRM, ARG\_314, 12.43, -0.07, 0, 0  
 1MJS, GLU\_283, 4.63, 0.21, -0.08, 0  
 2C13, GLU\_121, 4.5, 0.0, 0, 0  
 1EVB, ASP\_214, 3.72, 0, -0.08, 0  
 3B21, ARG\_119, 12.56, -1.94, 0.2  
 2OKO, ARG\_32, 12.5, 0.0, 0, 0  
 1J85, HIS\_60, 2.02, 0, -1.46, -3.02  
 2XHC, LYS\_17, 10.43, -0.07, 0, 0  
 1TJE, TYR\_155, 13.27, 0.07, 0.8, 2.4  
 2D25, ARG\_664, 12.16, -2.17, 0.1, 83  
 2C13, HIS\_206, 6.88, 0.8, 0, -0.42  
 2D0A, ARG\_167, 12.15, -0.35, 0, 0  
 3HUE, LYS\_14, 10.5, 0.0, 0, 0  
 2FBI, TYR\_113, 9.78, 0.94, 0, -1.16  
 1EW4, ASP\_27, 3.84, 0.14, -0.1, 0  
 3EX9, ARG\_24, 11.94, -0.56, 0, 0  
 2O4D, ASP\_58, 3.8, 0.07, -0.07, 0  
 3M3P, HIS\_28, 6.47, 0.04, 0, -0.07  
 3CN5, TYR\_159, 10.0, 0.0, 0, 0  
 3LQE, ASP\_512, 3.2, 0.21, -0.81, 0  
 1R5Q, LYS\_15, 10.08, -0.42, 0, 0  
 3ETU, LYS\_32, 10.29, -0.21, 0, 0  
 3BB7, TYR\_165, 10, 0.0, 0, 0

3EVP,GLU\_269,3.84,0.14,-0.8,0  
 2DFL,LYS\_232,10.5,0,0,0  
 4EZB,HIS\_229,6.29,0,0,-0.21  
 3ZXY,ASP\_125,3.87,0.07,0,0  
 3ETV,TYR\_238,10.78,0.27,0,0.51  
 3FHF,LYS\_79,10.43,-0.07,0,0  
 2JHY,GLU\_163,4.12,0.42,-0.8,0  
 1CHD,ARG\_255,11.87,-0.63,0,0  
 3CGW,LYS\_234,10.01,-0.49,0,0  
 3LJC,ASP\_123,3.29,0.63,-1.15,0  
 2CW4,TYR\_90,11.88,0.91,-0.8,1.77  
 2V4X,LYS\_17,10.5,0,0,0  
 1EQ6,ARG\_72,12.15,-0.35,0,0  
 1YTQ,ARG\_97,12.22,-0.28,0,0  
 4E6S,HIS\_43,7.02,0.8,0,-0.28  
 3BJV,GLU\_35,4.19,0.49,-0.8,0  
 1TWU,ARG\_27,11.87,-0.63,0,0  
 1NWA,GLU\_138,2.03,0.7,-3.18,0  
 2WB8,LYS\_727,10.5,0,0,0  
 2Q12,ASP\_122,1.33,0.84,-3.31,0  
 2QEV,ARG\_89,11.31,-1.19,0,0  
 2CBE,HIS\_17,6.5,0.21,0,-0.21  
 2RQY,HIS\_156,6.95,0.66,0,-0.21  
 1AIL,ARG\_38,12.29,-0.21,0,0  
 3GG6,CYS\_43,8.59,-0.41,0,0  
 2B3M,CYS\_142,10.16,0,0,1.16  
 3IO0,ARG\_290,12.08,-0.42,0,0  
 2FBQ,GLU\_147,4.78,0.28,0,0  
 3CAN,LYS\_48,10.5,0,0,0  
 3CNU,GLU\_3,3.93,0.14,-0.71,0  
 1Z3X,ARG\_196,12.29,-0.21,0,0  
 1YOK,TYR\_6,9.69,0,-0.31,0  
 2WOZ,CYS\_419,9.37,-0.49,0,0.86  
 1KCM,HIS\_136,6.43,0,0,-0.07  
 2OGQ,GLU\_460,3.97,0.21,-0.74,0  
 1W7B,LYS\_148,10.36,-0.14,0,0  
 3JSN,ARG\_165,11.44,-2.57,0,1.52  
 3T5B,HIS\_182,4.22,0,0,-2.28  
 1Y2Q,GLU\_37,3.81,0.14,-0.83,0  
 2G3A,TYR\_24,9.27,0.07,-0.8,0  
 3OAT,LYS\_503,10.5,0,0,0  
 3Q1C,ASP\_162,3.62,0.35,-0.53,0  
 3Q2C,TYR\_77,10.07,0.07,0,0  
 2RJD,GLU\_313,3.72,0.28,-1.06,0  
 3E5T,CYS\_172,8.98,-1.3,0,1.28  
 3QKY,GLU\_235,4.21,0.42,-0.71,0  
 2YX0,ASP\_132,2.73,0.56,-1.63,0  
 100X,ARG\_33,12.36,-0.14,0,0  
 1IAP,ARG\_54,12.15,-0.35,0,0  
 3GYW,HIS\_168,6.63,0.27,0,-0.14  
 3F1X,ARG\_179,12.15,-0.35,0,0  
 3D9H,ASP\_220,3.73,0.14,-0.21,0  
 2ZOM,LYS\_328,10.5,0,0,0  
 1WP5,TYR\_126,11.16,1.88,-0.8,0.08  
 3IDW,ASP\_15,3.52,0.14,-0.42,0  
 3I4T,CYS\_223,8.42,-0.85,0,0.27  
 1Q2Y,GLU\_43,4.19,0.49,-0.8,0  
 1PVT,LYS\_42,10.5,0,0,0  
 2YYO,LYS\_38,10.5,0,0,0  
 2QEV,LYS\_136,10.43,-0.07,0,0  
 1J33,GLU\_145,4.05,0.35,-0.8,0  
 1C3K,GLU\_77,2.65,0.91,-2.76,0  
 1FO9,GLU\_309,0.91,2.34,-2.9,-3.03  
 3V1Q,ARG\_506,11.25,-1.25,0,0  
 2PGX,LYS\_85,10.5,0,0,0  
 2RFA,GLU\_80,2.87,0.8,-2.42,0  
 2H85,ASP\_335,4.08,0.28,0,0  
 2FPN,HIS\_87,6.5,0,0,0  
 1SIG,LYS\_300,10.5,0,0,0  
 2CXC,ARG\_49,11.87,-0.63,0,0  
 2IQT,LYS\_81,10.5,0,0,0  
 3CBN,ARG\_151,11.66,-0.84,0,0  
 3RLN,LYS\_623,10.43,-0.07,0,0  
 2W1R,LYS\_153,9.94,-0.56,0,0  
 2Q34,ARG\_176,12.22,-0.28,0,0  
 2DFL,HIS\_275,6.5,0,0,0  
 4DBX,LYS\_247,10.29,-0.21,0,0  
 1OST,LYS\_465,10.5,0,0,0  
 1XWM,ASP\_150,3.89,0.28,-0.19,0  
 2XMZ,GLU\_248,4.2,1.61,-1.91,0  
 3JZN,ASP\_317,3.94,0.14,0,0  
 3V75,GLU\_52,3.6,0.49,-1.39,0  
 2OPJ,GLU\_153,0.67,2.18,-1.21,-4.8  
 1YMS,TYR\_222,10,0,0,0  
 3GEC,ASP\_267,3.24,0.28,-0.84,0  
 4DVD,GLU\_50,4.12,0.14,-0.51,0  
 1O17,ASP\_54,2.25,0.63,-2.18,0  
 3EYE,ASP\_151,3.21,0.28,-0.87,0  
 2OPJ,ARG\_192,11.94,-0.56,0,0  
 1F2V,GLU\_49,4.02,0.07,-0.55,0  
 1SFE,CYS\_36,9.44,-0.65,0,1.09  
 1SJ8,GLU\_650,4.57,0.07,0,0  
 3VHJ,GLU\_146,3.76,0.49,-1.23,0  
 1WXQ,GLU\_132,4.05,0.35,-0.8,0  
 3QKY,ARG\_225,12.29,-0.21,0,0  
 3CRM,ASP\_20,3.74,0,-0.06,0  
 3RJZ,GLU\_114,3.55,0.49,-1.44,0  
 3PM2,ASP\_108,3.87,0.07,0,0  
 2GKG,ASP\_34,3.27,0.49,-1.02,0  
 3BQW,LYS\_344,10.22,-0.28,0,0  
 1PSW,GLU\_212,4.2,0.35,-0.65,0  
 3D9H,CYS\_117,8.41,-1.61,0,1.02  
 2QEV,TYR\_138,10.91,0.24,0,0.67  
 4F85,ARG\_200,12.08,-0.42,0,0  
 3LE4,ARG\_322,12.36,-0.14,0,0  
 2H85,TYR\_7,10,0,0,0  
 3BWT,LYS\_661,10.22,-0.28,0,0  
 3JSN,ARG\_97,12.08,-0.42,0,0  
 1KCM,GLU\_158,3.64,0.14,-1,0  
 2FG1,HIS\_83,7.23,0.8,0,-0.07  
 1H09,TYR\_164,13.22,0.07,0.76,2.39  
 2GEN,HIS\_126,6.29,0,0,-0.21  
 3LD1,ASP\_69,4.29,0.49,0,0  
 3KV0,ARG\_199,11.94,-0.56,0,0  
 1X8F,HIS\_40,6.62,0.19,0,-0.07  
 2RJD,ARG\_460,11.18,-1.32,0,0  
 3BCH,HIS\_131,7.28,0.84,0,-0.07  
 3CO1,LYS\_34,10.5,0,0,0  
 3IVF,LYS\_196,10.22,-0.28,0,0  
 2Q34,TYR\_198,10,0,0,0  
 3JSN,ASP\_89,3.83,0.28,-0.25,0  
 3H13,ASP\_325,2.94,0.35,-1.21,0  
 1MD6,GLU\_125,4.5,0,0,0  
 3CAX,LYS\_421,10.5,0,0,0  
 3O7K,GLU\_94,4.5,0,0,0  
 4H86,LYS\_48,10.08,-0.42,0,0  
 1HF8,ASP\_119,3.91,0.14,-0.03,0  
 1R53,TYR\_305,10.6,1.71,-1.12,0  
 3GE9,ARG\_62,12.5,0,0,0  
 3GA2,HIS\_77,6.46,0.03,0,-0.07  
 2XWS,ASP\_78,3.98,0.35,-0.17,0  
 2B3M,LYS\_31,9.66,-0.84,0,0  
 2ZQ5,GLU\_50,3.56,1.05,-1.98,0  
 3CRM,ASP\_82,3.1,0.35,-1.05,0  
 2CVB,ARG\_61,12.5,0,0,0  
 3H8Y,ARG\_70,12.5,0,0,0  
 3M9A,LYS\_43,10.22,-0.28,0,0  
 1GPP,HIS\_79,1.18,0.19,0,-5.51  
 3K1H,ASP\_116,3.56,0.07,-0.31,0  
 1L2F,LYS\_193,10.36,-0.14,0,0  
 1DZF,HIS\_146,6.22,0,0,-0.28  
 2Q98,GLU\_67,4.55,0.07,-0.02,0  
 1G8P,GLU\_261,4.5,0,0,0  
 1EDG,HIS\_162,4.98,0.73,0,-2.25  
 3FRR,TYR\_177,13.44,0.58,-0.48,3.35  
 1OTM,ASP\_134,2.25,0.28,-1.83,0  
 3F5D,LYS\_126,10.29,-0.21,0,0  
 2Q13,GLU\_67,4.14,0.42,-0.78,0  
 2F8H,LYS\_233,10.5,0,0,0  
 3EAZ,TYR\_116,12.04,0.11,-0.01,1.94  
 1WNH,TYR\_76,12.31,1.98,0,0.33  
 1NRI,ASP\_232,4.15,0.35,0,0  
 1DCF,ASP\_121,4.01,0.21,0,0  
 3CS1,GLU\_76,4.17,0.21,-0.54,0  
 2WB3,TYR\_290,10,0,0,0  
 3U0V,LYS\_42,10.5,0,0,0  
 1L2F,ASP\_299,2.59,0.63,-1.84,0  
 2OBI,GLU\_82,4.88,1.91,-1.53,0  
 1L2F,ARG\_51,11.87,-0.63,0,0  
 2BOJ,GLU\_307,4.41,0.07,-0.16,0  
 2B0A,LYS\_49,10.15,-0.35,0,0  
 2Z61,GLU\_177,4.4,0.7,-0.8,0  
 1GQE,LYS\_31,10.5,0,0,0  
 3FTT,LYS\_79,10.5,0,0,0  
 2BCF,LYS\_149,10.29,-0.21,0,0  
 2I88,ASP\_429,3.28,0.28,-0.8,0  
 2PWQ,HIS\_50,6.36,0,0,-0.14  
 3GOZ,LYS\_294,10.43,-0.07,0,0  
 2X5Y,TYR\_893,10.64,1.2,-0.8,0.24  
 2QHT,GLU\_65,4.5,0,0,0  
 3RKV,GLU\_323,4.59,0.21,-0.12,0  
 2FBQ,ARG\_103,13.36,-1.54,0,2.4  
 3OOP,GLU\_53,4.57,0.07,0,0  
 1UJ8,HIS\_10,6.5,0,0,0  
 3QKY,CYS\_117,9.97,-0.31,0,1.28  
 1R5S,LYS\_137,10.43,-0.07,0,0  
 1BGF,ARG\_70,12.43,-0.07,0,0  
 3VHJ,LYS\_3,10.43,-0.07,0,0  
 2VGY,ASP\_87,3.74,0,-0.06,0  
 2CWY,GLU\_70,4.25,0.07,-0.33,0  
 2RFA,LYS\_244,10.5,0,0,0  
 3IBT,HIS\_49,7.6,1.31,0,-0.21  
 2OGQ,HIS\_373,6.5,0,0,0  
 3IO0,GLU\_262,3.9,2.56,-0.8,-2.36  
 1D2K,LYS\_223,9.66,-0.84,0,0  
 1OLR,ASP\_111,4.08,0.28,0,0  
 1EW4,ASP\_25,3.8,0,0,0  
 2E3S,LYS\_578,10.29,-0.21,0,0  
 3ADO,GLU\_304,3.25,0.35,-1.6,0  
 1XDZ,ASP\_142,0.61,0.56,-3.75,0  
 3IRA,LYS\_39,10.22,-0.28,0,0  
 2A6B,ARG\_173,11.8,-0.7,0,0  
 4DNU,ARG\_121,12.36,-0.14,0,0  
 1JSX,GLU\_170,4.5,0,0,0  
 2F8H,ARG\_214,12.43,-0.07,0,0  
 1SJ8,ASP\_695,3.8,0,0,0  
 1R16,ASP\_151,1.65,0.77,-2.92,0  
 2P1W,GLU\_92,4.5,0,0,0  
 1MUF,LYS\_233,10.36,-0.14,0,0  
 3I4T,LYS\_24,10.5,0,0,0  
 2R51,HIS\_184,6.29,0,0,-0.21  
 1X7F,GLU\_277,4.57,0.07,0,0  
 3M7D,ARG\_151,12.61,-2.47,0,2.58  
 3CNU,LYS\_77,10.29,-0.21,0,0  
 2EHG,LYS\_101,10.5,0,0,0  
 2FD5,ARG\_11,12.01,-0.49,0,0  
 2ZQ5,ARG\_333,12.01,-0.49,0,0  
 1PNE,LYS\_53,10.5,0,0,0  
 1EYH,CYS\_96,10.77,0,0,1.77  
 1J33,ARG\_293,12.15,-0.35,0,0  
 2Z14,HIS\_88,6.5,0.14,0,-0.14  
 3PF6,GLU\_132,3.92,0.21,-0.79,0  
 1RL0,TYR\_183,13.27,0.07,0.8,2.4  
 2CN1,LYS\_32,10.22,-0.28,0,0  
 4F8A,GLU\_682,4.57,0.07,0,0  
 3ANJ,LYS\_96,10.29,-0.21,0,0  
 2FD5,LYS\_5,10.5,0,0,0  
 3RKV,ASP\_216,3.36,0.28,-0.72,0  
 1R5S,ARG\_32,12.5,0,0,0  
 2ZCO,LYS\_275,10.5,0,0,0  
 1T95,GLU\_171,3.38,0.42,-1.54,0  
 3RLE,CYS\_173,10.28,-0.01,-0.23,1.52  
 2X5Y,TYR\_819,8.22,0.72,-2.51,0  
 2CN1,LYS\_107,3.27,0.16,0,-3.39  
 2Q99,HIS\_91,0.84,0.01,-1.1,-4.57  
 1RWZ,ARG\_162,11.66,-0.84,0,0  
 3I82,ASP\_23,3.8,0.07,-0.07,0  
 1AM2,HIS\_41,8.18,0.31,2.86,-1.5  
 3ETU,TYR\_343,11.84,0.14,0,1.7  
 1WRU,LYS\_210,10.22,-0.28,0,0  
 3GA2,HIS\_35,6.5,0,0,0  
 1OST,LYS\_331,10.22,-0.28,0,0  
 2CXA,GLU\_156,6.88,3.37,-0.99,0  
 2Z61,ARG\_72,10.71,-1.79,0,0  
 3DHN,TYR\_197,12.07,2.94,-0.88,0  
 3PBH,LYS\_166,10.36,-0.14,0,0  
 4H86,LYS\_15,10.5,0,0,0  
 1HF8,ASP\_266,3.49,0.49,-0.8,0  
 1T3Y,LYS\_75,10.29,-0.21,0,0  
 2B61,LYS\_92,10.82,0,0,0.32  
 2JHY,ASP\_172,11.45,-1.05,0,0  
 1PV5,GLU\_113,4.17,0.28,-0.61,0  
 3D9H,LYS\_86,10.5,0,0,0  
 3UX2,GLU\_144,4.5,0,0,0  
 2X5Y,ASP\_896,4.19,0.14,0.25,0  
 1ZP2,HIS\_95,6.36,0,0,-0.14  
 3EAZ,LYS\_171,10.43,-0.07,0,0  
 1R53,GLU\_46,12.62,-1.37,0,1.49  
 1O6D,ARG\_50,11.87,-0.63,0,0  
 3JV1,LYS\_84,10.43,-0.07,0,0  
 1BKR,TYR\_19,10.21,0.21,0,0  
 1N81,GLU\_24,3.95,0.14,-0.69,0  
 1NAR,TYR\_174,11.58,3.15,-1.56,0  
 2GS5,HIS\_138,6.54,0.04,0,0  
 1PSW,LYS\_142,10.43,-0.07,0,0  
 1ZYL,ARG\_283,12.18,-1.61,0,1.29  
 3MIX,LYS\_547,10.29,-0.21,0,0  
 2BDV,ASP\_13,3.78,0.14,-0.15,0  
 2E3S,GLU\_575,4.05,0.35,-0.8,0  
 1W7B,GLU\_306,3.62,0.49,-1.37,0  
 2GZR,ARG\_180,12.36,-0.14,0,0  
 1WRU,ASP\_325,2.87,0.35,-1.28,0  
 2OEW,GLU\_272,4.05,0.35,-0.8,0  
 1Q8B,GLU\_72,4.25,0,-0.25,0  
 3LPZ,ARG\_60,12.29,-0.21,0,0  
 2R57,LYS\_206,10.36,-0.14,0,0  
 2P65,ARG\_33,12.01,-0.49,0,0  
 2D8N,LYS\_139,10.43,-0.07,0,0  
 3HVM,CYS\_52,11.39,0,0,2.39  
 1QYI,GLU\_192,3.71,0.35,-1.14,0  
 1MD6,LYS\_11,10.43,-0.07,0,0  
 1R16,ASP\_48,1.53,0.77,-3.03,0  
 2R2Y,ASP\_115,3.19,0.14,-0.75,0  
 1CHD,ASP\_231,3.25,0.21,-0.76,0  
 3CAX,GLU\_155,4.19,0.14,-0.45,0  
 1PGV,ARG\_382,12.08,-0.42,0,0

3OBS,ARG\_18,12.29,-0.21,0,0  
3E5T,GLU\_29,2.59,0.49,-2.4,0  
4F85,HIS\_229,6.43,0,0,-0.07  
3DZ1,TYR\_252,13.27,0.07,0.8,2.4  
2CL3,LYS\_173,10.29,-0.21,0,0  
2OJQ,GLU\_462,3.9,0.28,-0.88,0  
3KT9,TYR\_96,10.25,1.07,-0.82,0  
1QYI,TYR\_106,10.26,0.14,-2.61,2.73  
2EA9,CYS\_52,8.91,-0.09,0,0  
2H8O,CYS\_230,11.99,0,0,2.99  
2RFA,ARG\_155,12.08,-0.42,0,0  
3C38,TYR\_230,13.23,0.14,-0.38,3.47  
1KCM,LYS\_87,10.5,0,0,0  
3BJV,ASP\_93,3.09,0.77,-1.48,0  
1NWA,HIS\_50,6.15,0,0,-0.35  
2VGM,TYR\_316,10.61,0.61,0,0  
2HRZ,GLU\_248,4.5,0,0,0  
2ZQ5,GLU\_375,3.43,0.28,-1.35,0  
1XIP,ASP\_239,3.8,0,0,0  
1DCF,ARG\_45,12.36,-0.14,0,0  
1V43,LYS\_176,10.5,0,0,0  
1E55,ASP\_140,3.88,0.35,-0.27,0  
3ANJ,ASP\_224,2.43,0.49,-1.86,0  
2RIS,ARG\_143,12.08,-0.42,0,0  
3LD1,LYS\_66,10.29,-0.21,0,0  
2CIU,LYS\_135,10.29,-0.21,0,0  
3RKV,GLU\_317,3.69,0.35,-1.16,0  
1RAJ,ASP\_317,3.36,0.63,-1.07,0  
3MIX,ASP\_390,3.17,0,-0.63,0  
3EUR,LYS\_20,10.01,-0.49,0,0  
2NYC,HIS\_182,6.5,0,0,0  
3ETV,GLU\_90,4.71,0.21,0,0  
1ANU,TYR\_39,9.46,0,-0.54,0  
2Q12,HIS\_45,7.01,0.58,0,-0.07  
2H8O,HIS\_124,4.25,0.79,0,-3.05  
3TIR,GLU\_7,3.52,0.21,-1.18,0  
3ILC,ASP\_156,3.36,0.42,-0.86,0  
3TIR,GLU\_176,4.64,0.14,0,0  
3I82,LYS\_57,9.94,-0.56,0,0  
1G8P,ARG\_54,12.5,0,0,0  
1PSW,HIS\_104,6.8,0.3,0,0  
2G3A,ARG\_108,11.73,-0.77,0,0  
1CBY,GLU\_198,4.5,0,0,0  
1EW4,ARG\_53,11.38,-1.12,0,0  
1C3K,HIS\_26,6.62,0.12,0,0  
1W7B,TYR\_232,8.95,1.06,-2.11,0  
2P52,ASP\_256,1.46,0.98,-3.32,0  
1MTZ,ARG\_267,12.29,-0.21,0,0  
1SQW,ARG\_120,12.08,-0.42,0,0  
4FD6,HIS\_55,2.77,0,-1.17,-2.56  
1YTQ,HIS\_134,7.03,0.53,0,0  
4FCU,GLU\_205,1.48,0.91,-3.92,0  
2IQT,ARG\_76,12.01,-0.49,0,0  
3KB5,ARG\_282,11.17,-1.33,0,0  
1OTM,ASP\_233,4.08,0.28,0,0  
3BJV,LYS\_23,10.36,-0.14,0,0  
1TWU,ARG\_37,11.94,-0.56,0,0  
3COC,CYS\_311,8.87,-0.55,0,0.42  
3RFY,LYS\_244,10.15,-0.35,0,0  
3SMD,GLU\_60,3.37,0.28,-1.41,0  
1KCM,LYS\_209,10.5,0,0,0  
2YYO,ARG\_106,11.8,-0.7,0,0  
1W24,HIS\_13,6.5,0,0,0  
1OLR,TYR\_119,10.1,0.1,0,0  
1NIJ,ASP\_75,3.86,0.21,-0.15,0  
3M3P,GLU\_27,4.57,0.07,0,0  
3LJC,ASP\_188,2.2,0.63,-2.24,0  
3TOW,ARG\_92,11.36,-1.14,0,0  
3FIX,TYR\_163,10.43,1.87,-0.61,-0.83  
4EF5,CYS\_206,9.67,0,0,0.67  
2QK0,GLU\_35,3.68,0.77,-1.59,0  
3KB5,CYS\_456,11.01,0.38,-0.22,1.84  
3ETU,HIS\_153,7.16,0.8,0,-0.14  
2H14,LYS\_70,10.08,-0.42,0,0  
3G9T,GLU\_47,3.84,0.14,-0.8,0  
1DUN,ARG\_112,12.5,0,0,0  
1R53,ARG\_165,12.7,-1.8,0,2  
1GQE,LYS\_307,10.43,-0.07,0,0  
2EDM,ASP\_84,3.55,0.35,-0.6,0  
2W0G,LYS\_157,10.5,0,0,0  
3DSH,GLU\_423,4.5,0,0,0  
2PGE,TYR\_96,9.85,0.92,-1.07,0  
3Q6L,TYR\_20,11.31,1.48,-0.8,0.62  
1XAW,ASP\_437,3.86,0.14,-0.08,0  
3LJN,GLU\_124,4.57,0.07,0,0  
1NJ4,LYS\_62,10.36,-0.14,0,0  
1WP5,GLU\_157,3.32,0.35,-1.53,0  
2PGX,ARG\_132,13.06,-1.74,0,2.3  
3L7N,GLU\_212,3.21,0.35,-1.63,0  
3CAX,LYS\_319,10.5,0,0,0  
3FXH,ASP\_30,3.8,0,0,0  
1YR6,LYS\_137,10.43,-0.07,0,0  
3GV0,LYS\_291,10.08,-0.42,0,0  
2GZR,GLU\_165,4.7,1.58,-0.8,-0.58  
1RWZ,TYR\_236,12.44,2.44,0,0  
2XHC,LYS\_60,10.5,0,0,0  
3A2Z,ASP\_50,3.94,0.14,0,0  
1SUU,GLU\_628,4.5,0,0,0  
3U2R,GLU\_117,4.64,0.14,0,0  
1FO9,ARG\_189,11.38,-1.12,0,0  
2D59,GLU\_136,3.91,0.93,-1.52,0  
1DCF,CYS\_101,9.07,-0.38,0,0.45  
3F53,TYR\_135,10.07,0.07,0,0  
3OA7,GLU\_492,4.57,0.07,0,0  
1EYH,ARG\_63,10.98,-1.52,0,0  
2OGQ,ASP\_438,1.5,0.63,-2.93,0  
2B6P,CYS\_88,8.97,-0.1,0,0.07  
3H13,GLU\_398,4.5,0,0,0  
1XEU,GLU\_228,4.34,0.07,-0.23,0  
1J33,GLU\_304,5.33,1.96,-1.13,0  
1LPL,LYS\_137,10.36,-0.14,0,0  
1YTD,LYS\_375,10.43,-0.07,0,0  
2A0J,LYS\_95,10.22,-0.28,0,0  
3EX9,HIS\_73,4.21,0,0,-2.29  
3IRA,TYR\_24,13.25,0.42,-0.4,3.23  
2FC3,HIS\_65,6.62,0.26,0,-0.14  
1DVO,LYS\_56,10.5,0,0,0  
3JSN,LYS\_182,10.29,-0.21,0,0  
3I47,GLU\_35,4.78,0.28,0,0  
1TR9,ARG\_72,11.87,-0.63,0,0  
2Q34,GLU\_92,4.5,0,0,0  
2H14,HIS\_255,2.61,0.5,0,-4.39  
3LD1,ARG\_6,12.22,-0.28,0,0  
1GXN,TYR\_598,10.92,2.08,-1.16,0  
2IRM,GLU\_45,3.25,0.14,-1.39,0  
2F9F,ASP\_159,2.9,0.28,-1.19,0  
1BGF,LYS\_88,10.5,0,0,0  
3Q1C,ARG\_147,11.38,-1.12,0,0  
1O17,LYS\_188,10.5,0,0,0  
2DFL,LYS\_288,10.29,-0.21,0,0  
3BB7,LYS\_144,10.15,-0.35,0,0  
3PZ9,ARG\_145,11.8,-0.7,0,0  
3M66,ARG\_277,11.8,-0.7,0,0  
3ADO,LYS\_311,9.94,-0.56,0,0  
3C5V,LYS\_64,10.29,-0.21,0,0  
2H2W,GLU\_116,3.05,0.35,-1.8,0  
3GG6,GLU\_95,5.33,2.24,-1.13,-0.28  
1K95,CYS\_94,10.28,-0.08,0,1.36  
2PGE,LYS\_192,10.08,-0.42,0,0  
3BWT,GLU\_658,3.58,0.56,-1.47,0  
3S0A,HIS\_11,6.79,0.43,0,-0.14  
1GXN,HIS\_446,3.76,0,0,-2.74  
4EF5,ARG\_331,12.08,-0.42,0,0  
1SNT,HIS\_82,7.52,1.09,0,-0.07  
3ZRI,ARG\_141,11.73,-0.77,0,0  
1X7F,CYS\_359,11.06,0,0,2.06  
1MD6,GLU\_137,4.5,0,0,0  
3CAX,LYS\_356,10.43,-0.07,0,0  
1DCF,LYS\_100,10.15,-0.35,0,0  
1YTQ,TYR\_155,10.07,0.07,0,0  
2AZL,GLU\_71,6.11,2.23,0,-0.62  
1RIS,ARG\_290,11.94,-0.56,0,0  
3ELI,ARG\_137,12.01,-0.49,0,0  
1XIP,LYS\_310,10.01,-0.49,0,0  
2FPN,ARG\_77,12.01,-0.49,0,0  
1PDB,LYS\_54,9.73,-0.77,0,0  
2C2Y,ASP\_247,3.89,0.14,-0.05,0  
3R2E,ARG\_93,11.87,-0.63,0,0  
3CO1,LYS\_89,10.22,-0.28,0,0  
2CXA,GLU\_22,4.64,0.14,0,0  
2BLX,ARG\_549,11.87,-0.63,0,0  
3IU5,LYS\_128,10.5,0,0,0  
4GA2,ASP\_108,3.18,0.42,-1.04,0  
3H04,ARG\_172,13.68,-1.7,0,2.88  
3P2F,ARG\_25,11.94,-0.56,0,0  
3CSR,ARG\_96,13.16,-1.37,0,2.03  
2OJQ,LYS\_671,10.43,-0.07,0,0  
3BCY,LYS\_68,10.43,-0.07,0,0  
2IF4,HIS\_60,6.51,0.08,0,-0.07  
4FLE,ASP\_125,3.94,0.28,-0.14,0  
1ES9,ARG\_214,12.29,-0.21,0,0  
2Q5X,GLU\_848,3.98,0.28,-0.8,0  
4FZR,ARG\_97,12.08,-0.42,0,0  
3ANJ,GLU\_13,4.78,0.28,0,0  
2JKF,TYR\_115,12.01,0.07,0,1.94  
3V1Q,LYS\_612,10.22,-0.28,0,0  
2IQT,GLU\_243,4.57,0.07,0,0  
1P1L,ASP\_68,1.71,0.42,-2.51,0  
3ADO,TYR\_232,10.0,0,0,0  
3EZ7,ARG\_391,12.22,-0.28,0,0  
3LMF,LYS\_110,10.29,-0.21,0,0  
4ECC,LYS\_27,10.08,-0.42,0,0  
1GSZ,GLU\_180,4.05,0.35,-0.8,0  
3M7D,GLU\_259,4.5,0,0,0  
2I88,ASP\_422,3.72,0,-0.08,0  
1FO9,LYS\_180,10.5,0,0,0  
3FHF,GLU\_112,5.35,1.74,-0.97,0.08  
1L2H,LYS\_77,10.5,0,0,0  
3QKY,GLU\_86,3.98,0.28,-0.8,0  
3NR5,ARG\_67,12.5,0,0,0  
4EKU,TYR\_265,12.28,2.05,-0.03,0.27  
1A8Q,ASP\_87,3.73,0.56,-0.63,0  
2APL,LYS\_104,10.5,0,0,0  
3M16,HIS\_167,5.78,0.166,-2.38  
3GOZ,ASP\_263,3.45,0.49,-0.84,0  
3BWT,LYS\_619,10.08,-0.42,0,0  
1W7B,ARG\_196,12.29,-0.21,0,0  
2VGM,TYR\_268,9.08,0.14,-1.06,0  
1NAF,ASP\_189,2.64,0.7,-1.85,0  
2GKG,ARG\_44,11.87,-0.63,0,0  
2ILR,LYS\_447,10.15,-0.35,0,0  
1XKR,TYR\_193,11.58,0.07,-0.03,1.54  
3CRM,TYR\_60,12.94,0.28,0.26,2.4  
3MTT,LYS\_598,10.5,0,0,0  
4ANN,ASP\_31,4.22,0.42,0,0  
3VJ8,ASP\_85,1.21,1.19,-3.77,0  
1WPA,LYS\_501,10.01,-0.49,0,0  
1K95,TYR\_57,10.0,0,0,0  
2XJ4,GLU\_86,3.67,0.35,-1.18,0  
1V8E,HIS\_171,7.01,0.72,0,-0.21  
15BX,TYR\_149,10.0,0,0,0  
4AE7,ARG\_118,12.43,-3.1,0.3,0.3  
1LZL,GLU\_123,1.61,0.56,-3.45,0  
1GSZ,LYS\_75,10.22,-0.28,0,0  
4EUG,TYR\_19,13.48,0.28,0.8,2.4  
3CJW,GLU\_300,4.64,0.28,-0.14,0  
4FZN,TYR\_189,12.22,0.21,-0.4,2.4  
3C38,GLU\_161,4.5,0,0,0  
3DHN,HIS\_37,6.62,0.26,0,-0.14  
1Y0K,TYR\_45,13.16,0.21,0.55,2.4  
1ZBP,GLU\_247,4.5,0,0,0  
2G55,GLU\_149,2.7,0.55,-2.35,0  
1OIS,ARG\_278,12.5,0,0,0  
1X04,GLU\_202,4.5,0,0,0  
3V75,TYR\_109,10.86,0,0,0.86  
2EEY,ARG\_12,12.08,-0.42,0,0  
1YB2,LYS\_176,10.15,-0.35,0,0  
3LJI,ASP\_127,3.17,0.56,-1.19,0  
1GSZ,LYS\_196,4.78,0.28,0,0  
1GQE,LYS\_204,10.36,-0.14,0,0  
3LD1,GLU\_90,2.73,0.63,-2.4,0  
1Q46,LYS\_11,10.5,0,0,0  
2OGQ,ASP\_419,3.76,0,-0.04,0  
3GFP,ARG\_371,12.22,-0.28,0,0  
4ESS,ARG\_51,12.08,-0.42,0,0  
1P4X,HIS\_186,3.69,0,-2.81  
1JT9,ASP\_115,3.74,0,-0.06,0  
3BQW,ASP\_300,2.23,0.77,-2.34,0  
2F4Q,TYR\_289,6.23,0.32,-0.56,-3.53  
1UOH,GLU\_205,4.5,0,0,0  
2B0J,GLU\_36,3.95,0.56,-1.11,0  
1WYC,ASP\_207,1.7,0.49,-2.59,0  
4ESS,LYS\_135,10.22,-0.28,0,0  
2RIK,ARG\_227,12.43,-0.07,0,0  
2P5D,ASP\_2,3.7,0,-0.1,0  
4ETX,ARG\_234,12.43,-0.07,0,0  
1SNT,GLU\_257,4.5,0,0,0  
1T95,ASP\_57,16.0,0.49,-1.13,0  
3BWT,ASP\_715,2.66,0.56,-1.69,0  
4GCO,LYS\_209,10.5,0,0,0  
1H09,TYR\_232,10.76,0.07,0.0,69  
2AD1,LYS\_282,10.29,-0.21,0,0  
2FBI,ARG\_38,11.42,-1.08,0,0  
2QZQ,LYS\_148,10.43,-0.07,0,0  
1XAW,ASP\_466,3.91,0.28,-0.16,0  
1YW5,ARG\_18,12.5,0,0,0  
2G5X,GLU\_23,4.11,0.21,-0.6,0  
2DG7,GLU\_113,4.33,0.28,-0.45,0  
3GMS,GLU\_82,4.5,0,0,0  
4ETX,ARG\_367,12.08,-0.82,0.1,1  
3GW3,HIS\_358,6.74,1.6,2.18,-3.54  
1TJE,ASP\_54,3.12,0.56,-1.24,0  
1OTM,LYS\_133,10.43,-0.07,0,0  
2F4Q,ARG\_135,12.61,-2.29,0.2,2.4  
2FL7,TYR\_119,9.64,0.28,-1.27,0.63  
3OAT,ASP\_550,3.04,0.35,-1.12,0  
2CW4,ARG\_92,11.8,-0.7,0,0  
1GXN,ARG\_626,11.31,-1.19,0,0  
4FLE,TYR\_181,13.41,0.21,0.8,2.4  
3GW3,HIS\_266,6.36,0,0,-0.14  
2D25,ARG\_724,12.01,-0.49,0,0  
4DVD,LYS\_24,10.22,-0.28,0,0  
1NJ4,ARG\_39,11.73,-0.77,0,0  
3RFF,LYS\_106,10.08,-0.42,0,0  
1X8F,ASP\_175,4.01,0.21,0,0  
1R3F,TYR\_36,11.64,1.4,-0.18,0.42



1V43,ASP\_75,1.9,0.63,-2.53,0  
2AZL,GLU\_260,4.6,0.21,-0.11,0  
2R51,LYS\_33,10.5,0,0,0  
1MHN,TYR\_127,12.28,0.28,-0.4,2.4  
2H85,ARG\_224,12.01,-0.49,0,0  
1WOU,GLU\_13,4.5,0,0,0  
1Q46,LYS\_60,10.29,-0.21,0,0  
3F1X,ARG\_158,11.71,-0.42,0,-0.37  
1X9G,LYS\_138,10.5,0,0,0  
3LMF,CYS\_33,5.61,-3.46,0,0.07  
1NAR,GLU\_42,4.29,2.25,-2.46,0  
4D8L,ASP\_226,3.31,0.28,-0.78,0  
2E3C,ARG\_227,11.11,-1.39,0,0  
3GMS,ARG\_36,12.08,-0.42,0,0  
1PNE,ASP\_13,1.92,0.56,-2.44,0  
2X4L,LYS\_195,10.5,0,0,0  
1S1Y,GLU\_2,3.71,0.21,-1,0  
3BB7,ASP\_85,3.8,0,0,0  
2H8O,LYS\_86,10.5,0,0,0  
2OOK,HIS\_352,2.28,0,-1.21,-3.01  
1L2F,ASP\_151,3.47,0.28,-0.61,0  
3DSH,LYS\_397,10.29,-0.21,0,0  
1MML,LYS\_53,10.15,-0.35,0,0  
3CXS,LYS\_152,10.29,-0.21,0,0  
3FNI,ARG\_151,11.8,-0.7,0,0  
1XAW,TYR\_420,9.54,0.14,-0.8,0.2  
1LN4,GLU\_54,3.84,0.14,-0.8,0  
1I6O,LYS\_195,10.22,-0.28,0,0  
4EKU,ARG\_309,12.15,-0.35,0,0  
3RLE,GLU\_8,4.5,0,0,0  
1NRI,CYS\_90,10.9,-0.34,1.56,0.68  
2H3O,LYS\_54,10.36,-0.14,0,0  
3FWU,TYR\_99,9.89,0.71,-0.82,0  
3M66,TYR\_384,9.78,0.14,-0.43,0.07  
3GW3,HIS\_189,6.29,0,0,-0.21  
4EZB,HIS\_265,8.1,1.81,0,-0.21  
1O3X,ARG\_299,12.5,0,0,0  
1MTZ,LYS\_76,10.5,0,0,0  
1W24,TYR\_69,10.09,0.23,-0.47,0.33  
1PV5,GLU\_103,3.37,0.21,-1.34,0  
2WOZ,ARG\_335,12.08,-0.42,0,0  
1WRU,GLU\_198,4.64,0.14,0,0  
2ZCO,ASP\_52,3.87,0.07,0,0  
2QEV,GLU\_130,4.57,0.07,0,0  
2ZCO,TYR\_54,10,0,0,0  
3GOZ,HIS\_22,6.5,0,0,0  
3CRM,ARG\_43,11.73,-0.77,0,0  
3G9G,LYS\_149,10.22,-0.28,0,0  
2NYC,TYR\_316,10,0,0,0  
4ANN,ARG\_33,12.13,-1.77,0,1.4  
1YTQ,ASP\_175,3.28,0.49,-1.02,0  
2C13,GLU\_151,3.95,0.14,-0.69,0  
2HRZ,GLU\_278,4.09,0.21,-0.62,0  
2EFK,GLU\_34,4.02,0.07,-0.55,0  
3LMO,ASP\_66,4.06,0.28,-0.02,0  
3NZL,LYS\_77,10.29,-0.21,0,0  
3F53,HIS\_232,6.38,0.0,0.16,-0.28  
2YT4,LYS\_500,10.5,0,0,0  
1RKA,ARG\_218,12.36,-0.14,0,0  
2PWQ,ASP\_28,3.76,0.14,-0.18,0  
1Q2Y,ASP\_49,3.87,0.07,0,0  
3GS9,TYR\_298,10.19,0.99,-0.8,0  
2XWS,ARG\_2,12.01,-0.49,0,0  
3UOV,GLU\_170,4.3,0.56,-0.76,0  
1UAJ,ASP\_95,2.56,0.42,-1.66,0  
1EQ6,ASP\_110,4.08,0.28,0,0  
2W0G,CYS\_233,8.63,-0.37,0,0  
3CIV,HIS\_57,6.4,0.04,0,-0.14  
3Q2C,CYS\_74,8.96,-0.04,0,0

2E3S,GLU\_410,4.57,0.07,0,0  
3L3P,LYS\_412,10.22,-0.28,0,0  
1YW5,GLU\_124,3.98,0.28,-0.8,0  
2POY,GLU\_321,4.5,0,0,0  
2AXO,ASP\_173,3.94,0.14,0,0  
3CS1,CYS\_124,10.66,-0.41,-0.16,2.24  
1ILW,ASP\_27,3.37,0.35,-0.79,0  
1LN4,GLU\_57,4.5,0,0,0  
3LQE,TYR\_496,12.01,1.09,-0.31,1.24  
3UX2,CYS\_90,9.07,0,0,0.07  
3IVF,ASP\_94,2.05,0.49,-2.24,0  
2HXB,LYS\_20,10.5,0,0,0  
3PU6,GLU\_27,4.64,0.14,0,0  
3O48,TYR\_131,13.34,0.14,0.8,2.4  
2JHY,ARG\_120,12.08,-0.42,0,0  
2FXT,GLU\_415,4.57,0.07,0,0  
1X7F,TYR\_82,10,0,0,0  
3GOZ,GLU\_243,3.98,0.28,-0.8,0  
2WBB,ASP\_714,4.01,0.21,0,0  
2CL3,GLU\_117,3.91,0.21,-0.8,0  
3OBS,TYR\_82,10,0,0,0  
3CJW,ARG\_187,12.5,0,0,0  
2Q98,HIS\_138,6.15,0,0,-0.35  
2B0A,TYR\_47,11.02,1.02,0,0  
2A1V,ASP\_55,3.94,0.14,0,0  
1GPP,ASP\_438,3.22,0.21,-0.79,0  
1JKS,LYS\_261,10.5,0,0,0  
4EUG,LYS\_177,10.43,-0.07,0,0  
2QZQ,TYR\_161,10,0,0,0  
1QZN,CYS\_37,10.94,-0.65,0,2.59  
3P51,GLU\_120,4.57,0.07,0,0  
2I88,LYS\_461,10.5,0,0,0  
3FRR,ASP\_77,3.7,0.07,-0.17,0  
2F9F,GLU\_29,2.91,0.28,-1.87,0  
1OTM,HIS\_162,6.43,0,0,-0.07  
2WOZ,GLU\_331,4.5,0,0,0  
1XAW,HIS\_509,6.29,0,0,-0.21  
3E7P,GLU\_122,5.37,2.98,-1.6,-0.51  
1MUJ,CYS\_200,7.72,-1.28,0,0  
1SUU,ASP\_612,3.43,0.21,-0.58,0  
1MD6,TYR\_88,8.9,0.07,-1.17,0  
1ZBM,LYS\_155,10.43,-0.07,0,0  
3K8J,TYR\_47,9.79,1.09,-1.3,0  
4FH3,TYR\_298,10,0,0,0  
3EOD,LYS\_68,10.29,-0.21,0,0  
1X7F,GLU\_344,2.05,1.92,-1.97,-2.4  
2YWK,LYS\_50,10.43,-0.07,0,0  
2YWJ,ARG\_31,11.52,-0.98,0,0  
3GFP,GLU\_460,3.7,0.28,-1.08,0  
1Z3X,ARG\_132,11.45,-1.05,0,0  
3G9G,GLU\_129,3.74,0.28,-1.04,0  
1W24,ASP\_55,2.64,0.42,-1.58,0  
2A6B,ARG\_32,11.94,-0.56,0,0  
3ADO,ASP\_110,2.53,0.91,-2.19,0  
2QDJ,HIS\_129,7.12,1.6,1.97,-2.95  
2ZCX,GLU\_92,4.5,0,0,0  
2GAU,GLU\_59,3.98,0.28,-0.8,0  
3ADO,TYR\_200,10,0,0,0  
4DIU,ARG\_137,11.69,0.14,0,1.55  
3F1X,GLU\_110,4.5,0,0,0  
3F5D,LYS\_81,10.43,-0.07,0,0  
3H5T,ARG\_210,12.5,0,0,0  
3RJZ,HIS\_179,6.86,0.5,0,-0.14  
2E3H,ARG\_297,12.5,0,0,0  
3TRE,LYS\_104,9.87,-0.63,0,0  
1OGL,ARG\_13,12.15,-0.35,0,0  
2D7J,ARG\_18,12.29,-0.21,0,0  
3ETU,TYR\_344,9.63,0.07,-0.44,0  
3G9G,ASP\_123,3.45,0.49,-0.84,0

3IL3,GLU\_224,3.73,0.07,-0.84,0  
1WJG,ARG\_32,12.01,-0.49,0,0  
1SQH,GLU\_17,2.58,0.63,-2.55,0  
1S1Y,GLU\_5,4.5,0,0,0  
1X7F,TYR\_229,12.3,0.55,-0.65,2.4  
1X04,ASP\_84,3.21,0.14,-0.73,0  
1FKM,CYS\_486,10.95,-0.61,0.63,1.93  
2OEW,GLU\_66,3.86,0.56,-1.2,0  
2IF4,GLU\_174,3.01,0.56,-2.06,0  
2BDD,TYR\_38,11.64,0.07,0,1.57  
2FPN,HIS\_24,6.36,0,0,-0.14  
3GW3,ARG\_47,11.52,-0.98,0,0  
1XEU,ARG\_130,12.08,-0.42,0,0  
3JSN,GLU\_10,3.81,0.07,-0.76,0  
1EYH,GLU\_137,4.2,0.07,-0.37,0  
3ZTA,ASP\_100,2.94,0.42,-1.28,0  
2VGM,ASP\_206,3.8,0,0,0  
3UX2,GLU\_120,4.64,0.14,0,0  
1MIX,TYR\_199,10,0,0,0  
3PM2,LYS\_36,10.29,-0.21,0,0  
2IRM,CYS\_237,8.79,-1.26,-1.6,2.65  
2QEV,ARG\_104,12.15,-0.35,0,0  
2NQU,TYR\_133,10,0,0,0  
2EDM,TYR\_153,10.44,0.14,-0.01,0.31  
3KT9,GLU\_92,4.64,0.14,0,0  
2B0A,CYS\_70,10.58,-0.15,0,1.73  
4FZN,GLU\_264,4.5,0,0,0  
3P2F,GLU\_7,3.43,0.21,-1.28,0  
1SNT,ARG\_170,12.5,0,0,0  
2E3S,LYS\_522,10.5,0,0,0  
1G8P,GLU\_172,4.2,0.28,-0.58,0  
3M7O,ARG\_273,11.73,-0.77,0,0  
3LD1,ARG\_46,12.22,-0.28,0,0  
2PLQ,TYR\_255,12.62,0.9,-0.18,1.9  
3R87,GLU\_69,4.22,0.14,-0.42,0  
1L2F,CYS\_250,9.66,0,0,0.66  
2D2S,ARG\_592,11.94,-0.56,0,0  
3D9H,ARG\_180,12.15,-0.35,0,0  
3GG6,LYS\_93,10.22,-0.28,0,0  
1WP5,ARG\_40,9.57,-2.31,0,-0.62  
4EUG,LYS\_147,10.43,-0.07,0,0  
3ETV,LYS\_226,10.43,-0.07,0,0  
1IDK,GLU\_265,4.5,0,0,0  
1SQH,LYS\_166,10.5,0,0,0  
1X9G,GLU\_162,4.5,0,0,0  
3G9G,LYS\_113,10.43,-0.07,0,0  
3G9B,ARG\_140,12.08,-0.42,0,0  
2YWJ,ASP\_171,2.33,0.42,-1.89,0  
3EAZ,GLU\_90,3.4,0.14,-1.24,0  
1PV5,GLU\_121,4.64,0.14,0,0  
3RKV,ARG\_195,12.22,-0.28,0,0  
1BN6,LYS\_186,10.5,0,0,0  
4E8B,ARG\_190,10.76,-1.74,0,0  
1T3Y,GLU\_111,3.39,0.49,-1.6,0  
2EFK,HIS\_116,7.04,0.68,0,-0.14  
1Z9L,LYS\_3,10.22,-0.28,0,0  
3EUR,LYS\_64,10.22,-0.28,0,0  
3CZC,LYS\_21,10.22,-0.28,0,0  
2ILR,GLU\_506,2.45,0.35,-2.4,0  
1X7F,HIS\_13,7.03,0.67,0,-0.14  
2CVB,GLU\_81,4.57,0.07,0,0  
2RFA,HIS\_157,6.5,0,0,0  
3JRT,HIS\_84,6.43,0,0,-0.07  
4D8L,ARG\_200,11.94,-0.56,0,0  
2Q99,LYS\_173,10.5,0,0,0  
2WOZ,CYS\_389,9.43,-0.03,0,0.46  
1SQH,LYS\_284,10.5,0,0,0  
2OJQ,ASP\_605,3.98,0.28,-0.1,0  
2QDJ,LYS\_95,10.29,-0.21,0,0

3ASA,ASP\_18,4.06,0.49,-0.23,0  
2NRR,HIS\_474,6.36,0,0,-0.14  
3ADO,ASP\_8,3.52,0.56,-0.84,0  
3IU5,TYR\_144,11.42,1.21,-0.8,1.01  
1QQE,LYS\_85,10.36,-0.14,0,0  
1DTO,LYS\_91,10.5,0,0,0  
2GAU,ASP\_49,3.07,0.49,-1.22,0  
2F9F,LYS\_64,10.43,-0.07,0,0  
1LZL,HIS\_143,7.08,0.72,0,-0.14  
1J33,ARG\_39,12.22,-0.28,0,0  
1XEU,TYR\_266,11.52,0.21,-0.11,1.42  
2D59,TYR\_22,10.08,0,0,0.08  
2RFA,HIS\_122,2.6,1.57,0,-5.48  
3ZTA,HIS\_114,5.03,1.28,0,-2.75  
3PBH,ARG\_235,12.89,-1.56,0,1.95  
3ERF,GLU\_39,1.67,1.17,-1.6,-2.4  
1WNH,LYS\_50,7.16,0.8,0,-0.14  
2EYI,ASP\_226,3.97,0.21,-0.04,0  
2FM9,ASP\_200,1.47,0.63,-2.97,0  
2YXO,LYS\_49,10.5,0,0,0  
1JB3,ASP\_49,3.06,0.21,-0.95,0  
2IIA,HIS\_71,6.68,0.25,0,-0.07  
2D0A,ARG\_219,12.08,-0.42,0,0  
1ZBS,ARG\_249,11.87,-0.63,0,0  
1ZBP,ASP\_46,3.17,0.28,-0.91,0  
3RLN,ASP\_731,1.66,0.91,-3.04,0  
2QEV,GLU\_65,4.56,0.28,-0.22,0  
3LH5,TYR\_718,10,0,0,0  
2E3H,LYS\_213,10.5,0,0,0  
2Q5X,ASP\_824,3.76,0,-0.04,0  
3CIV,TYR\_278,12.23,2.23,0,0  
4ANN,ASP\_126,3.87,0.07,0,0  
3GA2,TYR\_175,11.96,0,0,1.95  
2ZCO,HIS\_278,6.5,0,0,0  
1G8P,GLU\_226,3.91,0.21,-0.8,0  
3K1H,TYR\_127,9.07,0.19,-1.12,0  
3R87,ASP\_15,2.48,0.77,-2.09,0  
3ELI,ASP\_122,2.95,0.14,-0.99,0  
3G9G,LYS\_59,10.43,-0.07,0,0  
2FBQ,GLU\_87,1.17,0.28,-3.61,0  
3G9B,LYS\_109,11.91,1.91,0,0  
1XTZ,HIS\_62,6.5,0,0,0  
2BCF,HIS\_134,7.09,0.8,0,-0.21  
1DOV,ASP\_113,3.94,0.21,-0.07,0  
1X7F,ASP\_84,3.94,0.14,0,0  
1YLN,ASP\_79,3.72,0,-0.08,0  
1E59,ASP\_189,4.01,0.21,0,0  
3CBN,ASP\_133,3.01,0.84,-1.64,0  
3PAC,TYR\_166,10,0,0,0  
3K8J,HIS\_255,6.99,0.49,0,0  
3IVF,CYS\_116,8.87,-0.2,0,0.07  
2Z84,GLU\_131,2.15,0.75,-3.1,0  
3D9H,GLU\_242,4.64,0.14,0,0  
3G6S,LYS\_159,10.5,0,0,0  
1EYH,TYR\_48,9.51,0,-0.49,0  
3O7K,TYR\_109,11.6,0.7,-0.12,1.02  
3QYB,LYS\_954,10.5,0,0,0  
1RKA,GLU\_176,3.98,0.21,-0.73,0  
2A6B,GLU\_167,4.68,0.18,0,0  
3CIV,HIS\_133,8.51,1.6,2.4,-1.99  
2POY,ARG\_10,11.8,-0.7,0,0  
2CXA,HIS\_193,6.5,0,0,0  
1HF8,CYS\_230,8.63,-0.44,0,0.07

1OGL,ASP\_185,3.32,0.7,-1.18,0  
 3RFF,ARG\_150,11.87,-0.63,0,0  
 1SQH,CYS\_109,10.49,-0.12,0.37,1.24  
 1J8B,GLU\_36,3.94,0.63,-1.19,0  
 1X04,LYS\_137,10.5,0,0,0  
 3E7P,LYS\_220,10.5,0,0,0  
 2D2S,GLU\_538,4.57,0.07,0,0  
 3PBH,HIS\_45,2.72,0.57,-0.86,-3.49  
 1ZCU,TYR\_221,10,0,0,0  
 4GA2,LYS\_46,10.15,-0.35,0,0  
 1O6D,GLU\_47,4.07,0.21,-0.64,0  
 1PSW,ARG\_180,11.1,-1.4,0,0  
 3RE9,LYS\_209,9.8,-0.7,0,0  
 3GT0,LYS\_163,10.5,0,0,0  
 3E27,GLU\_235,3.98,0.28,-0.8,0  
 1T07,ARG\_3,11.59,-0.91,0,0  
 3LPZ,HIS\_133,4.04,0,0,-2.46  
 3MEW,ASP\_196,3.16,0.07,-0.71,0  
 2PPN,LYS\_52,10.29,-0.21,0,0  
 1HF8,ARG\_66,11.66,-0.84,0,0  
 3RE9,ASP\_193,3.08,0.77,-1.49,0  
 3I47,LYS\_195,10.5,0,0,0  
 2AXO,LYS\_228,9.66,-0.84,0,0  
 2FZ4,GLU\_131,4.5,0,0,0  
 1WP5,GLU\_69,4.05,0.35,-0.8,0  
 3ZXY,ASP\_182,3.74,0,-0.06,0  
 1YM5,HIS\_192,3.83,0.11,0,-2.78  
 1WOU,TYR\_4,11.1,0,0,1.1  
 2VAN,ARG\_137,12.15,-0.35,0,0  
 2AZP,ARG\_41,12.36,-0.14,0,0  
 1SUU,TYR\_743,10.65,1.28,-0.71,0.08  
 4EF5,LYS\_289,10.29,-0.21,0,0  
 2QEV,GLU\_48,4.5,0,0,0  
 2B78,GLU\_256,4.5,0,0,0  
 4FH3,GLU\_287,4.64,0.14,0,0  
 2E3C,ASP\_389,3.59,0.28,-0.49,0  
 2IDC,GLU\_82,3.65,0.35,-1.2,0  
 1HF8,LYS\_202,10.43,-0.07,0,0  
 3IBT,ARG\_259,11.66,-0.84,0,0  
 3V75,ARG\_99,11.26,-1.24,0,0  
 2YT4,ARG\_630,13.9,-0.58,0.1,98  
 1SNT,CYS\_219,11.19,-1.52,0.3,71  
 1ZBM,ASP\_137,2.89,0.49,-1.4,0  
 1WYC,ASP\_127,4.15,0.35,0,0  
 1LTU,HIS\_22,6.5,0,0,0  
 3LJI,ARG\_96,12.01,-0.49,0,0  
 2HQ2,LYS\_19,10.15,-0.35,0,0  
 1NIJ,CYS\_67,10.93,-0.09,0.2,02  
 1RKA,ASP\_204,1.96,0.42,-2.26,0  
 3F1X,LYS\_300,10.5,0,0,0  
 2HXB,ASP\_38,3.46,0.42,-0.75,0  
 3M7G,ARG\_144,10.39,-3.01,0,0.9  
 3OBS,GLU\_51,4.5,0,0,0  
 2EEY,LYS\_68,10.5,0,0,0  
 1QYI,LYS\_308,10.5,0,0,0  
 1OIS,ASP\_176,3.35,0.35,-0.8,0  
 2YX0,GLU\_300,4.57,0.07,0,0  
 3CRM,HIS\_297,6.5,0,0,0  
 1R16,TYR\_290,13.31,0.35,0.2,96  
 2NRR,ARG\_394,11.87,-0.63,0,0  
 4DNU,TYR\_253,9.84,0.21,-0.37,0  
 2ZOM,ARG\_312,12.43,-0.07,0,0  
 3B79,ARG\_117,12.15,-0.35,0,0  
 2NYC,ASP\_210,4.05,0.28,-0.03,0  
 2WZ9,GLU\_71,3.95,0.21,-0.76,0  
 3BB7,LYS\_90,10.01,-0.49,0,0  
 2EFK,ASP\_168,2.04,0.21,-1.97,0  
 1SI7,TYR\_159,11.03,1.99,-0.02,-0.94  
 3EYE,LYS\_117,10.5,0,0,0  
 3V1Q,ARG\_585,12.15,-0.35,0,0  
 2PGX,LYS\_177,10.29,-0.21,0,0  
 3O16,GLU\_60,2.54,1.14,-3.1,0  
 1QYI,TYR\_209,10,0,0,0  
 3BWT,ASP\_743,3.25,0.35,-0.9,0  
 1K95,ARG\_103,12.5,0,0,0  
 3F6M,HIS\_110,6.36,0,0,-0.14  
 1XIP,GLU\_314,4.33,0.21,-0.38,0  
 1YR6,LYS\_180,10.36,-0.14,0,0  
 3OKQ,ASP\_609,3.88,0.14,-0.06,0  
 3B79,ARG\_47,11.94,-0.56,0,0  
 3EVN,TYR\_56,13.11,0.07,0.64,2.4  
 3JSN,GLU\_181,4.71,0.21,0,0  
 1DUN,TYR\_25,10,0,0,0  
 1U53,ASP\_91,2.18,0.35,-1.97,0  
 3Q1C,GLU\_282,3.07,0.82,-2.25,0  
 2RIK,TYR\_75,10,0,0,0  
 2D8N,LYS\_101,10.5,0,0,0  
 2O0K,TYR\_55,12.28,0.98,-0.13,1.44  
 1DVO,ARG\_171,12.01,-0.49,0,0  
 3ETU,ASP\_262,4.11,0.35,-0.04,0  
 2Z61,ASP\_111,3.57,0.14,-0.37,0  
 3QAV,ASP\_184,4.21,0.42,-0.01,0  
 3H5T,GLU\_344,4.5,0,0,0  
 2RJD,LYS\_239,10.5,0,0,0  
 3U2R,ASP\_85,3.86,0.14,-0.08,0  
 1PNE,LYS\_115,10.29,-0.21,0,0  
 1R15,GLU\_182,4.28,0,-0.22,0  
 1PVT,ASP\_200,3.56,0.56,-0.8,0  
 4EVF,LYS\_48,10.08,-0.42,0,0  
 1RLO,ASP\_38,3.36,0.07,-0.51,0  
 3L7N,ARG\_2,11.52,-0.98,0,0  
 3JZN,ARG\_120,12.68,-0.56,0,0.74  
 4FCU,LYS\_206,10.01,-0.49,0,0  
 3GS3,LYS\_270,10.5,0,0,0  
 3EGN,TYR\_423,11.47,0.19,0.1,28  
 3IL3,HIS\_83,4.49,0.52,1.06,-3.58  
 3GA2,GLU\_95,6.07,2.37,-0.8,0  
 4ETX,GLU\_416,4.57,0.14,-0.07,0  
 2FL7,TYR\_102,12.01,0.21,0.1,8  
 1NAF,LYS\_250,10.5,0,0,0  
 2NRR,GLU\_407,4.64,0.14,0,0  
 2EJB,GLU\_45,4.5,0,0,0  
 2A6B,GLU\_107,4.5,0,0,0  
 3GW3,TYR\_30,12.68,1,-0.72,2.4  
 2Q99,ARG\_110,10.62,-1.88,0,0  
 2HQ2,ARG\_60,12.22,-0.28,0,0  
 2EA9,HIS\_35,6.73,0.3,0,-0.07  
 3CIV,HIS\_24,6.36,0,0,-0.14  
 2YYO,ASP\_16,3.92,0.14,-0.02,0  
 3IVF,ASP\_46,4.08,0.28,0,0  
 2P0Y,HIS\_160,6.5,0,0,0  
 1HF8,ARG\_129,12.08,-0.42,0,0  
 1GQE,LYS\_284,10.43,-0.07,0,0  
 3GMS,HIS\_179,4.47,0.02,0,-2.05  
 2B3M,ARG\_123,11.8,-0.7,0,0  
 4DVD,ASP\_146,3.19,0.84,-1.45,0  
 2GEN,GLU\_180,2.31,0.21,-2.4,0  
 2OB1,ASP\_21,1.88,0.98,-2.9,0  
 1O5J,ARG\_70,12.15,-0.35,0,0  
 2G7O,GLU\_65,4.03,0.21,-0.68,0  
 1DZF,ARG\_212,12.29,-0.21,0,0  
 4FH3,ARG\_277,12.97,-0.29,0.0,76  
 1MTZ,TYR\_281,12.56,3.36,-0.8,0  
 3EAZ,ASP\_115,1.82,0.42,-2.4,0  
 1WXQ,ARG\_234,12.08,-0.42,0,0  
 1BKB,TYR\_108,9.54,0.07,-0.8,0.27  
 1NRI,CYS\_50,8.49,-0.82,0.0,31  
 3H6Q,TYR\_7,10.75,0.07,-0.22,0.89  
 1OST,TYR\_150,13.56,0.36,0.8,2.4  
 1DUP,ASP\_90,3.5,0.07,-0.37,0  
 3ERF,ARG\_34,13.51,-1.39,0,2.4  
 3EVP,LYS\_265,10.5,0,0,0  
 4ACJ,ASP\_765,1.29,1.26,-3.77,0  
 2ZOM,ARG\_278,12.08,-0.42,0,0  
 2VGM,LYS\_128,10.43,-0.07,0,0  
 2Q99,TYR\_37,9.4,0.07,-0.67,0  
 2JEO,GLU\_106,4.1,0.14,-0.54,0  
 3LD1,ARG\_266,13.68,-0.85,0.2,03  
 2FD5,GLU\_141,3.17,0.77,-2.09,0  
 1MUF,GLU\_97,4.3,0.63,-0.84,0  
 1YOY,LYS\_167,10.15,-0.35,0,0  
 2ZQ5,GLU\_188,3.57,2.6,-1.6,-1.93  
 2W2S,GLU\_202,1.25,1,-1.85,-2.4  
 1ES9,LYS\_118,10.5,0,0,0  
 1XIP,ASP\_331,3.87,0.07,0,0  
 3ETV,ARG\_220,12.08,-0.42,0,0  
 3IBT,ARG\_221,11.66,-0.84,0,0  
 3BCY,GLU\_20,4.57,0.07,0,0  
 3EJC,LYS\_119,8.62,-0.38,0,0  
 2RQY,TYR\_254,9.31,0.07,-0.76,0  
 2O0K,LYS\_148,10.36,-0.14,0,0  
 3EST,GLU\_16,4.64,0.14,0,0  
 1Q8B,LYS\_62,10.08,-0.42,0,0  
 1RKA,GLU\_143,3.34,2.15,-1.9,-1.41  
 1KCM,GLU\_159,4.36,0.4,-0.54,0  
 3FXH,GLU\_47,4.5,0,0,0  
 3BPV,TYR\_89,10,0,0,0  
 3CAN,LYS\_113,10.5,0,0,0  
 1WRU,ARG\_268,11.17,-1.33,0,0  
 3L3P,GLU\_447,4.5,0,0,0  
 3CJW,TYR\_181,11.01,1.81,-0.8,0  
 2WB8,HIS\_651,2.76,0.49,-4.23  
 4FZN,CYS\_55,9.74,0,0,0.74  
 1K95,GLU\_140,2.92,0.77,-2.35,0  
 3M16,LYS\_6,10.5,0,0,0  
 1J85,ARG\_74,11.52,-0.98,0,0  
 4EZB,ARG\_142,12.5,0,0,0  
 1XIP,HIS\_252,6.48,0.12,0,-0.14  
 2FC3,ARG\_27,11.52,-0.98,0,0  
 2FZ4,HIS\_41,6.43,0,0,-0.07  
 4AF2,ARG\_93,11.8,-0.7,0,0  
 1W7B,TYR\_75,11.21,0.07,0.1,14  
 2V4U,ASP\_507,4.01,0.21,0,0  
 1CHD,HIS\_173,6.5,0,0,0  
 1T6L,ARG\_54,11.52,-1.35,0,0.37  
 3F53,CYS\_133,8.91,-0.27,-1.2,1.39  
 1GQE,ARG\_256,12.5,0,0,0  
 2W1R,ASP\_107,3.89,0.14,-0.05,0  
 4GA2,LYS\_123,10.5,0,0,0  
 2VGM,TYR\_277,9.17,0.69,-0.11,-1.41  
 3DB9,ASP\_69,1.8,0.63,-2.63,0  
 3BQW,CYS\_202,9,0,0,0  
 2X4L,LYS\_313,10.36,-0.14,0,0  
 3LJI,GLU\_286,3.39,0.56,-1.67,0  
 3LJN,LYS\_133,10.43,-0.07,0,0  
 1WJG,HIS\_296,8.7,0.51,0,-0.14  
 1PNE,ARG\_74,12.15,-0.35,0,0  
 2V1L,ASP\_102,3.91,0.28,-0.17,0  
 3HYQ,GLU\_173,5.2,0.28,0.42,0  
 4EKU,ASP\_189,4.22,0.42,0,0  
 3M7G,TYR\_258,12.09,0.85,-0.31,1.56  
 2PLQ,ARG\_316,12.36,-0.14,0,0  
 3VHJ,LYS\_121,10.36,-0.14,0,0  
 3LJN,ARG\_182,11.73,-0.77,0,0  
 3EJC,LYS\_81,10.01,-0.49,0,0  
 3AZZ,HIS\_139,6.36,0,0,-0.14  
 3BA1,GLU\_2,3.9,0,-0.6,0  
 2W2S,ASP\_80,2.74,0.28,-1.34,0  
 3ULX,GLU\_69,2.5,0.91,-1.2,-1.71  
 2APL,LYS\_106,10.29,-0.21,0,0  
 3BPP,GLU\_174,4.39,0.42,-0.53,0  
 2HZZ,LYS\_137,11.01,0,0,0.5  
 1WP5,TYR\_16,10.56,0.07,0,0.49  
 1DZF,GLU\_36,3.84,0.28,-0.94,0  
 1T07,TYR\_22,10.07,0.07,0,0  
 2W2S,GLU\_193,4.5,0,0,0  
 2R51,ARG\_283,12.01,-0.49,0,0  
 3US6,GLU\_105,4.5,0,0,0  
 2R2Y,ARG\_92,11.17,-1.33,0,0  
 3I4T,GLU\_264,4.3,0.35,-0.55,0  
 4DEZ,TYR\_50,9.58,0.7,-0.34,-0.78  
 1J74,LYS\_108,10.5,0,0,0  
 4ETX,GLU\_379,4.5,0,0,0  
 15J8,ASP\_666,4.01,0.21,0,0  
 4DVD,GLU\_138,4.71,0.21,0,0  
 1R16,ARG\_57,11.96,-0.54,0,0  
 3ERF,ARG\_119,12.08,-0.42,0,0  
 2Q34,ASP\_102,3.94,0.14,0,0  
 2IN0,CYS\_1,4.44,-3.79,-1.19,0.41  
 3RFY,ARG\_194,12.15,-0.35,0,0  
 2A0J,ARG\_24,12.43,-0.07,0,0  
 2DFL,LYS\_80,10.5,0,0,0  
 3N2T,ASP\_151,3.68,0.42,-0.53,0  
 3JZ9,GLU\_505,3.39,0.49,-1.6,0  
 2OJQ,GLU\_570,4.42,0.35,-0.42,0  
 1J33,GLU\_184,3.91,0.42,-1.01,0  
 2IN0,GLU\_102,3.91,0.21,-0.8,0  
 2XMZ,LYS\_152,10.43,-0.07,0,0  
 3LQE,ASP\_443,4.15,0.35,0,0  
 1J8B,ASP\_71,3.99,0.28,-0.09,0  
 2HZZ,ARG\_279,12.01,-0.49,0,0  
 3YWF,ASP\_139,3.76,0,-0.04,0  
 3PZ9,CYS\_82,6.52,-4.13,0.1,65  
 2B0J,GLU\_344,4.5,0,0,0  
 2GZQ,LYS\_102,10.43,-0.07,0,0  
 3V4G,ARG\_12,12.5,0,0,0  
 2QVO,ARG\_72,12.29,-0.21,0,0  
 2PPN,LYS\_34,10.5,0,0,0  
 2X4J,LYS\_59,9.87,-0.63,0,0  
 1WRU,ARG\_12,12.08,-0.42,0,0  
 3CX5,ASP\_18,3.29,0.63,-1.13,0  
 2YLF,ARG\_83,12.15,-0.35,0,0  
 1PGV,ARG\_356,12.01,-0.49,0,0  
 3H6Q,ARG\_108,11.9,-0.6,0,0  
 1AT0,GLU\_262,3.78,0.42,-1.14,0  
 1P6F,LYS\_149,10.5,0,0,0  
 1C44,ASP\_79,4.2,0.42,-0.02,0  
 1YB2,ARG\_38,12.29,-0.21,0,0  
 1FQI,ASP\_334,3.21,0.21,-0.8,0  
 1DVO,LYS\_138,10.5,0,0,0  
 4DVD,TYR\_107,9.76,0,-0.24,0  
 3CCY,ASP\_137,3.17,0.28,-0.91,0  
 3N2T,GLU\_191,1.87,0.88,-1.11,-2.4  
 3CIV,GLU\_307,2.69,0.94,-2.75,0  
 3NJM,ASP\_74,2.98,0.49,-1.3,0  
 1O17,ASP\_79,3.72,0,-0.08,0  
 2EEY,ASP\_17,2.19,0.35,-1.96,0  
 2B0A,CYS\_181,11.3,0,0,2.3  
 2D7U,ASP\_243,3.9,0.35,-0.25,0  
 1NIJ,ASP\_219,3.75,0.21,-0.26,0  
 1Q8B,LYS\_100,10.15,-0.35,0,0  
 1YHJ,ASP\_38,3.88,0.14,-0.06,0  
 1ZBP,GLU\_233,4.57,0.28,-0.21,0  
 3RKV,GLU\_261,4.24,0.07,-0.33,0  
 3LD1,ASP\_127,2.78,0.49,-1.51,0  
 3M16,CYS\_90,9.52,0,0,0.52

1HF8,LYS\_166,10.5,0,0,0  
3DSH,ARG\_288,11.73,-0.77,0,0  
1FO9,CYS\_123,10.3,-1.13,0,2.43  
1DVO,LYS\_81,10.01,-0.49,0,0  
1XEU,ASP\_239,3.87,0.07,0,0  
3RE9,TYR\_99,11.52,1.57,-1.82,1.77  
3P2F,TYR\_24,10.52,0,0,0.52  
2JEO,ASP\_229,3.83,0.42,-0.39,0  
3NOK,ASP\_40,3.71,0.14,-0.23,0  
1NFN,ARG\_142,12.08,-0.42,0,0  
3ZXY,GLU\_212,4.57,0.07,0,0  
2AD1,GLU\_95,3.69,0.28,-1.09,0  
2EEY,ARG\_159,12.15,-0.35,0,0  
2OJQ,ARG\_686,12.15,-0.35,0,0  
3K8J,GLU\_257,4.15,0.14,-0.49,0  
1T9S,LYS\_107,10.5,0,0,0  
1ZCU,TYR\_14,11.81,0.63,0.1.18  
1Q2Y,LYS\_116,10.5,0,0,0  
2OEW,ASP\_141,2.8,0.21,-1.21,0  
3UPD,LYS\_92,10.5,0,0,0  
2YWX,GLU\_45,4.5,0,0,0  
1MUF,ASP\_328,3.35,0.35,-0.8,0  
3BQE,ASP\_332,3.77,0.14,-0.17,0  
1LFP,GLU\_243,4.71,0.21,0,0  
2Q13,ARG\_237,12.43,-0.07,0,0  
3BCH,ARG\_184,11.7,-1.03,0,0.23  
2C13,ARG\_30,11.31,-1.19,0,0  
1TR9,GLU\_175,4.57,0.07,0,0  
3BB7,LYS\_314,10.5,0,0,0  
1J85,ARG\_20,12.15,-0.35,0,0  
2RIK,GLU\_258,3.84,0.14,-0.8,0  
3ONH,CYS\_540,9.75,0,0,0.75  
3M7D,HIS\_271,6.5,0,0,0  
1MIX,LYS\_306,10.29,-0.21,0,0  
3LQE,GLU\_311,2.75,1.2,-1.47,-1.48  
1P1L,TYR\_6,10,0,0,0  
3BWT,LYS\_780,10.43,-0.07,0,0  
3CIV,GLU\_224,4.5,0,0,0  
2X4G,HIS\_139,6.5,0,0,0  
3F6F,GLU\_125,4.71,0.21,0,0  
2Q12,GLU\_95,4.64,0.14,0,0  
2WB8,HIS\_505,6.5,0,0,0  
2FZ4,GLU\_159,4.71,0.35,-0.14,0  
4H4J,HIS\_212,8.55,3.6,1.72,-3.27  
3AU3,LYS\_561,10.43,-0.07,0,0  
1ZBS,ASP\_222,3.62,0.14,-0.32,0  
3MIX,GLU\_412,4.21,0.14,-0.43,0  
1EV8,GLU\_14,3.98,0.28,-0.8,0  
1O9G,GLU\_111,3.77,0.07,-0.8,0  
1ZKZ,ASP\_23,3.73,0.56,-0.63,0  
1EDG,ARG\_357,10.2,-2.7,0,0.4  
3HQX,GLU\_59,4.48,0.28,-0.3,0  
1ZBP,GLU\_223,4.41,0.07,-0.16,0  
1RKA,GLU\_192,4.26,0.56,-0.8,0  
3C2E,HIS\_250,6.5,0,0,0  
157K,ARG\_128,12.22,-0.28,0,0  
1MTZ,ARG\_90,13.13,-1.19,0,1.82  
2W0G,ARG\_266,12.36,-0.14,0,0  
3EIZ,ASP\_125,3.71,0.07,-0.16,0  
1H4U,LYS\_504,10.43,-0.07,0,0  
3V3T,LYS\_47,10.43,-0.07,0,0  
3CS1,GLU\_82,4.05,0.35,-0.8,0  
3FKS,ASP\_143,3.35,0.35,-0.8,0  
1L2F,LYS\_16,10.43,-0.07,0,0  
1JSX,GLU\_172,3.42,0.63,-1.71,0  
3S0A,LYS\_41,10.43,-0.07,0,0  
1XKR,GLU\_177,3.68,0.35,-1.17,0  
1GSZ,ASP\_151,2.69,0.63,-1.74,0  
2OBI,CYS\_46,4.34,-4.86,0,0.21  
1RAJ,GLU\_427,4.5,0,0,0  
2BAA,TYR\_111,8.96,0.14,-1.18,0  
3J5N,LYS\_37,10.5,0,0,0  
1QQE,GLU\_176,4.05,0.35,-0.8,0  
3COU,ASP\_71,2.91,0.21,-1.11,0  
3C2E,ASP\_222,2.56,0.56,-1.81,0  
1ZBM,GLU\_197,4.29,0.28,-0.49,0  
2CWC,HIS\_199,6.22,0,0,-0.28  
2P1W,LYS\_53,10.5,0,0,0  
4E9E,LYS\_529,10.5,0,0,0  
4GA2,ARG\_58,12.43,-0.07,0,0  
1J33,ARG\_200,11.8,-0.7,0,0  
1PZC,ASP\_100,3.75,0.07,-0.12,0  
2FXT,ARG\_291,12.36,-0.14,0,0  
4H89,GLU\_151,4.5,0,0,0  
2P5D,ASP\_140,2.67,1.05,-2.18,0  
1U7U,ASP\_185,1.29,0.7,-3.21,0  
2EYI,TYR\_246,9.19,0,-0.81,0  
2PLQ,TYR\_20,11.29,1.29,0,0  
4ANN,HIS\_179,7.02,0.8,0,-0.28  
1GPP,ARG\_138,12.43,-0.07,0,0  
4D8L,ARG\_124,11.47,-3.25,0,2.22  
3BCH,LYS\_17,10.43,-0.07,0,0  
1ZBM,LYS\_226,10.08,-0.42,0,0  
3MIX,LYS\_330,9.73,-0.77,0,0  
1Q5Z,ASP\_593,3.32,0.14,-0.63,0  
2OYZ,ASP\_61,4.01,0.21,0,0  
3RJX,TYR\_325,11.07,0.28,0,0.79  
2ZQ5,ASP\_330,2.62,0.42,-1.6,0  
1T07,ARG\_19,12.15,-0.35,0,0  
2B0J,CYS\_322,9,0,0,0  
4EF5,LYS\_338,10.5,0,0,0  
1U7U,LYS\_247,10.29,-0.21,0,0  
3M16,LYS\_67,10.08,-0.42,0,0  
1TLV,TYR\_240,9.98,0.07,-0.09,0  
1NIJ,ARG\_242,12.29,-0.21,0,0  
2Q99,TYR\_183,10.17,0.17,0,0  
3F1X,GLU\_188,3.9,0.07,0,-0.67  
2O8P,GLU\_211,4.5,0,0,0  
2NSN,ARG\_35,12.43,-0.07,0,0  
2IQT,ASP\_154,3.98,0.21,-0.03,0  
1BGF,HIS\_95,7.22,0.86,0,-0.14  
3GYW,ARG\_82,11.26,-1.83,0,0.59  
1LZL,GLU\_281,4.85,0.35,0,0  
2AH5,GLU\_95,4.5,0,0,0  
1QYI,GLU\_130,3.15,0.56,-1.91,0  
3ERF,LYS\_60,10.43,-0.07,0,0  
3G9G,ARG\_195,11.52,-0.98,0,0  
1U7U,TYR\_337,10.55,0,0,0.55  
2JEO,ASP\_116,2.38,0.42,-1.84,0  
1HF8,ASP\_224,3.8,0,0,0  
3TMO,GLU\_189,4.5,0,0,0  
1G8P,LYS\_316,9.87,-0.63,0,0  
1U53,LYS\_186,10.22,-0.28,0,0  
2V4U,ARG\_481,11.87,-0.63,0,0  
2Q12,GLU\_14,4.18,0.21,-0.53,0  
2A6B,LYS\_48,10.5,0,0,0  
2VGY,ASP\_100,3.33,0.28,-0.75,0  
2XJ4,GLU\_88,4.26,0.56,-0.8,0  
3IV4,ASP\_61,3.78,0,-0.02,0  
1QYI,GLU\_112,0.25,0.83,-2.68,-2.4  
2OSA,LYS\_402,10.36,-0.14,0,0  
3RJZ,LYS\_175,10.15,-0.35,0,0  
3KEY,HIS\_429,6.29,0,-0.21  
3BQW,ASP\_256,3.39,0.07,-0.48,0  
3JZN,GLU\_325,1.7,0.77,-2.52,-1.05  
100X,ASP\_222,1.34,0.84,-3.29,0  
2H2W,TYR\_293,10,0,0,0  
1QQE,GLU\_125,2.82,0.37,-0.17,-1.87  
3RJX,ARG\_86,10.7,-1.8,0,0  
2NMU,GLU\_60,4.5,0,0,0  
3IVF,GLU\_186,4.57,0.07,0,0  
2H2W,CYS\_142,4.49,-5.67,-1.68,2.84  
1UCH,ASP\_167,3.74,0.07,-0.13,0  
3JZN,ARG\_216,12.16,-1.19,0,0.85  
3RVC,ASP\_101,3.94,0.14,0,0  
3AU3,ASP\_610,3.73,0.07,-0.14,0  
2F9F,LYS\_96,10.29,-0.21,0,0  
2G2D,ARG\_164,11.94,-0.56,0,0  
2EJX,GLU\_47,4.47,0.21,-0.24,0  
3LJI,GLU\_201,4.5,0,0,0  
1ZP2,GLU\_228,4.82,0.35,-0.03,0  
3ZXY,LYS\_284,10.5,0,0,0  
1VJG,ASP\_142,3.99,0.28,-0.09,0  
3JZN,CYS\_126,8.52,0,-1.85,1.37  
3M70,GLU\_64,4.04,0.49,-0.96,0  
1OI7,GLU\_110,4.02,0.28,-0.76,0  
3F6F,TYR\_128,11.27,0.07,-0.94,2.13  
1XDZ,ARG\_105,13.74,-1.16,0,2.4  
3GS9,ASP\_20,3.81,0.49,-0.48,0  
2WB8,ARG\_648,11.65,-3.25,0,2.4  
2ZOW,ASP\_82,4.01,0.21,0,0  
2DG7,HIS\_167,6.5,0,0,0  
1YR6,ASP\_132,3.11,0.35,-1.04,0  
3EOH,CYS\_9,8.59,-0.41,0,0  
2VGY,HIS\_109,6.64,1.6,1.94,-3.4  
3Q9P,ARG\_94,12.08,-0.42,0,0  
3N2T,ASP\_311,3.91,0.21,-0.1,0  
2V81,TYR\_180,12.07,0.26,-0.55,2.36  
4ANN,ARG\_111,12.29,-0.21,0,0  
1QQE,LYS\_51,10.5,0,0,0  
3Q2C,GLU\_86,4.57,0.07,0,0  
4AF2,GLU\_140,3.38,0.07,-1.18,0  
2W25,ASP\_194,3.99,0.21,-0.02,0  
1QQL,ARG\_122,12.15,-0.35,0,0  
3H6Q,LYS\_21,10.5,0,0,0  
1ZBP,ARG\_151,12.63,-2.89,0,3.02  
2FXT,LYS\_314,10.5,0,0,0  
1KCM,LYS\_5,10.15,-0.35,0,0  
3BB7,GLU\_78,4.5,0,0,0  
3ON1,ARG\_17,12.5,0,0,0  
2F4Q,ARG\_170,12.22,-0.28,0,0  
3ON1,LYS\_64,10.29,-0.21,0,0  
3ETU,LYS\_313,10.01,-0.49,0,0  
3O48,GLU\_127,3.91,0.21,-0.8,0  
1WP5,TYR\_108,10.94,0,0,0.94  
3F5D,HIS\_117,4.35,1.13,0,-3.28  
2OKT,HIS\_7,6.7,0,1.57,-1.37  
1PGV,ASP\_329,3.25,0.42,-0.97,0  
2YYO,LYS\_86,10.5,0,0,0  
3GT0,LYS\_100,10.29,-0.21,0,0  
3GYW,ASP\_80,2.83,0.42,-1.39,0  
3GE9,ASP\_205,3.13,0.07,-0.73,0  
1MIX,LYS\_322,10.5,0,0,0  
3OBS,LYS\_33,10.43,-0.07,0,0  
2GAU,ARG\_77,12.07,-2.83,0,2.4  
3F6M,ASP\_67,3.6,0.49,-0.69,0  
1FOI,TYR\_393,10,0,0,0  
3ADO,ASP\_291,2.1,0.77,-2.48,0  
1Z9L,LYS\_83,10.5,0,0,0  
2FZP,GLU\_195,2.77,0.84,-2.57,0  
2HP7,GLU\_206,4.5,0,0,0  
1WXQ,LYS\_233,10.43,-0.07,0,0  
1YB2,HIS\_173,6.45,0.16,0,-0.21  
4AF2,CYS\_82,10.64,-1.14,0.56,2.22  
2Z61,TYR\_62,10,0,0,0  
1PSW,GLU\_226,4.5,0,0,0  
3RJZ,LYS\_208,9.87,-0.63,0,0  
3CIV,ASP\_246,3.2,0.56,-1.16,0  
1MJS,LYS\_332,10.5,0,0,0  
3C6B,GLU\_246,4.64,0.14,0,0  
3CBN,ARG\_145,12.01,-0.49,0,0  
3TR,ASP\_155,4.0,0.21,-0.01,0  
1YTO,LYS\_167,10.43,-0.07,0,0  
1UCH,TYR\_141,10.01,0.21,-0.2,0  
2QZQ,ARG\_77,11.94,-0.56,0,0  
3A2Z,ASP\_182,2.8,0.42,-1.41,0  
1ILW,ARG\_13,11.87,-0.63,0,0  
3CNU,TYR\_34,12.01,2.01,0,0  
3LD1,LYS\_101,10.01,-0.49,0,0  
4FCU,CYS\_122,7.76,-1.6,0,0.36  
1R3F,HIS\_173,7.42,1.6,1.75,-2.43  
1MTZ,GLU\_26,3.98,0.14,-0.66,0  
1RI6,TYR\_103,10.7,0.07,0,0.63  
1MML,LYS\_12,11.94,-0.21,0,0  
1PVT,ARG\_31,10.47,-2.03,0,0  
4DEZ,ASP\_204,3.12,0.07,-0.76,0  
1PBV,ARG\_63,12.5,0,0,0  
2W0G,ASP\_229,3,0.35,-1.15,0  
2QOP,GLU\_122,4.49,0,-0.01,0  
1TJE,ARG\_12,11.94,-0.56,0,0  
3ETV,LYS\_78,10.22,-0.28,0,0  
1YB2,ASP\_150,2.98,0.63,-1.45,0  
3EGN,GLU\_449,4.44,0,-0.06,0  
3KT9,CYS\_51,7.53,-1.54,0,0.07  
1RKA,GLU\_130,4.57,0.07,0,0  
3GW3,ASP\_306,3.86,0.84,-0.78,0  
3C2E,HIS\_179,6.43,0,0,-0.07  
3NBI,TYR\_170,10.07,0.07,0,0  
1O5T,HIS\_257,6.36,0,0,-0.14  
1W7B,TYR\_275,9.79,0,-0.21,0  
2YWJ,GLU\_47,1.81,0.77,-3.45,0  
1NWA,ASP\_19,3.49,0.49,-0.8,0  
3Q1C,ASP\_123,2.35,0.42,-1.86,0  
3OKQ,GLU\_565,4.64,0.14,0,0  
1W24,HIS\_57,5.53,0.78,0,-1.75  
2AH5,ASP\_127,4.01,0.21,0,0  
1BYI,TYR\_218,10,0,0,0  
3CSV,CYS\_178,12.37,-0.02,0,3.39  
3JV1,LYS\_72,10.36,-0.14,0,0  
4ECC,ASP\_227,3.4,0.21,-0.61,0  
1RAJ,HIS\_336,6.5,0,0,0  
3RE9,HIS\_235,6.86,0.36,0,0  
2FL4,GLU\_24,4.71,0.21,0,0  
1J85,GLU\_8,3.77,0.63,-1.36,0  
1O5T,HIS\_336,10.22,5.31,2.94,-4.53  
3LJI,TYR\_262,12.93,0.27,-0.33,2.99  
3BWT,GLU\_771,4.07,0.28,-0.71,0  
1ZBP,LYS\_179,10.36,-0.14,0,0  
2D7U,LYS\_300,10.5,0,0,0  
1R7J,LYS\_18,10.5,0,0,0  
4H4J,GLU\_60,3.84,0.14,-0.8,0  
1V43,LYS\_193,10.22,-0.28,0,0  
2YYO,TYR\_20,10.58,0.14,-0.55,0.99  
2E3C,GLU\_274,4.57,0.07,0,0  
3ANJ,TYR\_46,10.07,0.07,0,0  
3ON1,ARG\_81,11.94,-0.56,0,0  
4DIU,GLU\_136,4.26,0.28,-0.52,0  
2FXT,ASP\_389,3.94,0.14,0,0  
2P65,ASP\_139,3.2,0.49,-1.09,0  
2WOZ,ASP\_477,1.87,0.49,-2.42,0  
1QQE,TYR\_31,10.2,0,0,0.2  
3CAX,LYS\_371,10.5,0,0,0  
1QQL,TYR\_41,10.46,0,-0.11,0.57  
2PGX,LYS\_185,10.36,-0.14,0,0  
3O48,TYR\_81,10.56,0.56,0,0  
2JKF,ASP\_118,3.1,0.35,-1.05,0

3TOW,LYS\_102,10.5,0,0,0  
2OB5,LYS\_120,10.22,-0.28,0,0  
1X9G,GLU\_186,4.71,0.21,0,0  
2G3A,ARG\_92,11.03,-1.47,0,0  
2CBE,GLU\_221,3.18,0.14,-1.46,0  
2D8N,LYS\_166,10.22,-0.28,0,0  
1RL0,ASP\_163,3.92,0.28,-0.16,0  
3GA2,TYR\_57,11.31,0,0,1.31  
3FHF,GLU\_9,4.57,0,0,0,0  
3FHF,GLU\_156,3.98,0.28,-0.8,0  
2Q13,CYS\_99,8.35,-0.72,0,0,0  
2E3S,ASP\_479,1.01,1.12,-3.91,0  
3CN5,ASP\_191,3.49,0.49,-0.8,0  
4F3J,ASP\_167,2.65,0.7,-1.85,0  
1YM5,HIS\_157,6.48,0.12,0,-0.14  
2V4X,GLU\_12,4.57,0,0,0,0  
2QDJ,LYS\_228,10.36,-0.14,0,0  
1TP6,HIS\_110,6.29,0,0,-0.21  
3OIP,LYS\_214,10.36,-0.14,0,0  
2B61,TYR\_156,11.95,0.97,0,0.98  
3RFF,GLU\_142,4.5,0,0,0,0  
1SIG,ARG\_364,11.59,-0.91,0,0  
3V75,HIS\_166,6.43,0,0,-0.07  
1ZHV,ASP\_101,3.82,0.07,-0.05,0  
1W24,HIS\_115,4.48,0.01,0.05,-2.09  
2BQQ,GLU\_118,2.23,0.7,-2.97,0  
4F8A,HIS\_689,6.43,0,0,-0.07  
3GA2,ASP\_154,3.75,0.35,-0.4,0  
2ZCO,ASP\_155,2.83,0.28,-1.25,0  
2B02,GLU\_455,4.12,0.42,-0.8,0  
4FCU,LYS\_149,10.5,0,0,0  
2QEV,HIS\_37,5.21,1.06,0,-2.35  
3U4K,ASP\_169,3.86,0.07,-0.01,0  
1DUN,ASP\_40,1.27,1.05,-3.59,0  
4DIU,ASP\_231,3.25,0.07,-0.63,0  
3L3P,GLU\_281,4.44,0.21,-0.27,0  
3LJN,CYS\_141,10.26,-0.67,0,1.92  
2F8H,LYS\_66,10.43,-0.07,0,0  
3EGN,CYS\_388,9,0,0,0  
2YT4,CYS\_627,4.19,-4.4,-1.91,1.5  
3U56,ASP\_52,3.02,0.28,-1.05,0  
2R57,GLU\_212,3.55,1.44,-2.39,0  
3HVV,CYS\_276,9.07,0,0,0.07  
2JHY,ASP\_201,4.29,0.49,0,0  
3BQW,ARG\_117,11.8,-0.7,0,0  
1R3F,ASP\_298,2.19,1.05,-2.66,0  
3P28,HIS\_133,1.54,0.74,-1.11,-4.59  
1YW5,LYS\_84,10.43,-0.07,0,0  
3E7P,ASP\_114,3.63,0.63,-0.8,0  
2GZQ,ASP\_30,4.01,0.42,-0.21,0  
1OLR,TYR\_183,8.79,0.15,-1.36,0  
3GYW,TYR\_135,10.64,0,0,0.64  
3Q6L,ASP\_72,3.25,0.28,-0.83,0  
3ERF,GLU\_144,0.01,0.7,-2.79,-2.4  
3PAC,ARG\_114,12.43,-0.07,0,0  
1OST,ASP\_239,4.01,0.21,0,0  
2BAA,ASP\_146,2.36,0.35,-1.79,0  
1H4U,GLU\_485,4.33,0.49,-0.66,0  
3GG6,GLU\_94,4.35,0.42,-0.57,0  
1UXO,GLU\_63,3.54,0.28,-1.24,0  
3V4G,GLU\_21,4.57,0,0,0,0  
2BV9,LYS\_151,10.36,-0.14,0,0  
3D9H,GLU\_237,3.36,0.77,-1.91,0  
3BPP,ASP\_68,2.69,0.28,-1.39,0  
3BQW,TYR\_167,6.70,0.53,-0.8,-2.06  
1G8P,ARG\_219,12.5,0,0,0  
2A1V,ASP\_64,2.83,0.49,-1.46,0  
4E9E,GLU\_450,2.7,1.41,-3.21,0  
2DFL,HIS\_236,3.14,0.4,0,-3.76  
1H09,TYR\_253,9.9,0.07,-0.17,0  
1M5I,TYR\_191,10,0,0,0  
1BKB,ARG\_116,12.22,-0.28,0,0  
2O8P,GLU\_118,3.91,0.21,-0.8,0  
2C13,GLU\_240,0.98,1.8,-3.06,-2.26  
3GS9,GLU\_32,3.17,1.74,-0.89,-2.18  
3DTE,ARG\_179,12.36,-0.14,0,0  
3B7X,ARG\_70,12.36,-0.14,0,0  
2QK1,TYR\_412,8.17,0.14,-1.97,0  
1WP5,GLU\_172,4.73,1.51,-0.85,-0.42  
3DTE,GLU\_20,4.04,0.21,-0.67,0  
1U7U,TYR\_400,9.94,0,-0.06,0  
3QKY,TYR\_125,13.56,0,-0.19,3.75  
3RKV,GLU\_264,4.78,0.28,0,0  
4AM1,LYS\_94,10.15,-0.35,0,0  
1XIPL,LYS\_19,10.5,0,0,0  
1PSW,GLU\_338,4.64,0.14,0,0  
3PZ9,LYS\_307,10.22,-0.28,0,0  
3OIP,ARG\_195,12.08,-0.42,0,0  
4EF5,TYR\_245,9.08,0.31,-1.23,0  
3M70,CYS\_87,8.99,-0.62,0,0.61  
3SMD,GLU\_56,1.7,0.77,-3.57,0  
2F9F,GLU\_33,4.22,0.14,-0.42,0  
2AHE,ARG\_176,11.17,-1.33,0,0  
1V43,ARG\_350,12.36,-0.14,0,0  
3Q1C,ASP\_249,1.71,0.49,-2.58,0  
4F8A,GLU\_633,4.57,0,0,0,0  
2EDM,LYS\_160,9.87,-0.63,0,0  
1FKM,HIS\_285,3.89,0.76,-3.37  
3Q2C,ARG\_49,12.01,-0.49,0,0  
2JEO,ASP\_95,3.42,0.42,-0.8,0  
4F85,HIS\_66,6.71,0.28,0,-0.07  
2YWJ,ASP\_147,2.69,0.49,-1.6,0  
2V4U,CYS\_413,7.15,-1.08,-1.07,0.3  
1CBY,TYR\_245,10.26,0,0,0.26  
2H85,TYR\_193,13.98,0.21,0.8,2.97  
3C5V,ARG\_201,10.23,-2.27,0,0  
2E3C,ASP\_394,3.64,0.14,-0.3,0  
1OGL,ARG\_218,12.01,-0.49,0,0  
2EJX,GLU\_69,3.75,0.42,-1.17,0  
3J5N,LYS\_93,10.08,-0.42,0,0  
3DZ1,ASP\_25,1.81,0.98,-2.96,0  
2C13,HIS\_14,6.25,0.03,0,-0.28  
3PM2,LYS\_162,10.43,-0.07,0,0  
3CBN,ARG\_87,11.66,-0.84,0,0  
3G9G,GLU\_106,4.78,0.28,0,0  
3U2A,ARG\_44,12.5,0,0,0  
4H4J,LYS\_95,10.5,0,0,0  
3RKV,ARG\_324,12.01,-0.49,0,0  
2QDJ,GLU\_125,4.5,0,0,0  
1JT9,LYS\_57,10.36,-0.14,0,0  
2B3M,LYS\_155,10.22,-0.28,0,0  
2X5Y,GLU\_757,3.76,0.21,-0.95,0  
3PZ9,ARG\_53,11.94,-0.56,0,0  
3ADO,ARG\_302,11.8,-0.7,0,0  
1C44,ASP\_70,2.81,0.35,-1.34,0  
3HUE,LYS\_299,10.5,0,0,0  
2FBI,LYS\_111,10.43,-0.07,0,0  
3F1X,HIS\_186,6.25,0.03,0,-0.28  
1RSS,ARG\_114,12.5,0,0,0  
3F5D,HIS\_188,6.82,0.32,0,0  
1RZ2,GLU\_193,4.64,0.28,-0.14,0  
3V75,TYR\_130,10,0,0,0  
1DTO,LYS\_66,10.43,-0.07,0,0  
3EJG,GLU\_112,4.78,0.28,0,0  
3RJZ,TYR\_11,11.4,2.33,-0.93,0  
3PZ9,TYR\_88,11.31,0,-0.06,1.37  
1CHD,HIS\_256,4.49,0.91,-1.19,-1.74  
2C13,ARG\_91,11.45,-1.05,0,0  
3GOZ,GLU\_295,4.71,0.21,0,0  
3UX2,GLU\_39,4.57,0.07,0,0  
3JRT,GLU\_66,4,0.14,-0.64,0  
3CRM,GLU\_229,4.5,0,0,0  
3B4D,ASP\_222,4.01,0.21,0,0  
2VGM,ASP\_274,3.92,0.28,-0.16,0  
2YT4,CYS\_514,6.62,-2.37,0,0  
3ADO,ASP\_115,3.07,0.07,-0.8,0  
4FZR,CYS\_347,10.17,-0.18,0,1.35  
2X4J,LYS\_85,10.29,-0.21,0,0  
3L0D,ARG\_104,12.29,-0.21,0,0  
2NMU,GLU\_83,5.21,0.58,-0.04,0.17  
1FQI,LYS\_336,9.8,-0.7,0,0  
1PBV,TYR\_171,10.82,0.82,0,0  
2D8N,LYS\_157,10.5,0,0,0  
3ONH,LYS\_447,10.5,0,0,0  
1YM5,TYR\_242,10.05,0.05,0,0  
1UW7,TYR\_66,9.99,0,-0.01,0  
3RHE,LYS\_43,10.5,0,0,0  
2V1L,ASP\_140,1.84,0.77,-2.73,0  
2QVT,ASP\_127,3.65,0,-0.15,0  
3EX9,ASP\_48,2.14,0.84,-2.5,0  
3V55,ARG\_354,12.01,-0.49,0,0  
3JSN,TYR\_219,13.21,2.55,0,0.65  
1EV8,ARG\_222,11.52,-0.98,0,0  
2CN1,HIS\_171,7.12,0.69,0,-0.07  
3EZ7,HIS\_230,4.32,0.8,0,-2.98  
3NBI,GLU\_185,3.64,0.21,-1.07,0  
3V55,ASP\_377,4.01,0.21,0,0  
3EJG,LYS\_2,10.5,0,0,0  
3GOZ,CYS\_236,9,0,0,0  
1J8B,ASP\_79,2.45,0.63,-1.97,0  
2G5X,LYS\_38,9.31,-1.19,0,0  
3M7D,GLU\_262,4.64,0.14,0,0  
3RJX,LYS\_300,10.36,-0.14,0,0  
1TD6,LYS\_50,10.36,-0.14,0,0  
3L0D,GLU\_148,3.8,0.28,-0.98,0  
3CCY,ARG\_129,12.29,-0.21,0,0  
2R57,ASP\_243,1.78,0.63,-2.66,0  
1UOH,LYS\_90,10.5,0,0,0  
1K95,ASP\_209,1.89,0.49,-2.4,0  
3H13,TYR\_479,10.49,0,0.49  
1NRI,GLU\_109,4.64,0.14,0,0  
1Q2Y,GLU\_34,5.13,0.63,0,0  
157K,HIS\_25,6.44,0.01,0,-0.07  
1SQW,TYR\_88,9.55,0.07,-0.8,0.28  
1J7G,LYS\_16,10.5,0,0,0  
1MUF,LYS\_111,10.43,-0.07,0,0  
3ODJ,TYR\_102,10,0,0,0  
3P28,ASP\_168,2.75,0.42,-1.46,0  
3LQE,GLU\_488,3.62,0.28,-1.16,0  
1YLN,LYS\_197,10.5,0,0,0  
2P5D,LYS\_43,10.01,-0.49,0,0  
1PGV,ARG\_283,11.94,-0.56,0,0  
3M16,GLU\_26,4.57,0.07,0,0  
2B78,TYR\_278,10,0,0,0  
4AM1,LYS\_151,10.29,-0.21,0,0  
1WXQ,ASP\_123,3.87,0.07,0,0  
2188,ASP\_446,3.86,0.63,-0.57,0  
1MIX,LYS\_300,9.94,-0.56,0,0  
3ONH,GLU\_546,4.5,0,0,0  
3AUF,ASP\_161,1.3,0.91,-3.41,0  
3RJZ,TYR\_19,12.98,0.07,0.51,2.4  
2G3A,GLU\_86,2.87,0.77,-2.4,0  
1VJG,ARG\_54,12.15,-0.35,0,0  
2VGM,CYS\_134,7.39,-0.76,-1.02,0.17  
1OST,ASP\_148,3.24,0.35,-0.91,0  
3IRA,GLU\_143,4.57,0.07,0,0  
3ANJ,ARG\_108,12.22,-0.28,0,0  
3GS9,GLU\_177,1.46,0.42,-3.46,0  
3V55,LYS\_523,10.22,-0.28,0,0  
2B02,GLU\_362,3.68,0.14,-0.96,0  
3IVF,GLU\_293,4.57,0.83,-0.76,0  
21RM,HIS\_346,6.5,0,0,0  
2ILR,TYR\_489,11.26,0.95,0,0.31  
1DZF,LYS\_43,10.36,-0.14,0,0  
2CWC,ARG\_72,12.08,-0.42,0,0  
1NKD,ASP\_34,3,0.21,-1.01,0  
2D8N,LYS\_37,10.15,-0.35,0,0  
1UOH,LYS\_221,10.5,0,0,0  
1NAF,GLU\_230,4.57,0.07,0,0  
3M9A,LYS\_54,10.5,0,0,0  
1PVT,LYS\_86,10.5,0,0,0  
1QQL,ARG\_18,12.15,-0.35,0,0  
1OI7,LYS\_57,10.36,-0.14,0,0  
3CN5,ARG\_112,12.5,0,0,0  
3ETU,HIS\_355,6.5,0,0,0  
2A1V,ASP\_31,2.27,0.42,-1.95,0  
2XJ4,LYS\_208,10.29,-0.21,0,0  
1X1E,ARG\_12,11.85,-0.65,0,0  
3DB9,ARG\_60,12.01,-0.49,0,0  
2P1W,HIS\_174,7.29,0.86,0,-0.07  
1FKM,LYS\_354,10.36,-0.14,0,0  
1UOH,ASP\_29,2.66,0.49,-1.63,0  
1YG2,GLU\_170,4.5,0,0,0  
3P51,ASP\_77,2.17,0.77,-2.4,0  
3ONT,GLU\_28,4.71,0.21,0,0  
2P1N,LYS\_31,10.5,0,0,0  
1R3D,HIS\_244,0.9,0,-1.92,-3.68  
3CJW,HIS\_265,6.5,0.14,0,-0.14  
1EYH,LYS\_23,10.08,-0.42,0,0  
4ACJ,LYS\_671,10.22,-0.28,0,0  
3T5B,CYS\_246,8.37,-2.08,0.65,0.8  
2G9D,ARG\_315,12.43,-0.07,0,0  
4GA2,GLU\_38,3.98,0.28,-0.8,0  
2P0Y,CYS\_217,9.14,0,0.14  
1X1E,ASP\_220,3.12,0.21,-0.89,0  
3F6F,GLU\_65,4.6,0.12,0,-0.02  
1MJS,ARG\_294,11.94,-0.56,0,0  
3ULX,ARG\_68,12.36,-0.14,0,0  
3IBT,ASP\_18,3.51,0.35,-0.64,0  
1ZYL,LYS\_158,10.5,0,0,0  
1JSX,TYR\_162,10.09,1.16,-1.19,0.12  
2FL7,TYR\_175,9.92,0,-0.14,0.06  
2GZQ,GLU\_40,3.91,0.21,-0.8,0  
4FH3,LYS\_56,10.08,-0.42,0,0  
1160,TYR\_158,10.49,0.28,-1.13,1.34  
1WXQ,GLU\_307,5.35,0.85,0,0  
3182,TYR\_176,9.64,0,-0.36,0  
1GQE,GLU\_170,4.5,0,0,0  
1D2K,ASP\_419,2.83,0.35,-1.31,0  
3EVB,ARG\_167,11.94,-0.56,0,0  
1WP5,ARG\_231,12.01,-0.49,0,0  
3U2R,ASP\_115,3.33,0.42,-0.89,0  
1MN3,LYS\_403,10.29,-0.21,0,0  
3QKY,ARG\_259,12.36,-0.14,0,0  
2AH5,LYS\_78,10.36,-0.14,0,0  
3182,HIS\_33,6.31,0.02,0,-0.21  
2X5Y,LYS\_775,10.29,-0.21,0,0  
2HXB,GLU\_39,3.69,0.07,-0.88,0  
4E8B,LYS\_118,10.5,0,0,0  
2V5B,HIS\_36,6.51,0.22,0,-0.21  
3A4C,ASP\_540,2.93,0.28,-1.15,0  
3OBS,ASP\_78,2.45,0.28,-1.63,0  
2CN1,GLU\_126,4.57,0.42,-0.35,0  
1MTZ,GLU\_84,3.32,0.42,-1.6,0  
1SNT,ASP\_80,3.59,0,-0.21,0  
3CAN,ARG\_89,12.36,-0.14,0,0



2D59,GLU\_143,4.5,0,0,0  
3U56,LYS\_73,10.22,-0.28,0,0  
2C13,HIS\_46,3.23,0.37,0,-3.64  
3EYE,ASP\_127,3.77,0,-0.03,0  
3ANJ,ARG\_150,12.22,-0.28,0,0  
3CAX,LYS\_287,10.01,-0.49,0,0  
1RHS,ARG\_131,11.73,-0.77,0,0  
2BLL,HIS\_330,3.16,0.91,-0.04,-4.21  
3EX9,ARG\_34,12.22,-0.28,0,0  
4FH3,ARG\_166,12.01,-0.49,0,0  
1OXZ,HIS\_186,6.5,0,0,0  
1DVO,ASP\_91,3.61,0.07,-0.26,0  
1TUL,CYS\_66,9.16,0,0,0.16  
1OIS,ARG\_337,11.94,-0.56,0,0  
2XMZ,GLU\_112,3.69,4.53,-2.95,-2.4  
3QKY,GLU\_181,4.53,0.07,-0.04,0  
1R7J,ARG\_25,12.01,-0.49,0,0  
3ZSL,LYS\_196,10.43,-0.07,0,0  
3ASA,CYS\_170,11.54,-2.39,1.77,3.16  
2Q99,TYR\_251,11.68,0,-0.27,1.95  
3G9T,ARG\_158,11.17,-1.33,0,0  
3EZ7,TYR\_69,12.68,0.28,0,2.4  
2FXT,GLU\_287,4.5,0,0,0  
1UAJ,GLU\_101,4.16,0.28,-0.62,0  
2BDV,HIS\_122,7.2,0.84,0,-0.14  
1R53,CYS\_18,5.03,-4.18,0,0.21  
2CBE,ASP\_32,2.75,1.05,-2.09,0  
2OBS,LYS\_3,10.5,0,0,0  
2RJD,CYS\_278,7.25,-1.89,0,0.14  
3B21,HIS\_191,4.76,0,0,-1.74  
2QVO,GLU\_65,4.57,0.07,0,0  
2FGG,LYS\_27,10.36,-0.14,0,0  
1SQW,ASP\_42,3.94,0.14,0,0  
1X9G,GLU\_50,3.35,0.56,-1.72,0  
1AD6,ASP\_394,2.97,0.56,-1.39,0  
3CX2,LYS\_193,9.73,-0.77,0,0  
2EFK,LYS\_273,10.43,-0.07,0,0  
3EYE,LYS\_75,10.29,-0.21,0,0  
2OBI,CYS\_75,6.56,-3.6,0,1.17  
1PZC,LYS\_46,10.43,-0.07,0,0  
1RSQ,ARG\_19,12.15,-0.35,0,0  
3C6B,CYS\_183,12.63,0,0,3.63  
1SIG,LYS\_329,10.43,-0.07,0,0  
3E0H,ASP\_137,0.99,0.77,-3.58,0  
1S7K,LYS\_53,10.5,0,0,0  
3FRR,LYS\_76,10.94,-0.09,0.2,0.3  
3PAC,CYS\_38,7.04,-2.24,0,0.28  
3IBT,ARG\_190,11.94,-0.56,0,0  
2ILR,LYS\_478,10.29,-0.21,0,0  
3LJI,LYS\_206,10.22,-0.28,0,0  
3OBS,LYS\_118,10.36,-0.14,0,0  
1X7F,GLU\_167,4.64,0.14,0,0  
3M16,ARG\_308,12.01,-0.49,0,0  
3IU5,GLU\_52,4.5,0,0,0  
1LZL,ARG\_119,11.52,-0.98,0,0  
3L3P,ASP\_295,3.82,0.14,-0.12,0  
1R9W,TYR\_288,11.58,1.58,0,0  
1OGL,GLU\_89,5.37,2.57,-1,-0.7  
1N81,ASP\_124,4.08,0.28,0,0  
2OEW,ARG\_205,11.8,-0.7,0,0  
3VJ8,CYS\_258,11.53,0.068,1.85  
1SJJ,ARG\_86,12.15,-0.35,0,0  
1R29,LYS\_47,9.66,-0.84,0,0  
2RJD,HIS\_423,5.64,-3.37,0,0  
3ASA,ASP\_165,2.55,0.7,-1.95,0  
1SQW,CYS\_36,8.67,-0.67,0,0.34  
3GE9,ARG\_182,11.94,-0.56,0,0  
3FK5,ARG\_313,12.43,-0.07,0,0  
3N2T,ASP\_35,3.34,0.7,-1.17,0  
3CBN,GLU\_98,3.61,0.42,-1.31,0  
1I60,HIS\_177,6.76,1.6,4.04,-5.38  
3PP8,ARG\_56,12.36,-0.14,0,0  
3K1H,GLU\_84,4.59,0.35,-0.26,0  
2R05,GLU\_170,4.64,0.14,0,0  
2XWS,ARG\_46,11.59,-0.91,0,0  
2Z61,ARG\_5,12.43,-0.07,0,0  
1DVO,TYR\_67,10,0,0,0  
2C13,GLU\_109,4.47,0.42,-0.45,0  
2H01,LYS\_81,10.29,-0.21,0,0  
2A4D,ARG\_199,11.24,-1.26,0,0  
2CWC,ARG\_194,12.22,-0.28,0,0  
1PSW,LYS\_207,10.36,-0.14,0,0  
3EVZ,TYR\_223,11.1,1.2,-0.1,0  
2RH3,ARG\_167,11.94,-0.56,0,0  
1MHN,CYS\_107,9.49,0.43,0,0.07  
1ZBS,TYR\_213,9.58,0,-0.42,0  
2PGX,GLU\_43,3.47,0.49,-1.52,0  
3N2T,ARG\_171,11.87,-0.63,0,0  
2EFK,GLU\_285,4.5,0,0,0  
3LD1,HIS\_29,6.36,0,0,-0.14  
1TXJ,ASP\_142,3.94,0.14,0,0  
2X4L,LYS\_346,10.5,0,0,0  
3T57,ARG\_187,11.87,-0.63,0,0  
3FFM,ASP\_71,3.3,0.42,-0.92,0  
3JSN,GLU\_140,3.91,0.21,-0.8,0  
2F9F,LYS\_157,10.15,-0.35,0,0  
2A4D,LYS\_148,10.5,0,0,0  
1OTM,ARG\_224,12.43,-0.07,0,0  
1DUN,LYS\_61,10.5,0,0,0  
3UV9,LYS\_362,10.43,-0.07,0,0  
2VGM,LYS\_200,10.15,-0.35,0,0  
3OOP,LYS\_52,10.5,0,0,0  
3MEW,GLU\_179,4.64,0.14,0,0  
1BKB,GLU\_124,3.95,0.28,-0.83,0  
1RHS,GLU\_148,4.19,0.49,-0.8,0  
1MTZ,HIS\_121,6.36,0,0,-0.14  
3CRM,LYS\_89,10.5,0,0,0  
2P0Y,ARG\_250,11.94,-0.56,0,0  
35MD,GLU\_34,4.12,0.42,-0.8,0  
3B4D,CYS\_205,9,0,0,0  
2QK1,LYS\_404,10.08,-0.42,0,0  
2RGY,ASP\_159,1.09,0.98,-3.69,0  
3GW3,LYS\_290,10.5,0,0,0  
3M70,CYS\_129,12.73,-0.88,2.97,1.64  
1I60,TYR\_30,8.94,0.27,0,-1.33  
2GKG,ASP\_87,3.84,0.07,-0.03,0  
2EYI,LYS\_198,10.5,0,0,0  
1RZ2,GLU\_113,4.26,0.21,-0.45,0  
2OGQ,LYS\_413,9.8,-0.7,0,0  
1X7F,LYS\_60,10.43,-0.07,0,0  
3H8Y,GLU\_13,4,0.14,-0.64,0  
3PBH,ARG\_3,12.08,-0.42,0,0  
4ETX,ARG\_291,12.5,0,0,0  
3JSN,TYR\_20,9.42,0.07,-0.65,0  
1RZ2,GLU\_60,4.64,0.14,0,0  
2XJ4,GLU\_192,3.98,0.28,-0.8,0  
1PSW,ARG\_113,10.31,-2.19,0,0  
4DBX,LYS\_121,10.43,-0.07,0,0  
3BQW,CYS\_241,10.19,0,0,1.19  
2VAN,ASP\_91,2.6,0,-1.2,0  
2A68,GLU\_92,7.18,2.68,0,0  
2AH5,GLU\_204,3,0.56,-2.06,0  
3LJI,HIS\_102,6.34,0.19,0,-0.35  
3BA1,ARG\_23,11.8,-0.7,0,0  
1LZL,ARG\_317,12.36,-0.14,0,0  
2OOK,ASP\_325,3.51,0.42,-0.71,0  
3GW3,LYS\_322,10.29,-0.21,0,0  
2OGQ,ARG\_518,12.5,0,0,0  
4ACJ,TYR\_661,11.09,0,0,1.09  
2E3S,ASP\_389,3.04,0.49,-1.26,0  
1DCF,LYS\_9,10.15,-0.35,0,0  
1O5J,TYR\_66,10.97,0.28,-0.8,1.49  
3H6Q,TYR\_91,10,0,0,0  
2IDC,ASP\_58,3.1,0.49,-1.19,0  
1J33,HIS\_285,6.56,0.06,0,0  
3IVF,ARG\_297,12.29,-0.21,0,0  
3ZXY,GLU\_234,3.94,0.21,-0.77,0  
2OGQ,CYS\_573,4.56,-4.88,0,0.44  
1V43,TYR\_139,10,0,0,0  
3I4T,ASP\_27,3.33,0.28,-0.75,0  
2AZP,HIS\_42,6.19,0.04,0,-0.35  
2HRZ,TYR\_5,10,0,0,0  
2Q13,LYS\_124,10.43,-0.07,0,0  
3M7G,GLU\_202,4.03,0.28,-0.75,0  
3H13,ASP\_409,1.79,0.91,-2.92,0  
3MIX,GLU\_489,1.94,0.65,-1.77,-1.43  
3CZC,GLU\_89,4.64,0.14,0,0  
2Z61,LYS\_365,10.5,0,0,0  
1L2F,LYS\_29,10.5,0,0,0  
1N4J,ASP\_284,3.33,0.35,-0.82,0  
3OIP,ARG\_83,12.43,-0.07,0,0  
2V5B,GLU\_242,3.94,0.63,-1.19,0  
2OKT,ARG\_189,12.5,0,0,0  
3CGW,GLU\_250,4.55,0.14,-0.09,0  
3CGW,ARG\_155,12.36,-0.14,0,0  
1QYI,ARG\_280,12.08,-0.42,0,0  
3PU6,GLU\_45,4.26,0.56,-0.8,0  
1Z9L,LYS\_110,10.29,-0.21,0,0  
1YR6,GLU\_173,4.5,0,0,0  
1J33,ARG\_284,12.36,-0.14,0,0  
2P0Y,HIS\_286,7.23,0.8,0,-0.07  
1MIX,TYR\_308,9.98,0.4,-0.42,0  
2C13,GLU\_106,4.57,0.07,0,0  
4ANN,GLU\_120,2.19,1.74,-2.22,-1.83  
3OKQ,ARG\_594,12.22,-0.28,0,0  
2X4G,GLU\_56,4.5,0,0,0  
2H2Z,CYS\_265,10.5,0,0,1.5  
2X4L,LYS\_162,10.5,0,0,0  
2IRM,GLU\_28,3.14,0.94,-0.04,-2.26  
1W7B,LYS\_324,10.5,0,0,0  
3AUF,GLU\_120,4,0.28,-0.78,0  
3LPZ,LYS\_215,10.5,0,0,0  
3R1X,GLU\_293,4.5,0,0,0  
2OBS,TYR\_3,10,0,0,0  
2OGQ,GLU\_391,4.78,0.28,0,0  
3E7P,LYS\_48,10.5,0,0,0  
1R53,ASP\_38,2.16,0.56,-2.21,0  
4GA2,TYR\_31,10,0,0,0  
3RE9,GLU\_113,3.98,0.21,-0.73,0  
1ZYI,GLU\_257,4.5,0,0,0  
1YB2,GLU\_122,2.58,0.49,-2.41,0  
3U0V,GLU\_188,4.13,0.42,-0.79,0  
3M3P,ASP\_167,4.01,0.21,0,0  
4ECC,GLU\_26,3.84,0.14,-0.8,0  
3ZSL,LYS\_176,10.36,-0.14,0,0  
2A6B,CYS\_68,10.45,0,0,1.45  
2QDJ,GLU\_119,3.33,0.35,-1.52,0  
3H5T,GLU\_211,4.5,0,0,0  
1OXZ,ARG\_255,12.22,-0.28,0,0  
2P1W,GLU\_241,4.19,0.49,-0.8,0  
2H85,HIS\_1,6.5,0,0,0  
4EZB,ASP\_214,2.51,0.56,-1.85,0  
3TMO,ARG\_208,12.01,-0.49,0,0  
2AH5,GLU\_135,4.78,0.28,0,0  
3A4C,ARG\_547,12.01,-0.49,0,0  
1SFE,ARG\_171,11.94,-0.56,0,0  
3RE9,GLU\_204,4.78,0.28,0,0  
1EV8,HIS\_207,5.36,1.14,0.56,-2.85  
2QV2,HIS\_273,11.88,4.57,4.54,-3.73  
3CAX,GLU\_467,3.99,0.07,-0.58,0  
2Z0M,TYR\_267,10,0,0,0  
3I0C,HIS\_219,6.28,1.6,0.87,-2.69  
1J85,ARG\_59,11.94,-0.56,0,0  
2IF4,ASP\_87,2.68,1.05,-2.17,0  
1LTU,ASP\_279,4.01,0.21,0,0  
3R1X,LYS\_101,10.29,-0.21,0,0  
4DNU,LYS\_123,10.15,-0.35,0,0  
3ETU,TYR\_124,9.62,0,-0.38,0  
2EFK,LYS\_253,10.5,0,0,0  
3I4T,TYR\_230,10.63,0.63,0,0  
4ACJ,ASP\_685,3.8,0,0,0  
2FL4,HIS\_4,7.77,1.27,0,0  
3I0O,LYS\_103,10.29,-0.21,0,0  
3CRM,ARG\_93,12.22,-0.28,0,0  
3QKY,GLU\_137,4.5,0,0,0  
1ZBS,ASP\_37,3.12,0.63,-1.3,0  
1P2F,ARG\_69,12.22,-0.28,0,0  
3CAX,LYS\_263,10.36,-0.14,0,0  
3BA1,GLU\_164,3.91,0.21,-0.8,0  
1ZBM,TYR\_212,9.32,0.07,-0.75,0  
1PBV,TYR\_235,9.9,0.14,-0.24,0  
3MEW,CYS\_145,9.23,0,0,0.23  
3H6Q,TYR\_146,13.9,0.63,0.8,2.47  
3F6F,LYS\_120,10.29,-0.21,0,0  
1KN3,ASP\_128,3.94,0.14,0,0  
3F1X,HIS\_71,6.83,0.47,0,-0.14  
4DBX,GLU\_268,4.73,0.49,-0.26,0  
3GW3,HIS\_220,2.14,0.01,-1,-3.37  
3HUE,TYR\_60,9.99,0.59,-0.7,0.11  
1SUU,LYS\_567,10.43,-0.07,0,0  
3CBN,ARG\_131,12.01,-0.49,0,0  
3EJG,ASP\_27,3.87,0.07,0,0  
2CWY,CYS\_74,6.63,-2.43,0,0.07  
1X04,LYS\_138,10.08,-0.42,0,0  
3ULX,TYR\_71,11.61,1.35,0,0.26  
3PP8,GLU\_101,4.78,0.28,0,0  
4EVF,GLU\_245,4.88,0.49,-0.11,0  
3QKY,TYR\_183,12.3,0.07,0.04,2.2  
3CAX,ASP\_372,3.85,0.14,-0.09,0  
3ZXY,ARG\_248,10.41,-2.09,0,0  
2PLQ,TYR\_305,13.34,0.14,0.8,2.4  
1KN3,CYS\_133,8.71,-0.37,0,0.08  
2VGM,LYS\_68,10.43,-0.07,0,0  
2AD1,TYR\_15,10,0,0,0  
1SNT,ARG\_152,12.29,-0.21,0,0  
1V6T,TYR\_27,9.6,0,-0.65,0.25  
2PGX,GLU\_8,2.38,0.28,-2.4,0  
3UC9,GLU\_70,4.64,0.14,0,0  
1A8Q,ASP\_78,2.93,0.77,-1.98,0.34  
3GE9,GLU\_124,4.71,0.21,0,0  
3RLN,TYR\_645,12.49,0.07,0.02,2.4  
3CNU,LYS\_46,10.36,-0.14,0,0  
1SBX,ARG\_120,11.94,-0.56,0,0  
3C2E,GLU\_67,4.5,0,0,0  
3ONH,ASP\_490,3.8,0,0,0  
1RHS,GLU\_49,4.49,0,-0.01,0  
2Z61,LYS\_294,10.5,0,0,0  
3GS9,HIS\_116,6.92,0.7,0,-0.28  
1OTM,TYR\_214,10.82,0,0,0.82  
3VJ8,LYS\_335,10.5,0,0,0  
1YLN,ASP\_31,3.2,0.21,-0.81,0  
2E3H,ARG\_229,11.87,-0.63,0,0  
3P2F,HIS\_85,6.5,0,0,0  
1W24,LYS\_24,10.5,0,0,0  
1DTO,GLU\_185,4.57,0.07,0,0  
4ACJ,HIS\_774,6.97,0.68,0,-0.21

4EUG, TYR\_110, 13.31, 0.11, 0.8, 2.4  
 1OXZ, LYS\_183, 10.5, 0, 0, 0  
 4FH3, ASP\_296, 2.51, 0.28, -1.57, 0  
 1AD6, LYS\_447, 10.29, -0.21, 0, 0  
 2188, ASP\_376, 3.39, 0.21, -0.62, 0  
 1PDB, LYS\_157, 10.5, 0, 0, 0  
 2QK0, CYS\_84, 8.82, -0.39, 0, 0.21  
 1W7B, TYR\_318, 10.21, 0, 0, 21, 0  
 2CBE, ASP\_162, 3.51, 0.28, -0.56, 0  
 4FLE, CYS\_163, 9.41, 0, 0, 0.41  
 2E3I, GLU\_94, 4.5, 0, 0, 0  
 3R2E, GLU\_21, 4.01, 0.63, -1.12, 0  
 2EHG, TYR\_88, 9.59, 0.07, -0.48, 0  
 2IN0, GLU\_424, 4.64, 0.14, 0, 0  
 1PZC, LYS\_59, 10.29, -0.21, 0, 0  
 3PP8, ARG\_29, 11.66, -0.84, 0, 0  
 3UAH, LYS\_343, 10.43, -0.07, 0, 0  
 4GA2, LYS\_28, 10.43, -0.07, 0, 0  
 1AD6, ASP\_527, 2.73, 0.56, -1.62, 0  
 3OKQ, ASP\_571, 3.87, 0.07, 0, 0  
 1OXZ, ARG\_299, 12.29, -0.21, 0, 0  
 2C2Y, ARG\_143, 12.91, -1.99, 0, 2.4  
 2DBN, TYR\_109, 12.19, 3.02, -0.83, 0  
 2Q98, ARG\_192, 12.22, -0.28, 0, 0  
 1EYH, GLU\_26, 4.64, 0.14, 0, 0  
 1J7G, LYS\_112, 9.94, -0.56, 0, 0  
 1Y2Q, HIS\_83, 6.5, 0, 0, 0  
 3IDW, ARG\_56, 12.08, -0.42, 0, 0  
 3V46, ARG\_337, 12.01, -0.49, 0, 0  
 1160, HIS\_26, 7.02, 0.8, 0, -0.28  
 2C13, LYS\_229, 10.29, -0.21, 0, 0  
 2X5Y, LYS\_770, 10.5, 0, 0, 0  
 1WYC, ASP\_368, 3.25, 0.28, -0.83, 0  
 4DNU, TYR\_246, 13.27, 0.07, 0.8, 2.4  
 3T1R, ARG\_27, 12.5, 0, 0, 0  
 1TR9, ARG\_70, 13, -1.29, 0, 1.79  
 2Q12, GLU\_198, 4.57, 0.07, 0, 0  
 1KCM, LYS\_186, 10.5, 0, 0, 0  
 2Z14, ASP\_12, 3.28, 0.35, -0.87, 0  
 2NSN, CYS\_61, 9, 0, 0, 0  
 3AU3, LYS\_435, 10.29, -0.21, 0, 0  
 1GPP, GLU\_422, 4, 0.42, -0.92, 0  
 3EZ7, CYS\_305, 9.43, 0, 0, 0.43  
 2P65, LYS\_66, 10.08, -0.42, 0, 0  
 1XEU, ASP\_67, 3.04, 0.91, -1.68, 0  
 3ELI, ASP\_88, 2.68, 0.35, -1.47, 0  
 216I, ARG\_102, 12.09, -2.01, 0, 1.6  
 3LJI, GLU\_204, 3.68, 0.35, -1.17, 0  
 3LH5, HIS\_767, 1.06, 0.08, -2.27, -3.25  
 2RJD, ARG\_269, 11.73, -0.77, 0, 0  
 3JZN, CYS\_150, 12.63, -0.11, 0, 3.74  
 3A2Z, TYR\_38, 12.08, 0.99, -0.56, 1.65  
 2ILR, GLU\_459, 3.97, 0.28, -0.82, 0  
 3LQE, CYS\_288, 8.77, -0.1, -1.89, 1.76  
 1BYI, GLU\_89, 3.63, 0.56, -1.43, 0  
 3T5B, TYR\_196, 9.34, 0.14, -0.8, 0  
 4F3J, ASP\_235, 3.76, 0.63, -0.67, 0  
 2DVK, ASP\_175, 2.94, 0.49, -1.34, 0  
 3U2R, GLU\_16, 3.7, 0.07, -0.87, 0  
 2IQT, GLU\_128, 3.84, 0.14, -0.8, 0  
 1LZL, HIS\_210, 3.62, 0.17, 0, -3.05  
 3RE9, HIS\_138, 2.32, 1.12, 0, -5.31  
 3GEC, CYS\_455, 9.07, 0, 0, 0.07  
 1PNE, ARG\_55, 11.19, -1.31, 0, 0  
 2VGM, TYR\_104, 9.8, 0.07, -0.27, 0  
 1F2V, ARG\_104, 12.15, -0.35, 0, 0  
 3IDW, TYR\_3, 11.73, 0, 0, 1.73  
 3M3P, CYS\_188, 9.42, -0.05, 0, 0.47  
 2BDV, GLU\_140, 4.5, 0, 0, 0  
 2A1V, GLU\_19, 4.01, 0.28, -0.77, 0  
 1ZCU, GLU\_117, 4.5, 0, 0, 0  
 1LTU, HIS\_110, 3.99, 0.95, 0, -3.46  
 3GG6, GLU\_82, 2.12, 1.12, -3.5, 0  
 1UX0, TYR\_184, 11.44, 1.55, -0.11, 0  
 2D0A, ARG\_224, 11.66, -0.84, 0, 0  
 1X7F, LYS\_316, 10.22, -0.28, 0, 0  
 2NRK, LYS\_166, 10.36, -0.14, 0, 0  
 2CIU, LYS\_120, 10.5, 0, 0, 0  
 1W7B, LYS\_246, 10.15, -0.35, 0, 0  
 1EDG, ASP\_278, 2.75, 0.63, -1.68, 0  
 2Q34, GLU\_256, 4.71, 0.21, 0, 0  
 2O0K, ARG\_114, 11.73, -0.77, 0, 0  
 2OGQ, ASP\_449, 2.63, 0.91, -2.08, 0  
 2IRM, HIS\_292, 4.94, 0.01, 0, -1.57  
 2OJQ, CYS\_691, 9.11, -0.2, 0, 0.31  
 2QHT, LYS\_145, 10.43, -0.07, 0, 0  
 2IXM, ASP\_95, 3.76, 0.07, -0.11, 0  
 3N2T, GLU\_122, 4.5, 0, 0, 0  
 2B61, ASP\_345, 3.72, 0, -0.08, 0  
 1QZN, LYS\_122, 10.36, -0.14, 0, 0  
 3V75, GLU\_186, 3.11, 0.21, -1.6, 0  
 1YR6, ASP\_186, 3.77, 0.14, -0.17, 0  
 1XEU, LYS\_273, 10.08, -0.42, 0, 0  
 3RFF, ASP\_46, 2.61, 0.49, -1.68, 0  
 1YG2, LYS\_145, 10.5, 0, 0, 0  
 3IU5, TYR\_127, 11.77, 0, 0, 1.77  
 4AM1, LYS\_118, 10.5, 0, 0, 0  
 3HUE, LYS\_206, 10.5, 0, 0, 0  
 3ULX, ARG\_78, 12.29, -0.21, 0, 0  
 4ACJ, HIS\_672, 6.67, 0.31, 0, -0.14  
 2YWX, LYS\_51, 10.43, -0.07, 0, 0  
 4FCU, GLU\_250, 3.61, 0.21, -1.1, 0  
 1UW7, ARG\_74, 12.36, -0.14, 0, 0  
 2CBE, GLU\_26, 4.64, 0.14, 0, 0  
 2VGM, LYS\_348, 10.36, -0.14, 0, 0  
 4GCO, ASP\_236, 3.96, 0.21, -0.05, 0  
 2JHY, HIS\_189, 4.1, 0.71, 0, -3.11  
 4AM1, GLU\_252, 3.91, 0.21, -0.8, 0  
 3RJK, LYS\_183, 10.43, -0.07, 0, 0  
 1T95, GLU\_157, 10.22, -0.28, 0, 0  
 3ASA, ARG\_136, 12.22, -0.28, 0, 0  
 3VHJ, ARG\_52, 11.72, -0.78, 0, 0  
 3CE7, GLU\_36, 3.73, 0.35, -1.12, 0  
 2X5Y, LYS\_813, 10.36, -0.14, 0, 0  
 3G9T, ARG\_236, 12.15, -0.35, 0, 0  
 1S1G, ASP\_233, 3.74, 0.35, -0.41, 0  
 1Z3X, LYS\_131, 10.5, 0, 0, 0  
 1CHD, GLU\_306, 4.5, 0, 0, 0  
 4F85, ASP\_246, 3.97, 0.63, -0.46, 0  
 1TJE, GLU\_176, 3.39, 0.49, -1.6, 0  
 4EVF, TYR\_30, 11.78, 0.07, 0, 1.71  
 2IXM, GLU\_301, 4.12, 0.42, -0.8, 0  
 1YTD, ARG\_329, 12.65, -2.25, 0, 2.4  
 3ETU, GLU\_353, 4.71, 0.21, 0, 0  
 3AU3, ARG\_402, 11.38, -1.12, 0, 0  
 3BA1, LYS\_224, 10.5, 0, 0, 0  
 1WXF, LYS\_207, 10.29, -0.21, 0, 0  
 3KT9, ARG\_13, 12.22, -0.28, 0, 0  
 2CXC, ARG\_28, 12.01, -0.49, 0, 0  
 1PGV, LYS\_251, 9.94, -0.56, 0, 0  
 3BCY, CYS\_142, 8.74, -1.11, 0, 0.85  
 1SQH, CYS\_215, 8.03, -1.11, 0, 0.14  
 3P2F, GLU\_90, 3.75, 0.07, -0.82, 0  
 3Q9P, LYS\_123, 10.43, -0.07, 0, 0  
 2ZQ5, HIS\_192, 8.02, 1.6, 2.4, -2.48  
 4D8L, TYR\_21, 10.59, 0.59, 0, 0  
 3IL3, GLU\_167, 4.39, 0.42, -0.53, 0  
 3FNI, ASP\_40, 1.43, 0.84, -3.21, 0  
 2QHT, ARG\_196, 11.59, -0.91, 0, 0  
 1QZN, TYR\_43, 10.67, 0.71, -0.04, 0  
 1ZHV, CYS\_48, 9.18, 0, 0, 0.18  
 1C44, LYS\_40, 10.29, -0.21, 0, 0  
 3V4G, ASP\_129, 2.94, 0.14, -1, 0  
 3H5T, ARG\_252, 12.22, -0.28, 0, 0  
 3ETV, ASP\_199, 3.94, 0.14, 0, 0  
 3EST, LYS\_181, 10.22, -0.28, 0, 0  
 1UAJ, ASP\_128, 2.88, 0.28, -1.2, 0  
 2F4Q, ARG\_239, 9.35, -2.81, 0, -0.34  
 1ZCU, LYS\_48, 10.5, 0, 0, 0  
 3RAZ, ASP\_76, 3.09, 0.77, -1.48, 0  
 4GA2, ARG\_113, 12.01, -0.49, 0, 0  
 3A7L, ASP\_21, 1.93, 0.42, -2.29, 0  
 3LJI, GLU\_282, 3.41, 0.42, -1.51, 0  
 2OPJ, TYR\_154, 10.78, 2.16, -0.48, -0.9  
 2HRZ, ARG\_226, 11.73, -0.77, 0, 0  
 2GAU, ARG\_26, 11.66, -0.84, 0, 0  
 2CL3, ARG\_90, 12.22, -0.28, 0, 0  
 2PGX, HIS\_66, 6.44, 0.01, 0, -0.07  
 2Q13, ARG\_121, 11.87, -0.63, 0, 0  
 1J5X, LYS\_113, 10.5, 0, 0, 0  
 1SUU, HIS\_556, 6.5, 0, 0, 0  
 2W0Z, TYR\_587, 10.44, 0, -0.35, 0.79  
 3EZ7, ASP\_340, 3.81, 0.14, -0.13, 0  
 1KN3, ARG\_132, 12.5, 0, 0, 0  
 2Z14, ASP\_79, 4.08, 0.28, 0, 0  
 4F8A, ASP\_642, 3.08, 0.7, -1.42, 0  
 3LH5, ARG\_579, 12.01, -0.49, 0, 0  
 3CIV, ARG\_99, 12.08, -0.42, 0, 0  
 4DBX, LYS\_99, 10.5, 0, 0, 0  
 2A0J, GLU\_112, 4.57, 0.07, 0, 0  
 3ZTA, ASP\_39, 3.16, 0.49, -1.13, 0  
 3E5T, GLU\_91, 4.08, 0.21, -0.63, 0  
 4FH3, ARG\_198, 12.15, -0.35, 0, 0  
 2HXB, TYR\_72, 10, 0, 0, 0  
 2F4Q, LYS\_264, 10.5, 0, 0, 0  
 2Y2T, TYR\_17, 10.3, 0.07, 0, 0.23  
 3LJC, ASP\_161, 3.44, 0.63, -1, 0  
 4AM1, ARG\_126, 5.14, -2.93, 0, -4.42  
 3N2T, LYS\_307, 10.5, 0, 0, 0  
 1YB2, ARG\_230, 11.8, -0.7, 0, 0  
 3M16, TYR\_193, 11.77, 0, 0, 1.77  
 2ZTY, GLU\_53, 4.5, 0, 0, 0  
 1J33, GLU\_27, 3.14, 0.7, -2.06, 0  
 1WLY, HIS\_138, 10.08, 4.33, 2.4, -3.15  
 3EZ7, GLU\_63, 4.78, 0.28, 0, 0  
 216I, GLU\_88, 4.64, 0.14, 0, 0  
 2AZL, TYR\_151, 11.41, 0.07, -0.33, 1.66  
 2VAN, LYS\_209, 10.5, 0, 0, 0  
 1XFK, TYR\_289, 9.66, 0.21, -1.35, 0.8  
 1JB3, LYS\_62, 10.22, -0.28, 0, 0  
 2B0J, HIS\_174, 0.7, 0.01, -0.4, -5.41  
 1Q8B, GLU\_39, 2.76, 0.91, -2.65, 0  
 2XHC, ARG\_209, 13.4, -1.47, 0, 2.37  
 1SNT, ASP\_215, 3.42, 0.42, -0.8, 0  
 1IAP, GLU\_141, 4.64, 0.14, 0, 0  
 1AM2, LYS\_92, 10.82, -0.56, 0, 0.88  
 1YLN, ARG\_57, 12.29, -0.21, 0, 0  
 2POL, ARG\_250, 11.94, -0.56, 0, 0  
 3CNU, GLU\_94, 3.74, 0.21, -0.97, 0  
 1UOH, LYS\_135, 10.08, -0.42, 0, 0  
 2CBE, LYS\_39, 10.43, -0.07, 0, 0  
 1RAJ, GLU\_254, 4.5, 0, 0, 0  
 1SQW, ARG\_30, 12.01, -0.49, 0, 0  
 2H2W, HIS\_75, 6.29, 0, 0, -0.21  
 2E3C, ARG\_409, 12.5, 0, 0, 0  
 1OIS, GLU\_329, 4.5, 0, 0, 0  
 3V55, ASP\_638, 3.76, 0.07, -0.11, 0  
 2E35, ASP\_440, 3.73, 0.14, -0.21, 0  
 3AU3, ARG\_463, 11.52, -0.98, 0, 0  
 1XTZ, LYS\_258, 10.5, 0, 0, 0  
 1R7J, LYS\_6, 10.5, 0, 0, 0  
 4ANN, LYS\_37, 9.94, -0.56, 0, 0  
 3GS9, CYS\_51, 7.76, -1.24, 0, 0  
 1SJV, ARG\_73, 12.29, -0.21, 0, 0  
 1Q8B, LYS\_82, 10.29, -0.21, 0, 0  
 1Y2Q, LYS\_31, 10.29, -0.21, 0, 0  
 3IOC, GLU\_247, 2.08, 0.95, -3.37, 0  
 2X5Y, HIS\_810, 5.36, 0.9, 0.57, -2.61  
 3ANJ, LYS\_329, 9.87, -0.63, 0, 0  
 2B6P, TYR\_178, 10, 0, 0, 0  
 4DBX, TYR\_189, 10.13, 0.64, -1.37, 0.86  
 2ZTY, GLU\_94, 3.46, 0.37, -1.41, 0  
 3O16, GLU\_227, 4.71, 0.21, 0, 0  
 2AXO, ARG\_132, 12.5, 0, 0, 0  
 4EKU, ARG\_242, 12.5, 0, 0, 0  
 2QK1, GLU\_555, 4.5, 0, 0, 0  
 2G3A, GLU\_88, 3.96, 0.28, -0.82, 0  
 1ZCE, CYS\_68, 8.51, -0.49, 0, 0  
 2H8O, GLU\_148, 4.71, 0.21, 0, 0  
 1ZCU, ASP\_112, 2.96, 0.28, -1.12, 0  
 1RLO, ARG\_180, 11.62, -3.42, 0, 2.54  
 2JHY, LYS\_199, 10.43, -0.07, 0, 0  
 3FWU, LYS\_15, 10.22, -0.28, 0, 0  
 1FO9, LYS\_381, 10.43, -0.07, 0, 0  
 2H2Z, CYS\_44, 8.98, -0.64, 0, 0.62  
 2D25, LYS\_731, 10.08, -0.42, 0, 0  
 2ZCO, LYS\_190, 10.5, 0, 0, 0  
 1O6D, HIS\_21, 6.43, 0, 0, -0.07  
 2OSA, LYS\_384, 10.29, -0.21, 0, 0  
 1O5T, TYR\_402, 11.67, 2.27, -0.61, 0  
 3F53, TYR\_277, 9.58, 0, -0.42, 0  
 3FNI, LYS\_87, 10.5, 0, 0, 0  
 1WRU, GLU\_128, 4.23, 0.26, -0.53, 0  
 2Z14, LYS\_103, 10.29, -0.21, 0, 0  
 2VGM, ASP\_363, 3.95, 0.28, -0.13, 0  
 2FZ4, TYR\_67, 13.37, 0.28, 0.69, 2.4  
 3KVO, GLU\_129, 4.19, 0.49, -0.8, 0  
 1MIX, LYS\_274, 10.43, -0.07, 0, 0  
 3DB9, ASP\_182, 3.42, 0.14, -0.52, 0  
 2G2D, ASP\_179, 3.85, 0.14, -0.09, 0  
 3CIV, TYR\_302, 9.81, 0.07, -0.77, 0.5  
 3LJI, ASP\_227, 3.93, 0.14, -0.01, 0  
 4FH3, HIS\_273, 1.48, 0.42, -2.63, -2.81  
 3ETU, ASP\_150, 3.87, 0.07, 0, 0  
 1O3X, TYR\_253, 13.41, 0.21, 0.8, 2.4  
 2P0Y, LYS\_161, 10.22, -0.28, 0, 0  
 1Z3X, GLU\_108, 2.52, 0.3, -0.17, -2.11  
 2Z0W, ARG\_76, 12.08, -0.42, 0, 0  
 2O8P, ASP\_165, 3.38, 0.35, -0.77, 0  
 2OGQ, ASP\_457, 2.98, 0.49, -2.21, 0  
 2ZCO, ASP\_32, 3.76, 0, -0.04, 0  
 1NAF, GLU\_203, 4.01, 0.07, -0.55, 0  
 2RIK, LYS\_194, 10.22, -0.28, 0, 0  
 3KB5, ARG\_371, 12.5, 0, 0, 0  
 1RIS, GLU\_197, 4.78, 0.28, 0, 0  
 1EDG, LYS\_313, 9.31, -1.19, 0, 0  
 2B0J, GLU\_27, 3.95, 0.44, -0.23, -0.76  
 4AE7, ARG\_189, 11.8, -0.7, 0, 0  
 2PLQ, TYR\_116, 12.36, 0.14, -0.18, 2.4  
 2GZQ, TYR\_91, 9.36, 0.4, 0, -1.04  
 3BJV, GLU\_130, 4.5, 0, 0, 0  
 3ASA, ASP\_223, 3.94, 0.14, 0, 0  
 1L2F, GLU\_165, 3.97, 0.27, -0.8, 0  
 1DOV, ARG\_98, 11.94, -0.56, 0, 0  
 2BT8, ARG\_262, 11.87, -0.63, 0, 0  
 2AZL, LYS\_41, 10.22, -0.28, 0, 0

3RJZ,ARG\_105,11.73,-0.77,0,0  
 3CAX,ASP\_333,2.43,0.63,-2,0  
 2Q34,TYR\_170,10,0,0,0  
 1H09,HIS\_14,6.76,0.26,0,0  
 2F9F,ASP\_144,3.89,0.14,-0.05,0  
 2GEN,TYR\_64,12.05,2.13,-0.08,0  
 3ETU,ASP\_161,3.35,0.35,-0.8,0  
 3JZN,GLU\_249,4.71,0.21,0,0  
 4EKU,ASP\_196,3.96,0.35,-0.19,0  
 2G9D,ASP\_131,3.48,0.14,-0.46,0  
 4GCO,GLU\_145,5.29,0.42,0.37,0  
 2IIA,LYS\_54,9.94,-0.56,0,0  
 1BN6,GLU\_202,4.5,0,0,0  
 3UC9,ARG\_48,12.36,-0.14,0,0  
 2QRX,LYS\_72,10.36,-0.14,0,0  
 2P1W,ARG\_111,12.01,-0.49,0,0  
 1EQ6,ASP\_96,3.69,0.07,-0.18,0  
 3IV4,GLU\_75,4.71,0.21,0,0  
 1YM5,GLU\_52,3.05,2.96,-2.06,-2.34  
 3AU3,GLU\_461,4.38,0.21,-0.33,0  
 2H14,GLU\_58,4.57,0.07,0,0  
 3UX2,ARG\_101,12.01,-0.49,0,0  
 1NJ4,ASP\_156,3.79,0,-0.01,0  
 2QV2,ARG\_271,12.22,-0.28,0,0  
 1RSS,TYR\_85,10,0,0,0  
 1WOU,ASP\_36,2.11,0.91,-2.6,0  
 3IL3,LYS\_60,10.15,-0.35,0,0  
 1OTM,ASP\_87,3.21,0.21,-0.8,0  
 3ETU,GLU\_51,4.5,0,0,0  
 1XAW,LYS\_501,10.5,0,0,0  
 3EX9,GLU\_157,4.5,0,0,0  
 3UAH,CYS\_332,10.48,-2.65,0.4,1.33  
 3JSN,TYR\_306,10.88,0,0.88  
 3CBN,HIS\_111,6.39,0.17,0,-0.28  
 1J33,ARG\_46,11.66,-0.84,0,0  
 2B2H,ASP\_214,3.76,0,-0.04,0  
 1SFE,ARG\_81,11.94,-0.56,0,0  
 2GVZ,ARG\_88,11.94,-0.56,0,0  
 2YT4,LYS\_689,9.8,-0.7,0,0  
 2F4Q,HIS\_218,6.43,0,0,-0.07  
 2FL4,ARG\_139,11.94,-0.56,0,0  
 3ELI,GLU\_61,4.57,0.07,0,0  
 1X7F,GLU\_17,3.66,0.35,-1.19,0  
 2EDM,ASP\_105,3.28,0.63,-1.15,0  
 4DBX,CYS\_213,8.75,-0.39,0,0.14  
 2X4G,ARG\_272,12.29,-0.21,0,0  
 2Q13,GLU\_11,4.5,0,0,0  
 2F4Q,LYS\_194,10.08,-0.42,0,0  
 2F4Q,GLU\_260,3.49,0,-1.01,0  
 1ZBS,ARG\_38,12.15,-0.35,0,0  
 2RIK,LYS\_49,10.5,0,0,0  
 1EW4,GLU\_44,3.72,0.35,-1.13,0  
 2AD1,LYS\_31,10.5,0,0,0  
 3RJZ,ARG\_28,12.5,0,0,0  
 2AH5,TYR\_81,10,0,0,0  
 2WOZ,LYS\_436,10.22,-0.28,0,0  
 3N2T,LYS\_262,9.87,-0.63,0,0  
 3HVV,ARG\_246,13.71,-0.55,0,1.76  
 4H4J,ASP\_188,4.15,0.35,0,0  
 1R9W,CYS\_290,9,0,0,0  
 2V4U,ASP\_365,2.93,0.35,-1.22,0  
 3IOO,ARG\_120,12.01,-0.49,0,0  
 2IXM,LYS\_242,10.29,-0.21,0,0  
 3PP8,ARG\_269,11.8,-0.7,0,0  
 1WLY,ARG\_235,12.36,-0.14,0,0  
 3GEC,ASP\_276,4.12,0.63,-0.3,0  
 1UJ8,ASP\_55,2.16,0.56,-2.2,0  
 2H2Z,LYS\_236,10.5,0,0,0  
 1DTO,LYS\_34,10.36,-0.14,0,0  
 2VAN,LYS\_148,10.08,-0.42,0,0  
 2O8P,LYS\_61,10.5,0,0,0  
 1YLN,GLU\_188,4.12,0.42,-0.8,0  
 1I60,TYR\_199,11.96,2.68,-0.8,0.08  
 1M5I,ARG\_197,12.15,-0.35,0,0  
 3IU5,GLU\_104,4.5,0,0,0  
 2VGM,ASP\_185,2.92,0.42,-1.3,0  
 2EJB,LYS\_116,10.22,-0.28,0,0  
 3G6S,LYS\_197,10.22,-0.28,0,0  
 1SQW,TYR\_95,9.64,0,-0.36,0  
 1XAW,ARG\_519,12.08,-0.42,0,0  
 4E8B,ASP\_155,3.1,0.21,-0.91,0  
 2APL,TYR\_115,13.41,0.21,0.8,2.4  
 3EIZ,ARG\_89,11.73,-0.77,0,0  
 3EZ7,GLU\_222,4.57,0.07,0,0  
 3QKY,GLU\_254,4.22,0.14,-0.42,0  
 1RKA,HIS\_17,6.43,0,0,-0.07  
 1XKR,ASP\_70,3.02,0.42,-1.2,0  
 4DBX,LYS\_171,10.5,0,0,0  
 4AM1,ARG\_294,12.08,-0.42,0,0  
 3FNI,LYS\_109,10.43,-0.07,0,0  
 3RJX,LYS\_41,10.43,-0.07,0,0  
 3AUF,ARG\_26,11.73,-0.77,0,0  
 3G9G,GLU\_220,4.54,0.35,-0.3,0  
 3E5T,GLU\_215,3.29,3.29,-1.6,-2.91  
 1L3K,ARG\_55,12.15,-0.35,0,0  
 1RAJ,GLU\_364,3.98,0.28,-0.8,0  
 1SUU,LYS\_749,10.5,0,0,0  
 1C44,ASP\_41,4.01,0.21,0,0  
 2V4U,ASP\_470,3.92,0.21,-0.09,0  
 3OA7,GLU\_446,4.28,0.21,-0.43,0  
 3F7M,ARG\_225,11.94,-0.56,0,0  
 1FKM,ARG\_254,11.59,-0.91,0,0  
 2B02,ARG\_409,12.01,-0.49,0,0  
 3PZ9,ARG\_38,11.45,-1.05,0,0  
 1WYC,HIS\_58,7.15,0.72,0,-0.07  
 1O6D,ARG\_115,12.01,-0.49,0,0  
 4ECC,ARG\_116,11.32,-3.03,0,1.85  
 3ONT,GLU\_69,4.71,0.21,0,0  
 1ANU,ASP\_114,4.01,0.21,0,0  
 1O9G,ARG\_108,8.2,-1.9,0,-2.4  
 2GZQ,GLU\_63,4.57,0.07,0,0  
 1ZKZ,LYS\_96,10.22,-0.28,0,0  
 4HDE,ASP\_142,2.73,0.56,-1.63,0  
 3CAX,ARG\_419,11.94,-0.56,0,0  
 3Q2C,GLU\_11,3.75,0.21,-0.97,0  
 1NWA,GLU\_140,4.71,0.21,0,0  
 1H4U,CYS\_373,9,0,0,0  
 1MIX,TYR\_270,12.95,0.84,0.2,1.91  
 3RFY,ARG\_238,12.63,-3.09,0,3.21  
 2H2W,ARG\_98,12.22,-0.28,0,0  
 3LJN,GLU\_18,4.5,0,0,0  
 4DVD,ARG\_71,12.01,-0.49,0,0  
 3CIV,GLU\_121,4.19,0.84,-1.15,0  
 2Q99,LYS\_312,8.17,-0.7,0,-1.63  
 2ATR,GLU\_32,4.64,0.14,0,0  
 1MN3,GLU\_405,4.13,0.35,-0.72,0  
 2D7J,LYS\_87,10.5,0,0,0  
 4F85,ASP\_74,3.43,0.21,-0.58,0  
 2D8N,LYS\_63,10.36,-0.14,0,0  
 2XHC,HIS\_64,7.16,0.8,0,-0.14  
 3ETV,ASP\_347,4.2,0.42,-0.02,0  
 1ZP2,GLU\_124,4.12,0.42,-0.8,0  
 1QQE,ARG\_220,12.36,-0.14,0,0  
 1I60,ARG\_166,12.01,-0.49,0,0  
 1R3D,LYS\_207,10.5,0,0,0  
 1SQH,GLU\_295,3.24,0.42,-1.68,0  
 1PNE,ASP\_54,1.16,0.42,-3.06,0  
 1WP5,LYS\_141,10.5,0,0,0  
 3FXH,CYS\_103,10.77,-0.09,0,1.86  
 1GPP,LYS\_427,10.5,0,0,0  
 2RIS,LYS\_141,10.5,0,0,0  
 2CIU,LYS\_180,10.43,-0.07,0,0  
 2FBJ,ARG\_41,13.07,-0.59,0,1.16  
 1PNE,ARG\_136,11.87,-0.63,0,0  
 3GS9,GLU\_247,4.5,0,0,0  
 1XWM,TYR\_159,11.95,0.05,1.91  
 4D8L,ASP\_170,3.8,0,0,0  
 4AF2,ASP\_151,3.88,0.21,-0.13,0  
 2IQT,TYR\_288,10,0,0,0  
 3GE9,LYS\_165,10.08,-0.42,0,0  
 2G9D,ASP\_279,3.69,0.35,-0.46,0  
 1J8B,LYS\_89,10.5,0,0,0  
 2GZQ,GLU\_9,3.02,0.63,-2.11,0  
 3GEC,CYS\_502,7.8,-1.41,0,0.21  
 3CBN,GLU\_162,4.34,0.21,-0.37,0  
 2B0J,GLU\_229,3.98,0.28,-0.8,0  
 1WLY,HIS\_192,6.43,0.07,0,-0.14  
 1J74,TYR\_143,9.02,0.21,-1.19,0  
 2XWS,ARG\_89,12.22,-0.28,0,0  
 3LJL,LYS\_260,10.22,-0.28,0,0  
 1PF6,ARG\_139,12.5,0,0,0  
 1BN6,ASP\_89,3.94,0.14,0,0  
 3BCY,HIS\_91,6.5,0,0,0  
 3F1X,TYR\_261,10,0,0,0  
 3OIP,ASP\_145,3.11,0.49,-1.18,0  
 3RJZ,ARG\_84,11.94,-0.56,0,0  
 2FD5,LYS\_4,10.5,0,0,0  
 2V4X,ASP\_82,3.63,0.21,-0.38,0  
 2YWX,GLU\_16,4.71,0.21,0,0  
 1O6D,ARG\_4,11.8,-0.7,0,0  
 2NSN,ASP\_73,3.27,0.35,-0.88,0  
 1NAF,GLU\_219,4.41,0.21,-0.3,0  
 2D7U,ARG\_55,11.48,-1.05,0,0.03  
 2OSA,ASP\_373,3.74,0.07,-0.13,0  
 2B02,GLU\_435,4.57,0.07,0,0  
 3BB7,LYS\_105,10.5,0,0,0  
 4FD6,LYS\_213,10.29,-0.21,0,0  
 1HF8,ARG\_246,11.59,-0.91,0,0  
 1FQJ,ARG\_305,12.15,-0.35,0,0  
 3L7N,LYS\_125,10.22,-0.28,0,0  
 1ZYL,LYS\_176,10.29,-0.21,0,0  
 2CW4,GLU\_88,4.06,0.42,-0.86,0  
 3IVF,ASP\_54,3.8,0,0,0  
 1SJ8,CYS\_709,11.19,0.134,0.85  
 3T57,ARG\_149,12.22,-0.28,0,0  
 2V81,TYR\_137,10.04,0.07,-0.03,0  
 1XTZ,HIS\_222,1.53,0,-2.12,-2.85  
 2A6B,GLU\_76,4.5,0,0,0  
 1WP5,LYS\_274,10.15,-0.35,0,0  
 1JKS,ARG\_254,12.29,-0.21,0,0  
 1C3K,GLU\_69,4.51,0.21,-0.2,0  
 3RJZ,TYR\_199,10,0,0,0  
 2OOK,LYS\_305,10.29,-0.21,0,0  
 3OOP,GLU\_41,4.78,0.36,-0.08,0  
 1AKO,HIS\_16,6.43,0.07,0,-0.14  
 4EZB,GLU\_242,4.54,0.35,-0.31,0  
 2YT4,TYR\_519,12.25,1.62,0,0.63  
 3CXS,LYS\_167,10.01,-0.49,0,0  
 2VGM,LYS\_66,10.01,-0.49,0,0  
 3GS3,GLU\_54,4.57,0.07,0,0  
 4ESS,GLU\_13,3.98,0.28,-0.8,0  
 2B0J,LYS\_2,9.59,-0.91,0,0  
 3OOP,ASP\_31,3.31,0.28,-0.77,0  
 1W24,HIS\_117,4.29,1.19,0.52,-3.92  
 3M9A,CYS\_93,8.55,-0.52,0,0.07  
 2PGX,ARG\_241,11.87,-0.63,0,0  
 1NJ4,LYS\_84,10.5,0,0,0  
 2H2Z,TYR\_37,10.48,0.8,-0.31,0  
 1RWZ,ARG\_37,11.87,-0.63,0,0  
 2CIU,ASP\_129,3.8,0,0,0  
 1WP5,ARG\_74,12.29,-0.21,0,0  
 3RFF,ARG\_65,12.01,-0.49,0,0  
 2WZ9,GLU\_59,3.98,0.28,-0.8,0  
 1OGL,LYS\_106,10.5,0,0,0  
 1ZCE,LYS\_101,10.5,0,0,0  
 2IQT,ASP\_180,2.83,0.28,-1.25,0  
 1YR6,ARG\_177,12.36,-0.14,0,0  
 3IOC,HIS\_305,6.43,2.09,2.15,-4.3  
 3LPZ,ARG\_319,12.5,0,0,0  
 2FXT,GLU\_295,4.46,0.21,-0.25,0  
 1YB2,ARG\_221,12.22,-0.28,0,0  
 1MTZ,TYR\_176,9.72,0.14,-0.42,0  
 3FTT,LYS\_6,10.29,-0.21,0,0  
 2OB5,HIS\_49,6.69,0.41,0,-0.21  
 1R9W,ASP\_275,3.86,0.07,-0.01,0  
 3GT0,GLU\_103,4.5,0,0,0  
 3CAX,TYR\_448,10.65,0.45,-0.85,1.05  
 1OLR,TYR\_128,13.29,0.89,0.2,4  
 3EIZ,LYS\_175,10.5,0,0,0  
 2H30,CYS\_71,8.87,-0.95,-0.17,0.99  
 1SJ8,ASP\_661,4.01,0.21,0,0  
 1K95,LYS\_125,10.08,-0.42,0,0  
 3B79,LYS\_123,10.29,-0.21,0,0  
 1FQI,ASP\_399,4.21,0.42,-0.01,0  
 1G8P,GLU\_267,4.64,0.14,0,0  
 1E5S,TYR\_258,10,0,0,0  
 1EYH,HIS\_67,6.36,0,0,-0.14  
 1O0X,LYS\_54,10.5,0,0,0  
 2RH3,LYS\_198,10.5,0,0,0  
 2G3A,ASP\_36,3.64,0,-0.16,0  
 3HVM,ARG\_33,11.8,-0.7,0,0  
 2RD,TYR\_427,13.58,0.38,0.8,2.4  
 1YB2,LYS\_182,10.29,-0.21,0,0  
 3BPP,CYS\_120,9.34,-1.92,0.2,26  
 1QZN,ASP\_147,2.39,0.98,-2.4,0  
 1Q46,TYR\_141,10.4,0,0.4  
 2CBE,ASP\_41,1.77,0.56,-2.6,0  
 2OOK,ASP\_34,4.01,0.21,0,0  
 1YM5,HIS\_295,6.43,0,0,-0.07  
 1J33,GLU\_135,2.77,0.84,-2.56,0  
 3EJG,LYS\_47,10.43,-0.07,0,0  
 1Z3X,HIS\_39,6.5,0,0,0  
 3EVZ,GLU\_57,3.56,0.49,-1.43,0  
 2YQJ,LYS\_93,10.43,-0.07,0,0  
 1V43,ARG\_150,12.78,-0.91,0,1.19  
 1YW5,ASP\_42,2.87,0.35,-1.27,0  
 2P1W,ASP\_112,3.58,0.21,-0.43,0  
 3FNI,ARG\_20,12.22,-0.28,0,0  
 3C2E,ARG\_115,12.15,-0.35,0,0  
 1DZF,LYS\_201,9.8,-0.7,0,0  
 2EA9,CYS\_92,9.66,-1.2,0,1.86  
 1U3Y,LYS\_272,10.43,-0.07,0,0  
 2W0G,ASP\_254,3.99,0.21,-0.02,0  
 1DVO,ARG\_101,12.22,-0.28,0,0  
 3BPV,ARG\_140,11.59,-0.91,0,0  
 1WP5,LYS\_228,10.08,-0.42,0,0  
 1MIX,GLU\_350,4.07,0.21,-0.64,0  
 2BDV,ASP\_179,2.94,0.49,-1.34,0  
 1YDL,ARG\_56,12.08,-0.42,0,0  
 1UCH,LYS\_210,10.29,-0.21,0,0  
 3ODJ,GLU\_49,4.12,0.42,-0.8,0  
 2OJQ,ASP\_434,4.15,0.35,0,0  
 3V55,LYS\_593,10.5,0,0,0  
 3HVM,HIS\_46,6.82,0.6,0,-0.28  
 3GEC,TYR\_377,11.41,1.41,0,0  
 2O8I,HIS\_97,6.5,0,0,0

3BJV,ARG\_77,11.66,-0.84,0,0  
2A1V,GLU\_32,4.64,0.14,0,0  
2QOP,ARG\_140,12.43,-0.07,0,0  
3M7D,GLU\_15,3.08,0.56,-1.99,0  
2RIK,TYR\_130,12.79,0.07,0.03,2.69  
3H5T,GLU\_346,4.57,0.07,0,0  
2IIA,GLU\_41,4.5,0,0,0  
2PIM,ARG\_105,12.01,-0.49,0,0  
3CO1,ASP\_19,3.57,0.14,-0.37,0  
3G9G,TYR\_193,10.74,0,0,0.74  
2CW4,ARG\_8,12.36,-0.14,0,0  
4F8A,ARG\_662,12.29,-0.21,0,0  
2BAA,ARG\_114,12.14,-2.76,0,2.4  
3ODJ,ASP\_183,2.27,0.63,-2.17,0  
3BB7,ARG\_43,12.08,-0.42,0,0  
2YXO,CYS\_58,5.23,-5.18,-0.52,1.93  
4EVF,ASP\_129,4.08,0.28,0,0  
4DNU,HIS\_49,3.09,0.4,0,-3.81  
3C38,TYR\_234,11.17,0.07,-0.31,1.41  
2P4D,HIS\_109,3.08,0.71,0,-4.13  
3EAZ,HIS\_155,7.23,0.8,0,-0.07  
1TJE,ASP\_22,2.13,0.28,-1.95,0  
1RWZ,ASP\_85,2.98,0.35,-1.17,0  
1QSZ,ARG\_550,11.52,-0.98,0,0  
3HZQ,LYS\_85,10.29,-0.21,0,0  
1RWZ,HIS\_175,7.28,0.92,0,-0.14  
2OJQ,ARG\_456,12.43,-0.07,0,0  
3OA7,GLU\_468,3.36,0.14,-1.28,0  
1P4X,LYS\_72,10.5,0,0,0  
3JZ9,ASP\_387,3.08,0.14,-0.86,0  
3GMS,ASP\_193,2.62,1.19,-2.37,0  
1WNH,GLU\_59,4.57,0.07,0,0  
1J74,LYS\_72,10.5,0,0,0  
2Q13,LYS\_351,10.36,-0.14,0,0  
3GOZ,LYS\_274,10.5,0,0,0  
1L2H,LYS\_74,10.5,0,0,0  
3ASA,TYR\_350,10.34,0.22,0,0.12  
2XWS,LYS\_26,10.29,-0.21,0,0  
3UPD,LYS\_19,10.5,0,0,0  
1HF8,CYS\_48,8.8,-0.2,0,0  
1GQE,LYS\_314,10.43,-0.07,0,0  
1RL0,LYS\_156,9.94,-0.56,0,0  
1N81,ARG\_36,12.5,0,0,0  
2HZZ,CYS\_160,11.32,-0.12,0,2.44  
4ETX,GLU\_238,4.5,0,0,0  
4GCO,CYS\_220,8.01,-1.39,0,0.39  
2D59,ASP\_14,2.02,0.28,-2.06,0  
1NAF,GLU\_257,4.04,0.28,-0.74,0  
2D7U,ARG\_335,13.41,-0.81,0,1.72  
3F5D,LYS\_129,10.5,0,0,0  
3RNV,LYS\_453,9.8,-0.7,0,0  
2I88,LYS\_403,10.5,0,0,0  
1GXN,ARG\_567,12.01,-0.49,0,0  
1W7B,TYR\_238,9.27,0.07,-0.8,0  
1DOV,GLU\_82,4.61,0.21,-0.1,0  
3GFP,ARG\_369,11.94,-0.56,0,0  
1NFN,GLU\_70,2.45,0.35,-2.4,0  
2Q98,LYS\_190,10.22,-0.28,0,0  
3FHF,TYR\_86,10.26,0,0,0.26  
2CBE,LYS\_149,10.01,-0.49,0,0  
3GVO,ASP\_235,3.09,0.21,-0.92,0  
4F8A,ARG\_704,12.43,-0.07,0,0  
3NR5,ASP\_133,1.52,0.7,-2.98,0  
1SJ8,GLU\_748,4.64,0.28,-0.14,0  
1LTU,ASP\_235,4.08,0.28,0,0  
2Z61,ARG\_230,11.93,-0.57,0,0  
2Q07,ASP\_362,3.84,0.14,-0.1,0  
2E3S,GLU\_431,0.83,1.03,-4.71,0  
4AE7,LYS\_99,10.36,-0.14,0,0  
2EHG,LYS\_13,10.43,-0.07,0,0  
1ZBM,GLU\_186,4.24,0.28,-0.54,0  
2B0J,CYS\_250,8.24,0,-1.8,1.04  
2RH3,LYS\_137,9.94,-0.56,0,0  
4EKU,GLU\_19,4.57,0.07,0,0  
3T58,GLU\_242,4.57,0.07,0,0  
4F85,GLU\_279,4.64,0.14,0,0  
3HNX,GLU\_72,4.5,0,0,0  
2EJB,ASP\_28,4.01,0.21,0,0  
3PBH,ARG\_21,11.97,-3.83,0.3,29  
4FZN,ARG\_69,11.8,-0.7,0,0  
2FBQ,ARG\_160,11.1,-1.4,0,0  
1RI6,LYS\_316,10.22,-0.28,0,0  
3C5V,ARG\_288,12.69,-1.5,0,1.69  
2OJQ,GLU\_561,4.5,0,0,0  
2O8I,ARG\_61,12.15,-0.35,0,0  
3GA2,HIS\_131,1.13,0,-1.44,-3.93  
2PLQ,HIS\_232,7.15,1,1.8,-2.15  
1DVO,GLU\_106,4.57,0.07,0,0  
2H85,LYS\_181,9.59,-0.91,0,0  
3QKY,ARG\_180,12.43,-0.07,0,0  
3G59,GLU\_262,4.25,0.21,0,-0.46  
1JB3,ARG\_10,11.26,-1.24,0,0  
2V5B,GLU\_133,3.15,0.56,-1.92,0  
2HRZ,CYS\_296,8.19,-0.92,0,0.11  
2IDC,HIS\_36,6.43,0,0,-0.07  
2EFK,ASP\_23,3.75,0.35,-0.4,0  
2QK1,TYR\_446,10.07,0.07,0,0  
1R53,ASP\_236,4.01,0.21,0,0  
3M7G,ASP\_119,3.94,0.14,0,0  
3LJC,ARG\_99,12.36,-0.14,0,0  
2BV9,ASP\_113,3.74,0.28,-0.34,0  
4FCU,ARG\_158,11.87,-0.63,0,0  
2R05,LYS\_128,11.11,-0.77,0,1.38  
2GZR,TYR\_208,10.54,1.7,-1.46,0.3  
3IVF,GLU\_63,4.71,0.21,0,0  
2XHC,GLU\_23,4.85,0.35,0,0  
2I6I,TYR\_137,10.42,0,0,0.42  
3A0X,GLU\_668,4.99,0.49,0,0  
1IDK,TYR\_229,12.04,0.46,0,1.58  
2H30,LYS\_148,10.29,-0.21,0,0  
3ELI,GLU\_146,4.5,0,0,0  
2X5Y,LYS\_774,10.15,-0.35,0,0  
1V8E,ARG\_29,12.43,-0.07,0,0  
2B0J,LYS\_273,10.5,0,0,0  
3EZ7,ARG\_145,10.97,-1.54,0,0.01  
1C44,LYS\_29,10.29,-0.21,0,0  
1HUFLYS\_26,10.22,-0.28,0,0  
2IF4,GLU\_96,4.64,0.14,0,0  
2OGQ,HIS\_524,2.48,0.71,-0.87,-3.86  
1D2K,TYR\_344,11.21,0.21,0,1  
2A4D,GLU\_115,4.94,0.21,0.23,0  
3LD1,LYS\_293,10.5,0,0,0  
2IXM,ARG\_41,12.08,-0.42,0,0  
1QQE,LYS\_14,10.15,-0.35,0,0  
1DCF,GLU\_50,4.64,0.14,0,0  
2JEO,ARG\_122,11.87,-0.63,0,0  
3IL3,HIS\_15,6.48,0.12,0,-0.14  
2ILR,CYS\_319,9.43,0,0,0.43  
2RJD,LYS\_310,10.5,0,0,0  
3LMO,ASP\_85,3.28,0.35,-0.87,0  
3G9G,GLU\_171,4.5,0,0,0  
2O8I,TYR\_107,10.63,0.82,-0.4,0.21  
2RIK,ARG\_143,11.8,-0.7,0,0  
2FG1,GLU\_59,4.5,0,0,0  
1FKM,ASP\_462,2.36,0.42,-1.85,0  
3QKY,TYR\_177,10,0,0,0  
1I60,LYS\_2,10.29,-0.21,0,0  
2FM9,LYS\_157,10.5,0,0,0  
3C5V,LYS\_203,10.43,-0.07,0,0  
1K95,LYS\_169,10.43,-0.07,0,0  
1QV1,LYS\_141,10.29,-0.21,0,0  
3L7N,LYS\_38,10.5,0,0,0  
2DFL,ASP\_170,3.36,0.14,-0.58,0  
1IDK,ASP\_309,4.16,0.42,-0.06,0  
1S7K,TYR\_121,13.31,1.15,-0.94,3.1  
2BLL,GLU\_640,4.05,0.35,-0.8,0  
3I47,ARG\_131,12.01,-0.49,0,0  
3BPV,GLU\_25,4.32,0.42,-0.6,0  
3VJ8,CYS\_289,11.61,-0.31,0,2.92  
2YLF,CYS\_65,12.26,0,0.73,2.53  
3L3P,ARG\_471,12.15,-0.35,0,0  
3V46,GLU\_360,0.91,0.84,-2.08,-2.35  
2RIK,TYR\_166,12.45,0.79,0,1.66  
3U56,CYS\_97,10.46,0,0,1.46  
2ZCO,GLU\_198,4.05,0.35,-0.8,0  
3LE4,LYS\_342,10.5,0,0,0  
1NIJ,GLU\_39,4.5,0,0,0  
2IDC,LYS\_10,10.5,0,0,0  
1YLN,ASP\_157,3.15,0.21,-0.86,0  
1X9G,LYS\_170,9.8,-0.7,0,0  
3UV1,GLU\_71,4.5,0,0,0  
3O16,LYS\_61,10.22,-0.28,0,0  
2PGE,ASP\_115,2.36,0.7,-2.14,0  
1MML,ARG\_121,11.73,-0.77,0,0  
3F5D,ASP\_12,2.98,0.42,-1.24,0  
2OOK,GLU\_357,4.64,0.14,0,0  
3EJG,LYS\_94,10.43,-0.07,0,0  
2Q07,TYR\_447,10.23,0.45,-0.77,0.55  
3BPP,ASP\_168,3.46,0.42,-0.76,0  
3C38,ASP\_121,1.48,0.35,-2.67,0  
4HDE,ASP\_104,3.83,0.07,-0.04,0  
3FHF,LYS\_88,10.5,0,0,0  
1RKA,HIS\_213,4.52,1.49,0,-3.47  
3RJX,LYS\_176,10.29,-0.21,0,0  
4DNU,LYS\_329,10.43,-0.07,0,0  
3TIR,HIS\_51,5.86,0,0.87,-1.51  
3JZN,ASP\_144,3.94,0.14,0,0  
3V55,ARG\_551,12.15,-0.35,0,0  
3K9I,ASP\_156,3.16,0.28,-0.92,0  
3BCY,HIS\_130,6.29,0,0,-0.21  
2YWX,LYS\_144,10.5,0,0,0  
1QQL,LYS\_32,10.46,-0.56,0,0.52  
3OBS,ASP\_40,3.34,0.42,-0.87,0  
2JEO,TYR\_144,10,0,0,0  
3CRM,HIS\_240,6.36,0,0,-0.14  
2CXA,CYS\_200,8.46,-0.54,0,0  
1YTQ,LYS\_171,10.5,0,0,0  
3V3T,ARG\_306,12.43,-0.07,0,0  
2Z84,CYS\_119,8.86,-0.42,0,0.27  
4FCU,ARG\_84,11.87,-0.63,0,0  
2FG2,ASP\_72,3.22,0.42,-1,0  
1H4U,ARG\_620,12.29,-0.21,0,0  
1RWZ,LYS\_100,10.29,-0.21,0,0  
3CBN,ARG\_41,12.29,-0.21,0,0  
2Q98,GLU\_70,4.5,0,0,0  
2G5X,TYR\_69,12.03,1.04,-0.8,1.79  
1MML,ARG\_116,12.5,0,0,0  
3DTE,LYS\_15,10.36,-0.14,0,0  
1NAR,GLU\_32,0.49,0.64,-1.6,-3.06  
3LD1,GLU\_57,4.37,0.49,-0.62,0  
3M16,GLU\_260,4.71,0.21,0,0  
3G59,TYR\_222,10.69,0,0,0.69  
1SUU,TYR\_740,10,0,0,0  
3IL3,ASP\_289,2.75,0.98,-2.03,0  
2Q12,LYS\_70,10.5,0,0,0  
1R3F,HIS\_218,6.5,0,0,0  
1ZCE,HIS\_72,7.82,1.53,0,-0.21  
3RLE,GLU\_119,4.5,0,0,0  
2QK1,GLU\_543,4.07,0.07,-0.5,0  
2IF4,ARG\_288,12.36,-0.14,0,0  
2JEO,GLU\_53,4.05,0.14,-0.59,0  
1G5Z,LYS\_165,10.08,-0.42,0,0  
2B61,ARG\_352,11.66,-0.84,0,0  
4FZR,ASP\_110,4.07,0.35,-0.08,0  
1RKA,ARG\_288,12.08,-0.42,0,0  
2CL3,ARG\_63,9.66,-1.2,0,-1.64  
3IPZ,CYS\_151,9,0,0,0  
1L2F,ASP\_184,2.63,0.42,-1.59,0  
1SIG,TYR\_421,12.39,0.28,-0.31,2.42  
3L3P,TYR\_402,12.1,0.88,0,1.22  
3CXS,LYS\_55,10.29,-0.21,0,0  
3M66,ASP\_378,2.4,0.56,-1.96,0  
3EVZ,GLU\_146,4.5,0,0,0  
4E9E,GLU\_198,3.41,0.35,-1.44,0  
3BQE,ARG\_311,11.87,-0.63,0,0  
2FXT,LYS\_379,10.5,0,0,0  
3IUS,LYS\_96,9.94,-0.56,0,0  
2V4U,TYR\_336,10.26,0.26,0,0  
3T58,LYS\_320,12.01,-0.49,0,0  
3CJW,GLU\_210,4.76,0.77,-0.51,0  
1TLV,HIS\_269,5,0.81,0,-2.31  
1T3Y,LYS\_93,10.29,-0.21,0,0  
2O8P,CYS\_112,9.06,-0.81,0,0.87  
4H4J,ARG\_256,12.22,-2.24,0,1.96  
1T6L,HIS\_185,6.29,0,0,-0.21  
3IPZ,LYS\_94,10.43,-0.07,0,0  
4E8B,GLU\_53,3.98,0.28,-0.8,0  
1O5T,ARG\_464,10.92,-1.58,0,0  
2RH3,GLU\_124,4.05,0.35,-0.8,0  
1RSS,LYS\_60,10.5,0,0,0  
350A,GLU\_5,3.24,0.35,-1.61,0  
3MIX,GLU\_323,4.02,0.49,-0.97,0  
2EDM,GLU\_176,3.22,0.49,-1.77,0  
3A7L,ASP\_108,2.55,0.49,-1.74,0  
1RWZ,ARG\_241,11.8,-0.7,0,0  
2EEY,GLU\_91,4.64,0.14,0,0  
3BJV,GLU\_72,3.92,0.49,-1.07,0  
1GXN,TYR\_360,9.97,0.07,-0.1,0  
2BV9,TYR\_98,14,0.52,0.8,2.68  
1FKM,LYS\_313,10.29,-0.21,0,0  
1OLR,LYS\_62,9.45,-1.05,0,0  
2Q12,CYS\_99,8.73,-0.27,0,0  
3G9G,GLU\_107,4.71,0.21,0,0  
1ANU,ASP\_65,4.0,0.21,0,0  
1MD6,CYS\_66,10.07,0,0,1.07  
3GMS,HIS\_284,5.11,0,0,-1.39  
2WZ9,GLU\_55,3.84,0.14,-0.8,0  
1Q5Z,ARG\_627,12.01,-0.49,0,0  
2FZP,TYR\_271,9.76,0,-0.67,0.43  
4DND,ASP\_60,3.82,0.07,-0.05,0  
1BKR,GLU\_92,3.98,0.28,-0.8,0  
2FBQ,GLU\_8,3.98,0.28,-0.8,0  
2RFA,LYS\_229,10.08,-0.42,0,0  
1GQE,ARG\_212,12.36,-0.14,0,0  
4DNU,HIS\_67,7.33,0.9,0,-0.07  
3RNL,ASP\_652,3.22,0.28,-0.86,0  
3FHF,ARG\_57,12.08,-0.42,0,0  
3CCY,ASP\_192,3.28,0.28,-0.8,0  
3I4T,TYR\_10,10.82,0,-0.87,1.69  
3EJG,GLU\_80,4.5,0,0,0  
1E5S,ARG\_248,10.42,-2.08,0,0  
1KBK,TYR\_99,10,0,0,0  
3ON1,LYS\_28,10.5,0,0,0  
2O8P,LYS\_190,10.5,0,0,0  
3EJG,LYS\_56,10.22,-0.28,0,0  
4E5S,ARG\_56,12.43,-0.07,0,0



3GW3,GLU\_13,4.5,0,0,0  
1YW5,LYS\_141,10.29,-0.21,0,0  
2G9D,CYS\_156,10.08,-1.64,0.72,1.99  
1Q2Y,HIS\_77,6.36,0,0,-0.14  
3V55,CYS\_591,9.07,0,0,0.07  
3MIX,ASP\_327,3.91,0.14,-0.03,0  
3L7N,ASP\_135,3.35,0.21,-0.65,0  
2QV2,TYR\_246,10.24,0,-0.58,0.82  
2RGY,ARG\_190,12.43,-0.07,0,0  
2H2W,GLU\_236,3.56,4.17,-2.71,-2.4  
3K8J,LYS\_192,9.94,-0.56,0,0  
4E9E,ARG\_442,11.52,-0.98,0,0  
2OGQ,GLU\_455,3.91,0.14,-0.73,0  
2CXC,LYS\_123,10.43,-0.07,0,0  
3FK5,CYS\_114,9.4,0,0,0.4  
1X04,ASP\_41,3.42,0.42,-0.8,0  
3VJ8,CYS\_43,12.25,-0.12,1.93,1.43  
1DTP,ASP\_174,3.42,0.42,-0.8,0  
2RJD,GLU\_425,4.5,0,0,0  
2E3S,LYS\_425,10.5,0,0,0  
3R87,TYR\_30,13.73,0.53,0.8,2.4  
2FZ4,LYS\_109,10.43,-0.07,0,0  
1O59,TYR\_200,13.09,0.28,0.53,2.28  
2G3A,GLU\_31,4.57,0,0,0.07,0  
3T5B,TYR\_107,11.48,0,0,1.48  
3IL3,LYS\_255,10.5,0,0,0  
3M70,HIS\_59,6.45,0.16,0,-0.21  
2QEV,LYS\_116,9.87,-0.63,0,0  
3LJC,ASP\_67,3.13,0.21,-0.88,0  
1ANU,GLU\_45,3.81,0.07,-0.76,0  
3T5B,ARG\_344,11.87,-0.63,0,0  
1C44,LYS\_18,10.43,-0.07,0,0  
1SIG,ASP\_313,3.19,0.28,-0.89,0  
3GS3,ASP\_32,3.84,0.07,-0.03,0  
4FH3,GLU\_123,4.5,0,0,0  
1TWU,TYR\_103,10.55,0.14,-0.8,1.21  
2CYG,GLU\_303,4.5,0,0,0  
2EJB,GLU\_132,4.5,0,0,0  
1FKM,ASP\_415,3.61,0,-0.19,0  
1TD6,HIS\_280,0.72,0,-2.21,-3.57  
1X91,ARG\_117,12.5,0,0,0  
3H5T,HIS\_266,6.78,0.56,0,-0.28  
1MIX,GLU\_386,4.5,0,0,0  
1UAJ,TYR\_136,10.07,0.07,0,0  
2OGQ,GLU\_488,4.3,0.56,-0.76,0  
1YB2,LYS\_129,10.29,-0.21,0,0  
3H13,ASP\_304,4.02,0.28,-0.06,0  
4FD6,LYS\_61,10.29,-0.21,0,0  
1U53,ARG\_75,13.4,-1.38,0.2,2.28  
4EVF,TYR\_269,10.78,0.78,0,0  
1O59,GLU\_80,4.71,0.21,0,0  
3OOP,GLU\_81,4.57,0.07,0,0  
3BJV,TYR\_43,10.6,2.03,-1.43,0  
1MHN,LYS\_97,10.5,0,0,0  
1F2V,ARG\_101,12.43,-0.07,0,0  
4F8A,GLU\_596,4.71,0.21,0,0  
3N2T,ARG\_260,11.73,-0.77,0,0  
2Z61,TYR\_354,9.8,0,-0.2,0  
2IQT,HIS\_253,7.16,0.8,0,-0.14  
2OSA,GLU\_377,4.36,0.14,-0.28,0  
1TUL,GLU\_92,4.57,0.07,0,0  
2P1W,LYS\_208,10.29,-0.21,0,0  
3L7N,ASP\_136,3.35,0.35,-0.8,0  
2D7U,TYR\_192,10,0,0,0  
3J5N,HIS\_12,4.97,0.1,2.3,-2.77  
1G8P,ARG\_18,12.5,0,0,0  
2H2W,ASP\_249,3.9,0.07,-0.14,0.17  
1Q46,ARG\_74,12.08,-0.42,0,0  
1PV5,GLU\_244,4.11,0.28,-0.67,0  
2B61,ASP\_37,3.7,0,-0.1,0  
3OBS,TYR\_17,10,0,0,0  
3P2F,ARG\_135,11.87,-0.63,0,0  
2IRM,TYR\_233,12.17,1.7,-0.8,1.27  
2B61,ARG\_212,11.98,-2.3,0,1.78  
4EUG,LYS\_184,10.5,0,0,0  
3M3P,HIS\_247,7.2,0.77,0,-0.07  
4ESS,ARG\_157,12.29,-0.21,0,0  
3MEW,ASP\_194,4.01,0.21,0,0  
3J5N,ARG\_61,9.05,-3.45,0,0  
1N81,GLU\_113,4.57,0.07,0,0  
2OEW,ASP\_292,3.87,0.07,0,0  
1SJ8,ASP\_564,3.63,0.28,-0.44,0  
3C6B,GLU\_267,4.21,0.35,-0.64,0  
1ZCE,ASP\_80,2.98,0.42,-1.23,0  
1RKA,LYS\_91,10.5,0,0,0  
4H89,GLU\_4,3.96,0.42,-0.96,0  
2Q12,ARG\_154,12.5,0,0,0  
1QQE,TYR\_174,10.14,0.14,0,0  
3GS3,HIS\_234,7.34,0.84,0,0  
1TJE,HIS\_125,7.16,1.06,1.7,-2.1  
2QHT,TYR\_127,10.05,0.07,-0.02,0  
3TMO,TYR\_301,10.14,0.14,0,0  
2G2D,ASP\_38,3.08,0.35,-1.08,0  
1LPL,ASP\_204,3.77,0,-0.03,0  
1SJV,GLU\_101,4.29,0.21,-0.42,0  
2APL,GLU\_40,4.51,0.28,-0.27,0  
1K95,TYR\_153,10.75,0.99,-0.24,0  
3IVF,HIS\_283,2.64,0.05,0,-3.91  
2R0S,TYR\_251,11.18,1.99,-0.68,-0.13  
1WPA,TYR\_481,13.07,0.07,0.6,2.4  
3BQE,ASP\_339,3.35,0.35,-0.8,0  
1E5S,LYS\_166,10.5,0,0,0  
1WRU,ASP\_78,3.8,0,0,0  
3OOP,ARG\_99,11.94,-0.56,0,0  
2WB3,ARG\_242,12.5,0,0,0  
1TP6,ARG\_35,13.53,-1.37,0.2,4  
3IAT,LYS\_148,10.5,0,0,0  
2IDC,GLU\_116,3.95,0.21,-0.76,0  
1JT9,TYR\_184,10,0,0,0  
2JHY,GLU\_154,4.5,0,0,0  
3HZQ,ASP\_51,4.22,0.42,0,0  
3JV1,ASP\_98,3.75,0.07,-0.12,0  
3PU6,LYS\_2,9.94,-0.56,0,0  
3H5T,GLU\_261,4.71,0.21,0,0  
3BQE,ASP\_240,2.2,0.21,-1.81,0  
4F85,TYR\_77,10.08,0,-0.15,0.23  
2RIK,GLU\_169,4.47,0,-0.03,0  
2E3C,ARG\_239,12.01,-0.49,0,0  
1HF8,LYS\_40,10.36,-0.14,0,0  
3FHF,HIS\_-3,6.5,0,0,0  
2G9D,ASP\_118,3.3,0.21,-0.71,0  
2NPK,ASP\_154,3.36,0.28,-0.72,0  
1GXN,TYR\_648,12.4,0.21,0.2,1.9  
2VGM,LYS\_221,10.43,-0.07,0,0  
2RFA,LYS\_63,10.22,-0.28,0,0  
3C6B,ASP\_103,2.55,0.42,-1.66,0  
2EEY,GLU\_9,4.5,0,0,0  
1M5I,GLU\_192,3.87,0.35,-0.99,0  
1XKR,GLU\_151,4.57,0.07,0,0  
1WXF,GLU\_252,4.12,0.42,-0.8,0  
1RHS,GLU\_169,4.32,0.07,-0.25,0  
2R51,GLU\_69,4.32,0.49,-0.67,0  
1TD6,TYR\_256,11.26,0,-0.76,2.03  
1X7F,ARG\_262,12.01,-0.49,0,0  
2Q12,GLU\_239,4.57,0.07,0,0  
3M9A,ARG\_17,12.43,-0.07,0,0  
1Y0K,ASP\_49,3.09,0.56,-1.27,0  
3PU6,ASP\_130,3.2,0.35,-0.95,0  
3M7G,GLU\_240,4.71,0.21,0,0  
2OEW,LYS\_101,10.43,-0.07,0,0  
1DTP,LYS\_177,10.5,0,0,0  
1N81,TYR\_108,11.36,2.33,-0.48,-0.5  
2RJD,CYS\_363,9.68,-1.44,1.1,1.02  
3BA1,LYS\_306,10.5,0,0,0  
2IQT,ASP\_286,3.83,0.14,-0.11,0  
1T95,ARG\_183,11.87,-0.63,0,0  
1AD6,GLU\_554,4.69,0.28,-0.09,0  
3ERF,LYS\_40,9.38,-1.12,0,0  
4FZP,ASP\_258,3.36,0.07,-0.51,0  
3ADO,TYR\_35,9.82,0,-0.18,0  
4AM1,CYS\_271,8.91,-4.32,1.3,2.93  
3UAH,TYR\_220,9.39,0.09,-0.07,-0.63  
2Q13,TYR\_68,10.54,0,0,0.54  
1FQI,GLU\_419,4.5,0,0,0  
2IXM,HIS\_127,6.36,0,0,-0.14  
3PZ9,ASP\_64,3.83,0.14,-0.11,0  
2ZQ5,LYS\_80,10.29,-0.21,0,0  
1JSX,ARG\_52,12.15,-0.35,0,0  
2QVO,GLU\_61,4.56,0.07,-0.01,0  
3EX9,ARG\_65,12.22,-0.28,0,0  
3CIV,GLU\_118,4.78,0.28,0,0  
2B0J,GLU\_221,4.5,0,0,0  
3EVZ,LYS\_220,10.5,0,0,0  
3V46,LYS\_263,10.22,-0.28,0,0  
2X5Y,HIS\_737,6.36,0,0,-0.14  
1JKS,HIS\_166,1.81,0.26,-2.24,-2.71  
1DZF,GLU\_21,4.25,1.35,-1.6,0  
1ZCE,GLU\_66,3.82,0.35,-1.03,0  
1BKR,HIS\_60,6.43,0,0,-0.07  
2XWS,TYR\_115,10,0,0,0  
2GS5,GLU\_124,4.78,0.28,0,0  
2QK1,HIS\_378,6.54,0.04,0,0  
1ZP2,GLU\_91,4.5,0,0,0  
2X4L,LYS\_157,10.29,-0.21,0,0  
3K9I,TYR\_124,10,0,0,0  
3VJ8,TYR\_46,13.41,0.21,0.8,2.4  
3ERF,HIS\_164,7.21,0.78,0,-0.07  
2RJD,LYS\_235,10.36,-0.14,0,0  
3GMS,TYR\_276,12.16,0,0.2,16  
3KB5,GLU\_344,4.52,0.14,-0.12,0  
2QK1,GLU\_464,4.57,0.07,0,0  
2WB8,LYS\_768,10.15,-0.35,0,0  
2R0S,ASP\_37,3.42,0.42,-0.8,0  
1KN3,LYS\_148,10.5,0,0,0  
1I60,HIS\_200,12.91,4.8,8.13,-6.52  
1RZ2,ASP\_103,4.0,0.21,-0.01,0  
2R4Q,GLU\_263,3.91,0.21,-0.8,0  
1MML,HIS\_126,6.5,0,0,0  
3IU5,ARG\_79,12.15,-0.35,0,0  
2B78,HIS\_254,2.83,1.44,0,-5.11  
1MIX,ARG\_303,12.08,-0.42,0,0  
1X04,ASP\_31,3.58,0.07,-0.29,0  
2VAN,ARG\_213,12.08,-0.42,0,0  
2FG1,ARG\_101,11.8,-0.7,0,0  
2P1W,ARG\_91,12.95,-1.55,0,2  
3ADO,LYS\_130,10.5,0,0,0  
3R1X,TYR\_64,12.17,0.14,-0.19,2.22  
1DZF,ASP\_41,3.95,0.21,-0.06,0  
1LPL,ASP\_192,1.38,0.49,-2.91,0  
3CX2,LYS\_190,10.5,0,0,0  
2R57,GLU\_299,4.5,0,0,0  
3DTE,TYR\_246,10.53,0,0.53  
2BDV,ARG\_23,12.43,-0.07,0,0  
3HUE,LYS\_76,10.5,0,0,0  
1X8F,LYS\_268,10.36,-0.14,0,0  
1T07,ARG\_54,12.22,-0.28,0,0  
1J74,LYS\_8,10.5,0,0,0  
1RHS,GLU\_227,3.18,0.35,-1.67,0  
2RJD,TYR\_386,11.29,0,0,1.29  
2P4D,GLU\_154,1.41,0.7,-3.78,0  
1BYI,HIS\_154,6.5,0,0,0  
2RIS,ARG\_66,10.6,-1.9,0,0  
1GXN,TYR\_412,13.34,0.14,0.8,2.4  
3M7G,GLU\_256,4.83,0.42,-0.09,0  
3BA1,LYS\_178,10.36,-0.14,0,0  
2NSN,ASP\_99,3.8,0.07,-0.07,0  
1RLO,TYR\_89,9.94,0.45,0,-0.51  
1YW5,ASP\_90,3.93,0.14,-0.01,0  
2CXA,CYS\_174,10.41,0,0,1.41  
3BPP,ASP\_188,2.99,0.49,-1.3,0  
3T5B,GLU\_152,4.78,0.28,0,0  
3PZ9,ASP\_341,3.89,0.21,-0.12,0  
1EDG,LYS\_127,10.29,-0.21,0,0  
1NJ4,LYS\_273,10.5,0,0,0  
3LJN,GLU\_121,4.5,0,0,0  
3EJG,ARG\_93,11.94,-0.56,0,0  
3M7G,GLU\_51,3.65,0.42,-1.27,0  
3DZ1,LYS\_73,10.5,0,0,0  
2AHE,TYR\_154,10.26,0.21,-0.8,0.85  
1PVT,GLU\_230,1.93,0.71,-1.9,-1.37  
3U4K,TYR\_152,10.37,0.41,-0.04,0  
2W0G,ARG\_264,11.87,-0.63,0,0  
2QDJ,ARG\_71,11.73,-0.77,0,0  
1WP5,GLU\_266,3.17,0.56,-1.88,0  
2QVT,ARG\_43,11.49,-1.01,0,0  
2D0A,LYS\_230,10.5,0,0,0  
1J33,LYS\_41,10.29,-0.21,0,0  
1T3Y,ARG\_117,11.8,-0.7,0,0  
2X4L,GLU\_136,2.49,0.77,-2.79,0  
3B4D,TYR\_181,10.14,0.14,0,0  
3CE7,GLU\_88,2.87,0.63,-2.26,0  
3DHN,GLU\_46,4.64,0.14,0,0  
2OKT,LYS\_314,10.5,0,0,0  
1J7G,ASP\_127,3.31,0.21,-0.7,0  
2EDM,GLU\_112,3.73,0.7,-1.47,0  
3K8J,ARG\_222,12.43,-0.07,0,0  
3PAC,LYS\_25,10.29,-0.21,0,0  
2V8C,ASP\_58,3.45,0.42,-0.77,0  
2D7U,ARG\_227,10.49,-2.01,0,0  
2E3C,ARG\_298,13.63,-2.53,0.3,66  
1T3J,LYS\_707,10.5,0,0,0  
1MJS,GLU\_238,1.99,1.34,-2.06,-1.79  
2R0S,LYS\_72,10.43,-0.07,0,0  
1DZF,CYS\_47,9,0,0,0  
1I60,LYS\_266,10.29,-0.21,0,0  
2FM9,HIS\_226,6.72,0.29,0,-0.07  
3B79,TYR\_118,10.07,0.07,0,0  
2WB8,HIS\_477,6.43,0,0,-0.07  
3HUE,LYS\_172,10.29,-0.21,0,0  
3M3P,ARG\_155,12.01,-0.49,0,0  
3ZSL,CYS\_173,10,-0.66,0,1.66  
1X04,ASP\_128,3.42,0.28,-0.66,0  
2POL,GLU\_76,4.64,0.14,0,0  
4H4J,LYS\_247,10.29,-0.21,0,0  
2E3S,GLU\_498,4.56,0.28,-0.22,0  
3ASA,ASP\_183,2.6,0.28,-1.48,0  
3N0K,TYR\_8,9.91,0.14,-0.23,0  
3U0V,ARG\_64,11.8,-0.7,0,0  
4EZB,GLU\_146,2.52,0.42,-2.4,0  
1QZN,LYS\_86,10.29,-0.21,0,0  
1RZ2,LYS\_44,10.5,0,0,0  
3GE9,GLU\_180,4.06,0.7,-1.15,0  
3CN5,HIS\_62,6.43,0,0,-0.07  
3R2E,ARG\_74,11.8,-0.7,0,0  
2X4G,GLU\_97,4.5,0,0,0  
2OBI,LYS\_48,10.43,-0.07,0,0

30KQ,ASP\_590,3.37,0.28,-0.7,0  
4E9E,ARG\_492,12.15,-0.35,0,0  
3BQW,LYS\_265,10.43,-0.07,0,0  
2D7J,TYR\_68,10.88,1.1,-0.22,0  
2FL7,LYS\_99,10.5,0,0,0  
3T8R,GLU\_34,4.57,0.07,0,0  
4FD6,LYS\_107,10.5,0,0,0  
2X4L,ARG\_320,11.17,-3.82,0.2,49  
3CJW,GLU\_251,3.59,2.08,-0.76,-2.23  
1L3K,GLU\_126,4.92,0.42,0,0  
2ZTY,HIS\_177,6.46,0.03,0,-0.07  
3U2A,ARG\_69,11.31,-1.19,0,0  
3T57,LYS\_70,10.29,-0.21,0,0  
2IN0,ARG\_82,12.08,-0.42,0,0  
3RRQ,ASP\_105,2.69,0.49,-1.6,0  
4FZR,CYS\_175,10.55,-0.47,1.16,0.86  
1Z3X,GLU\_-1,4.41,0.56,-0.65,0  
3KB5,ARG\_401,12.29,-0.21,0,0  
1PV5,GLU\_177,4.5,0,0,0  
2X4G,HIS\_67,6.5,0,0,0  
2IRM,GLU\_42,4.64,0.14,0,0  
2FBQ,ASP\_107,0.55,1.05,-4.3,0  
3L3P,LYS\_266,10.43,-0.07,0,0  
2NRR,HIS\_472,6.43,0,0,-0.07  
3L3P,HIS\_355,6.5,0,0,0  
2HNG,ARG\_109,12.29,-0.21,0,0  
4DND,ASP\_44,3.72,0,-0.08,0  
3PBH,HIS\_28,7.42,1.06,0,-0.14  
2R57,CYS\_223,9.38,-0.47,0,0.85  
3H9W,GLU\_58,4.5,0,0,0  
1BKB,LYS\_42,10.5,0,0,0  
2RIS,LYS\_187,10.43,-0.07,0,0  
2IDC,GLU\_120,3.16,0.42,-1.76,0  
3BWT,LYS\_591,10.5,0,0,0  
2X4J,GLU\_112,3.85,0.35,-1,0  
1DVO,ASP\_145,2.48,1.12,-2.44,0  
1U53,LYS\_101,10.29,-0.21,0,0  
3A0X,TYR\_680,10,0,0,0  
2ILR,LYS\_499,10.29,-0.21,0,0  
3B7X,ASP\_41,3.78,0.21,-0.22,0  
1ZBP,CYS\_242,8.94,-0.06,0,0  
3GEC,GLU\_506,4.56,0.14,-0.08,0  
3KEY,LYS\_417,10.43,-0.07,0,0  
1NAR,ARG\_271,12.43,-0.07,0,0  
1WLY,ARG\_48,10.96,-1.54,0,0  
1ZKZ,GLU\_36,4.54,0.28,-0.24,0  
1SFE,ASP\_43,2.8,0.56,-1.56,0  
4H4J,GLU\_138,5.7,1.2,0,0  
3GOZ,ASP\_250,3.46,0.28,-0.62,0  
1YW5,HIS\_130,7.06,1.05,0,-0.49  
3CCY,ARG\_136,11.94,-0.56,0,0  
2DFL,LYS\_87,10.08,-0.42,0,0  
2CII,TYR\_204,10.89,0,-0.57,1.46  
3O16,ARG\_19,11.8,-0.7,0,0  
2FD5,ASP\_3,2.18,0.77,-2.39,0  
1YTQ,ASP\_172,2.2,0.35,-1.95,0  
2AZL,LYS\_214,10.5,0,0,0  
3FWU,ASP\_44,2.92,0.49,-1.38,0  
3GS3,HIS\_76,6.5,0,0,0  
3EVP,LYS\_75,10.5,0,0,0  
1T95,GLU\_80,4.7,0.21,-0.01,0  
2PLQ,ARG\_2,12.01,-0.49,0,0  
2FC3,LYS\_24,10.29,-0.21,0,0  
3ADO,CYS\_78,6.63,-2.44,0,0.07  
1NIJ,ASP\_46,3.56,0.56,-0.8,0  
1T95,ASP\_30,2.41,0.63,-2.02,0  
1YM5,LYS\_124,10.5,0,0,0  
1ZP2,TYR\_63,13.41,0.21,0.8,2.4  
1R3F,GLU\_97,3.97,0.35,-0.88,0  
1GPP,GLU\_16,4.12,0.35,-0.74,0  
3PP8,HIS\_230,3.07,0.7,-0.03,-4.1  
3NR5,CYS\_116,9.86,-0.04,0,0.9  
1OI7,GLU\_281,4.56,0.07,-0.01,0  
1VJG,ARG\_137,12.01,-0.49,0,0  
3LMO,GLU\_21,3.79,0.28,-0.99,0  
3H6Q,GLU\_139,4.8,0.42,-0.12,0  
2QHT,GLU\_191,4.5,0,0,0  
2R51,TYR\_41,10.07,0.07,0,0  
1W24,GLU\_125,4.5,0,0,0  
3NOK,GLU\_106,4.5,0,0,0  
3LJN,ARG\_47,12.22,-0.28,0,0  
3JZN,TYR\_280,9.94,0.07,-0.13,0  
2ZTY,ARG\_39,12.08,-0.42,0,0  
1UJ8,ARG\_20,11.66,-0.84,0,0  
2P52,ASP\_183,1.58,0.77,-3,0  
3LH5,ASP\_780,1.3,0.7,-3.2,0  
2Q07,ASP\_375,3.08,0.42,-1.14,0  
2OKT,HIS\_338,6.43,0,0,-0.07  
3FWU,HIS\_104,6.29,0,0,-0.21  
1WXQ,TYR\_368,10,0,0,0  
2E3C,ASP\_256,3.54,0.42,-0.68,0  
3LQE,GLU\_447,3.76,0.14,-0.88,0  
1XWM,ASP\_61,3.91,0.21,-0.1,0  
3GS3,LYS\_95,10.15,-0.35,0,0  
2ATR,GLU\_137,4.5,0,0,0  
1EV8,ASP\_193,3.72,0,-0.08,0  
3BQE,HIS\_350,4.56,0.92,0.79,-3.65  
2CL3,GLU\_127,4.12,0.35,-0.73,0  
3ONH,ASP\_514,1.69,0.98,-3.09,0  
1DVO,ASP\_167,2.6,0.35,-1.55,0  
3L3P,GLU\_486,4.53,0.28,-0.25,0  
3IRA,HIS\_54,6.89,0.53,0,-0.14  
1PNE,GLU\_46,1.13,1.05,-4.42,0  
1DZF,HIS\_153,4.87,0.8,0,-2.43  
2Q12,GLU\_28,4.57,0.07,0,0  
3IV4,GLU\_46,4.5,0,0,0  
3CX5,LYS\_2,10.5,0,0,0  
1V6T,HIS\_223,10.38,1.6,5.48,-3.2  
1ZYL,ARG\_49,12.36,-0.14,0,0  
1XFK,HIS\_28,6.91,0.55,0,-0.14  
3U0V,ARG\_80,12.63,-2.52,0.2,65  
2IRM,LYS\_125,10.15,-0.35,0,0  
3VJ8,ASP\_159,3.7,0.14,-0.24,0  
2P4D,ASP\_91,3.76,0,-0.04,0  
3RRQ,GLU\_84,4.5,0,0,0  
2V5B,GLU\_168,5.98,2.9,-1.42,0  
3GT0,TYR\_49,9.56,0.14,-0.58,0  
1O5T,HIS\_445,10.16,4.24,2.76,-3.33  
1MD6,GLU\_40,4.38,0.07,-0.19,0  
1T95,ASP\_47,4.07,0.28,-0.01,0  
3C38,TYR\_262,9.53,0.68,-1.15,0  
3I47,HIS\_25,6.43,0,0,-0.07  
1X9G,LYS\_75,10.5,0,0,0  
2EJX,HIS\_99,3.88,0.66,0,-3.28  
3QAV,ASP\_136,3.65,0.42,-0.57,0  
2F8H,ARG\_25,12.14,-1.26,0,0.9  
1RL0,LYS\_211,10.43,-0.07,0,0  
1TXJ,GLU\_35,3.36,1.59,-2.73,0  
3UC9,GLU\_99,4.78,0.28,0,0  
1RKA,GLU\_200,4.18,0,-0.32,0  
1SIG,TYR\_430,10.58,0.58,0,0  
4E8B,HIS\_8,4.82,0.68,0,-2.36  
2EJB,HIS\_108,2.81,0.01,0,-3.7  
2IDC,ARG\_174,12.5,0,0,0  
3RE9,ASP\_150,2.81,0.49,-1.49,0  
1MHN,TYR\_130,10,0,0,0  
3OA7,ARG\_505,12.5,0,0,0  
1P4X,CYS\_61,9.87,-0.12,0,0.99  
4DIU,ARG\_135,12.15,-0.35,0,0  
2ZCX,LYS\_80,10.43,-0.07,0,0  
1A8Q,LYS\_209,10.29,-0.21,0,0  
1BYI,GLU\_211,4.64,0.14,0,0  
3EVN,GLU\_147,4.57,0.07,0,0  
2E3C,ASP\_334,3.35,0.35,-0.8,0  
1ZCU,HIS\_28,6.43,0.21,0,-0.28  
3IO0,LYS\_210,10.43,-0.07,0,0  
4DVD,HIS\_92,6.41,0.05,0,-0.14  
4EUG,GLU\_52,3.02,0.7,-2.18,0  
1Q8B,GLU\_94,4.57,0.07,0,0  
3RLN,LYS\_594,10.5,0,0,0  
1J33,GLU\_229,3.2,4.35,-3.26,-2.4  
1MD6,ARG\_9,12.43,-0.07,0,0  
2Q13,LYS\_160,10.5,0,0,0  
3NOK,LYS\_71,10.43,-0.07,0,0  
2I6I,ASP\_25,12.22,-0.28,0,0  
2XWS,GLU\_97,2.66,0.56,-2.4,0  
1ATO,GLU\_268,4.12,0.42,-0.8,0  
1O59,LYS\_261,10.22,-0.28,0,0  
1XWM,GLU\_202,3.94,0.63,-1.19,0  
2R51,GLU\_254,4.05,0.28,-0.73,0  
2RJD,CYS\_264,3.18,-3.6,-2.4,0.18  
2B3M,ARG\_77,12.5,0,0,0  
1QQL,TYR\_63,10.14,0.14,0,0  
2APL,HIS\_71,6.63,0.13,0,0  
1FHL,TYR\_319,10,0,0,0  
2EJB,GLU\_66,4.16,0.63,-0.97,0  
1XDZ,ARG\_147,11.24,-2.87,0,1.61  
3QYB,LYS\_958,10.36,-0.14,0,0  
2CXA,ARG\_136,12.22,-0.28,0,0  
3G6S,TYR\_196,11.11,0,0,1.11  
1X9G,HIS\_59,6.31,0.45,-0.5,-0.14  
2AXO,LYS\_66,10.29,-0.21,0,0  
3BWT,TYR\_839,9.62,0,-0.38,0  
3JRT,ASP\_5,3.76,0.14,-0.18,0  
1UW7,ASP\_50,4.01,0.21,0,0  
1SFE,TYR\_115,11.21,0.33,0,0.88  
3FFM,GLU\_110,4.92,0.42,0,0  
2EJX,ASP\_117,3.14,0.21,-0.87,0  
2W0G,LYS\_154,10.15,-0.35,0,0  
3LJN,GLU\_178,3.21,0.67,-0.49,-1.46  
2FG1,HIS\_119,2.86,0,0,-3.64  
1QVI,GLU\_211,3.51,2.49,-1.47,-2  
4H4J,ASP\_104,3.87,0.07,0,0  
3PBH,ARG\_41,12.42,-4.21,0.4,14  
1YOK,LYS\_124,10.5,0,0,0  
3VJ8,ARG\_279,11.73,-0.77,0,0  
1G8P,TYR\_234,10.62,0.42,0,0.2  
2QOP,ARG\_105,12.22,-0.28,0,0  
3M16,HIS\_54,7.23,1.01,0,-0.28  
3GFP,ASP\_310,3.21,0.21,-0.8,0  
2E3C,GLU\_238,3.94,0.56,-1.12,0  
2ZQ5,HIS\_363,6.5,0,0,0  
3M7D,ARG\_304,12.29,-0.21,0,0  
1NIJ,GLU\_239,4.64,0.14,0,0  
3O16,ARG\_225,12.15,-0.35,0,0  
4ECC,ARG\_121,12.22,-0.28,0,0  
3RJX,GLU\_212,4.08,0,-0.42,0  
3LOD,ARG\_85,11.94,-0.56,0,0  
2O4D,LYS\_61,10.43,-0.07,0,0  
2XHC,LYS\_62,10.5,0,0,0  
1G8P,GLU\_136,4.52,0.14,-0.12,0  
2EDM,LYS\_75,10.15,-0.35,0,0  
1ZKZ,ARG\_110,11.45,-1.05,0,0  
2E3I,ASP\_100,1.27,0.56,-3.09,0  
3G9T,ASP\_248,3.14,0.7,-1.36,0  
2AH5,GLU\_155,3.8,0.42,-1.12,0  
3H04,CYS\_96,9.08,-0.05,0,0.13  
2W0G,HIS\_211,4.28,0.8,0,-3.02  
1U7U,ASP\_210,4.36,0.56,0,0  
2WZ9,TYR\_80,9.79,0.1,-0.31,0  
1UOH,HIS\_78,3.01,1.24,0,-4.72  
1OTM,TYR\_96,10,0,0,0  
2X4L,GLU\_323,4.17,3.01,-1.59,-1.75  
3M3P,LYS\_97,10.15,-0.35,0,0  
3ERF,GLU\_62,4.5,0,0,0  
1RKA,HIS\_157,6.43,0,0,-0.07  
3F6F,HIS\_51,6.65,0.42,0,-0.28  
3FHF,ARG\_121,12.5,0,0,0  
1XDZ,ASP\_136,3.77,0,-0.03,0  
3OKQ,LYS\_561,10.36,-0.14,0,0  
2P65,ASP\_74,3.63,0.07,-0.24,0  
3CNU,ASP\_48,2.06,0.49,-2.23,0  
2AHE,LYS\_103,10.15,-0.35,0,0  
2G9D,LYS\_134,10.29,-0.28,0,0  
1JT9,LYS\_124,10.29,-0.21,0,0  
4FH3,GLU\_92,4.89,0.39,0,0  
3IPZ,GLU\_166,4.5,0.14,-0.14,0  
3PZ9,TYR\_318,12.92,3.4,-0.8,0.32  
1O0X,ARG\_169,12.08,-0.42,0,0  
3RRQ,ARG\_114,12.15,-0.35,0,0  
1DZF,ASP\_159,3.78,0,-0.02,0  
2RJD,ASP\_415,4.15,0.35,0,0  
2OEW,LYS\_327,10.5,0,0,0  
2V4U,ARG\_425,11.8,-0.7,0,0  
1UCH,LYS\_72,10.29,-0.21,0,0  
1A8Q,ASP\_178,3.29,0.35,-0.86,0  
2X4L,LYS\_218,10.5,0,0,0  
1LTU,HIS\_41,6.43,0,0,-0.07  
3NR5,HIS\_69,7.16,0.8,0,-0.14  
2WB8,CYS\_487,9.7,-0.53,0,1.23  
1YB2,GLU\_137,4.64,0.14,0,0  
1QQE,ASP\_139,3.87,0.14,-0.07,0  
2Z0M,LYS\_179,10.22,-0.28,0,0  
1NJ4,LYS\_219,9.87,-0.63,0,0  
3F1X,ARG\_50,12.56,-2.55,0.2,61  
3G9T,CYS\_64,7.1,-2.54,0,0.64  
1A8Q,TYR\_47,9.9,0.21,-0.3,0  
2D59,LYS\_58,10.5,0,0,0  
3M9A,GLU\_37,4.5,0,0,0  
3U2R,GLU\_96,4.5,0,0,0  
1DTO,HIS\_0,6.43,0,0,-0.07  
2G9D,ASP\_18,3.08,0.07,-0.79,0  
2RIS,ARG\_106,11.21,-1.29,0,0  
2RGY,CYS\_124,9,0,0,0  
2XHC,LYS\_111,9.94,-0.56,0,0  
2OJQ,ASP\_572,3.86,0.14,-0.08,0  
2RGY,HIS\_234,7.48,1.05,0,-0.07  
1G8P,ARG\_289,9.58,-1.09,0,-1.83  
3GMS,TYR\_200,10.63,0.0,0.63  
2RIK,LYS\_224,9.94,-0.56,0,0  
2B0J,GLU\_288,3.91,0.21,-0.8,0  
2EFK,GLU\_119,3.98,0.28,-0.8,0  
2BDV,ARG\_165,11.29,-1.23,0,0.02  
3RAZ,ARG\_136,11.87,-0.63,0,0  
3HZQ,CYS\_32,8.75,-0.25,0,0  
3GS3,CYS\_46,8.95,-0.05,0,0  
1CBY,GLU\_192,2.11,1.05,-1.04,-2.4  
2CYG,ASP\_230,2.67,0.7,-1.83,0  
3BPV,ARG\_87,12.29,-0.21,0,0  
3DHN,ASP\_59,3.69,0.07,-0.18,0  
1SNT,HIS\_239,4.89,0.8,-0.72,-1.69  
3BCH,CYS\_163,11.87,-0.49,0.3,36  
2NRR,GLU\_486,3.25,0.35,-1.6,0  
1GPP,ARG\_42,12.08,-0.42,0,0  
3JZ9,LYS\_461,10.43,-0.07,0,0  
3UX2,ASP\_42,3.33,0.28,-0.75,0

4EKU,GLU\_220,4.5,0,0,0  
 1V43,LYS\_113,10.43,-0.07,0,0  
 3GA2,CYS\_192,9.37,-1.45,0,1.82  
 2BQQ,ASP\_75,3.61,0,-0.19,0  
 1N81,ARG\_185,12.7,-3.18,0,3.38  
 2F8H,CYS\_102,11.21,-0.96,1.32,1.86  
 3CXS,ARG\_181,12.5,0,0,0  
 1QZN,ASP\_99,3.14,0.14,-0.8,0  
 3HUE,HIS\_242,7.26,0.83,0,-0.07  
 1N81,ARG\_70,11.87,-0.63,0,0  
 3GE9,LYS\_218,10.36,-0.14,0,0  
 1GXN,LYS\_440,10.22,-0.28,0,0  
 2XMZ,LYS\_81,9.87,-0.63,0,0  
 2IDC,LYS\_168,10.29,-0.21,0,0  
 3IPZ,GLU\_162,4.5,0,0,0  
 3IRA,GLU\_59,3.72,0.35,-1.13,0  
 1ZHV,ARG\_52,11.24,-1.26,0,0  
 1WXQ,TYR\_244,11.09,1.51,0.24,-0.66  
 2IRM,TYR\_62,10.46,1.39,-0.93,0  
 1J7G,ARG\_39,12.01,-0.49,0,0  
 2QHT,LYS\_182,10.5,0,0,0  
 1NAR,LYS\_233,10.5,0,0,0  
 4H86,LYS\_81,10.5,0,0,0  
 2ZOM,GLU\_266,4.5,0,0,0  
 2Z84,LYS\_198,10.15,-0.35,0,0  
 3ASA,ARG\_69,11.66,-0.84,0,0  
 2AD1,LYS\_70,8.96,-1.54,0,0  
 3DSH,GLU\_392,4.57,0.07,0,0  
 2CWY,GLU\_34,4.64,0.14,0,0  
 1WXQ,ARG\_373,12.49,-0.76,0,0.75  
 3UAH,GLU\_467,4.57,0.07,0,0  
 2OJQ,ARG\_469,11.94,-0.56,0,0  
 3F1X,ARG\_293,12.29,-0.21,0,0  
 3I47,HIS\_182,6.36,0,-0.14  
 3GFP,TYR\_308,11.15,0.07,0,1.08  
 3IVF,ARG\_277,12.5,0,0,0  
 2P4D,ASP\_80,1.37,0.56,-2.99,0  
 3H5T,ASP\_337,3.8,0,0,0  
 2HRZ,TYR\_103,10.07,0.07,0,0  
 3LD1,ARG\_100,12.01,-0.49,0,0  
 1TJE,ASP\_26,3.2,0.28,-0.88,0  
 1GSZ,HIS\_162,7.09,0.8,0,-0.21  
 1TJE,ASP\_64,2.75,0.49,-1.54,0  
 1DOV,HIS\_231,6.47,0.11,0,-0.14  
 1ZYL,LYS\_292,10.5,0,0,0  
 3ODJ,TYR\_93,11.22,1.91,-1.05,0.37  
 1PBV,ARG\_218,11.94,-0.56,0,0  
 3ON1,LYS\_78,10.5,0,0,0  
 2XHC,LYS\_230,10.15,-0.35,0,0  
 3CGW,ARG\_208,13.18,-0.31,0,0.99  
 3EIZ,LYS\_149,10.43,-0.07,0,0  
 1PSW,LYS\_263,10.5,0,0,0  
 3JZ9,ASP\_395,2.88,0.42,-1.34,0  
 4F3J,TYR\_151,11.33,0.24,-1.3,2.4  
 1RI6,GLU\_189,4.57,0.07,0,0  
 1QQE,GLU\_254,4.5,0,0,0  
 2IRM,CYS\_41,9,0,0,0  
 1XIP,LYS\_24,9.73,-0.77,0,0  
 1XEU,ASP\_154,3.22,0.56,-1.14,0  
 2PWQ,ASP\_118,3.52,0.07,-0.35,0  
 2CXA,GLU\_137,4.5,0,0,0  
 2QZQ,TYR\_53,11.81,0,0,1.81  
 3CBN,ASP\_49,3.46,0.28,-0.62,0  
 3B21,LYS\_175,10.22,-0.28,0,0  
 2ZCO,GLU\_264,4.5,0,0,0  
 3GS3,LYS\_97,10.29,-0.21,0,0  
 1R53,LYS\_19,10.5,0,0,0  
 2EDM,ASP\_132,3.08,0.35,-1.07,0  
 3US6,ASP\_110,3.63,0,-0.17,0  
 2ZCO,GLU\_193,4.57,0.07,0,0  
 3F7M,ARG\_320,12.5,0,0,0  
 4ESS,LYS\_91,10.36,-0.14,0,0  
 2RJD,GLU\_204,4.5,0,0,0  
 4FCU,HIS\_220,6.6,0.24,0,-0.14  
 1X04,ASP\_158,3.43,0,-0.37,0  
 3MIX,ARG\_650,12.5,0,0,0  
 3LQE,TYR\_399,10,0,0,0  
 2B2H,TYR\_57,9.55,0.35,-0.8,0  
 3RFY,TYR\_333,12.77,0,0.37,2.4  
 2G7O,GLU\_72,4.5,0,0,0  
 1SNT,ARG\_123,11.73,-0.77,0,0  
 1X1E,ARG\_34,12.36,-0.14,0,0  
 1TD6,ASP\_202,3.7,0,-0.1,0  
 3I4T,LYS\_166,9.8,-0.7,0,0  
 3E0H,ASP\_121,3.64,0,-0.16,0  
 3K8J,ASP\_71,3.73,0.28,-0.35,0  
 3GYW,TYR\_71,9.7,0,-0.3,0  
 3M70,TYR\_218,9.78,0.07,-0.37,0.08  
 4HDE,GLU\_184,3.69,0.21,-1.02,0  
 1OLR,GLU\_194,4.57,0.07,0,0  
 3PZ9,LYS\_304,10.5,0,0,0  
 2JHY,ASP\_183,1.42,1.12,-3.52,0  
 2OB5,GLU\_98,4.71,0.21,0,0  
 3H13,LYS\_249,10.5,0,0,0  
 2POL,GLU\_27,2.35,0.21,-1.22,-1.14  
 3LPZ,ASP\_86,1.95,0.56,-2.41,0  
 3EAZ,HIS\_134,6.36,0,-0.14  
 3BQW,HIS\_187,6.29,0,0,-0.21  
 3A2Z,ASP\_34,3.07,0.7,-1.42,0  
 2Y2T,LYS\_52,10.5,0,0,0  
 3IOO,HIS\_104,6.5,0,0,0  
 3B79,GLU\_58,4.5,0,0,0  
 3VJ8,ARG\_119,12.29,-0.21,0,0  
 2ZCX,HIS\_187,6.29,0,0,-0.21  
 1UW7,ARG\_39,12.01,-0.49,0,0  
 1XEU,LYS\_173,10.15,-0.35,0,0  
 3GE9,HIS\_75,6.5,0,0,0  
 2H8O,TYR\_120,10.76,0.76,0,0  
 1ANU,LYS\_128,10.5,0,0,0  
 3PM2,LYS\_79,10.5,0,0,0  
 1DVO,GLU\_157,3.36,0.35,-1.49,0  
 2GS5,GLU\_14,4.57,0.07,0,0  
 2HXB,ASP\_45,2.28,0.7,-2.22,0  
 1WXQ,GLU\_184,4.78,0.28,0,0  
 1MIX,GLU\_335,4.73,0.56,-0.34,0  
 3J5N,LYS\_157,10.15,-0.35,0,0  
 1PVT,GLU\_46,4.5,0,0,0  
 1X9G,GLU\_81,4.64,0.14,0,0  
 1TWU,ARG\_14,11.8,-0.7,0,0  
 3CBN,HIS\_104,6.22,0,0,-0.28  
 1TR9,ARG\_323,12.5,0,0,0  
 2W25,HIS\_74,6.79,0.36,0,-0.07  
 3DTE,ASP\_33,2.63,0.42,-1.58,0  
 3LMO,GLU\_26,3.83,0.56,-1.22,0  
 2F4Q,ARG\_137,12.72,-1.01,0,1.23  
 3AU3,CYS\_520,8.63,-1.37,0,1  
 1Q46,GLU\_98,4.64,0.14,0,0  
 3O7K,ARG\_124,11.52,-0.98,0,0  
 3BB7,LYS\_46,10.36,-0.14,0,0  
 3FTT,TYR\_20,12.43,0.07,0.2,3.6  
 1O3X,ASP\_204,3.28,0.28,-0.8,0  
 3M7G,ARG\_187,12.15,-0.35,0,0  
 3CAX,ARG\_173,12.36,-0.14,0,0  
 1LFP,ARG\_30,12.22,-1.56,0,1.28  
 3RJX,TYR\_287,9.74,0,-0.26,0  
 3J5N,ASP\_237,3.05,0.14,-0.89,0  
 3M7G,ASP\_75,3.4,0.49,-0.88,0  
 1RI6,CYS\_194,11.53,-0.85,0.29,3.09  
 2IQT,LYS\_28,10.5,0,0,0  
 4AF2,GLU\_98,4.19,0.49,-0.8,0  
 2G7O,ARG\_119,12.29,-0.21,0,0  
 2C13,ARG\_148,11.94,-0.56,0,0  
 1WP5,TYR\_62,11.04,1.04,0,0  
 2Z61,LYS\_156,9.87,-0.63,0,0  
 3F1X,ASP\_104,3.3,0,-0.5,0  
 1X6J,GLU\_70,3.7,0.28,-1.08,0  
 1N81,HIS\_44,6.13,0,1.53,-1.9  
 2VGM,LYS\_187,10.43,-0.07,0,0  
 1IAP,ARG\_158,11.52,-0.98,0,0  
 2YLF,ASP\_38,3.28,0.21,-0.73,0  
 4EKU,GLU\_101,4.15,0.49,-0.84,0  
 4E8B,CYS\_142,6.69,-2.39,-0.71,0.8  
 1R3D,ARG\_14,12.22,-0.28,0,0  
 2WB3,GLU\_292,4.57,0.07,0,0  
 2X4L,ASP\_100,3.85,0.07,-0.02,0  
 2CYG,TYR\_168,10,0,0,0  
 4ETX,TYR\_195,9.14,0.28,-1.14,0  
 1MML,GLU\_176,4.52,0.35,-0.32,0  
 1X8F,ASP\_281,2.73,0.7,-1.76,0  
 3VJ8,LYS\_248,10.29,-0.21,0,0  
 3RRQ,GLU\_46,3.51,0.63,-1.62,0  
 4FH3,GLU\_131,4.51,0.21,-0.2,0  
 1NIJ,LYS\_58,10.01,-0.49,0,0  
 3M66,HIS\_231,7.51,1.15,0,-0.14  
 1X8F,ARG\_226,11.94,-0.56,0,0  
 4H89,ASP\_112,3.22,0.35,-0.93,0  
 2YXO,TYR\_309,10.33,1.67,-0.07,-1.27  
 1BKB,CYS\_30,7.93,-1.34,0,0.27  
 1C44,LYS\_67,10.08,-0.42,0,0  
 1HUF,LYS\_75,10.5,0,0,0  
 3OOP,LYS\_97,10.43,-0.07,0,0  
 2E0T,ASP\_202,3.42,0.42,-0.8,0  
 2Y2T,ASP\_15,3.99,0.28,-0.09,0  
 2AD1,ARG\_145,12.43,-0.07,0,0  
 2BCF,ARG\_222,12.15,-0.35,0,0  
 1CBY,TYR\_53,10,0,0,0  
 2IF4,LYS\_262,10.36,-0.14,0,0  
 3EVN,LYS\_321,10.29,-0.21,0,0  
 1P2F,ARG\_201,12.5,0,0,0  
 4EVF,ARG\_249,13.1,-1.8,0,2.4  
 3GEC,LYS\_378,10.01,-0.49,0,0  
 1KW4,GLU\_76,4.78,0.28,0,0  
 3GW3,ARG\_122,11.94,-0.56,0,0  
 1XTZ,GLU\_55,3.84,0.14,-0.8,0  
 1X1E,ASP\_55,3.06,0.49,-1.23,0  
 2OSA,GLU\_300,4.57,0.07,0,0  
 2B3M,LYS\_141,10.43,-0.07,0,0  
 4F85,GLU\_142,4.55,0.07,-0.02,0  
 3CS1,LYS\_59,10.36,-0.14,0,0  
 2FG1,GLU\_136,4.05,0.35,-0.8,0  
 3N2T,HIS\_201,6.36,0,0,-0.14  
 1H09,TYR\_220,10,0,0,0  
 1X1E,GLU\_38,4.5,0,0,0  
 3QAV,ASP\_221,2.48,0.42,-1.74,0  
 2R51,ARG\_22,11.38,-1.12,0,0  
 1TLV,ASP\_151,2.53,0.35,-1.62,0  
 1R15,ARG\_158,12.15,-0.35,0,0  
 1Q46,LYS\_105,10.29,-0.21,0,0  
 4H89,GLU\_31,4.57,0.07,0,0  
 1RLQ,ARG\_69,11.66,-0.84,0,0  
 1JYH,CYS\_130,9.97,-0.93,0,1.9  
 2RJD,GLU\_475,4.26,0.56,-0.8,0  
 3O16,GLU\_117,4.71,0.21,0,0  
 2YWJ,GLU\_14,4.62,0.07,0.0,0.05  
 3V3T,TYR\_160,12.81,3.28,-0.47,0  
 3IOO,TYR\_189,7.52,0.24,-0.59,-2.13  
 1AIL,LYS\_67,10.15,-0.35,0,0  
 1O0X,LYS\_55,10.08,-0.42,0,0  
 3B4D,ASP\_170,3.36,0.21,-0.65,0  
 2B0J,HIS\_294,6.5,0,0,0  
 3ULX,LYS\_129,10.29,-0.21,0,0  
 2POL,ASP\_22,7.03,0.21,-1.28,0  
 2IF4,ASP\_286,2.86,0.7,-1.65,0  
 1G8P,GLU\_305,4.85,0.35,0,0  
 2H2Z,HIS\_172,3.62,0.95,0,-3.83  
 1LN4,ARG\_68,12.08,-0.42,0,0  
 1P4X,GLU\_125,4.5,0,0,0  
 2QVO,ARG\_67,12.5,0,0,0  
 3H04,GLU\_229,4.26,0.56,-0.8,0  
 1YTD,ARG\_243,10.92,-1.58,0,0  
 4H89,HIS\_158,6.5,0,0,0  
 3V75,GLU\_111,4.57,0.07,0,0  
 1O17,ARG\_18,12.08,-0.42,0,0  
 2I88,LYS\_377,11.87,-0.07,0,0  
 1ZBP,GLU\_18,4.6,0.14,-0.04,0  
 3GEC,HIS\_247,6.5,0,0,0  
 3OKQ,ASP\_568,3.95,0.21,-0.06,0  
 2WB3,ASP\_287,3.16,0.56,-1.2,0  
 3DEZ,ASP\_114,3.77,0.35,-0.38,0  
 2F19,ARG\_15,11.87,-0.63,0,0  
 2H01,GLU\_146,4.13,0.07,-0.44,0  
 1Z9L,LYS\_85,10.5,0,0,0  
 4ETX,ARG\_323,12.13,-0.79,0,0.42  
 3EZ7,GLU\_186,3.68,0.35,-1.17,0  
 3CS1,ARG\_88,11.87,-0.63,0,0  
 2YXO,TYR\_309,10.33,1.67,-0.07,-1.27  
 2FD4,GLU\_482,4.78,0.28,0,0  
 3LE4,HIS\_312,6.15,0,0,-0.35  
 2P4D,TYR\_88,10,0,0,0  
 3T5B,GLU\_284,4.38,0.14,-0.26,0  
 1JYH,LYS\_28,10.22,-0.28,0,0  
 3ODJ,ASP\_47,4.03,0.28,-0.05,0  
 1MTZ,ARG\_201,12.22,-0.28,0,0  
 3PU6,GLU\_28,4.64,0.14,0,0  
 1U7U,ARG\_321,13.39,-1.51,0,2.4  
 3M7G,CYS\_68,12.42,-0.19,0,3.61  
 2YWK,LYS\_38,10.29,-0.21,0,0  
 1ZBM,ASP\_221,2.37,0.49,-1.92,0  
 1YW5,HIS\_72,7.93,3.6,2.11,-4.28  
 1NIJ,TYR\_233,9.01,0.21,-1.19,0  
 3IV4,LYS\_68,10.43,-0.07,0,0  
 1EDG,LYS\_280,10.5,0,0,0  
 3RFY,GLU\_144,3.84,0.14,-0.8,0  
 3GE9,ASP\_125,3.05,0.56,-1.31,0  
 3G9G,TYR\_19,12.55,0,0.15,2.4  
 1P6F,LYS\_20,10.08,-0.42,0,0  
 1ZBM,LYS\_215,10.15,-0.35,0,0  
 1ZCE,LYS\_144,10.43,-0.07,0,0  
 2XJ4,TYR\_159,11.43,2.89,-1.46,0  
 3L3P,ASP\_340,12.36,-0.14,0,0  
 2RIK,GLU\_187,4.64,0.14,0,0  
 1BGF,ARG\_110,12.5,0,0,0  
 3M70,LYS\_285,9.94,-0.56,0,0  
 4GCO,ARG\_164,12.15,-0.35,0,0  
 3IL3,HIS\_180,7.08,0.79,0,-0.21  
 3RJZ,LYS\_141,10.36,-0.14,0,0  
 4FD6,ARG\_44,12.29,-0.21,0,0  
 3VJ8,GLU\_261,2.38,1.08,-3.2,0  
 2R57,CYS\_332,9.7,-0.1,0,0.8  
 2PGX,ARG\_68,12.22,-0.28,0,0  
 3IBT,ASP\_88,3.76,0.14,-0.18,0  
 2OQG,GLU\_398,3.95,0.49,-1.05,0  
 4FH3,GLU\_329,2.24,1.76,-1.62,-2.4  
 2H2W,GLU\_245,3.73,1.81,-0.75,-1.84  
 2OPI,TYR\_55,11.02,0,0,1.02  
 2VGM,LYS\_64,10.36,-0.14,0,0

2OSA,ASP\_327,2.31,0.42,-1.91,0  
 2OEW,GLU\_273,4.51,0.81,-0.8,0  
 2POL,GLU\_145,4.5,0,0,0  
 1J85,GLU\_143,1.93,0.63,-3.2,0  
 1ES5,LYS\_124,10.15,-0.35,0,0  
 200K,GLU\_105,4.57,0.07,0,0  
 2YX0,LYS\_190,10.5,0,0,0  
 2FPN,GLU\_101,4.63,0.42,-0.29,0  
 3M66,ARG\_261,11.52,-0.98,0,0  
 2H30,LYS\_104,10.29,-0.21,0,0  
 1L2F,ASP\_70,2.9,0.63,-1.52,0  
 2RIS,LYS\_46,10.15,-0.35,0,0  
 1L3K,GLU\_35,4.51,0.28,-0.27,0  
 2Q13,ASP\_122,1.19,0.77,-3.38,0  
 3CXS,TYR\_151,10.07,0.07,0,0  
 1T6L,ARG\_32,11.8,-0.7,0,0  
 3ETU,ASP\_56,3.87,0.07,0,0  
 3BWT,GLU\_803,4.57,0.83,-0.76,0  
 4D8L,ASP\_160,3.29,0.14,-0.64,0  
 3OOP,LYS\_133,10.5,0,0,0  
 3KT9,LYS\_80,10.5,0,0,0  
 3BPP,TYR\_87,11.53,0.99,0.54  
 3BPP,ARG\_220,12.08,-0.42,0,0  
 2Q5X,GLU\_739,3.58,0.14,-1.06,0  
 2DVK,ARG\_43,13.12,-0.34,0.096  
 2AZL,GLU\_157,4.5,0,0,0  
 1SUU,LYS\_607,10.5,0,0,0  
 2H85,CYS\_102,6.49,-4.31,1.35,0.46  
 1MD6,GLU\_86,4.57,0.07,0,0  
 2BOJ,TYR\_213,10,0,0,0  
 2G9D,CYS\_60,11.88,0,0.288  
 1WRU,ASP\_95,3.32,0.35,-0.82,0  
 3JV1,GLU\_179,4.43,0,-0.07,0  
 3EUR,LYS\_96,10.5,0,0,0  
 3ADO,LYS\_51,10.29,-0.21,0,0  
 4AM1,LYS\_175,10.43,-0.07,0,0  
 2YLF,GLU\_210,4.64,0.14,0,0  
 3QAV,GLU\_212,4.64,0.14,0,0  
 1R9W,HIS\_270,2.73,0.59,0,-4.36  
 1KCM,ASP\_234,1.79,1.05,-3.05,0  
 1L3K,LYS\_52,10.5,0,0,0  
 1Q46,TYR\_38,12.77,1.05,-0.73,2.45  
 2X4G,TYR\_144,9.88,0,-0.12,0  
 1FHL,TYR\_295,11.85,2.65,-0.8,0  
 2OGQ,CYS\_405,7.95,-1.19,0,0.14  
 1X1E,ARG\_16,12.01,-0.49,0,0  
 1FKM,TYR\_466,9.47,0,-0.53,0  
 1R3D,HIS\_240,5.22,1.84,1.99,-5.11  
 2RIK,TYR\_259,12.41,0.63,0.178  
 2J8A,GLU\_334,4.78,0.28,0,0  
 1TD6,TYR\_75,10,0,0,0  
 1S7K,CYS\_155,8.88,-0.12,0,0  
 1Q8B,LYS\_26,10.43,-0.07,0,0  
 3UPD,ARG\_320,8.8,-3.7,0,0  
 3CIV,ARG\_248,12.36,-0.14,0,0  
 3AUF,GLU\_8,4.55,1.12,-1.07,0  
 2APL,HIS\_55,6.43,0,0,-0.07  
 1EDG,ARG\_208,12.63,-2.27,0.24  
 1YIB,LYS\_220,10.29,-0.21,0,0  
 2F9F,ASP\_138,2.54,0.56,-1.82,0  
 3TMO,GLU\_204,4.5,0.07,-0.07,0  
 1WYC,GLU\_41,0.24,1.27,-1.57,-3.96  
 1DZF,ARG\_155,12.86,-1.8,0.2,16  
 3M7G,ARG\_151,12.66,-2.24,0.24  
 3PAC,LYS\_161,10.15,-0.35,0,0  
 3CRM,ARG\_68,11.94,-0.56,0,0  
 3M3P,HIS\_248,6.17,0.02,0,-0.35  
 2O8P,ARG\_11,11.45,-1.05,0,0  
 1GPP,GLU\_415,3.69,0.28,-1.09,0  
 1XTZ,LYS\_155,10.43,-0.07,0,0  
 2QRX,ASP\_164,2.6,0.42,-1.62,0  
 2RJU,CYS\_205,8.39,-0.61,0,0  
 1ZBM,ASP\_64,3.23,0.14,-0.71,0  
 3EJG,LYS\_158,10.5,0,0,0  
 3CS1,LYS\_22,10.22,-0.28,0,0  
 3F7M,HIS\_119,6.81,0.66,0,-0.35  
 3EJG,GLU\_98,3.86,0.49,-1.13,0  
 2ZTY,ARG\_33,12.22,-0.28,0,0  
 3EIZ,LYS\_147,10.5,0,0,0  
 1ZBM,LYS\_249,10.43,-0.07,0,0  
 2R51,ARG\_95,12.5,0,0,0  
 3IL3,ARG\_151,12.15,-0.35,0,0  
 2WB8,GLU\_541,4.73,0.57,-0.34,0  
 2Q12,TYR\_190,10,0,0,0  
 200K,ARG\_321,10.26,-2.24,0,0  
 3M70,GLU\_200,4.39,0.28,-0.39,0  
 1DTO,ARG\_7,12.36,-0.14,0,0  
 3QKY,ARG\_114,13.07,-1.38,0.195  
 2P0Y,LYS\_12,10.36,-0.14,0,0  
 1SUU,GLU\_784,4.57,0.35,-0.28,0  
 4E9E,TYR\_530,13.41,0.21,0.8,2.4  
 2EYH,HIS\_20,6.5,0,0,0  
 1SJY,ASP\_114,3.66,0.07,-0.21,0  
 1X8F,ASP\_16,3.33,0.28,-0.75,0  
 3KEY,ASP\_469,4.15,0.35,0,0  
 3IV4,ASP\_92,3.33,0.35,-0.82,0  
 3ELI,LYS\_26,9.73,-0.77,0,0  
 1WRU,GLU\_266,3.75,0.68,-1.18,-0.25  
 1BKB,GLU\_34,4.71,0.21,0,0  
 2P65,ARG\_27,11.59,-0.91,0,0  
 2O8P,ASP\_155,3.94,0.21,-0.07,0  
 2RIK,CYS\_74,13.82,0.39,0.88  
 3CIV,ARG\_237,12.15,-0.35,0,0  
 2FC3,GLU\_21,4.13,0.35,-0.72,0  
 1RZ2,ARG\_68,12.5,-2.12,0.2,12  
 1IAP,ARG\_161,11.88,-0.62,0,0  
 1UXO,GLU\_169,2.76,0.77,-2.23,-0.28  
 1WXF,LYS\_193,9.95,-0.28,0,-0.27  
 3VJ8,LYS\_45,10.43,-0.07,0,0  
 3BCH,CYS\_148,10.41,-0.97,0,2.38  
 3IOO,GLU\_175,4.64,0.14,0,0  
 2NRK,TYR\_88,10.66,1.07,0,-0.41  
 2EFK,GLU\_37,4.71,0.21,0,0  
 2WB3,TYR\_340,10.92,0,0.092  
 1X04,GLU\_220,4.5,0,0,0  
 2NRK,LYS\_136,10.29,-0.21,0,0  
 2XMX,LYS\_205,10.08,-0.42,0,0  
 1UJ8,ARG\_39,12.22,-0.28,0,0  
 1SUU,ARG\_771,12.22,-0.28,0,0  
 3KB5,ASP\_459,3.75,0.63,-0.68,0  
 3IVF,LYS\_58,10.29,-0.21,0,0  
 1QQL,GLU\_60,4.78,0.28,0,0  
 1TR9,ARG\_18,12.01,-0.49,0,0  
 1WXF,GLU\_20,4.5,0,0,0  
 2JHY,GLU\_106,1.81,0.84,-3.53,0  
 4F85,GLU\_266,3.98,0.28,-0.8,0  
 2J8A,LYS\_357,10.22,-0.28,0,0  
 1GXN,ARG\_481,11.45,-1.05,0,0  
 3ETU,TYR\_97,10.62,0.66,-0.03,0  
 3CAX,ARG\_158,11.45,-1.05,0,0  
 2H2Z,TYR\_118,8.92,0.07,-1.15,0  
 3ASA,GLU\_194,4.5,0,0,0  
 1PSW,GLU\_346,2.24,0.89,-0.8,-2.35  
 1Y2Q,ARG\_32,12.15,-0.35,0,0  
 2APL,ARG\_84,12.29,-0.21,0,0  
 2YT4,TYR\_597,10,0,0,0  
 2OB5,ASP\_6,0.88,0.63,-3.55,0  
 1EYH,ARG\_114,12.5,0,0,0  
 3DSH,ARG\_247,12.01,-0.49,0,0  
 1ZBP,GLU\_267,4.5,0,0,0  
 2YWK,GLU\_6,2.59,0.49,-2.4,0  
 3UX2,ASP\_128,3.44,0.28,-0.64,0  
 1PV5,HIS\_204,6.52,0.16,-0.14  
 2O8P,GLU\_44,4.64,0.14,0,0  
 1QQE,GLU\_35,3.84,0.14,-0.8,0  
 2CN1,ARG\_45,11.52,-0.98,0,0  
 4EKU,GLU\_182,2.29,3.07,-1.6,-3.68  
 3FK5,ARG\_139,12.29,-0.21,0,0  
 4EVF,LYS\_18,10.36,-0.14,0,0  
 1PDB,TYR\_182,10.79,0.56,0,0.23  
 1H09,ASP\_205,3.09,0.84,-1.55,0  
 3LJC,ASP\_61,3.55,0.14,-0.39,0  
 1X1E,LYS\_62,10.5,0,0,0  
 2OGQ,GLU\_401,4.71,0.21,0,0  
 3H13,GLU\_461,3.31,0.28,-1.47,0  
 2QRX,ARG\_117,11.94,-0.56,0,0  
 2G9D,ASP\_271,4.1,0.42,-0.12,0  
 3KV0,ARG\_112,11.38,-1.12,0,0  
 2NYC,ASP\_312,4.01,0.21,0,0  
 2RIK,GLU\_133,4.5,0,0,0  
 2HZW,GLU\_117,4.64,0.14,0,0  
 4DEZ,ASP\_117,3.18,0.07,-0.69,0  
 4DND,GLU\_66,4.5,0,0,0  
 1F2V,ARG\_191,12.15,-0.35,0,0  
 3NBI,GLU\_36,4.57,0.07,0,0  
 3V1Q,ARG\_560,12.01,-0.49,0,0  
 3M7G,GLU\_161,2.38,0.28,-2.4,0  
 1LPL,ARG\_212,11.24,-1.26,0,0  
 3I4T,TYR\_3,10,0,0,0  
 3R2E,GLU\_33,4.04,0.28,-0.74,0  
 3LJC,ARG\_33,11.94,-0.56,0,0  
 1PBV,TYR\_186,13.27,0.07,0.8,2.4  
 1OXZ,ARG\_265,12.5,0,0,0  
 1UW7,ARG\_111,12.5,0,0,0  
 2GYZ,ASP\_24,3.93,0.14,-0.01,0  
 3I4T,ARG\_220,11.17,-1.33,0,0  
 3K8U,TYR\_37,10,0,0,0  
 1AD6,GLU\_533,4.5,0,0,0  
 3HUE,ASP\_194,2.79,0.7,-1.71,0  
 1SI7,ASP\_221,3.01,0.7,-1.49,0  
 2FB6,ASP\_76,3.81,0.14,-0.13,0  
 3ERF,LYS\_223,10.43,-0.07,0,0  
 2WB3,ARG\_268,12.5,0,0,0  
 3V75,HIS\_182,6.22,0,0,-0.28  
 2AD1,ASP\_185,3.8,0.21,-0.21,0  
 2QK1,ARG\_497,11.73,-0.77,0,0  
 1XTD,ASP\_131,3.42,0.42,-0.8,0  
 1WXF,ARG\_140,12.08,-0.42,0,0  
 1TWU,TYR\_84,10.07,0.07,0,0  
 2FC3,GLU\_113,3.98,0.28,-0.8,0  
 2QZQ,LYS\_115,10.5,0,0,0  
 4EZB,CYS\_64,8.9,-0.1,0,0  
 1FQI,HIS\_391,6.61,0.18,0,-0.07  
 2IXM,LYS\_249,10.5,0,0,0  
 1YTD,ASP\_19,2.91,0.35,-1.24,0  
 3N2T,GLU\_74,4.09,0.35,-0.76,0  
 4GCO,GLU\_152,4.71,0.21,0,0  
 1L2H,CYS\_71,8.95,-1.6,0.155  
 3FHF,ASP\_104,3.14,0.28,-0.94,0  
 2HZW,HIS\_182,2.84,0.69,0,-4.34  
 2O8P,TYR\_180,10.65,0,0.65  
 4DNU,ASP\_192,3.94,0.21,-0.07,0  
 3O48,GLU\_128,4.64,0.14,0,0  
 3GS9,GLU\_142,4.78,0.28,0,0  
 4H4J,LYS\_78,10.5,0,0,0  
 2XMX,LYS\_225,10.5,0,0,0  
 1K95,ARG\_75,12.08,-0.42,0,0  
 2FPN,ASP\_69,2.26,0.77,-2.31,0  
 3GS3,HIS\_210,6.33,0.04,0,-0.21  
 3B7X,GLU\_23,2.14,0.49,-2.85,0  
 3CRM,ARG\_80,11.8,-0.7,0,0  
 1WXF,TYR\_185,10.98,0.59,0.39  
 3ZXY,GLU\_191,4.57,0.07,0,0  
 1SI7,ARG\_335,11.47,-2.1,0.107  
 1UAJ,ARG\_114,11.59,-0.91,0,0  
 3NR5,HIS\_0,6.5,0,0,0  
 3RLN,ARG\_751,12.15,-0.35,0,0  
 1KN3,GLU\_36,4.5,0,0,0  
 2EHG,LYS\_93,10.29,-0.21,0,0  
 3VJ8,TYR\_339,11.59,0,0.159  
 3LMO,LYS\_49,10.5,0,0,0  
 3RNV,LYS\_378,10.43,-0.07,0,0  
 1O0X,GLU\_79,1.94,1.79,-1.95,-2.4  
 2D7U,ASP\_168,3.44,0.42,-0.79,0  
 4E8B,ARG\_74,12.22,-0.28,0,0  
 2XMX,HIS\_33,6.23,1.8,-4.65  
 1I60,HIS\_59,6.93,0.5,0,-0.07  
 3M7D,ARG\_231,13.49,-1.41,0.2,4  
 2ZCX,ASP\_195,2.74,0.77,-1.83,0  
 1BYL,ASP\_67,3.75,0.07,-0.12,0  
 3M16,HIS\_159,8.38,1.7,1.81,-1.62  
 2CL3,ASP\_72,3.75,0.07,-0.12,0  
 1BYL,HIS\_164,6.6,0.1,0,0  
 3M7D,ASP\_160,3.77,0,-0.03,0  
 3E5T,ARG\_10,12.5,0,0,0  
 1R3D,HIS\_99,6.51,0.01,0,0  
 3GS9,GLU\_195,4.5,0,0,0  
 2RGY,ASP\_225,3.32,0.28,-0.76,0  
 1TLV,HIS\_237,6.5,0,0,0  
 2EJB,ARG\_118,12.43,-0.07,0,0  
 1OXZ,LYS\_250,10.29,-0.21,0,0  
 2GZT,TYR\_75,10,0,0,0  
 3I4T,TYR\_187,10.45,0.52,-0.07,0  
 1XEU,GLU\_284,4.57,0.07,0,0  
 2BV9,ASP\_78,3.03,0.35,-1.12,0  
 2YT4,ARG\_670,12.43,-0.07,0,0  
 2IQT,GLU\_129,2.45,0.35,-2.4,0  
 3Q98,HIS\_97,6.43,0,0,-0.07  
 1SQW,GLU\_123,4.21,0,-0.29,0  
 2YYO,GLU\_26,4.1,0.77,-1.17,0  
 2A0J,LYS\_53,10.29,-0.21,0,0  
 2XHC,ASP\_323,3.56,0.56,-0.8,0  
 3GOZ,LYS\_249,10.36,-0.14,0,0  
 3IV4,ASP\_185,3.8,0.21,-0.21,0  
 2V5B,LYS\_157,10.5,0,0,0  
 2HXB,LYS\_6,10.36,-0.14,0,0  
 3GA2,TYR\_233,10.07,0.07,0,0  
 1DVO,TYR\_133,8.44,1.41,-1.53,-1.44  
 3EAZ,HIS\_84,4.37,0.94,0,-3.07  
 2QEW,CYS\_127,11.62,-0.31,0.2,93  
 3Q6L,LYS\_101,10.43,-0.07,0,0  
 3V3T,TYR\_68,10,0,0,0  
 1O6D,GLU\_107,4.5,0,0,0  
 3V75,GLU\_69,3.32,0.42,-1.6,0  
 3M3P,ARG\_227,11.8,-0.7,0,0  
 2ZCO,TYR\_214,11.46,0.14,-0.28,1.59  
 1DOV,LYS\_120,10.15,-0.35,0,0  
 1EYH,ARG\_124,11.45,-1.05,0,0  
 3HUE,TYR\_319,11.27,0,0.127  
 1RI6,CYS\_131,8.52,-2.93,0.2,45  
 3RLE,GLU\_24,4.5,0,0,0  
 1AD6,ARG\_445,10.93,-1.57,0,0  
 2BDD,CYS\_33,5.74,-3.26,0,0  
 4FZR,HIS\_84,6.7,0.27,0,-0.07  
 3H13,GLU\_434,3.92,0.42,-1,0  
 1X04,GLU\_170,4.5,0,0,0



4FD6,LYS\_145,10.01,-0.49,0,0  
1X04,LYS\_150,10.22,-0.28,0,0  
3COU,GLU\_91,4.19,0.49,-0.8,0  
2IDC,ARG\_148,12.08,-0.42,0,0  
2QDJ,GLU\_54,4.18,0.35,-0.67,0  
1YR6,LYS\_80,10.29,-0.21,0,0  
1ANU,LYS\_98,10.29,-0.21,0,0  
1GQE,HIS\_281,6.29,0,0,-0.21  
2HP7,TYR\_171,10,0,0,0  
3ON1,LYS\_51,10.08,-0.42,0,0  
2FM9,ARG\_100,12.08,-0.42,0,0  
3ADO,GLU\_97,1.31,1.53,-2.46,-2.25  
3QKY,TYR\_214,11.71,0.75,0.39,0.58  
3EX9,GLU\_137,4.47,0.28,-0.31,0  
1ZCE,LYS\_49,10.01,-0.49,0,0  
1Y2Q,ASP\_96,3.63,0.49,-0.66,0  
1R3F,ASP\_186,3.9,0.21,-0.11,0  
3N2T,ARG\_7,12.29,-0.21,0,0  
1QYI,TYR\_276,11.44,0,-0.76,2.19  
4F3J,ARG\_110,10.99,-1.51,0,0  
1X9G,GLU\_58,4.15,0.7,-1.05,0  
1QQL,HIS\_124,6.36,0,0,-0.14  
1KCM,ARG\_147,11.94,-0.56,0,0  
2BQQ,TYR\_58,10.07,0.14,-0.07,0  
3A2Z,GLU\_61,0.91,2.79,-3.98,-2.4  
2AD1,HIS\_109,0.82,0,0,-5.68  
3HNX,GLU\_60,3.96,0.14,-0.68,0  
3GYW,TYR\_259,10,0,0,0  
2YJW,ASP\_149,3.53,0.14,-0.41,0  
3GMS,TYR\_22,9.72,0,-0.28,0  
4H4J,LYS\_182,9.66,-0.84,0,0  
2WOZ,TYR\_354,10,0,0,0  
1GXN,TYR\_575,9.43,0.99,-1.56,0  
4AM1,LYS\_189,10.5,0,0,0  
1SUU,ARG\_520,11.66,-0.84,0,0  
1T6L,GLU\_138,4.5,0,0,0  
2WB3,LYS\_306,10.5,0,0,0  
1U7U,LYS\_318,10.43,-0.07,0,0  
2D7U,TYR\_270,10,0,0,0  
1LTU,ASP\_79,2.9,0.63,-1.53,0  
2FZ4,GLU\_66,4.2,0.35,-0.65,0  
3ADO,ASP\_114,1.87,0.63,-2.57,0  
1X1E,LYS\_160,10.5,0,0,0  
3BQW,LYS\_251,10.22,-0.28,0,0  
2NRK,TYR\_120,13.41,0.21,0.8,2.4  
4H86,GLU\_80,4.64,0.14,0,0  
3HQX,LYS\_13,10.5,0,0,0  
3TOW,ASP\_83,3.48,0.77,-1.09,0  
2VGM,GLU\_234,3.44,0.49,-1.55,0  
3GG6,TYR\_72,10.41,1.17,0,-0.76  
3GT0,LYS\_48,10.36,-0.14,0,0  
3F5D,LYS\_50,10.43,-0.07,0,0  
4DEZ,HIS\_7,4.17,1.61,0.87,-4.82  
2Q13,TYR\_161,12.76,0.07,0.29,2.4  
1U3Y,ARG\_281,11.52,-0.98,0,0  
3TIR,ARG\_89,12.5,0,0,0  
1XFK,HIS\_288,6.5,0,0,0  
2H14,HIS\_310,2.95,0,0,-3.55  
2FXT,ASP\_336,4.08,0.28,0,0  
1SI7,TYR\_9,10,0,0,0  
4ESS,ARG\_159,11.59,-0.91,0,0  
3LE4,GLU\_301,4.64,0.14,0,0  
4FCU,GLU\_81,3.07,0.56,-1.99,0  
2AXO,TYR\_114,9.24,0.45,-1.2,0  
3RFY,LYS\_378,10.5,2,0,0  
1Y0K,GLU\_75,4.37,0.49,-0.62,0  
2OSA,LYS\_275,10.43,-0.07,0,0  
4DNU,LYS\_225,10.36,-0.14,0,0  
1PGV,ARG\_255,12.08,-0.42,0,0  
200K,ASP\_183,4.08,0.28,0,0  
2E3H,ARG\_298,11.66,-0.84,0,0  
350A,TYR\_46,10.99,0.99,0,0  
3ANJ,HIS\_113,3.98,0,-1.13,-1.39  
3CE7,GLU\_45,4.62,0.28,-0.16,0  
1ZBP,ARG\_49,12.36,-0.14,0,0  
1TUL,ASP\_31,4.3,0.42,0.08,0  
1TWU,LYS\_134,10.5,0,0,0  
2FD5,ARG\_115,11.94,-0.56,0,0  
2DG7,GLU\_9,4,0,0,-0.5  
3PM2,TYR\_67,10.82,0.14,-1.48,2.16  
1M5I,ASP\_209,2.47,0.84,-2.17,0  
2ZTY,GLU\_71,5.31,0.97,-0.15,0  
1YB2,ARG\_145,12.5,0,0,0  
4AM1,TYR\_203,9.33,0,-0.71,0.04  
200K,HIS\_24,6.34,0.19,0,-0.35  
3D9H,ASP\_224,3.02,0.56,-1.35,0  
2NMU,GLU\_117,2.53,1.26,-3.23,0  
2O4D,ARG\_112,12.08,-0.42,0,0  
2P4D,LYS\_130,10.5,0,0,0  
3R2E,ASP\_31,3.12,0.42,-1.1,0  
1R5S,TYR\_18,10.34,0.0.34,0  
4EUG,ARG\_179,11.8,-0.7,0,0  
3F6M,CYS\_124,9.14,0,0,0.14  
2H85,HIS\_95,2.72,0.04,0,-3.82  
3PM2,LYS\_119,10.5,0,0,0  
1Z3X,ASP\_204,2.27,0.49,-2.01,0  
3ODJ,HIS\_65,4.03,0.32,0,-2.79  
1Y0K,ARG\_31,11.66,-0.84,0,0  
3RUX,ARG\_303,13.3,-1.47,0,2.27  
3T57,GLU\_245,3.88,0.21,-0.83,0  
1X7F,GLU\_51,4.57,0.07,0,0  
3BWT,HIS\_569,6.5,0,0,0  
3JSN,LYS\_155,10.36,-0.14,0,0  
2D25,ASP\_651,3.76,0.07,-0.11,0  
1TXD,GLU\_866,3.84,0.14,-0.8,0  
2WB8,ASP\_707,2.85,0.28,-1.24,0  
3T8R,ASP\_113,4.01,0.21,0,0  
3EJC,LYS\_38,10.5,0,0,0  
3ETV,GLU\_63,4.64,0.14,0,0  
200K,GLU\_208,5.21,0.71,0,0  
1TLV,GLU\_255,4.5,0,0,0  
3GMS,ASP\_106,3.57,0.14,-0.37,0  
3GS9,ASP\_101,3.24,0.21,-0.76,0  
2AZL,GLU\_266,3.91,0.21,-0.8,0  
1K95,GLU\_67,4.47,0.14,-0.17,0  
1PGV,GLU\_350,4.57,0.07,0,0  
2EYI,LYS\_79,10.5,0,0,0  
2A1V,LYS\_118,10.5,0,0,0  
2I88,TYR\_396,11.18,1.21,-0.03,0  
2OPJ,ARG\_280,11.59,-0.91,0,0  
3OOP,LYS\_115,10.5,0,0,0  
2OBI,LYS\_20,10.5,0,0,0  
2OKT,LYS\_2,10.43,-0.07,0,0  
2YWJ,GLU\_17,4.57,0.07,0,0  
3C5V,ARG\_222,12.29,-0.21,0,0  
2RH3,LYS\_148,10.5,0,0,0  
1XEU,CYS\_141,9.07,0.0,0.07  
2J8A,LYS\_332,10.01,-0.49,0,0  
2Q98,ARG\_129,12.29,-0.21,0,0  
1Q8B,LYS\_21,10.5,0,0,0  
1IAP,HIS\_80,2.96,0.57,0,-4.11  
3E0H,ASP\_122,3.94,0.28,-0.14,0  
1X91,ASP\_61,1.39,0.7,-3.11,0  
2HX8,LYS\_15,10.5,0,0,0  
3H5T,GLU\_77,2.13,2.43,-2.4,-2.4  
2XMZ,GLU\_60,4.57,0.07,0,0  
2PGE,ASP\_95,3.56,0.07,-0.31,0  
2P65,ASP\_85,1.6,0.42,-2.62,0  
3GW3,LYS\_15,10.5,0,0,0  
2G9D,GLU\_306,4.57,0.07,0,0  
3HVW,ASP\_312,3.78,0.21,-0.23,0  
3UV9,TYR\_401,10.14,0.14,0,0  
1OSJ,LYS\_42,10.43,-0.07,0,0  
3ZSL,ARG\_162,11.94,-0.56,0,0  
3DSH,ASP\_309,3.8,0,0,0  
3LD1,CYS\_60,8.92,-0.15,0,0.07  
2BDD,GLU\_152,4.64,0.14,0,0  
3Q6L,LYS\_108,10.29,-0.21,0,0  
3M16,GLU\_275,4.71,0.21,0,0  
1R53,ARG\_337,12.5,0,0,0  
1YM5,ARG\_236,13.33,-1.35,0,2.18  
1MUS,GLU\_305,3.91,0.21,-0.8,0  
2ILR,CYS\_345,10.75,-0.04,0,1.79  
2YXO,ARG\_283,12.5,0,0,0  
1Z9L,GLU\_5,4.5,0,0,0  
3I82,ASP\_170,3.87,0.07,0,0  
2RIS,LYS\_16,10.01,-0.49,0,0  
2GKG,ASP\_55,2.42,0.21,-1.59,0  
3NR5,ASP\_124,3.41,0.42,-0.81,0  
1MTZ,GLU\_97,3.98,0.28,-0.8,0  
3LQE,ARG\_431,11.81,-2.31,0,1.62  
3GV0,GLU\_170,3.3,0.35,-1.55,0  
3RE9,TYR\_239,13.1,0.14,0.56,2.4  
2DG7,GLU\_18,4.38,0.21,-0.33,0  
3RFY,LYS\_189,10.5,0,0,0  
4DVD,LYS\_139,10.5,0,0,0  
3BPV,ARG\_44,12.36,-0.14,0,0  
1DOV,ARG\_129,12.43,-0.07,0,0  
1NJ4,GLU\_351,4.5,0,0,0  
3C5V,CYS\_105,10.24,0,0,1.24  
2V4U,ARG\_453,11.59,-0.91,0,0  
3IL3,GLU\_170,4.5,0,0,0  
1UXQ,GLU\_111,1.49,0.49,-3.5,0  
2PLQ,ASP\_68,2.55,0.49,-1.74,0  
2GZQ,TYR\_153,13.15,0.28,0.48,2.4  
3PAC,ASP\_66,3.66,0.14,-0.28,0  
2R51,LYS\_143,10.36,-0.14,0,0  
2WOZ,HIS\_337,2.16,0.51,0,-4.85  
1R3F,GLU\_61,4.3,0.14,-0.34,0  
2P5D,TYR\_65,12.35,0.97,0,1.38  
2BLL,GLU\_397,4.0,21,-0.71,0  
1G5Z,ASP\_188,3.8,0.56,-0.56,0  
2BQQ,TYR\_64,10,0,0,0  
2BTH,ASP\_283,3.85,0.28,-0.23,0  
3BFM,GLU\_159,4.92,0.42,0,0  
2IRM,GLU\_345,4.57,0.07,0,0  
1QQH,ASP\_126,3.88,0.21,-0.13,0  
4ACJ,ARG\_657,11.73,-0.77,0,0  
4FLE,TYR\_116,9.96,0.37,-0.41,0  
1X1E,HIS\_101,0.34,0.99,-2.4,-4.75  
2BQQ,ASP\_93,1.65,0.84,-2.99,0  
3M66,LYS\_415,10.5,0,0,0  
3MTT,ASP\_566,3.39,0.07,-0.48,0  
3GS9,ASP\_121,2.9,0.42,-1.32,0  
3RZJ,TYR\_22,10.07,0.07,0,0  
3HKX,ASP\_44,3.81,0.14,-0.13,0  
3K85,HIS\_337,6.39,0.1,0,-0.21  
4FH3,ASP\_254,3.42,0.07,-0.45,0  
1KCM,LYS\_105,10.43,-0.07,0,0  
2Z84,GLU\_109,4.5,0,0,0  
3BWT,GLU\_818,3.75,0.42,-1.17,0  
1SUU,ASP\_763,2.62,0.77,-1.96,0  
1V43,HIS\_343,6.29,0,0,-0.21  
3AU3,GLU\_477,4.19,0.49,-0.8,0  
3ZTA,ASP\_113,3.67,0.49,-0.62,0  
2C2Y,HIS\_215,6.36,0,0,-0.14  
2WB8,CYS\_467,10.77,0.04,1.31  
2B2H,LYS\_292,10.5,0,0,0  
2QVT,GLU\_79,3.67,0.63,-1.46,0  
1Q46,GLU\_116,4.07,0,-0.43,0  
1SBX,GLU\_145,4.5,0,0,0  
3F1X,HIS\_30,6.36,0,0,-0.14  
3IBT,TYR\_212,10.68,0.68,0,0  
2JEO,LYS\_58,10.5,0,0,0  
1JKS,ARG\_54,12.36,-0.14,0,0  
1MTZ,ASP\_187,3.78,0,-0.02,0  
4AM1,LYS\_38,10.15,-0.35,0,0  
1N81,TYR\_125,9.35,0.3,-0.95,0  
2A6B,LYS\_83,10.5,0,0,0  
3F53,ARG\_268,12.15,-0.35,0,0  
1YTD,ASP\_216,2.75,0.28,-1.33,0  
1QQL,ARG\_47,12.29,-0.21,0,0  
2Q13,LYS\_212,10.5,0,0,0  
1O5T,ARG\_318,12.43,-0.07,0,0  
1AD6,ARG\_556,12.43,-0.07,0,0  
157K,TYR\_166,10,0,0,0  
2EJX,CYS\_40,9.14,0,0,0.14  
3F6M,ARG\_115,12.36,-0.14,0,0  
3CAN,CYS\_77,6.68,-1.6,0.0.28  
1AM2,GLU\_155,1.37,0.68,-0.54,-3.27  
1FKM,LYS\_407,10.01,-0.49,0,0  
3BCH,ARG\_120,12.22,-0.28,0,0  
2Q99,TYR\_169,11.3,0.67,0.48,0.14  
4AF2,ARG\_66,11.73,-0.77,0,0  
2IF4,HIS\_73,6.38,0.02,0,-0.14  
3I0O,TYR\_249,10,0,0,0  
3UX2,GLU\_64,4.64,0.14,0,0  
1X7F,ASP\_61,4.0,21,-0.01,0  
3RLE,ARG\_30,12.08,-0.42,0,0  
4E9E,ARG\_512,11.3,-1.2,0,0  
3AUF,ARG\_104,12.29,-0.21,0,0  
2IRM,HIS\_175,6.6,0.17,0,-0.07  
2E0T,ASP\_135,3.19,0.28,-0.89,0  
3CGW,GLU\_24,4.07,0.42,-0.85,0  
3CE7,GLU\_96,4.05,0.35,-0.8,0  
1Q5Z,GLU\_573,3.98,0.28,-0.8,0  
3BCY,LYS\_112,10.43,-0.07,0,0  
1DCF,HIS\_49,6.29,0,0,-0.21  
1J33,LYS\_18,9.87,-0.63,0,0  
4AM1,LYS\_29,10.22,-0.28,0,0  
2IF4,ASP\_281,3.39,0.28,-0.69,0  
3OKQ,GLU\_654,4.64,0.14,0,0  
3NZL,CYS\_66,8.98,-0.09,0.0.07  
2OSA,ARG\_403,12.22,-0.28,0,0  
3B21,GLU\_29,4.57,0.07,0,0  
1UOH,GLU\_225,4.05,0.35,-0.8,0  
1RAJ,LYS\_200,10.5,0,0,0  
2P0Y,TYR\_78,10,0,0,0  
2GZR,HIS\_66,7.16,0.87,0,-0.21  
2FL7,CYS\_177,10.01,-0.38,0,1.39  
3QKY,TYR\_217,12.51,0.21,-0.1,2.4  
3QKY,TYR\_50,9.49,0,-0.51,0  
3B7X,CYS\_123,9.21,0,0,0.21  
3BB7,CYS\_227,12.87,-0.03,0,3.9  
1PSW,ARG\_334,12.36,-0.14,0,0  
2FBQ,ASP\_185,3.95,0.21,-0.06,0  
1PDB,ARG\_91,11.59,-0.91,0,0  
2OSA,TYR\_357,9.34,0.14,-0.8,0  
4F3J,LYS\_170,10.15,-0.35,0,0  
1N81,HIS\_28,6.5,0,0,0  
3CBN,CYS\_124,2.05,-7.16,0,0.21  
2R51,ARG\_199,12.08,-0.42,0,0  
3DZ1,ARG\_299,12.29,-0.21,0,0  
1IDK,ASP\_324,3.44,0.07,-0.43,0  
1DVO,HIS\_117,6.29,0,0,-0.21  
1T3Y,ARG\_73,12.22,-0.28,0,0

3AU3,ARG\_653,11.73,-0.77,0,0  
2QK1,LYS\_428,10.36,-0.14,0,0  
1SFE,ARG\_105,12.22,-0.28,0,0  
2O8PLYS\_151,10.5,0,0,0  
3CBN,GLU\_45,9.45,1.48,1.21,2.27  
3IV4,GLU\_17,4.22,0.28,-0.56,0  
1S7K,ARG\_52,12.08,-0.42,0,0  
3IVF,ASP\_369,2.82,0.63,-1.61,0  
3BPP,ASP\_61,3.44,0.42,-0.78,0  
3HZQ,GLU\_7,4.5,0,0,0  
1X7F,GLU\_258,4.57,0.07,0,0  
3L3P,GLU\_359,4.57,0.07,0,0  
1GQE,ARG\_337,12.76,-1.99,0,2.25  
3P2F,GLU\_18,2.43,0.35,-2.42,0  
1TR9,ARG\_77,11.47,-1.03,0,0  
2OBI,ARG\_16,3.32,0.42,-1.6,0  
3MTT,GLU\_482,4.5,0,0,0  
1T07,HIS\_11,6.88,0.52,0,-0.14  
3F1X,GLU\_183,4.23,0.49,-0.76,0  
3CAN,GLU\_165,4.19,0.07,-0.38,0  
3O48,GLU\_71,3.98,0.28,-0.8,0  
2B2H,LYS\_294,10.36,-0.14,0,0  
2B6P,LYS\_238,10.5,0,0,0  
3G9G,ARG\_174,11.94,-0.56,0,0  
2V4X,GLU\_72,3.91,0.49,-1.08,0  
2VGM,GLU\_310,3.98,0.28,-0.8,0  
3H04,ASP\_196,2.68,0.21,-1.33,0  
1PSW,LYS\_195,10.01,-0.49,0,0  
3LMF,GLU\_95,3.68,0.35,-1.17,0  
2RGY,CYS\_272,12.02,0,0,3.02  
2NYC,ASP\_299,1.42,1.12,-3.49,0  
3LPZ,ARG\_290,12.29,-0.21,0,0  
1ZP2,ARG\_97,12.15,-0.35,0,0  
3ETU,GLU\_322,4.64,0.14,0,0  
3DZ1,LYS\_269,10.15,-0.35,0,0  
2WB8,ARG\_552,12.08,-0.42,0,0  
1XKR,GLU\_156,4.8,0.86,-0.56,0  
2Z84,HIS\_120,6.36,0,0,-0.14  
3IV4,ARG\_60,11.94,-0.56,0,0  
3EVN,LYS\_281,10.29,-0.21,0,0  
3TIR,GLU\_39,4.38,0.7,-0.82,0  
3G9G,GLU\_96,4.26,0.56,-0.8,0  
3B79,LYS\_61,10.5,0,0,0  
2HP7,ARG\_53,12.43,-0.07,0,0  
4GA2,LYS\_78,10.29,-0.21,0,0  
3BWT,ASP\_683,3.01,0.56,-1.35,0  
2WB8,ASP\_589,2.84,0.28,-1.24,0  
1GPP,GLU\_428,3.56,0.21,-1.15,0  
1A8Q,ASP\_222,1.26,0.63,-3.16,0  
2E3S,GLU\_450,3.43,0.35,-1.42,0  
3PU6,GLU\_72,4.39,0.28,-0.39,0  
2H30,GLU\_108,3.91,0.28,-0.87,0  
3BQE,GLU\_325,3.69,0.42,-1.23,0  
2BT8,ASP\_252,3.4,0.7,-1.1,0  
2FC3,GLU\_55,5.02,0.52,0,0  
3VJ8,CYS\_147,11.6,0,0,2.6  
1V43,ARG\_68,12.29,-0.21,0,0  
1LFP,GLU\_149,4.51,0.21,-0.2,0  
2YLF,ARG\_89,12.01,-0.49,0,0  
200K,GLU\_50,4.57,0.07,0,0  
3I0C,ARG\_337,12.08,-0.42,0,0  
3C01,LYS\_95,10.5,0,0,0  
3DB9,ARG\_94,11.87,-0.63,0,0  
2OB5,LYS\_105,10.36,-0.14,0,0  
3BA1,ARG\_232,11.96,-2.48,0,1.94  
3M66,GLU\_400,4.78,0.28,0,0  
3B4D,HIS\_191,6.36,0,0,-0.14  
1DOV,ASP\_205,4.04,0.28,-0.04,0  
3L7N,GLU\_12,6.73,2.9,0,-0.67  
2GEN,CYS\_178,9,0,0,0  
1YTQ,HIS\_132,6.22,0,0,-0.28  
3E7P,LYS\_113,10.5,0,0,0  
1YM5,LYS\_108,10.5,0,0,0  
1XKR,LYS\_32,10.01,-0.49,0,0  
4AE7,HIS\_221,7.79,2.45,2.1,-3.26  
2P5D,GLU\_13,2.52,0.42,-2.4,0  
3T5B,ARG\_119,12.08,-0.42,0,0  
1XTZ,LYS\_151,10.29,-0.21,0,0  
1L2F,LYS\_187,10.5,0,0,0  
1NIJ,HIS\_134,7.09,0.8,0,-0.21  
3CZC,LYS\_93,10.5,0,0,0  
1WPS,LYS\_205,10.5,0,0,0  
2Q13,CYS\_341,9.07,0,0,0.07  
1NJ4,ASP\_295,2.97,0.28,-1.12,0  
1JKS,HIS\_73,6.29,0,0,-0.21  
2Z0M,LYS\_23,10.08,-0.42,0,0  
2BLL,TYR\_443,10.1,0.07,-0.45,0.48  
1XAW,ASP\_465,3.89,0.14,-0.05,0  
1GXN,TYR\_595,11.06,1.06,0,0  
1RLO,TYR\_249,9.9,0,-0.1,0  
1R9W,LYS\_318,10.15,-0.35,0,0  
4DNU,HIS\_339,0.63,0.55,0,-6.42  
2Q12,TYR\_181,13.56,0.36,0.8,2.4  
2Z84,HIS\_110,6.43,0,0,-0.07  
3ETV,GLU\_239,4.57,0.07,0,0  
3P28,ASP\_125,3.87,0.07,0,0  
3GEC,LYS\_445,10.5,0,0,0  
1R9W,GLU\_309,3.98,0.28,-0.8,0  
2E3C,TYR\_235,10,0,0,0  
4ESS,HIS\_75,8.28,3.6,2.4,-4.22  
3CIV,GLU\_112,4.71,0.21,0,0  
3GT0,LYS\_114,10.01,-0.49,0,0  
3HVM,LYS\_250,10.15,-0.35,0,0  
1YM5,CYS\_107,5.95,-4.13,0,1.08  
1EV8,HIS\_212,8.05,0.38,1.31,-0.14  
4EUG,ARG\_156,10.91,-1.59,0,0  
1O5J,TYR\_5,10.07,0.07,0,0  
1EW4,ARG\_20,11.59,-0.91,0,0  
1XIP,ASP\_151,2.57,0.42,-1.66,0  
3BZT,LYS\_317,10.5,0,0,0  
2EYI,GLU\_75,4.8,0.35,-0.05,0  
1AKO,TYR\_135,11.36,0.14,0,1.22  
3KVO,ASP\_90,2.52,0.28,-1.56,0  
1PZC,LYS\_55,10.15,-0.35,0,0  
2PGX,HIS\_151,7.23,0.87,0,-0.14  
3KEY,ASP\_390,2.51,0.49,-1.78,0  
4DIU,GLU\_146,4.5,0,0,0  
2B61,ARG\_231,12.36,-0.14,0,0  
3AU3,GLU\_536,4.34,0.21,-0.37,0  
2JHY,ASP\_140,3.31,0.28,-0.77,0  
4E9E,HIS\_567,5.17,1.42,0,-2.75  
3ZRI,GLU\_22,4.57,0.07,0,0  
2PGX,ARG\_219,10.95,-1.55,0,0  
3R2E,LYS\_106,10.5,0,0,0  
1X91,ASP\_114,3.35,0.35,-0.8,0  
3EVZ,GLU\_189,2.98,0.84,-2.36,0  
3M70,GLU\_48,4.71,0.21,0,0  
1O9G,ARG\_118,12.22,-0.28,0,0  
1PSW,ARG\_42,12.15,-0.35,0,0  
2A4D,ARG\_200,12.01,-0.49,0,0  
1ES9,ASP\_20,2.83,0.42,-1.38,0  
2GZQ,GLU\_103,4.51,0.14,-0.13,0  
2IQT,LYS\_222,10.36,-0.14,0,0  
1IDK,ASP\_207,2.23,0.7,-2.27,0  
3NZL,ARG\_23,12.29,-0.21,0,0  
2W2S,HIS\_128,6.57,0.21,0,-0.14  
3FFM,GLU\_87,4.5,0,0,0  
2A0J,LYS\_119,10.5,0,0,0  
2IRM,TYR\_241,10.07,0.07,0,0  
1XDZ,LYS\_48,10.43,-0.07,0,0  
3F1X,TYR\_139,10.11,0,0,0.11  
2Q5X,ASP\_773,4.03,0.28,-0.05,0  
1U74,GLU\_18,4.48,1.95,-1.97,0  
3JZ9,ARG\_390,11.31,-1.19,0,0  
3BPV,ARG\_41,11.31,-1.19,0,0  
3V55,LYS\_545,10.36,-0.14,0,0  
1UW7,ASP\_78,3.87,0.07,0,0  
2V4U,LYS\_535,10.29,-0.21,0,0  
2Q98,LYS\_124,10.36,-0.14,0,0  
2B0J,GLU\_78,4.71,0.21,0,0  
3ANJ,GLU\_324,3.91,0.21,-0.8,0  
3GW3,HIS\_349,8.05,1.7,0,-0.14  
1QQL,ARG\_38,12.5,0,0,0  
1Z3X,ASP\_10,3.75,0.07,-0.12,0  
15I7,GLU\_25,3.78,0.14,-0.87,0  
3FK5,ARG\_70,12.15,-0.35,0,0  
3C5V,GLU\_57,4.01,0.14,-0.63,0  
3OOP,GLU\_7,4.71,0.21,0,0  
1XEU,LYS\_207,10.43,-0.07,0,0  
2ZQ5,HIS\_17,4.4,0.86,0,-2.96  
3ZTA,ARG\_131,12.01,-0.49,0,0  
1X1E,ASP\_103,3.34,0.42,-0.88,0  
2R4Q,LYS\_242,10.5,0,0,0  
1H4U,ASP\_427,3.45,0.35,-0.71,0  
3C01,HIS\_69,6.43,0,0,-0.07  
3C6B,LYS\_68,10.5,0,0,0  
3T5B,LYS\_288,10.43,-0.07,0,0  
3DB9,TYR\_23,10,0,0,0  
3HUE,LYS\_210,10.5,0,0,0  
3G9G,LYS\_37,10.5,0,0,0  
4DNU,GLU\_158,4.5,0,0,0  
3BPV,CYS\_38,10.07,-0.04,0,1.11  
1L3K,ASP\_115,3.8,0,0,0  
3ELI,GLU\_15,3.62,0.07,-0.95,0  
3C6B,GLU\_214,4.64,0.14,0,0  
1WPA,LYS\_488,10.29,-0.21,0,0  
2BDD,LYS\_153,10.29,-0.21,0,0  
1DVO,LYS\_37,10.5,0,0,0  
1TXJ,LYS\_106,10.15,-0.35,0,0  
1OTM,ASP\_140,4.15,0.35,0,0  
2F4Q,ARG\_156,11.87,-0.63,0,0  
1C3K,LYS\_19,10.5,0,0,0  
2P1W,ARG\_231,12.01,-0.49,0,0  
2Z84,ARG\_133,11.94,-0.56,0,0  
3GT0,GLU\_59,4.13,0.21,-0.58,0  
3I0O,LYS\_240,10.29,-0.21,0,0  
2GZR,HIS\_188,1.67,0.86,-1.87,-3.82  
2IDC,GLU\_166,4.03,0,-0.47,0  
1C44,LYS\_68,10.5,0,0,0  
3RLE,LYS\_65,10.43,-0.07,0,0  
1YOY,ARG\_144,11.8,-0.7,0,0  
4EVF,GLU\_141,4.12,0.35,-0.73,0  
2FBI,ARG\_62,12.36,-0.14,0,0  
1YTD,LYS\_206,10.36,-0.14,0,0  
1YR6,GLU\_72,4.06,0.49,-0.93,0  
1EDG,ASP\_3,2.83,0.56,-1.53,0  
2HXB,ASP\_89,1.6,0.77,-2.97,0  
3ON1,LYS\_87,10.29,-0.21,0,0  
2ATR,GLU\_121,1.31,0.63,-3.82,0  
1JKS,GLU\_294,4.19,0.35,-0.66,0  
3JV1,ASP\_157,2.16,0.35,-1.99,0  
2CN1,LYS\_217,10.5,0,0,0  
3Q1C,ARG\_364,9.35,-4.54,0,1.39  
1J8B,GLU\_27,4.5,0,0,0  
1XTD,ASP\_135,3.17,0.35,-0.98,0  
2DVK,GLU\_72,2.55,0.77,-2.72,0  
1DVO,LYS\_57,10.22,-0.28,0,0  
4EUG,GLU\_97,4.54,0.84,-0.8,0  
2FPN,ARG\_115,11.94,-0.56,0,0  
3AUF,GLU\_193,4.02,0.35,-0.83,0  
3CNS,TYR\_259,10.02,0.02,0,0  
2VGM,LYS\_207,10.36,-0.14,0,0  
3HVM,LYS\_317,10.36,-0.14,0,0  
3GS9,ASP\_199,3.41,0.42,-0.81,0  
3M66,GLU\_332,4.78,0.28,0,0  
3F1X,GLU\_106,3.72,0.14,-0.92,0  
3FTT,LYS\_76,9.73,-0.77,0,0  
1P4X,HIS\_227,6.5,0,0,0  
1EYH,GLU\_152,4.5,0,0,0  
2CWC,ASP\_78,2.8,0.91,-1.91,0  
1JKS,LYS\_45,10.08,-0.42,0,0  
1X9G,GLU\_187,4.5,0,0,0  
1R3F,ASP\_118,3.09,0.21,-0.92,0  
2QRX,ARG\_507,12.01,-0.32,0,0  
2QV2,TYR\_116,10.6,1.36,-0.75,0  
1R29,TYR\_111,9.98,0.07,-1.1,1.01  
3EIZ,ASP\_168,3.21,0.42,-1.01,0  
3GS9,HIS\_90,2.45,0.8,0,-4.85  
3RLN,ARG\_612,10.58,-1.92,0,0  
3GEC,CYS\_511,8.64,-0.5,0.0,14  
3DHN,LYS\_179,10.36,-0.14,0,0  
1ATO,GLU\_388,4.5,0,0,0  
3JZ9,GLU\_516,4.5,0,0,0  
2V4X,TYR\_93,10,0,0,0  
3HVM,GLU\_180,4.85,0.35,0,0  
1O0X,ARG\_57,12.01,-0.49,0,0  
2BT8,ARG\_185,12.15,-0.35,0,0  
1TD6,GLU\_257,4.12,0.42,-0.8,0  
1X6J,GLU\_68,3.93,0.21,-0.78,0  
4E8B,ARG\_5,10.54,-1.96,0,0  
4EZB,GLU\_121,1.73,2.21,-3.94,-1.04  
3ELI,ASP\_91,2.95,0.35,-1.2,0  
1U7U,ARG\_344,12.29,-0.21,0,0  
1W24,ARG\_104,12.43,-0.07,0,0  
3HNX,ASP\_89,3.83,0.07,-0.04,0  
2AXO,GLU\_162,4.71,0.21,0,0  
2B0J,ASP\_194,0.56,1.05,-4.29,0  
1LZL,TYR\_269,12.19,2.19,0,0  
2D7J,GLU\_62,3.67,0.8,-1.63,0  
157K,HIS\_20,4.13,0.07,0,-2.44  
1PVT,GLU\_212,3.84,1.68,-2.34,0  
3DB9,ASP\_264,3.94,0.14,0,0  
3H04,LYS\_245,10.22,-0.28,0,0  
1WXF,ARG\_156,2.59,1.81,2.2,-4.92  
3ASA,GLU\_86,4.35,0.07,-0.22,0  
2IF4,GLU\_86,4.73,1.14,-0.91,0  
3JZN,LYS\_408,10.5,0,0,0  
2PPN,LYS\_73,10.29,-0.21,0,0  
3K8J,GLU\_56,2.82,0.49,-2.17,0  
3EZ7,ARG\_290,12.29,-0.21,0,0  
1EYH,ARG\_135,12.43,-0.07,0,0  
1R5Q,ARG\_82,11.94,-0.56,0,0  
3C6B,LYS\_2,10.5,0,0,0  
3JZN,GLU\_195,2.25,4.12,-2.02,-4.35  
1X7F,GLU\_332,4.32,0.42,-0.6,0  
1R9W,GLU\_345,3.91,0.21,-0.8,0  
2YWJ,TYR\_173,10,0,0,0  
1XDZ,GLU\_179,3.36,0.56,-1.7,0  
1X7F,HIS\_251,6.5,0,0,0  
3RFF,GLU\_22,3.91,0.21,-0.8,0  
1R16,HIS\_186,3.67,0,0,-2.83  
1P4X,ARG\_10,12.01,-0.49,0,0  
2QZQ,ARG\_24,11.87,-0.63,0,0  
1UCH,HIS\_26,6.15,0,0,-0.35  
3V7S,ARG\_250,12.15,-0.35,0,0  
3HKX,ARG\_48,12.22,-0.28,0,0

3MEW,LYS\_161,10.36,-0.14,0,0  
2CYG,TYR\_336,11.27,2.07,-0.8,0  
4DND,ASP\_63,3.76,0.07,-0.11,0  
4FZR,LYS\_211,10.43,-0.07,0,0  
3IOC,GLU\_260,4.2,0.49,-0.79,0  
4EKU,ARG\_184,11.73,-0.77,0,0  
1VSM,HIS\_103,6.36,0,0,-0.14  
2P65,ASP\_22,3.75,0,-0.05,0  
3KB5,LYS\_389,10.5,0,0,0  
4EF5,ARG\_191,11.8,-0.7,0,0  
1AIL,ARG\_37,11.94,-0.56,0,0  
2QV2,LYS\_188,10.29,-0.21,0,0  
1PSW,HIS\_274,3.03,0,0,-3.47  
1X04,CYS\_86,5.83,-3.31,0,0,14  
3HVM,LYS\_121,10.36,-0.14,0,0  
1C44,ASP\_53,0.86,0.98,-3.92,0  
3K8J,HIS\_132,7.07,0.57,0,0  
1XIP,ASP\_111,2.97,0.21,-1.04,0  
1TD6,GLU\_208,4.5,0,0,0  
3RE9,ASP\_69,1.02,0.49,-3.28,0  
2V4X,TYR\_102,10,0,0,0  
3H13,HIS\_328,6.5,0,0,0  
1WUG,LYS\_99,10.5,0,0,0  
2R4Q,LYS\_264,10.29,-0.21,0,0  
1UJ8,LYS\_36,10.29,-0.21,0,0  
1QVI,GLU\_219,4.26,0.28,-0.52,0  
2G5X,TYR\_148,9.26,0,-0.74,0  
3J5N,GLU\_261,4.5,0,0,0  
3MIT,ARG\_574,11.87,-0.63,0,0  
2J8A,ARG\_319,12.08,-0.42,0,0  
1R53,LYS\_311,10.5,0,0,0  
2OJQ,GLU\_406,4.07,0.86,-1.29,0  
2D7U,HIS\_43,1.58,1.6,-0.98,-5.54  
1WXQ,LYS\_262,10.5,0,0,0  
2ILR,TYR\_500,10.4,1.01,-0.61,0  
3U56,LYS\_129,10.29,-0.21,0,0  
3KV0,GLU\_181,4.5,0,0,0  
2CIU,ARG\_137,12.5,0,0,0  
2AD1,ASP\_222,3.5,0.42,-0.72,0  
1X04,LYS\_114,10.29,-0.21,0,0  
2R6Y,ARG\_233,11.87,-0.63,0,0  
4F3J,GLU\_202,4.5,0,0,0  
2IF4,GLU\_152,4.13,1.01,-1.38,0  
1X1E,GLU\_180,4.61,0.49,-0.38,0  
2AZL,LYS\_276,10.5,0,0,0  
4ECC,GLU\_29,4.57,0.07,0,0  
3H8Y,TYR\_45,10,0,0,0  
2YWJ,LYS\_57,10.43,-0.07,0,0  
3T5B,LYS\_293,9.8,-0.7,0,0  
3F7M,LYS\_362,9.66,-0.84,0,0  
2JKF,GLU\_42,4.5,0,0,0  
2NRK,ARG\_86,12.96,-1.35,0,1.81  
2NSN,GLU\_56,4.5,0,0,0  
1DUN,LYS\_35,10.22,-0.28,0,0  
1PGV,GLU\_372,4.57,0.07,0,0  
1R16,CYS\_216,8.68,-3.46,2.4,0.74  
1NJ4,ASP\_154,3.87,0.07,0,0  
2FM9,LYS\_213,10.29,-0.21,0,0  
1SNT,ASP\_306,2.94,0.28,-1.14,0  
3CNU,GLU\_6,3.94,0.14,-0.7,0  
2OKT,HIS\_340,6.5,0,0,0  
2FBQ,GLU\_193,4.57,0.07,0,0  
4DBL,ASP\_238,3.4,0.42,-0.82,0  
1TLV,LYS\_134,10.43,-0.07,0,0  
1DTP,CYS\_40,8.86,-0.22,-0.58,0.65  
3V3T,GLU\_257,4.64,0.14,0,0  
3T8R,ASP\_39,3.88,0.28,-0.2,0  
2OJQ,ASP\_411,3.4,0,-0.4,0  
3NBI,GLU\_37,4.67,0.28,-0.11,0  
3ADO,HIS\_242,6.36,0,0,-0.14  
2AH5,TYR\_193,10.2,0,0,0.2  
3C6B,ARG\_90,13.44,-1.46,0,2.4  
1V8E,HIS\_55,3.08,0,-1.8,-1.62  
1O9G,ARG\_46,11.94,-0.56,0,0  
3LJI,ASP\_268,3.33,0.35,-0.82,0  
4H89,TYR\_76,9.99,1.15,-1.16,0  
2YWJ,ASP\_109,3.57,0,-0.23,0  
2GAU,GLU\_137,3.24,1.44,-0.3,-2.4  
1OXZ,TYR\_294,9.7,0.14,-0.44,0  
2QDJ,ASP\_338,3.92,0.14,-0.02,0  
1Z3X,CYS\_122,9.5,-0.03,0,0.53  
2X4G,ARG\_119,11.46,-1.04,0,0  
3CCY,ARG\_39,12.01,-0.49,0,0  
1TR9,GLU\_257,3.14,0.42,-1.78,0  
3Q1C,LYS\_271,9.8,-0.7,0,0  
2QOP,ARG\_107,11.66,-0.84,0,0  
2A0J,GLU\_115,4.57,0.07,0,0  
2OEW,CYS\_250,9.54,0,0,0.54  
3QAV,TYR\_186,11.73,0.67,-0.07,1.14  
3TMO,ASP\_322,3.87,0.07,0,0  
1OLR,ASP\_222,4.01,0.21,0,0  
3IAT,HIS\_91,7.76,2.25,2.08,-3.07  
3BA1,CYS\_203,10.03,-0.44,0,1.47  
2H14,LYS\_67,10.5,0,0,0  
1X1E,GLU\_93,2.4,0.56,-2.65,0  
1R53,ASP\_369,3.21,0.21,-0.8,0  
3T57,ARG\_250,11.73,-0.77,0,0  
3LH5,HIS\_524,4.69,1.6,1.05,-4.47  
4DVD,GLU\_167,4.71,0.21,0,0  
2B78,GLU\_319,4.61,0.21,-0.1,0  
3N0K,GLU\_39,4.64,0.14,0,0  
1S17,ASP\_143,2.69,0.84,-1.95,0  
3G9T,CYS\_179,9.12,-1.43,0.51,1.04  
2OKT,TYR\_83,13.17,1.15,-0.05,2.07  
3UC9,GLU\_144,1.2,1.5,-2.4,-2.4  
2E35,LYS\_370,10.29,-0.21,0,0  
2A1V,GLU\_66,4.5,0,0,0  
3FWU,HIS\_49,6.5,0,0,0  
2OBI,TYR\_53,13.12,1.86,0,1.26  
1O59,HIS\_94,6.89,0.53,0,-0.14  
4DEZ,LYS\_230,10.36,-0.14,0,0  
3AU3,CYS\_451,8.68,-0.32,0,0  
1PSW,HIS\_199,6.01,0,0,-0.49  
3FHF,ARG\_89,10.83,-1.67,0,0  
1AKO,ARG\_200,11.81,-1.37,0,0.68  
4E8B,ARG\_88,12.5,0,0,0  
1VSM,LYS\_164,10.22,-0.28,0,0  
3EZ7,HIS\_136,6.43,0,0,-0.07  
2OSA,LYS\_316,10.15,-0.35,0,0  
2FL7,ASP\_113,3.8,0,0,0  
2F9F,CYS\_11,8.97,-0.03,0,0  
3GFP,LYS\_340,9.94,-0.56,0,0  
3V1Q,TYR\_519,10.73,0,0,0.73  
1WOU,CYS\_64,6.89,-2.25,0,0.14  
4EVF,HIS\_228,4.68,0,-0.15,-1.67  
3AU3,HIS\_444,6.43,0,0,-0.07  
3TIR,ASP\_87,3.33,0.56,-1.03,0  
3FNI,ASP\_46,2.56,0.42,-1.67,0  
2XMZ,ASP\_139,3.27,0.21,-0.74,0  
4GCO,ASP\_201,3.87,0.07,0,0  
1TJE,LYS\_122,10.5,0,0,0  
2PGX,ASP\_160,3.85,0.14,-0.09,0  
1WP5,TYR\_64,9.09,0,-0.91,0  
1O5T,GLU\_386,3.93,0.35,-0.92,0  
1L2F,TYR\_181,11.54,0.07,0,1.47  
3ADO,GLU\_257,4.39,0,-0.11,0  
3K9I,ARG\_123,12.08,-0.42,0,0  
3GA2,LYS\_105,10.29,-0.21,0,0  
3UV9,LYS\_371,10.5,0,0,0  
3CAX,TYR\_349,12.59,0,0,19.2,4  
1RZ2,ASP\_225,2.7,0.56,-1.66,0  
1V43,ARG\_124,12.36,-0.14,0,0  
1O17,HIS\_23,3.06,0,-0.71,-2.73  
3LH5,LYS\_760,10.15,-0.35,0,0  
1WYC,ARG\_302,12.22,-0.28,0,0  
3FK5,LYS\_277,10.5,0,0,0  
2ZTY,LYS\_42,10.5,0,0,0  
1YW5,LYS\_54,10.01,-0.49,0,0  
3F6F,TYR\_72,13.34,0.21,0.73,2.4  
3UC9,HIS\_53,7.13,0.69,0,-0.07  
3OOP,ASP\_61,2.23,0.56,-2.13,0  
2PPN,ASP\_79,3.29,0.07,-0.58,0  
2H85,GLU\_128,4.5,0,0,0  
3AUF,GLU\_45,3.78,0.35,-1.06,0  
2R51,LYS\_201,10.5,0,0,0  
1R3F,GLU\_227,4.5,0,0,0  
2D7U,GLU\_310,4.46,0.21,-0.25,0  
3BZT,LYS\_290,10.22,-0.28,0,0  
3F53,ASP\_275,3.99,0.21,-0.02,0  
3BQW,TYR\_314,11.75,0.07,-0.7,2.38  
2Q34,HIS\_114,3.75,0.07,0,-2.82  
3JZN,ASP\_155,2.22,0.56,-2.14,0  
2QEV,HIS\_91,3.44,0.94,0,-4  
1GPP,TYR\_48,12.53,0,0,13.2,4  
1ZBP,GLU\_121,4.5,0,0,0  
1JSX,HIS\_91,4.47,0,0,-2.03  
1R16,LYS\_4,10.15,-0.35,0,0  
2CXC,ARG\_37,13.2,-1.7,0,2,4  
2PWQ,ARG\_102,11.38,-1.12,0,0  
1R3D,TYR\_198,9.93,0,-0.07,0  
2OJQ,GLU\_567,4.5,0,0,0  
3CAN,GLU\_112,3.84,0.14,-0.8,0  
3H9W,HIS\_65,6.15,0,0,-0.35  
1TWU,CYS\_34,7.78,-1.29,0,0.07  
3K1H,GLU\_105,4.5,0,0,0  
1WLY,TYR\_148,10,0,0,0  
1DVO,ARG\_129,11.94,-0.56,0,0  
3E7P,HIS\_164,6.43,0,0,-0.07  
3M70,TYR\_248,11.42,0.07,0,1.35  
3GV0,HIS\_153,1.81,0,-0.61,-4.08  
2W1R,ARG\_79,11.94,-0.56,0,0  
3PZ9,TYR\_340,10.31,0,0,0.31  
1IDK,ARG\_349,11.89,-0.61,0,0  
3FXH,LYS\_67,10.5,0,0,0  
1L3K,HIS\_168,4.39,0.89,0,-3  
3FRR,LYS\_171,10.36,-0.14,0,0  
4DND,GLU\_13,4.57,0.07,0,0  
1X6J,ARG\_8,12.36,-0.14,0,0  
3H5T,ASP\_186,3.6,0.35,-0.54,0  
3HVW,GLU\_182,4.33,0.21,-0.38,0  
3OBS,LYS\_108,10.29,-0.21,0,0  
1AM2,GLU\_141,4.71,0.21,0,0  
3L7N,ASP\_198,3.8,0,0,0  
4AE7,CYS\_63,5.37,-4.06,0,0.43  
3V55,LYS\_665,10.36,-0.14,0,0  
1O59,LYS\_19,10.5,0,0,0  
2DFL,LYS\_27,9.94,-0.56,0,0  
1LFP,TYR\_174,11.26,1.26,0,0  
4ETX,GLU\_348,2.25,0.56,-2.81,0  
2GYZ,ARG\_30,12.15,-0.35,0,0  
3F53,GLU\_84,4.4,0.21,-0.31,0  
3BWT,GLU\_813,4.37,0.49,-0.62,0  
2W25,GLU\_135,4.08,0.21,-0.63,0  
3M7D,HIS\_56,1.71,0.36,-0.68,-4.48  
3OA7,LYS\_14,10.5,0,0,0  
2D7J,LYS\_45,10.36,-0.14,0,0  
1FHL,GLU\_16,0.8,0.47,-2.4,-1.77  
3IOC,LYS\_258,10.15,-0.35,0,0  
2BAA,ARG\_18,10.49,-2.01,0,0  
2IXM,GLU\_298,4.78,0.28,0,0  
3GV0,ARG\_141,12.43,-0.07,0,0  
3H8Y,ASP\_66,3.59,0.07,-0.28,0  
2OJQ,ARG\_422,12.36,-0.14,0,0  
4EUG,ARG\_49,12.29,-0.21,0,0  
3DHN,ASP\_156,2.35,0.84,-2.29,0  
1UXO,TYR\_178,12.67,0.35,-0.59,2.91  
2PWQ,GLU\_15,4.5,0,0,0  
3HOX,HIS\_105,6.85,0.63,0,-0.28  
2V81,ARG\_181,11.94,-0.56,0,0  
1O17,GLU\_259,4.42,0.35,-0.43,0  
1C3K,LYS\_104,10.22,-0.28,0,0  
1Q8B,GLU\_45,4.09,1.19,-1.6,0  
1NKD,GLU\_49,4.5,0,0,0  
1FKM,HIS\_335,6.5,0,0,0  
2G2D,ARG\_64,12.5,0,0,0  
2XHC,TYR\_235,10.17,0.17,0,0  
4AF2,LYS\_24,10.08,-0.42,0,0  
2ZQ5,ARG\_37,12.08,-0.42,0,0  
1R3D,TYR\_232,11.69,0.07,0,1.62  
2B78,ASP\_41,3.53,0.14,-0.41,0  
1RSS,ARG\_94,12.08,-0.42,0,0  
4FZR,GLU\_366,3.33,0.84,-2.01,0  
2Q34,GLU\_231,4.71,0.21,0,0  
3L7N,HIS\_8,7.09,3.41,2.4,-5.22  
2F4Q,HIS\_180,6.36,0,0,-0.14  
3H6Q,ARG\_55,11.8,-0.7,0,0  
2VGM,TYR\_111,13.91,0.42,0.79,2.71  
1PDB,CYS\_6,11.09,0,0,2.09  
3EVP,ASP\_260,3.94,0.14,0,0  
1WPA,LYS\_462,10.22,-0.28,0,0  
3Q1C,TYR\_388,12.67,1.31,-0.06,1.42  
2R05,ASP\_75,3.07,0.07,-0.8,0  
1EV8,GLU\_248,4.17,0.14,-0.47,0  
3V55,LYS\_621,10.08,-0.42,0,0  
2O8P,LYS\_189,10.29,-0.21,0,0  
3PBH,TYR\_16,9.27,0.07,-0.8,0  
1NJ4,GLU\_18,3.98,0.21,-0.73,0  
1MIX,GLU\_342,4.64,0.14,0,0  
1V43,LYS\_14,10.22,-0.28,0,0  
2CN1,GLU\_79,4.99,0.49,0,0  
1W7B,LYS\_212,10.5,0,0,0  
3EOD,LYS\_96,9.87,-0.63,0,0  
3T5B,ASP\_232,2.61,0.63,-1.82,0  
2P0Y,GLU\_119,4.57,0.07,0,0  
2CYG,TYR\_132,10.07,0.07,0,0  
3ON1,ARG\_15,12.43,-0.07,0,0  
3UC9,ASP\_167,3.93,0.28,-0.15,0  
2HRZ,GLU\_210,2.84,0.84,-2.5,0  
2AHE,GLU\_138,4.48,0.14,-0.16,0  
1D2K,LYS\_278,10.08,-0.42,0,0  
2B61,ASP\_158,4.01,0.21,0,0  
2Z61,ASP\_16,2.95,0.42,-1.27,0  
1CHD,LYS\_269,10.5,0,0,0  
2FD4,LYS\_435,10.5,0,0,0  
3GMS,ASP\_271,3.61,0.14,-0.33,0  
3LJI,LYS\_71,10.48,-0.16,0,1.64  
2Z61,CYS\_122,11.42,0,0,2.42  
3U56,ASP\_70,2.77,0.35,-1.38,0  
3BQW,GLU\_225,4.44,0.28,-0.34,0  
2V4U,CYS\_559,9,0,0,0  
2O8P,LYS\_89,10.29,-0.21,0,0  
3BA1,LYS\_67,10.29,-0.21,0,0  
3K8U,LYS\_90,10.22,-0.28,0,0  
2FXT,GLU\_300,3.96,0.53,-1.07,0  
1SUU,TYR\_614,10.84,0,-0.25,1.09  
3I47,GLU\_206,4.2,0.14,-0.44,0

2NRR,TYR\_406,10.07,0.07,0,0  
 3EUR,LYS\_126,10.08,-0.42,0,0  
 1QSZ,CYS\_589,9.11,-0.01,0,0.12  
 3MTT,TYR\_464,10,0,0,0  
 3V1Q,HIS\_592,4.61,1.75,0,-3.64  
 3V1Q,TYR\_522,12.22,0.42,0,1.8  
 2DOA,HIS\_295,4.5,0.05,0,-2.05  
 1H09,ASP\_324,3.7,0.07,-0.17,0  
 2F8H,ARG\_178,12.01,-0.49,0,0  
 4DEZ,HIS\_58,6.36,0,0,-0.14  
 2HNG,HIS\_79,7.09,0,8,0,-0.21  
 1XAW,ARG\_459,12.22,-0.28,0,0  
 3LD1,LYS\_81,10.5,0,0,0  
 1YLN,LYS\_205,10.29,-0.21,0,0  
 2BV9,ARG\_277,12.15,-0.35,0,0  
 2ZQ5,ARG\_134,11.94,-0.56,0,0  
 3HUE,LYS\_12,10.5,0,0,0  
 2W2S,GLU\_132,4.5,0,0,0  
 2PLQ,ASP\_70,3.72,0,-0.08,0  
 3GYW,LYS\_194,10.15,-0.35,0,0  
 4FCU,ARG\_189,11.63,-0.87,0,0  
 1GPP,GLU\_19,3.07,0.84,-2.27,0  
 4FH3,ARG\_286,12.5,0,0,0  
 3UX2,TYR\_77,12.83,0,-0.1,2.94  
 2OGQ,ARG\_483,11.87,-0.63,0,0  
 3CAX,TYR\_435,10.26,0,-0.72,0.98  
 3NR5,GLU\_110,3.12,0.45,-1.83,0  
 3U2R,ARG\_86,11.94,-0.56,0,0  
 1PGV,ARG\_296,12.22,-0.28,0,0  
 1H4U,GLU\_538,3.91,0.21,-0.8,0  
 2C2Y,LYS\_20,10.5,0,0,0  
 3A7L,ASP\_38,3.94,0.14,0,0  
 4F8A,ASP\_632,3.94,0.14,0,0  
 3DB9,TYR\_152,10.07,0.07,0,0  
 3EAZ,CYS\_119,3.83,-3.73,-2.8,1.36  
 1R53,GLU\_140,3.98,2.06,-0.8,-1.78  
 1NAF,GLU\_271,4.57,0.07,0,0  
 1LZL,ARG\_242,11.89,-0.91,0,0.3  
 3UC9,GLU\_75,3.05,0.35,-1.8,0  
 3BPV,ARG\_66,12.5,0,0,0  
 2PWQ,LYS\_67,10.5,0,0,0  
 3C2E,GLU\_153,4.01,1.4,-1.89,0  
 2B02,ASP\_452,4.01,0.21,0,0  
 1QQL,LYS\_128,10.5,0,0,0  
 3FXH,LYS\_4,10.5,0,0,0  
 2EDM,LYS\_88,10.08,-0.42,0,0  
 2ZOM,GLU\_11,2.73,0.56,-2.33,0  
 2E0T,ASP\_63,2.92,0.84,-1.72,0  
 3H5T,ASP\_205,3.07,0.35,-1.08,0  
 4ETX,HIS\_258,6.58,0.15,0,-0.07  
 2VAN,LYS\_289,10.22,-0.28,0,0  
 3BA1,LYS\_85,10.08,-0.42,0,0  
 1H09,LYS\_183,10.01,-0.49,0,0  
 3GEC,GLU\_474,4.44,0,-0.06,0  
 2NMU,GLU\_112,4.57,0.07,0,0  
 1RAJ,TYR\_81,12.09,2.44,0,-0.35  
 2QRX,HIS\_135,3.93,0.42,0,-2.99  
 2F8H,TYR\_331,10.72,1.58,-0.8,-0.06  
 4F85,ARG\_242,12.29,-0.21,0,0  
 2D2S,LYS\_751,10.15,-0.35,0,0  
 3O48,TYR\_99,11.24,0.22,-0.29,1.31  
 2WOZ,ASP\_506,3.8,0,0,0  
 1O9G,ARG\_78,12.36,-0.14,0,0  
 1WPA,HIS\_509,6.29,0,0,-0.21  
 4EZB,ARG\_195,12.36,-0.14,0,0  
 3OBS,GLU\_116,4.5,0,0,0  
 4AM1,HIS\_90,2.59,0.89,0,-4.8  
 2XHC,LYS\_19,10.29,-0.21,0,0  
 2OKT,ASP\_206,3.95,0.21,-0.06,0  
 2H14,ASP\_157,2.16,0.63,-2.27,0  
 2FL4,LYS\_7,10.5,0,0,0  
 3RHE,LYS\_23,10.29,-0.21,0,0  
 3ONT,LYS\_141,10.5,0,0,0  
 1T6L,ASP\_149,4.01,0.21,0,0  
 1GPP,ASP\_31,1.23,0.84,-3.4,0  
 1P4X,LYS\_76,10.5,0,0,0  
 3GOZ,GLU\_157,3.04,0.49,-1.95,0  
 2QVO,GLU\_55,4.5,0.21,-0.31  
 4GCO,CYS\_186,9.31,0,0,0,0  
 2B61,LYS\_234,10.36,-0.14,0,0  
 1Z3X,GLU\_184,4.64,0.14,0,0  
 2NYC,CYS\_202,9.55,-0.04,0,0.59  
 1SIG,ARG\_373,12.08,-0.42,0,0  
 2VAN,ASP\_263,1.88,0.77,-2.69,0  
 3I82,ARG\_213,12.01,-0.49,0,0  
 2D7J,ARG\_15,12.22,-0.28,0,0  
 3EVP,ASP\_287,4.01,0.21,0,0  
 3EZ7,HIS\_223,6.52,0.02,0,0  
 1Y0K,GLU\_15,4.71,0.21,0,0  
 1OLR,ASP\_169,2.52,0.56,-1.84,0  
 3IDW,ARG\_28,11.73,-0.77,0,0  
 2X4L,TYR\_236,9.29,0,-0.71,0  
 3ZXY,GLU\_240,4.3,0.28,-0.48,0  
 1R16,GLU\_59,4.75,0.28,-0.03,0  
 1D7O,ARG\_165,11.87,-0.63,0,0  
 2EJX,GLU\_44,3.73,0.14,-0.91,0  
 3ULX,ASP\_131,3.94,0.14,0,0  
 3PBH,ASP\_11,3.39,0.28,-0.69,0  
 3G9G,GLU\_85,3.46,0.49,-1.53,0  
 2JHY,GLU\_121,4.48,0.07,-0.09,0  
 1L2F,GLU\_88,4.26,0.07,-0.31,0  
 1R3F,GLU\_311,4.5,0,0,0  
 3MEW,ARG\_282,12.15,-0.35,0,0  
 3SMD,LYS\_78,10.5,0,0,0  
 2V4X,LYS\_128,10.22,-0.28,0,0  
 1AKO,ARG\_189,12.15,-0.35,0,0  
 1GPP,CYS\_17,8.09,-0.91,0,0  
 4FLE,GLU\_132,4.5,0,0,0  
 3O48,LYS\_126,10.5,0,0,0  
 1ZYL,GLU\_22,4.5,0,0,0  
 2VGM,HIS\_250,6.22,0,0,-0.28  
 2RH3,TYR\_99,11.11,0.43,0,0.68  
 1SUU,GLU\_565,4.85,0.35,0,0  
 3MTT,GLU\_504,4.54,0.07,-0.03,0  
 1SIG,ARG\_385,12.5,0,0,0  
 3OOP,GLU\_47,3.08,0.56,-1.98,0  
 2PLQ,HIS\_10,6.5,0,0,0  
 3GS9,TYR\_93,10.9,1.04,-0.14,0  
 3F1X,CYS\_146,5.41,-3.73,0,0.14  
 2OPJ,ARG\_17,13.43,-2.29,0,3.22  
 1YLN,ARG\_211,11.52,-0.98,0,0  
 1O59,TYR\_68,10.81,0.07,-0.4,1.13  
 1WXF,TYR\_255,10.62,0.27,-0.08,0.43  
 2D7U,GLU\_249,3.69,1.95,-0.36,-2.4  
 3K1H,LYS\_136,10.5,0,0,0  
 2CBE,TYR\_194,10.32,3.01,-1.93,-0.77  
 3MEW,LYS\_136,10.5,0,0,0  
 2B0A,GLU\_134,4.64,0.14,0,0  
 1NIJ,ARG\_93,11.94,-0.56,0,0  
 1J33,ARG\_144,11.8,-0.7,0,0  
 2IXM,ARG\_99,12.5,0,0,0  
 3EAZ,ASP\_123,3.92,0.14,-0.02,0  
 2G3A,GLU\_12,3.82,0,-0.68,0  
 1O0X,GLU\_16,4.57,0.07,0,0  
 2NMU,ARG\_17,11.8,-0.7,0,0  
 2H2W,TYR\_150,13.34,0.14,0.8,2.4  
 3PAC,GLU\_101,3.91,0.14,-0.73,0  
 1XEU,ASP\_237,2.56,1.05,-2.3,0  
 1UCH,ASP\_216,3.56,0.56,-0.8,0  
 4DBL,LYS\_280,10.22,-0.28,0,0  
 3IU5,LYS\_139,10.43,-0.07,0,0  
 1AK1,LYS\_44,10.43,-0.07,0,0  
 1V8E,LYS\_21,10.29,-0.21,0,0  
 2I88,GLU\_373,4.61,0.14,-0.03,0  
 2ZCX,GLU\_38,4.32,0.07,-0.25,0  
 1PVT,GLU\_140,4.5,0,0,0  
 2VGY,ASP\_54,3.84,0.07,-0.03,0  
 3QAV,LYS\_121,10.36,-0.14,0,0  
 3L3P,ARG\_524,11.8,-0.7,0,0  
 2VC8,LYS\_46,10.43,-0.07,0,0  
 1RAJ,LYS\_322,10.29,-0.21,0,0  
 3B21,ASP\_103,3.8,0,0,0  
 3CJW,ARG\_397,12.43,-0.07,0,0  
 2FD4,ASP\_473,3.21,0.21,-0.8,0  
 4EVF,LYS\_120,10.22,-0.28,0,0  
 3I47,GLU\_246,3.39,0.56,-1.66,0  
 3UOV,ASP\_103,3.37,0.42,-0.85,0  
 3QKY,TYR\_101,9.84,0.25,-0.41,0  
 4DND,GLU\_97,4.73,0.21,0.02,0  
 2HRZ,LYS\_306,10.36,-0.14,0,0  
 3CBN,TYR\_122,10,0,0,0  
 1L2F,GLU\_148,4.64,0.14,0,0  
 1OIS,LYS\_167,10.08,-0.42,0,0  
 2FBQ,HIS\_197,6.43,0,0,-0.07  
 3IVF,TYR\_373,9.63,0,-0.37,0  
 2H2Z,ARG\_76,12.43,-0.07,0,0  
 2QHT,LYS\_50,10.5,0,0,0  
 2JKF,ASP\_151,2.92,0.42,-1.31,0  
 1H4U,TYR\_440,9.43,0.14,-0.71,0  
 1MD6,TYR\_115,10.49,0.49,0,0  
 2A0J,HIS\_113,6.56,0.33,0,-0.28  
 3BPV,ASP\_51,1.5,0.63,-2.92,0  
 2QVO,LYS\_13,10.15,-0.35,0,0  
 1AK1,TYR\_47,11.5,1.75,-0.8,0.55  
 3UAH,HIS\_198,6.47,0.11,0,-0.14  
 1UXO,GLU\_48,4.57,0.07,0,0  
 2HXB,GLU\_105,4.18,0.56,-0.88,0  
 2A0J,ASP\_43,2.76,0.07,-1.11,0  
 2A6B,GLU\_89,4.64,0.14,0,0  
 2WB8,LYS\_659,10.5,0,0,0  
 3M66,GLU\_201,4.5,0,0,0  
 3ONT,GLU\_114,3.84,0.14,-0.8,0  
 1DCF,HIS\_1,6.43,0,0,-0.07  
 2H8O,LYS\_207,10.29,-0.21,0,0  
 2CXA,TYR\_93,10,0,0,0  
 3P51,LYS\_38,10.5,0,0,0  
 2HNG,ASP\_47,3.08,0.56,-1.28,0  
 2OEW,ARG\_306,11.94,-0.56,0,0  
 2B2H,ASP\_3,3.61,0.07,-0.26,0  
 2OBI,GLU\_163,1.86,0.56,-3.2,0  
 1MN3,LYS\_402,10.5,0,0,0  
 2ROS,ASP\_79,3.78,0.35,-0.37,0  
 2D2S,ASP\_696,3.84,0.21,-0.17,0  
 2JKF,TYR\_5,10,0,0,0  
 1DZF,GLU\_33,4.5,0,0,0  
 1YOY,ARG\_161,12.43,-0.07,0,0  
 4DBL,ARG\_205,11.66,-0.84,0,0  
 2R57,HIS\_377,5.61,4.63,-1.84,-3.68  
 2O4D,HIS\_55,8.06,1.6,2.82,-2.86  
 1H4U,TYR\_559,11.14,1.14,0,0  
 3UV9,HIS\_363,7.31,1.16,0,-0.35  
 157K,GLU\_77,4.64,0.14,0,0  
 3O7K,ARG\_153,11.73,-0.77,0,0  
 2B61,HIS\_135,7.43,1.29,0,-0.35  
 1XWM,GLU\_140,4.06,0.36,-0.8,0  
 1L2H,LYS\_93,10.5,0,0,0  
 3BQW,LYS\_75,10.5,0,0,0  
 3CSR,TYR\_3,11.1,0,0,1.1  
 3CE7,LYS\_99,10.29,-0.21,0,0  
 2PWQ,LYS\_12,10.5,0,0,0  
 3F1X,GLU\_168,4.98,0.48,0,0  
 1XTZ,ARG\_23,12.29,-0.21,0,0  
 1YTQ,LYS\_120,10.29,-0.21,0,0  
 1YLN,TYR\_218,8.16,0.14,-1.98,0  
 2CBE,ASP\_110,2.56,0.7,-1.94,0  
 1ZKZ,GLU\_31,3.35,0.21,-1.36,0  
 3C2E,LYS\_48,10.36,-0.14,0,0  
 3G9G,TYR\_247,8.6,0.14,-1.55,0  
 3LPZ,GLU\_22,4.5,0,0,0  
 1OTM,TYR\_170,10.21,0.21,0,0  
 3CAX,LYS\_413,10.43,-0.07,0,0  
 3RLN,HIS\_694,6.78,0.28,0,0  
 1R15,ARG\_275,12.5,0,0,0  
 2QZQ,ASP\_129,3.94,0.14,0,0  
 2V1L,TYR\_107,10,0,0,0  
 2E0T,ARG\_139,12.29,-0.21,0,0  
 1YTD,LYS\_14,10.43,-0.07,0,0  
 1TP6,ASP\_23,4.15,0.35,0,0  
 3GS3,ARG\_215,12.01,-0.49,0,0  
 1V43,GLU\_252,3.37,0.35,-1.48,0  
 1LZL,GLU\_224,4.57,0.07,0,0  
 4EVF,LYS\_12,10.01,-0.49,0,0  
 1J85,LYS\_90,10.5,0,0,0  
 2BV9,TYR\_208,8.8,0.35,-1.55,0  
 3PM2,LYS\_42,10.5,0,0,0  
 1R29,ASP\_17,3.85,0.21,-0.15,0  
 1O6D,ARG\_2,12.43,-0.07,0,0  
 1GPP,GLU\_108,3.98,0.28,-0.8,0  
 2OEW,GLU\_282,4.5,0,0,0  
 2YWJ,LYS\_30,10.08,-0.42,0,0  
 1GPP,HIS\_453,8.9,1.6,3.84,-3.04  
 3MEW,GLU\_201,4.54,0.21,-0.17,0  
 3RKV,ARG\_287,10.94,-1.56,0,0  
 3F7M,ARG\_156,10.42,-2.08,0,0  
 3SMD,TYR\_126,10.24,0.24,0,0  
 3CJW,ARG\_218,12.08,-0.42,0,0  
 3PU6,ASP\_40,3.22,0.14,-0.72,0  
 3LJ,GLU\_28,2.97,0.21,-1.73,0  
 1MUF,ASP\_256,4.035,-0.15,0  
 1AKO,HIS\_38,6.85,0.42,0,-0.07  
 2FXT,LYS\_333,10.08,-0.42,0,0  
 2VGM,ASP\_61,3.19,0.14,-0.75,0  
 4HDE,LYS\_117,10.5,0,0,0  
 3JVI,ARG\_51,12.5,0,0,0  
 2AZP,LYS\_252,10.5,0,0,0  
 1KCM,GLU\_54,2,0.7,-3.2,0  
 2GEN,HIS\_131,6.93,0.49,0,-0.07  
 1R15,TYR\_184,10,0,0,0  
 2AD1,GLU\_121,4.78,0.28,0,0  
 2G9D,HIS\_121,7.16,0.8,0,-0.14  
 1EYH,TYR\_75,10,0,0,0  
 1O59,LYS\_209,10.5,0,0,0  
 3UC9,GLU\_69,4.5,0,0,0  
 1SFE,ARG\_160,12.11,-1.65,0,1.26  
 3V1Q,CYS\_635,9.68,-0.41,0.24,0.84  
 1IAP,LYS\_93,9.87,-0.63,0,0  
 1M5I,GLU\_190,4.71,0.21,0,0  
 4F85,ARG\_197,11.52,-0.98,0,0  
 1AD6,CYS\_489,11.53,0,0,2.53  
 2CBE,GLU\_14,3.53,0.7,-1.68,0  
 2WB3,LYS\_362,10.5,0,0,0  
 3TIR,GLU\_217,2.57,0.49,-2.42,0  
 3DTE,TYR\_172,10.58,1.38,-0.8,0  
 4AF2,ARG\_47,11.66,-0.84,0,0  
 2Z84,ASP\_87,4.11,0.42,-0.11,0  
 1K95,CYS\_76,9.36,0,0,0.36



2EYI,GLU\_257,4.57,0.07,0,0  
 4E9E,GLU\_575,4.57,0.07,0,0  
 1D7O,TYR\_102,11.71,0.99,-0.8,1.52  
 1Q2Y,HIS\_44,5.62,1.75,0.41,-3.04  
 2V4U,HIS\_323,6.15,0.0,-0.35  
 2QK1,LYS\_552,10.43,-0.07,0,0  
 3FWU,GLU\_72,3.8,0.49,-1.19,0  
 2HRZ,ARG\_63,11.73,-0.77,0,0  
 3IRA,GLU\_136,3.5,0.49,-1.49,0  
 4AE7,HIS\_158,6.5,0,0,0  
 3JZ9,LYS\_466,10.15,-0.35,0,0  
 4DBX,ASP\_145,2.98,0.35,-1.17,0  
 3C2E,CYS\_47,7.66,-2.29,0,0.95  
 3EYE,ARG\_14,12.36,-0.14,0,0  
 3RNV,ARG\_456,11.87,-0.63,0,0  
 2FBI,ARG\_79,12.43,-0.07,0,0  
 2CWY,GLU\_25,4.5,0,0,0  
 1MJS,GLU\_396,1.32,0.89,-2.4,-1.67  
 3IL3,ARG\_248,11.8,-0.7,0,0  
 2A1V,HIS\_89,6.36,0,-0.14  
 1NAR,LYS\_182,10.5,0,0,0  
 2CBE,LYS\_127,10.29,-0.21,0,0  
 2E3S,ASP\_510,3.71,0,-0.09,0  
 2QVT,LYS\_145,10.15,-0.35,0,0  
 1MN3,LYS\_410,10.5,0,0,0  
 4H89,TYR\_160,10,0,0,0  
 1W7B,TYR\_235,11.88,0.28,-0.8,2.4  
 1RAJ,TYR\_326,9.35,0,-0.65,0  
 3F5D,ASP\_54,2.41,0.42,-1.81,0  
 3GG6,ASP\_55,3.49,0.49,-0.8,0  
 1VJG,ARG\_136,11.71,-2.15,0,1.36  
 1SIG,LYS\_371,10.08,-0.42,0,0  
 1PDB,LYS\_46,9.52,-0.98,0,0  
 3GFP,HIS\_355,6.54,0.04,0,0  
 2WB8,HIS\_630,3.1,0,0,-3.4  
 1U7U,ASP\_279,3.94,0.14,0,0  
 3R87,ARG\_35,10.85,-2.29,0,0.64  
 2G9D,ARG\_177,10.22,-2.28,0,0  
 1XFK,ARG\_163,12.08,-0.42,0,0  
 2I6I,HIS\_95,1.59,0.81,0,-5.71  
 3GOZ,HIS\_254,6.43,0,0,-0.07  
 3BB7,GLU\_98,2.81,1.01,-2.7,0  
 3RVC,CYS\_116,8.5,-0.64,0,0.14  
 3VJ8,TYR\_73,12.62,2.62,0,0  
 2QHT,HIS\_82,2.24,0.92,0,-5.18  
 3RE9,HIS\_244,6.43,0,0,-0.07  
 2OGQ,GLU\_569,4.7,0.21,-0.01,0  
 2H8O,ARG\_328,12.08,-0.42,0,0  
 1O3X,CYS\_256,9.58,0,0,0.58  
 3H13,TYR\_451,10,0,0,0  
 2GYZ,ASP\_82,2.1,1.12,-2.81,0  
 2H85,CYS\_333,8.81,-0.26,0,0.07  
 3IPZ,LYS\_89,10.43,-0.07,0,0  
 3T5B,LYS\_103,10.08,-0.42,0,0  
 1YDL,LYS\_17,9.8,-0.7,0,0  
 2HNG,LYS\_67,10.43,-0.07,0,0  
 3DHN,LYS\_49,10.5,0,0,0  
 1DZF,CYS\_214,9.62,0.48,0,0.14  
 2XWS,GLU\_22,2.45,0.35,-2.4,0  
 1NIJ,ASP\_191,3.01,0.14,-0.93,0  
 3BQE,ASP\_264,2.78,0.21,-1.23,0  
 3QKY,LYS\_58,10.43,-0.07,0,0  
 3RFY,LYS\_123,10.29,-0.21,0,0  
 4F85,ARG\_80,11.17,-1.33,0,0  
 2OGQ,TYR\_445,10.14,0.14,0,0  
 1D2K,LYS\_261,10.36,-0.14,0,0  
 1DUP,ASP\_92,3.63,0.14,-0.31,0  
 4AE7,LYS\_138,10.22,-0.28,0,0  
 3ADO,ARG\_177,12.5,0,0,0  
 1PSW,ARG\_121,12.64,-2.26,0,2.4  
 1YLN,CYS\_207,8.35,-0.72,0,0.07  
 1TUL,LYS\_37,9.8,-0.7,0,0  
 2D7U,ARG\_213,11.59,-0.91,0,0  
 3U2A,GLU\_106,4.5,0,0,0  
 1MIX,TYR\_241,12.12,0.31,-0.49,2.3  
 2Q34,ARG\_157,12.29,-0.21,0,0  
 1D7O,TYR\_158,11.65,0.07,-0.4,1.98  
 2CWC,LYS\_5,10.5,0,0,0  
 2R51,LYS\_286,10.36,-0.14,0,0  
 1WP5,LYS\_59,9.8,-0.7,0,0  
 1ES9,ASP\_192,1.57,1.05,-3.28,0  
 3GW3,CYS\_294,8.9,-0.17,0,0.07  
 2YWX,GLU\_154,4.55,0.14,-0.09,0  
 1OIS,LYS\_248,10.08,-0.42,0,0  
 1S7K,TYR\_66,10,0,0,0  
 3H04,TYR\_60,9.89,0.88,-0.99,0  
 1TR9,LYS\_275,10.22,-0.28,0,0  
 3RFF,GLU\_132,4.11,0.14,-0.53,0  
 1X6J,ASP\_66,2.14,0.63,-2.29,0  
 2H2W,TYR\_193,10.45,0,0,0.45  
 1Z9L,ASP\_37,3.94,0.14,0,0  
 2QVO,ASP\_30,3.7,0,-0.1,0  
 3RJZ,TYR\_120,11.59,0,0,1.59  
 1WJG,LYS\_23,10.36,-0.14,0,0  
 2CBE,LYS\_45,10.36,-0.14,0,0  
 1BN6,GLU\_219,4.23,1.67,-1.19,-0.75  
 3GS3,GLU\_62,4.02,0.07,-0.55,0  
 4DEZ,GLU\_126,4.64,0.14,0,0  
 1WPA,TYR\_420,9.61,0.21,-0.8,0.2  
 3GW3,ASP\_197,3.95,0.28,-0.13,0  
 3ONH,CYS\_452,8.79,-0.35,0,0.14  
 3UX2,LYS\_111,10.5,0,0,0  
 4H4J,TYR\_152,10.44,0.44,0,0  
 3BQW,TYR\_266,10.48,0.07,0,0.41  
 2V4U,LYS\_306,10.29,-0.21,0,0  
 3DB9,ARG\_221,12.5,0,0,0  
 3CCY,HIS\_66,3.49,0,0,-3.01  
 1OGL,HIS\_72,6.51,0.01,0,0  
 3F1X,GLU\_149,3.72,0.07,-0.85,0  
 2NYC,ASP\_197,3.85,0.14,-0.09,0  
 2IN0,GLU\_78,3.49,0.91,-1.93,0  
 1AK1,TYR\_83,13.93,0.07,0.8,3.06  
 2GEN,GLU\_50,2.45,0.35,-2.4,0  
 1O5T,LYS\_102,10.5,0,0,0  
 1LTU,ARG\_4,12.5,0,0,0  
 3H04,LYS\_207,10.5,0,0,0  
 2G9D,ARG\_138,12.08,-0.42,0,0  
 2CWC,ARG\_40,11.94,-0.56,0,0  
 1RKA,GLU\_107,3.86,0.07,-0.71,0  
 3RJZ,LYS\_102,10.43,-0.07,0,0  
 2GQV,LYS\_33,10.22,-0.28,0,0  
 1SQW,TYR\_92,9.27,0.07,-0.8,0  
 1YLN,ASP\_66,3.12,0.07,-0.75,0  
 3HUE,LYS\_262,10.5,0,0,0  
 3BQW,CYS\_63,10,0,0,1  
 3E5T,ARG\_92,11.09,-3.95,0,2.54  
 1WXF,LYS\_31,9.87,-0.63,0,0  
 2ZTY,LYS\_92,10.36,-0.14,0,0  
 2X4G,ARG\_170,11.8,-0.7,0,0  
 3EVN,GLU\_280,4.67,0.42,-0.25,0  
 2QHT,TYR\_19,12.88,0.21,0.22,2.45  
 3CBN,GLU\_160,4.5,0,0,0  
 3L0D,TYR\_79,11.54,0.14,0,1.4  
 4EF5,ARG\_253,11.66,-0.84,0,0  
 1TXJ,ASP\_129,3.77,0.07,-0.1,0  
 2IF4,GLU\_120,0.28,0.7,-1.59,-3.32  
 1AM2,TYR\_162,12.82,0.42,0,2.4  
 2D2S,ASP\_561,3.87,0.07,0,0  
 3C6B,ASP\_264,4.11,0.42,-0.1,0  
 3EVZ,LYS\_61,10.08,-0.42,0,0  
 3EJC,LYS\_82,10.29,-0.21,0,0  
 1SIG,ASP\_173,3.72,0,-0.08,0  
 1L2H,GLU\_83,1.86,0.56,-3.2,0  
 1NJ4,GLU\_179,6.15,3.25,-1.6,0  
 2YLF,CYS\_62,13.69,-0.15,1.8,3.03  
 2F4Q,ASP\_305,3.41,0.07,-0.46,0  
 3FS3,TYR\_79,10.039,0,-0.39  
 1TXJ,GLU\_137,4.71,0.21,0,0  
 3C2E,HIS\_281,2.26,0.1,-0.52,-3.82  
 3G9G,LYS\_242,10.15,-0.35,0,0  
 1SI7,LYS\_13,10.15,-0.35,0,0  
 2PLQ,CYS\_178,10.22,-1.3,0.69,1.84  
 1NAF,TYR\_253,13.42,0.28,0.74,2.4  
 2B3M,ARG\_81,11.87,-0.63,0,0  
 3HXK,ASP\_120,2.09,0.98,-2.69,0  
 3QAV,GLU\_114,3.94,0.14,-0.7,0  
 3CXS,LYS\_131,9.94,-0.56,0,0  
 1SNT,TYR\_181,10.98,0.95,0,0.03  
 1TXJ,GLU\_153,4.5,0,0,0  
 4DNU,GLU\_88,4.13,0.42,-0.79,0  
 3IRA,LYS\_158,10.29,-0.21,0,0  
 2G5S,ARG\_108,12.22,-0.28,0,0  
 1WJG,ARG\_70,11.87,-0.63,0,0  
 2ILR,CYS\_477,9.29,-0.05,0,0.34  
 1BN6,HIS\_70,6.24,0.02,0,-0.28  
 2PP6,ARG\_11,12.29,-0.21,0,0  
 1NWA,LYS\_6,10.29,-0.21,0,0  
 3VJ8,GLU\_137,4.5,0,0,0  
 4H4J,LYS\_262,10.22,-0.28,0,0  
 3G6S,GLU\_89,4.23,0.21,-0.48,0  
 3FTT,GLU\_153,4.5,0,0,0  
 3LJN,GLU\_15,3.99,0,-0.51,0  
 1OGL,ARG\_268,12.08,-0.42,0,0  
 2QEV,ARG\_126,12.43,-0.07,0,0  
 3BCY,HIS\_144,6.15,0,0,-0.35  
 3ZXY,ARG\_93,12.08,-0.42,0,0  
 3IVF,HIS\_228,2.54,0,-3.96  
 3CN5,ARG\_39,12.08,-0.42,0,0  
 1LFP,HIS\_12,6.81,0.52,0,-0.21  
 2QV2,GLU\_170,4.5,0,0,0  
 4FZN,HIS\_136,3.73,1.6,1.96,-6.33  
 3L7N,ARG\_24,11.87,-0.63,0,0  
 1MIX,ARG\_297,12.22,-0.28,0,0  
 2F9F,ARG\_57,12.5,0,0,0  
 3AU3,GLU\_578,4.71,0.21,0,0  
 3A4C,LYS\_509,10.5,0,0,0  
 2YWJ,GLU\_25,4.64,0.14,0,0  
 1ZCE,GLU\_24,4.71,0.21,0,0  
 3ANJ,ASP\_326,2.5,0.77,-2.08,0  
 1YTQ,ARG\_144,11.94,-0.56,0,0  
 1RSS,ARG\_102,12.36,-0.14,0,0  
 1PBV,GLU\_228,4.5,0,0,0  
 2A0J,GLU\_131,4.42,0.35,-0.43,0  
 3K1H,ASP\_104,4.01,0.21,0,0  
 1V43,ASP\_275,4.08,0.28,0,0  
 3IVF,ARG\_195,12.08,-0.42,0,0  
 2QVO,GLU\_12,3.97,0.28,-0.81,0  
 1V43,LYS\_121,10.5,0,0,0  
 1EQ6,TYR\_67,13.48,0.27,0.3,2.1  
 1F2V,HIS\_83,6.43,0,0,-0.07  
 1NAF,ASP\_204,3.23,0.07,-0.64,0  
 1RLO,GLU\_139,3.9,0.49,-1.09,0  
 4GA2,LYS\_47,10.36,-0.14,0,0  
 2DVK,LYS\_104,10.29,-0.21,0,0  
 3P28,GLU\_76,4.5,0,0,0  
 4DVD,ASP\_158,2.79,0.14,-1.15,0  
 3IPZ,ARG\_126,12.15,-0.35,0,0  
 1R5Q,GLU\_63,3.32,0.42,-1.6,0  
 3DSH,ARG\_263,10.31,-2.19,0,0  
 1S17,CYS\_90,9.51,-0.87,0,1.37  
 3EZ7,ARG\_345,11.73,-0.77,0,0  
 2RIK,LYS\_141,10.01,-0.49,0,0  
 2V4U,ASP\_505,3.74,0,-0.06,0  
 1J7G,LYS\_61,10.5,0,0,0  
 1TLV,TYR\_188,10,0,0,0  
 3FHF,GLU\_185,4.19,0.35,-0.66,0  
 3FHF,TYR\_159,9.41,0.21,-0.8,0  
 3V75,ASP\_206,3.45,0.21,-0.56,0  
 2Q13,ARG\_46,12.5,0,0,0  
 2GZR,ASP\_126,1.9,0.35,-2.25,0  
 2BDD,LYS\_124,10.15,-0.35,0,0  
 3H6Q,TYR\_120,10.04,0,-0.54,0.57  
 3B7X,ARG\_104,11.94,-0.56,0,0  
 3L0S,ARG\_333,12.43,-0.07,0.8,2.4  
 3QAV,LYS\_6,10.15,-0.35,0,0  
 1WOU,HIS\_16,6.5,0,0,0  
 3ETU,LYS\_149,10.5,0,0,0  
 2RIS,LYS\_125,10.29,-0.21,0,0  
 3ETU,ASP\_335,3.75,0.42,-0.48,0  
 1PGV,ASP\_237,4.05,0.28,-0.03,0  
 3EYE,GLU\_67,4.39,0,-0.11,0  
 3Q1C,ARG\_231,12.01,-0.49,0,0  
 3HUE,ARG\_16,13.22,-1.68,0,2.4  
 1PVT,ASP\_33,2.01,0.56,-2.35,0  
 3CAX,LYS\_334,10.22,-0.28,0,0  
 3L0S,ARG\_571,12.43,-0.07,0,0  
 2OB5,LYS\_122,10.22,-0.28,0,0  
 1QQE,ASP\_130,3.7,0.49,-0.59,0  
 3BB7,GLU\_240,4.39,0.35,-0.46,0  
 2EYI,CYS\_41,11.3,-0.15,0,2.45  
 3K9I,GLU\_125,4.57,0.07,0,0  
 1NAR,ASP\_154,2.53,0.7,-1.97,0  
 3FWU,ASP\_93,3.22,0.28,-0.86,0  
 3EVP,LYS\_289,10.36,-0.14,0,0  
 3T5B,ARG\_9,11.87,-0.63,0,0  
 2OEW,LYS\_215,10.5,0,0,0  
 1EQ6,LYS\_208,10.22,-0.28,0,0  
 3EAZ,GLU\_100,3.98,0.28,-0.8,0  
 1PDB,HIS\_87,5.43,0.85,0,-1.92  
 2B3M,GLU\_45,4.57,0.07,0,0  
 1SQH,ARG\_11,12.08,-0.42,0,0  
 3I00,ASP\_88,3.28,0.28,-0.8,0  
 3T57,ARG\_275,11.94,-0.56,0,0  
 3G6S,LYS\_130,10.15,-0.35,0,0  
 1EV8,LYS\_120,9.59,-0.91,0,0  
 3DB9,ASP\_215,3.2,0.56,-1.16,0  
 4EVF,ASP\_176,3.35,0.21,-0.66,0  
 1VJG,ASP\_44,3.94,0.14,0,0  
 1L2F,ARG\_227,11.88,-3.02,0,2.4  
 2EYI,HIS\_28,6.5,0,0,0  
 2W1R,ASP\_116,3.21,0.21,-0.8,0  
 1E5S,LYS\_254,10.22,-0.28,0,0  
 1IAP,GLU\_105,3.93,0.21,-0.77,0  
 3LH5,GLU\_665,4.64,0.14,0,0  
 1YTD,HIS\_182,8.02,0.3,3.4,-1.81  
 3C6B,LYS\_36,10.43,-0.07,0,0  
 1XTD,ARG\_79,12.15,-0.35,0,0  
 3L3P,GLU\_375,3.78,1.06,-1.78,0  
 3H5T,ARG\_226,12.29,-0.21,0,0  
 1J8B,HIS\_50,7.15,0.71,0,-0.07  
 1JKS,GLU\_59,3.8,0.07,-0.77,0  
 1R16,CYS\_248,10.16,-3.07,1.01,3.22  
 1ZYL,ARG\_127,11.87,-0.63,0,0  
 3KT9,LYS\_59,10.22,-0.28,0,0  
 3DSH,GLU\_418,4.63,0.21,-0.08,0  
 3LPZ,TYR\_182,13.34,0.14,0.8,2.4

1H09,ASP\_67,2.79,0.56,-1.57,0  
1ZBP,GLU\_117,4.09,0.07,-0.48,0  
2O8P,CYS\_144,8.95,-0.12,0,0.07  
2QEV,LYS\_108,10.15,-0.35,0,0  
1U7U,LYS\_403,10.22,-0.28,0,0  
4DBX,ARG\_41,12.01,-0.49,0,0  
2ZCO,LYS\_186,10.29,-0.21,0,0  
3TRE,ASP\_26,3.7,0.49,-0.59,0  
2BAA,LYS\_220,10.5,0,0,0  
2QVT,TYR\_141,11.71,0.07,-0.17,1.81  
3FTT,ARG\_27,11.54,-0.96,0,0  
3HNX,ASP\_5,3.88,0.21,-0.14,0  
1UOH,LYS\_18,10.43,-0.07,0,0  
1PSW,TYR\_85,8.34,1.34,-0.8,-2.2  
2QK1,ARG\_335,11.73,-0.77,0,0  
2BLL,ARG\_472,12.22,-0.28,0,0  
3CSR,TYR\_155,10,0,0,0  
4DIU,LYS\_154,10.5,0,0,0  
1VJG,ARG\_71,12.01,-0.49,0,0  
3M3P,GLU\_110,0.37,2.46,-4.81,-1.78  
4EZB,ASP\_217,3.96,0.28,-0.12,0  
4ETX,ARG\_246,12.22,-0.28,0,0  
3T57,HIS\_199,5.5,0.1,2.5,-2.25  
3ASA,ARG\_309,11.45,-1.73,0,0.68  
3LJI,TYR\_38,10.07,0.07,0,0  
2VGM,LYS\_46,10.43,-0.07,0,0  
2CXA,ARG\_114,12.5,0,0,0  
1MTZ,ASP\_268,4.01,0.21,0,0  
3P51,ASP\_26,2.12,0.35,-2.03,0  
1X8F,GLU\_279,4.5,0,0,0  
3HST,ASP\_238,3.67,0.28,-0.41,0  
3M16,ARG\_307,12.01,-0.49,0,0  
4EZB,GLU\_159,4.57,0.07,0,0  
1V43,ARG\_148,11.91,-0.59,0,0  
1S17,LYS\_118,10.22,-0.28,0,0  
1AKO,TYR\_248,9.59,1.08,-1.49,0  
1X6J,ASP\_2,3.31,0.35,-0.84,0  
4DNU,ARG\_323,12.22,-0.28,0,0  
3CSR,TYR\_87,10,0,0,0  
3CRM,ASP\_262,3.57,0.56,-0.79,0  
1LPL,ASP\_227,3.87,0.07,0,0  
3T8R,LYS\_62,10.5,0,0,0  
3C38,GLU\_98,4.5,0,0,0  
4EVF,ASP\_281,2.13,0.56,-2.22,0  
1XEU,GLU\_123,4.28,0.49,-0.71,0  
1P6F,ARG\_164,11.87,-0.63,0,0  
3F5D,ARG\_144,12.15,-0.35,0,0  
1SQH,ASP\_161,3.12,0.07,-0.75,0  
3F7M,ARG\_116,13.09,-1.81,0,2.4  
3V55,ARG\_719,10.45,-2.05,0,0  
3IV4,LYS\_42,10.29,-0.21,0,0  
2XHC,LYS\_69,10.22,-0.28,0,0  
1CBY,ASP\_196,3.07,0.77,-1.5,0  
2P1W,TYR\_236,10.66,0.66,0,0  
1Q46,ARG\_53,12.43,-0.07,0,0  
4H86,TYR\_153,10.58,0.58,0,0  
1YG2,GLU\_24,4.5,0.24,-0.24,0  
2EDM,ASP\_93,3.07,0.21,-0.94,0  
2RFA,GLU\_46,4.71,0.21,0,0  
2R51,ARG\_131,12.01,-0.49,0,0  
2ZOM,ARG\_298,13.1,-0.63,0,1.23  
1UCH,ARG\_66,12.83,-0.49,0,0.82  
1TR9,ARG\_67,11.94,-0.56,0,0  
2EYI,LYS\_195,10.43,-0.07,0,0  
1O59,HIS\_149,4.27,1.2,0,-3.43  
3ONT,GLU\_109,4.71,0.21,0,0  
1NAF,ARG\_180,12.5,0,0,0  
2ATR,LYS\_96,10.43,-0.07,0,0  
3G9T,ARG\_60,11.8,-0.7,0,0  
2H30,LYS\_180,10.5,0,0,0  
1O6D,ARG\_42,12.5,0,0,0  
1G5Z,LYS\_184,10.5,0,0,0  
2O8I,TYR\_26,10.21,0.21,0,0  
2D7J,GLU\_168,2.58,3.18,-2.73,-2.36  
4ACJ,GLU\_637,3.06,0.56,-2,0  
1FQI,LYS\_344,10.29,-0.21,0,0  
2JKF,CYS\_122,9.87,-0.62,0,1.49  
1DUN,ARG\_13,12.43,-0.07,0,0  
3ZSL,ASP\_239,1.85,0.35,-2.3,0  
3E7P,LYS\_256,9.94,-0.56,0,0  
1JKS,LYS\_29,10.29,-0.21,0,0  
2WZ9,GLU\_69,4.78,0.28,0,0  
1X9G,GLU\_157,4.71,0.63,-0.42,0  
2OKT,HIS\_112,6.74,0.73,0,-0.49  
1U53,TYR\_153,10.21,0.85,-1.43,0.78  
1KCM,LYS\_128,10.5,0,0,0  
2W1R,ASP\_154,2.8,0.21,-1.22,0  
1YIB,ASP\_190,3.69,0.07,-0.18,0  
2AXO,TYR\_82,10.55,0.91,-0.36,0  
4F85,ASP\_155,3.45,0.49,-0.84,0  
2OOK,ASP\_79,3.84,0.49,-0.45,0  
1T6L,LYS\_192,10.43,-0.07,0,0  
2Q07,LYS\_339,9.8,-0.7,0,0  
1BKB,LYS\_107,10.43,-0.07,0,0  
2D8N,HIS\_68,1.84,0.52,-1.7,-3.48  
2EFK,ASP\_200,3.83,0.28,-0.25,0  
1RKA,ASP\_66,2.99,0.63,-1.45,0  
1ZHV,LYS\_8,10.5,0,0,0  
3BB7,GLU\_282,1.78,1.02,-1.6,-2.15  
1J85,ARG\_46,12.36,-0.14,0,0  
1SNT,HIS\_18,6.66,0.3,0,-0.14  
3ONT,CYS\_67,8.79,-0.28,0,0.07  
1DTO,TYR\_155,10,0,0,0  
1P4X,HIS\_185,0.65,0,-2.4,-3.45  
2V81,GLU\_187,3.45,0.14,-1.19,0  
1LN4,ARG\_86,11.66,-0.84,0,0  
1DCF,LYS\_112,10.08,-0.42,0,0  
1FO9,ARG\_393,11.73,-0.77,0,0  
4GA2,ASP\_77,3.02,0.07,-0.85,0  
4EKU,LYS\_57,10.22,-0.28,0,0  
2BDD,ARG\_36,12.36,-0.14,0,0  
1RIG,ARG\_152,11.94,-0.56,0,0  
2CIU,LYS\_217,10.5,0,0,0  
1R3D,HIS\_53,3.04,1,0,-4.46  
3OIP,GLU\_176,4.18,0.28,-0.6,0  
3M16,CYS\_246,11.24,-1.14,1.19,2.18  
3E7P,LYS\_257,9.52,-0.98,0,0  
1ZBP,GLU\_128,4.5,0,0,0  
2GZR,ASP\_100,3.35,0.35,-0.8,0  
3O48,TYR\_82,12.91,0.94,0.2,1.77  
2QRX,LYS\_64,10.5,0,0,0  
2F4Q,TYR\_55,12.61,0.02,21,2.4  
2FC3,GLU\_88,4.5,0,0,0  
3JZN,CYS\_84,7.17,-2.19,0,0.36  
2ZOM,LYS\_161,10.36,-0.14,0,0  
1WNH,HIS\_211,6.48,0.12,0,-0.14  
2VGY,CYS\_113,9.34,-0.2,0.054  
2XHC,LYS\_227,10.08,-0.42,0,0  
2DFL,ARG\_157,11.15,-1.35,0,0  
3BPP,GLU\_191,3.53,0.77,-1.74,0  
1JB3,ARG\_40,12.08,-0.42,0,0  
2PP6,ARG\_78,12.22,-0.28,0,0  
1O5J,LYS\_56,10.15,-0.35,0,0  
2OKT,LYS\_131,10.5,0,0,0  
2FPN,GLU\_116,4.54,1.34,-1.3,0  
1OXZ,LYS\_210,9.94,-0.56,0,0  
1R53,CYS\_221,11.39,-1.44,0.3,3.53  
2ZOM,LYS\_176,10.08,-0.42,0,0  
1TLV,HIS\_159,0.75,0,-1.8,-3.95  
2CXA,HIS\_73,6.43,0,0,-0.07  
1GXN,LYS\_405,10.29,-0.21,0,0  
3CQ1,HIS\_57,6.5,0,0,0  
3SMD,LYS\_77,10.43,-0.07,0,0  
2YWK,CYS\_56,6.94,-2.06,0,0  
4FD6,LYS\_188,10.36,-0.14,0,0  
2NRK,GLU\_69,4.06,0,-0.44,0  
2YX0,ARG\_29,11.87,-0.63,0,0  
3HUE,CYS\_291,9,0,0,0  
3M3P,GLU\_45,3.67,0.35,-1.18,0  
3IV4,GLU\_16,4.5,0,0,0  
4DEZ,GLU\_135,4.5,0,0,0  
1X9G,ASP\_119,3.2,0.28,-0.87,0  
1BGF,LYS\_84,10.5,0,0,0  
1ANU,LYS\_28,10.36,-0.14,0,0  
3KB5,ARG\_368,10.9,-1.6,0,0  
1T6L,HIS\_56,6.5,0,0,0  
1PDB,GLU\_171,4.57,0.14,-0.07,0  
3C2E,ASP\_25,3.8,0,0,0  
2A1V,LYS\_37,10.36,-0.14,0,0  
2WB3,ARG\_330,11.66,-0.84,0,0  
3N2T,GLU\_66,3.6,0.52,-0.14,-1.28  
3HUE,ASP\_269,3.12,0.49,-1.16,0  
1H09,ASP\_136,2.57,0.56,-1.79,0  
2IQT,ASP\_109,3.71,0,-0.09,0  
2A0J,HIS\_70,6.43,0,0,-0.07  
2HNG,GLU\_97,3.78,0.07,-0.79,0  
3MTT,GLU\_465,4.64,0.14,0,0  
1O59,CYS\_282,9.07,0,0,0.07  
2OOK,LYS\_60,10.5,0,0,0  
3BQE,ASP\_219,3.26,0.28,-0.82,0  
2B02,ARG\_440,12.22,-0.28,0,0  
2OSA,GLU\_313,4.5,0,0,0  
1FQI,ARG\_295,12.22,-0.28,0,0  
1EV8,TYR\_153,10,0,0,0  
1XKR,LYS\_54,10.5,0,0,0  
2BV9,ARG\_265,11.59,-0.91,0,0  
2I88,LYS\_379,10.15,-0.35,0,0  
1SJJ,LYS\_78,10.29,-0.21,0,0  
4EKU,TYR\_166,10.06,0,-0.51,0.58  
2V4U,ASP\_435,3.69,0.63,-0.74,0  
1DTO,TYR\_178,11.72,0,0,1.72  
2YT4,ARG\_663,12.15,-0.35,0,0  
1Q8B,ARG\_61,11.73,-0.77,0,0  
1CBY,TYR\_213,11.7,1.7,0,0  
1RWZ,LYS\_79,10.29,-0.21,0,0  
3HKX,TYR\_166,10.65,0,0,0.65  
2OEW,GLU\_35,4.54,0.21,-0.17,0  
1A8Q,LYS\_234,10.43,-0.07,0,0  
2FL4,ASP\_78,0.88,0.7,-3.62,0  
2Z14,LYS\_29,10.43,-0.07,0,0  
2QV2,ARG\_130,12.01,-0.49,0,0  
3CAN,GLU\_82,2.95,0.35,-1.9,0  
1SNT,ARG\_204,12.5,0,0,0  
2I88,ASP\_456,3.87,0.07,0,0  
2WOZ,ARG\_464,12.08,-0.42,0,0  
2RGY,CYS\_145,9.02,-0.19,0,0.21  
1WYC,ARG\_190,12.36,-0.14,0,0  
2E3S,TYR\_381,10,0,0,0  
1TD6,ASP\_151,2.22,0.63,-2.21,0  
4EF5,ARG\_281,12.5,0,0,0  
3BB7,GLU\_273,3.56,0.35,-1.29,0  
4ETX,ARG\_330,13.24,-2.37,0,3.11  
2OBI,ARG\_33,12.01,-0.49,0,0  
1TWU,GLU\_109,4.64,0.14,0,0  
1PSW,GLU\_164,3.95,0.21,-0.76,0  
1OTM,ARG\_184,12.43,-0.07,0,0  
2FBI,ASP\_75,3.38,0.49,-0.92,0  
2QRX,CYS\_59,8.43,-1.05,0,0.47  
3G53,ASP\_209,3.45,0,-0.35,0  
1A8Q,ASP\_74,1.07,0.56,-3.29,0  
3BPP,HIS\_107,2.05,0.6,0,-5.06  
1EDG,ASP\_126,0.94,0.28,-2.06,-1.08  
1J33,GLU\_239,3.55,0.56,-1.51,0  
2OKT,GLU\_94,4.05,0.14,-0.59,0  
4E6S,HIS\_64,6.36,0,0,-0.14  
3FXH,TYR\_56,10,0,0,0  
2CWY,ARG\_56,12.36,-0.14,0,0  
3EVP,LYS\_119,10.5,0,0,0  
1UOH,GLU\_120,3.39,0.07,-1.18,0  
1YG2,HIS\_128,6.43,0,0,-0.07  
2P52,LYS\_117,10.5,0,0,0  
1R53,ASP\_339,4.22,0.42,0,0  
2BAA,TYR\_230,13.41,0.21,0.8,2.4  
1WP5,HIS\_125,6.6,0.1,0,0  
3S0A,LYS\_102,10.01,-0.49,0,0  
1RIS,GLU\_246,3.72,0.14,-0.92,0  
1J85,CYS\_83,9,0,0,0  
1RI6,HIS\_314,7.01,0.58,0,-0.07  
2D7J,LYS\_40,10.22,-0.28,0,0  
2Q99,ASP\_281,2.97,0.49,-1.31,0  
3H04,HIS\_237,6.36,0,0,-0.14  
3JSN,HIS\_49,6.45,0.16,0,-0.21  
2W0G,TYR\_174,10.14,0.21,-0.07,0  
1H09,TYR\_293,10,0,0,0  
3VJ8,GLU\_250,3.76,0.35,-1.09,0  
1SBX,GLU\_183,4.11,0.28,-0.67,0  
3Q9P,GLU\_119,4.11,0.28,-0.67,0  
4E88,GLU\_162,3.53,0.63,-1.6,0  
2PLQ,LYS\_197,10.22,-0.28,0,0  
1WRU,CYS\_118,10.6,0,0,1.6  
3QAV,ASP\_63,2.4,0.84,-2.24,0  
2EHG,TYR\_132,11.79,0.0,1.79  
1FKM,ARG\_370,11.7,-0.8,0,0  
2A0J,ARG\_82,11.59,-0.91,0,0  
2P1W,GLU\_184,3.1,9.5,-3.44,0  
1YDL,GLU\_11,4.5,0,0,0  
2CN1,HIS\_145,7.2,0.84,0,-0.14  
2YWK,LYS\_158,10.29,-0.21,0,0  
3F53,TYR\_54,10.28,0,0.28  
2WB8,GLU\_554,4.02,0.25,-0.73,0  
3GS9,TYR\_308,10,0,0,0  
2QDJ,LYS\_329,10.5,0,0,0  
4F85,GLU\_78,3.63,0.56,-1.43,0  
3HVM,GLU\_145,4.75,4.36,-1.84,-2.27  
2BLL,ARG\_505,13.03,-1.87,0,2.4  
1DTO,ASP\_122,3.87,0.07,0,0  
2V1L,ASP\_54,3.21,0.21,-0.8,0  
3MEW,TYR\_260,10.65,1.74,-1.09,0  
3DTE,TYR\_58,10,0,0,0  
2VGM,ASP\_202,3.7,0.7,-0.8,0  
2DVK,ARG\_27,11.24,-1.26,0,0  
3V4G,GLU\_150,4.57,0.07,0,0  
3AU3,ASP\_539,3.64,0,-0.17,0  
1O6D,ARG\_39,11.8,-0.7,0,0  
2FL4,LYS\_106,10.43,-0.07,0,0  
3CAX,LYS\_410,10.5,0,0,0  
4ECC,ARG\_86,11.87,-0.63,0,0  
2I88,ASP\_473,2.7,0.42,-1.52,0  
1MIX,LYS\_364,10.5,0,0,0  
1Z9L,ARG\_38,11.94,-0.56,0,0  
2B0J,HIS\_52,5.04,0.93,0,-2.39  
3KEY,TYR\_459,10,0,0,0  
3H8Y,ARG\_15,12.08,-0.42,0,0  
1IAP,GLU\_203,4.64,0.14,0,0  
1NJ4,GLU\_251,2.93,0.35,-1.92,0  
2EFK,TYR\_205,10,0,0,0

2HP7,GLU\_60,4.05,0.35,-0.8,0  
 4E8B,GLU\_122,4.5,0,0,0  
 1ZP2,CYS\_92,8.41,-0.59,0,0  
 3RHE,ASP\_80,3.26,0.28,-0.82,0  
 1E59,GLU\_38,4.71,0.21,0,0  
 1TWU,HIS\_56,6.37,0.01,0,-0.14  
 2CN1,TYR\_96,10.77,0.07,-0.37,1.07  
 3RE9,LYS\_116,10.15,-0.35,0,0  
 1R3F,LYS\_31,10.5,0,0,0  
 3ETU,TYR\_226,10.99,0.29,0,0.7  
 3NZL,LYS\_65,10.01,-0.49,0,0  
 3JV1,ASP\_177,4.01,0.21,0,0  
 1VSM,ARG\_95,12.5,0,0,0  
 2OKT,ASP\_39,2.88,0.49,-1.41,0  
 1UOH,HIS\_177,3.88,1.36,0,-3.98  
 1RKA,ASP\_67,1.27,0.98,-3.51,0  
 1WLY,GLU\_257,3.96,0.56,-1.1,0  
 2Q34,GLU\_158,4.57,0.07,0,0  
 3IV4,GLU\_106,4.57,0.07,0,0  
 2XHC,LYS\_4,10.5,0,0,0  
 2A6B,GLU\_212,8.18,3.68,0,0  
 3BQW,TYR\_191,10,0,0,0  
 3OOP,ASP\_107,3.97,0.21,-0.04,0  
 2PGE,HIS\_235,6.43,0,0,-0.07  
 1UAJ,ASP\_135,3.21,0.21,-0.8,0  
 1MTZ,ASP\_222,3.42,0.42,-0.8,0  
 2OEW,LYS\_298,10.36,-0.14,0,0  
 3FRR,LYS\_38,10.43,-0.07,0,0  
 3CRM,ARG\_213,11.94,-0.56,0,0  
 2AHE,ARG\_142,12.29,-0.21,0,0  
 3I4T,GLU\_183,4.5,0,0,0  
 1ZP2,GLU\_225,4.57,0.07,0,0  
 3EZ7,LYS\_286,10.5,0,0,0  
 2YT4,ARG\_696,9.81,-2.69,0,0  
 4EVF,LYS\_295,10.5,-0.35,0,0  
 4ACJ,GLU\_714,4.5,0,0,0  
 1RAJ,LYS\_311,9.87,-0.63,0,0  
 2ZCO,ASP\_109,3.91,0.14,-0.03,0  
 1NAR,LYS\_197,10.5,0,0,0  
 2FL7,ASP\_205,3.42,0.42,-0.8,0  
 3RHE,LYS\_89,10.5,0,0,0  
 1XWM,TYR\_206,9.84,0,-0.16,0  
 1P4X,LYS\_178,10.5,0,0,0  
 2RFA,GLU\_184,4.85,0.35,0,0  
 3MTT,LYS\_541,10.5,0,0,0  
 1YB2,ASP\_93,2.89,0.14,-1.05,0  
 1UOH,LYS\_30,10.5,0,0,0  
 1R53,ARG\_132,10.8,-1.7,0,0  
 2B0J,LYS\_182,10.36,-0.14,0,0  
 3C2E,ARG\_143,12.15,-0.35,0,0  
 3T5B,ASP\_396,4.08,0.28,0,0  
 3H13,TYR\_423,12.44,3.26,-1.29,0.46  
 2OOK,ARG\_95,12.36,-0.14,0,0  
 3DTE,ARG\_107,12.5,0,0,0  
 2B0A,GLU\_186,4.5,0,0,0  
 1V43,GLU\_261,4.75,0.28,-0.03,0  
 1L2F,GLU\_171,4.57,0.07,0,0  
 4EVF,GLU\_33,3.11,0.42,-1.82,0  
 1PSW,TYR\_135,13.87,1.85,0.2,0.2  
 1XKR,GLU\_42,4.64,0.14,0,0  
 2P1W,HIS\_106,5.36,1.6,1.07,-3.8  
 1O6D,ARG\_28,11.87,-0.63,0,0  
 2FZP,GLU\_252,3.54,0.56,-1.52,0  
 1F09,ARG\_427,12.22,-0.28,0,0  
 2RGY,GLU\_323,3.09,0.33,-0.99,-0.75  
 4FD6,GLU\_156,4.05,0.35,-0.8,0  
 2P65,ASP\_51,3.81,0.07,-0.06,0  
 2A1V,CYS\_17,9.71,-1.05,0,1.76  
 1ZP2,HIS\_176,6.5,0,0,0  
 2ZCX,GLU\_145,3.53,0.42,-1.39,0  
 2EYI,GLU\_57,4.59,0.35,-0.26,0  
 3R87,ASP\_83,3.94,0.14,0,0  
 1X9G,CYS\_156,10.06,0,0,1.06  
 1GXN,TYR\_518,11.1,0.07,0,1.03  
 3BCH,HIS\_193,7.16,0.87,0,-0.21  
 1MUF,ASP\_161,3.87,0.07,0,0  
 1X7F,LYS\_170,10.36,-0.14,0,0  
 4H86,ASP\_27,3.61,0.21,-0.4,0  
 1WYC,ASP\_384,2.59,0.42,-1.63,0  
 2RJD,LYS\_480,10.43,-0.07,0,0  
 1C44,LYS\_100,10.5,0,0,0  
 1SIG,ASP\_191,4.15,0.35,0,0  
 3C38,LYS\_142,10.29,-0.21,0,0  
 2FC3,ASP\_58,3.94,0.14,0,0  
 1DTO,ASP\_153,2.86,0.7,-1.63,0  
 2ZTY,TYR\_22,10,0,0,0  
 1DZF,LYS\_91,10.5,0,0,0  
 3NR5,ASP\_22,3.86,0.14,-0.08,0  
 1RLO,ASP\_29,1.92,0.63,-2.51,0  
 2OPJ,CYS\_54,10.85,-0.51,0,2.36  
 2AD1,ASP\_27,3.88,0.21,-0.13,0  
 2H2W,ARG\_180,11.94,-0.56,0,0  
 4H89,ARG\_144,12.36,-0.14,0,0  
 1VSM,GLU\_157,4.57,0.07,0,0  
 3MEW,ARG\_165,11.94,-0.56,0,0  
 1X1E,GLU\_92,4.5,0,0,0  
 2EFK,GLU\_92,4.5,0,0,0  
 3CBN,HIS\_164,6.5,0,0,0  
 3CRM,ARG\_95,12.01,-0.49,0,0  
 4FH3,LYS\_240,10.08,-0.42,0,0  
 3GMS,GLU\_319,4.71,0.21,0,0  
 1XDZ,TYR\_225,10.57,0.07,0,0.5  
 2P52,ASP\_181,2.88,0.98,-1.9,0  
 2X4J,LYS\_20,10.29,-0.21,0,0  
 1EV8,GLU\_223,4.57,0.07,0,0  
 1YTQ,GLU\_138,2.84,0.42,-2.09,0  
 3LD1,CYS\_356,6.9,-2.18,0,0.07  
 1FKM,HIS\_327,6.49,0.14,0,-0.14  
 2Z61,TYR\_261,10.82,0,0,0.82  
 1LPL,GLU\_153,3.78,0.21,-0.93,0  
 4HDE,GLU\_38,3.91,0.21,-0.8,0  
 2ZQ5,TYR\_160,10,0,0,0  
 2AZP,CYS\_73,8.66,-0.52,0,0.18  
 1LZL,TYR\_220,9.88,0.07,-0.19,0  
 1X8F,LYS\_2,10.5,0,0,0  
 1J83,GLU\_12,4.96,0.49,-0.03,0  
 3ILC,ARG\_139,11.8,-0.7,0,0  
 1MIX,LYS\_196,10.5,0,0,0  
 3T5B,GLU\_296,4.54,0.14,-0.1,0  
 1KCM,LYS\_55,10.5,0,0,0  
 2ZQ5,CYS\_266,10.23,-0.07,0,1.3  
 3G9G,ARG\_98,12.22,-0.28,0,0  
 1ZHV,ASP\_56,3.46,0.21,-0.55,0  
 3GOZ,LYS\_153,10.01,-0.49,0,0  
 1NRI,ARG\_149,12.22,-0.28,0,0  
 2X5Y,GLU\_739,3.27,0.56,-1.79,0  
 3MM4,ARG\_987,11.83,-0.67,0,0  
 3ZXY,ASP\_175,2.13,1.05,-2.73,0  
 2PLQ,ASP\_294,3.48,0.14,-0.46,0  
 1NAF,LYS\_183,10.5,0,0,0  
 2R05,GLU\_302,4.18,0.35,-0.67,0  
 4AM1,LYS\_180,9.94,-0.56,0,0  
 1YR6,TYR\_64,13.44,0,-0.43,3.87  
 2ZCO,ASP\_5,2.1,0.35,-2.06,0  
 2AXO,GLU\_160,4.62,0.07,0.05,0  
 1SQH,ASP\_8,1.65,1.05,-3.2,0  
 1KCM,GLU\_46,4.57,0.07,0,0  
 1XKR,ASP\_103,2.08,0.63,-2.35,0  
 1ZKZ,CYS\_73,9,0,0,0  
 1TJE,ARG\_123,12.15,-0.35,0,0  
 2APL,GLU\_64,4.5,0,0,0  
 3Q1C,GLU\_392,0.42,1.52,-3.2,-2.4  
 3V55,ASP\_522,3.14,0.14,-0.8,0  
 2Q98,ASP\_41,3.21,0.21,-0.8,0  
 1ZYL,GLU\_300,4.5,0,0,0  
 1DOV,GLU\_88,4.5,0,0,0  
 1ILW,GLU\_107,4.52,0.48,-1.43,0.97  
 2R51,ARG\_247,12.22,-0.28,0,0  
 2QV2,TYR\_279,12.03,1.07,-0.16,1.12  
 3OIP,LYS\_205,10.29,-0.21,0,0  
 1S7K,HIS\_149,6.36,0,0,-0.14  
 2WOZ,LYS\_303,9.94,-0.56,0,0  
 2GZQ,ARG\_161,11.7,-1.84,0,1.04  
 1SJ8,CYS\_575,9.07,0,0,0.07  
 2VAN,TYR\_173,10.44,0.6,-0.16,0  
 3N0K,GLU\_122,4.05,0.35,-0.8,0  
 2A6B,GLU\_112,4.64,0.14,0,0  
 2B0A,LYS\_105,10.22,-0.28,0,0  
 2P65,ARG\_79,11.24,-1.26,0,0  
 1BYI,GLU\_48,4.07,0,-0.43,0  
 2IF4,ASP\_48,3.04,0.42,-1.18,0  
 3EVZ,ARG\_237,13.49,-1.17,0.2,1.6  
 1I60,LYS\_17,10.29,-0.21,0,0  
 1CHD,GLU\_317,3.81,0.07,-0.76,0  
 2E0T,ARG\_81,12.5,0,0,0  
 3G9G,TYR\_40,9.67,0.14,-0.47,0  
 2H2W,ARG\_248,12.15,-0.35,0,0  
 1MTZ,ASP\_154,3.46,0.49,-0.83,0  
 1O5J,LYS\_71,10.36,-0.14,0,0  
 3I4T,LYS\_227,10.36,-0.14,0,0  
 3L3P,GLU\_468,4.64,0.14,0,0  
 2CXK,LYS\_103,10.36,-0.14,0,0  
 1NJ4,TYR\_297,11.66,0,0,1.66  
 1YTQ,HIS\_180,7.29,0.79,0,0  
 1U7U,ARG\_248,11.66,-0.84,0,0  
 3V3T,ARG\_149,12.15,-0.35,0,0  
 3K8J,LYS\_151,10.5,0,0,0  
 4DEZ,ARG\_129,13.01,-0.63,0.1,1.4  
 2H14,LYS\_81,9.87,-0.63,0,0  
 2B78,GLU\_302,4.5,0,0,0  
 1T95,ARG\_196,12.43,-0.07,0,0  
 2WB3,LYS\_368,10.5,0,0,0  
 3QKY,HIS\_67,7.54,1.32,0,-0.28  
 2QDJ,CYS\_169,10.58,-0.01,0,1.59  
 2I6I,ASP\_49,3.13,0.28,-0.95,0  
 3V75,ARG\_263,11.87,-0.63,0,0  
 1MML,ASP\_83,3.28,0.28,-0.8,0  
 3I4T,GLU\_47,4.5,0,0,0  
 3DHN,LYS\_5,10.5,0,0,0  
 1O59,TYR\_170,11.8,0.14,-0.8,2.46  
 4DNU,TYR\_201,10,0,0,0  
 1O9G,ARG\_42,11.52,-0.98,0,0  
 2FXT,ARG\_294,12.43,-0.07,0,0  
 1MD6,LYS\_92,10.5,0,0,0  
 3UV9,ASP\_368,1.74,0.49,-2.55,0  
 1EQ6,LYS\_144,10.5,0,0,0  
 3ANJ,LYS\_333,10.43,-0.07,0,0  
 1UAJ,HIS\_0,6.5,0,0,0  
 3RE9,GLU\_76,4.31,0.21,-0.4,0  
 3CN5,HIS\_210,1.36,0.09,0,-5.23  
 3I0O,ASP\_108,2.4,0.63,-2.03,0  
 2DVK,ARG\_78,11.94,-0.56,0,0  
 3V55,ARG\_465,11.8,-0.7,0,0  
 1MD6,TYR\_100,10,0,0,0  
 3NBI,CYS\_30,9.86,0,0,0.86  
 1FKM,ASP\_259,2.81,0.63,-1.61,0  
 3EGN,ASP\_445,2.4,0.42,-1.82,0  
 2CN1,LYS\_284,10.5,0,0,0  
 3EVZ,ARG\_70,11.82,-2.6,0,1.93  
 2FGI,GLU\_106,4.74,0.49,-0.25,0  
 1A8Q,LYS\_171,10.5,0,0,0  
 1WYC,ARG\_234,12.65,-2.25,0.2,4  
 2RIS,LYS\_119,10.5,0,0,0  
 2GZQ,LYS\_140,10.5,0,0,0  
 1TLV,LYS\_127,10.01,-0.49,0,0  
 4ACJ,TYR\_717,10.55,1.51,-1.19,0.23  
 3IL3,LYS\_256,10.22,-0.28,0,0  
 1XEU,ARG\_170,11.87,-0.63,0,0  
 1OTM,ASP\_189,3.29,0.42,-0.93,0  
 4EKU,LYS\_284,10.5,0,0,0  
 2V81,GLU\_119,4.5,0,0,0  
 2FM9,CYS\_69,9.71,-0.42,0,1.13  
 3DHN,ASP\_126,3.54,0,-0.26,0  
 3ZXY,ARG\_50,12.29,-0.21,0,0  
 1TD6,LYS\_138,10.43,-0.07,0,0  
 1O5T,LYS\_204,10.5,0,0,0  
 3GS9,GLU\_232,4.56,0.21,-0.15,0  
 2B0J,LYS\_30,10.5,0,0,0  
 1X04,ASP\_32,3.79,0,-0.01,0  
 3IUR,ARG\_23,12.5,0,0,0  
 4FZN,ASP\_167,3.74,0,-0.06,0  
 2B0J,LYS\_151,10.22,-0.28,0,0  
 2IQT,ARG\_270,12.5,0,0,0  
 3CO1,LYS\_84,10.08,-0.42,0,0  
 1WNH,GLU\_2,4.21,0.42,-0.7,0  
 3BQW,ARG\_50,12.29,-0.35,0,0  
 3FK5,HIS\_13,0.98,0,-1.99,-3.53  
 1JT9,HIS\_56,7.05,0.69,0,-0.14  
 1DVO,LYS\_119,10.5,0,0,0  
 1JYH,GLU\_9,4.5,0,0,0  
 1R3F,GLU\_217,3.11,0.35,-1.74,0  
 2DVK,GLU\_50,4.5,0,0,0  
 2ZQ5,TYR\_127,10.22,0.22,0,0  
 3IL3,GLU\_49,3.1,0.56,-1.96,0  
 2HRZ,GLU\_2,3.98,0.28,-0.8,0  
 3T8R,LYS\_6,10.43,-0.07,0,0  
 3EJG,HIS\_64,6.29,0,0,-0.21  
 3TIR,ASP\_200,3.35,0.28,-0.73,0  
 3O48,GLU\_92,3.96,0.21,-0.74,0  
 3EVN,HIS\_298,6.37,0.01,0,-0.14  
 1XDZ,GLU\_37,4.78,0.28,0,0  
 3B21,LYS\_41,10.01,-0.49,0,0  
 1PNE,TYR\_128,10.11,0,-0.6,0.71  
 3ONT,TYR\_20,9.79,0.21,-0.41,0  
 3ZXY,ARG\_237,12.43,-0.07,0,0  
 3ONH,GLU\_492,4.5,0,0,0  
 2IXM,LYS\_183,10.43,-0.07,0,0  
 2G9D,ASP\_337,3.79,0.21,-0.22,0  
 1AK1,TYR\_125,12.31,2.31,0,0  
 3LME,LYS\_26,10.5,0,0,0  
 1XEU,TYR\_277,10,0,0,0  
 4DNU,ASP\_294,2.76,0.35,-1.39,0  
 1TR9,HIS\_165,10.82,4.3,3.12,-3.1  
 3QAV,ASP\_214,3.79,0,-0.01,0  
 1U7U,GLU\_395,4.23,0.21,-0.48,0  
 3Q2C,ASP\_89,3.18,0.21,-0.83,0  
 2D7U,TYR\_288,10.84,0.08,0,0.76  
 1FKM,ASP\_594,2.94,0.56,-1.42,0  
 4EZB,ARG\_288,12.15,-0.35,0,0  
 3JRT,GLU\_92,4.5,0,0,0  
 1LTU,LYS\_165,10.5,0,0,0  
 3Q2C,ARG\_25,11.8,-0.7,0,0  
 3RNV,TYR\_455,9.21,0.07,-0.86,0  
 2E3C,HIS\_338,6.43,0,0,-0.07  
 2O4D,GLU\_31,1.48,0.49,-3.51,0  
 1G8P,HIS\_314,3.97,0.1,0,-2.63

1J8B,LYS\_12,10.43,-0.07,0,0  
2JHY,ASP\_93,2.2,0.7,-2.29,0  
3BA1,GLU\_300,4.06,0.35,-0.79,0  
3BQE,ASP\_259,3.12,0.35,-1.03,0  
4ETX,ARG\_374,12.36,-0.14,0,0  
1RAJ,TYR\_334,9.76,0.14,-1.14,0.76  
1X8F,LYS\_189,10.43,-0.07,0,0  
2WOG,LYS\_227,10.43,-0.07,0,0  
2WOZ,GLU\_505,4.57,0.07,0,0  
1AK1,LYS\_34,9.66,-0.84,0,0  
3UV9,GLU\_366,3.64,0.49,-1.35,0  
1Q5Z,ASP\_591,3.94,0.14,0,0  
2HP7,GLU\_50,4.5,0,0,0  
2YWX,GLU\_24,4.64,0.14,0,0  
2QRX,GLU\_67,4.5,0,0,0  
3GV0,ARG\_204,13.86,-1.04,0,2.4  
2PPN,ASP\_11,1.23,0.91,-3.48,0  
1PGV,GLU\_281,2.24,0.77,-3.03,0  
3IBT,CYS\_105,9.97,-0.99,0,1.96  
1WLJ,GLU\_180,3.85,0.07,-0.72,0  
2CIU,LYS\_161,10.43,-0.07,0,0  
3E0H,LYS\_12,10.36,-0.14,0,0  
3EVP,LYS\_203,9.87,-0.63,0,0  
3ILC,LYS\_157,9.94,-0.56,0,0  
1PBV,ASP\_183,3.83,0.07,-0.04,0  
1GPP,LYS\_97,10.43,-0.07,0,0  
1WNH,TYR\_158,11.94,0.51,0,1.43  
1UOH,TYR\_112,12.24,0.46,-0.51,2.29  
1FQJ,LYS\_378,10.5,0,0,0  
2APL,ASP\_120,2.66,0.35,-1.49,0  
1ZBM,ASP\_151,2.52,0.42,-1.7,0  
1X9G,ARG\_27,12.29,-0.21,0,0  
3ERF,ASP\_179,3.87,0.07,0,0  
4ECC,HIS\_163,4.87,1.6,0.78,-4.01  
1R3F,TYR\_251,10.53,0,0,0.53  
2P4D,ARG\_20,12.22,-0.28,0,0  
2IXM,LYS\_38,9.87,-0.63,0,0  
1G8P,TYR\_274,10,0,0,0  
1UCH,LYS\_120,10.29,-0.21,0,0  
1NIJ,ARG\_310,13.76,-0.99,0,2.25  
2RIS,GLU\_32,4.67,0.28,-0.11,0  
1NAF,ARG\_214,11.66,-0.84,0,0  
1W24,LYS\_50,10.29,-0.21,0,0  
1AT0,CYS\_258,4.85,-2.27,-2.4,0.51  
1YR6,ARG\_22,12.22,-0.28,0,0  
1C3K,ASP\_139,4.17,0.7,-0.33,0  
1JT9,LYS\_50,10.43,-0.07,0,0  
3V75,GLU\_44,3.85,0.07,-0.72,0  
1XEU,LYS\_132,10.5,0,0,0  
2QHT,GLU\_60,3.85,0.14,-0.8,0  
3C38,HIS\_74,6.68,0.32,0,-0.14  
3EX9,ARG\_41,12.17,-2.73,0,2.4  
1GXN,LYS\_497,10.29,-0.21,0,0  
3K9I,GLU\_94,3.95,0.28,-0.83,0  
1ZP2,ARG\_217,13.73,-0.95,0,2.18  
3U2R,ARG\_9,12.5,0,0,0  
3K9I,HIS\_107,6.5,0,0,0  
4DBX,CYS\_34,10.7,-0.02,0.33,1.38  
3NBI,GLU\_193,4.57,0.07,0,0  
2Z14,ARG\_112,11.94,-0.56,0,0  
2H8O,ARG\_78,11.66,-0.84,0,0  
3PM2,GLU\_75,3.9,0.35,-0.95,0  
2ZQ5,ARG\_7,12.22,-0.28,0,0  
3KV0,TYR\_169,9.96,0.76,-0.8,0  
4EZB,ARG\_175,12.43,-0.07,0,0  
3ANJ,ARG\_17,11.03,-1.47,0,0  
2H85,LYS\_149,10.5,0,0,0  
3EGN,ARG\_452,11.73,-0.77,0,0  
3GYW,HIS\_232,6.36,0,0,-0.14  
3H9W,HIS\_131,6.38,0.02,0,-0.14  
3UC9,CYS\_32,8.95,-0.05,0,0  
2ZCO,ARG\_85,11.94,-0.56,0,0  
1O0X,HIS\_236,5.47,2.04,3.36,-6.43  
1T95,GLU\_42,4.5,0,0,0  
3P28,LYS\_118,10.5,0,0,0  
2OGQ,ARG\_441,11.92,-1.57,0,0.99  
2FC3,TYR\_6,9.59,0.42,-1.15,0.32  
2YX0,ARG\_227,12.08,-0.42,0,0  
3AUF,ASP\_53,3.21,0.21,-0.8,0  
1XDZ,GLU\_114,4.5,0,0,0  
3ULX,ARG\_85,12.01,-0.49,0,0  
3CSR,ARG\_138,11.8,-0.7,0,0  
2W8B,CYS\_478,4.36,-3.6,-2.34,1.3  
3IBT,GLU\_135,4.99,0.49,0,0  
4D8L,HIS\_79,3.31,0.67,0,-3.86  
3C38,GLU\_200,2.38,0.28,-2.4,0  
2HXB,TYR\_48,9.93,0.07,-0.14,0  
3G6S,LYS\_85,10.29,-0.21,0,0  
1O9G,GLU\_185,4.35,0.42,-0.57,0  
3HZQ,LYS\_93,10.5,0,0,0  
3ULX,CYS\_162,12.73,-0.53,1.19,3.07  
1F09,LYS\_232,10.15,-0.35,0,0  
3EZ7,GLU\_36,4.78,0.28,0,0  
2BV9,ASP\_47,3.48,0.35,-0.67,0  
1R16,GLU\_276,1.85,1.35,-4,0  
1X7F,HIS\_136,6.26,0.11,0,-0.35  
1U53,LYS\_117,10.22,-0.28,0,0  
2F8H,HIS\_194,6.36,0,0,-0.14  
3M3P,GLU\_178,1.06,3.46,-2.7,-4.21  
2INO,HIS\_429,7.1,0.67,0,-0.07  
3LH5,LYS\_567,10.5,0,0,0  
1XEU,GLU\_165,4.57,0.07,0,0  
3CCY,ASP\_156,3.82,0.14,-0.12,0  
3C38,HIS\_237,7.49,1.12,0,-0.14  
3RFY,ASP\_249,3.92,0.14,-0.02,0  
3EJC,ASP\_21,3.35,0.84,-1.29,0  
1XKR,GLU\_58,2.97,0.35,-1.88,0  
1SUU,GLU\_697,4.5,0,0,0  
1AK1,LYS\_102,10.5,0,0,0  
3QAV,GLU\_51,4.5,0,0,0  
3C38,ARG\_115,12.76,-2.14,0,2.4  
4ACJ,ASP\_747,1.93,0.84,-2.71,0  
3F6F,ARG\_6,12.29,-0.21,0,0  
3CAN,ARG\_30,12.29,-0.21,0,0  
1TXJ,TYR\_150,11.33,0,0,1.33  
3M7G,GLU\_171,4.31,0.52,-0.71,0  
3NJM,LYS\_56,10.43,-0.07,0,0  
3ULX,ASP\_25,4.13,0.35,-0.03,0  
2EYI,GLU\_225,4.5,0,0,0  
3A2Z,ASP\_41,2.68,0.42,-1.54,0  
2GKG,GLU\_9,0.76,0.9,-2.24,-2.4  
2VGM,GLU\_381,4.83,0.28,0.05,0  
1VJG,CYS\_27,9,0,0,0  
2G7O,LYS\_123,10.5,0,0,0  
1SIG,LYS\_299,10.5,0,0,0  
3H04,TYR\_52,12.12,0.86,-0.27,1.53  
1R1S,ARG\_177,11.63,-0.87,0,0  
2B02,CYS\_400,9.25,-0.15,0,0.4  
4ETX,TYR\_354,10.47,0,-0.26,0.73  
3GG6,GLU\_91,6.94,1.58,-0.71,1.57  
2B02,HIS\_367,5.77,4.31,0,-5.04  
3KEY,LYS\_456,10.15,-0.35,0,0  
1QYI,GLU\_152,4.57,0.07,0,0  
3BA1,GLU\_286,3.32,0,-1.18,0  
2XHC,LYS\_225,10.43,-0.07,0,0  
2GKG,GLU\_40,2.45,0.35,-2.4,0  
3HQX,ARG\_57,11.73,-0.77,0,0  
2WZ9,HIS\_37,8.17,4.4,2,-4.73  
2EYV,ARG\_38,12.29,-0.21,0,0  
1WXQ,ASP\_201,3.56,0,-0.24,0  
3BWT,GLU\_769,2.03,1.52,-3.99,0  
3EVP,ARG\_81,12.22,-0.28,0,0  
2QOP,ARG\_22,12.29,-0.21,0,0  
2INO,LYS\_27,10.43,-0.07,0,0  
3R87,LYS\_117,10.5,0,0,0  
1DVO,LYS\_176,10.36,-0.14,0,0  
3VJ8,ASP\_351,3.2,0.07,-0.67,0  
4HDE,GLU\_134,4.5,0,0,0  
3G9T,LYS\_31,10.36,-0.14,0,0  
3IVF,LYS\_295,10.01,-0.49,0,0  
3O7K,ARG\_112,11.94,-0.56,0,0  
3T5B,ASP\_156,3.77,0.21,-0.24,0  
2G7O,LYS\_68,10.29,-0.21,0,0  
2EJY,ARG\_143,12.22,-0.28,0,0  
1WJL,HIS\_122,7.16,0.8,0,-0.14  
3PP8,ARG\_27,12.36,-0.14,0,0  
2Q98,TYR\_28,13.34,0.14,0.8,2.4  
2C2Y,HIS\_103,7.52,1.16,0,-0.14  
2PLQ,ARG\_306,12.15,-0.35,0,0  
1CBY,LYS\_26,10.08,-0.42,0,0  
2H2Z,HIS\_246,4.27,0,0,-2.23  
1H09,LYS\_195,10.5,0,0,0  
2JKF,GLU\_168,4.05,0.35,-0.8,0  
2AHE,ASP\_237,3.77,0.07,-0.1,0  
2FXT,LYS\_260,10.5,0,0,0  
3NZL,ARG\_71,12.22,-0.28,0,0  
1GPP,TYR\_130,9.34,0.14,-0.8,0  
1P4X,ARG\_90,12.29,-0.21,0,0  
4ANN,TYR\_97,10.53,0,-0.05,0.58  
3G9B,TYR\_128,10,0,0,0  
4HDE,GLU\_90,3.98,0.21,-0.73,0  
2IDC,LYS\_165,9.87,-0.63,0,0  
3B7X,ARG\_109,12.15,-0.35,0,0  
2WB3,TYR\_317,10,0,0,0  
1Q42,LYS\_47,10.08,-0.42,0,0  
2VGM,TYR\_32,13.35,0.57,0.38,2.4  
3V1Q,GLU\_607,4.5,0,0,0  
4AE7,TYR\_229,9.97,0.11,-0.14,0  
3LJJ,ARG\_95,13.88,-1.02,0,2.4  
3ADO,ASP\_303,3.42,0.56,-0.94,0  
1F09,ARG\_307,10.08,-4.35,0,1.93  
4H86,LYS\_41,10.5,0,0,0  
2RGY,ARG\_138,11.8,-0.7,0,0  
2188,CYS\_505,8.78,-1.89,0,1.66  
3V3T,GLU\_136,3.52,0.56,-1.55,0  
2OJQ,GLU\_603,4.16,0.56,-0.9,0  
3S0A,LYS\_59,10.5,0,0,0  
2B6P,GLU\_254,4.5,0,0,0  
3P28,TYR\_231,11.09,0,0,1.09  
3K9I,LYS\_102,10.5,0,0,0  
2QV2,LYS\_81,10.36,-0.14,0,0  
3CIV,ARG\_37,12.22,-0.28,0,0  
1P2F,HIS\_145,6.43,0,0,-0.07  
3GEC,CYS\_241,7.84,-1.23,0,0.07  
3KV0,ASP\_191,3.87,0.21,-0.14,0  
1P6F,TYR\_75,10.85,0.85,0,0  
4E8B,TYR\_7,10.17,0,0,1.0,0  
1FHL,TYR\_151,10.11,0.11,0,0  
3PU6,GLU\_79,4.05,0.21,-0.66,0  
2FZP,HIS\_295,7.43,1.07,0,-0.14  
2F8H,ARG\_222,12.08,-0.42,0,0  
1UAJ,GLU\_222,4.2,0.77,-1.08,0  
3IOC,ARG\_282,12.01,-0.49,0,0  
1OTM,LYS\_62,10.43,-0.07,0,0  
4DIU,LYS\_121,10.5,0,0,0  
2DG7,ARG\_135,11.8,-0.7,0,0  
3P28,ASP\_213,3.63,0.56,-0.73,0  
1T95,LYS\_41,10.5,0,0,0  
2CVB,LYS\_166,10.5,0,0,0  
1AKO,GLU\_185,4.57,0.07,0,0  
1NAF,ASP\_285,4.11,0.35,-0.04,0  
1KW4,ARG\_51,12.5,0,0,0  
4GA2,TYR\_52,13.27,0.07,0.8,2.4  
3IRA,LYS\_125,10.36,-0.14,0,0  
1KW4,LYS\_74,10.5,0,0,0  
3FHF,TYR\_196,11.74,0.13,0,1.61  
2WOZ,TYR\_545,10.48,0.48,0,0  
2QV2,LYS\_25,10.29,-0.21,0,0  
3BCH,ARG\_155,12.5,0,0,0  
1EDG,ARG\_319,11.17,-3.21,0,1.88  
2JEO,HIS\_226,6.5,0,0,0  
3DSH,GLU\_363,4.5,0,0,0  
3O7K,ASP\_58,3.71,0,-0.09,0  
1EYH,GLU\_19,4.28,0.07,-0.29,0  
2IQT,ASP\_273,3.04,0.07,-0.83,0  
1DUN,GLU\_73,4.06,0.49,-0.93,0  
2EFK,GLU\_184,4.57,0.07,0,0  
1TP6,HIS\_46,6.5,0,0,0  
2FPN,LYS\_85,10.5,0,0,0  
1Y2Q,TYR\_79,11.02,1.02,0,0  
3ELI,ARG\_127,11.94,-0.56,0,0  
3O48,ARG\_76,11.94,-0.56,0,0  
2AZL,GLU\_164,4.67,0.17,0,0  
1SJ8,GLU\_734,4.68,0.21,-0.03,0  
2D2S,ARG\_532,12.43,-0.07,0,0  
2H01,CYS\_44,7.49,-1.51,0,0  
3D9H,GLU\_131,4.5,0,0,0  
4ETX,GLU\_251,4.99,0.49,0,0  
1P2F,ARG\_110,12.23,-1.34,0,1.07  
1QZN,ASP\_73,3.15,0,-0.65,0  
1NFN,LYS\_143,10.5,0,0,0  
3DHN,GLU\_206,4.29,0.28,-0.49,0  
1NIJ,LYS\_86,10.36,-0.14,0,0  
1J7G,GLU\_115,4.64,0.14,0,0  
2GZR,LYS\_104,10.43,-0.07,0,0  
2Q5X,GLU\_832,4.5,0,0,0  
2EHG,ARG\_65,12.5,0,0,0  
2FBI,GLU\_96,4.5,0,0,0  
3LPZ,ARG\_32,12.36,-0.14,0,0  
2EJX,GLU\_125,3.81,0.28,-0.97,0  
1PDB,ASP\_145,2.43,0.77,-2.14,0  
1X9G,CYS\_112,10.86,0.19,0.4,1.27  
1PVT,TYR\_88,10.53,0.53,0,0  
2X5Y,CYS\_867,9.26,-0.01,0,0.27  
1S17,ARG\_122,12.43,-0.07,0,0  
3BWT,GLU\_622,3.98,0.35,-0.87,0  
3A2Z,TYR\_197,10.58,0,0,0.58  
3IV4,TYR\_81,11.57,0.07,0,1.5  
2Q99,ARG\_233,11.8,-0.7,0,0  
3V46,GLU\_363,4.78,0.28,0,0  
1TJE,TYR\_219,9.49,0.07,-0.58,0  
3HNX,ARG\_103,12.36,-0.14,0,0  
3LJC,GLU\_240,4.5,0,0,0  
1E8V,TYR\_164,10,0,0,0  
2GAU,GLU\_47,4.85,0.35,0,0  
4F85,ASP\_298,3.35,0.35,-0.8,0  
1LPL,ASP\_202,3.67,0.21,-0.34,0  
2D0A,HIS\_235,3.41,1.19,0,-4.28  
2IQT,LYS\_188,10.43,-0.07,0,0  
3G9T,LYS\_134,10.5,0,0,0  
3V46,ARG\_393,12.5,0,0,0  
3KEY,LYS\_464,10.43,-0.07,0,0  
1XDZ,LYS\_164,10.36,-0.14,0,0  
3F6F,HIS\_59,7.23,0.8,0,-0.07  
3RKV,LYS\_301,10.29,-0.21,0,0  
2OJQ,GLU\_679,4.78,0.28,0,0



3AU3,ARG\_657,11.87,-0.63,0,0  
 1NAR,ASP\_59,2.62,0.49,-1.68,0  
 3CIV,ARG\_312,12.01,-0.49,0,0  
 2VGM,TYR\_300,10.0,0,0  
 4ESS,CYS\_49,3.43,-3.76,-2.4,0.59  
 2H01,LYS\_7,10.43,-0.07,0,0  
 3P2F,CYS\_147,8.95,-0.05,0,0  
 2P0L,TYR\_19,13.34,0.14,0.8,2.4  
 3LH5,GLU\_528,4.63,0.14,-0.01,0  
 2Q98,CYS\_199,9.59,0.59,0,0  
 1X1E,ARG\_96,12.22,-0.28,0,0  
 1R7J,GLU\_75,4.76,0.28,-0.02,0  
 2CXA,GLU\_201,4.71,0.21,0,0  
 1MN3,GLU\_406,4.57,0.07,0,0  
 1YG2,ASP\_144,3.82,0.21,-0.19,0  
 2R0S,ASP\_205,2.69,0.49,-1.6,0  
 3V55,GLU\_556,3.98,0.28,-0.8,0  
 1DUP,ASP\_39,4.01,0.21,0,0  
 2BV9,TYR\_179,12.0,62,0.1,38  
 1OST,LYS\_154,10.5,0,0,0  
 2YX0,TYR\_199,12.48,3,-0.99,0.47  
 3IVF,LYS\_15,10.29,-0.21,0,0  
 3CCY,TYR\_51,9.48,0.14,-0.66,0  
 3V3T,HIS\_191,6.7,0.41,0,-0.21  
 3F6M,ARG\_85,11.94,-0.56,0,0  
 3CNU,GLU\_19,4.12,0.42,-0.8,0  
 3C6B,HIS\_37,5.37,0.87,0.28,-2.28  
 3G65,ARG\_69,12.58,-2.32,0,2.4  
 3G9G,GLU\_3,4.5,0,0,0  
 1ES9,GLU\_88,1.21,3.16,-2.23,-4.22  
 3TOW,ASP\_135,0.79,1.05,-4.04,0  
 2GZR,HIS\_52,7.08,0.79,0,-0.21  
 3FHF,ARG\_22,11.87,-0.63,0,0  
 1TLV,LYS\_60,10.43,-0.07,0,0  
 2CXV,TYR\_8,13.27,0.07,0.8,2.4  
 3JSN,ASP\_288,3.76,0,-0.04,0  
 1PDB,LYS\_155,10.36,-0.14,0,0  
 3IU5,GLU\_105,4.57,0.07,0,0  
 3ANJ,ASP\_133,3.01,0.77,-1.56,0  
 1EV8,ARG\_99,11.77,-0.73,0,0  
 2IRM,GLU\_266,1.21,0.22,-1.6,-1.91  
 3H04,HIS\_230,2.19,0,-2.4,-1.91  
 4EKU,ARG\_148,12.01,-0.49,0,0  
 3ZXY,ARG\_141,12.15,-0.35,0,0  
 2I6I,ARG\_145,12.08,-0.42,0,0  
 1DOV,LYS\_87,10.43,-0.07,0,0  
 2FM9,ASP\_108,4.01,0.21,0,0  
 1AK1,GLU\_170,4.5,0,0,0  
 1YM5,LYS\_270,9.8,-0.7,0,0  
 3H04,ASP\_118,3.94,0.14,0,0  
 1YLN,LYS\_231,10.29,-0.21,0,0  
 1PBV,ARG\_162,11.52,-0.98,0,0  
 3T5B,TYR\_391,13.27,0.28,-0.31,3.31  
 2CIU,TYR\_214,9.51,0,-0.49,0  
 2EEY,CYS\_132,9.42,0,0,0.42  
 3KEY,LYS\_338,10.5,0,0,0  
 3OA7,GLU\_9,4.64,0.14,0,0  
 2B3M,ASP\_146,3.91,0.14,-0.03,0  
 3DHN,ASP\_185,1.74,1.05,-3.11,0  
 1RI6,ASP\_229,2.45,0.14,-1.49,0  
 2Q13,TYR\_48,9.94,0,-0.15,0.09  
 2V5B,TYR\_211,10.8,1.35,-0.55,0  
 2E0T,GLU\_104,3.93,0.49,-1.06,0  
 1YTD,GLU\_376,3.88,0.21,-0.83,0  
 3GEC,HIS\_403,6.5,0,0,0  
 2QV2,LYS\_154,10.22,-0.28,0,0  
 3Q1C,GLU\_77,4.05,0.35,-0.8,0  
 1RI6,LYS\_49,10.36,-0.14,0,0  
 2XHC,ARG\_275,11.94,-0.56,0,0  
 1AM2,ARG\_49,12.08,-0.42,0,0  
 2OPJ,ARG\_124,12.5,0,0,0  
 2O4D,ARG\_4,12.5,0,0,0  
 2CXK,GLU\_63,4.5,0,0,0  
 2Q13,ARG\_238,12.01,-0.49,0,0  
 1Y2Q,GLU\_74,4.5,0,0,0  
 1AKO,ARG\_14,13.55,-1.35,0,2.4  
 1V43,GLU\_319,4.12,0.42,-0.8,0  
 2HNG,ASP\_20,4.01,0.21,0,0  
 2I6I,LYS\_30,10.36,-0.14,0,0  
 1LN4,CYS\_73,8.12,-1.34,0,0.46  
 3LD1,ARG\_201,11.45,-1.05,0,0  
 2BAA,ASP\_12,3.27,0.28,-0.81,0  
 3IBT,LYS\_61,10.5,0,0,0  
 2G9D,ARG\_322,9.86,-1.95,0,-0.69  
 350A,ARG\_9,11.94,-0.56,0,0  
 3V4G,ASP\_8,3.75,0,-0.05,0  
 3V55,TYR\_389,10.62,0,0,0.62  
 3R87,TYR\_12,10,0,0,0  
 1NWA,GLU\_52,5.74,2.03,-0.79,0  
 4FCU,ASP\_50,4.13,0.7,-0.37,0  
 2DVK,LYS\_23,10.5,0,0,0  
 3P28,LYS\_59,10.5,0,0,0  
 1MTZ,GLU\_7,3.84,0.14,-0.8,0  
 3LQE,ARG\_537,12.5,0,0,0  
 1W24,LYS\_173,10.43,-0.07,0,0  
 2X4L,ARG\_214,12.29,-0.21,0,0  
 3C5V,LYS\_119,10.15,-0.35,0,0  
 1UOH,LYS\_213,9.94,-0.56,0,0  
 2CN1,TYR\_98,10.62,0,0,0.62  
 1VSM,ARG\_158,12.29,-0.21,0,0  
 2RFA,ARG\_146,11.87,-0.63,0,0  
 1NRI,LYS\_102,10.29,-0.21,0,0  
 1MHN,GLU\_121,4.64,0.14,0,0  
 2P4D,TYR\_7,10,0,0,0  
 1O5J,ARG\_19,12.01,-0.49,0,0  
 1SUU,LYS\_514,10.29,-0.21,0,0  
 1QYI,TYR\_257,10.07,0.07,0,0  
 1RI6,ASP\_168,3.94,0.14,0,0  
 2A6B,GLU\_200,4.57,0.07,0,0  
 1SFE,ARG\_33,12.36,-0.14,0,0  
 3B21,HIS\_96,7.48,1.11,0,-0.14  
 4FZR,ARG\_76,12.5,0,0,0  
 3HUE,ARG\_114,12.27,-0.23,0,0  
 2CVB,GLU\_10,4.59,0.28,-0.19,0  
 2QRX,HIS\_36,6.5,0,0,0  
 1V8E,ASP\_48,2.03,0.91,-2.68,0  
 2PWQ,LYS\_27,10.5,0,0,0  
 3DHN,LYS\_66,10.29,-0.21,0,0  
 1RHS,ARG\_7,11.8,-0.7,0,0  
 1LTU,ARG\_115,11.66,-0.84,0,0  
 1N81,LYS\_170,10.15,-0.35,0,0  
 1PDB,ASP\_21,3.43,0.14,-0.51,0  
 2CL3,GLU\_81,5.54,3.07,0,-2.03  
 3P2F,ARG\_151,11.87,-0.63,0,0  
 2BDV,ARG\_137,12.5,0,0,0  
 3TMO,HIS\_279,6.43,0,0,-0.07  
 3EVN,ARG\_263,12.01,-0.49,0,0  
 1WYC,ARG\_301,11.87,-0.63,0,0  
 4ANN,GLU\_93,2.38,0.28,-2.4,0  
 1FKM,GLU\_472,4.56,0.28,-0.22,0  
 1TD6,LYS\_56,10.15,-0.35,0,0  
 2B0A,ARG\_180,12.15,-0.35,0,0  
 1J7G,ARG\_53,12.36,-0.14,0,0  
 2OKT,TYR\_56,9.33,1.95,-0.49,-2.14  
 1HF8,GLU\_187,3.7,0.28,-1.08,0  
 3BJV,LYS\_20,10.5,0,0,0  
 1SIG,ASP\_167,3.8,0,0,0  
 2PGX,HIS\_27,7.41,1.12,0,-0.21  
 2X4G,TYR\_238,13.09,0.23,-0.38,3.25  
 3VHJ,HIS\_67,3.44,1.35,0,-4.41  
 1X04,ARG\_223,12.08,-0.42,0,0  
 1DQO,TYR\_83,9.41,0.21,-0.8,0  
 1STG,GLU\_146,4.57,0.07,0,0  
 1NRI,ASP\_183,1.55,0.42,-2.66,0  
 2IQT,CYS\_183,6.97,-2.03,0,0  
 2QZQ,HIS\_84,6.83,0.33,0,0  
 3T5B,ASP\_317,2.97,0.7,-1.52,0  
 1WNH,TYR\_180,12.75,2.75,0,0  
 1Q2Y,ARG\_78,12.01,-0.49,0,0  
 2DG7,ARG\_46,12.5,0,0,0  
 1R6Y,CYS\_37,6.58,-2.49,0,0.07  
 1H4U,TYR\_431,10,0,0,0  
 3M70,HIS\_265,6.43,0,0,-0.07  
 2BAA,ARG\_215,13.88,-3.11,0,4.49  
 1OIS,LYS\_256,9.73,-0.77,0,0  
 3BWT,GLU\_598,4.05,0.35,-0.8,0  
 3UV9,CYS\_451,7.4,-1.6,0,0  
 1C3K,ASP\_50,1.64,1.19,-3.35,0  
 2BDD,LYS\_78,10.22,-0.28,0,0  
 2NYC,LYS\_315,10.36,-0.14,0,0  
 2GAU,GLU\_171,3.76,0.35,-1.09,0  
 3PM2,GLU\_91,3.08,0.42,-1.84,0  
 3V3T,ASP\_135,3.69,0,-0.11,0  
 1KCM,ASP\_242,3.24,0.07,-0.63,0  
 3ASA,HIS\_351,6.36,0,0,-0.14  
 3GFP,TYR\_347,9.41,0.21,-0.8,0  
 2O4D,GLU\_64,1.91,0.42,-3.01,0  
 4ANN,GLU\_52,3.6,0.28,-1.18,0  
 3P51,CYS\_37,7.63,-0.84,-1.18,0.65  
 1ZBP,ARG\_72,12.29,-0.21,0,0  
 1TXJ,GLU\_132,4.57,0.07,0,0  
 3NZL,GLU\_68,4.05,0.35,-0.8,0  
 1EV8,ASP\_246,1.02,0.77,-3.55,0  
 1X8F,GLU\_157,4.64,0.14,0,0  
 1WLY,ARG\_262,10.89,-1.61,0,0  
 1O9G,LYS\_231,10.5,0,0,0  
 1WPA,GLU\_480,3.92,0.21,-0.79,0  
 3M7G,GLU\_221,4.4,0.14,-0.24,0  
 2O8P,ASP\_85,3.73,0.07,-0.14,0  
 2QK0,ARG\_36,11.52,-0.98,0,0  
 1YTQ,TYR\_78,10.23,0.07,-1.17,1.33  
 3GYW,ARG\_268,12.22,-0.28,0,0  
 3OKQ,GLU\_593,4.78,0.28,0,0  
 2H14,LYS\_159,10.5,0,0,0  
 1TD6,HIS\_35,6.41,0.05,0,-0.14  
 1TD6,GLU\_153,3.91,0.21,-0.8,0  
 4DNU,HIS\_118,7.22,0.79,0,-0.07  
 3T8R,GLU\_21,3.72,0.35,-1.13,0  
 3V1Q,ARG\_609,12.5,0,0,0  
 2YX0,GLU\_23,4.5,0,0,0  
 2OBI,LYS\_105,9.87,-0.63,0,0  
 1J7G,LYS\_35,10.43,-0.07,0,0  
 3HNX,CYS\_83,9.2,0.13,0,0.07  
 2E3S,LYS\_594,10.36,-0.14,0,0  
 2EYI,GLU\_189,3.49,0.77,-1.78,0  
 4AE7,ARG\_223,11.52,-0.98,0,0  
 1OIS,CYS\_273,8.86,-0.82,0,0.68  
 1V43,HIS\_293,4.96,0.08,1.25,-2.88  
 2RIK,LYS\_279,10.5,0,0,0  
 1ES9,LYS\_37,10.43,-0.07,0,0  
 2P5D,LYS\_39,9.66,-0.84,0,0  
 1YTD,ASP\_173,3.87,0.07,0,0  
 1GVP,ARG\_80,11.87,-0.63,0,0  
 1X9G,GLU\_94,4.5,0,0,0  
 3RE9,GLU\_84,4.5,0,0,0  
 3DHN,HIS\_210,6.81,0.59,0,-0.28  
 1L3K,GLU\_117,4.4,0.7,-0.8,0  
 1SIG,CYS\_291,10.02,-0.09,0,1.11  
 2OSA,TYR\_360,12.74,0.66,-0.32,2.4  
 1QZN,TYR\_157,9.28,0.67,-1.38,0  
 3HUE,ASP\_72,1.96,0.91,-2.75,0  
 1ZCU,GLU\_78,3.95,0.49,-1.04,0  
 3LJN,LYS\_308,10.36,-0.14,0,0  
 3L3P,ASP\_493,4.15,0.7,-0.35,0  
 2OEW,GLU\_79,3.39,1.04,0,-2.15  
 3P28,HIS\_169,7.44,1.15,0,-0.21  
 2ZQ5,ASP\_45,3.88,0.14,-0.06,0  
 2Q13,LYS\_158,10.5,0,0,0  
 2X4G,HIS\_26,1.88,0,-1.63,-2.98  
 3D9H,ASP\_116,3.9,0.14,-0.04,0  
 2NRK,LYS\_62,10.29,-0.21,0,0  
 3A4C,ARG\_493,12.08,-0.42,0,0  
 2RIK,TYR\_115,10.7,0.69,0,0.01  
 2VGE,LYS\_91,6.94,0.51,0,-0.07  
 1NKD,GLU\_24,4.57,0.07,0,0  
 1XTZ,LYS\_148,10.43,-0.07,0,0  
 4DBX,HIS\_202,6.46,1.02,2.86,-3.92  
 1LZL,ASP\_25,3.49,0.42,-0.73,0  
 3U2A,GLU\_74,3.18,0.28,-1.6,0  
 3GFP,LYS\_47,10.5,0,0,0  
 2BDD,LYS\_43,10.5,0,0,0  
 3AUF,GLU\_187,3.72,0.56,-1.34,0  
 3T8R,ARG\_59,12.5,0,0,0  
 2B3M,GLU\_30,4.5,0,0,0  
 3HQX,GLU\_64,3.34,0.35,-1.51,0  
 2VGE,HIS\_119,6.36,0,0,-0.14  
 3FK5,ARG\_269,11.87,-0.63,0,0  
 3U2R,HIS\_130,6.5,0,0,0  
 2AZL,GLU\_117,4.85,0.35,0,0  
 1NFN,GLU\_96,4.4,0.49,-0.59,0  
 1BKB,TYR\_11,10.79,0.14,-0.41,1.06  
 2F9F,LYS\_51,10.36,-0.14,0,0  
 3C2E,GLU\_212,4.34,0.14,-0.3,0  
 2YWJ,ARG\_101,11.94,-0.56,0,0  
 1MUF,GLU\_163,4.78,0.28,0,0  
 2FD4,GLU\_531,3.9,0.84,-1.44,0  
 2FZP,ARG\_210,12.01,-0.49,0,0  
 1SIG,TYR\_148,12.19,0,0,2.19  
 2B78,LYS\_351,10.5,0,0,0  
 1K95,ARG\_166,12.5,0,0,0  
 2CVB,GLU\_60,4.04,0.28,-0.74,0  
 2C13,LYS\_105,10.01,-0.49,0,0  
 3CAN,GLU\_93,4.41,0.21,-0.3,0  
 1TR9,LYS\_151,10.5,0,0,0  
 1OGL,CYS\_230,9.72,0,0,0.72  
 2FD4,ASP\_439,2.04,0.63,-2.39,0  
 1DQO,GLU\_141,4.15,0.07,-0.42,0  
 3EJG,CYS\_157,8.91,-0.16,0,0.07  
 4FCU,GLU\_56,4.64,0.14,0,0  
 2AZP,HIS\_10,6.56,0.06,0,0  
 3M7G,ASP\_124,3.85,0.21,-0.16,0  
 1DUP,ARG\_71,11.73,-0.77,0,0  
 3Q1C,TYR\_313,10,0,0,0  
 1AT0,ARG\_283,11.87,-0.63,0,0  
 2B3M,GLU\_33,4.5,0,0,0  
 2CWC,LYS\_43,10.5,0,0,0  
 3DTE,ARG\_17,11.94,-0.56,0,0  
 2QRX,ASP\_51,2.61,0.63,-1.82,0  
 2FC3,GLU\_116,3.84,0.14,-0.8,0  
 2D7U,ASP\_148,3.35,0.56,-1.01,0  
 2F9F,GLU\_78,3.84,0.14,-0.8,0  
 1MIX,TYR\_373,10.07,0.07,0,0  
 3HYQ,LYS\_55,11.01,-0.21,0,0.72  
 2G9D,ARG\_268,11.45,-1.05,0,0  
 2O8P,LYS\_185,10.43,-0.07,0,0  
 2EJX,LYS\_9,10.29,-0.21,0,0

4EUG,GLU\_30,1.86,0.56,-3.2,0  
 2B6P,TYR\_105,9.5,0.07,-0.57,0  
 3FXH,ASP\_60,3.59,0.07,-0.28,0  
 3EJG,TYR\_151,10.95,0,0,0.95  
 2JEO,ARG\_169,12.09,-2.22,0,1.81  
 3Q2C,ARG\_72,12.08,-0.42,0,0  
 2H2W,HIS\_84,8.15,1.6,2.3,-2.25  
 4DBX,TYR\_37,9.4,0,-0.6,0  
 1PDB,ASP\_168,2.49,0.7,-2.01,0  
 2A6B,LYS\_98,10.43,-0.07,0,0  
 2IXM,GLU\_156,6.15,4.76,-3.12,0  
 2PIM,ARG\_12,12.01,-0.49,0,0  
 1RI6,LYS\_269,9.94,-0.56,0,0  
 3N2T,HIS\_88,7.16,0.8,0,-0.14  
 3RNV,HIS\_430,6.5,0,0,0  
 2QEV,GLU\_75,4.64,0.14,0,0  
 4GA2,ARG\_10,11.19,-1.99,-0.8,0  
 1OIS,ASP\_321,3.87,0.07,0,0  
 3H04,LYS\_145,10.5,0,0,0  
 3B7X,GLU\_88,4.26,0.21,-0.45,0  
 4DNU,ARG\_338,11.75,-0.75,0,0  
 3EVP,ASP\_177,3.21,0.21,-0.8,0  
 1Q42,TYR\_168,11.19,-1.99,-0.8,0  
 3NZL,GLU\_41,4.57,0.07,0,0  
 4DNU,TYR\_90,11.31,0.07,0,1.24  
 1OTM,LYS\_114,10.5,0,0,0  
 4ACJ,GLU\_643,4.5,0,0,0  
 1UAJ,GLU\_239,3.93,0.21,-0.78,0  
 3EUR,ASP\_127,3.94,0.14,0,0  
 1FO9,ARG\_429,11.59,-0.91,0,0  
 4FZN,ARG\_208,12.22,-0.28,0,0  
 2E0T,LYS\_181,10.43,-0.07,0,0  
 2NSN,GLU\_80,2.84,1.19,-2.85,0  
 2FXT,GLU\_413,3.81,0.28,-0.98,0  
 1YOK,ARG\_8,11.94,-0.56,0,0  
 3CX5,CYS\_128,9.07,0,0,0.07  
 1SI7,ASP\_60,3.84,0.35,-0.31,0  
 2R57,HIS\_262,6.15,0,0,-0.35  
 3I0C,GLU\_190,4.57,0.07,0,0  
 3V4G,ASP\_113,3.25,0.14,-0.69,0  
 1X7F,LYS\_249,10.36,-0.14,0,0  
 2CI3,HIS\_172,8.65,1.6,5.41,-4.86  
 3M3P,GLU\_133,2.6,0.63,-2.53,0  
 1K95,GLU\_92,4.5,0,0,0  
 2H2W,LYS\_203,10.43,-0.07,0,0  
 2ZQ5,TYR\_365,9.26,0,-0.74,0  
 3LJC,GLU\_222,4.64,0.14,0,0  
 2FPN,ARG\_73,12.01,-0.49,0,0  
 1UXO,LYS\_135,10.5,0,0,0  
 1YW5,LYS\_82,10.5,0,0,0  
 1XEU,GLU\_282,4.71,0.21,0,0  
 1IDK,ASP\_160,2.76,0.35,-1.39,0  
 3LJI,TYR\_53,10.48,1.57,-0.9,-0.18  
 3BWT,ASP\_663,3.46,0.14,-0.48,0  
 1RI6,GLU\_334,3.66,0.14,-0.98,0  
 3IL3,ASP\_101,3.99,0.28,-0.09,0  
 1FO9,TYR\_356,11.69,2.79,-1.1,-0.01  
 1O3X,LYS\_210,10.15,-0.35,0,0  
 3V75,LYS\_116,10.15,-0.35,0,0  
 1J33,LYS\_263,10.22,-0.28,0,0  
 1QYI,LYS\_228,10.22,-0.28,0,0  
 1WLY,ARG\_167,11.94,-0.56,0,0  
 1R7J,GLU\_68,4.2,0,-0.3,0  
 2IRM,HIS\_335,5.31,1.6,1.39,-4.18  
 3KT2,GLU\_21,4.64,0.14,0,0  
 3GOZ,LYS\_102,10.43,-0.07,0,0  
 2GZQ,ARG\_83,13.74,-0.84,0,2.08  
 3M7G,ARG\_148,12.73,-2.76,0,2.99  
 2BOJ,ARG\_101,11.16,-1.4,0,0.06  
 3PZ9,GLU\_250,2.49,0.77,-2.78,0  
 1X7F,ASP\_349,3.11,0.21,-0.9,0  
 2I6I,GLU\_23,4.71,0.21,0,0  
 2QDJ,GLU\_275,4.75,0.35,-0.1,0  
 3ERF,LYS\_199,10.15,-0.35,0,0  
 3EVP,TYR\_264,11.79,2.59,-0.8,0  
 4FH3,LYS\_150,10.08,-0.42,0,0  
 1G8P,ARG\_177,12.15,-0.35,0,0  
 1O59,HIS\_109,6.42,0.2,0,-0.28  
 2PP6,ARG\_62,12.08,-0.42,0,0  
 3FHF,GLU\_61,4.5,0,0,0  
 1W7B,ARG\_304,12.65,-1.3,0,1.45  
 2D7U,GLU\_84,4.55,2.76,-2.68,-0.03  
 2CL3,TYR\_45,10.07,0.54,-0.47,0  
 3GMS,LYS\_4,10.36,-0.14,0,0  
 3KEY,CYS\_451,11.51,-0.14,1.2,1.45  
 3V75,ARG\_260,12.5,0,0,0  
 3U2R,ARG\_50,12.29,-0.21,0,0  
 4EKU,LYS\_60,10.5,0,0,0  
 1SJ8,HIS\_541,6.36,0,0,-0.14  
 3V3T,GLU\_153,4.17,0.28,-0.61,0  
 1NAR,GLU\_280,4.09,2.97,-3.38,0  
 1TWU,ARG\_4,12.5,0,0,0  
 1SIG,ARG\_397,12.5,0,0,0  
 2Z61,ARG\_363,11.52,-0.98,0,0  
 1SJ8,HIS\_663,6.43,0,0,-0.07  
 3ASA,ARG\_90,12.01,-0.49,0,0  
 3RVC,GLU\_186,4.64,0.14,0,0  
 3GMS,ASP\_223,3.59,0.07,-0.28,0  
 1PSW,TYR\_28,12.95,0.26,-0.8,3.49  
 2B3M,LYS\_37,10.01,-0.49,0,0  
 2YWK,ARG\_10,11.24,-1.26,0,0  
 2NRK,ASP\_144,2.3,0.35,-1.84,0  
 3V75,ASP\_117,3.08,0.56,-1.28,0  
 1TR9,GLU\_95,4.27,0.57,-0.8,0  
 3AU3,GLU\_403,4.28,0.14,-0.36,0  
 1ANU,GLU\_17,3.84,0.14,-0.8,0  
 3PAC,ARG\_167,12.29,-0.21,0,0  
 2NSN,ARG\_27,11.73,-0.77,0,0  
 3CZC,LYS\_19,10.15,-0.35,0,0  
 1YOK,ASP\_204,3.67,0,-0.13,0  
 3RJJ,LYS\_32,10.29,-0.21,0,0  
 1TLV,TYR\_80,11.37,0,0,1.37  
 2FM9,LYS\_113,10.36,-0.14,0,0  
 2AZP,TYR\_137,13.27,0.14,0.65,2.48  
 4EUG,LYS\_57,9.87,-0.63,0,0  
 2B3M,GLU\_132,4.53,0.07,-0.04,0  
 1C3K,LYS\_124,10.5,0,0,0  
 3IU5,TYR\_54,10.22,0.25,-0.03,0  
 3CCY,ARG\_103,11.94,-0.56,0,0  
 3BQW,LYS\_290,10.43,-0.07,0,0  
 1SQW,LYS\_18,10.43,-0.07,0,0  
 4EUG,LYS\_170,10.43,-0.07,0,0  
 1PNE,LYS\_90,10.36,-0.14,0,0  
 2WB8,ARG\_486,11.8,-0.7,0,0  
 3IPZ,TYR\_142,10.1,0.9,-0.8,0  
 1DVO,LYS\_40,10.5,0,0,0  
 1T95,GLU\_23,4.05,0.35,-0.8,0  
 1ILW,GLU\_169,3.86,0.21,-0.85,0  
 2VAN,ARG\_333,13.15,-2.47,0,3.12  
 1MTZ,TYR\_16,10,0,0,0  
 2OKT,ARG\_29,10.92,-4.02,0,2.44  
 2EYI,GLU\_114,4.06,0.49,-0.93,0  
 2RIK,HIS\_196,6.5,0,0,0  
 4ACJ,ASP\_640,3.94,0.14,0,0  
 2YT4,GLU\_536,4.5,0,0,0  
 1JKS,LYS\_46,9.8,-0.7,0,0  
 2VGY,TYR\_40,10.16,0.16,0,0  
 3ASA,HIS\_33,6.36,0,0,-0.14  
 3BA1,ASP\_63,3.21,0.21,-0.8,0  
 3CX5,ARG\_129,11.66,-0.84,0,0  
 4ETX,ASP\_229,3.92,0.14,-0.02,0  
 1P2F,GLU\_20,4.78,0.28,0,0  
 3RNV,ASP\_398,3.8,0.07,-0.07,0  
 2H2W,HIS\_281,4.15,0.6,0,-2.95  
 1TR9,ARG\_130,13.18,-1.72,0,2.4  
 4ECC,ASP\_203,3.46,0.28,-0.62,0  
 1EQ6,GLU\_85,1,2.27,-3.96,-1.82  
 4E8B,GLU\_113,4.05,0.35,-0.8,0  
 1Z3X,HIS\_82,6.5,0,0,0  
 1V6T,TYR\_170,10.78,1.92,-1.14,0  
 1U53,ASP\_51,1.92,0.63,-2.51,0  
 2Z61,ASP\_316,2.83,0.7,-1.67,0  
 1BYI,TYR\_31,10.08,0,0,0.08  
 3GG6,GLU\_164,3.91,0.21,-0.8,0  
 1RWZ,LYS\_12,9.94,-0.56,0,0  
 1YTQ,ASP\_127,2.63,0.63,-1.8,0  
 2B78,ARG\_246,12.89,-0.28,0,0.67  
 1L2H,LYS\_88,10.5,0,0,0  
 2Z84,HIS\_177,11.41,3.6,3.92,-2.61  
 1H4U,HIS\_545,6.51,0.01,0,0  
 2QHT,ASP\_7,2.53,0.49,-1.76,0  
 2YT4,LYS\_629,10.29,-0.21,0,0  
 3CBN,ASP\_66,2.6,0.63,-1.83,0  
 1QZN,GLU\_123,4.64,0.14,0,0  
 3M7G,ASP\_6,3.74,0.28,-0.34,0  
 3L3P,ASP\_256,3.55,0.14,-0.39,0  
 3CCY,GLU\_72,4.46,0.21,-0.25,0  
 1KN3,LYS\_179,10.5,0,0,0  
 2QK1,ASP\_326,2.24,0.7,-2.26,0  
 4FH3,LYS\_282,10.5,0,0,0  
 3FNI,CYS\_136,9.43,-0.46,0,0.89  
 1WPA,GLU\_469,3.6,0.14,-1.04,0  
 3QAV,TYR\_99,9.94,0,-0.06,0  
 3IRA,GLU\_62,4.78,0.28,0,0  
 3UPD,ARG\_167,11.8,-0.7,0,0  
 1RH5,GLU\_17,3.86,0.07,-0.71,0  
 3G9T,ASP\_254,2.23,0.49,-2.06,0  
 3OA7,TYR\_549,10,0,0,0  
 3E7P,HIS\_221,7.06,0.63,0,-0.07  
 3BCY,GLU\_64,5.13,0.63,0,0  
 3LMF,ARG\_109,11.8,-0.7,0,0  
 3DB9,ASP\_107,2.39,0.49,-1.9,0  
 3JRT,ASP\_151,2.43,0.56,-1.93,0  
 2D8N,ASP\_112,3.99,0.14,0.04,0  
 3C6B,GLU\_290,3.98,0.28,-0.8,0  
 1U7U,GLU\_330,4.38,0.63,-0.75,0  
 1C44,LYS\_30,10.01,-0.49,0,0  
 3BWT,HIS\_576,6.5,0,0,0  
 3PZ9,TYR\_247,9.98,0.21,-0.23,0  
 1R53,ARG\_209,12.29,-0.21,0,0  
 2OJQ,ARG\_373,12.01,-0.49,0,0  
 1R3D,ARG\_112,12.15,-0.35,0,0  
 1MTZ,ARG\_143,11.8,-0.7,0,0  
 1ZKZ,TYR\_32,10.21,0.21,0,0  
 3EUR,GLU\_48,4.5,0,0,0  
 3H13,CYS\_406,10.39,-1.02,0,2.4  
 1X7F,ASP\_103,1.49,0.56,-2.88,0  
 2AZP,ARG\_289,11.66,-0.84,0,0  
 1YG2,ARG\_155,11.94,-0.56,0,0  
 3JRT,ARG\_103,11.94,-0.56,0,0  
 2ZCO,LYS\_270,10.5,0,0,0  
 3BPP,TYR\_221,10.2,0,0,0.2  
 2IF4,LYS\_194,10.08,-0.42,0,0  
 2RIK,CYS\_261,8.53,-1.6,0,1.13  
 3L3P,ARG\_349,11.8,-0.7,0,0  
 2IRM,CYS\_277,5.09,-3.98,0,0.07  
 3GS9,GLU\_34,4.78,0.28,0,0  
 3O16,GLU\_96,3.72,0.14,-0.92,0  
 2NRR,LYS\_419,10.5,0,0,0  
 2WOZ,LYS\_399,10.5,0,0,0  
 1SIG,TYR\_425,10,0,0,0  
 4H4J,TYR\_106,11.73,1.01,0,0.72  
 1SJY,GLU\_103,4.57,0.07,0,0  
 2G9D,LYS\_162,10.01,-0.49,0,0  
 3TOW,CYS\_147,9,0,0,0  
 2NSN,LYS\_46,10.5,0,0,0  
 3ODJ,GLU\_81,1.77,1.26,-3.98,0  
 1JSX,HIS\_153,6.69,0.54,0,-0.35  
 1HF8,ASP\_235,3.28,0.28,-0.8,0  
 3BPP,TYR\_233,10,0,0,0  
 1MD6,LYS\_78,10.22,-0.28,0,0  
 2WOZ,GLU\_429,3.49,0.48,-0.94,-0.55  
 2EFK,ASP\_264,1.37,0.98,-3.41,0  
 2D9H,HIS\_74,2.68,1.26,0,-5.08  
 1LTU,LYS\_53,10.5,0,0,0  
 3U0V,LYS\_110,10.5,0,0,0  
 1O59,TYR\_210,7.92,0.07,0,-2.15  
 4ANN,ASP\_84,3.53,0.28,-0.54,0  
 2WOZ,TYR\_438,10,0,0,0  
 1WXQ,ASP\_100,12.22,-0.28,0,0  
 1DVO,GLU\_164,3.56,0.56,-1.5,0  
 2CXA,ARG\_205,12.5,0,0,0  
 2CBE,GLU\_106,5.93,4.02,-1.99,-0.61  
 1SUU,GLU\_655,2.29,-3.01,-2.4  
 4EF5,ARG\_220,12.08,-0.42,0,0  
 2D61,HIS\_284,11.73,-0.77,0,0  
 1KW4,ASP\_20,3.74,0,-0.06,0  
 3R2E,CYS\_50,9,0,0,0  
 2QHT,ARG\_25,12.08,-0.42,0,0  
 4DVD,ASP\_49,3.64,0.21,-0.37,0  
 3A4C,ASP\_536,3.09,0.35,-1.06,0  
 1X7F,TYR\_292,9.96,0,-0.04,0  
 3RJJ,LYS\_207,10.5,0,0,0  
 3DHN,LYS\_151,10.29,-0.21,0,0  
 3UC9,GLU\_162,4.12,0.07,-0.45,0  
 2CXC,ASP\_113,3.31,0.42,-0.91,0  
 1MUF,LYS\_158,10.36,-0.14,0,0  
 4E65,ARG\_24,12.5,0,0,0  
 1UJ8,LYS\_15,10.15,-0.35,0,0  
 1U7U,LYS\_345,10.29,-0.21,0,0  
 2CBE,ASP\_175,3.8,0,0,0  
 1J33,CYS\_94,10.76,0,0,1.76  
 3IVF,GLU\_34,4.2,0.21,-0.51,0  
 2EHG,ARG\_136,12.43,-0.07,0,0  
 2APL,ASP\_119,2.3,0.84,-2.35,0  
 3M66,GLU\_296,4.85,0.35,0,0  
 4F3J,TYR\_233,11.96,0.07,0,1.89  
 1R3D,HIS\_135,4.4,0,-0.11,-2  
 2BLL,LYS\_587,10.5,0,0,0  
 1UJ8,HIS\_8,6.36,0,0,-0.14  
 1WJG,TYR\_9,11.41,0,-0.07,1.48  
 2E3C,GLU\_249,4.78,0.28,0,0  
 2FGG,HIS\_6,6.5,0,0,0  
 2FD5,ASP\_143,3.77,0,-0.03,0  
 2X5Y,LYS\_755,10.15,-0.35,0,0  
 1WJG,LYS\_167,10.29,-0.21,0,0  
 2VAN,ARG\_126,11.66,-0.84,0,0  
 3K1H,GLU\_78,4.64,0.14,0,0  
 1BYI,ARG\_3,12.22,-0.28,0,0  
 1DCF,GLU\_128,4.96,0.7,-0.24,0  
 3I4T,LYS\_106,10.5,0,0,0  
 3QKY,ARG\_96,12.22,-0.28,0,0  
 2YWX,ARG\_138,12.43,-0.07,0,0  
 2AHE,LYS\_257,10.5,0,0,0  
 3AUF,ARG\_196,12.5,0,0,0  
 3CX2,ASP\_163,2.57,0.28,-1.51,0

3CZC,ASP\_80,2.98,0.56,-1.37,0  
3TOW,ARG\_145,11.8,-0.7,0,0  
2F4Q,ARG\_114,12.43,-0.07,0,0  
3BJV,HIS\_111,4.81,0,0,-1.69  
3P28,CYS\_22,10.72,-1.28,-0.03,3.04  
2D0A,LYS\_307,10.36,-0.14,0,0  
3M7D,TYR\_268,13.41,0.21,0.8,2.4  
1SNT,GLU\_376,4.12,0.35,-0.73,0  
3GMS,ASP\_113,3.6,0,-0.2,0  
2WB3,LYS\_379,9.94,-0.56,0,0  
1SBX,LYS\_119,10.5,0,0,0  
3IDW,ASP\_53,2.87,0.63,-1.56,0  
1J85,ASP\_41,2.38,0.49,-1.91,0  
2F4Q,ARG\_261,12.43,-0.07,0,0  
2Y2T,ASP\_75,2.99,0.63,-1.45,0  
3CO1,GLU\_94,4.5,0,0,0  
3L3P,ARG\_494,12.22,-0.28,0,0  
2NYC,LYS\_185,10.5,0,0,0  
3A7L,GLU\_76,4.57,0.07,0,0  
1RIS,GLU\_276,4.5,0,0,0  
3KEY,GLU\_406,4.5,0,0,0  
4DNU,LYS\_269,10.29,-0.21,0,0  
2VAN,LYS\_234,11.78,-0.42,0,1.7  
2FBI,GLU\_73,4.05,0.35,-0.8,0  
2XWS,TYR\_111,10.0,0,0,0  
4AF2,HIS\_6,7.05,0.7,0,-0.14  
1SBX,HIS\_89,6.5,0,0,0  
1BYI,GLU\_137,3.52,0.54,-1.52,0  
3KT9,CYS\_5,9.65,-0.07,0,0.72  
3B7H,ASP\_69,3.07,0.07,-0.8,0  
2R0S,TYR\_318,11.46,0.14,0,1.32  
2EFK,ARG\_27,12.43,-0.07,0,0  
1EDG,ASP\_281,3.14,0.56,-1.22,0  
2O8P,GLU\_188,4.22,0.49,-0.77,0  
3LPZ,ARG\_257,12.08,-0.42,0,0  
1P4X,LYS\_151,10.43,-0.07,0,0  
2QOP,GLU\_61,4.4,0.21,-0.31,0  
3ASA,ARG\_340,12.5,0,0,0  
2R0S,ASP\_109,2.48,0.7,-2.02,0  
3E0H,TYR\_102,10.13,0.21,-0.56,0.48  
3D9H,ARG\_144,11.8,-0.7,0,0  
3RJX,TYR\_39,13.34,0.14,0.8,2.4  
3KB5,ARG\_444,12.5,0,0,0  
1EV8,ARG\_166,13.27,-0.62,0,1.39  
1TWU,GLU\_30,4.19,0.49,-0.8,0  
4DNU,TYR\_248,12.94,2.94,0,0  
2GZR,ASP\_272,3.8,0,0,0  
1GXN,ARG\_468,12.85,-1.64,0,1.99  
3UOV,CYS\_12,7.47,-1.67,0,0.14  
2AXO,TYR\_85,8.79,0.28,-1.49,0  
3IPZ,GLU\_146,4.64,0.14,0,0  
2H01,ASP\_125,2.35,1.05,-2.5,0  
2WB8,LYS\_618,10.43,-0.07,0,0  
3KV0,ARG\_184,12.01,-0.49,0,0  
1R3F,ARG\_271,11.94,-0.56,0,0  
1ANU,ASP\_40,2.77,0.63,-1.66,0  
1Z3X,ASP\_47,3.4,0.49,-0.89,0  
3ODJ,HIS\_134,6.63,0.13,0,0  
4EF5,GLU\_339,4.45,0.28,-0.33,0  
3CZC,CYS\_8,4.03,-5.05,0,0.07  
2D2S,HIS\_611,6.5,0,0,0  
3CCY,LYS\_85,10.15,-0.35,0,0  
2XWS,GLU\_105,3.77,0.07,-0.8,0  
1S7K,ARG\_124,11.94,-0.56,0,0  
1EV8,GLU\_195,4.5,0,0,0  
1JT9,CYS\_219,8.97,-0.03,0,0  
1V43,ASP\_279,3.82,0.07,-0.05,0  
1UJ8,ASP\_54,3.51,0.07,-0.36,0  
3M66,LYS\_274,10.29,-0.21,0,0  
3C2E,LYS\_144,10.43,-0.07,0,0  
3MTT,ARG\_587,12.29,-0.21,0,0  
1OIS,ASP\_141,2.74,0.14,-1.2,0  
2CN1,GLU\_259,4.5,0,0,0  
3BWT,ASP\_562,3.67,0,-0.13,0  
2HRZ,ASP\_61,3.39,0.28,-0.69,0  
2B2H,TYR\_284,12.22,0.07,0.2,1.5  
3HNX,ASP\_36,3.29,0.42,-0.93,0  
1RLO,ASP\_81,1.34,0.91,-3.37,0  
1V43,LYS\_82,10.29,-0.21,0,0  
3RJZ,LYS\_129,10.5,0,0,0  
3CIV,ASP\_60,3.05,-1.36,0  
4DNU,LYS\_165,10.08,-0.42,0,0  
1SFE,GLU\_32,4.15,0.07,-0.42,0  
1V43,GLU\_334,4.78,0.49,-0.21,0  
2CYG,ARG\_232,12.5,0,0,0  
3RLE,CYS\_103,1.18,-6.31,-1.76,0.25  
1LTU,TYR\_232,10.96,0.96,0,0  
2H85,GLU\_91,4.14,0.14,-0.5,0  
3GYW,ASP\_223,3.86,0.07,-0.01,0  
3E7P,ASP\_165,4.05,0.35,-0.1,0  
2PWQ,GLU\_94,4.64,0.14,0,0  
2V4X,TYR\_116,9.62,1.05,-1.43,0  
2H01,ARG\_61,11.8,-0.7,0,0  
2E0T,TYR\_113,9.92,0.72,-0.8,0  
2B61,ARG\_61,11.73,-0.77,0,0  
2R0S,ASP\_311,3.15,0.28,-0.93,0  
1PVT,GLU\_72,4.55,0.14,-0.09,0  
1XIP,HIS\_70,6.29,0,0,-0.21  
2X5Y,LYS\_849,9.87,-0.63,0,0  
2WOZ,TYR\_317,10.69,0.69,0,0  
1SJ8,LYS\_687,10.5,0,0,0  
4DBX,TYR\_288,13.0,0.07,0.03,2.91  
3DTE,ARG\_72,12.08,-0.42,0,0  
1PVT,ARG\_6,12.36,-0.14,0,0  
2QVO,LYS\_7,10.08,-0.42,0,0  
1RKA,GLU\_214,4.64,0.14,0,0  
1V6T,ASP\_123,2.97,0.21,-1.04,0  
2G9D,GLU\_146,3.8,0.35,-1.05,0  
4H86,ASP\_108,2.27,0.35,-1.87,0  
3B21,GLU\_44,3.98,0.28,-0.8,0  
2D0A,ARG\_258,12.15,-0.35,0,0  
1AKO,CYS\_241,7.27,-2.21,0,0.48  
2CXC,LYS\_90,10.5,0,0,0  
1RLO,GLU\_99,2.7,0.63,-2.43,0  
2EEY,LYS\_137,10.08,-0.42,0,0  
2G2D,ASP\_148,3.8,0.07,-0.05,0  
3UAH,ARG\_204,10.32,-2.18,0,0  
2CXV,TYR\_23,11.22,1.22,0,0  
3M70,ASP\_54,3.37,0.35,-0.78,0  
3LJC,ARG\_17,11.37,-1.13,0,0  
2YWK,LYS\_43,10.5,0,0,0  
3CAX,ARG\_428,12.5,0,0,0  
1V43,GLU\_128,4.71,0.21,0,0  
2PGX,ARG\_101,10.48,-1.7,0,-0.32  
4DBX,LYS\_113,10.29,-0.21,0,0  
2O8P,TYR\_137,10.97,0.85,0.12  
1LZL,ARG\_263,13.99,-0.91,0.2,4  
4ETX,GLU\_357,3.79,0.21,-0.92,0  
3IRA,ARG\_81,11.52,-0.98,0,0  
3V1Q,GLU\_545,3.31,0.35,-1.54,0  
1YG2,ARG\_148,11.94,-0.56,0,0  
3VJ8,ASP\_145,2.9,0.49,-1.4,0  
2AZP,TYR\_185,10.14,0.14,0,0  
3B21,LYS\_132,10.43,-0.07,0,0  
2R4Q,LYS\_193,10.5,0,0,0  
3DB9,ARG\_173,11.01,-1.53,0,0.04  
1V8E,ARG\_10,11.87,-0.63,0,0  
2B6P,GLU\_250,3.8,0.21,-0.91,0  
3GS3,GLU\_65,4.57,0.07,0,0  
3ADO,ASP\_226,4.08,0.28,0,0  
2D2S,HIS\_701,1.99,0.15,-0.29,-4.37  
3CS1,GLU\_29,4.71,0.21,0,0  
3B7H,LYS\_55,10.43,-0.07,0,0  
3UV9,CYS\_380,8.36,-2.59,0.05,1.9  
2XHC,LYS\_24,10.5,0,0,0  
4DVD,ASP\_163,3.21,0.28,-0.87,0  
3ZXY,HIS\_30,8.74,2.52,0,-0.28  
2EHG,LYS\_82,10.22,-0.28,0,0  
1L3K,LYS\_130,10.43,-0.07,0,0  
3I47,TYR\_230,10.0,0,0,0  
2AXO,HIS\_125,6.29,0,0,-0.21  
2CXV,ARG\_49,12.43,-0.07,0,0  
2ZQ5,ARG\_214,11.19,-1.31,0,0  
3UAH,LYS\_246,10.5,0,0,0  
1X04,LYS\_167,10.36,-0.14,0,0  
2GAU,CYS\_127,8.92,-0.22,0,0.14  
2DFL,LYS\_235,10.5,0,0,0  
2A0J,GLU\_52,3.38,1.47,-2.59,0  
1NIJ,LYS\_168,10.22,-0.28,0,0  
1O17,HIS\_63,6.22,0,0,-0.28  
3VJ8,TYR\_341,10.4,0.16,-0.8,-1.04  
3K8J,ARG\_152,11.45,-1.05,0,0  
1WNH,LYS\_167,10.29,-0.21,0,0  
3F6F,GLU\_25,4.5,0,0,0  
2H85,GLU\_113,2.79,0.56,-2.27,0  
1R2Z,TYR\_124,10.63,0,0,0.63  
3LH5,ARG\_740,13.62,-1.28,0.2,4  
3MTT,TYR\_467,11.55,0,0,1.55  
1KN3,GLU\_16,4.03,-0.85,0  
3ETU,ASP\_37,3.83,0.07,-0.04,0  
1X6J,HIS\_10,7.19,0.69,0,0  
1Q42,GLU\_154,4.64,0.14,0,0  
2EFK,ARG\_179,12.22,-0.28,0,0  
3FFM,HIS\_77,6.43,0,0,-0.07  
2H80,LYS\_145,10.5,0,0,0  
2DBN,LYS\_22,10.43,-0.07,0,0  
3OOP,ARG\_88,12.5,0,0,0  
1RIS,GLU\_225,1.08,1.78,-3.19,-2.01  
3NZL,HIS\_75,6.5,0,0,0  
2OJQ,GLU\_645,3.04,0.42,-1.88,0  
2P5D,GLU\_110,4.5,0,0,0  
3H5T,ASP\_297,3.25,0.63,-1.18,0  
2OGQ,CYS\_372,8.3,-0.7,0,0  
2CXV,GLU\_56,4.64,0.14,0,0  
1QQE,ASP\_98,3.4,0.14,-0.54,0  
1WPA,ARG\_434,11.94,-0.56,0,0  
1SUU,TYR\_558,11.55,0,0,1.55  
1UAJ,LYS\_14,10.43,-0.07,0,0  
3ILC,CYS\_151,10.99,0,0,1.99  
3F7M,HIS\_171,6.39,0,-0.11,0  
2GAU,LYS\_227,10.5,0,0,0  
3CNU,GLU\_20,4.5,0,0,0  
3DHN,TYR\_175,12.73,0.41,0.03,2.29  
1IDK,ASP\_77,3.68,0.84,-0.96,0  
2VGM,LYS\_165,10.36,-0.14,0,0  
3ON1,GLU\_101,4.54,0.04,0,0  
3LD1,LYS\_271,10.29,-0.21,0,0  
2OPJ,CYS\_266,12.13,-0.24,2.24,1.13  
3F53,TYR\_71,9.69,0,-0.31,0  
1N81,ARG\_144,12.5,0,0,0  
3ETV,TYR\_94,10.8,0,-0.45,1.25  
3PP8,GLU\_183,3.29,0.56,-1.77,0  
1PGV,ARG\_376,11.73,-0.77,0,0  
1F2V,CYS\_45,6.97,-2.72,0,0.69  
1MTZ,LYS\_28,10.22,-0.28,0,0  
3PBH,HIS\_49,6.62,0.19,0,-0.07  
2F8H,TYR\_148,13.92,0.72,0.8,2.4  
3FTT,GLU\_126,5.16,1.07,-0.28,-0.12  
2Z0W,CYS\_64,9,-0.21,0,0.21  
1J7G,LYS\_87,10.5,0,0,0  
3CAN,GLU\_123,3.98,0.28,-0.8,0  
2QHT,LYS\_170,10.29,-0.21,0,0  
1YR6,GLU\_113,3.98,0.28,-0.8,0  
2BV9,TYR\_247,13.95,0.89,0.66,2.4  
1Q46,GLU\_99,4.64,0.14,0,0  
3C5V,ARG\_371,12.5,0,0,0  
1Q2Y,GLU\_33,4.5,0,0,0  
1C44,GLU\_15,4.57,0.07,0,0  
3CAX,ARG\_376,12.29,-0.21,0,0  
1J74,LYS\_24,10.29,-0.21,0,0  
3ETU,ARG\_44,12.36,-0.14,0,0  
3CCY,LYS\_172,10.01,-0.49,0,0  
2W2S,ARG\_167,12.43,-0.07,0,0  
3LH5,LYS\_702,10.01,-0.49,0,0  
2QDJ,GLU\_280,4.28,0.21,-0.43,0  
2J8A,TYR\_253,11.6,0.2,0,1.4  
3CAX,GLU\_417,4.24,0.42,-0.68,0  
1XIP,GLU\_14,4.15,0.14,-0.49,0  
2D59,GLU\_79,3.24,0.7,-1.96,0  
1IAP,HIS\_228,5.09,0,0,-1.41  
2GZQ,LYS\_180,10.29,-0.21,0,0  
1BN6,ARG\_97,12.22,-0.28,0,0  
1P2F,ARG\_63,12.36,-0.14,0,0  
1MTZ,HIS\_264,5.18,0,0,-1.32  
3A0X,LYS\_699,9.8,-0.7,0,0  
1O59,ARG\_179,12.02,-2.65,0.2,16  
3L7N,HIS\_143,8.77,3.85,3.45,-5.03  
1WPA,LYS\_494,10.43,-0.07,0,0  
3T5B,TYR\_301,13.95,1.66,-0.11,2.4  
1QQL,GLU\_90,3.3,0.42,-1.62,0  
1LPL,GLU\_186,4.5,0,0,0  
1NJ4,GLU\_342,4.39,0.21,-0.32,0  
3DZ1,ASP\_21,2.63,0.63,-1.8,0  
3C6B,ASP\_230,3.34,0.07,-0.53,0  
1LZL,GLU\_190,8.07,4.37,-0.8,0  
1T07,TYR\_10,11.52,0.07,0,1.45  
2OSA,ASP\_371,2.59,0.42,-1.63,0  
3UAH,HIS\_420,6.29,0,0,-0.21  
3LJN,LYS\_26,10.29,-0.21,0,0  
3IBT,CYS\_31,7.84,-3.6,0.2,44  
3ZSL,ARG\_151,11.94,-0.56,0,0  
3HYQ,GLU\_42,4.32,0,-0.18,0  
1ZP2,GLU\_90,3.18,0.28,-1.6,0  
220M,ASP\_296,2.38,0.63,-2.04,0  
4DND,GLU\_49,4.71,0.21,0,0  
3I47,TYR\_93,10.0,0,0,0  
3O16,GLU\_141,4.23,0.42,-0.69,0  
1J74,GLU\_130,3.15,0.49,-1.84,0  
3RKV,ASP\_239,1.21,0.56,-3.15,0  
1N4A,ARG\_344,11.73,-0.77,0,0  
3IRA,LYS\_9,10.5,0,0,0  
4EZB,ARG\_127,12.36,-0.14,0,0  
1YW5,TYR\_49,8.43,1.58,-2.1,-1.04  
1WJG,LYS\_3,10.5,0,0,0  
3C38,TYR\_266,10.44,0.07,0.37,0  
3D9H,GLU\_251,4.77,0.28,-0.01,0  
1WPA,ASP\_466,3.87,0.14,-0.07,0  
3KV0,GLU\_205,3.76,0.35,-1.09,0  
2Q99,LYS\_65,10.43,-0.07,0,0  
2D59,TYR\_112,9.34,0.14,-0.8,0  
3CN5,LYS\_237,9.87,-0.63,0,0  
3GS3,LYS\_45,10.15,-0.35,0,0  
3ETU,ASP\_187,3.75,0,-0.05,0  
1F09,ARG\_192,12.5,0,0,0  
3H13,CYS\_426,9.87,0,0,0.87  
3L7N,ASP\_195,3.94,0.14,0,0

2WB8,ARG\_732,11.87,-0.63,0,0  
 2V1L,GLU\_61,3.65,0.38,-1.23,0  
 3E7P,LYS\_37,10.5,0,0,0  
 3BCH,LYS\_89,10.43,-0.07,0,0  
 3BQE,ASP\_275,2.07,0.7,-2.42,0  
 1T3Y,LYS\_4,10.22,-0.28,0,0  
 2IN0,GLU\_20,3.35,1.05,-2.2,0  
 3CE7,ASP\_14,3.42,0.49,-0.87,0  
 3C0C,GLU\_345,4.64,0.14,0,0  
 1WXQ,ARG\_299,11.45,-1.05,0,0  
 1YM5,HIS\_185,6.5,0,0,0  
 1AIL,LYS\_70,10.5,0,0,0  
 1BKR,LYS\_15,10.43,-0.07,0,0  
 4E6S,GLU\_84,4.92,0.42,0,0  
 3FTT,HIS\_170,6.36,0,0,-0.14  
 2OKT,LYS\_238,10.5,0,0,0  
 3R87,ASP\_40,2.86,0.42,-1.36,0  
 2GKG,LYS\_96,10.5,0,0,0  
 3E7P,LYS\_245,9.94,-0.56,0,0  
 2AHE,ASP\_246,4.01,0.21,0,0  
 1R3D,GLU\_69,4.78,0.28,0,0  
 2VGM,LYS\_322,10.5,0,0,0  
 3EGN,LYS\_396,10.5,0,0,0  
 1S18,GLU\_621,4.58,0.49,-0.41,0  
 3LJC,HIS\_172,5.01,0,0,-1.49  
 1QQE,GLU\_12,4.5,0,0,0  
 1XAW,TYR\_467,12.11,0,0,2.11  
 1FQI,GLU\_349,4.5,0,0,0  
 4EVF,ARG\_293,12.22,-0.28,0,0  
 1U7U,ARG\_206,12.15,-0.35,0,0  
 2PGX,ARG\_164,11.17,-1.33,0,0  
 3DZ1,LYS\_229,10.43,-0.07,0,0  
 3UX2,TYR\_117,13.27,0.07,0.8,2.4  
 3BZT,HIS\_265,7.24,0.81,0,-0.07  
 2FBQ,ARG\_9,12.08,-0.42,0,0  
 3B79,GLU\_92,4.4,0.7,-0.8,0  
 2G5X,ASP\_7,2.76,0.14,-1.18,0  
 1R22,GLU\_48,3.93,0.21,-0.79,0  
 1WNH,HIS\_138,3.67,0.49,0,-3.32  
 4ECC,ASP\_127,4.02,0.28,-0.06,0  
 2OBI,ARG\_152,10.55,-1.95,0,0  
 3K8J,TYR\_190,10,0,0,0  
 2A6B,LYS\_45,10.5,0,0,0  
 2YT4,HIS\_685,8.13,4.38,1.91,-4.65  
 1TWU,ARG\_127,11.73,-0.77,0,0  
 1WLY,LYS\_10,10.43,-0.07,0,0  
 3EGN,ARG\_502,12.5,0,0,0  
 1XTD,LYS\_38,10.36,-0.14,0,0  
 3M3P,ASP\_64,3.87,0.07,0,0  
 1YR6,ARG\_90,12.15,-0.35,0,0  
 1FHL,ASP\_127,3.86,0.07,-0.01,0  
 1DOV,ARG\_211,11.73,-0.77,0,0  
 1RHS,LYS\_45,10.43,-0.07,0,0  
 1U7U,ARG\_384,12.01,-0.49,0,0  
 2V5B,ARG\_55,12.29,-0.21,0,0  
 3IVF,GLU\_350,4.35,0.07,-0.22,0  
 3L0D,HIS\_84,6.75,0.39,0,-0.14  
 3V3T,GLU\_232,4.05,0.35,-0.8,0  
 3P51,LYS\_39,10.22,-0.28,0,0  
 2CWY,GLU\_35,3.97,0.42,-0.95,0  
 2FGG,ASP\_57,3.7,0.49,-0.58,0  
 3GT0,LYS\_202,10.5,0,0,0  
 1EDG,ASP\_160,2.4,0.63,-2.03,0  
 1NFN,GLU\_45,4.57,0.07,0,0  
 2C2Y,ARG\_67,11.94,-0.56,0,0  
 2EJX,GLU\_98,4.73,0.28,-0.05,0  
 3K8J,ASP\_265,4.07,0.28,-0.01,0  
 1JT9,LYS\_160,10.15,-0.35,0,0  
 1S18,ASP\_760,2.14,0.63,-2.28,0  
 1RAJ,LYS\_228,10.36,-0.14,0,0  
 4ECC,LYS\_207,10.29,-0.21,0,0  
 3CAX,LYS\_338,10.36,-0.14,0,0  
 3GS9,ARG\_239,12.01,-0.49,0,0  
 1GXN,TYR\_569,12.08,0,2.08  
 3CNS,LYS\_161,10.08,-0.42,0,0  
 1D2K,ARG\_120,11.73,-0.77,0,0  
 1YR6,GLU\_58,3.28,0.28,-1.5,0  
 1RSS,GLU\_113,3.41,0.7,-1.79,0  
 3HUE,CYS\_117,8.2,-1.55,0,0.75  
 1WLY,TYR\_197,10.19,0.19,0,0  
 1CHD,TYR\_226,11.02,0.73,-1.18,1.47  
 2RIS,CYS\_91,10.75,0,0.08,1.67  
 1RHS,ASP\_92,3.87,0.07,0,0  
 2Q12,GLU\_67,4.5,0,0,0  
 1KCM,GLU\_181,4.78,0.28,0,0  
 3V55,GLU\_680,4.5,0,0,0  
 1W7B,CYS\_262,10.89,-0.03,-0.65,2.58  
 2FBQ,ASP\_12,3.32,0.35,-0.83,0  
 2PGE,ARG\_18,12.5,0,0,0  
 1SQH,LYS\_26,10.36,-0.14,0,0  
 3LMF,ARG\_102,12.22,-0.28,0,0  
 1R3F,GLU\_167,3.2,0.14,-1.44,0  
 4FH3,GLU\_43,4.57,0.07,0,0  
 3P28,LYS\_166,10.5,0,0,0  
 2H01,ASP\_14,3.4,0.07,-0.47,0  
 3SMD,HIS\_16,7.16,0.8,0,-0.14  
 3ZXV,GLU\_106,4.57,0.07,0,0  
 2I6I,ARG\_6,12.29,-0.21,0,0  
 3D9H,GLU\_253,3.56,0.14,-1.08,0  
 1P4X,TYR\_188,10,0,0,0  
 3LH5,LYS\_695,10.43,-0.07,0,0  
 1YM5,LYS\_207,10.5,0,0,0  
 3CAX,ARG\_194,12.79,-2.11,0,2.4  
 1A8Q,ARG\_54,10.42,-4.76,0,2.68  
 3LQE,ASP\_366,3.94,0.21,-0.07,0  
 3NR5,LYS\_146,10.22,-0.28,0,0  
 3OA7,ASP\_569,3.91,0.28,-0.17,0  
 3V46,LYS\_366,10.22,-0.28,0,0  
 1YIB,ASP\_244,3.73,0.42,-0.49,0  
 2F19,TYR\_21,9.27,0.07,-0.8,0  
 3ELI,ARG\_92,12.22,-0.28,0,0  
 3V4G,LYS\_146,10.29,-0.21,0,0  
 3GS3,CYS\_60,7.21,-1.93,0,0.14  
 1ZBS,CYS\_123,8.53,-1.94,0,1.47  
 2FBQ,LYS\_78,10.43,-0.07,0,0  
 2YT4,GLU\_518,3.37,0.21,-1.34,0  
 1RKA,GLU\_273,4.27,0.28,-0.51,0  
 3RKV,GLU\_234,3.74,0.21,-0.97,0  
 3ODJ,HIS\_56,3.18,1.42,0,-4.74  
 3CCY,HIS\_106,2.61,0,-0.85,-3.04  
 1H09,TYR\_120,10,0,0,0  
 2BDV,ARG\_33,12.01,-0.49,0,0  
 1SQH,ARG\_142,12.08,-0.42,0,0  
 3G9T,ASP\_265,4.06,0.35,-0.09,0  
 2H30,HIS\_181,6.5,0,0,0  
 3CBN,ARG\_77,11.87,-0.63,0,0  
 2WOZ,LYS\_431,10.43,-0.07,0,0  
 1R3F,ARG\_75,11.94,-0.56,0,0  
 1EQ6,LYS\_147,10.43,-0.07,0,0  
 1AM2,TYR\_102,9.87,0,-0.13,0  
 3NR5,TYR\_61,10.83,0,0,0.83  
 2W1R,TYR\_133,12.47,0.55,0,1.92  
 3CCY,GLU\_56,4.64,0.14,0,0  
 3P28,GLU\_209,3.84,0.14,-0.8,0  
 3C38,GLU\_209,3.16,0.7,-2.04,0  
 3LJI,GLU\_107,4.71,0.21,0,0  
 2H85,LYS\_110,10.5,0,0,0  
 3CRM,ARG\_223,9.48,-2.23,0,-0.79  
 1H4U,ARG\_383,12.5,0,0,0  
 3GS9,GLU\_292,4.18,0.42,-0.74,0  
 3N2T,ARG\_315,11.87,-0.63,0,0  
 3EIZ,CYS\_115,5.17,-3.91,0,0.07  
 3F6F,ASP\_58,1.81,0.63,-2.62,0  
 2BAA,ASP\_95,2.78,0.28,-1.3,0  
 1P6F,LYS\_61,10.08,-0.42,0,0  
 1RKA,ARG\_74,11.94,-0.56,0,0  
 2W1R,LYS\_96,10.08,-0.42,0,0  
 1NRI,ARG\_113,12.5,0,0,0  
 1A8Q,TYR\_182,10.27,0,0,0.27  
 1JSX,HIS\_53,4.47,0,-0.01,-2.02  
 3C6B,TYR\_180,8.91,2.39,-1.08,-2.4  
 3EJC,LYS\_12,10.5,0,0,0  
 3F6F,LYS\_76,10.22,-0.28,0,0  
 1R6Y,ARG\_17,12.01,-0.49,0,0  
 3BJV,ARG\_70,12.29,-0.21,0,0  
 1BKB,ASP\_95,1.33,1.19,-3.66,0  
 1R15,ARG\_106,12.5,0,0,0  
 3IVF,ASP\_55,3.38,0.77,-1.18,0  
 1UAJ,TYR\_181,10,0,0,0  
 2CYG,ASP\_99,3.39,0.35,-0.77,0  
 1NAF,ASP\_451,3.91,0.21,-0.1,0  
 3CAX,GLU\_140,4.78,0.28,0,0  
 2V5B,HIS\_188,1.86,1.03,0,-5.66  
 2EVI,HIS\_184,6.34,0.05,0,-0.21  
 2EDM,ASP\_127,3.42,0,-0.38,0  
 3JRT,GLU\_74,5.05,0.65,-0.1,0  
 1NAF,GLU\_246,4.15,0.07,-0.42,0  
 3K8J,ARG\_78,11.87,-0.63,0,0  
 2FL4,TYR\_112,9.95,0.07,-0.8,0.68  
 1L3K,LYS\_105,10.29,-0.21,0,0  
 3CIV,ARG\_168,11.8,-0.7,0,0  
 2AOJ,ASP\_93,2.0,7,-2.49,0  
 1OXZ,LYS\_295,10.29,-0.21,0,0  
 2CW4,ARG\_111,12.29,-0.21,0,0  
 1XFK,LYS\_147,10.5,0,0,0  
 3OKQ,GLU\_653,4.71,0.21,0,0  
 3A2Z,GLU\_193,3.64,0.28,-1.14,0  
 1R53,ASP\_26,3.46,0.35,-0.69,0  
 3ULX,ASP\_157,3.94,0.14,0,0  
 2H2W,LYS\_76,10.5,0,0,0  
 3ONH,ASP\_533,3.27,0.28,-0.81,0  
 1NJ4,HIS\_216,6.08,0,0,-0.42  
 3FFM,CYS\_38,8.2,-0.95,0,0.14  
 1X7F,CYS\_37,11.7,0,1.18,1.52  
 3RAZ,GLU\_129,1.58,0.56,-1.08,-2.4  
 3B7H,GLU\_42,4.5,0,0,0  
 2POL,ASP\_195,3.29,0.21,-0.72,0  
 3CCY,GLU\_83,4.5,0,0,0  
 1WPA,GLU\_456,4.78,0.28,0,0  
 1XEU,LYS\_72,10.5,0,0,0  
 1QQH,LYS\_173,10.5,0,0,0  
 2A4D,GLU\_96,4.5,0,0,0  
 3GFP,TYR\_455,10,0,0,0  
 2EHG,LYS\_122,10.5,0,0,0  
 1TR9,ARG\_258,11.52,-0.98,0,0  
 1R9W,ARG\_294,12.08,-0.42,0,0  
 2F19,ARG\_27,12.5,0,0,0  
 1CBY,LYS\_199,10.01,-0.49,0,0  
 3DSH,CYS\_388,10.22,-1.4,1.21,1.42  
 2I88,LYS\_362,9.94,-0.56,0,0  
 1JYH,GLU\_4,4.5,0,0,0  
 1A8Q,LYS\_263,10.15,-0.35,0,0  
 3M16,GLU\_242,4.93,0.56,-0.12,0  
 1ES9,ARG\_160,11.87,-0.63,0,0  
 3BWT,ASP\_671,3.38,0.35,-0.76,0  
 3M70,GLU\_160,4.03,0.14,-0.61,0  
 3RJZ,ARG\_133,12.08,-0.42,0,0  
 2AHE,LYS\_124,10.43,-0.07,0,0  
 2X4G,GLU\_313,3.45,0.49,-1.54,0  
 2O0K,ARG\_162,12.43,-0.07,0,0  
 2VGM,LYS\_264,10.01,-0.49,0,0  
 3CGW,LYS\_87,10.22,-0.28,0,0  
 2PGE,GLU\_274,3.67,0.21,-1.04,0  
 1ZHV,TYR\_14,10.26,0.45,-1.19,1  
 1U53,LYS\_140,10.29,-0.21,0,0  
 2BCF,TYR\_258,9.82,0,-0.18,0  
 2A6B,ASP\_93,3.12,0.49,-1.17,0  
 1WYC,GLU\_336,4.5,0,0,0  
 3E7P,LYS\_72,10.43,-0.07,0,0  
 4DIU,HIS\_53,0.64,0.87,-1.49,-5.25  
 3K1H,LYS\_38,10.43,-0.07,0,0  
 2POL,GLU\_46,3.08,0.65,-2.07,0  
 1YB2,HIS\_238,7.03,0.6,0,-0.07  
 4FLE,LYS\_24,10.5,0,0,0  
 1A8Q,GLU\_160,3.98,0.28,-0.8,0  
 2GAU,ASP\_223,3.8,0,0,0  
 3ELI,HIS\_87,6.62,0.4,0,-0.28  
 2PGE,ASP\_144,2.83,0.14,-1.11,0  
 2YX0,ARG\_224,11.73,-0.77,0,0  
 3V55,LYS\_367,10.36,-0.14,0,0  
 1WXQ,LYS\_188,10.01,-0.49,0,0  
 3D9H,GLU\_140,4.52,1.57,-1.55,0  
 1W24,GLU\_44,4.57,0.07,0,0  
 2QHT,LYS\_175,10.29,-0.21,0,0  
 1KCM,LYS\_179,10.36,-0.14,0,0  
 3F1X,HIS\_201,6.04,0,-0.46,0  
 1OXZ,ASP\_274,3.56,0,-0.24,0  
 2VGM,GLU\_186,4.57,0.07,0,0  
 4DNU,ARG\_286,11.52,-0.98,0,0  
 2YLF,ARG\_92,12.15,-0.35,0,0  
 2IXM,TYR\_45,11.38,0.51,0,0.87  
 2AD1,ASP\_196,3.8,0.07,-0.07,0  
 1M5I,GLU\_140,4.05,0.35,-0.8,0  
 3BWT,CYS\_738,9.78,-0.43,0,1.21  
 1ILW,ASP\_110,3.87,0.07,0,0  
 3RFY,ASP\_186,3.73,0.28,-0.35,0  
 2OJQ,LYS\_525,10.22,-0.28,0,0  
 3TMO,ARG\_187,12.5,0,0,0  
 1D2K,HIS\_251,2.91,0.29,0,-3.88  
 1R15,ARG\_260,12.08,-0.42,0,0  
 3ETU,ARG\_193,12.01,-0.49,0,0  
 2IF4,GLU\_173,2.25,0.7,-2.95,0  
 3ON1,LYS\_5,10.5,0,0,0  
 1BYI,LYS\_2,10.36,-0.14,0,0  
 1PSW,CYS\_262,11.12,-0.63,0,2.75  
 1MIX,ARG\_277,12.5,0,0,0  
 3CSV,ASP\_299,3.55,0.49,-0.74,0  
 1GXN,TYR\_616,11.15,0,0,1.15  
 3MIX,HIS\_482,2.46,0.11,-1.34,-2.8  
 4F8A,LYS\_577,10.29,-0.21,0,0  
 2RJD,GLU\_522,4.57,0.07,0,0  
 3EAZ,ARG\_89,12.01,-0.49,0,0  
 1NIJ,LYS\_318,10.36,-0.14,0,0  
 2WB3,ASP\_337,2.85,0.7,-1.65,0  
 3M9A,GLU\_92,4.71,0.21,0,0  
 2IF4,GLU\_197,4.71,0.21,0,0  
 2EHG,GLU\_133,4.28,0.21,-0.43,0  
 3I82,ASP\_206,3.8,0.07,-0.07,0  
 3LH5,GLU\_664,3.4,0.63,-1.74,0  
 1UXO,LYS\_146,10.5,0,0,0  
 1WYC,GLU\_28,4.64,0.14,0,0  
 3ADO,LYS\_178,10.5,0,0,0  
 1AM2,GLU\_96,4.64,0.14,0,0  
 3JSN,ASP\_36,3.87,0.07,0,0  
 3LQE,ARG\_268,9.78,-2.72,0,0  
 3B21,LYS\_51,10.36,-0.14,0,0



1X1E,GLU\_209,1.39,0.42,-3.53,0  
3B21,GLU\_113,2.07,1.12,-3.55,0  
3T57,LYS\_76,10.36,-0.14,0,0  
2CW4,ASP\_82,3.92,0.7,-0.58,0  
1L2F,GLU\_294,4.5,0,0,0  
3C5V,GLU\_361,4.22,0.07,-0.35,0  
1W7B,LYS\_279,10.43,-0.07,0,0  
1N14,GLU\_65,2.23,0.76,-0.8,-2.23  
3MEW,LYS\_140,10.5,0,0,0  
1160,GLU\_21,4.57,0.07,0,0  
2CW4,LYS\_57,10.29,-0.21,0,0  
2E3S,GLU\_446,3.92,2,-2.31,-0.28  
3C6B,ASP\_63,2.54,0.35,-1.61,0  
3I4T,TYR\_34,10.23,0,0,0.23  
3V5S,LYS\_543,10.5,0,0,0  
1ZP2,ASP\_130,3.87,0.07,0,0  
1T07,LYS\_9,9.8,-0.7,0,0  
3R1X,GLU\_317,6.13,2.83,-1.21,0  
3C5V,LYS\_293,10.5,0,0,0  
1T07,GLU\_61,4.57,0.07,0,0  
1N81,TYR\_166,12.55,0.15,0,2.4  
2X4G,ARG\_231,12.22,-0.28,0,0  
2BV9,ASP\_85,3.49,0.56,-0.87,0  
2CYG,GLU\_122,7.64,1.24,-0.8,2.7  
2JKF,GLU\_111,4.5,0,0,0  
2OEW,LYS\_48,10.43,-0.07,0,0  
3ADO,ARG\_197,12.29,-0.21,0,0  
1L3K,GLU\_24,4.5,0,0,0  
1X91,LYS\_24,10.43,-0.07,0,0  
1RHS,ARG\_29,11.31,-1.19,0,0  
1TUL,TYR\_69,11.7,0.65,-0.66,1.71  
1A8Q,ASP\_82,3.77,0.07,-0.1,0  
3BQE,ARG\_272,11.73,-0.77,0,0  
1OST,ARG\_106,12.22,-0.28,0,0  
1N14,LYS\_254,10.15,-0.35,0,0  
1H4U,HIS\_370,6.08,0,0,-0.42  
2OEW,HIS\_249,4.35,0.75,0,-2.9  
2ILR,GLU\_448,4.64,0.14,0,0  
3EIZ,LYS\_95,10.22,-0.28,0,0  
2AZP,ARG\_104,12.15,-0.35,0,0  
4F85,ASP\_287,2.53,0.91,-2.19,0  
1UW7,LYS\_52,10.15,-0.35,0,0  
3DHN,ASP\_165,4.01,0.35,-0.14,0  
1FKM,LYS\_302,10.22,-0.28,0,0  
1AK1,TYR\_216,10.14,0.14,0,0  
1GVP,TYR\_26,9.0,0.07,-0.16,0  
1BKR,CYS\_12,10.23,-0.16,0,1.39  
1SQH,ARG\_73,12.22,-0.28,0,0  
2QZQ,GLU\_127,4.21,0.49,-0.78,0  
3BB7,TYR\_312,9.26,0.28,-1.02,0  
3V1Q,GLU\_501,4.4,0.7,-0.8,0  
3B79,GLU\_60,4.57,0.07,0,0  
21XM,CYS\_164,11,0,-0.09,2.09  
2QEV,ASP\_44,3.07,0.07,-0.8,0  
1PGV,ARG\_384,12.5,0,0,0  
2A1V,ASP\_12,1.42,0.98,-3.36,0  
3F1X,LYS\_298,10.5,0,0,0  
2W2S,ASP\_145,4.01,0.21,0,0  
2FD5,LYS\_176,10.36,-0.14,0,0  
3AU3,GLU\_443,4.4,0.07,-0.17,0  
1AK1,LYS\_130,10.29,-0.21,0,0  
4DIU,TYR\_133,10.1,1.19,-1.1,0  
4FH3,GLU\_303,2.51,0.49,-2.48,0  
1TXD,GLU\_877,4.32,0.49,-0.67,0  
3EGN,GLU\_387,4.5,0,0,0  
3CS1,ASP\_112,3.68,0.07,-0.19,0  
4AM1,ARG\_124,8.94,-2.72,0,-0.84  
3IU5,TYR\_85,10.14,0.14,0,0  
1L2F,ASP\_84,4.32,0.77,-0.25,0  
2G3A,ASP\_105,3.27,0.35,-0.88,0  
3C38,ASP\_97,3.52,0.56,-0.84,0  
3IL3,GLU\_172,3.96,0.21,-0.75,0  
2HP7,GLU\_90,3.85,0.14,-0.79,0  
1GQE,LYS\_282,10.29,-0.21,0,0  
2E0T,ARG\_192,12.43,-0.07,0,0  
2YLF,TYR\_49,13.49,0.56,0.53,2.4  
3BA1,GLU\_238,4.53,1.19,-1.16,0  
3HUE,GLU\_67,3.62,0.28,-1.15,0  
3D9H,GLU\_75,5.37,0.87,0,0  
3T57,LYS\_131,10.29,-0.21,0,0  
3EYE,TYR\_124,10.07,0.07,0,0  
3ADO,ARG\_50,12.01,-0.49,0,0  
2G5X,LYS\_12,10.5,0,0,0  
2JKF,LYS\_124,10.43,-0.07,0,0  
2QK1,ASP\_331,3.5,0.42,-0.72,0  
2QDJ,GLU\_184,4.44,0.07,-0.13,0  
3GW3,ARG\_332,11.73,-0.77,0,0  
1T6L,LYS\_113,10.29,-0.21,0,0  
2AZL,ARG\_129,11.87,-0.63,0,0  
3LD1,LYS\_284,10.36,-0.14,0,0  
1L2F,LYS\_125,10.36,-0.14,0,0  
2YWX,LYS\_23,10.5,0,0,0  
1O0X,ARG\_216,11.87,-0.63,0,0  
2CN1,GLU\_69,4.64,0.14,0,0  
3BB7,TYR\_235,12.2,2.36,-0.16,0  
2H2W,LYS\_224,10.29,-0.21,0,0  
3CIV,GLU\_56,4.14,0.28,-0.64,0  
1WYC,ASP\_105,1.08,0.35,-3.07,0  
2IIA,ARG\_6,11.94,-0.56,0,0  
2IRM,ASP\_154,3.94,0.14,0,0  
3JZN,LYS\_400,10.43,-0.07,0,0  
1ZP2,ARG\_51,11.8,-0.7,0,0  
4ECC,ASP\_73,3.81,0.49,-0.48,0  
1U3Y,ARG\_305,12.5,0,0,0  
4EZB,ASP\_204,3.22,0.28,-0.86,0  
2E3S,ARG\_544,11.03,-1.47,0,0  
1SFE,ARG\_151,12.15,-0.35,0,0  
3CIV,GLU\_291,4.78,0.28,0,0  
3L7N,ASP\_45,3.85,0.07,-0.02,0  
4D8L,ARG\_199,11.66,-0.84,0,0  
2ZQ5,LYS\_306,9.8,-0.7,0,0  
2G9D,ARG\_233,12.08,-0.42,0,0  
3BQE,ARG\_244,12.5,0,0,0  
1R1S,GLU\_211,4.4,0.21,-0.31,0  
1GPP,LYS\_113,10.29,-0.21,0,0  
2HP7,GLU\_117,5.39,2.55,-1.13,-0.53  
2XHC,GLU\_27,4.5,0,0,0  
2HXB,CYS\_30,9,0,0,0  
3I47,TYR\_217,10.1,0,0,0.1  
2G2D,CYS\_39,10.69,0,0,1.69  
1AKO,HIS\_25,5.35,0.11,1.57,-2.83  
3I0C,TYR\_237,10,0,0,0  
2P6S,ARG\_96,12.22,-0.28,0,0  
3P28,LYS\_110,10.01,-0.49,0,0  
2D7J,LYS\_140,10.36,-0.14,0,0  
3HYQ,GLU\_143,4.43,0.14,-0.21,0  
3HNX,LYS\_67,10.5,0,0,0  
1E5S,LYS\_221,10.43,-0.07,0,0  
1LPL,LYS\_217,10.22,-0.28,0,0  
1SIG,LYS\_392,10.43,-0.07,0,0  
2OBI,TYR\_169,10,0,0,0  
1X7F,LYS\_287,9.94,-0.56,0,0  
3G59,ASP\_24,3.65,0.07,-0.22,0  
1TR9,GLU\_16,3.95,0.14,-0.69,0  
2XWS,GLU\_29,3.98,0.28,-0.8,0  
2Q5X,GLU\_781,3.8,0.35,-1.05,0  
1T07,HIS\_0,6.48,0.12,0,-0.14  
3Q6L,GLU\_15,4.42,0.14,-0.22,0  
3F6F,TYR\_112,10.39,0.07,-0.22,0.54  
1PGV,GLU\_349,2.38,0.28,-2.4,0  
1OXZ,GLU\_219,4.71,0.21,0,0  
1CHD,ARG\_348,12.5,0,0,0  
1PBV,GLU\_134,4.31,0.07,-0.26,0  
2DG7,ARG\_136,12.01,-0.49,0,0  
2D7J,LYS\_133,10.01,-0.49,0,0  
3PAC,CYS\_108,12.9,-0.74,2.4,2.24  
2QV2,GLU\_16,4.5,0,0,0  
3K9I,TYR\_59,10,0,0,0  
3EUR,GLU\_29,4.05,0.35,-0.8,0  
2FG1,TYR\_54,10,0,0,0  
1U3Y,LYS\_315,10.43,-0.07,0,0  
2E3S,GLU\_407,4.72,0.35,-0.13,0  
1TLV,LYS\_141,10.01,-0.49,0,0  
1ANU,ARG\_23,12.22,-0.28,0,0  
1XDZ,ASP\_209,3.06,0.21,-0.95,0  
1XEU,CYS\_218,9.96,0,0,0.96  
3LQE,CYS\_240,12.19,0.04,2.04,1.12  
3C5V,TYR\_70,10.86,1.35,-0.8,0.31  
2ZCO,ARG\_188,11.66,-0.84,0,0  
1U7U,ASP\_394,3.08,0.07,-0.79,0  
3R87,ASP\_66,2.89,0.35,-1.26,0  
3CXS,LYS\_15,10.5,0,0,0  
2D2S,LYS\_703,10.43,-0.07,0,0  
2ZCX,ARG\_42,13.97,-0.59,0,2.06  
2D59,LYS\_77,10.5,0,0,0  
2D7J,TYR\_22,11.48,0,0,1.48  
2RIK,LYS\_118,10.5,0,0,0  
1MTZ,LYS\_233,10.29,-0.21,0,0  
3DSH,TYR\_303,9.95,0,-0.05,0  
2EHG,ARG\_137,12.43,-0.07,0,0  
1XFK,GLU\_99,4.5,0,0,0  
1WYC,GLU\_372,4.5,0,0,0  
3CJW,ARG\_293,12.15,-0.35,0,0  
1EV8,GLU\_137,3.92,0.42,-1,0  
3CAN,ASP\_176,3.27,0.35,-0.88,0  
2Q5X,TYR\_785,8.76,0.38,-1.62,0  
2Q12,ASP\_243,3.8,0,0,0  
2C13,GLU\_249,4.92,0.42,0,0  
3BCY,ASP\_45,1.19,0.49,-3.1,0  
2NYC,LYS\_246,10.5,0,0,0  
1X8F,TYR\_174,10,0,0,0  
1AM2,ARG\_138,12.43,-0.07,0,0  
3ASA,ASP\_42,3.63,0.63,-0.8,0  
2PWQ,ARG\_6,11.66,-0.84,0,0  
3Q6L,ASP\_48,3.87,0.07,0,0  
3ASA,TYR\_300,9.04,0.14,-1.09,0  
2ZCO,LYS\_272,10.01,-0.49,0,0  
3PBH,ARG\_40,11.38,-1.12,0,0  
3HVM,HIS\_302,7.1,0.81,0,-0.21  
3S0A,GLU\_94,4.64,0.14,0,0  
3C2E,TYR\_34,10,0,0,0  
3JZN,GLU\_125,4.05,0.28,-0.73,0  
2XJ4,GLU\_272,3.91,0.21,-0.8,0  
2CWC,TYR\_91,10,0,0,0  
1NAF,GLU\_188,4.5,0,0,0  
1JT9,TYR\_254,10,0,0,0  
2FC3,GLU\_28,4.01,0.35,-0.84,0  
2JEO,TYR\_84,10.16,0.16,0,0  
1S1Y,ARG\_137,12.01,-0.49,0,0  
2QV2,ARG\_311,10.67,-1.83,0,0  
3GYW,ASP\_192,3.94,0.28,-0.14,0  
1XTD,ASP\_82,3.89,0.21,-0.12,0  
3R1X,LYS\_71,10.5,0,0,0  
3JZN,CYS\_330,10.3,-0.12,0,1.42  
2FPN,ARG\_13,12.15,-0.35,0,0  
3U2A,GLU\_105,4.57,0.07,0,0  
1UXO,TYR\_11,10,0,0,0  
2OJQ,GLU\_623,4.71,0.21,0,0  
1NIJ,GLU\_37,5.8,1.19,-0.5,0.6  
3V7S,ARG\_9,12,-2.02,0,1.52  
3V5S,GLU\_700,4.5,0,0,0  
3V46,ARG\_369,11.45,-1.05,0,0  
3N2T,LYS\_245,10.43,-0.07,0,0  
1P2F,TYR\_59,10.16,0.16,0,0  
3L7N,GLU\_234,4.5,0,0,0  
3ONH,TYR\_469,10.27,0.46,-0.22,0.03  
1SFE,ASP\_64,2.73,0.63,-1.7,0  
3H13,TYR\_244,11.72,0.54,-1.22,2.4  
1PSW,ARG\_109,12.22,-0.28,0,0  
3O16,CYS\_82,10.64,-0.02,0,1.66  
1E59,GLU\_85,4.64,0.14,0,0  
3KV0,GLU\_95,2.36,1.26,-3.4,0  
3CSR,LYS\_15,10.43,-0.07,0,0  
2BDV,ASP\_109,3.51,0.63,-0.92,0  
2H2W,TYR\_246,10.07,0.07,0,0  
2OJQ,LYS\_438,10.5,0,0,0  
3LD1,ARG\_303,11.52,-0.98,0,0  
3EVN,HIS\_80,3.1,2.59,0,-5.99  
2V81,ASP\_74,2.73,0.49,-1.57,0  
3U2R,ARG\_82,12.08,-0.42,0,0  
3HVW,GLU\_225,4.57,0.07,0,0  
1NAR,ASP\_183,3.89,0.14,-0.05,0  
2QDJ,GLU\_166,3.98,0.42,-0.94,0  
1AT0,TYR\_295,10,0,0,0  
3COU,ASP\_177,3.4,0,-0.4,0  
1E5S,LYS\_122,10.43,-0.07,0,0  
3GG6,GLU\_110,4.5,0,0,0  
3GA2,GLU\_14,4.5,0,0,0  
1IAP,GLU\_213,4.57,0.07,0,0  
3G9T,GLU\_261,4.23,1.12,-1.39,0  
1IDK,LYS\_12,10.5,0,0,0  
3TMO,ASP\_238,2.72,0.14,-1.21,0  
2Q13,HIS\_175,6.22,0,0,-0.28  
2QZQ,GLU\_96,3.27,0.63,-1.86,0  
1ILW,ARG\_122,11.94,-0.56,0,0  
1ZBM,CYS\_156,9.42,-1.97,1.63,0.75  
3OKQ,CYS\_676,8.9,-0.17,0,0.07  
1C44,GLU\_22,4.5,0.28,-0.28,0  
3I4T,CYS\_40,8.7,-0.54,0,0.42  
2FPN,GLU\_164,4.57,0.07,0,0  
2V81,TYR\_56,10.17,0.14,-0.17,0.2  
2IQT,CYS\_127,9.44,-0.1,0,0.54  
1MD6,ASP\_154,3.81,0.07,-0.06,0  
1R29,ARG\_13,12.5,0,0,0  
1Z3X,LYS\_46,10.29,-0.21,0,0  
3FRR,LYS\_27,10.43,-0.07,0,0  
3CXS,HIS\_77,6.5,0,0,0  
3E7P,GLU\_228,4.41,0.21,-0.3,0  
2QZQ,GLU\_28,4.05,0.35,-0.8,0  
1QQH,HIS\_70,6.52,0.02,0,0  
3T57,GLU\_290,4.28,0.14,-0.36,0  
1SUU,CYS\_691,8.89,-0.11,0,0  
3T8R,TYR\_126,11.2,0,0,1.2  
1UJ8,ASP\_52,4.01,0.35,-0.14,0  
2Q99,ARG\_204,12.08,-0.42,0,0  
2YX0,LYS\_263,10.29,-0.21,0,0  
1RKA,GLU\_268,4.54,0.07,-0.03,0  
3C5V,LYS\_133,10.43,-0.07,0,0  
1X7F,LYS\_318,10.01,-0.49,0,0  
2WB8,GLU\_213,6.24,0.47,0,1.27  
2ZCO,TYR\_215,12.51,1.31,-1.21,2.4  
3CB9,LYS\_165,10.5,0,0,0  
2GAU,CYS\_38,8.14,-1.09,0,0.23  
2Q12,ASP\_49,3.54,0.28,-0.54,0  
3ERF,ASP\_97,2.47,0.7,-2.04,0  
3P2F,HIS\_6,4.75,0,0,-1.75

1AM2,ASP\_171,3.32,0.49,-0.98,0  
2AXO,LYS\_220,10.43,-0.07,0,0  
1UCH,ARG\_186,13.2,-1.06,0,1.76  
1Z9L,ARG\_50,12.5,0,0,0  
3OIP,LYS\_135,10.43,-0.07,0,0  
1XIP,ASP\_15,3.94,0.14,0,0  
2G5X,LYS\_215,10.5,0,0,0  
2Q13,CYS\_328,8.16,-1.18,0,0.34  
1O0X,TYR\_70,10.07,0.07,0,0  
2JKF,ASP\_8,2.81,0.21,-1.21,0  
1YTD,ASP\_190,3.41,0.7,-1.09,0  
3EJC,LYS\_5,10.5,0,0,0  
3EVP,GLU\_282,4.5,0,0,0  
3EVN,ARG\_295,12.36,-0.14,0,0  
1MTZ,ARG\_202,11.13,-1.37,0,0  
1U3Y,CYS\_270,9.35,-0.15,0,0.5  
2QVT,ASP\_134,2.98,0.21,-1.03,0  
3UC9,ASP\_126,3.71,0,-0.09,0  
3T5B,ARG\_370,12.5,0,0,0  
3EX9,GLU\_68,4.5,0,0,0  
3JZ9,GLU\_381,4.33,0.21,-0.38,0  
1ZBM,ASP\_78,3.28,0.28,-0.8,0  
3BA1,LYS\_141,10.5,0,0,0  
3BB7,ASP\_97,3.28,0.28,-0.8,0  
3HUE,LYS\_188,10.5,0,0,0  
2E3S,ARG\_442,11.86,-2.65,0,2.02  
1P4X,GLU\_229,4.78,0.28,0,0  
1YR6,ASP\_26,3.99,0.21,-0.02,0  
1SQH,LYS\_28,10.29,-0.21,0,0  
3HNX,ASP\_27,3.87,0.07,0,0  
3P28,HIS\_29,7.32,1.03,0,-0.21  
3M3P,ARG\_235,11.59,-0.91,0,0  
1JKS,ASP\_250,2.76,0.56,-1.6,0  
2I88,ASP\_347,3.59,0.14,-0.35,0  
3VJ8,ARG\_77,12.93,-1.7,0,2.14  
2R0S,TYR\_93,10.14,0.14,0,0  
2B0J,GLU\_216,4.64,0.14,0,0  
2DFL,LYS\_143,10.15,-0.35,0,0  
2AXO,LYS\_142,10.5,0,0,0  
1DTP,TYR\_131,13.8,0.6,0.8,2.4  
3U2R,LYS\_111,10.29,-0.21,0,0  
3GA2,TYR\_120,11.99,0.37,0.01,1.61  
3JRT,ASP\_30,3.93,0.21,-0.08,0  
4DNU,HIS\_287,3.86,3.93,0,-6.57  
3V5S,TYR\_690,11.41,0.07,-0.02,1.36  
3EJG,GLU\_145,4.64,0.14,0,0  
3V1Q,LYS\_628,10.43,-0.07,0,0  
2O4D,ARG\_86,12.01,-0.49,0,0  
2VAN,ARG\_254,12.92,-2.25,0,2.67  
1PSW,ASP\_82,2.85,0.35,-1.3,0  
3CBN,ARG\_91,12.08,-0.42,0,0  
2AHS,ASP\_189,3.69,0,-0.11,0  
1QVI,LYS\_348,10.36,-0.14,0,0  
3FRR,LYS\_130,10.5,0,0,0  
3D9H,HIS\_91,6.43,0,0,-0.07  
3LMO,LYS\_68,10.5,0,0,0  
2FZ4,ARG\_192,11.94,-0.56,0,0  
1DCF,CYS\_59,9.27,-2.42,2.4,0.28  
2BT8,HIS\_287,6.36,0,0,-0.14  
3H6Q,HIS\_121,3.43,0.8,0,-3.87  
3V4G,LYS\_117,10.5,0,0,0  
2Q98,ASP\_160,2.64,0.28,-1.45,0  
3GOZ,CYS\_273,8.54,-0.89,0,0.43  
3V7S,GLU\_56,4.5,0,0,0  
3UC9,GLU\_46,4.5,0,0,0  
2FBQ,GLU\_210,4.5,0,0,0  
2D59,GLU\_47,4.85,0.35,0,0  
3LQE,ASP\_348,1.92,0.84,-2.72,0  
1N81,HIS\_142,7.05,0.69,0,-0.14  
3M3P,GLU\_194,2.89,0.79,-2.4,0  
1T9S,TYR\_216,10.0,0,0,0  
1LTU,LYS\_248,10.5,0,0,0  
3F5D,ASP\_170,2.96,0.56,-1.4,0  
3CAN,HIS\_138,6.36,0,0,-0.14  
2HRZ,ASP\_31,3.45,0.49,-0.84,0  
3LJI,ASP\_91,4.01,0.21,0,0  
1MJS,HIS\_398,7.81,1.6,1.67,-1.96  
3HUE,GLU\_227,4.71,0.21,0,0  
2IDC,LYS\_35,10.5,0,0,0  
2H2W,ARG\_132,12.15,-0.35,0,0  
2IQT,HIS\_169,7.16,0.8,0,-0.14  
3RJZ,ARG\_159,11.73,-0.77,0,0  
1CHD,LYS\_212,9.73,-0.77,0,0  
3IVF,GLU\_317,0.73,1.03,-2.4,-2.4  
1A8Q,ASP\_70,3.03,0.42,-1.2,0  
3M7G,ARG\_102,10.64,-3.95,0,2.09  
3DSH,TYR\_246,11.43,1.43,0,0  
1IAP,GLU\_187,3.99,0.14,-0.64,0  
1H09,LYS\_121,10.43,-0.07,0,0  
1AK1,LYS\_152,10.08,-0.42,0,0  
2QRX,GLU\_151,1.05,0.83,-2.39,-1.88  
2RGY,ARG\_284,12.01,-0.49,0,0  
2H01,LYS\_28,10.5,0,0,0  
1J74,ARG\_101,12.29,-0.21,0,0  
1PVT,LYS\_180,9.8,-0.7,0,0  
2R0S,LYS\_219,10.29,-0.21,0,0  
2Q98,ARG\_103,12.22,-0.28,0,0  
1R3D,HIS\_243,5.38,1.6,2.81,-5.53  
2WOZ,LYS\_583,10.5,0,0,0  
2WZ9,HIS\_104,6.54,0.04,0,0  
3CAX,GLU\_304,3.27,0.56,-1.79,0  
3JV1,GLU\_61,4.64,0.14,0,0  
1WYC,ASP\_250,3.28,0.35,-0.87,0  
1OGL,ARG\_34,12.36,-0.14,0,0  
3PP8,GLU\_2,3.58,0.42,-1.34,0  
1V43,ARG\_266,11.94,-0.56,0,0  
3EAZ,HIS\_128,9.99,3.66,2.01,-2.18  
3DSH,GLU\_400,3.78,0.21,-0.93,0  
2WB3,ASP\_346,2.95,0.35,-1.2,0  
3A0X,GLU\_608,4.33,0,-0.17,0  
1TWU,LYS\_99,10.22,-0.28,0,0  
3T5B,ARG\_195,11.94,-0.56,0,0  
2CVB,GLU\_184,4.5,0,0,0  
3B7X,ASP\_31,2.04,1.19,-2.95,0  
3F7M,ARG\_268,12.5,0,0,0  
2C13,GLU\_191,4.5,0,0,0  
1P1L,HIS\_74,4.14,1,0,-3.36  
3K8J,CYS\_178,10.59,-0.01,0.45,1.16  
3C6B,LYS\_16,10.29,-0.21,0,0  
3I0C,ARG\_249,12.08,-0.42,0,0  
1WXQ,HIS\_125,6.42,0.06,0,-0.14  
1ZBM,TYR\_80,9.73,0.3,-0.88,0.3  
4ACJ,GLU\_796,3.11,1.59,-2.99,0  
2WZ9,LYS\_58,9.87,-0.63,0,0  
1QQH,CYS\_176,8.38,-0.69,0,0.07  
2B3M,LYS\_22,10.5,0,0,0  
2ZQ5,GLU\_379,4.5,0,0,0  
1RSS,GLU\_74,2.58,0.84,-2.76,0  
1SNT,ASP\_201,1.1,0.98,-3.68,0  
1LPL,ARG\_199,11.66,-0.84,0,0  
3V5S,TYR\_490,13.69,0.92,0.37,2.4  
4D8L,ARG\_187,12.22,-0.28,0,0  
3BQW,ASP\_228,3.35,0.28,-0.72,0  
3Q6L,ASP\_112,3.74,0.07,-0.13,0  
2IXM,GLU\_134,1.92,1.4,-3.97,0  
3B7X,TYR\_22,10.55,0.62,-0.46,0.39  
1J7G,GLU\_40,4.5,0,0,0  
1RHS,HIS\_94,2.83,0,0,-3.67  
2JKF,HIS\_174,7.3,0.8,0,0  
1Q46,HIS\_108,3.72,0.05,0,-2.83  
3UAH,TYR\_426,11.72,2.57,-0.85,0  
1XDZ,LYS\_135,10.5,0,0,0  
3K1H,ASP\_95,3.15,0.49,-1.14,0  
1WXF,ARG\_142,11.58,-0.92,0,0  
2NSN,LYS\_78,10.08,-0.42,0,0  
3UAH,TYR\_259,9.93,0,-0.07,0  
1N81,LYS\_180,10.5,0,0,0  
3P28,ARG\_48,8.46,-4.04,0,0  
1BKB,HIS\_43,6.5,0,0,0  
3M70,LYS\_16,10.43,-0.07,0,0  
3BB7,ASP\_184,3.24,0.56,-1.12,0  
1C3K,TYR\_107,13.47,0.28,0.79,2.4  
4FH3,TYR\_281,9.9,0,-0.1,0  
3EVZ,GLU\_208,4.36,0.07,-0.21,0  
3E2Z,GLU\_66,4.5,0,0,0  
1SQH,ARG\_65,11.98,-0.91,0,0.39  
3E7P,LYS\_92,10.5,0,0,0  
4FCU,GLU\_136,4.57,0.07,0,0  
1L2F,ASP\_10,3.83,0.14,-0.11,0  
4GA2,TYR\_37,10.0,0,0,0  
2Z61,LYS\_53,10.43,-0.07,0,0  
1MJS,ASP\_309,3.22,0.07,-0.65,0  
3GA2,GLU\_101,4.27,0,-0.23,0  
1PV5,GLU\_133,4.5,0,0,0  
4DEZ,ASP\_96,3.9,0.14,-0.04,0  
2BCF,HIS\_65,6.15,0,0,-0.35  
1K9S,GLU\_72,4.07,0.63,-1.06,0  
3B7X,ARG\_44,11.87,-0.63,0,0  
3NZL,LYS\_31,10.5,0,0,0  
3A4C,GLU\_555,2.45,0.35,-2.4,0  
1J85,LYS\_151,10.43,-0.07,0,0  
3CZC,GLU\_23,3.24,0.21,-1.47,0  
3DB9,LYS\_63,10.43,-0.07,0,0  
2HXB,GLU\_77,4.5,0,0,0  
3ASA,GLU\_220,3.15,1.4,-2.74,0  
3G59,TYR\_291,10.0,0,0,0  
3BCY,GLU\_67,4.5,0,0,0  
3VJ8,ASP\_327,4.05,0.28,-0.03,0  
2A1V,GLU\_102,4.71,0.21,0,0  
1NAR,TYR\_184,10.0,0,0,0  
1UAJ,CYS\_178,7.73,-1.27,0,0  
3G59,ASP\_56,3.06,0.28,-1.02,0  
1WPA,ASP\_461,3.55,0.35,-0.6,0  
2W1R,HIS\_162,6.48,0.05,0,-0.07  
2ZCO,ASP\_195,2.54,0.35,-1.61,0  
1SI7,ASP\_150,3.28,0.35,-0.87,0  
2EFK,ARG\_157,12.22,-0.28,0,0  
2QVQ,LYS\_76,10.36,-0.14,0,0  
3OIP,LYS\_202,9.45,-1.05,0,0  
2EJX,LYS\_39,10.01,-0.49,0,0  
4FZR,GLU\_156,3.42,0.49,-1.56,0  
1XAW,ASP\_492,3.94,0.14,0,0  
3CXS,ARG\_180,12.22,-0.28,0,0  
2POY,ARG\_289,12.43,-0.07,0,0  
2NRK,GLU\_163,3.84,0.14,-0.8,0  
1YTO,TYR\_170,9.91,0.14,-1.19,0.96  
3HXK,ASP\_34,2.96,0.28,-1.12,0  
1Y2Q,LYS\_124,10.43,-0.07,0,0  
2POY,ASP\_190,3.81,0.56,-0.55,0  
3AZZ,CYS\_173,9.07,0,0,0.07  
1SQH,ARG\_77,11.8,-0.7,0,0  
3JZN,LYS\_311,11.71,-2.04,0.66,4.09  
3F6F,LYS\_129,10.5,0,0,0  
3CRM,HIS\_246,6.43,0,0,-0.07  
3H5T,HIS\_189,4.84,0.65,0,-2.32  
3LMF,GLU\_96,4,0.14,-0.64,0  
3DB9,ARG\_48,12.43,-0.07,0,0  
3JZN,LYS\_344,10.43,-0.07,0,0  
3IVF,GLU\_276,2.75,0.84,-2.59,0  
1R53,TYR\_208,13.02,0,0,0.301  
3KVO,CYS\_162,9.72,0,0,0.72  
1PVT,TYR\_47,11.8,1.17,-0.3,0.93  
3LJN,GLU\_258,4.32,0.21,-0.39,0  
1W24,LYS\_73,10.15,-0.35,0,0  
3KT9,ARG\_29,11.31,-1.19,0,0  
2QDJ,LYS\_63,10.29,-0.21,0,0  
2V4U,GLU\_349,4.64,0.14,0,0  
3BA1,HIS\_235,2.65,0.47,0,-4.32  
1O59,GLU\_315,4.17,0.21,-0.54,0  
3F6F,TYR\_4,13.12,0.07,0.65,2.4  
2RGY,ARG\_206,12.22,-0.28,0,0  
1V43,GLU\_369,4.71,0.21,0,0  
3ZRI,TYR\_84,10.0,0,0,0  
2HXB,ARG\_85,10.15,-0.35,0,0  
1SQH,ARG\_180,12.01,-0.49,0,0  
2Q34,TYR\_73,10.0,0,0,0  
3G59,GLU\_39,4.13,0.35,-0.72,0  
2A4D,ASP\_116,1.08,1.05,-3.77,0  
3JRT,TYR\_64,10.14,1.69,-1.15,-0.39  
2OKT,ASP\_258,3.14,0.35,-1.01,0  
2GZQ,TYR\_32,12.74,0.07,0.27,2.4  
1XTZ,LYS\_35,10.5,0,0,0  
3CCY,TYR\_168,9.38,0,-0.62,0  
2XHC,TYR\_224,13.15,0.14,0.61,2.4  
2Q12,HIS\_100,6.36,0,0,-0.14  
1G5Z,HIS\_141,7.3,0.87,0,-0.07  
2AZP,HIS\_110,6.81,0.52,0,-0.21  
3BQW,GLU\_278,4.64,0.14,0,0  
2IRM,CYS\_250,9.22,-0.25,0,0.47  
3CNU,LYS\_35,10.22,-0.28,0,0  
3DSH,HIS\_260,6.36,0,0,-0.14  
2ZCO,LYS\_97,10.43,-0.07,0,0  
2DFL,ASP\_46,3.95,0.28,-0.13,0  
1Q8B,GLU\_30,4.5,0.14,-0.14,0  
3L7N,ASP\_132,3.42,0.42,-0.8,0  
1ZBM,GLU\_30,4.57,0.07,0,0  
1SZL,ASP\_107,11.73,-0.77,0,0  
1SQW,TYR\_19,11.59,1.72,-0.13,0  
2GZR,TYR\_83,10.16,0.21,-0.05,0  
3CS1,LYS\_174,10.5,0,0,0  
3QAV,GLU\_80,4.57,0.07,0,0  
1VJG,GLU\_92,4.14,0.28,-0.65,0  
1MML,TYR\_146,11.33,0.07,0,1.26  
4H86,ASP\_25,4.08,0.28,0,0  
4DBX,LYS\_49,9.94,-0.56,0,0  
3GG6,GLU\_101,4.69,0.28,-0.09,0  
2FL4,TYR\_108,13.68,0.14,0.27,3.27  
3E5T,ASP\_98,3.11,0.49,-1.18,0  
1H4U,TYR\_577,10.75,2.08,-0.22,-1.12  
2HRZ,HIS\_241,6.29,0,0,-0.21  
1PSW,LYS\_223,10.5,0,0,0  
1XDZ,GLU\_34,4.5,0,0,0  
1PSW,TYR\_21,11.42,2.22,-0.8,0  
3UX2,GLU\_76,4.64,0.14,0,0  
2RIK,ARG\_230,12.15,-0.35,0,0  
3F5D,GLU\_139,4.5,0,0,0  
3M7D,GLU\_18,3.58,0.35,-1.28,0  
3K9I,LYS\_163,10.5,0,0,0  
1KCM,GLU\_124,2.45,0.35,-2.4,0  
3Q1C,GLU\_132,3.87,0.07,-0.7,0  
1UAJ,LYS\_32,9.94,-0.56,0,0  
2EAF,ARG\_146,12.01,-0.49,0,0  
3RKV,ASP\_206,4.01,0.21,0,0  
3F5D,GLU\_173,3.59,0.7,-1.6,0  
2AD1,GLU\_279,4.5,0,0,0  
1V43,LYS\_30,10.5,0,0,0

3EX9,ARG\_38,10.86,-1.64,0,0  
2ZCO,GLU\_162,5.87,1.37,0,0  
1UOH,LYS\_69,10.15,-0.35,0,0  
3FXH,ASP\_88,3.1,0.28,-0.98,0  
2X4G,ASP\_324,3.52,0.14,-0.43,0  
200K,ASP\_32,3.28,0.28,-0.8,0  
3T8R,GLU\_73,4.71,0.21,0,0  
2P1W,ARG\_217,12.87,-0.84,0,1.21  
3G9T,LYS\_252,10.22,-0.28,0,0  
3IVF,LYS\_343,10.5,0,0,0  
3UX2,LYS\_136,10.29,-0.21,0,0  
4ACJ,ASP\_687,3.87,0.07,0,0  
3CAX,CYS\_399,8.97,-0.1,0,0.07  
4FD6,CYS\_218,9.59,0,0,0.59  
3DZ1,ASP\_20,3.03,0.21,-0.98,0  
2H85,TYR\_324,10.34,1.25,-0.91,0  
1MML,ARG\_205,12.08,-0.42,0,0  
3G9T,ASP\_43,1.35,0.49,-2.94,0  
1Q46,ASP\_150,3.46,0.49,-0.83,0  
3ANJ,LYS\_91,10.5,0,0,0  
3ETU,TYR\_274,10.16,0,0,0.16  
1J74,ARG\_81,12.15,-0.35,0,0  
2P5D,LYS\_131,10.29,-0.21,0,0  
1ZBM,HIS\_143,2.37,0,-0.23,-3.91  
3GE9,ARG\_97,12.5,0,0,0  
1R22,TYR\_215,11.87,0.49,0,1.38  
3I0C,HIS\_140,4.85,0.54,-2.19  
3OOP,GLU\_44,4.05,0.35,-0.8,0  
2X4L,ASP\_111,3.02,0.56,-1.34,0  
1SBX,GLU\_106,4.62,0.21,-0.09,0  
2RGY,ARG\_143,12.36,-0.14,0,0  
1WYC,ARG\_205,11.59,-0.91,0,0  
2C2Y,ASP\_83,3.33,0.42,-0.89,0  
1WOU,LYS\_35,10.29,-0.21,0,0  
4F3J,GLU\_132,4.5,0,0,0  
2Q99,LYS\_35,10.43,-0.07,0,0  
1PVT,TYR\_51,10.65,0.85,-0.2,0  
1H4U,HIS\_513,6.5,0,0,0  
3I4T,LYS\_202,10.5,0,0,0  
3IRA,TYR\_47,9.55,0,-0.45,0  
2X4G,ASP\_51,11.87,-0.63,0,0  
1OI7,GLU\_7,4.5,0,0,0  
1O9G,ARG\_198,11.87,-0.63,0,0  
3GYW,TYR\_56,11.8,0,0,13.1.67  
1FHL,GLU\_329,4.57,0.07,0,0  
1PV5,HIS\_214,9.99,4.84,2.26,-3.6  
2LHC,LYS\_159,10.43,-0.07,0,0  
3RFY,ARG\_196,11.66,-0.84,0,0  
1Q5Z,GLU\_554,3.98,0.28,-0.8,0  
3CGW,TYR\_251,10.27,1.12,-0.14,-0.72  
2BDV,LYS\_8,10.01,-0.49,0,0  
1W24,LYS\_181,10.15,-0.35,0,0  
2RIS,ASP\_122,3.07,0.49,-1.22,0  
3BQE,CYS\_207,9.36,-3.76,2.69,1.43  
1XTD,LYS\_50,10.36,-0.14,0,0  
1WLJ,TYR\_104,9.77,1.89,-1.45,-0.66  
1U7U,ASP\_377,3.34,0.42,-0.88,0  
4DBX,ARG\_125,12.08,-0.42,0,0  
2Z84,HIS\_35,7.16,0.8,0,-0.14  
2BLL,LYS\_381,10.5,0,0,0  
3GOZ,TYR\_262,10.07,0.07,0,0  
3CAX,LYS\_445,10.15,-0.35,0,0  
3UX2,ARG\_82,12.15,-0.35,0,0  
3G65,LYS\_193,10.43,-0.07,0,0  
3CCY,ASP\_174,3.44,0.07,-0.43,0  
2E3H,ASP\_216,3.3,0.56,-1.06,0  
3C6B,LYS\_269,10.15,-0.35,0,0  
2FC3,ASP\_71,3.17,0.56,-1.2,0  
1R3F,ASP\_113,3.28,0.07,-0.59,0  
1ZBM,ARG\_43,12.22,-0.28,0,0  
1AM2,ARG\_68,12.29,-0.21,0,0  
1YG2,TYR\_41,9.7,0.14,-0.44,0  
3ASA,TYR\_256,12.82,0.59,0.22,2  
2P65,ARG\_102,11.94,-0.56,0,0  
2B0J,ASP\_157,3.79,0,-0.01,0  
1ZBS,GLU\_272,4.4,0.07,-0.17,0  
2ZQ5,ASP\_319,3.6,0.42,-0.61,0  
1LTU,ASP\_11,1.85,0.49,-2.44,0  
1WLJ,ARG\_321,11.16,-1.34,0,0  
2P0L,ASP\_7,2.94,0.42,-1.28,0  
3F7M,LYS\_161,10.5,0,0,0  
2W0G,CYS\_203,8.75,-0.32,0,0.07  
3RVC,GLU\_153,4.5,0,0,0  
1Q46,LYS\_127,10.43,-0.07,0,0  
2XMX,ASP\_80,4.01,0.21,0,0  
2EJB,GLU\_180,4.5,0,0,0  
2C2Y,GLU\_279,2.59,0.49,-2.4,0  
1R53,ARG\_127,12.43,-0.07,0,0  
2P5D,GLU\_48,0.24,1.34,-3.2,-2.4  
1XTD,ASP\_104,3.48,0.42,-0.74,0  
2XWS,GLU\_95,4.64,0.14,0,0  
1MD6,ARG\_101,11.87,-0.63,0,0  
3JZ9,ASP\_459,4.01,0.21,0,0  
3V75,GLU\_145,4.57,0.07,0,0  
3EGN,LYS\_434,10.43,-0.07,0,0  
2RIS,ASP\_179,3.25,0.21,-0.76,0  
3RJZ,HIS\_225,7.96,1.6,0,-0.14  
3DSH,ASP\_298,3.09,0.21,-0.92,0  
1X8F,LYS\_156,10.5,0,0,0  
2RIS,HIS\_188,6.98,0.55,0,-0.07  
3ASA,ARG\_376,11.59,-0.91,0,0  
1L3K,HIS\_33,2.57,0.22,-1.41,-2.75  
2CI3,GLU\_117,4.05,0.35,-0.8,0  
3UPD,TYR\_193,9.96,0,-0.42,0.38  
2P0Y,ASP\_80,3.94,0.14,0,0  
2RFA,LYS\_66,10.5,0,0,0  
1HF8,GLU\_213,3.94,0.56,-1.12,0  
2AZL,TYR\_200,9.46,0.59,0,-1.13  
3T8R,TYR\_65,11.33,0.14,-0.8,1.99  
1D0T,LYS\_180,10.36,-0.14,0,0  
2GZR,ARG\_217,12.43,-0.07,0,0  
3M16,HIS\_299,6.5,0,0,0  
3LD1,ASP\_305,1.26,0.63,-3.17,0  
3BPP,GLU\_153,4.64,0.14,0,0  
4HDE,ASP\_93,3.87,0.07,0,0  
1LTU,ASP\_73,3.07,0.42,-1.15,0  
2I88,LYS\_346,10.22,-0.28,0,0  
4FCU,GLU\_61,3.98,0.28,-0.8,0  
3CCY,ASP\_53,3.86,0.07,-0.01,0  
4AF2,ARG\_110,11.94,-0.56,0,0  
3U4K,ASP\_68,1.51,0.98,-3.27,0  
1UXO,ARG\_79,11.17,-1.33,0,0  
1SNT,TYR\_354,12.95,1.52,0,1.43  
2JHY,LYS\_178,10.43,-0.07,0,0  
4GCO,CYS\_254,9.07,0,0,0.07  
2H2W,ARG\_252,12.29,-0.21,0,0  
2B78,GLU\_134,4.71,0.21,0,0  
2BLL,ARG\_591,11.45,-1.05,0,0  
2B0J,LYS\_99,10.36,-0.14,0,0  
2QV2,ARG\_251,12.01,-0.49,0,0  
3CAN,ASP\_139,3.94,0.14,0,0  
3CS1,ARG\_99,11.38,-1.12,0,0  
4DVD,ASP\_87,3.27,0.28,-0.81,0  
4FH3,ASP\_371,3.94,0.14,0,0  
3UC9,TYR\_50,11.19,0.59,-0.49,1.09  
3TOW,LYS\_149,10.29,-0.21,0,0  
2AXO,TYR\_102,10.94,0.07,0,0.87  
3N2T,ARG\_104,12.15,-0.35,0,0  
4ANN,ARG\_109,11.94,-0.56,0,0  
2DOA,ASP\_77,3.21,0.35,-0.94,0  
3JZ9,LYS\_377,10.22,-0.28,0,0  
2P52,GLU\_255,0.29,1.39,-3.2,-2.4  
1MIX,GLU\_276,3.35,0.77,-1.93,0  
2X4G,GLU\_163,3.41,0.28,-1.37,0  
3HVM,CYS\_220,8.65,-0.49,0,0.14  
2YYO,HIS\_81,1.73,0.01,0,-4.78  
3O48,LYS\_123,10.43,-0.07,0,0  
1OIS,ARG\_308,13.78,-0.89,0,2.17  
3RLN,GLU\_622,4.5,0,0,0  
1N81,TYR\_197,10,0,0,0  
2I88,GLU\_518,4.64,0.14,0,0  
3F7M,ASP\_216,3.39,0.35,-0.76,0  
2W0G,GLU\_250,4.5,0,0,0  
2FM9,LYS\_217,10.43,-0.07,0,0  
1X8F,LYS\_265,10.29,-0.21,0,0  
3Q1C,GLU\_116,4.57,0.07,0,0  
2P1W,HIS\_51,6.43,0,0,-0.07  
1H4U,GLU\_471,4.2,1.58,-1.88,0  
3H5T,LYS\_338,10.5,0,0,0  
4EVF,LYS\_263,10.01,-0.49,0,0  
4DNU,TYR\_298,10,0,0,0  
1SJV,TYR\_131,10,0,0,0  
1GXN,GLU\_535,5.4,3.3,-1.98,-0.42  
1NKD,TYR\_51,9.34,0.14,-0.8,0  
1PZC,GLU\_54,4.49,0.07,-0.08,0  
4ETX,ASP\_320,3.36,0.21,-0.65,0  
2Q12,HIS\_140,6.59,0.23,0,-0.14  
4ETX,GLU\_290,4.57,0.07,0,0  
2XHC,LYS\_306,10.5,0,0,0  
1WRU,TYR\_305,10.07,0.07,0,0  
3GW3,GLU\_67,1.85,0.35,-3,0  
4ESS,ASP\_50,2.6,0.49,-1.69,0  
3B79,ASP\_33,3.8,0,0,0  
2Q07,LYS\_334,10.15,-0.35,0,0  
4ETX,ARG\_415,12.22,-0.28,0,0  
2PGE,GLU\_171,5.17,0.56,0.11,0  
1DZF,GLU\_66,4.5,0,0,0  
3ULX,ARG\_40,12.08,-0.42,0,0  
2QV2,GLU\_147,4.57,0.07,0,0  
2OSA,ARG\_442,11.94,-0.56,0,0  
3MEW,ARG\_246,12.01,-0.49,0,0  
2PGE,ARG\_230,12.43,-0.07,0,0  
3PM2,GLU\_125,4.55,0.07,-0.02,0  
1I60,LYS\_254,10.15,-0.35,0,0  
1H4U,TYR\_540,11.42,2.1,-0.08,-0.61  
1TP6,ARG\_7,12.5,0,0,0  
2IRM,GLU\_259,4.99,0.49,0,0  
2GQV,ASP\_28,3.09,0.49,-1.19,0  
3EZ7,GLU\_142,4.19,0.49,-0.8,0  
3G9T,GLU\_289,4.64,0.14,0,0  
2G7O,GLU\_107,2.59,0.49,-2.4,0  
3EZ7,LYS\_324,10.5,0,0,0  
2IF4,GLU\_248,4.12,0.28,-0.66,0  
2YLF,HIS\_216,7.16,0.8,0,-0.14  
4FZR,TYR\_195,10.27,0.28,-0.01,0  
1R3F,GLU\_98,4.33,0.07,-0.24,0  
2FPN,ARG\_195,12.22,-0.28,0,0  
2H8O,CYS\_116,11.25,0,0,2.25  
1A8Q,HIS\_107,4.79,0.8,0,-2.51  
2J8A,HIS\_321,6.44,0.01,0,-0.07  
3OAA,ASP\_558,2.85,0.21,-1.16,0  
1XKR,CYS\_118,10.67,-0.34,0,2.01  
2IDC,LYS\_143,10.5,0,0,0  
1X6J,ASP\_50,3.77,0.07,-0.1,0  
1ZP2,LYS\_30,10.5,0,0,0  
3GT0,GLU\_47,4.27,0.35,-0.58,0  
3D9H,HIS\_46,7.15,0.86,0,-0.21  
2H2Z,CYS\_85,9.43,-0.48,0.02,0.88  
4DEZ,CYS\_70,8.19,-0.81,0,0  
1OLR,ASP\_118,2.44,0.63,-1.99,0  
1P1L,LYS\_37,10.43,-0.07,0,0  
3CE7,ASP\_81,3.91,0.21,-0.1,0  
4ANN,ASP\_202,4.03,0.28,-0.05,0  
3CX2,LYS\_185,10.5,0,0,0  
1U7U,ARG\_199,11.66,-0.84,0,0  
3U2R,ASP\_84,3.99,0.28,-0.09,0  
3H13,ARG\_456,12.15,-0.35,0,0  
4E88,ASP\_164,2.5,0.35,-1.65,0  
2W0Z,ASP\_311,2.85,0.21,-1.16,0  
2QV2,ASP\_48,3.35,0.28,-0.73,0  
1Y0K,ASP\_74,2.21,0.91,-2.5,0  
2IF4,GLU\_193,4.33,0.42,-0.59,0  
1A8Q,TYR\_13,12.01,0,0,2.01  
2C6B,ARG\_184,11.95,-0.84,0,0.29  
2Z0M,LYS\_221,10.5,0,0,0  
2ZQ5,ASP\_149,3.59,0.07,-0.28,0  
2X4L,GLU\_343,2.8,0.7,-2.4,0  
3CN5,TYR\_262,10,0,0,0  
3KT9,HIS\_14,6.5,0,0,0  
1NWA,HIS\_76,1.66,0.89,-0.01,-5.72  
1ZCU,GLU\_143,4.5,0,0,0  
4FZN,LYS\_193,10.22,-0.28,0,0  
1X8F,HIS\_241,8.53,1.6,2.19,-1.76  
3JRT,ASP\_145,3.08,0.14,-0.86,0  
2CWC,ARG\_278,12.08,-0.42,0,0  
3C6B,LYS\_181,9.8,-0.7,0,0  
3V3T,GLU\_297,4.5,0,0,0  
3BZT,GLU\_331,4.44,0.14,-0.2,0  
2AHE,LYS\_254,10.5,0,0,0  
3GEC,ARG\_422,12.22,-0.28,0,0  
3H5T,GLU\_264,4.71,0.21,0,0  
2BLL,CYS\_439,6.38,-2.84,0,0.21  
2X4G,ARG\_75,11.94,-0.56,0,0  
2GZQ,GLU\_156,1.86,0.56,-3.2,0  
2DVK,HIS\_65,7.3,0.87,0,-0.07  
2RH3,TYR\_106,10,0,0,0  
2HXB,TYR\_114,10.87,1.85,-0.98,0  
3RJX,HIS\_109,7.16,0.8,0,-0.14  
2GZQ,LYS\_100,10.01,-0.49,0,0  
1MML,LYS\_62,10.5,0,0,0  
2Q13,TYR\_283,9.27,0.07,-0.8,0  
1N81,ASP\_176,3.63,0,-0.17,0  
2V81,TYR\_100,13.27,0.07,0.8,2.4  
2XMX,ARG\_200,12.29,-0.21,0,0  
2CL3,GLU\_34,4.6,0.21,-0.11,0  
2IRM,ASP\_16,3.8,0,0,0  
1LZL,GLU\_302,4.78,0.28,0,0  
2HXB,GLU\_102,3.16,1.89,-3.23,0  
1P6F,ARG\_168,11.87,-0.63,0,0  
3U2A,GLU\_109,4.57,0.07,0,0  
1R29,ASP\_63,3.11,0.42,-1.11,0  
3L7N,TYR\_218,10.76,0.8,-0.04,0  
1LZL,ARG\_272,12.09,-0.41,0,0  
3FHF,TYR\_92,10.2,0,0,0.2  
1BKR,ASP\_84,3.81,0.07,-0.05,0  
2FL7,HIS\_72,3.77,0.64,0,-3.37  
1UJ8,GLU\_51,4.5,0,0,0  
3L7N,TYR\_206,10.07,0.07,0,0  
1AD6,LYS\_429,10.43,-0.07,0,0  
2QDJ,ASP\_109,3.28,0.28,-0.8,0  
1R2Z,TYR\_39,10.05,0.07,-0.92,0.9  
2DFL,HIS\_304,6.5,0,0,0  
1RLO,ARG\_28,12.15,-0.35,0,0  
1Q42,HIS\_102,7.04,0.61,0,-0.07  
3CJW,CYS\_260,8.96,-0.6,-0.21,0.77  
3FRR,LYS\_151,10.29,-0.21,0,0

1WXQ,LYS\_163,10.43,-0.07,0,0  
3HNX,GLU\_22,3.32,0.42,-1.6,0  
4DIU,TYR\_84,12.06,0.21,-0.55,2.4  
2C13,ASP\_205,3.8,0,0,0  
1GVP,LYS\_3,10.5,0,0,0  
2AHE,GLU\_141,3.91,0.21,-0.8,0  
1Q42,LYS\_14,10.29,-0.21,0,0  
3G9T,HIS\_86,5.94,1.83,2.4,-4.79  
1SNT,HIS\_202,7.9,1.54,0,-0.14  
2Q07,HIS\_348,3.23,0.74,0,-4.01  
2EHG,GLU\_11,4.57,0.07,0,0  
1BKB,GLU\_28,3.15,1.19,-2.53,0  
2GYZ,ARG\_92,12.36,-0.14,0,0  
2FXT,ARG\_255,11.31,-1.19,0,0  
1MML,HIS\_214,6.29,0,0,-0.21  
3B7H,GLU\_6,3.17,0.35,-1.68,0  
3E5T,GLU\_97,3.45,0.28,-1.33,0  
2IF4,TYR\_218,10,0,0,0  
3G6S,ARG\_156,11.94,-0.56,0,0  
2FPN,TYR\_47,11.81,0.33,0,1.48  
1TR9,GLU\_290,4.57,0.07,0,0  
1SI7,HIS\_69,6.29,0,0,-0.21  
1160,LYS\_119,10.36,-0.14,0,0  
1OGL,TYR\_193,11.44,0.91,0,0.53  
2R0S,ASP\_137,3.8,0,0,0  
3V1Q,ARG\_550,11.94,-0.56,0,0  
3Q1C,ARG\_98,13.72,-1.18,0,2.4  
2P52,TYR\_226,10,0,0,0  
3KV0,GLU\_130,3.53,0.77,-1.74,0  
1ZYL,TYR\_152,11.83,2.39,-0.11,-0.44  
3M70,LYS\_266,10.36,-0.14,0,0  
3P29,TYR\_46,10.36,1.9,-1.54,0  
2ZTY,HIS\_161,2.53,0.1,0,-4.07  
3UC9,ASP\_174,2.81,0.63,-1.63,0  
3QKY,TYR\_190,13.15,0.7,0.21,2.25  
3P2F,ARG\_154,12.08,-0.42,0,0  
2NRR,GLU\_464,4.71,0.21,0,0  
2OBI,LYS\_99,10.22,-0.28,0,0  
2YT4,LYS\_510,9.94,-0.56,0,0  
2Z14,HIS\_71,7.23,0.94,0,-0.21  
2YLF,ARG\_47,12.36,-0.14,0,0  
2X4G,ASP\_331,3.59,0.14,-0.35,0  
3GV0,ARG\_209,11.87,-0.63,0,0  
1A8Q,ASP\_212,3.22,0.42,-1,0  
2FXT,ARG\_370,12.43,-0.07,0,0  
1YTD,LYS\_280,10.5,0,0,0  
2R57,GLU\_305,3.91,0.21,-0.8,0  
2Z14,ASP\_106,2.55,0.49,-1.74,0  
1QQE,TYR\_148,11.3,0.31,0,0.99  
1Q42,HIS\_91,6.36,0,0,-0.14  
1JB3,HIS\_127,6.37,0.08,0,-0.21  
4FZR,GLU\_209,4.5,0,0,0  
1R3F,ASP\_10,3.44,0.14,-0.5,0  
2Z0M,GLU\_323,0.97,0.94,-2.71,-1.76  
2CWC,ARG\_82,11.45,-1.05,0,0  
2OGQ,CYS\_428,7.92,-2.24,0.63,0.53  
2B3M,ASP\_62,2.72,0.49,-1.56,0  
1Z9L,ASP\_11,3.94,0.14,0,0  
2PGX,ASP\_30,4.01,0.21,0,0  
1R3F,GLU\_278,4.5,0,0,0  
1HF8,ARG\_92,11.52,-0.98,0,0  
1VJG,CYS\_35,10.73,0,0,1.73  
1T6L,LYS\_73,10.15,-0.35,0,0  
3FFM,GLU\_45,4.4,0.35,-0.45,0  
3PBH,TYR\_183,10.73,1.94,-0.89,-0.31  
2OSA,ASP\_310,3.8,0,0,0  
3IVF,GLU\_335,4.38,0,-0.13,0  
2Q07,ARG\_359,11.87,-0.63,0,0  
200K,HIS\_12,2.55,0,0,-3.95  
3EVZ,ASP\_206,3.89,0.35,-0.26,0  
3CXS,ARG\_118,11.94,-0.56,0,0  
1Q46,TYR\_101,10.33,0.33,0,0  
3O7K,ARG\_108,12.22,-0.28,0,0  
2X4J,TYR\_95,12.34,0.23,-0.29,2.4  
1SUU,GLU\_546,4.78,0.35,-0.07,0  
4D8L,HIS\_251,7.1,1.67,4.11,-5.19  
2EJB,LYS\_40,10.5,0,0,0  
1X6J,CYS\_49,9.04,-0.03,0,0.07  
3IDW,ARG\_50,12.5,0,0,0  
3QAV,LYS\_81,10.5,0,0,0  
1JB3,GLU\_23,3.19,0.56,-1.87,0  
2R51,GLU\_26,4.57,0.07,0,0  
2FBQ,TYR\_134,10.29,0.45,-0.8,0.64  
3ETV,GLU\_241,4.57,0.07,0,0  
2ZQ5,ARG\_109,12.29,-0.21,0,0  
1ZP2,HIS\_136,6.5,0,0,0  
1NAR,GLU\_66,4.72,0.28,-0.06,0  
1U3Y,CYS\_310,9,0,0,0  
4F3J,LYS\_142,10.15,-0.35,0,0  
1R53,GLU\_256,1.56,1.06,-2,-2  
2VGM,LYS\_167,10.36,-0.14,0,0  
1TR9,TYR\_11,10,0,0,0  
2ZCO,ASP\_210,3.89,0.14,-0.05,0  
2XMZ,HIS\_31,5.61,1.25,0,-2.14  
3EVN,TYR\_284,10,0,0,0  
1TD6,GLU\_24,3.64,0.49,-1.34,0  
3MTT,TYR\_577,10.28,0.14,0.14,0  
2Z14,GLU\_23,3.87,0.28,-0.91,0  
2B78,ARG\_315,11.52,-0.98,0,0  
3RJK,LYS\_190,10.29,-0.21,0,0  
2EFK,HIS\_177,6.43,0,0,-0.07  
2Q07,ARG\_433,12.01,-0.49,0,0  
3EX9,GLU\_140,7.48,2.98,0,0  
2YYO,GLU\_155,3.49,2.19,-3.21,0  
1LFL,LYS\_14,10.29,-0.21,0,0  
3DHN,ASP\_196,0.84,1.19,-4.16,0  
1RHS,HIS\_280,7.37,1.01,0,-0.14  
2FL7,ASP\_188,3.35,0.63,-1.08,0  
2OSA,GLU\_374,4.99,0.21,0.28,0  
3J5N,ASP\_3,2.39,0.28,-1.69,0  
1DUP,GLU\_129,4.5,0,0,0  
3MIX,ASP\_495,3.86,0.14,-0.08,0  
1WP5,GLU\_5,4.57,0.07,0,0  
2B78,GLU\_169,4.29,0.63,-0.84,0  
3RLE,ASP\_53,4.01,0.21,0,0  
2QDJ,LYS\_94,10.22,-0.28,0,0  
3CBN,ASP\_73,3.45,0.07,-0.42,0  
3RJK,LYS\_273,10.43,-0.07,0,0  
3LD1,ARG\_339,12.29,-0.21,0,0  
4FZN,GLU\_226,3.51,0.21,-1.2,0  
3G9G,LYS\_219,10.36,-0.14,0,0  
2X5Y,CYS\_831,7.11,-2.37,0,0.48  
2OBI,HIS\_60,4.06,0,0,-2.44  
4DBX,TYR\_284,10.37,0,0,0.37  
3LD1,ARG\_359,12.29,-0.21,0,0  
3PZ9,ASP\_379,3.87,0.07,0,0  
1X7F,TYR\_115,10.36,0.07,-0.77,1.06  
3EJC,HIS\_124,7.39,1.25,0,-0.35  
2OJQ,TYR\_485,12.5,0.24,-0.14,2.4  
1QQL,TYR\_94,10.02,0.07,-0.05,0  
1WPA,ASP\_518,3.37,0.42,-0.85,0  
2GKG,ARG\_46,12.01,-0.49,0,0  
1QYI,HIS\_358,6.43,0,0,-0.07  
1F2V,GLU\_33,4.5,0,0,0  
3K1H,GLU\_144,4.5,0,0,0  
4EKU,LYS\_54,10.5,0,0,0  
3IU5,TYR\_134,10,0,0,0  
2OKT,HIS\_336,6.5,0,0,0  
2OSA,HIS\_400,5.34,1.6,1.85,-4.61  
1T3Y,LYS\_7,10.36,-0.14,0,0  
2E3C,GLU\_237,4.43,0.35,-0.42,0  
1CBY,ASP\_179,2.29,0.98,-2.49,0  
3E5T,GLU\_7,4.5,0,0,0  
3T5B,CYS\_307,11.91,0,0,2.91  
3L7N,GLU\_112,2.86,1.9,-1.84,-1.7  
3I47,HIS\_237,6.5,0,0,0  
1WOU,GLU\_5,3.65,0.28,-1.13,0  
1NFN,HIS\_140,6.43,0,0,-0.07  
3GS9,ASP\_9,1.9,1.19,-3.09,0  
1MD6,CYS\_121,7.98,-2.06,0,1.04  
3HST,GLU\_34,4.12,0.63,-1.01,0  
3CAX,TYR\_129,10.19,0.19,0,0  
1YOY,GLU\_134,1.04,1.15,-2.4,-2.21  
3CX2,GLU\_240,4.26,0.56,-0.8,0  
4FCU,GLU\_118,3.37,0.42,-0.85,0  
3B4D,TYR\_217,10,0,0,0  
2CWY,ASP\_80,2.68,0.42,-1.54,0  
2I6I,LYS\_89,10.43,-0.07,0,0  
1TR9,GLU\_326,4.2,0.28,-0.58,0  
1AKO,GLU\_85,4.53,0.07,-0.04,0  
3GW3,GLU\_130,4.74,0.28,-0.04,0  
2OYZ,GLU\_59,3.15,0.63,-1.98,0  
1GPP,GLU\_425,4.51,0.14,-0.13,0  
2BDD,GLU\_76,4.5,0,0,0  
2QV2,ARG\_10,12.01,-0.49,0,0  
3MIX,HIS\_340,7.69,1.26,0,-0.07  
3Q1C,GLU\_312,4.64,0.14,0,0  
3KT9,LYS\_57,10.5,0,0,0  
2CN1,TYR\_261,11.44,1.22,-0.12,0.34  
1XKR,ARG\_6,11.8,-0.7,0,0  
1OGL,TYR\_198,11.52,1.52,0,0  
3EVP,GLU\_190,4.5,0,0,0  
2X5Y,TYR\_814,11.46,0.07,0,1.39  
2Z0M,TYR\_96,10.12,0,0,0.12  
3ONT,ASP\_55,0.66,0.77,-3.91,0  
2QV2,LYS\_93,10.29,-0.21,0,0  
3M7G,ASP\_121,2.97,0.21,-1.04,0  
3RJK,GLU\_54,4.78,2.9,-2.62,0  
4DIU,ASP\_172,3.52,0.21,-0.49,0  
3HVM,TYR\_217,10.04,0.84,-0.8,0  
1ZBM,ARG\_4,11.94,-0.56,0,0  
3KB5,ARG\_326,12.22,-0.28,0,0  
3A7L,TYR\_70,13.79,0,0,12.3.68  
1TWU,TYR\_47,10,0,0,0  
2WOZ,LYS\_406,10.22,-0.28,0,0  
3ERF,ARG\_210,11.8,-0.7,0,0  
2C13,LYS\_198,10.5,0,0,0  
2IXM,LYS\_302,10.36,-0.14,0,0  
3GFP,HIS\_422,5.68,0.82,0,-1.64  
2PGE,ARG\_151,11.73,-0.77,0,0  
1R7J,LYS\_86,10.5,0,0,0  
3KB5,GLU\_392,4.19,0.49,-0.8,0  
3T5B,ARG\_140,12.01,-0.49,0,0  
1PVT,LYS\_112,10.43,-0.07,0,0  
2F4Q,TYR\_307,8.61,0.21,-1.6,0  
2I6I,GLU\_115,2.45,0.35,-2.4,0  
4FZR,CYS\_216,8.4,-2.64,0,2.04  
1R2Z,TYR\_105,13.01,0.61,0,2.4  
3I4T,CYS\_193,11.57,0,0,2.57  
3BQE,LYS\_281,10.15,-0.35,0,0  
2X4J,LYS\_53,10.08,-0.42,0,0  
1ZBH,GLU\_63,3.88,0.35,-0.97,0  
2E3P,ASP\_254,1.78,0.49,-2.52,0  
3ULX,LYS\_53,10.29,-0.21,0,0  
1FHL,LYS\_175,10.43,-0.07,0,0  
2FL4,ARG\_74,11.89,-0.61,0,0  
3BCY,LYS\_50,10.22,-0.28,0,0  
1JB3,CYS\_123,8.9,-0.1,0,0  
2YWJ,LYS\_63,10.5,0,0,0  
1QQE,TYR\_80,11.47,0.64,0,0.83  
1XEU,LYS\_62,10.22,-0.28,0,0  
3M7D,ASP\_303,3.92,0.14,-0.02,0  
1YR6,HIS\_112,4.83,1.01,0,-2.68  
3BPP,ASP\_228,1.51,0.84,-3.12,0  
2R57,LYS\_265,10.15,-0.35,0,0  
2Q12,TYR\_168,10.07,0.07,0,0  
3A0X,LYS\_628,10.29,-0.21,0,0  
1RWZ,LYS\_118,10.5,0,0,0  
2GZR,GLU\_101,4.5,0,0,0  
3RJK,GLU\_179,4.78,0.28,0,0  
1O5J,HIS\_0,7.26,0.83,0,-0.07  
2OPJ,ARG\_67,11.31,-1.19,0,0  
2E3I,ARG\_126,11.66,-0.84,0,0  
1Y2Q,GLU\_62,3.96,0.21,-0.75,0  
3HVM,TYR\_193,13.21,0.14,0.71,2.36  
3K9I,GLU\_160,4.5,0,0,0  
3BA1,HIS\_211,7.02,0.8,0,-0.28  
1WRU,LYS\_132,10.43,-0.07,0,0  
2B6P,TYR\_23,13.69,4.01,-0.32,0  
3OIP,CYS\_177,9,0,0,0  
3HVV,ARG\_315,13.09,-1.78,0,2.37  
2V5B,LYS\_113,10.08,-0.42,0,0  
3COU,GLU\_124,2.89,0.79,-2.4,0  
3PP8,ASP\_68,3.34,0.21,-0.67,0  
1P2F,LYS\_148,10.43,-0.07,0,0  
2EHG,ARG\_118,12.5,0,0,0  
1BYI,TYR\_4,12.18,0.48,0,1.7  
1CBY,ASP\_39,2.39,0.63,-2.04,0  
3EZZ,GLU\_293,4.57,0.07,0,0  
3CBN,LYS\_76,10.08,-0.42,0,0  
3G53,ARG\_216,11.66,-0.84,0,0  
1R3D,GLU\_172,4.59,0.77,-0.68,0  
3B7X,ARG\_28,12.5,0,0,0  
2FPN,GLU\_9,4.78,0.28,0,0  
2EFK,ARG\_121,11.94,-0.56,0,0  
1TLV,ARG\_214,11.66,-0.84,0,0  
3BCH,ARG\_41,11.87,-0.63,0,0  
1E59,ARG\_127,11.94,-0.56,0,0  
1FO9,TYR\_350,10.67,1.65,-0.98,0  
3RLN,TYR\_635,11.24,0.14,-0.18,1.28  
200K,LYS\_40,10.08,-0.42,0,0  
3P2F,CYS\_196,9,0,0,0  
3EZZ,HIS\_131,4.06,0,0,-2.44  
1JKS,TYR\_191,9.27,0.07,-0.8,0  
3ERF,LYS\_66,10.22,-0.28,0,0  
4ESS,GLU\_132,3.51,0.49,-1.48,0  
1MML,TYR\_271,10,0,0,0  
2D8N,LYS\_196,10.22,-0.28,0,0  
3GW3,ARG\_113,11.59,-0.91,0,0  
1XIPT,TYR\_279,9.91,3.38,-1.45,-2.02  
3PM2,ARG\_43,12.01,-0.49,0,0  
1J7G,GLU\_47,4.5,0,0,0  
1DOV,ASP\_185,3.31,0.21,-0.69,0  
2OSA,ARG\_321,11.29,-0.21,0,0  
2CVB,TYR\_4,11.04,1.1,-0.06,0  
3CF6,LYS\_82,10.5,0,0,0  
4EVF,ARG\_161,12.22,-0.28,0,0  
1OGL,LYS\_66,10.43,-0.07,0,0  
1X1E,GLU\_190,4.5,0,0,0  
2BDV,HIS\_65,6.5,0,0,0  
3FTT,ARG\_46,12.08,-0.42,0,0  
3FTT,ASP\_14,3.22,0.56,-1.14,0  
2YT4,ASP\_605,0.9,0.7,-3.6,0  
3PBH,LYS\_130,10.43,-0.07,0,0  
2H85,ASP\_310,3.39,0.42,-0.83,0  
1Y2Q,LYS\_21,10.5,0,0,0



4F85,HIS\_235,5.72,1.79,1.53,-4.1  
1UCH,TYR\_85,8.79,1.61,-0.94,-1.88  
3MIX,CYS\_583,11.44,0.1,1.1,1.34  
3RKV,ARG\_227,12.29,-0.21,0,0  
2B61,LYS\_256,10.43,-0.07,0,0  
2YT4,LYS\_640,10.43,-0.07,0,0  
2ZCO,GLU\_76,4.64,0.14,0,0  
3PBH,ARG\_252,11.54,-0.96,0,0  
1O9G,ARG\_112,11.61,-0.89,0,0  
2E3H,GLU\_233,4.5,0,0,0  
3BWT,LYS\_682,10.22,-0.28,0,0  
2B2H,LYS\_144,10.15,-0.35,0,0  
2WB3,LYS\_327,10.36,-0.14,0,0  
3F53,HIS\_227,4.83,0.22,0,-1.89  
2Q99,ARG\_71,11.45,-1.05,0,0  
2Z0M,GLU\_143,4.71,0.21,0,0  
2D7J,HIS\_166,11.22,5.2,3.94,-4.42  
1W24,ARG\_14,11.59,-0.91,0,0  
2D7J,GLU\_173,3.81,0.42,-1.11,0  
1P4X,HIS\_77,6.5,0,0,0  
4FCU,LYS\_2,10.36,-0.14,0,0  
2G55,LYS\_73,10.5,0,0,0  
3DZ1,ASP\_159,3.74,0.35,-0.41,0  
2QVO,LYS\_11,10.5,0,0,0  
2EFK,ASP\_214,3.9,0.14,-0.04,0  
3DHN,ARG\_214,12.55,-2.19,0,2.24  
2EHG,GLU\_52,6.68,2.29,-0.95,0.84  
3DZ1,ARG\_113,12.5,0,0,0  
3A4C,GLU\_508,4.5,0,0,0  
3LQE,GLU\_303,3.17,0.63,-1.96,0  
1SUU,ARG\_790,11.87,-0.63,0,0  
1OGL,ARG\_204,12.06,-0.44,0,0  
3EGN,GLU\_395,4.16,0.21,-0.55,0  
1YB2,TYR\_62,11.68,1.37,-0.39,0.69  
1R7J,GLU\_65,4.64,0.14,0,0  
1X9G,ASP\_171,2.87,0.21,-1.14,0  
3LPZ,HIS\_177,6.43,0,0,-0.07  
2P1W,TYR\_83,10,0,0,0  
3IVF,LYS\_98,10.5,0,0,0  
3AUF,HIS\_175,4.02,0.16,0,-2.64  
1DT9,HIS\_113,6.5,0,0,0  
3H8Y,ARG\_83,12.5,0,0,0  
4AM1,GLU\_59,4.5,0,0,0  
2W1R,GLU\_61,4.25,0.21,-0.46,0  
2Q34,GLU\_81,4.64,0.14,0,0  
1OGL,HIS\_20,5.05,0.63,0.43,-2.52  
3EVN,ARG\_19,12.22,-0.28,0,0  
3OIP,GLU\_82,4.57,0.07,0,0  
3V3T,LYS\_4,10.22,-0.28,0,0  
2Q07,ARG\_384,11.94,-0.56,0,0  
1RSQ,ASP\_80,3.8,0,0,0  
2XMZ,GLU\_214,3.77,0.35,-1.08,0  
2PWQ,LYS\_39,10.22,-0.28,0,0  
2F8H,HIS\_87,4.32,0.89,-0.37,-2.7  
3MTT,ARG\_458,12.01,-0.49,0,0  
3G59,TYR\_62,13.25,0.1,0.3,1.4  
1WJG,GLU\_27,4.57,0.07,0,0  
1R29,ARG\_94,12.5,0,0,0  
1J33,ARG\_148,11.87,-0.63,0,0  
1P1L,LYS\_20,10.5,0,0,0  
4DNU,GLU\_216,4.71,0.21,0,0  
2E3C,LYS\_229,10.01,-0.49,0,0  
3HQX,CYS\_65,9.09,-0.62,0,0.71  
2AHE,CYS\_189,11.3,-0.33,0,2.63  
1X91,HIS\_88,0.7,0.53,0,0  
3CRM,TYR\_315,9.23,0,-0.77,0  
1MIX,LYS\_263,10.36,-0.14,0,0  
3JZN,LYS\_385,10.36,-0.14,0,0  
2P65,ARG\_176,12.22,-0.28,0,0  
4EUG,LYS\_94,10.36,-0.14,0,0  
1O17,GLU\_58,3.26,0.35,-1.6,0  
2E3C,CYS\_328,9.38,-0.27,-1.45,2.1  
1T6L,ASP\_109,3.87,0.07,0,0  
2BLL,GLU\_617,4.5,0,0,0  
2FXT,LYS\_278,10.29,-0.21,0,0  
2YWXX,LYS\_140,10.43,-0.07,0,0  
3LQE,TYR\_525,11.91,0,0,1.91  
1PVT,LYS\_76,10.43,-0.07,0,0  
2IQT,ARG\_10,12.01,-0.49,0,0  
1WOU,GLU\_122,4.5,0,0,0  
3O16,GLU\_215,4.57,0.07,0,0  
2B0J,ARG\_192,11.59,-0.91,0,0  
3FNI,GLU\_137,3.39,0.49,-1.6,0  
1RAJ,ASP\_89,4.08,0.28,0,0  
1EDG,ASP\_68,2.82,0.7,-1.69,0  
1EDG,LYS\_61,10.5,0,0,0  
2QK0,LYS\_71,10.5,0,0,0  
2YWXX,GLU\_46,4.1,0.49,-0.89,0  
2RIK,GLU\_240,4.64,0.14,0,0  
2H85,TYR\_225,13.34,0.14,0.8,2.4  
3ANJ,CYS\_176,8.57,-2.37,0.07,1.87  
2NSN,ASP\_54,1.49,0.42,-2.72,0  
2IQT,GLU\_4,4.57,0.07,0,0  
3HUE,GLU\_287,4.85,0.35,0,0  
3V3T,LYS\_155,10.43,-0.07,0,0  
2Q13,ARG\_338,11.66,-0.84,0,0  
1JSX,GLU\_48,4.5,0,0,0  
1N81,GLU\_91,4.5,0,0,0  
2P0Y,ASP\_76,4.01,0.21,0,0  
1YM5,ASP\_140,3.8,0.07,-0.07,0  
3VJ8,ARG\_218,13.16,-1.74,0,2.4  
2FBQ,GLU\_80,4.5,0,0,0  
2H01,CYS\_68,13.07,-0.14,1.79,2.42  
2B61,GLU\_348,3.88,0.28,-0.9,0  
2V5B,GLU\_248,4.72,0.35,-0.13,0  
3V55,CYS\_596,5.98,-3.03,0,0  
2PGX,ARG\_118,12.01,-0.49,0,0  
1WXQ,ASP\_97,3.9,0.28,-0.18,0  
2ZQ5,GLU\_342,2.96,0.21,-1.76,0  
1JT9,HIS\_132,3.78,0.59,0,-3.32  
3JZ9,TYR\_368,11.59,2.39,-0.8,0  
1U7U,GLU\_256,2.13,0.49,-2.86,0  
3G59,CYS\_113,9.15,-0.8,0,0.95  
3I47,HIS\_60,6.32,0.03,0,-0.21  
1HF8,TYR\_88,10,0,0,0  
3RKV,GLU\_268,1.66,0.4,-1.6,-1.64  
3CS1,ARG\_49,11.8,-0.7,0,0  
1YLN,ARG\_165,12.22,-0.28,0,0  
2X4L,GLU\_261,3.84,0.14,-0.8,0  
3DTE,ARG\_19,11.87,-0.63,0,0  
2VAN,TYR\_271,11.65,0,0,1.65  
2H85,LYS\_46,10.22,-0.28,0,0  
1Q2Y,TYR\_65,11.45,0,0,1.45  
1XEU,ASP\_156,4.03,0.35,-0.12,0  
2Q12,GLU\_216,4.77,0.35,-0.08,0  
1D2K,LYS\_149,9.94,-0.56,0,0  
1BN6,HIS\_283,7.51,3.2,3.78,-5.98  
1UXO,HIS\_9,3.71,0.99,0,-3.78  
3VJ8,ARG\_203,11.66,-0.84,0,0  
1C44,LYS\_8,10.29,-0.21,0,0  
1Q2Y,HIS\_117,7.25,0.82,0,-0.07  
1YTD,ASP\_229,2.91,0.14,-1.04,0  
2NRK,GLU\_161,2.44,0.9,-0.8,-2.16  
2V4U,HIS\_517,3.18,0.98,0,-4.3  
3OBS,LYS\_36,10.5,0,0,0  
3G9G,TYR\_183,13.34,0.14,0.8,2.4  
2QEV,GLU\_88,4.57,0.07,0,0  
2RIS,GLU\_95,4.5,0,0,0  
3M7D,ARG\_287,12.5,0,0,0  
2CVB,ASP\_15,1.88,0.63,-2.55,0  
3JZN,ASP\_338,3.042,-1.23,0  
2WZ9,LYS\_110,10.5,0,0,0  
3ZYX,ASP\_157,3.89,0.14,-0.05,0  
4H86,LYS\_107,10.5,0,0,0  
4FD6,LYS\_219,10.15,-0.35,0,0  
2EFK,TYR\_231,10,0,0,0  
3TOW,ASP\_154,3.88,0.35,-0.27,0  
1FHL,GLU\_279,4.5,0,0,0  
2G3A,ASP\_33,3.94,0.21,-0.07,0  
3IL3,ARG\_127,12.15,-0.35,0,0  
3EVP,ASP\_123,2.55,0.63,-1.88,0  
1SFE,GLU\_22,4.74,0.42,-0.18,0  
2CW4,LYS\_5,10.5,0,0,0  
3QAV,ASP\_91,2.64,0.49,-1.65,0  
4DND,GLU\_41,4.5,0,0,0  
4HDE,ASP\_166,1.68,0.84,-2.97,0  
2AD1,GLU\_275,4.64,0.14,0,0  
2BLL,ARG\_415,11.87,-0.63,0,0  
2PLQ,ASP\_109,4.22,0.42,0,0  
3C38,ARG\_203,11.94,-0.56,0,0  
1WYC,ARG\_89,12.15,-0.35,0,0  
2EJB,GLU\_117,4.05,0.35,-0.8,0  
3I0C,HIS\_145,4.09,0.8,0,-3.21  
2CWC,ARG\_162,11.45,-1.05,0,0  
3KV0,GLU\_40,3.0,28,-1.78,0  
2G5X,ASP\_121,2.25,0.42,-1.97,0  
3G6S,ARG\_147,11.39,-1.11,0,0  
3EX9,GLU\_72,4.2,0.14,-0.44,0  
1X8F,ASP\_180,3.52,0.35,-0.63,0  
1H09,CYS\_108,11.2,-0.21,0,2.41  
1L2H,LYS\_55,10.22,-0.28,0,0  
2Q13,LYS\_350,10.29,-0.21,0,0  
2AD1,ASP\_264,4.08,0.28,0,0  
2A1V,ASP\_51,3.19,0.35,-0.96,0  
3Q1C,HIS\_250,6.32,0.03,0,-0.21  
1G8P,TYR\_149,13.68,1.35,-0.07,2.4  
1SIG,TYR\_137,13.69,1.1,0.31,2.28  
1JKS,TYR\_208,9.44,0.5,-1.75,0.69  
3V1Q,LYS\_622,10.5,0,0,0  
1XTD,LYS\_96,10.5,0,0,0  
4AM1,LYS\_9,10.43,-0.07,0,0  
1OST,LYS\_114,10.36,-0.14,0,0  
1TMO,LYS\_175,10.5,0,0,0  
3TMO,TYR\_299,12.94,0.14,0.33,2.47  
3FHF,GLU\_25,3.58,0.49,-1.41,0  
4AM1,LYS\_164,10.29,-0.21,0,0  
2W1R,LYS\_90,10.36,-0.14,0,0  
3H8Y,GLU\_53,4.57,0.07,0,0  
3O7K,GLU\_154,3.98,0.28,-0.8,0  
2IQT,GLU\_265,4.02,0.56,-1.04,0  
2DGT,ARG\_180,12.5,0,0,0  
1YG2,ASP\_94,2.35,0.84,-2.3,0  
1BKR,LYS\_78,10.22,-0.28,0,0  
3TMO,HIS\_240,6.9,0.61,0,-0.21  
2AZL,GLU\_30,4.64,0.14,0,0  
3CS1,GLU\_175,4.5,0,0,0  
2BDD,ASP\_114,4.11,0.35,-0.05,0  
3RLN,GLU\_609,4.71,0.21,0,0  
1WLY,ARG\_254,12.15,-0.35,0,0  
3M9A,CYS\_23,7.54,-1.6,0,0.14  
1NAR,LYS\_210,10.22,-0.28,0,0  
2QHT,ARG\_43,11.45,-1.05,0,0  
1R7J,LYS\_3,10.5,0,0,0  
1OIS,ARG\_307,12.01,-0.49,0,0  
2Z61,TYR\_176,12.58,2.49,-0.62,0.7  
1O5J,ARG\_97,11.94,-0.56,0,0  
3DHN,GLU\_154,4.5,0,0,0  
2FC3,LYS\_83,9.94,-0.56,0,0  
2NYC,ASP\_190,4.15,0.35,0,0  
2AZL,LYS\_138,10.36,-0.14,0,0  
3ETU,TYR\_81,10.62,0.62,0,0  
2Q13,GLU\_255,4.36,0.21,-0.35,0  
2FG1,ARG\_122,11.59,-0.91,0,0  
1UOH,HIS\_137,6.23,0.08,0,-0.35  
1MIX,GLU\_291,4.15,0.21,-0.56,0  
3GG6,HIS\_157,6.49,0.06,0,-0.07  
3MTT,LYS\_572,10.29,-0.21,0,0  
3N2T,LYS\_147,10.36,-0.14,0,0  
2P1W,ARG\_90,12.43,-0.07,0,0  
2F4Q,GLU\_10,4.57,0.07,0,0  
2R4Q,GLU\_260,4.05,0.35,-0.8,0  
1CBY,LYS\_201,10.5,0,0,0  
3M3P,CYS\_49,8.89,-1.2,0,1.09  
1J8B,LYS\_43,10.29,-0.21,0,0  
2GZQ,TYR\_118,11.38,1.38,0,0  
3BA1,GLU\_208,3.62,0.42,-1.3,0  
1O3X,LYS\_213,10.43,-0.07,0,0  
2YX0,GLU\_312,3.41,0.28,-1.37,0  
2EYI,ARG\_133,11.73,-0.77,0,0  
2Q13,GLU\_95,4.85,0.35,0,0  
1AK1,TYR\_17,12.17,0.62,0,1.55  
3BB7,ASP\_193,2.77,0.49,-1.52,0  
2Z61,TYR\_292,12.98,0.14,0.44,2.4  
3C0C,ASP\_322,3.72,0.07,-0.15,0  
2VGM,TYR\_230,13.31,0.21,0.35,2.75  
1NAR,ARG\_6,11.58,-3.7,0,2.79  
3MEW,TYR\_269,11.54,0,-0.21,1.75  
2O8P,ASP\_148,3.32,0.07,-0.55,0  
3CCY,TYR\_99,9.26,0.14,-0.88,0  
3K1H,ARG\_35,11.52,-0.98,0,0  
3M66,LYS\_363,10.5,0,0,0  
2IF4,ASP\_223,3.67,0.07,-0.2,0  
2WB8,HIS\_563,10.35,3.6,2.34,-2.09  
1AIL,GLU\_55,4.5,0,0,0  
3BWT,GLU\_700,4.31,0.42,-0.61,0  
2HRZ,HIS\_10,3.7,0.63,0,-3.43  
1XWM,ARG\_92,12.01,-0.49,0,0  
2F4Q,ASP\_300,3.27,0.14,-0.67,0  
2ZCX,ARG\_136,12.29,-0.21,0,0  
1IDK,ARG\_188,11.94,-0.56,0,0  
3TOW,ARG\_164,12.01,-0.49,0,0  
2G55,GLU\_123,4.5,0,0,0  
2IRM,ARG\_354,12.59,-1.79,0,1.88  
1UCH,ASP\_38,3.58,0.35,-0.57,0  
3ZXY,ARG\_107,11.66,-0.84,0,0  
2P52,TYR\_123,10.7,0.72,-0.02,0  
1X7F,ASP\_194,3.13,0.49,-1.16,0  
1ZCE,GLU\_17,4.5,0.14,-0.14,0  
3D9H,LYS\_228,10.5,0,0,0  
3ZTA,CYS\_51,10.28,-0.26,0,1.54  
1EQ6,GLU\_65,3.61,0.26,-1.15,0  
3H04,HIS\_216,5.1,1.6,1.79,-4.8  
1WXQ,TYR\_382,12.32,0.07,-0.15,2.4  
2WZ9,GLU\_107,4.3,0.49,-0.69,0  
1H09,LYS\_311,10.36,-0.14,0,0  
1ZKZ,ASP\_48,4.12,0.21,0,1.11,0  
3GMS,LYS\_309,10.29,-0.21,0,0  
2PGE,ARG\_122,12.53,-2.37,0,2.4  
1NJ4,ASP\_293,3.47,0.07,-0.4,0  
1OST,HIS\_375,6.29,0,0,-0.21  
3CIV,ARG\_210,12.08,-0.42,0,0  
2XWS,GLU\_93,4.0,0.14,-0.64,0  
3V3T,ASP\_27,3.24,0.14,-0.69,0  
1OST,HIS\_170,2.75,0,0,-3.75  
1MIX,GLU\_346,4.57,0.07,0,0  
2Z61,ASP\_283,3.14,0.7,-1.35,0

3AUF, TYR\_42,9.38,0.07,-0.8,0.11  
 1NIJ, GLU\_204,0.28,1.84,-1.6,-4.46  
 3IBT, CYS\_182,10.81,0,0,1.81  
 4EKU, GLU\_243,2.33,1.25,-1.76,-1.65  
 3EAZ, ASP\_161,3.21,0.21,-0.8,0  
 3IU5, ARG\_74,12.5,0,0,0  
 3K1H, ASP\_36,3.21,0.21,-0.8,0  
 1BKB, ARG\_49,12.29,-0.21,0,0  
 3RJZ, GLU\_80,4.64,0.14,0,0  
 3DZ1, TYR\_265,13.55,0.35,0.8,2.4  
 1J74, GLU\_59,3.88,0.35,-0.97,0  
 2FBI, ARG\_16,11.94,-0.56,0,0  
 3TOW, ARG\_168,12.22,-0.28,0,0  
 1GPP, GLU\_125,3.85,0.35,-1,0  
 3L0D, LYS\_100,10.29,-0.21,0,0  
 2ZTY, LYS\_76,10.43,0.07,0,0  
 3HVM, GLU\_91,4.03,0.28,-0.75,0  
 3NR5, GLU\_10,4.57,0.07,0,0  
 2XHC, ASP\_148,3.04,0.42,-1.18,0  
 1H4U, ARG\_525,11.52,-0.98,0,0  
 1X04, LYS\_77,10.36,-0.14,0,0  
 1NJ4, GLU\_274,3.39,0.49,-1.6,0  
 3JSN, TYR\_169,11.15,1.52,-0.51,0.14  
 1QYI, HIS\_39,7.83,1.47,0,-0.14  
 1SJJ, HIS\_96,4.19,0.1,0,-2.41  
 2EFK, GLU\_270,4.85,0.35,0,0  
 3I0C, GLU\_138,0.54,1.19,-2.75,-2.4  
 2H2W, LYS\_197,10.15,-0.35,0,0  
 2F4Q, CYS\_291,7.05,-2.86,-0.36,1.27  
 4AE7, ASP\_65,3.2,0.14,-0.74,0  
 2FPN, LYS\_145,10.36,-0.14,0,0  
 4F85, ARG\_146,12.43,-0.07,0,0  
 1ZKZ, GLU\_100,4.85,0.35,0,0  
 2QDJ, TYR\_325,10.88,0.65,-1.38,1.61  
 2ZTY, GLU\_61,3.91,0.21,-0.8,0  
 1TD6, TYR\_119,13.51,0.33,0.8,2.38  
 1YOY, GLU\_59,4.09,0.28,-0.69,0  
 2QRX, TYR\_85,12.96,1.25,-0.77,2.48  
 1T95, GLU\_68,4.19,0.49,-0.8,0  
 4GCO, ASP\_158,3.94,0.42,-0.28,0  
 3ONT, TYR\_59,13.27,0.07,0.8,2.4  
 1WNH, GLU\_94,4.5,0,0,0  
 3CE7, CYS\_28,9.98,0,0,0.98  
 1ZBS, LYS\_257,10.5,0,0,0  
 1MUF, GLU\_214,4.31,0,-0.19,0  
 3DTE, ASP\_224,3.93,0.14,-0.01,0  
 3UV9, LYS\_467,10.36,-0.14,0,0  
 1TJE, CYS\_35,9.97,-0.06,0,1.03  
 3ETU, LYS\_230,10.5,0,0,0  
 2O8I, GLU\_151,2.75,0.83,-2.4,-0.18  
 4EKU, GLU\_146,4.5,0,0,0  
 4H86, TYR\_70,11.82,2.43,-0.61,0  
 1ANU, ASP\_82,3.94,0.14,0,0  
 3F6M, ASP\_127,3.86,0.28,-0.22,0  
 3RJX, ARG\_304,12.15,-0.35,0,0  
 1SI7, LYS\_190,10.43,-0.07,0,0  
 2QEV, GLU\_80,4.08,0.35,-0.77,0  
 3ODJ, TYR\_53,11.77,0.14,0,1.63  
 2I88, TYR\_421,10.14,0.14,0,0  
 2HRZ, ASP\_98,3.1,0.42,-1.12,0  
 1WLY, LYS\_316,10.22,-0.28,0,0  
 3RLE, TYR\_135,10.31,0.31,0,0  
 1MTZ, ARG\_153,11.87,-0.63,0,0  
 3PM2, ASP\_112,3.75,0,-0.05,0  
 2H8O, HIS\_109,4.29,0.96,0,-3.17  
 2XJ4, ARG\_120,12.29,-0.21,0,0  
 2APL, TYR\_45,12.36,0.14,-0.8,3.02  
 2ATR, ARG\_136,12.22,-0.28,0,0  
 3ETV, GLU\_79,3.84,0.14,-0.8,0  
 3RLE, LYS\_68,10.29,-0.21,0,0  
 3Q6L, ASP\_78,3.58,0.07,-0.29,0  
 1H4U, TYR\_612,11.52,0.35,-0.23,1.41  
 2IQT, ARG\_242,11.75,-0.75,0,0  
 3T5B, GLU\_350,3.36,0.81,-1.94,0  
 3CZC, CYS\_39,9.07,0,0,0.07  
 2GKG, GLU\_31,3.54,0.63,-1.59,0  
 4DNU, LYS\_304,10.5,0,0,0  
 1GQE, TYR\_326,9.89,2.68,-1.6,-1.19  
 1R53, GLU\_171,4.5,0,0,0  
 2E3S, CYS\_503,7.16,-3.6,0,1.76  
 4F3J, ARG\_198,12.15,-0.35,0,0  
 2V81, TYR\_200,10.14,0.14,0,0  
 1R15, ARG\_247,13.87,-1.03,0,2.4  
 2B3M, LYS\_21,10.5,0,0,0  
 4FCU, GLU\_211,3.3,2.11,-3.31,0  
 1AKO, ARG\_209,12.01,-0.49,0,0  
 3HUE, ASP\_74,3.8,0,0,0  
 1ZBM, GLU\_190,2.99,0.56,-2.07,0  
 1J85, ARG\_129,12.43,-0.07,0,0  
 3V75, ARG\_274,12.08,-0.42,0,0  
 2IN0, ARG\_417,11.73,-0.77,0,0  
 3RE9, ASP\_177,2.6,0.77,-1.97,0  
 3BCY, HIS\_87,3.52,0,0,-2.98  
 3K8U, TYR\_33,9.72,0,-0.28,0  
 2W0Z, HIS\_298,6.5,0,0,0  
 1G8P, GLU\_244,4.5,0,0,0  
 1YM5, ASP\_32,3.41,0.56,-0.95,0  
 2VAN, HIS\_212,6.55,0.19,0,-0.14  
 3T5B, ARG\_29,12.01,-0.49,0,0  
 2QDJ, GLU\_287,3.34,0.28,-1.44,0  
 3FRR, ASP\_180,3.03,0.42,-1.19,0  
 3OIP, ARG\_200,12.15,-0.35,0,0  
 3AU3, ASP\_556,1.67,0.63,-2.75,0  
 3VHJ, LYS\_37,10.29,-0.21,0,0  
 2Q34, GLU\_238,4.71,0.21,0,0  
 1SUU, ASP\_798,3.87,0.07,0,0  
 2V5B, GLU\_158,3.75,0.42,-1.17,0  
 2ZCX, LYS\_21,10.29,-0.21,0,0  
 1TLV, LYS\_187,9.94,-0.56,0,0  
 2QV2, ASP\_258,3.05,0.07,-1.23,0  
 1G5Z, GLU\_117,4.5,0,0,0  
 3B21, TYR\_170,10.19,0,0,0.19  
 2XHC, ARG\_181,12.5,0,0,0  
 3C2E, HIS\_124,6.64,0.14,0,0  
 2B78, TYR\_50,11.79,2.59,-0.8,0  
 2DVK, ARG\_96,12.29,-0.21,0,0  
 1PV5, GLU\_213,4.5,0,0,0  
 4H4J, LYS\_27,10.5,0,0,0  
 2YWJ, LYS\_65,10.15,-0.35,0,0  
 2Z14, TYR\_21,11.69,0,0,1.69  
 3BBL, HIS\_226,2.18,0,0,-4.32  
 1LPL, CYS\_152,8.87,-0.95,0,0.82  
 1BKB, LYS\_114,10.22,-0.28,0,0  
 2QEV, ARG\_69,12.08,-0.42,0,0  
 2QK1, LYS\_363,10.36,-0.14,0,0  
 1F2V, ARG\_189,11.8,-0.7,0,0  
 3OBS, TYR\_68,10,0,0,0  
 3MEW, GLU\_173,3.78,0.42,-1.14,0  
 1R9W, TYR\_268,11.03,1.03,0,0  
 1PZC, GLU\_43,4.33,0.63,-0.8,0  
 4FLE, HIS\_9,3.19,0.54,0,-3.85  
 3V4G, ASP\_90,2.95,0.14,-0.99,0  
 2EJK, GLU\_7,3.98,0.28,-0.8,0  
 1AKO, GLU\_23,4.5,0,0,0  
 4FZN, ARG\_68,12.22,-0.28,0,0  
 1OIS, GLU\_274,3.95,0.14,-0.69,0  
 1RZ2, GLU\_178,3.7,0.28,-1.08,0  
 2NYC, LYS\_279,10.43,-0.07,0,0  
 3HNX, CYS\_23,7.66,-1.6,0,0.26  
 1L2H, LYS\_65,10.5,0,0,0  
 1WYC, ARG\_76,11.84,-0.66,0,0  
 2BV9, GLU\_21,3.84,0.14,-0.8,0  
 3EJG, ASP\_82,3.38,0.35,-0.77,0  
 3Q2C, GLU\_34,4.64,0.14,0,0  
 2AH5, TYR\_100,10,0,0,0  
 2AHE, GLU\_113,4.5,0,0,0  
 1YTD, LYS\_346,10.43,-0.07,0,0  
 3ZXY, ASP\_130,4.04,0.28,-0.04,0  
 2G9D, TYR\_334,9.6,0,-0.56,0.16  
 1SFE, ASP\_90,3.3,0.84,-1.34,0  
 3GA2, LYS\_2,10.5,0,0,0  
 2P1W, HIS\_203,6.24,1.31,0,-1.57  
 1ZHV, ASP\_51,3.58,0,-0.22,0  
 1LTU, GLU\_133,4.89,0.4,-0.01,0  
 2BQQ, ARG\_76,12.15,-0.35,0,0  
 3SMD, GLU\_87,4.57,0.07,0,0  
 1X9G, LYS\_178,10.5,0,0,0  
 1DZF, ARG\_177,12.29,-0.21,0,0  
 2V81, CYS\_108,10.02,0,0,1.02  
 1WXQ, LYS\_318,10.5,0,0,0  
 2NSX, GLU\_53,4.5,0,0,0  
 3EZ7, GLU\_304,4.5,0,0,0  
 3ASA, TYR\_14,9.37,0.14,-0.77,0  
 3ZRI, GLU\_110,4.64,0.14,0,0  
 2BAA, ARG\_211,12.01,-0.49,0,0  
 3F5D, TYR\_21,10,0,0,0  
 2EFK, TYR\_28,9.82,0.36,-0.54,0  
 3D9H, ASP\_36,3.39,0.14,-0.55,0  
 3D9H, HIS\_146,5.17,1.16,0,-2.49  
 1YG2, ARG\_14,12.5,0,0,0  
 2E3C, ASP\_373,3.85,0.07,-0.02,0  
 2PGE, HIS\_299,3.25,0,0,-3.25  
 3LD1, LYS\_70,10.5,0,0,0  
 4D8L, ASP\_203,3.29,0.35,-0.86,0  
 2P1W, GLU\_54,2.59,0.49,-2.4,0  
 1IAP, TYR\_186,11.98,0,0,1.98  
 2EJB, CYS\_7,12.04,0,0,3.04  
 1PSW, HIS\_201,4.02,0.9,0,-3.38  
 2EHG, GLU\_104,4.57,0.07,0,0  
 1ZP2, LYS\_210,10.29,-0.21,0,0  
 3F6M, TYR\_83,9.16,0.35,-1.19,0  
 1RHS, ASP\_82,3.87,0.14,-0.07,0  
 2BLL, GLU\_342,4.33,0.63,-0.8,0  
 3EUR, GLU\_139,4.78,0.28,0,0  
 1XKR, GLU\_169,4.57,0.07,0,0  
 2GZQ, CYS\_70,8.6,-1.03,0,0.64  
 3CAX, ARG\_387,13.15,-1.55,0,2.2  
 2FZP, ARG\_253,11.94,-0.56,0,0  
 3IVF, ARG\_33,11.45,-1.05,0,0  
 2ZOM, GLU\_327,3.77,0.56,-1.29,0  
 2WB8, TYR\_717,10.29,0.92,-0.8,0.17  
 3R2E, ARG\_68,12.22,-0.28,0,0  
 3K9I, LYS\_71,10.5,0,0,0  
 3TRE, LYS\_34,10.5,0,0,0  
 1JB3, ASP\_82,3.07,0.7,-1.44,0  
 3EJC, HIS\_37,8.08,2.14,0,-0.56  
 1J8B, ASP\_58,2.63,0.42,-1.59,0  
 1IAP, ARG\_124,11.8,-0.7,0,0  
 4FLE, ASP\_152,3.25,0.49,-1.04,0  
 2QZQ, ASP\_51,3.92,0.14,-0.02,0  
 3IL3, TYR\_117,9.41,0.14,-0.73,0  
 2RIK, GLU\_199,4.78,0.28,0,0  
 3CZC, TYR\_51,10.75,0,0,0.75  
 3ASA, LYS\_141,10.43,-0.07,0,0  
 1WLY, TYR\_317,8.69,0.07,-1.38,0  
 3CE7, GLU\_69,4.57,0.07,0,0  
 1QQL, LYS\_69,10.29,-0.21,0,0  
 4ANN, LYS\_87,10.15,-0.35,0,0  
 3JRT, GLU\_12,4.64,0.14,0,0  
 4F85, TYR\_240,10.95,2.72,-2.09,0.32  
 3V4G, LYS\_102,10.43,-0.07,0,0  
 2FB6, GLU\_163,4.5,0,0,0  
 2PLQ, TYR\_145,10,0,0,0  
 2B61, TYR\_108,9.82,0.38,-0.56,0  
 3C38, GLU\_255,4.71,0.21,0,0  
 2Q98, TYR\_44,9.95,0.05,-0.1,0  
 2Z84, CYS\_62,10.63,-0.15,0,1.78  
 2G9D, TYR\_334,9.6,0,-0.56,0.16  
 1TXJ, TYR\_167,11.27,0.14,-0.69,1.82  
 2X4L, GLU\_185,3.75,0.42,-1.17,0  
 2DVK, GLU\_146,4.5,0,0,0  
 3T5B, TYR\_393,11.65,0.07,-0.05,1.63  
 2G9D, HIS\_210,4.8,0,-1.7  
 1QQE, CYS\_35,3.69,0.21,-0.32,0  
 4GCO, GLU\_249,4.57,0.07,0,0  
 2R2Y, LYS\_34,10.5,0,0,0  
 1LTU, ARG\_50,12.24,-1.54,0,1.28  
 4F3J, GLU\_173,4.64,0.14,0,0  
 2GKG, ASP\_45,4.08,0.28,0,0  
 2OEW, CYS\_76,9.89,-0.85,0.23,1.51  
 1G8P, GLU\_198,4.5,0,0,0  
 1X7F, ARG\_164,11.73,-0.77,0,0  
 1W24, TYR\_179,11.84,0.07,-0.14,1.91  
 4EVF, LYS\_211,10.5,0,0,0  
 3I0O, HIS\_102,7.34,0.98,0,-0.14  
 1ZYL, ASP\_210,11.87,-0.63,0,0  
 1N81, TYR\_23,10.77,0.07,-0.8,1.5  
 1XEU, TYR\_247,9.68,0,-0.32,0  
 1MUF, TYR\_287,10.81,2.16,-1.16,-0.18  
 1SFE, CYS\_135,10.51,-0.13,0.14,1.51  
 3M66, LYS\_404,10.36,-0.14,0,0  
 1QQE, CYS\_160,10.06,0,0,1.06  
 2X4L, GLU\_258,3.03,1.23,-2.7,0  
 2H85, GLU\_21,4.64,0.14,0,0  
 2FZ4, GLU\_187,4.47,0.21,-0.24,0  
 3I0O, ASP\_166,2.2,0.28,-1.87,0  
 3AU3, CYS\_527,10.58,-0.2,0,1.78  
 1NAR, GLU\_95,4.57,0.07,0,0  
 1O9G, ASP\_156,3.34,0.49,-0.95,0  
 2GZQ, HIS\_18,6.54,0.11,-0.07  
 2ZQ5, ASP\_369,2.81,0.49,-1.47,0  
 1WP5, GLU\_271,3.98,0.28,-0.8,0  
 3OA7, LYS\_541,10.29,-0.21,0,0  
 1QQL, ARG\_218,12.15,-0.35,0,0  
 3PU6, GLU\_70,4.5,0,0,0  
 3GT0, GLU\_128,4.64,0.14,0,0  
 3U2R, ASP\_81,3.52,0.63,-0.91,0  
 2EJX, TYR\_57,11.32,1.32,0,0  
 2OEW, LYS\_265,10.15,-0.35,0,0  
 1NAR, GLU\_121,12.5,0,0,0  
 2POL, GLU\_83,4.71,0.21,0,0  
 3ASA, ARG\_110,13.33,-0.84,0,1.67  
 2P65, LYS\_7,10.36,-0.14,0,0  
 1LPL, LYS\_173,10.5,0,0,0  
 3A2Z, ARG\_45,12.36,-0.14,0,0  
 2VAN, GLU\_216,4.64,0.14,0,0  
 1XEU, GLU\_122,4.57,0.07,0,0  
 1V43, GLU\_268,4.24,0.42,-0.68,0  
 3M3P, ASP\_37,2.18,0.91,-2.53,0  
 1AK1, ARG\_30,11.45,-1.05,0,0  
 3QKY, TYR\_63,9.64,0.35,-0.8,0.09  
 2R4Q, HIS\_215,6.56,0.06,0,0  
 2B78, LYS\_245,10.5,0,0,0  
 3TOW, TYR\_66,10.43,0.03,0,0.4  
 1Q46, GLU\_155,4.64,0.14,0,0  
 1T95, HIS\_180,6.29,0,-0.21

2OKT,LYS\_16,10.08,-0.42,0,0  
 2H14,ASP\_172,4.15,0.35,0,0  
 3OIP,TYR\_132,9.48,0.28,-0.8,0  
 157K,ASP\_177,2.79,0.42,-1.43,0  
 4DBX,GLU\_262,4.17,0.14,-0.47,0  
 1FQI,HIS\_379,6.49,0.13,0,-0.14  
 3F1X,LYS\_24,10.15,-0.35,0,0  
 1XTD,GLU\_163,4.05,0.21,-0.66,0  
 1AII,CYS\_13,9.03,-0.18,0,0.21  
 2R57,GLU\_308,3.28,0.28,-1.5,0  
 3OIP,HIS\_136,6.43,0,0,-0.07  
 2NSN,LYS\_24,10.5,0,0,0  
 1Q46,LYS\_96,10.29,-0.21,0,0  
 2EJB,LYS\_59,10.43,-0.07,0,0  
 2VAN,ARG\_222,12.5,0,0,0  
 2FXT,GLU\_373,1.71,1.21,-1.6,-2.4  
 2BLI,GLU\_366,4.57,0.07,0,0  
 3UX2,HIS\_89,6.55,0.05,0,0  
 3NBI,LYS\_78,10.5,0,0,0  
 1V6T,ASP\_202,4.03,0.28,-0.06,0  
 3V55,ASP\_530,3.87,0.07,0,0  
 1TD6,ASP\_118,3.67,0.07,-0.2,0  
 4E8B,GLU\_140,5.05,1.54,-0.99,0  
 1ZBM,TYR\_103,10,0,0,0  
 1PDB,GLU\_123,4.15,0.21,-0.56,0  
 3CAX,ASP\_457,2.54,0.77,-2.04,0  
 2Z84,ASP\_47,1.17,0.77,-3.4,0  
 3DB9,GLU\_104,4.13,0.28,-0.65,0  
 3BJV,ARG\_131,11.94,-0.56,0,0  
 1YDL,ARG\_5,12.22,-0.28,0,0  
 1XFK,ARG\_150,11.66,-0.84,0,0  
 3K8U,TYR\_97,11.53,1.53,0,0  
 2QV2,ASP\_145,3.87,0.07,0,0  
 1SQW,HIS\_40,6.43,0,0,-0.07  
 3GG6,HIS\_161,6.5,0,0,0  
 4GCO,TYR\_137,10,0,0,0  
 3F6F,TYR\_153,11.38,1.77,-0.8,0.41  
 1FQI,ASP\_371,3.67,0.14,-0.27,0  
 3BWT,HIS\_732,6.36,0,0,-0.14  
 3LJN,ARG\_199,12.08,-0.42,0,0  
 1AK1,TYR\_196,12.31,2.45,-0.14,0  
 2CYG,GLU\_310,9.33,2.8,1.39,0.64  
 2NYC,LYS\_289,10.5,0,0,0  
 3P2F,CYS\_65,8.71,-0.29,0,0  
 4F3J,ARG\_103,12.5,0,0,0  
 3LJC,LYS\_35,10.43,-0.07,0,0  
 1UW7,ARG\_55,12.36,-0.14,0,0  
 2OKT,ARG\_246,12.1,-2.82,0,2.42  
 2GZR,ASP\_45,3.74,0.35,-0.41,0  
 2OB5,GLU\_103,3.98,0.28,-0.8,0  
 1XAW,TYR\_474,11.32,0,0,1.32  
 2B0J,ASP\_269,3.49,0.49,-0.8,0  
 1OTM,ASP\_200,3.09,0.42,-1.13,0  
 2OYZ,TYR\_65,9.82,0.07,-0.76,0.51  
 2PPN,GLU\_31,3.55,0.35,-1.29,0  
 3BJV,TYR\_54,10,0,0,0  
 2I88,TYR\_367,11.49,2.29,-0.8,0  
 3ONH,ASP\_474,4.17,0.42,-0.05,0  
 3P28,ASP\_85,3.2,0.07,-0.67,0  
 3CN5,CYS\_91,8.93,-0.14,0,0.07  
 2X4G,GLU\_297,4.5,0,0,0  
 3GG6,ASP\_140,0.39,1.12,-3.36,-1.17  
 3F6F,CYS\_201,6.24,-2.14,-2.4,1.78  
 3H5T,GLU\_164,4.5,0,0,0  
 3LJC,ASP\_105,4.18,0.42,-0.04,0  
 1PSW,GLU\_111,3.81,0.35,-1.04,0  
 3DTE,ARG\_255,13.79,-1.02,0,2.31  
 2NRR,ARG\_466,12.5,0,0,0  
 3CAX,LYS\_432,10.5,0,0,0  
 3K9I,TYR\_154,10.14,0.14,0,0  
 2FD4,LYS\_520,10.36,-0.14,0,0  
 3GFP,HIS\_361,6.36,0,0,-0.14  
 2Z0M,ASP\_84,3.8,0,0,0  
 4GA2,ASP\_59,2.47,0.7,-2.03,0  
 1M5I,ARG\_187,11.94,-0.56,0,0  
 3QKY,TYR\_197,10.26,0.32,0,-0.06  
 1TP6,ARG\_17,11.8,-0.7,0,0  
 2G9D,ARG\_179,12.01,-0.49,0,0  
 3EVZ,GLU\_125,4.15,0.07,-0.42,0  
 1TLV,HIS\_207,6.29,0,0,-0.21  
 3L3P,GLU\_338,4.5,0,0,0  
 2FPN,TYR\_180,10,0,0,0  
 3BQW,ASP\_323,3.74,0,-0.06,0  
 3P28,ASP\_162,2.5,0.7,-2,0  
 3H13,CYS\_259,8.23,-2.11,0,1.34  
 3L3P,ASP\_372,3.65,0,-0.15,0  
 3UAH,CYS\_470,9,0,0,0  
 1RKA,ASP\_202,3.4,0.77,-1.17,0  
 1V43,LYS\_36,10.5,0,0,0  
 3U56,ARG\_135,12.01,-0.49,0,0  
 1RI6,TYR\_193,10.43,1.13,-0.7,0  
 3ON1,CYS\_56,9.36,-0.05,0,0.41  
 4EZB,ARG\_280,12.15,-0.35,0,0  
 2OEW,CYS\_90,9,0,0,0  
 2E35,LYS\_550,10.43,-0.07,0,0  
 3MEW,TYR\_238,11.03,0,0,1.03  
 2EFK,HIS\_203,6.51,0.01,0,0  
 3IF5,ASP\_41,2.41,0.63,-2.03,0  
 1TXD,GLU\_794,4.57,0.07,0,0  
 1JKS,GLU\_84,1.93,0.77,-3.34,0  
 1O0X,TYR\_171,10.6,0.6,0,0  
 3D9H,GLU\_188,4.7,0.42,-0.22,0  
 3I47,ARG\_39,12.36,-0.14,0,0  
 1WXQ,GLU\_179,4.71,0.21,0,0  
 1SQH,LYS\_136,10.08,-0.42,0,0  
 3F5D,TYR\_123,10,0,0,0  
 1P4X,HIS\_244,7.31,1.6,1.54,-2.33  
 2IDC,CYS\_99,10.21,-0.56,0,1.77  
 1T3Y,LYS\_131,10.36,-0.14,0,0  
 2B6P,GLU\_244,4.38,0.14,-0.26,0  
 1L2F,TYR\_130,7.59,0.28,-2.69,0  
 2B2H,ASP\_364,2.89,0.28,-1.19,0  
 2Q13,LYS\_66,10.5,0,0,0  
 1X8F,TYR\_69,10.28,0.28,0,0  
 2ZQ5,LYS\_170,3.65,0.39,-1.24,0  
 2QEV,LYS\_95,9.94,-0.56,0,0  
 3BCH,LYS\_40,10.43,-0.07,0,0  
 2F19,GLU\_93,4.71,0.21,0,0  
 3ZTA,ARG\_95,12.5,0,0,0  
 2XJ4,LYS\_63,10.36,-0.14,0,0  
 2P65,ARG\_177,11.8,-0.7,0,0  
 1LFP,LYS\_247,10.5,0,0,0  
 1XAW,LYS\_494,10.22,-0.28,0,0  
 3RE9,ARG\_229,11.94,-0.56,0,0  
 4AM1,LYS\_354,10.5,0,0,0  
 1L2H,ARG\_11,12.08,-0.42,0,0  
 3AUF,TYR\_5,10,0,0,0  
 3BQE,HIS\_248,3.64,0.9,0,-3.76  
 1Z3X,GLU\_141,4.78,0.28,0,0  
 1GXN,ARG\_588,12.36,-0.14,0,0  
 3DHN,GLU\_23,3.58,0.56,-1.47,0  
 3O16,ARG\_71,12.22,-0.28,0,0  
 4E65,GLU\_50,3.51,0.14,-1.13,0  
 2D0A,ARG\_212,12.36,-0.14,0,0  
 2RFA,GLU\_116,3.77,0.07,-0.8,0  
 3JSN,TYR\_23,10.22,0.22,0,0  
 3LH5,CYS\_744,8.41,-0.66,0,0.07  
 1X8F,GLU\_239,1.62,3.56,-2.41,-4.03  
 2RFA,ARG\_75,11.73,-0.77,0,0  
 3RKV,TYR\_253,9.21,0.13,-0.8,-0.12  
 3DZ1,LYS\_232,10.22,-0.28,0,0  
 3JV1,GLU\_140,4.57,0.07,0,0  
 4ECC,ASP\_134,3.44,0.21,-0.57,0  
 2GSX,LYS\_150,10.22,-0.28,0,0  
 1MTZ,LYS\_194,10.22,-0.28,0,0  
 2VGM,TYR\_80,11.59,0.14,-0.24,1.69  
 3O48,LYS\_63,10.5,0,0,0  
 2E3H,TYR\_269,10.49,0,0,0.49  
 3M7D,ARG\_112,11.43,-0.66,0,-0.41  
 1X6J,GLU\_19,3.68,0.14,-0.96,0  
 2WOZ,CYS\_46,1.725,-0.85,-1.02,0.12  
 3O47,LYS\_48,10.15,-0.35,0,0  
 3QAV,CYS\_18,7.15,-3.89,0.2,0.4  
 2PGE,CYS\_180,11.23,0.53,-0.11,1.81  
 3LPZ,ARG\_84,11.94,-0.56,0,0  
 2E3H,GLU\_248,4.64,0.14,0,0  
 2PWQ,ASP\_89,3.19,0.07,-0.68,0  
 3GG6,ARG\_84,11.94,-0.56,0,0  
 1RI5,ARG\_210,12.29,-0.21,0,0  
 1OXZ,GLU\_246,5.2,0.7,0,0  
 2ZOM,HIS\_75,4.44,0,-2.06  
 3NJM,ASP\_116,3.73,0.14,-0.21,0  
 1QQE,GLU\_258,4.57,0.07,0,0  
 1JYH,ASP\_104,3.94,0.14,0,0  
 2GAU,GLU\_23,4.57,0.07,0,0  
 1QLL,GLU\_82,3.98,0.28,-0.8,0  
 4EVF,ASP\_6,3.97,0.21,-0.04,0  
 3DZ1,ASP\_131,3.79,0.14,-0.15,0  
 3B79,ARG\_89,12.43,-0.07,0,0  
 2W0G,GLU\_156,3.91,0.21,-0.8,0  
 2H2W,HIS\_234,11.21,5.2,4.64,-5.13  
 3O47,GLU\_476,4.57,0.07,0,0  
 1UW7,ARG\_10,12.36,-0.14,0,0  
 1NIJ,LYS\_159,9.94,-0.56,0,0  
 1LPL,GLU\_140,4.57,0.07,0,0  
 3RFY,ARG\_145,12.36,-0.14,0,0  
 3V46,HIS\_353,7.5,1.14,0,-0.14  
 3P51,GLU\_78,3.98,0.28,-0.8,0  
 3EUR,ARG\_3,12.5,0,0,0  
 3BB7,LYS\_285,10.5,0,0,0  
 1KCM,LYS\_168,10.22,-0.28,0,0  
 3EVN,GLU\_282,8.63,3.72,-0.5,0.91  
 3GOZ,LYS\_270,10.5,0,0,0  
 1MHN,ASP\_105,2.07,0.63,-2.37,0  
 1E59,GLU\_111,3.23,0.35,-1.61,0  
 2WOZ,ASP\_574,3.76,0.07,-0.11,0  
 1RAJ,GLU\_227,4.22,0.14,-0.42,0  
 3HVM,ARG\_83,9.19,-5.17,0,1.86  
 1RI6,ASP\_129,3.3,0.28,-0.78,0  
 3PU6,ARG\_24,12.15,-0.35,0,0  
 3DSH,ASP\_313,11.73,-0.77,0,0  
 2OJQ,LYS\_627,10.43,-0.07,0,0  
 1UAJ,GLU\_225,4.57,0.07,0,0  
 3MIX,CYS\_636,13.31,0.258,1.73  
 1V6T,TYR\_95,10,0,0,0  
 1T6L,TYR\_253,12.62,1.04,0.45,1.13  
 1YB,TYR\_247,13.34,0.14,0.8,2.4  
 2JKF,ASP\_60,3.35,0.35,-0.8,0  
 1SQW,GLU\_6,4.5,0,0,0  
 1DOV,GLU\_183,3.86,0.28,-0.93,0  
 2AD1,ASP\_217,3.28,0.35,-0.87,0  
 1KN3,GLU\_172,4.64,0.14,0,0  
 2X4G,ARG\_60,11.1,-1.4,0,0  
 1G8P,ARG\_145,11.32,-1.18,0,0  
 3NBI,LYS\_188,10.36,-0.14,0,0  
 1JKS,LYS\_258,10.43,-0.07,0,0  
 1JSX,TYR\_180,10.07,0.07,0,0  
 3BPV,LYS\_61,10.5,0,0,0  
 4DBX,TYR\_264,12.57,0.07,-0.68,3.19  
 3Q9P,GLU\_108,4.5,0,0,0  
 3E27,CYS\_303,7.33,-1.68,0,0  
 4ACI,TYR\_734,13.1,0.21,0.49,2.4  
 1DVO,ARG\_121,11.87,-0.63,0,0  
 1PV5,GLU\_117,4.5,0,0,0  
 2HRZ,ARG\_175,12.08,-0.42,0,0  
 1VSM,LYS\_116,10.08,-0.42,0,0  
 2AD1,GLU\_57,4.64,0.14,0,0  
 3O48,LYS\_97,10.29,-0.21,0,0  
 3M66,ASP\_151,3.79,0,-0.01,0  
 157K,TYR\_172,9.64,0.07,-0.43,0  
 3B21,ARG\_121,11.45,-1.05,0,0  
 1WRU,ARG\_242,12.29,-0.21,0,0  
 3EVN,LYS\_58,10.5,0,0,0  
 3C2E,ARG\_150,11.94,-0.68,0.84,0  
 3T5B,HIS\_178,1.58,0,0,-4.92  
 1VJG,TYR\_48,10,0,0,0  
 4E5S,ASP\_10,2.19,0.56,-2.17,0  
 2OKT,GLU\_274,7.31,4.01,-1.6,0.4  
 3OKQ,LYS\_608,10.29,-0.21,0,0  
 157K,ASP\_179,3.79,0,-0.01,0  
 2FZ4,ASP\_63,3.48,0,-0.32,0  
 2Z61,TYR\_350,11.21,2.34,-0.41,-0.73  
 3UAH,TYR\_423,12.81,0.28,0.13,2.4  
 2C2Y,ASP\_18,3.46,0.42,-0.76,0  
 1D2K,TYR\_276,11.89,2.69,-0.8,0  
 3RRQ,ARG\_147,12.22,-0.28,0,0  
 1WYC,ASP\_24,3.93,0.14,-0.01,0  
 3CNU,HIS\_58,6.43,0,0,-0.07  
 2OSA,ARG\_290,11.94,-0.56,0,0  
 2BV9,TYR\_121,10,0,0,0  
 2QHT,LYS\_187,10.15,-0.35,0,0  
 1RW7,ARG\_10,12.36,-0.14,0,0  
 3DB9,ARG\_156,12.43,-0.07,0,0  
 1SUU,LYS\_694,10.5,0,0,0  
 3ZTA,ARG\_112,12.36,-0.14,0,0  
 2OSA,LYS\_409,10.5,0,0,0  
 2G9D,ARG\_7,12.01,-0.49,0,0  
 2F9F,ASP\_83,0.83,0.49,-3.46,0  
 1CHD,ASP\_329,2.09,0.63,-2.34,0  
 1P2F,ARG\_203,12.01,-0.49,0,0  
 2F19,ARG\_34,11.87,-0.63,0,0  
 3N0K,GLU\_69,4.5,0,0,0  
 2GAU,TYR\_58,11.18,0,0,1.18  
 1GK,ASP\_126,2.89,0.63,-1.54,0  
 1UAJ,HIS\_244,6.49,0.06,0,-0.07  
 1OIS,GLU\_183,2.74,1.2,-0.79,-2.17  
 1OTM,GLU\_36,4.36,0.07,-0.21,0  
 1WRU,ARG\_176,11.73,-0.77,0,0  
 2Q99,HIS\_214,7.09,0.8,0,-0.21  
 3FKE,ASP\_45,4.08,0.28,0,0  
 2C2Y,ARG\_129,12.15,-0.35,0,0  
 3KT9,ARG\_9,11.38,-1.12,0,0  
 3DHN,LYS\_52,10.43,-0.07,0,0  
 1BKR,HIS\_73,6.69,0.26,0,-0.07  
 3H9W,LYS\_23,10.15,-0.35,0,0  
 2HXB,LYS\_83,10.15,-0.35,0,0  
 2Z61,ARG\_286,11.74,-1.49,0,0.73  
 1DVO,GLU\_75,3.55,0.28,-1.23,0  
 4ECC,GLU\_197,1.32,0.82,-1.6,-2.4  
 1UOH,ARG\_85,11.66,-0.84,0,0  
 2P0L,LYS\_17,10.15,-0.35,0,0  
 1LFP,HIS\_6,5.29,0.94,0,-2.15  
 1YLN,TYR\_83,10.95,0,-0.19,1.14  
 2ZQ5,HIS\_235,5.32,4.08,1.63,-6.89  
 2FXT,LYS\_381,10.43,-0.07,0,0  
 2AZP,ARG\_140,12.22,-0.28,0,0

2RFA,ASP\_223,2.62,0.49,-1.67,0  
 3LH5,HIS\_703,3.06,0,0,-3.44  
 1YW5,LYS\_43,10.36,-0.14,0,0  
 3ERF,ARG\_173,11.94,-0.56,0,0  
 1D2K,ARG\_190,12.25,-2,0,1.75  
 2QZQ,ASP\_65,3.3,0.42,-0.92,0  
 1EV8,GLU\_82,4.71,0.21,0,0  
 1CHD,HIS\_265,6.23,0.48,1.34,-2.08  
 2OYZ,HIS\_21,6.5,0,0,0  
 3OBS,TYR\_113,11.29,0.21,-1.02,2.09  
 2V1L,ARG\_117,12.43,-0.07,0,0  
 4DNU,GLU\_53,4.64,0.14,0,0  
 1W7B,GLU\_82,4.64,0.14,0,0  
 2CBE,HIS\_64,2.91,0,-0.08,-3.51  
 3ASA,HIS\_195,7.06,0.84,0,-0.28  
 3U4K,ASP\_59,2.43,0.42,-1.79,0  
 1ANU,ASP\_71,3.56,0,-0.24,0  
 2YYO,ASP\_117,4.08,0.28,0,0  
 2W0G,TYR\_155,9.27,0.07,-0.8,0  
 2FPN,ASP\_175,3.48,0.14,-0.46,0  
 4E9E,LYS\_539,9.8,-0.7,0,0  
 4H89,ARG\_120,12.5,0,0,0  
 1RSS,LYS\_136,10.22,-0.28,0,0  
 2WB8,GLU\_640,3.78,3.12,-3.84,0  
 2Q5X,LYS\_791,10.15,-0.35,0,0  
 2RIK,GLU\_209,3.98,0.28,-0.8,0  
 2I88,LYS\_433,10.29,-0.21,0,0  
 3EVP,ASP\_234,3.68,0.21,-0.33,0  
 1JB3,CYS\_74,7.82,-1.17,0,0  
 2F4Q,GLU\_16,4.76,0.28,-0.02,0  
 3H04,LYS\_44,10.22,-0.28,0,0  
 2J8A,LYS\_312,10.5,0,0,0  
 1PGV,GLU\_325,4.05,0.35,-0.8,0  
 2I6I,HIS\_64,4.1,1.08,0,-3.48  
 2QEV,CYS\_81,7.44,-2.29,0,0.73  
 2IRM,HIS\_121,6.5,0,0,0  
 3E5T,ARG\_179,12.08,-0.42,0,0  
 1XKR,LYS\_85,10.15,-0.35,0,0  
 1GPP,LYS\_39,10.29,-0.21,0,0  
 3LPZ,ASP\_123,3.11,0.14,-0.83,0  
 4FZR,ARG\_25,12.08,-0.42,0,0  
 1OI7,GLU\_130,3.49,0.35,-1.36,0  
 1RLO,ASP\_230,2.61,0.7,-1.9,0  
 3F6M,LYS\_11,10.5,0,0,0  
 3H5T,GLU\_234,4.5,0,0,0  
 4DBX,GLU\_152,4.78,0.28,0,0  
 3GM5,HIS\_2,7.39,1.03,0,-0.14  
 2Z0M,LYS\_219,10.5,0,0,0  
 1I60,HIS\_179,4.5,0.05,0,-2.05  
 3NOK,LYS\_83,10.29,-0.21,0,0  
 4ETX,HIS\_302,6.44,1.6,2.16,-3.83  
 2OEW,ARG\_290,12.29,-0.21,0,0  
 3T8R,GLU\_84,4.15,0.14,-0.48,0  
 2R51,LYS\_34,10.29,-0.21,0,0  
 2JEO,ASP\_207,3.13,0.42,-1.09,0  
 2B0J,HIS\_340,7.31,0.81,0,0  
 2GEN,CYS\_150,8.94,-0.06,0,0  
 1SJB,ASP\_525,3.15,0.49,-1.14,0  
 1KCM,CYS\_192,11.69,-0.31,1.16,1.84  
 4FLE,HIS\_173,7.7,1.6,2.4,-2.8  
 3VHJ,TYR\_137,9.9,0.07,-0.27,0.11  
 2BLL,TYR\_344,10.3,0.14,-0.8,0.96  
 2YLF,TYR\_139,10,0,0,0  
 1WYC,HIS\_346,3.94,0,-2.56  
 3LJC,GLU\_139,4.71,0.21,0,0  
 3F5D,ASP\_40,4.08,0.28,0,0  
 2Q12,GLU\_131,4.64,0.14,0,0  
 3H13,ARG\_472,12.08,-0.42,0,0  
 3EVZ,LYS\_209,10.5,0,0,0  
 2OEW,TYR\_258,10.47,0.47,0,0  
 2P5D,GLU\_135,4.5,0,0,0  
 1X04,GLU\_37,4.71,0.21,0,0  
 3L3P,LYS\_315,10.36,-0.14,0,0  
 3BA1,TYR\_125,10.29,0.28,0,0.01  
 3MTT,ASP\_461,3.83,0.07,-0.04,0  
 1FO9,LYS\_186,10.15,-0.35,0,0  
 3DSH,ASP\_439,2.28,0.77,-2.3,0  
 1JB3,GLU\_119,4.52,0.14,-0.12,0  
 2OPJ,ARG\_281,12.43,-0.07,0,0  
 1SNT,ASP\_358,3.87,0.07,0,0  
 3GG6,LYS\_130,9.59,-0.91,0,0  
 1TXJ,ASP\_11,2.06,0.98,-2.71,0  
 2F19,GLU\_86,3.54,0.21,-1.17,0  
 1TR9,ARG\_310,12.08,-0.42,0,0  
 2NRR,LYS\_414,10.08,-0.42,0,0  
 2G55,ARG\_112,11.8,-0.7,0,0  
 1R7J,GLU\_64,4.64,0.14,0,0  
 2INO,ARG\_18,12.29,-0.21,0,0  
 1EDG,HIS\_254,5.57,1.6,3.37,-5.9  
 3RE9,LYS\_89,10.43,-0.07,0,0  
 1OXZ,ARG\_207,12.36,-0.14,0,0  
 3UAH,LYS\_242,10.5,0,0,0  
 1TR9,ARG\_55,11.3,-1.2,0,0  
 1U7U,ARG\_399,11.87,-1.19,0,0.56  
 3ETV,ASP\_173,3.19,0.21,-0.82,0  
 3VJ8,HIS\_173,4.95,0.8,0,-2.35  
 3VJ8,ARG\_66,11.87,-0.63,0,0  
 2DVK,TYR\_62,13.12,0.07,0.66,2.4  
 1O3X,GLU\_219,4.5,0,0,0  
 2DFL,GLU\_309,2.85,0.18,-0.8,-1.03  
 1RLO,TYR\_4,9.27,0.07,-0.8,0  
 1Y2Q,HIS\_130,6.5,0,0,0  
 3ZTA,GLU\_132,4.57,0.07,0,0  
 3M70,LYS\_101,9.59,-0.91,0,0  
 2AHE,LYS\_60,10.5,0,0,0  
 2P1W,ASP\_57,3.8,0,0,0  
 3FWU,TYR\_68,9.62,0.51,-0.89,0  
 1AK1,LYS\_127,10.43,-0.07,0,0  
 1PSW,LYS\_125,10.5,0,0,0  
 2ATR,ASP\_51,3.87,0.07,0,0  
 1Q46,GLU\_158,4.5,0,0,0  
 3ZTA,ASP\_88,3.68,0.07,-0.19,0  
 2D7U,ARG\_258,13.41,-1.47,0,2.38  
 1YDL,GLU\_59,4.33,0.14,-0.31,0  
 3EVN,TYR\_242,10,0,0,0  
 2QK1,HIS\_544,6.5,0,0,0  
 3S0A,LYS\_27,10.29,-0.21,0,0  
 1DUN,ASP\_14,3.72,0,-0.08,0  
 3V55,TYR\_417,10,0,0,0  
 1SNT,HIS\_210,7.34,0.91,0,-0.07  
 1Z3X,LYS\_185,10.5,0,0,0  
 1P4X,HIS\_6,6.5,0,0,0  
 1R5Q,GLU\_55,4.66,0.07,0.09,0  
 1NAF,LYS\_176,10.5,0,0,0  
 1O5T,LYS\_111,10.22,-0.28,0,0  
 2NMU,GLU\_79,1.18,1.52,-2.44,-2.4  
 3U0V,CYS\_128,5.3,-3.96,-3.02,3.27  
 2EJX,GLU\_121,4.64,0.14,0,0  
 3P51,ARG\_20,11.73,-0.77,0,0  
 3IU5,GLU\_150,4.71,0.21,0,0  
 1R7J,LYS\_62,10.36,-0.14,0,0  
 1NFN,GLU\_132,3.41,0.35,-1.44,0  
 4FH3,LYS\_42,10.5,0,0,0  
 2A4D,LYS\_192,10.29,-0.21,0,0  
 2B61,GLU\_320,4.12,0.42,-0.8,0  
 1A8Q,GLU\_206,3.91,0.21,-0.8,0  
 3EYE,LYS\_153,10.15,-0.35,0,0  
 4GA2,LYS\_61,10.5,0,0,0  
 2ZQ5,ASP\_316,4.31,0.28,0.23,0  
 1PVT,HIS\_81,6.5,0.35,0,-0.35  
 3EIZ,HIS\_111,6.58,0.15,0,-0.07  
 1BKB,LYS\_39,10.43,-0.07,0,0  
 2BQ,ARG\_78,12.5,0,0,0  
 2P52,HIS\_175,6.5,0,0,0  
 1WXQ,LYS\_155,10.43,-0.07,0,0  
 1RLO,LYS\_195,10.43,-0.07,0,0  
 2DG7,ARG\_52,12.01,-0.49,0,0  
 1XFK,ARG\_62,11.59,-0.91,0,0  
 3GVO,GLU\_134,4.71,0.21,0,0  
 3Q1C,GLU\_357,4.15,0.56,-0.91,0  
 3ELI,LYS\_75,10.22,-0.28,0,0  
 2IXM,LYS\_27,10.43,-0.07,0,0  
 1DVO,ARG\_61,12.22,-0.28,0,0  
 1H4U,GLU\_563,4.5,0,0,0  
 3V4G,ASP\_57,9.66,-2.84,0,0  
 2F8H,HIS\_206,6.43,0,0,-0.07  
 1TJE,ASP\_116,1.87,0.77,-2.7,0  
 3LJC,GLU\_203,3.91,0.21,-0.8,0  
 1O0X,TYR\_109,9.97,0,-0.03,0  
 2POY,HIS\_129,6.43,0,0,-0.07  
 3GEC,GLU\_382,2.45,0.56,-2.61,0  
 2POL,ARG\_80,12.08,-0.42,0,0  
 3G9G,GLU\_189,3.61,0.84,-1.72,0  
 2OEW,TYR\_233,10,0,0,0  
 4GA2,TYR\_42,10.07,0.07,0,0  
 1R6Y,TYR\_84,11.22,1.22,0,0  
 1R3F,ASP\_92,3.8,0,0,0  
 2YLF,LYS\_201,10.43,-0.07,0,0  
 1BN6,ASP\_198,3.23,0.21,-0.78,0  
 1J33,ARG\_211,10.98,-1.52,0,0  
 3L3P,LYS\_350,10.29,-0.21,0,0  
 2PAD,HIS\_143,6.43,0,0,-0.07  
 3QAV,ARG\_199,13.7,-1.2,0.2,4  
 1YOK,LYS\_63,10.36,-0.14,0,0  
 2R2Y,ARG\_84,11.87,-0.63,0,0  
 1FKM,LYS\_431,10.36,-0.14,0,0  
 3EZ7,TYR\_38,10.07,0.07,0,0  
 1NAR,HIS\_34,2.83,1.6,-0.6,-4.66  
 3K8U,ARG\_93,11.8,-0.7,0,0  
 1BKB,LYS\_47,10.08,-0.42,0,0  
 1RHS,LYS\_66,10.36,-0.14,0,0  
 2PGE,ARG\_147,11.87,-0.63,0,0  
 2B02,ASP\_377,0.16,1.12,-4.76,0  
 2ZCX,ASP\_222,4.04,0.28,-0.04,0  
 3HVM,ARG\_267,11.52,-0.98,0,0  
 2QHT,CYS\_170,8.96,-0.11,0,0.07  
 1WRU,ARG\_126,12.36,-0.14,0,0  
 3OIP,TYR\_27,10.84,0.24,0,0.6  
 1XAW,LYS\_521,10.22,-0.28,0,0  
 1U7U,HIS\_370,7.02,0.8,0,-0.28  
 3OKQ,LYS\_660,10.5,0,0,0  
 1RHS,GLU\_61,3.91,0.21,-0.8,0  
 1P2F,ARG\_190,12.36,-0.14,0,0  
 3Q6L,ASP\_88,3.87,0.07,0,0  
 3Q6L,ASP\_19,3.78,0,-0.02,0  
 2BLL,GLU\_633,4.5,0,0,0  
 2OJQ,LYS\_690,10.29,-0.21,0,0  
 2R2Y,ASP\_54,1.92,0.56,-2.44,0  
 3CX2,GLU\_165,3.84,0.14,-0.8,0  
 1AIL,ASP\_34,3.1,0.42,-1.12,0  
 2DG7,GLU\_99,4.16,0.14,-0.48,0  
 3EUR,ASP\_77,3.76,0,-0.04,0  
 3HKX,TYR\_270,10,0,0,0  
 2Z0M,ARG\_102,12.15,-0.35,0,0  
 3O16,GLU\_226,4.57,0.07,0,0  
 3EVN,HIS\_51,7.27,0.84,0,-0.07  
 3V4G,LYS\_15,10.29,-0.21,0,0  
 4ECC,ASP\_36,3.19,0.07,-0.68,0  
 3LH5,ARG\_748,11.87,-0.63,0,0  
 2CWY,ARG\_52,12.08,-0.42,0,0  
 1DZF,ARG\_192,12.5,0,0,0  
 1KCM,LYS\_202,10.43,-0.07,0,0  
 2H80,ARG\_89,9.67,-3.19,0,0.36  
 2DVK,ARG\_128,12.08,-0.42,0,0  
 1LTU,GLU\_184,5.27,4.2,-1.62,-1.81  
 1WNH,ARG\_48,12.29,-0.21,0,0  
 2OSA,GLU\_408,4.26,0.35,-0.59,0  
 3MTT,LYS\_500,10.5,0,0,0  
 2F19,ASP\_48,3.8,0,0,0  
 1TLV,HIS\_220,6.31,0.02,0,-0.21  
 2XHC,GLU\_20,4.85,0.35,0,0  
 2OGQ,ARG\_456,12.5,0,0,0  
 1D2K,TYR\_230,11.33,0.14,0,1.19  
 2VGM,LYS\_138,10.65,0,0.65  
 1YM5,ASP\_129,4.01,0.21,0,0  
 3LJC,TYR\_116,11.45,0,1.45  
 3FK5,LYS\_316,9.87,-0.63,0,0  
 3Q1C,TYR\_367,12.64,3.44,-0.8,0  
 1IDK,ASP\_331,3.85,0.07,-0.02,0  
 1J79,TYR\_86,10.68,0,0.68  
 3ZXY,CYS\_81,7.88,-2.78,0,1.66  
 2PLQ,CYS\_246,9.75,-0.34,0,1.09  
 2ZCX,ARG\_193,12.08,-0.42,0,0  
 3VJ8,GLU\_123,4.46,0.35,-0.39,0  
 3JZ9,ARG\_453,12.5,0,0,0  
 1XTZ,HIS\_260,6.66,0.23,0,-0.07  
 1PBV,TYR\_114,10.94,0.94,0,0  
 4F85,ARG\_116,12.15,-0.35,0,0  
 3L3P,ARG\_306,12.01,-0.49,0,0  
 1Q46,ASP\_163,3.87,0.07,0,0  
 3N2T,LYS\_200,10.43,-0.07,0,0  
 1XZ7,HIS\_260,6.66,0.23,0,-0.07  
 2H85,LYS\_204,10.5,0,0,0  
 3EVN,HIS\_93,3.9,0.48,0,-3.08  
 2P1W,HIS\_88,2.8,0.8,-2.34,-2.16  
 2RFA,GLU\_113,4.5,0,0,0  
 4EQU,HIS\_358,6.5,0,0,0  
 1W7B,ARG\_284,11.59,-0.91,0,0  
 1EQ6,GLU\_190,4.3,0.21,-0.41,0  
 3NR5,TYR\_121,12.74,0.46,0.2,28  
 3UPD,ARG\_248,13.2,-0.62,0,1.32  
 1N81,LYS\_37,10.36,-0.14,0,0  
 2CL3,TYR\_208,13.41,0.21,0.8,2.4  
 2F8H,HIS\_6,6.45,0.02,0,-0.07  
 3BCH,ARG\_205,12.15,-0.35,0,0  
 2YX0,ARG\_184,10.49,-2.17,0,0.16  
 3CAX,LYS\_285,10.08,-0.42,0,0  
 3F6F,ASP\_27,2.63,0.07,-1.24,0  
 3PM2,ASP\_73,2.89,0.49,-1.41,0  
 1W7B,LYS\_80,10.5,0,0,0  
 3U2R,ARG\_78,12.5,0,0,0  
 3H6Q,ASP\_72,0.37,0.7,-4.12,0  
 1SQW,TYR\_45,10,0,0,0  
 2RJD,GLU\_209,4.41,0,-0.09,0  
 2H14,LYS\_162,10.5,0,0,0  
 1OLR,ARG\_217,12.43,-0.07,0,0  
 3U0V,HIS\_90,6.43,0,0,-0.07  
 3IL3,GLU\_195,4.57,0.07,0,0  
 3R87,HIS\_37,6.43,0,0,-0.07  
 3G65,TYR\_78,9.97,0.21,-0.24,0  
 1Q5Z,GLU\_616,4.5,0,0,0  
 3ULX,ARG\_76,12.62,-0.35,0.0,47  
 2QVT,HIS\_129,2.97,0.05,0,-3.58  
 1EDG,ASP\_188,3.84,0.14,-0.1,0  
 2B0J,LYS\_209,11.14,-0.21,0,0.85  
 1J7G,ASP\_57,2.27,1.12,-2.64,0



1NIJ,GLU\_27,4.85,0.35,0,0  
2P5D,LYS\_22,10.43,-0.07,0,0  
15NT,ASP\_60,3.05,0.7,-1.45,0  
4HDE,LYS\_58,10.43,-0.07,0,0  
3N2T,GLU\_258,4.64,0.14,0,0  
3HUE,LYS\_94,10.36,-0.14,0,0  
1SI7,ARG\_299,8.69,-3.81,0,0  
2HRZ,ARG\_294,12.5,0,0,0  
3JZN,ASP\_421,1.35,0.49,-2.94,0  
3CIV,LYS\_276,10.08,-0.42,0,0  
3RKV,ASP\_294,3.59,0.07,-0.28,0  
1QQE,LYS\_13,10.5,0,0,0  
3QAV,LYS\_135,10.01,-0.49,0,0  
3BB7,ARG\_149,11.87,-0.63,0,0  
3IV4,ASP\_9,3.79,0,-0.01,0  
3ULX,ASP\_158,3.6,0.21,-0.41,0  
3GVW,TYR\_276,10.27,0.14,-0.86,0.98  
1RWZ,ARG\_16,12.08,-0.42,0,0  
1YM5,ASP\_65,3.04,0.42,-1.17,0  
3O16,TYR\_154,10.03,0.07,-0.04,0  
3LJC,ARG\_192,10.15,-1.76,0,-0.59  
2H85,ARG\_61,12.71,-1.59,0,1.8  
1R7J,ASP\_81,3.92,0.21,-0.09,0  
1MD6,GLU\_80,4.78,0.28,0,0  
2E3C,HIS\_432,2.14,0,-1.68,-2.68  
1MUF,TYR\_110,12.29,0.14,-0.25,2.4  
2GZR,ARG\_296,11.7,-0.8,0,0  
2P52,TYR\_202,11.26,1.02,-1.12,1.37  
3H6Q,ARG\_95,12.29,-0.21,0,0  
3DZ1,ASP\_132,2.57,0.42,-1.66,0  
2O8P,GLU\_22,4.05,0.35,-0.8,0  
3GS3,ASP\_164,3.87,0.07,0,0  
3R1X,LYS\_33,10.43,-0.07,0,0  
2R2Y,GLU\_111,3.53,0.56,-1.53,0  
2X4G,CYS\_112,10.85,-0.06,0.191  
3GFP,GLU\_314,4.57,0.07,0,0  
1WYC,GLU\_228,5.6,2.97,-1.87,0  
3ASA,LYS\_375,10.43,-0.07,0,0  
2GAU,ARG\_143,12.08,-0.42,0,0  
1MTZ,LYS\_11,10.5,0,0,0  
2H85,GLU\_56,2.14,1.16,-1.12,-2.4  
2Q99,LYS\_229,10.5,0,0,0  
2H30,ARG\_170,12.22,-0.28,0,0  
1PSW,GLU\_347,4.57,0.07,0,0  
2P1W,TYR\_158,11.55,0.77,0,0.78  
2JKF,GLU\_57,4.5,0,0,0  
2AH5,LYS\_177,10.22,-0.28,0,0  
2OEW,LYS\_334,10.29,-0.21,0,0  
1KCM,LYS\_31,10.5,0,0,0  
1UCH,LYS\_61,10.43,-0.07,0,0  
4ETX,GLU\_173,4.71,0.21,0,0  
3FHF,GLU\_35,3.13,0.49,-1.86,0  
3JZ9,LYS\_476,10.29,-0.21,0,0  
3U2R,GLU\_125,4.29,0.14,-0.35,0  
1EV8,TYR\_252,10.44,0.44,0,0  
1LN4,LYS\_92,10.36,-0.14,0,0  
1N81,ARG\_74,12.01,-0.49,0,0  
1PVT,GLU\_22,4.5,0,0,0  
1RIS,LYS\_42,10.5,0,0,0  
1GXN,ARG\_346,11.59,-0.91,0,0  
4ANN,GLU\_173,4.78,0.28,0,0  
1YB2,ASP\_234,3.8,0.49,-0.49,0  
1RZ2,LYS\_69,10.43,-0.07,0,0  
1DZF,ARG\_162,12.5,0,0,0  
2R2Y,ASP\_78,3.94,0.14,0,0  
2CE6,ARG\_67,11.87,-0.63,0,0  
1RAJ,ARG\_456,12.43,-0.07,0,0  
1ZBP,LYS\_25,10.5,0,0,0  
2QV2,LYS\_142,10.5,0,0,0

2RJD,GLU\_213,4.5,0,0,0  
1J33,ARG\_202,11.94,-0.56,0,0  
1BYI,LYS\_148,10.08,-0.42,0,0  
4GCO,TYR\_159,9.97,0,-0.03,0  
2FD5,LYS\_94,10.22,-0.28,0,0  
1MUF,ASP\_259,3.95,0.42,-0.27,0  
2CBE,HIS\_122,1.63,0.95,0,-5.82  
2FPN,LYS\_70,10.5,0,0,0  
3M66,HIS\_213,6.56,0.48,0,-0.42  
1RHS,ASP\_219,3.91,0.14,-0.03,0  
4E6S,HIS\_36,6.29,0,0,-0.21  
1O59,ARG\_270,12.08,-0.42,0,0  
3HUE,LYS\_104,10.43,-0.07,0,0  
3AU3,CYS\_417,11.42,0.13,1.12  
3UPD,LYS\_271,10.36,-0.14,0,0  
2B61,ASP\_353,3.0,49,-1.3,0  
2FPN,GLU\_96,4.63,0.57,-0.44,0  
1CBY,HIS\_163,6.54,0.04,0,0  
2JEO,ASP\_90,3.89,0.14,-0.05,0  
1NJ4,LYS\_339,10.5,0,0,0  
1MD6,LYS\_37,10.5,0,0,0  
2P4D,TYR\_39,10,0,0,0  
3UPD,CYS\_203,10.18,-0.03,0,1.21  
1XDZ,ARG\_151,12.08,-0.42,0,0  
1YTD,LYS\_383,10.43,-0.07,0,0  
3IOC,HIS\_233,3.17,0,0,-3.33  
2OBI,TYR\_153,13.96,0.76,0.8,2.4  
1OIS,LYS\_149,9.8,-0.7,0,0  
1T3J,HIS\_690,6.43,0,0,-0.07  
3C2E,TYR\_4,10,0,0,0  
3LOD,ASP\_6,3.7,0.14,-0.24,0  
3F6F,TYR\_99,10,0,0,0  
1MD6,TYR\_19,13.34,0.14,0.8,2.4  
2V81,ARG\_96,11.73,-0.77,0,0  
1TWU,GLU\_105,3.84,0.14,-0.8,0  
2O0K,LYS\_83,10.29,-0.21,0,0  
3H04,HIS\_36,3.22,1.06,1.06,-5.4  
1TUL,ASP\_26,2.82,0.63,-1.61,0  
1G5Z,CYS\_129,8.94,-0.23,0.17  
2IXM,LYS\_296,10.43,-0.07,0,0  
3LJC,GLU\_232,4.43,0.21,-0.28,0  
3PU6,GLU\_32,3.87,0.14,-0.77,0  
3KB5,HIS\_458,6.15,0,0,-0.35  
1PZC,LYS\_77,10.36,-0.14,0,0  
1P4X,ARG\_214,12.5,0,0,0  
1ZBP,GLU\_52,4.5,0,0,0  
3O48,TYR\_93,10.07,0.07,0,0  
3O48,GLU\_58,4.54,0.49,-0.45,0  
1GXN,GLU\_553,3.32,0.42,-1.6,0  
2CXV,LYS\_68,10.15,-0.35,0,0  
1FKM,ASP\_402,3.81,0.14,-0.13,0  
1RHS,LYS\_292,10.5,0,0,0  
3M70,GLU\_4,4.5,0,0,0  
2ZCO,LYS\_221,10.29,-0.21,0,0  
2BAA,LYS\_87,10.15,-0.35,0,0  
2C13,TYR\_160,13.1,0.07,0.63,2.4  
2EEY,ASP\_130,3.94,0.14,0,0  
2INO,HIS\_73,1.97,1.05,-1.08,-4.5  
2FD5,GLU\_137,3.97,0.14,-0.67,0  
1XFK,CYS\_31,9,0,0,0  
1XIPL,LYS\_33,10.5,0,0,0  
2G5S,LYS\_126,10.43,-0.07,0,0  
1W7B,LYS\_308,10.29,-0.21,0,0  
1BYI,GLU\_115,5.03,3.48,-1.6,-1.35  
1DVO,LYS\_46,10.29,-0.21,0,0  
1YR6,ARG\_51,11.73,-0.77,0,0  
2Z14,GLU\_25,4.57,0.07,0,0  
2F4Q,LYS\_265,10.5,0,0,0  
1GQE,HIS\_265,6.29,0,0,-0.21

3OOP,LYS\_18,10.5,0,0,0  
2Z14,GLU\_24,3.41,0.28,-1.37,0  
2ILR,GLU\_443,4.5,0,0,0  
3CQ1,GLU\_16,4.78,0.28,0,0  
2OEW,ARG\_51,12.08,-0.42,0,0  
1Q5Z,LYS\_599,10.36,-0.14,0,0  
1KCM,LYS\_219,10.43,-0.07,0,0  
3H04,TYR\_178,12.18,0.14,0,2.04  
3CBN,TYR\_96,12.15,0.3,1.85  
3FHF,LYS\_100,10.5,0,0,0  
1QQH,TYR\_169,9.79,1.71,-1.92,0  
3HYQ,ASP\_43,3.87,0.07,0,0  
1SFE,HIS\_70,7.09,0.8,0,-0.21  
2CWC,ARG\_11,12.71,-2.09,0,2.3  
1P4X,ASP\_212,3.23,0.56,-1.14,0  
1RAJ,ASP\_455,3.74,0.07,-0.13,0  
1CHD,HIS\_233,2.87,0,0,-3.63  
3CS1,LYS\_25,10.5,0,0,0  
2YT4,HIS\_625,6.43,0,0,-0.07  
3GMS,LYS\_277,10.29,-0.21,0,0  
2FZ4,ARG\_60,11.8,-0.7,0,0  
1YB2,GLU\_165,5.29,1.88,-1.09,0  
2QK1,ASP\_411,3.8,0,0,0  
3R1X,GLU\_98,4.5,0,0,0  
3BZT,GLU\_276,3.98,0.28,-0.8,0  
3MEW,LYS\_200,10.5,0,0,0  
3R87,HIS\_18,6.5,0,0,0  
3IVF,LYS\_272,10.5,0,0,0  
1H4U,GLU\_448,3.03,0.28,-1.75,0  
3EVZ,TYR\_203,5.83,1.35,-1.31,-4.21  
2JHY,TYR\_149,10.07,0.07,0,0  
1K95,ASP\_208,3.87,0.07,0,0  
3D9H,HIS\_139,2.51,1.7,-1.13,-4.55  
3LJC,LYS\_211,10.43,-0.07,0,0  
4ETX,CYS\_343,7.7,-2.62,0,1.33  
2Q07,ARG\_439,12.36,-0.14,0,0  
4FZN,GLU\_92,1.57,1.49,-2.16,-2.26  
1RZ2,LYS\_100,10.5,0,0,0  
3UPD,CYS\_62,8.55,-0.52,0.07  
3VJ8,ARG\_367,12.01,-0.49,0,0  
1U74,LYS\_133,10.29,-0.21,0,0  
2O8I,ARG\_24,12.01,-0.49,0,0  
1ZKZ,TYR\_97,10,0,0,0  
1SI7,ARG\_71,12.15,-0.35,0,0  
1J33,ARG\_119,11.66,-0.84,0,0  
1RZ2,GLU\_201,3.04,0.42,-1.88,0  
2WOZ,TYR\_450,10.48,0.48,0,0  
2NMU,TYR\_56,10,0,0,0  
2QVT,GLU\_78,4.5,0,0,0  
1Y2Q,ARG\_34,11.87,-0.63,0,0  
2ILR,GLU\_449,3.89,0.35,-0.96,0  
1Y2Q,LYS\_90,10.5,0,0,0  
1TWU,GLU\_90,4.71,0.21,0,0  
3Q1C,ASP\_165,2.19,0.56,-2.18,0  
2ILR,GLU\_427,4.5,0,0,0  
3F53,HIS\_115,6.43,0,0,-0.07  
1Y2Q,ARG\_137,12.08,-0.42,0,0  
2OJQ,ARG\_475,12.5,0,0,0  
1Z3X,TYR\_38,10.03,0.07,-0.04,0  
2I88,LYS\_381,9.87,-0.63,0,0  
2Q13,LYS\_153,10.5,0,0,0  
3IOC,TYR\_246,11.07,1.33,-0.56,0.3  
3M16,TYR\_202,9.24,0.14,-0.9,0  
2W2S,GLU\_134,4.28,0.91,-1.13,0  
1Q5Z,LYS\_601,10.15,-0.35,0,0  
2FGG,ARG\_44,12.29,-0.21,0,0  
4AE7,TYR\_55,10.07,0.07,0,0  
3IVF,CYS\_336,8.39,-1.03,0,0.41  
3IL3,GLU\_258,4.64,0.14,0,0

3IOC,ARG\_217,12.01,-0.49,0,0  
2QOP,LYS\_39,10.5,0,0,0  
3BPV,LYS\_49,10.36,-0.14,0,0  
2WOZ,ARG\_597,12.15,-0.35,0,0  
1QQL,GLU\_45,4.57,0.07,0,0  
2D59,HIS\_48,7.1,0.88,0,-0.28  
1R16,ARG\_112,12.29,-0.21,0,0  
2ZQ5,ARG\_344,12.22,-0.28,0,0  
3JZN,TYR\_154,10,0,0,0  
2H2Z,ARG\_105,12.52,-1.19,0,1.21  
3P28,LYS\_53,10.29,-0.21,0,0  
1WPA,ARG\_483,12.01,-0.49,0,0  
1AKO,ARG\_12,12.15,-0.35,0,0  
1DUP,CYS\_36,8.62,-0.38,0,0  
3CBN,GLU\_93,4.24,0.42,-0.68,0  
3UPD,HIS\_-20,6.5,0,0,0  
3UPD,HIS\_431,2.3,0.56,-2.06,0  
3UC9,ASP\_63,4.22,0.42,0,0  
2VAN,ASP\_124,1.08,0.63,-3.35,0  
2GKG,HIS\_98,7.38,0.88,0,0  
3ZXY,LYS\_246,10.43,-0.07,0,0  
2Q13,GLU\_165,4.63,0.42,-0.29,0  
1YW5,GLU\_23,3.66,0.14,-0.98,0  
1V8E,ASP\_68,1.86,0.49,-2.43,0  
3ZSL,TYR\_221,12.02,1.34,-1.16,1.84  
3MTT,ARG\_469,12.01,-0.49,0,0  
2B78,ASP\_287,1.67,0.42,-2.55,0  
3GE9,HIS\_134,6.5,0,0,0  
3LJH,HIS\_272,6.36,0,0,-0.14  
1MTZ,LYS\_228,10.43,-0.07,0,0  
4EKU,GLU\_124,4.5,0,0,0  
2HNG,GLU\_12,3.5,0.14,-1.14,0  
4ANN,ASP\_68,4.01,0.21,0,0  
3MIX,ARG\_487,12.08,-0.42,0,0  
1N81,GLU\_167,4.29,3.08,-1.81,0  
3N2T,ASP\_251,3.79,0.14,-0.15,0  
1XIPL,LYS\_155,10.5,0,0,0  
4FLE,TYR\_103,10,0,0,0  
3M70,GLU\_165,2.8,0.7,-2.4,0  
2C13,ARG\_18,13.22,-1.27,0,1.99  
1SIQH,CYS\_132,9.05,-0.59,0.63  
3CO1,HIS\_73,7.37,1.01,0,-0.14  
3M3P,HIS\_249,6.96,0.46,0,0  
3UPD,TYR\_36,13.41,0.21,0.8,2.4  
3ZXY,ASP\_14,3.09,0.49,-1.21,0  
1P6F,ASP\_126,3.26,0.14,-0.68,0  
2CYG,GLU\_264,4.29,3.08,-1.81,-1.48  
2B61,ASP\_242,3.45,0.49,-0.84,0  
2POY,HIS\_275,6.36,0,0,-0.14  
3EOD,CYS\_57,10.95,0,1.95  
2Q99,ASP\_162,3.18,0.21,-0.8,-0.03  
2CBE,ASP\_19,3.87,0.07,0,0  
1WJG,TYR\_118,9.39,0,-0.61,0  
3F7M,ASP\_130,1.92,0.42,-2.29,0  
2FGG,GLU\_18,4.0,0.14,-0.64,0  
2FB6,LYS\_16,10.22,-0.28,0,0  
3BPV,ARG\_86,12.15,-0.35,0,0  
2IXM,GLU\_114,4.5,0,0,0  
3T5B,CYS\_153,8.52,-0.99,0,0.51  
1NKD,GLU\_28,4.78,0.28,0,0  
3LQE,GLU\_356,4.64,0.14,0,0  
1P6F,TYR\_79,10.35,0.35,0,0  
2IXM,TYR\_232,11.11,0.07,0,1.04  
1YR6,ARG\_191,12.36,-0.14,0,0  
2V5B,ARG\_196,12.15,-0.35,0,0  
2CYG,ASP\_86,3.73,0.49,-0.55,0  
2Q99,ARG\_69,11.94,-0.56,0,0  
4AE7,LYS\_89,10.5,0,0,0  
2AD1,LYS\_38,10.29,-0.21,0,0

1SQH,GLU\_117,4.19,0.49,-0.8,0  
2BQQ,CYS\_127,11.09,0,0,2.09  
2F8H,ASP\_256,2.94,0.07,-0.93,0  
3PM2,ARG\_52,11.59,-0.91,0,0  
1ZBS,ASP\_208,3.38,0.49,-0.91,0  
2ZQ5,ARG\_380,11.8,-0.7,0,0  
2HRZ,CYS\_166,8.92,-1.44,-0.65,2.01  
1P4X,LYS\_152,10.36,-0.14,0,0  
3EIZ,ASP\_126,2.39,0.49,-1.9,0  
2YWK,TYR\_27,9.76,0,-0.24,0  
3PAC,LYS\_93,10.43,-0.07,0,0  
2Q12,LYS\_212,10.5,0,0,0  
1EV8,ARG\_243,12.15,-0.35,0,0  
1XTZ,LYS\_22,9.65,-0.35,0,-0.5  
1TLV,CYS\_242,9.75,0,0,0.75  
1SQH,HIS\_188,7.47,0.97,0,0  
2OOK,ARG\_144,13.05,-1.13,0,1.68  
2E3S,CYS\_518,8.82,-0.18,0,0  
1L3K,HIS\_156,8.85,1.72,3.35,-2.73  
3ASA,HIS\_324,3.87,0.05,0.36,-3.04  
4F8A,HIS\_670,4.41,0.62,0,-2.71  
4DEZ,LYS\_193,10.15,-0.35,0,0  
2E3C,ARG\_442,12.43,-0.07,0,0  
3NR5,LYS\_44,9.87,-0.63,0,0  
1NWA,HIS\_0,6.29,0,0,-0.21  
2VAN,ASP\_160,3.85,0.07,-0.02,0  
4ANN,GLU\_34,4.08,0.21,-0.63,0  
1MIX,GLU\_237,4.62,0.63,-0.51,0  
1TJE,TYR\_14,12.99,0.14,0.45,2.4  
1WP5,ASP\_206,2.92,0.35,-1.23,0  
2AHE,ASP\_87,2.65,0.42,-1.57,0  
3CO1,ASP\_120,1.93,0.56,-2.43,0  
1EV8,HIS\_186,3.7,0,0,-2.8  
1GPP,TYR\_432,11.81,0,0,1.82  
2WOG,ARG\_166,11.94,-0.56,0,0  
3CAN,LYS\_158,10.29,-0.21,0,0  
3GW3,GLU\_218,6.93,4.18,-1.76,0  
2RH3,ARG\_89,12.36,-0.14,0,0  
4FZR,ASP\_98,3.81,0.07,-0.06,0  
2Q34,TYR\_70,10.77,0.07,-0.25,0.95  
1F09,LYS\_374,10.5,0,0,0  
3FRR,LYS\_48,10.36,-0.14,0,0  
3G9T,ASP\_264,3.35,0,-0.45,0  
3ASA,HIS\_299,6.5,0,0,0  
1N81,LYS\_120,10.5,0,0,0  
2X5Y,GLU\_780,2.53,0.35,-2.32,0  
1TR9,ASP\_214,2.25,0.49,-2.04,0  
1O17,GLU\_267,4.21,0.21,-0.5,0  
2P1W,HIS\_32,6.22,0,0,-0.28  
3DHN,GLU\_195,2.99,0.77,-2.29,0  
3M70,LYS\_123,10.01,-0.49,0,0  
4E8B,LYS\_126,10.43,-0.07,0,0  
3E0H,ASP\_41,3.34,0.21,-0.67,0  
1ZBS,CYS\_168,9,0,0,0  
2B61,LYS\_286,10.43,-0.07,0,0  
3BWT,HIS\_719,6.3,0.08,0,-0.28  
2Q07,LYS\_484,10.5,0,0,0  
2V4U,ARG\_311,11.66,-0.84,0,0  
3G9T,HIS\_274,2.89,0.04,0,-3.65  
4FLE,HIS\_122,6.52,0.23,0,-0.21  
3B21,HIS\_98,4.66,0.27,0,-2.11  
1ZYL,LYS\_171,9.8,-0.7,0,0  
2QHT,HIS\_41,0.86,0.01,-1.04,-4.6  
1ZBS,CYS\_114,11.53,0,0,2.53  
3H04,ASP\_76,2.75,0.42,-1.47,0  
2RFA,ARG\_262,11.94,-0.56,0,0  
2E3S,ARG\_517,12.22,-0.28,0,0  
2YWX,GLU\_9,4.5,0,0,0  
3KTR,HIS\_21,7.42,1.13,0,-0.21  
1W24,GLU\_65,4.71,0.21,0,0  
2R4Q,CYS\_178,2.6,-6.61,0,0.21  
1SUU,LYS\_748,10.5,0,0,0  
2Q5X,TYR\_755,10,0,0,0  
1WYC,ASP\_285,2.03,0.63,-2.4,0  
3DB9,ASP\_49,3.55,0.42,-0.67,0  
2O0K,LYS\_46,10.29,-0.21,0,0  
2WB3,ASP\_344,3.94,0.14,0,0  
1XKR,HIS\_0,7.1,0.6,0,0  
2VGM,GLU\_286,3.86,0.14,-0.78,0  
2IF4,ARG\_182,12.08,-0.42,0,0  
1RHS,HIS\_255,1.13,0.3,0,-5.67  
3U2A,ASP\_68,0.93,0.7,-3.57,0  
2ZQ5,ARG\_213,12.07,-0.56,0,0.13  
2EFK,LYS\_215,10.29,-0.21,0,0  
1ZCU,ASP\_177,3.44,0.63,-0.99,0  
1YR6,GLU\_62,2.52,0.42,-2.4,0  
3A2Z,ASP\_181,3.87,0.07,0,0  
3O48,ASP\_67,3.83,0.07,-0.04,0  
1MTZ,HIS\_42,3.44,1.6,0.29,-4.95  
3LD1,TYR\_341,9.87,0,-0.13,0  
3F7M,ASP\_269,2.99,0.35,-1.16,0  
3N2T,HIS\_63,6.78,1.99,0.85,-2.56  
1QQE,CYS\_86,8.92,-0.52,0.18,0.26  
1D2K,TYR\_196,11.66,0.53,-0.68,1.81  
3RNV,ARG\_369,11.87,-0.63,0,0  
2RIS,GLU\_13,4.62,0.21,-0.09,0  
2Q07,ARG\_354,12.08,-0.42,0,0  
3HZQ,GLU\_55,4.39,0,-0.11,0  
3IVF,ASP\_208,2.86,0.28,-1.22,0  
2EA9,ASP\_18,4.01,0.21,0,0  
3KEY,ARG\_312,11.94,-0.56,0,0  
2VGM,TYR\_192,10.42,0.42,0,0  
3OAT,ARG\_439,12.15,-0.35,0,0  
1PBV,GLU\_54,4.5,0,0,0  
4GA2,ARG\_64,11.94,-0.56,0,0  
1UXO,GLU\_82,3.2,0.63,-1.93,0  
1O59,ARG\_183,11.09,-1.41,0,0  
1PDB,LYS\_80,10.5,0,0,0  
3FHF,GLU\_72,3.68,0.35,-1.17,0  
2B6P,ARG\_152,10.96,-1.54,0,0  
2JKF,ASP\_58,4.03,0.49,-0.26,0  
2FGG,GLU\_5,4.57,0.07,0,0  
1PSW,ASP\_141,3.62,0,-0.18,0  
2Z84,CYS\_43,6.85,-3.09,-0.27,1.21  
2CBE,ASP\_139,2.58,0.49,-1.71,0  
2VAN,ARG\_183,11.31,-1.19,0,0  
2B0J,TYR\_11,12.6,2.08,-0.76,1.27  
2C13,LYS\_110,10.36,-0.14,0,0  
3J5N,HIS\_75,3.9,0.67,0.6,-3.87  
2ILR,ASP\_286,3.79,0.14,-0.15,0  
4E5S,GLU\_123,4.57,0.07,0,0  
3F5D,TYR\_14,10.22,0.07,-0.8,0.95  
3UAH,ARG\_374,11.28,-2.67,0,1.45  
1J74,GLU\_36,4.45,0.42,-0.47,0  
1HF8,TYR\_237,10.31,0.21,-0.16,0.26  
2EFK,GLU\_185,4.6,0.07,0.03,0  
2B61,ASP\_59,2.3,0.63,-2.13,0  
2ZCO,ASP\_253,3.12,0.07,-0.75,0  
2ILR,ARG\_381,12.22,-0.28,0,0  
2O0K,TYR\_295,10.11,0,0,0.11  
1AK1,ASP\_241,3.14,0.14,-0.8,0  
3HUE,TYR\_180,10.81,0.95,-0.14,0  
1T95,LYS\_59,10.43,-0.07,0,0  
1NWA,ARG\_166,11.73,-0.77,0,0  
2NSN,CYS\_39,8.77,-0.23,0,0  
2H85,CYS\_116,8.47,-0.53,0,0  
1YTD,ARG\_94,11.82,-2.77,0,2.08  
2O0K,ARG\_245,12.5,0,0,0  
3I0O,GLU\_140,4.5,0,0,0  
3L7N,GLU\_185,3.6,0.14,-1.04,0  
2CN1,HIS\_198,2.49,0,0,-4.01  
2YXO,ARG\_319,11.87,-0.63,0,0  
2B0A,LYS\_80,10.5,0,0,0  
2AD1,HIS\_203,7.21,0.71,0,0  
2YWJ,TYR\_178,11.29,0.44,-0.03,0.88  
1VSM,ARG\_132,12.22,-0.28,0,0  
1QQE,HIS\_132,7.02,0.66,0,-0.14  
1R16,GLU\_270,3.25,0.35,-1.6,0  
3MIX,ARG\_387,11.87,-0.63,0,0  
2B3M,LYS\_75,10.5,0,0,0  
3C5V,CYS\_347,11.85,-0.91,2.4,1.36  
1YG2,GLU\_49,4.5,0,0,0  
1M5I,LYS\_150,10.5,0,0,0  
1ZBP,LYS\_262,9.87,-0.63,0,0  
2AD1,LYS\_178,10.36,-0.14,0,0  
3O16,LYS\_138,10.5,0,0,0  
3DHN,HIS\_224,6.61,0.11,0,0  
1DUN,LYS\_10,10.5,0,0,0  
3HVW,TYR\_240,13.72,0.52,0.8,2.4  
2GZQ,LYS\_125,10.36,-0.14,0,0  
3QKY,TYR\_119,13.41,0.21,0.8,2.4  
3M7D,CYS\_68,12.13,-0.37,0.3,5.1  
3CCY,ARG\_150,12.29,-0.21,0,0  
2V4U,LYS\_466,10.36,-0.14,0,0  
2FG1,GLU\_142,2.71,0.49,-2.29,0  
1O59,LYS\_21,10.08,-0.42,0,0  
4FH3,ASP\_258,4.08,0.28,0,0  
2FL7,LYS\_97,10.22,-0.28,0,0  
1NAR,LYS\_236,10.29,-0.21,0,0  
1O17,TYR\_158,11.2,1.2,0,0  
3ZTA,LYS\_124,10.29,-0.21,0,0  
2H85,ASP\_202,3.55,0.28,-0.53,0  
1WXQ,TYR\_124,11.64,0.14,-0.72,2.22  
2ILR,LYS\_296,10.29,-0.21,0,0  
2B0J,LYS\_58,10.29,-0.21,0,0  
1E55,LYS\_186,10.43,-0.07,0,0  
3M7G,GLU\_122,4.25,0.77,-1.02,0  
4DEZ,ASP\_177,3.86,0.07,-0.01,0  
1L2F,LYS\_223,10.36,-0.14,0,0  
3FWU,ARG\_28,11.73,-0.77,0,0  
1D2K,LYS\_138,10.36,-0.14,0,0  
1S1Y,TYR\_145,11.26,0.91,-0.29,0.64  
1OGL,ARG\_93,13,-0.65,0,1.15  
2VGM,LYS\_237,10.5,0,0,0  
3DTE,ARG\_238,11.73,-0.77,0,0  
3OIP,GLU\_48,4.5,0,0,0  
3CAN,CYS\_13,8.79,-0.21,0,0  
2P5D,GLU\_21,4.37,0.07,-0.2,0  
2WOZ,TYR\_8,9.78,0.14,-0.36,0  
2WOZ,ASP\_407,2.08,0.63,-2.35,0  
1OST,HIS\_140,3.42,0.89,0,-3.97  
3RLE,HIS\_29,6.43,0,0,-0.07  
2B78,ARG\_24,12.5,0,0,0  
3LPZ,TYR\_203,9.56,1.49,-1.79,-0.14  
1WLY,GLU\_284,4.5,0,0,0  
1FOV,ARG\_131,11.43,-1.07,0,0  
4EVF,LYS\_59,10.5,0,0,0  
2O8P,TYR\_94,10,0,0,0  
2AXO,LYS\_70,10.5,0,0,0  
4E9E,GLU\_522,3.83,0.42,-1.09,0  
3UPD,HIS\_274,5.15,1.6,2.88,-5.83  
2EJB,ARG\_83,11.45,-1.05,0,0  
2X14,ARG\_258,12.5,0,0,0  
2CE6,LYS\_87,9.73,-0.77,0,0  
1H4U,ARG\_617,12.43,-0.07,0,0  
2HRZ,GLU\_223,4.25,0.14,-0.39,0  
2ZOM,ASP\_148,3.37,0.14,-0.56,0  
1W7B,LYS\_115,10.22,-0.28,0,0  
3A0X,GLU\_640,4.5,0,0,0  
3VHU,ASP\_141,3.09,0.35,-1.05,0  
2F4Q,LYS\_122,9.8,-0.7,0,0  
1YTQ,LYS\_29,7.04,0.68,0,-0.14  
3KB5,ASP\_421,3.12,0.14,-0.82,0  
2H2Z,CYS\_38,11.29,-0.53,0.2,82  
3EGN,TYR\_489,13.01,0.14,0.61,2.26  
3IL3,ASP\_102,3.21,0.21,-0.8,0  
1ZCU,ASP\_61,3.66,0.63,-0.76,0  
2Q12,ASP\_109,3.87,0.35,-0.28,0  
1WYC,TYR\_140,10.66,0.07,-1.12,1.71  
1XFK,HIS\_195,3.98,0.66,0,-3.18  
3M70,ASP\_228,3.8,0,0,0  
4DBX,ARG\_265,12.01,-0.49,0,0  
1YR6,GLU\_57,3.36,0,-1.14,0  
3ADO,LYS\_249,3.73,0.14,-0.91,0  
1W24,LYS\_127,10.43,-0.07,0,0  
2YWK,ARG\_78,12.01,-0.49,0,0  
3V3T,CYS\_143,11.21,0,-0.33,2.54  
4ECC,ARG\_102,11.66,-0.84,0,0  
4DNU,GLU\_224,2.45,0.35,-2.4,0  
1C44,LYS\_38,10.5,0,0,0  
3LD1,CYS\_362,9,0,0,0  
3L7N,GLU\_211,4.5,0,0,0  
3BWT,HIS\_779,6.59,0.09,0,0  
1V43,ARG\_233,12.22,-0.28,0,0  
4FH3,TYR\_221,10.57,1.33,0,-0.76  
3U2A,GLU\_100,12.08,-0.42,0,0  
4DBX,TYR\_282,10.55,0.35,0,0.2  
1S18,GLU\_542,4.5,0,0,0  
2P4D,ARG\_102,12.29,-0.21,0,0  
2DVK,LYS\_33,10.43,-0.07,0,0  
2XHC,TYR\_114,8.98,0.85,0,-1.87  
1RHZ,LYS\_165,10.5,0,0,0  
1JYH,TYR\_143,13.27,0,0,3.27  
1TD6,CYS\_67,11.01,-0.21,0,2.22  
1GQE,ARG\_52,12.08,-0.42,0,0  
2OJQ,GLU\_651,4.15,0.07,-0.42,0  
2XHC,LYS\_205,10.5,0,0,0  
1P4X,GLU\_160,3.02,0.56,-2.04,0  
1Z9L,ASP\_112,3.41,0.7,-1.08,0  
3CZC,ASP\_52,2.82,0.42,-1.4,0  
2H2Z,ARG\_298,12.2,-0.95,0.0,65  
3Q6L,CYS\_118,10.8,0,-0.28,2.08  
3ONT,GLU\_110,3.98,0.28,-0.8,0  
1ILW,ASP\_84,4.01,0.21,0,0  
3LJN,GLU\_239,4.57,0.07,0,0  
1WXQ,CYS\_50,8,-1.07,0,0.07  
1PGV,ARG\_332,12.29,-0.21,0,0  
1VJG,ASP\_133,1.68,0.7,-2.82,0  
3HVW,GLU\_258,4.64,0.14,0,0  
2AD1,LYS\_283,10.43,-0.07,0,0  
3HNX,GLU\_57,4.78,0.28,0,0  
3BQW,GLU\_302,2.38,0.28,-2.4,0  
3PP8,ASP\_241,3.25,0.35,-0.9,0  
1JKS,GLU\_64,4.82,2.82,-0.84,-1.66  
1V8E,ARG\_185,11.94,-0.56,0,0  
3CAN,CYS\_170,9.5,-0.08,0,0.58  
3TOW,LYS\_143,10.22,-0.28,0,0  
3IRA,LYS\_7,10.5,0,0,0  
4FH3,LYS\_46,10.5,0,0,0  
2P65,GLU\_101,4.57,0.07,0,0  
3DHN,HIS\_207,6.5,0.14,0,-0.14  
2CYG,GLU\_314,0.63,1.99,-3.46,-2.4  
2BDV,ARG\_57,11.87,-0.63,0,0  
2IF4,ASP\_41,3.77,0.14,-0.17,0  
1ZCE,GLU\_127,4.5,0,0,0  
2PLQ,CYS\_332,9,0,0,0

3DB9,GLU\_114,2.73,0.63,-2.4,0  
2QOP,ARG\_45,12.5,0,0,0  
3U4K,LYS\_163,10.36,-0.14,0,0  
1X7F,ARG\_272,11.87,-0.63,0,0  
3MEW,CYS\_287,8.65,-0.35,0,0  
2Q98,ARG\_10,12.01,-0.49,0,0  
3V55,GLU\_418,2.66,0.56,-2.4,0  
2H01,ASP\_24,3.02,0.42,-1.2,0  
3IL3,LYS\_213,10.22,-0.28,0,0  
3ETU,LYS\_170,10.5,0,0,0  
1NFN,LYS\_75,9.94,-0.56,0,0  
4EVF,GLU\_64,5.2,0.7,0,0  
2P5D,GLU\_138,4.46,0.14,-0.18,0  
3RLN,LYS\_674,10.43,-0.07,0,0  
3O16,HIS\_132,6.39,0.03,0,-0.14  
3QAV,LYS\_45,10.08,-0.42,0,0  
1V6T,LYS\_99,10.5,0,0,0  
2X4L,LYS\_208,10.5,0,0,0  
3UOV,GLU\_92,3.49,0.14,-1.15,0  
1U3Y,HIS\_304,6.43,0,0,-0.07  
3V55,LYS\_358,10.36,-0.14,0,0  
4FCU,LYS\_144,9.52,-0.98,0,0  
1XFK,GLU\_96,4.5,0,0,0  
3ANJ,ARG\_196,12.36,-0.14,0,0  
1X91,LYS\_35,10.22,-0.28,0,0  
2B78,LYS\_82,10.15,-0.35,0,0  
1SBX,ASP\_144,3.9,0.14,-0.04,0  
2CXC,ARG\_13,12.22,-0.28,0,0  
2G5X,ASP\_18,1.69,0.14,-0.73,-1.52  
2I88,ASP\_398,3.48,0.07,-0.38,0  
1SFE,ARG\_148,13.1,-1.8,0,2.4  
2CVG,ARG\_103,12.15,-0.35,0,0  
1QSZ,ARG\_564,11.66,-0.84,0,0  
2OPJ,ARG\_307,12.22,-0.28,0,0  
1R29,ARG\_98,12.22,-0.28,0,0  
1LFP,LYS\_13,10.5,0,0,0  
1IAP,ASP\_123,3.89,0.21,-0.12,0  
1WXQ,ARG\_212,12.15,-0.35,0,0  
2CWY,HIS\_21,5.25,0,0,-1.25  
3IVF,ASP\_397,3.75,0.14,-0.19,0  
2DOA,LYS\_37,10.43,-0.07,0,0  
1EDG,ARG\_299,12.29,-0.21,0,0  
2Z14,GLU\_46,4.43,0,-0.07,0  
1ZYL,GLU\_250,4.5,0,0,0  
3ETV,HIS\_165,7.94,1.58,0,-0.14  
1WYC,ASP\_106,2.92,0.28,-1.16,0  
3RXX,GLU\_229,5.39,1.59,-0.7,0  
3Q1C,ASP\_191,3.21,0.7,-1.3,0  
2ZOM,ASP\_180,4.05,0.28,-0.03,0  
2D7U,ARG\_141,12.08,-0.42,0,0  
3COU,GLU\_83,4.5,0,0,0  
1WNH,TYR\_205,10,0,0,0  
3Q1C,HIS\_304,7.05,0.69,0,-0.14  
3IL3,LYS\_130,10.5,0,0,0  
2YWJ,LYS\_122,10.29,-0.21,0,0  
1NWA,HIS\_47,5.41,1.62,0,-2.71  
3P2F,HIS\_161,6.68,0.25,0,-0.07  
2DVK,ARG\_59,12.36,-0.14,0,0  
1EQ6,ARG\_58,12.29,-0.21,0,0  
1X7F,GLU\_327,4.71,0.21,0,0  
2R51,HIS\_84,6.22,0,0,-0.28  
3GW3,ASP\_123,3.19,0.56,-1.17,0  
1DTO,LYS\_172,10.29,-0.21,0,0  
1MTZ,GLU\_276,3.84,2.49,-3.14,0  
3D9H,ARG\_252,12.15,-0.35,0,0  
3N2T,ASP\_102,2.09,0.84,-2.55,0  
2V81,GLU\_202,4.05,0.35,-0.8,0  
4FZN,LYS\_119,10.43,-0.07,0,0  
2E3I,ARG\_107,11.45,-1.05,0,0  
1YTD,ARG\_83,11.66,-0.84,0,0  
3O48,ARG\_75,12.15,-0.35,0,0  
2H2W,ARG\_227,11.91,-0.59,0,0  
2ZCO,GLU\_279,4.78,0.28,0,0  
1JYH,ASP\_120,1.72,0.21,-2.99,0  
3GMS,HIS\_260,6.76,0.26,0,0  
3U4K,GLU\_154,4.36,0.28,-0.42,0  
1L2F,GLU\_21,3.98,0.28,-0.8,0  
2FD4,GLU\_542,3.92,0.42,-1,0  
3OA7,LYS\_516,10.43,-0.07,0,0  
2YT4,LYS\_565,10.29,-0.21,0,0  
1TLV,GLU\_168,4.5,0,0,0  
1V43,LYS\_283,10.5,0,0,0  
3U0V,LYS\_215,10.43,-0.07,0,0  
4DBX,ARG\_52,11.8,-0.7,0,0  
1KCM,HIS\_116,1.57,0.6,-0.92,-4.61  
3ASA,LYS\_182,10.22,-0.28,0,0  
2GAU,TYR\_56,10.76,0.65,-0.54,0.65  
1RHS,LYS\_174,10.5,0,0,0  
3CRM,ARG\_293,12.5,0,0,0  
2FG1,ARG\_96,11.73,-0.77,0,0  
2ZQ5,GLU\_173,3.65,2.75,-1.2,-2.4  
1LZL,GLU\_196,4.71,0.21,0,0  
3EX9,HIS\_22,7.06,0.56,0,0  
3ULX,HIS\_30,6.68,0.18,0,0  
1SQH,HIS\_159,7.67,1.39,0,-0.21  
1ZYL,TYR\_302,12.15,1,0,1.15  
3GYW,HIS\_227,6.52,0.09,0,-0.07  
3CCY,ASP\_114,3.12,0.14,-0.83,0  
2IN0,HIS\_30,6.43,0,0,-0.07  
2EDM,ARG\_64,11.31,-1.19,0,0  
2OEW,GLU\_14,4.26,0.07,-0.31,0  
2CL3,GLU\_69,4.05,0.35,-0.8,0  
3ETU,ASP\_40,3.1,0.28,-0.98,0  
2D7J,TYR\_101,11.45,0.43,0,1.02  
3O7K,GLU\_30,4.57,0.07,0,0  
2XJ4,HIS\_250,6.88,0.45,0,-0.07  
2D7U,LYS\_147,10.29,-0.21,0,0  
3GEC,ARG\_283,11.94,-0.56,0,0  
200K,ASP\_265,3.8,0,0,0  
2G7O,LYS\_112,10.43,-0.07,0,0  
3QKY,ARG\_133,12.01,-0.49,0,0  
2GKG,ASP\_74,3.82,0.07,-0.05,0  
3KVO,ASP\_167,3.67,0.07,-0.2,0  
2WBB,ARG\_692,10.55,-2.18,0,0.23  
2IQT,GLU\_275,3.77,0.07,-0.8,0  
1X8F,ARG\_218,12.36,-0.14,0,0  
2IRM,GLU\_228,4.5,0,0,0  
3M7D,ARG\_135,8.88,-1.79,0,-1.83  
2CN1,LYS\_119,10.5,0,0,0  
1R6Y,ASP\_45,3.2,0.7,-1.3,0  
2YWJ,GLU\_62,4.5,0,0,0  
2D7U,ARG\_259,11.24,-1.26,0,0  
4H4J,ARG\_99,13.29,-1.47,0,2.26  
2E0T,TYR\_106,11.27,0.99,0,0.28  
3AU3,CYS\_681,8.84,-0.23,0,0.07  
1Y0K,ARG\_25,12.5,0,0,0  
2CL3,LYS\_122,10.22,-0.28,0,0  
3E7P,GLU\_237,5.71,1.69,-0.48,0  
2QZQ,LYS\_157,10.5,0,0,0  
3LPZ,GLU\_175,4.64,0.14,0,0  
1UAI,LYS\_83,10.15,-0.35,0,0  
1P6F,ARG\_145,12.01,-0.49,0,0  
1ZP2,ASP\_207,2.35,0.63,-2.08,0  
2OJQ,GLU\_635,4.64,0.14,0,0  
2VGY,TYR\_47,10.23,0.19,0,0.04  
3ASA,ASP\_344,3.39,0.14,-0.55,0  
3AUF,ARG\_49,12.08,-0.42,0,0  
2CE6,GLU\_57,2.01,0.28,-2.76,0  
3RLE,TYR\_166,13.49,0.32,0.77,2.4  
1EQ6,LYS\_34,10.5,0,0,0  
2PGE,ARG\_309,11.94,-0.56,0,0  
3LJI,HIS\_83,4.53,0.81,0,-2.78  
2Q99,ASP\_178,3.21,0.21,-0.8,0  
3NR5,ASP\_126,3.07,0.28,-1.01,0  
3RFY,ASP\_310,4.08,0.28,0,0  
3MTT,GLU\_492,4.64,0.14,0,0  
1KW4,LYS\_64,10.5,0,0,0  
3OIP,ASP\_150,2.38,0.35,-1.77,0  
3E27,GLU\_190,4.5,0,0,0  
1UOH,LYS\_95,10.36,-0.14,0,0  
1N81,ASP\_95,3.27,0.35,-0.88,0  
3M66,TYR\_301,12.16,2.16,0,0  
2HP7,LYS\_226,10.5,0,0,0  
3KB5,ASP\_329,2.82,0.91,-1.89,0  
3A0X,CYS\_634,9.19,0.12,0,0.07  
2R2Y,GLU\_81,4.57,0.07,0,0  
1MUF,HIS\_116,6.36,0,0,-0.14  
2O8P,LYS\_124,10.43,-0.07,0,0  
3ONT,ASP\_112,3.93,0.14,-0.01,0  
1L3K,ARG\_31,11.73,-0.77,0,0  
3RXX,TYR\_156,13.35,0.15,0.8,2.4  
3BQW,TYR\_77,10,0,0,0  
3TMO,ASP\_192,3.47,0.49,-0.82,0  
2A4D,ARG\_87,11.63,-0.91,0,0.04  
2A0J,CYS\_47,9.67,0,0,0.67  
2IQT,GLU\_45,3.9,0.42,-1.02,0  
3A0T,GLU\_339,4.44,0.07,-0.13,0  
1R16,HIS\_93,4.79,0.02,0,-1.73  
4H4J,HIS\_178,6.3,0.01,0,-0.21  
1X91,GLU\_84,4.57,0.07,0,0  
4GCO,GLU\_168,4.05,0.35,-0.8,0  
2A1V,ASP\_96,2.22,0.77,-2.36,0  
1HUF,HIS\_83,7.26,0.34,0.49,-0.07  
3EVZ,LYS\_106,10.5,0,0,0  
2PP6,ARG\_10,12.36,-0.14,0,0  
2R2Y,CYS\_80,9.2,-0.03,0,0.23  
3IRA,ARG\_4,11.87,-0.63,0,0  
3CS1,TYR\_125,10.64,1.84,0,-1.2  
1EDG,TYR\_116,11.06,0.43,0,0.63  
3BQW,TYR\_159,12.82,1.86,-0.68,1.64  
1H09,ARG\_212,12.36,-0.14,0,0  
3KVO,GLU\_105,4.64,0.14,0,0  
3HFH,GLU\_162,4.71,0.21,0,0  
2A0J,LYS\_127,10.36,-0.14,0,0  
4ECC,GLU\_109,2.11,1.33,-1.92,-1.8  
1UXO,LYS\_121,9.73,-0.77,0,0  
1D2K,TYR\_113,10.69,0.69,0,0  
1Q8B,HIS\_52,7.16,0.8,0,-0.14  
1SFE,LYS\_124,10.5,0,0,0  
2EYJ,LYS\_98,10.22,-0.28,0,0  
3V46,CYS\_338,9.35,0,-1.11,1.46  
3B4D,GLU\_234,4.5,0,0,0  
1MUF,GLU\_271,4.5,0,0,0  
1CHD,ARG\_273,12.43,-0.07,0,0  
4H89,ASP\_66,3.87,0.07,0,0  
3E7P,ARG\_98,11.73,-0.77,0,0  
1WXQ,LYS\_364,10.5,0,0,0  
3E7P,GLU\_25,3.04,0.7,-0.48,-1.69  
1O9G,HIS\_6,6.5,0.07,0,-0.07  
1O6D,ARG\_59,12.01,-0.49,0,0  
2A4D,TYR\_134,10.85,0.86,-0.31,0.3  
3E27,LYS\_81,10.29,-0.21,0,0  
2BAA,ARG\_183,11.87,-0.63,0,0  
1AK1,ARG\_46,12.46,-0.54,0,0.5  
3P51,TYR\_5,13.13,0.21,0.52,2.4  
1V6T,TYR\_65,9.63,0.52,-1.2,0.31  
3VJ8,LYS\_41,10.08,-0.42,0,0  
1LZL,CYS\_133,12.29,0,0,3.29  
1NWA,ASP\_113,3.29,0.42,-0.93,0  
1WJG,ARG\_16,12.29,-0.21,0,0  
2RJD,GLU\_312,4.5,0,0,0  
4AF2,GLU\_113,3.28,0.56,-1.78,0  
3ETU,HIS\_116,0.07,0.71,-2.34,-4.8  
4FZR,LYS\_189,9.66,-0.84,0,0  
1O9G,GLU\_114,4.71,0.21,0,0  
1RKA,ASP\_302,3.5,0.49,-0.79,0  
3CXS,TYR\_85,10.47,0.47,0,0  
3ZSL,ASP\_178,3.86,0.07,-0.01,0  
1V6T,LYS\_120,10.5,0,0,0  
1NAF,ARG\_207,12.01,-0.49,0,0  
3PP8,HIS\_77,6.99,0.63,0,-0.14  
3U0V,ASP\_106,3.98,0.21,-0.03,0  
1YB2,LYS\_130,10.36,-0.14,0,0  
1YM5,LYS\_293,10.43,-0.07,0,0  
3BPP,ARG\_66,12.29,-0.21,0,0  
1GQE,ARG\_278,12.5,0,0,0  
2RIK,GLU\_102,3.98,0.28,-0.8,0  
3CZC,LYS\_87,10.15,-0.35,0,0  
2BDV,GLU\_197,3.99,0.07,-0.58,0  
1QYI,GLU\_109,4.5,0,0,0  
3ETU,LYS\_201,10.5,0,0,0  
1X04,ARG\_217,12.29,-0.21,0,0  
3HQX,HIS\_8,6.5,0,0,0  
1SJV,ASP\_147,3.23,0.28,-0.85,0  
2V4U,GLU\_483,0.21,2.45,-2.54,-4.21  
1RWZ,ARG\_231,12.15,-0.35,0,0  
3Q6L,ARG\_109,11.66,-0.84,0,0  
3LJN,GLU\_220,3.73,0.07,-0.83,0  
3BPV,ASP\_113,3.92,0.21,-0.09,0  
3RFF,ASP\_19,2.49,0.56,-1.86,0  
1F2V,ARG\_8,12.08,-0.42,0,0  
1XWM,GLU\_18,4.08,0.35,-0.77,0  
3CIV,ARG\_190,12.5,0,0,0  
3GA2,ARG\_81,12.43,-0.07,0,0  
2B78,GLU\_373,4.11,0.14,-0.53,0  
2G9D,HIS\_63,2.29,1.6,-0.95,-4.85  
3I4T,GLU\_211,4.57,0.07,0,0  
4EUG,TYR\_66,11.6,2.34,-0.74,0  
3OIP,CYS\_93,9.67,-0.08,0,0.75  
2P65,ASP\_98,2.94,0.49,-1.34,0  
2A4D,LYS\_142,10.29,-0.21,0,0  
1UXO,LYS\_187,10.36,-0.14,0,0  
2VCH,ARG\_39,12.43,-0.07,0,0  
3HVV,ARG\_187,12.15,-0.35,0,0  
4EVF,ARG\_35,10.51,-2.94,0.95  
2WOZ,HIS\_445,6.29,0,0,-0.21  
1J33,GLU\_134,3.54,0.35,-1.31,0  
4ACJ,ASP\_794,4.08,0.28,0,0  
3CJW,ARG\_228,11.05,-1.45,0,0  
2QVO,TYR\_66,12.09,0.14,0,0.85  
3TRE,ARG\_40,12.29,-0.21,0,0  
1AKO,LYS\_49,10.5,0,0,0  
2DVK,CYS\_40,6.63,-2.26,-0.96,0.85  
3CJW,ARG\_366,11.73,-0.77,0,0  
1Z9L,HIS\_0,6.5,0,0,0  
1YR6,TYR\_129,11.29,1.29,0,0  
3ETV,GLU\_344,4.47,0.14,-0.17,0  
3CAX,TYR\_461,10.07,0.07,0,0  
1EQ6,LYS\_97,10.43,-0.07,0,0  
2FGG,ARG\_35,12.08,-0.42,0,0  
1KN3,LYS\_150,10.77,-0.14,0,0.41  
2PIM,ASP\_41,2.93,0.7,-1.57,0  
1OLR,LYS\_26,10.22,-0.28,0,0  
1MUF,HIS\_310,4.23,1.6,1.82,-5.69  
1N81,CYS\_109,10.43,0,1,1.43  
3RLE,ASP\_57,3.29,0.35,-0.86,0

1TLV,LYS\_115,10.5,0,0,0  
3UPD,LYS\_288,10.15,-0.35,0,0  
1V6T,LYS\_189,10.22,-0.28,0,0  
3OBS,GLU\_138,4.57,0.07,0,0  
1KN3,HIS\_15,6.51,0.01,0,0  
2EEY,ARG\_26,11.17,-1.33,0,0  
3U4K,ARG\_37,12.22,-0.28,0,0  
1RAJ,LYS\_431,10.5,0,0,0  
3VJ8,LYS\_117,10.5,0,0,0  
2P0L,ARG\_38,11.66,-0.84,0,0  
2X4G,GLU\_63,4.57,0.07,0,0  
3K1H,GLU\_42,3.65,0.35,-1.2,0  
1Q46,ASP\_16,4.01,0.21,0,0  
4F3J,HIS\_244,6.15,0,0,-0.35  
2AXO,GLU\_144,4.57,0.07,0,0  
1ES9,GLU\_157,3.65,0.63,-1.48,0  
2RS1,TYR\_116,9.58,0.07,-0.49,0  
1ZYL,TYR\_37,10.07,0.07,0,0  
1YR6,GLU\_45,4.5,0,0,0  
4DBX,LYS\_97,9.94,-0.56,0,0  
4ESS,ARG\_3,11.87,-0.63,0,0  
3TRE,CYS\_22,8.98,-0.2,0.019  
1T95,GLU\_26,3.65,0.28,-1.13,0  
1MUF,LYS\_107,10.5,0,0,0  
1MUF,ASP\_306,3.5,0.21,-0.51,0  
2DG7,ARG\_3,12.36,-0.14,0,0  
1HUF,ASP\_106,3.65,0.84,-0.99,0  
3F5D,ASP\_191,4.05,0.28,-0.03,0  
2OEW,ASP\_299,3.71,0,-0.09,0  
1OST,CYS\_394,7.28,-2.41,0,0.68  
1KW4,ASP\_37,3.73,0,-0.07,0  
2FBI,HIS\_30,6.93,0.64,0,-0.21  
2FGG,HIS\_20,6.43,0,0,-0.07  
1AM2,GLU\_55,4.57,0.07,0,0  
2D59,GLU\_138,4.71,0.21,0,0  
2CWC,ARG\_180,11.8,-0.7,0,0  
1NWA,TYR\_148,9.42,0.07,-0.65,0  
3DTE,ASP\_215,3.8,0.35,-0.35,0  
1TD6,LYS\_220,10.5,0,0,0  
4E9E,GLU\_559,4.38,0.21,-0.33,0  
3I0C,LYS\_314,10.01,-0.49,0,0  
1DZF,GLU\_148,4.5,0,0,0  
3BPV,CYS\_131,9,0,0,0  
2FXT,LYS\_355,10.22,-0.28,0,0  
3HVM,TYR\_249,11.52,0.77,-0.65,1.4  
1G8P,GLU\_222,3.49,0,-1.01,0  
2D2S,ASP\_525,3.2,0.07,-0.67,0  
2XHC,LYS\_270,10.43,-0.07,0,0  
3BJV,LYS\_136,10.43,-0.07,0,0  
1DUP,ASP\_47,2.96,0.35,-1.19,0  
3LQE,ARG\_228,12.22,-0.28,0,0  
2PGX,GLU\_145,4.71,0.21,0,0  
1GQE,ARG\_116,12.51,-2.0,2.01  
1ANU,ASP\_50,3.61,0.21,-0.4,0  
2F9F,LYS\_165,10.5,0,0,0  
3U2A,ARG\_61,11.8,-0.7,0,0  
3G9G,GLU\_232,4.71,0.21,0,0  
1JT9,ARG\_158,11.5,-1,0,0  
3LH5,ARG\_677,12.01,-0.49,0,0  
3A2Z,GLU\_166,4.57,0.28,-0.21,0  
4FCU,CYS\_58,9.72,0,0,0.72  
3BQW,ARG\_116,12.08,-0.42,0,0  
4AM1,LYS\_98,10.36,-0.14,0,0  
1JKS,GLU\_182,4.74,1.03,-0.79,0  
1YTQ,ASP\_102,3.21,0.21,-0.8,0  
4DND,ASP\_5,4.04,0.35,-0.11,0  
1GPP,ARG\_35,11.1,-1.4,0,0  
2IQT,LYS\_118,10.43,-0.07,0,0  
3FTT,LYS\_179,10.29,-0.21,0,0  
2FD5,LYS\_80,10.29,-0.21,0,0  
2FD5,ARG\_9,11.94,-0.56,0,0  
1WXQ,ASP\_381,3.93,0.14,-0.01,0  
3M3P,HIS\_231,5.57,0.58,0,-1.51  
1L2F,TYR\_59,12.48,0.1,1.2,39  
3H5T,TYR\_30,10.07,0.07,0,0  
4EVF,ASP\_125,2.97,0.35,-1.18,0  
2RGY,GLU\_245,3.92,0.42,-1,0  
2CW4,CYS\_119,10.28,-0.32,0,1.6  
2FB6,LYS\_31,10.08,-0.42,0,0  
2B78,TYR\_115,13.67,3.26,-0.96,1.38  
1SNT,ARG\_78,12.36,-0.14,0,0  
1H4U,HIS\_497,6.36,0,0,-0.14  
2YT4,LYS\_525,10.5,0,0,0  
4ECC,LYS\_210,10.08,-0.42,0,0  
3Q6L,ASP\_111,3.94,0.14,0,0  
3BQE,ASP\_352,3.64,0.14,-0.3,0  
3CNU,GLU\_24,4.64,0.14,0,0  
3QKY,LYS\_120,10.5,0,0,0  
3G6S,ASP\_206,3.62,0.07,-0.25,0  
3GEC,TYR\_253,10.04,0.07,-0.03,0  
3OA7,LYS\_4,10.43,-0.07,0,0  
3L3P,ASP\_528,3.67,0.49,-0.63,0  
4ESS,ARG\_90,11.94,-0.56,0,0  
2WB8,ASP\_596,3.48,0.07,-0.39,0  
1F2V,LYS\_122,10.43,-0.07,0,0  
2BDV,GLU\_80,4.33,0.63,-0.8,0  
1TP6,ARG\_60,12.15,-0.35,0,0  
2AZL,LYS\_152,10.29,-0.21,0,0  
1TLV,LYS\_177,10.5,0,0,0  
3HUE,HIS\_150,3.62,0,0,-2.88  
1LFP,LYS\_16,10.29,-0.21,0,0  
1OIS,HIS\_299,6.43,0,0,-0.07  
3LQE,TYR\_317,10.06,0.69,-0.75,0.12  
2BT8,HIS\_223,7.13,0.77,0,-0.14  
3VJ8,LYS\_170,10.15,-0.35,0,0  
1PBV,GLU\_119,3.91,0.21,-0.8,0  
1YDL,GLU\_25,4.57,0.07,0,0  
3E5T,LYS\_227,10.5,0,0,0  
2P0L,GLU\_143,4.64,0.14,0,0  
3EX9,GLU\_131,4.78,0.28,0,0  
3GE9,GLU\_24,4.5,0,0,0  
3F7M,GLU\_147,3.22,0.7,-1.99,0  
3SMD,ARG\_89,11.94,-0.56,0,0  
3M16,CYS\_160,13.25,0.19,2.05,2.01  
1LZL,LYS\_20,10.36,-0.14,0,0  
1FO9,TYR\_365,10.81,0.81,0,0  
4DBX,LYS\_255,10.29,-0.21,0,0  
2D0A,LYS\_266,10.22,-0.28,0,0  
1PSW,HIS\_225,7.46,1.03,0,-0.07  
1TLV,LYS\_244,10.22,-0.28,0,0  
3LJC,ARG\_212,11.94,-0.56,0,0  
1C44,LYS\_46,10.15,-0.35,0,0  
3QAV,TYR\_193,10.74,0.74,0,0  
2AHE,GLU\_213,3.76,0.35,-1.09,0  
2H01,LYS\_159,10.36,-0.14,0,0  
2QEV,ASP\_137,3.51,0.42,-0.71,0  
3LJC,ASP\_205,3.88,0.21,-0.13,0  
4HDE,LYS\_174,10.5,0,0,0  
1WRU,LYS\_232,10.5,0,0,0  
3CS1,ARG\_50,11.1,-2,0,0.6  
3HNX,ARG\_24,12.08,-0.42,0,0  
1EW4,ASP\_23,4.07,0.28,-0.01,0  
2RGY,ARG\_175,10.38,-2.12,0,0  
2Q34,TYR\_137,10.28,1.86,-1.58,0  
1OST,ARG\_381,11.8,-0.7,0,0  
1T3J,LYS\_700,10.29,-0.21,0,0  
2E3I,ASP\_56,2.52,0.07,-1.35,0  
2CXC,LYS\_83,10.29,-0.21,0,0  
1MTZ,TYR\_198,9.26,0.17,-0.65,-0.26  
3ERF,LYS\_110,10.43,-0.07,0,0  
2DVK,GLU\_108,3.98,0.28,-0.8,0  
2A0J,LYS\_22,9.45,-1.05,0,0  
2W1R,HIS\_72,6.81,0.52,0,-0.21  
1Ri6,ASP\_209,1.98,1.19,-3.02,0  
4FH3,ARG\_139,12.5,0,0,0  
3JRT,LYS\_101,10.22,-0.28,0,0  
3Q9P,GLU\_166,3.93,0.35,-0.92,0  
3KB5,LYS\_279,10.5,0,0,0  
1LZL,ASP\_245,2.45,0.63,-1.98,0  
4AF2,ARG\_133,10.28,-2.22,0,0  
3QAV,GLU\_133,4.5,0,0,0  
1TUL,ASP\_21,3.17,0.56,-1.19,0  
1NFN,ARG\_136,12.15,-0.35,0,0  
2H01,ASP\_56,3.78,0,-0.02,0  
1BVI,LYS\_45,10.5,0,0,0  
1H4U,CYS\_588,9,0,0,0  
1XDZ,TYR\_56,10.79,0.77,0,0.02  
1WYC,ARG\_278,12.55,-1.74,0,1.79  
2H85,TYR\_237,10.82,0.89,-0.07,0  
3GEC,HIS\_429,6.29,0,0,-0.21  
3IUS,CYS\_69,9.06,-0.28,0,0.34  
4FH3,ASP\_249,1.49,0.77,-3.07,0  
1Q5Z,LYS\_581,10.5,0,0,0  
4E9E,ASP\_510,3.28,0.28,-0.8,0  
1TR9,LYS\_300,10.43,-0.07,0,0  
1IAP,HIS\_101,7.1,0.74,0,-0.14  
1DUN,GLU\_78,4.64,0.14,0,0  
1J33,GLU\_288,4.57,0.07,0,0  
1CBY,LYS\_216,10.43,-0.07,0,0  
2JKF,ASP\_13,3.93,0.21,-0.08,0  
2NRK,LYS\_28,10.5,0,0,0  
4ANN,GLU\_106,4.39,0,-0.11,0  
1X8F,ARG\_36,12.36,-0.14,0,0  
3CZC,GLU\_90,4.71,0.21,0,0  
1YTQ,ASP\_191,4.01,0.21,0,0  
2OJQ,LYS\_574,10.36,-0.14,0,0  
1X9G,GLU\_108,4.39,0.9,-1.01,0  
3Q1C,ASP\_238,2.35,0.56,-2.02,0  
3C2E,CYS\_162,9.62,-0.71,0,1.34  
2H2Z,GLU\_240,5.15,0.65,0,0  
1X1E,GLU\_208,4.19,0.49,-0.8,0  
2Q12,HIS\_180,6.43,0,0,-0.07  
2YLF,GLU\_124,2.92,0.35,-1.93,0  
3EAZ,GLU\_154,4.5,0,0,0  
1QVI,LYS\_315,10.15,-0.35,0,0  
3RJX,GLU\_270,4.71,0.21,0,0  
2ILR,ARG\_460,11.31,-1.19,0,0  
1TD6,ASP\_31,3.8,0,0,0  
2QZQ,ASP\_146,1.24,0.84,-3.39,0  
1Ri6,ARG\_231,11.73,-0.77,0,0  
1DCF,LYS\_24,10.43,-0.07,0,0  
4EVF,GLU\_156,3.37,0.56,-1.7,0  
2AD1,TYR\_194,8.4,0.8,0,-2.4  
1X8F,HIS\_202,4.48,1.6,0.67,-4.29  
2Q5X,ASP\_870,2.69,0.35,-1.47,0  
2Q07,ARG\_269,12.08,-0.42,0,0  
1F2V,ARG\_22,12.01,-0.49,0,0  
1Q42,ARG\_114,11.8,-0.7,0,0  
2G3A,GLU\_111,4.62,0.49,-0.37,0  
1XEU,HIS\_160,6.43,0,0,-0.07  
2O8P,LYS\_29,10.43,-0.07,0,0  
3G6S,LYS\_157,10.22,-0.28,0,0  
3B21,ASP\_171,3.24,0.56,-1.12,0  
3TMO,GLU\_284,4.85,0.35,0,0  
3TOW,LYS\_89,10.43,-0.07,0,0  
1PBV,LYS\_57,10.5,0,0,0  
3ANJ,GLU\_374,2.44,0.98,-3.04,0  
3VJ8,ASP\_245,2.42,0.84,-2.22,0  
2Q99,CYS\_97,10.87,0,0.67,1.2  
2CVB,ASP\_137,2.34,0.91,-2.37,0  
3MTT,ASP\_547,4.08,0.28,0,0  
4MZN,GLU\_267,4.71,0.21,0,0  
3EZ7,HIS\_95,6.5,0,0,0  
3NR5,ASP\_108,3.03,0.14,-0.91,0  
1QYI,GLU\_271,4.0,0.14,-0.64,0  
4DNU,ARG\_15,12.29,-0.21,0,0  
3GW3,GLU\_115,4.57,0.07,0,0  
2CWC,LYS\_77,10.5,0,0,0  
2XJ4,TYR\_31,12.44,0.73,0.27,1.44  
2QDJ,LYS\_319,10.15,-0.35,0,0  
2B0J,GLU\_207,6.05,3.6,-2.05,0  
2DG7,GLU\_22,4.4,0.63,-0.73,0  
2CBE,CYS\_206,9.76,-0.58,0,1.33  
3H13,ARG\_268,12.08,-0.42,0,0  
1MD6,TYR\_149,10,0,0,0  
3PBH,TYR\_75,10,0,0,0  
4AM1,ARG\_244,11.8,-0.7,0,0  
3VHJ,GLU\_29,3.79,0.42,-1.13,0  
2R0S,TYR\_92,10.49,0.49,0,0  
3IUS,LYS\_78,11.94,-0.56,0,0  
3BQW,TYR\_227,10.14,0.14,0,0  
3OIP,LYS\_75,10.08,-0.42,0,0  
3PP8,ARG\_181,12.22,-0.28,0,0  
2QRX,ARG\_183,12.08,-0.42,0,0  
1X7F,GLU\_303,4.57,0.07,0,0  
3P13,GLU\_116,3.98,0.28,-0.8,0  
3JZN,ASP\_91,1.38,0.28,-2.7,0  
2CBE,ARG\_246,10.07,-2.43,0,0  
2OKT,ARG\_157,11.94,-0.56,0,0  
2FXT,ASP\_244,3.87,0.07,0,0  
3EVP,GLU\_253,3.76,0.14,-0.88,0  
3RUX,GLU\_90,4.93,0.8,0,-2.37  
1RHS,ASP\_238,1.79,0.77,-2.78,0  
1NAR,GLU\_98,4.71,0.21,0,0  
3ADO,GLU\_189,3.37,0.7,-1.83,0  
2E3H,LYS\_252,10.36,-0.14,0,0  
2ZCX,ARG\_33,13.69,-1.21,0,2.4  
3L7N,CYS\_178,11.27,-1.22,0,3.49  
4ETX,ASP\_450,3.57,0.14,-0.37,0  
2ZCO,TYR\_73,9.83,0,-0.17,0  
2E3S,GLU\_456,2.52,0.42,-2.4,0  
3CX2,ARG\_238,11.59,-0.91,0,0  
3PBH,CYS\_42,11.24,0.02,2.22  
3Q1C,GLU\_276,3.91,0.21,-0.8,0  
2CYG,ARG\_138,12.15,-0.35,0,0  
1N81,TYR\_65,12.08,0,0.2,0.8  
1R2Z,GLU\_54,4.48,0.28,-0.3,0  
1PV5,HIS\_48,6.36,0,0,-0.14  
3V46,LYS\_361,9.66,-0.84,0,0  
4KEU,CYS\_180,10.9,-0.01,0,1.91  
3V1Q,ARG\_657,12.15,-0.35,0,0  
1O6D,LYS\_24,10.5,0,0,0  
1QQE,LYS\_183,10.5,0,0,0  
1EDG,LYS\_15,10.5,0,0,0  
1PSW,GLU\_78,4.57,0.07,0,0  
2GZQ,ARG\_85,12.36,-0.14,0,0  
4D8L,ARG\_63,11.31,-1.19,0,0  
2R57,LYS\_326,10.29,-0.21,0,0  
1NJ4,GLU\_249,4.96,0.68,-0.21,0  
1Q46,ARG\_63,12.29,-0.21,0,0  
3V1Q,ARG\_650,11.45,-1.05,0,0  
3H6Q,ASP\_35,4.22,0.42,0,0  
3ETU,LYS\_133,10.5,0,0,0  
2R2Y,ARG\_104,11.94,-0.56,0,0  
3GMS,GLU\_304,4.5,0.21,-0.21,0  
1BGF,HIS\_32,6.5,0,0,0



1Y2Q,GLU\_50,3.15,0.63,-1.98,0  
1JSX,LYS\_33,10.5,0,0,0  
2IF4,GLU\_160,3.26,0.47,-0.37,-1.34  
1NAF,ARG\_255,12.29,-0.21,0,0  
3ZTA,TYR\_107,9.83,0.26,-0.43,0  
1ZBS,ARG\_152,11.62,-0.88,0,0  
3NOK,LYS\_13,10.36,-0.14,0,0  
3V55,CYS\_441,4.75,-4.25,0,0  
3AU3,GLU\_425,4.85,0.35,0,0  
2XHC,LYS\_3,10.5,0,0,0  
3KB5,ARG\_409,11.52,-0.98,0,0  
3GFP,ASP\_370,3.84,0.21,-0.17,0  
2AD1,HIS\_226,6.5,0,0,0  
2VAN,GLU\_203,4.52,0.07,-0.05,0  
2H2W,TYR\_168,10.19,1.28,-1.28,0.2  
2V1L,HIS\_28,6.43,0,0,-0.07  
3EIZ,LYS\_113,10.5,0,0,0  
3CJW,GLU\_379,4.02,0.63,-1.11,0  
4DEZ,GLU\_118,4.64,0.14,0,0  
2AHE,ASP\_65,3.29,0.28,-0.79,0  
1LTU,ASP\_245,3.94,0.14,0,0  
1KCM,ARG\_49,4.64,0.14,0,0  
4FLE,ARG\_164,11.8,-0.7,0,0  
1XFK,ARG\_317,12.15,-0.35,0,0  
3AUF,HIS\_128,6.5,0,0,0  
1JB3,GLU\_121,4.57,0.07,0,0  
4FZR,ARG\_67,11.87,-0.63,0,0  
2ZCO,GLU\_71,4.12,0.42,-0.8,0  
2B2H,GLU\_323,4.5,0,0,0  
2DFL,ARG\_295,11.17,-1.33,0,0  
1ZBS,LYS\_74,10.43,-0.07,0,0  
2CXA,ASP\_105,3.8,0,0,0  
2QEV,LYS\_120,10.5,0,0,0  
1XEU,LYS\_116,10.29,-0.21,0,0  
3BCY,LYS\_94,10.36,-0.14,0,0  
1N81,ASP\_155,2.07,0.63,-2.36,0  
2B02,GLU\_453,4.64,0.14,0,0  
3GV0,TYR\_118,9.65,0,-0.35,0  
2QZQ,LYS\_170,9.73,-0.77,0,0  
3A2Z,ASP\_194,3.11,0.21,-0.9,0  
3GOZ,GLU\_41,4.78,0.28,0,0  
2FPN,LYS\_34,10.5,0,0,0  
3F5D,ARG\_29,11.66,-0.84,0,0  
3EUR,TYR\_71,12.86,0.21,-1.04,3.7  
2RIK,LYS\_63,10.5,0,0,0  
1L2F,LYS\_100,10.29,-0.21,0,0  
1JT9,TYR\_128,10,0,0,0,0  
2P1W,LYS\_175,10.22,-0.28,0,0  
3QAV,GLU\_160,4.5,0,0,0  
2V4X,ARG\_85,12.5,0,0,0  
2AD1,ASP\_218,3.65,0,-0.15,0  
1J7G,TYR\_108,13.47,0.14,0.8,2.53  
2GEN,ARG\_179,12.01,-0.49,0,0  
1WNH,GLU\_92,3.84,0.14,-0.8,0  
2CWC,ARG\_234,12.01,-0.49,0,0  
1GQE,LYS\_109,10.43,-0.07,0,0  
3HST,ASP\_78,3.77,0,-0.03,0  
1R3D,ARG\_108,12.01,-0.49,0,0  
2FD5,HIS\_47,6.5,0,0,0  
1T95,LYS\_20,10.36,-0.14,0,0  
2V1L,ASP\_69,2.32,0.35,-1.83,0  
2Q98,GLU\_93,4.64,0.14,0,0  
4DNU,ARG\_368,11.94,-0.56,0,0  
3M66,GLU\_185,3.91,0.21,-0.8,0  
1KCM,CYS\_231,10.39,0,-0.01,1.4  
1MHN,GLU\_147,4.57,0.07,0,0  
3CIV,GLU\_172,4.5,0,0,0  
2RIK,TYR\_156,12.91,0.14,0.37,2.4  
4F8A,TYR\_699,9.74,0.07,-0.33,0  
3RHE,ASP\_101,3.8,0,0,0  
3GW3,ARG\_362,12.08,-0.42,0,0  
1ZBP,GLU\_39,5.16,1.6,-0.94,0  
3QAV,LYS\_150,10.43,-0.07,0,0  
2Q99,ARG\_273,9.97,-1.84,0,-0.69  
3S0A,LYS\_111,10.22,-0.28,0,0  
1SQW,ARG\_80,12.36,-0.14,0,0  
2RIS,TYR\_15,11.73,2.85,-1.13,0  
2W1R,ASP\_64,2.67,0.35,-1.48,0  
3BA1,TYR\_172,9.01,0.14,-1.13,0  
3F6F,TYR\_5,10,0,0,0,0  
4FZN,ASP\_95,2.14,0.49,-2.14,0  
2YWJ,LYS\_53,10.5,0,0,0  
3B79,GLU\_87,4.5,0,0,0  
4FLE,TYR\_74,10.09,1.09,-1,0  
3H8Y,GLU\_97,4.5,0,0,0  
4DEZ,ARG\_22,12.01,-0.49,0,0  
3B7X,GLU\_106,1.36,0.87,-1.61,-2.4  
1U3Y,CYS\_259,4.85,-4.29,0,0.14  
1X1E,ARG\_206,12.08,-0.42,0,0  
3IVF,ASP\_205,1.03,0.77,-3.54,0  
1SQM,GLU\_259,3.18,0.51,-0.08,-1.75  
3CGW,ARG\_274,11.94,-0.56,0,0  
1EV8,LYS\_259,10.5,0,0,0  
1T95,ASP\_221,3.83,0.14,-0.11,0  
1I60,TYR\_275,13.18,0.28,0.5,2.4  
4FH3,GLU\_376,4.5,0,0,0  
3UPD,LYS\_33,10.01,-0.49,0,0  
3F1X,TYR\_57,10.07,0.07,0,0  
2ILR,LYS\_425,10.36,-0.14,0,0  
2G9D,ARG\_276,12.36,-0.14,0,0  
4H4J,LYS\_164,10.36,-0.14,0,0  
3T5B,ARG\_87,12.36,-0.14,0,0  
2PGE,ARG\_117,12.29,-0.21,0,0  
1EV8,GLU\_74,4.57,0.07,0,0  
1DVO,GLU\_50,4.14,0.42,-0.78,0  
1L3K,LYS\_179,10.29,-0.21,0,0  
2JEO,HIS\_88,6.36,0,0,-0.14  
2ILR,LYS\_282,10.5,0,0,0  
2CI3,GLU\_77,5.4,0.3,-1.73,-1.8  
3M66,TYR\_229,13.69,0.49,0.8,2.4  
3H13,HIS\_335,6.15,0,0,-0.35  
2H14,LYS\_272,10.5,0,0,0  
3GA2,ARG\_182,12.22,-0.28,0,0  
3ETV,LYS\_332,10.15,-0.35,0,0  
3C6B,LYS\_223,10.36,-0.14,0,0  
1CBY,LYS\_29,10.5,0,0,0  
3QAV,LYS\_84,10.5,0,0,0  
2D59,TYR\_59,9.8,0,-0.2,0  
2CYG,GLU\_251,3.89,0.42,-1.02,0  
2BLL,HIS\_340,6.89,0.53,0,-0.14  
3FTT,HIS\_132,6.5,0,0,0  
3EZ7,LYS\_261,10.08,-0.42,0,0  
1Ri6,HIS\_24,6.36,0,0,-0.14  
2OEW,HIS\_279,8.2,1.6,1.96,-1.86  
4H86,TYR\_137,10.25,0,0,0.25  
2IF4,ARG\_167,12.15,-0.35,0,0  
1PZC,GLU\_13,4.46,0.28,-0.32,0  
3N2T,ARG\_155,12.15,-0.35,0,0  
3GFP,LYS\_474,10.5,0,0,0  
2XMZ,ARG\_174,10.41,-2.47,0.0,38  
2EHG,TYR\_53,10.84,0.91,-0.07,0  
3BA1,CYS\_10,9.56,-0.25,0,0.81  
2EJB,ARG\_126,12.01,-0.49,0,0  
3RUX,TYR\_267,8.6,0.14,-1.55,0  
3CIV,LYS\_286,10.5,0,0,0  
2GAU,GLU\_185,0.79,1.24,-2.55,-2.4  
2Z14,GLU\_54,2.67,0.7,-2.53,0  
3L0D,CYS\_133,8.36,-0.64,0,0  
1GXN,ARG\_417,11.73,-0.77,0,0  
4FZR,TYR\_356,10.9,0,-0.21,1.11  
1F09,GLU\_276,3.63,0.14,-1.01,0  
3U4K,LYS\_90,9.94,-0.56,0,0  
4DBX,GLU\_86,4.5,0,0,0  
1AIL,LYS\_20,10.29,-0.21,0,0  
1XTZ,HIS\_152,6.66,0.16,0,0  
3F1X,CYS\_153,9,0,0,0  
3PZ9,LYS\_125,10.5,0,0,0  
2PWQ,ASP\_60,3.45,0.42,-0.77,0  
1CHD,ASP\_216,2.78,0.28,-1.3,0  
1XIP,LYS\_84,10.43,-0.07,0,0  
2F19,ASP\_30,3.94,0.14,0,0  
2YLF,ARG\_37,12.22,-0.28,0,0  
2ZOM,ARG\_306,10.71,-1.79,0,0  
3HZQ,LYS\_3,10.5,0,0,0  
3EVN,HIS\_285,2.82,0,0,-3.68  
3G9B,LYS\_116,10.29,-0.21,0,0  
3RKV,ASP\_212,3.81,0.07,-0.06,0  
3LMF,ASP\_82,3.35,0.35,-0.8,0  
3B7H,HIS\_65,6.5,0,0,0  
3GS9,ARG\_64,12.08,-0.42,0,0  
1KJS,LYS\_222,9.66,-0.84,0,0  
2O0K,TYR\_237,10.1,0.1,0,0  
3JSN,ARG\_133,11.83,-0.9,0,0.23  
1NAR,ASP\_94,3.81,0.49,-0.48,0  
1YW5,ARG\_81,12.08,-0.42,0,0  
1BKR,ASP\_6,3.96,0.35,-0.19,0  
3TOW,CYS\_161,8.85,-0.33,-0.11,0.29  
2RJD,GLU\_456,3.65,2.75,-3.6,0  
2AD1,HIS\_174,0.1,0,-2.11,-4.29  
3R1X,ARG\_76,11.8,-0.7,0,0  
3ELI,GLU\_142,4.85,0.35,0,0  
2CL3,GLU\_181,4.5,0,0,0  
2E3C,GLU\_220,3.92,0.21,-0.79,0  
3H13,ASP\_269,3.89,0.21,-0.12,0  
3HYQ,ASP\_168,2.79,0.7,-1.72,0  
2CBE,ASP\_34,3.13,0.63,-1.3,0  
2B0A,HIS\_40,9.95,3.2,3.65,-3.4  
2ZQ5,HIS\_271,6.43,0,0,-0.07  
1R3D,ARG\_95,9.53,-2.91,0,-0.06  
1L3K,LYS\_78,10.5,0,0,0  
4FZN,ARG\_109,11.8,-0.7,0,0  
1SNT,ARG\_56,11.39,-1.11,0,0  
3CIV,GLU\_164,4.12,0.42,-0.8,0  
2CYG,GLU\_322,4.15,0.57,0,-0.92  
2EJX,ASP\_124,2.41,0.84,-2.23,0  
3IV4,CYS\_30,5.69,-3.38,0,0.07  
3HST,GLU\_246,1.06,2.4,-3.44,-2.4  
1XIP,GLU\_261,4.07,1.04,-1.47,0  
2BQQ,TYR\_138,8.92,0.58,-2.9,1.25  
3BQW,GLU\_105,3.56,0.63,-1.57,0  
2R4Q,LYS\_171,10.36,-0.14,0,0  
1GQE,TYR\_24,10,0,0,0  
2QK1,LYS\_486,10.29,-0.21,0,0  
4EF5,ASP\_297,3.73,0.21,-0.28,0  
3P28,GLU\_174,6.34,2.64,-0.8,0  
4ETX,ARG\_382,11.59,-0.91,0,0  
2JKF,LYS\_164,9.94,-0.56,0,0  
4AF2,LYS\_33,10.5,0,0,0  
4H86,GLU\_170,3.42,0.14,-1.22,0  
2AZPHIS\_293,6.43,0,0,-0.07  
1YW5,GLU\_108,4.5,0,0,0  
1QLL,ARG\_24,11.31,-1.19,0,0  
1ILW,ARG\_152,12.43,-0.07,0,0  
2CWY,ARG\_36,11.38,-1.12,0,0  
2AD1,GLU\_65,4.78,0.28,0,0  
2YWJ,LYS\_27,10.15,-0.35,0,0  
1NIJ,ASP\_82,3.28,0.35,-0.87,0  
3A0X,LYS\_750,10.01,-0.49,0,0  
1R53,LYS\_287,10.5,0,0,0  
2EFK,ARG\_143,11.94,-0.56,0,0  
2APL,ASP\_39,3.94,0.21,-0.07,0  
3F6F,ASP\_87,2.38,0.35,-1.76,0  
1YB2,TYR\_110,10,0,0,0,0  
2CIU,GLU\_136,3.08,0.91,-2.33,0  
1H09,TYR\_17,10.26,0.07,0.19,0  
3G9B,LYS\_96,9.94,-0.56,0,0  
2EYJ,LYS\_153,10.5,0,0,0  
1BKR,LYS\_5,10.15,-0.35,0,0  
3PZ9,GLU\_308,4.5,0,0,0  
2BDV,GLU\_16,3.52,0.21,-1.19,0  
3C6B,TYR\_279,10,0,0,0,0  
3EVZ,GLU\_216,4.63,0.14,-0.01,0  
1T95,ARG\_115,12.01,-0.49,0,0  
3E7P,ASP\_199,4.85,0.35,0,0  
3V3T,GLU\_170,4.8,0.58,-0.28,0  
3AUF,GLU\_180,4.51,0.07,-0.06,0  
2CWC,TYR\_267,11.21,0.83,0.0,38  
3LD1,ARG\_281,12.22,-0.28,0,0  
1SIG,ASP\_125,3.21,0.21,-0.8,0  
1T95,ARG\_237,12.08,-0.42,0,0  
1WNH,ARG\_12,11.66,-0.84,0,0  
3K8U,TYR\_82,9.55,0.35,-0.8,0  
3UC9,GLU\_182,4.57,0.07,0,0  
1VJG,ARG\_10,11.8,-0.7,0,0  
3GE9,CYS\_14,7.05,-2.3,0.0,34  
3LMO,GLU\_86,2.45,0.35,-2.4,0  
3ASA,GLU\_303,4.57,0.07,0,0  
3KEY,ASP\_335,3.29,0.07,-0.58,0  
1MJS,ARG\_291,12.01,-0.49,0,0  
1XDZ,CYS\_90,11,-0.01,0,2.01  
2FG1,CYS\_103,9.15,-1.4,0.1,55  
2BDV,LYS\_106,10.43,-0.07,0,0  
2G9D,ARG\_225,12.5,0,0,0  
3GOZ,ARG\_146,13.66,-1.24,0,2.4  
1SQW,ARG\_43,12.15,-0.35,0,0  
3GS3,GLU\_36,4.71,0.21,0,0  
3V75,ASP\_174,2.24,0.84,-2.4,0  
2FDV,LYS\_188,10.43,-0.07,0,0  
2GZQ,GLU\_64,4.57,0.07,0,0  
3IPZ,LYS\_77,10.5,0,0,0  
1O9G,ARG\_75,12.22,-0.28,0,0  
1R6Y,LYS\_82,10.29,-0.21,0,0  
2IF4,ARG\_75,11.59,-0.91,0,0  
2FZ4,HIS\_118,10.02,-0.7,0,-2.52  
1D2K,TYR\_81,9.43,0.07,-0.64,0  
3V4G,GLU\_20,4.12,0.42,-0.8,0  
1WRU,ARG\_330,12.15,-0.35,0,0  
3JSN,GLU\_48,4.64,0.14,0,0  
3JSN,TYR\_275,9.91,0.71,-0.8,0  
2ILR,GLU\_467,3.62,0.21,-1.08,0  
3C38,TYR\_185,9.28,0,-0.72,0  
1WLJ,CYS\_233,10.48,0,-0.06,1.54  
1OXZ,GLU\_271,4.57,0.07,0,0  
3GE9,TYR\_60,10.21,0.21,0,0  
2JKF,ASP\_31,2.87,0.49,-1.42,0  
1FHL,CYS\_118,10.02,-0.7,0,1.72  
3HZQ,TYR\_63,10,0,0,0,0  
2OEW,GLU\_45,4.46,0.21,-0.25,0  
2P5D,LYS\_89,10.22,-0.28,0,0  
2ZQ5,ARG\_92,12.08,-0.42,0,0  
3CCY,ARG\_73,12.08,-0.42,0,0  
2H2Z,HIS\_164,0.42,0,-0.22,-5.85  
3CGW,CYS\_239,8.99,-0.59,0,0.58  
1PDB,ARG\_65,10.89,-1.61,0,0  
3HUE,GLU\_124,3.78,0.56,-1.29,0  
2IF4,GLU\_276,3.88,0.28,-0.9,0

4FD6,GLU\_157,4.3,0.35,-0.55,0  
 3P29,LYS\_118,10.22,-0.28,0,0  
 3RLN,ASP\_576,4.05,0.28,-0.03,0  
 2ILR,LYS\_528,10.15,-0.35,0,0  
 1NWA,ARG\_22,11.73,-0.77,0,0  
 3ETU,ARG\_267,11.54,-1.21,0,0.25  
 2B0A,CYS\_42,6.42,-3.37,0,0.79  
 3B21,ARG\_79,11.24,-1.26,0,0  
 2P0Y,GLU\_293,4.8,0.49,-0.19,0  
 3M7D,ASP\_365,3.43,0.14,-0.51,0  
 3GW3,ARG\_148,12.5,0,0,0  
 2Z0W,LYS\_51,10.5,0,0,0  
 1NFN,CYS\_112,9.91,-0.06,0,0.97  
 2OEW,LYS\_202,10.43,-0.07,0,0  
 1S1Y,ARG\_124,11.59,-0.91,0,0  
 2GZQ,CYS\_167,9.07,0,0,1.68  
 2CX1,ASP\_21,2.75,0.63,-0.67,0  
 1QQE,TYR\_134,9.47,0.07,-0.6,0  
 2P1W,CYS\_182,9.35,0,0,0.35  
 2DVK,HIS\_94,7.01,0.58,0,-0.07  
 3V3T,LYS\_302,9.87,-0.63,0,0  
 3N2T,ARG\_40,11.8,-0.7,0,0  
 2C2Y,ASP\_13,3.41,0.35,-0.74,0  
 2B2H,LYS\_361,10.29,-0.21,0,0  
 1T6L,LYS\_158,10.5,0,0,0  
 2NRK,GLU\_71,4.05,0.35,-0.8,0  
 3EGN,GLU\_393,3.51,0.42,-1.41,0  
 2APL,LYS\_15,10.15,-0.35,0,0  
 2AZL,ARG\_90,13.42,-1.48,0,2.4  
 2Y0O,ARG\_158,12.29,-0.21,0,0  
 1AK1,ARG\_31,12.15,-0.35,0,0  
 2P4D,TYR\_124,13.41,0.43,0.58,2.4  
 1RWZ,LYS\_65,9.73,-0.77,0,0  
 2P4D,LYS\_40,10.43,-0.07,0,0  
 3LH5,GLU\_570,4.0,14,-0.64,0  
 3IU5,ASP\_108,2.7,0.49,-1.59,0  
 2P0L,ASP\_25,4.01,0.21,0,0  
 3CGW,CYS\_277,9.19,-0.23,0,0.42  
 3RNV,LYS\_340,10.36,-0.14,0,0  
 4F8A,TYR\_609,13.43,1.3,-2.4,12  
 3M66,LYS\_350,10.5,0,0,0  
 3S0A,TYR\_110,13.41,0.21,0.8,2.4  
 1AK1,GLU\_20,3.79,0.21,-0.92,0  
 2VG1,GLU\_112,1.02,1.46,-3,-1.94  
 3M7G,LYS\_248,10.5,0,0,0  
 2R0S,LYS\_95,10.5,0,0,0  
 1JKS,LYS\_121,10.36,-0.14,0,0  
 3C38,GLU\_105,4.43,0.07,-0.14,0  
 2F19,ARG\_95,11.94,-0.56,0,0  
 3G9B,CYS\_55,8.57,-0.43,0,0  
 3PU6,CYS\_7,11,-0.18,0,2.18  
 3CS1,TYR\_71,9.95,0,-0.05,0  
 3M66,LYS\_186,10.29,-0.21,0,0  
 3B79,ASP\_109,4.06,0.35,-0.09,0  
 2PP6,ASP\_6,3.87,0.07,0,0  
 1AKO,GLU\_183,1.04,2.52,-3.58,-2.4  
 1J33,ARG\_279,11.94,-0.56,0,0  
 2CWC,TYR\_141,10.0,0.39,-0.39,0  
 1Q2Y,LYS\_52,10.5,0,0,0  
 3RFF,GLU\_98,1.76,0.46,-0.8,-2.4  
 3TMO,GLU\_197,4.64,0.14,0,0  
 2IQT,ASP\_38,3.45,0.28,-0.63,0  
 3Q6L,LYS\_82,10.29,-0.21,0,0  
 3FWU,ASP\_55,3.69,0.14,-0.25,0  
 1EW4,HIS\_7,6.66,0.3,0,-0.14  
 1WXQ,ARG\_311,11.94,-0.56,0,0  
 2P0L,ASP\_236,3.94,0.21,-0.07,0  
 2H8O,ARG\_293,11.87,-0.63,0,0  
 3BWT,ASP\_594,3.17,0.28,-0.91,0  
 2BV9,TYR\_167,8.64,0.5,-0.66,-1.2  
 3BB7,LYS\_358,10.22,-0.28,0,0  
 2AZP,ARG\_17,13.92,-1.91,0,3.33  
 3C2E,CYS\_66,10,0,0,1  
 3CS1,GLU\_106,4.78,0.28,0,0  
 4E9E,ARG\_468,12.29,-0.21,0,0  
 2FZ4,GLU\_147,4.17,0.21,-0.54,0  
 2R4Q,GLU\_223,4.57,0.07,0,0  
 3ONT,LYS\_134,10.36,-0.14,0,0  
 4FH3,ASP\_82,3.85,0.07,-0.02,0  
 2VAN,GLU\_288,4.35,0,-0.15,0  
 2P0L,TYR\_121,10.45,0.61,-0.16,0  
 1WRU,ARG\_270,11.59,-0.91,0,0  
 3I4T,HIS\_205,6.82,0.46,0,-0.14  
 3CCY,TYR\_49,10.07,0.07,0,0  
 2WOZ,LYS\_494,10.15,-0.35,0,0  
 3A7L,LYS\_11,10.36,-0.14,0,0  
 3ETV,LYS\_343,10.36,-0.14,0,0  
 3GEC,LYS\_500,10.5,0,0,0  
 1CHD,LYS\_205,10.43,-0.07,0,0  
 2R2Y,LYS\_113,10.5,0,0,0  
 2HXB,ASP\_150,4.01,0.21,0,0  
 4D8L,ARG\_70,11.66,-0.84,0,0  
 3CAN,GLU\_130,3.84,0.14,-0.8,0  
 1ILW,ASP\_88,3.53,0.21,-0.48,0  
 3GE9,GLU\_130,4.5,0,0,0  
 3U2R,ARG\_121,12.01,-0.49,0,0  
 3C6B,GLU\_93,3.81,0.42,-1.11,0  
 2Z14,TYR\_39,12.31,0.14,-0.3,2.47  
 2CVB,LYS\_49,10.29,-0.21,0,0  
 1O5T,LYS\_264,10.36,-0.14,0,0  
 3H5T,LYS\_292,10.29,-0.21,0,0  
 2Z0M,LYS\_331,10.22,-0.28,0,0  
 1MJS,LYS\_408,10.43,-0.07,0,0  
 3BWT,HIS\_721,6.43,0,0,-0.07  
 2CWY,TYR\_18,10,0,0,0  
 4AM1,TYR\_89,10.83,1.41,-0.05,-0.53  
 2FZ4,LYS\_37,10.43,-0.07,0,0  
 3TRE,LYS\_47,10.15,-0.35,0,0  
 2GYZ,ARG\_63,12.22,-0.28,0,0  
 2R2Y,LYS\_44,10.5,0,0,0  
 1YTO,LYS\_41,10.29,-0.21,0,0  
 2P4D,ARG\_13,11.87,-0.63,0,0  
 3EJC,ARG\_155,11.73,-0.77,0,0  
 2Z61,LYS\_265,10.22,-0.28,0,0  
 3DTE,GLU\_102,4.57,0.07,0,0  
 3O7K,ARG\_115,12.01,-0.49,0,0  
 3US6,ASP\_12,3.84,0.14,-0.1,0  
 3E7P,TYR\_146,12.3,0.28,-0.38,2.4  
 1P2F,LYS\_129,10.08,-0.42,0,0  
 1IAP,ASP\_211,3.05,0.63,-1.38,0  
 2YLF,ARG\_147,11.52,-0.98,0,0  
 1F2V,ARG\_127,12.22,-0.28,0,0  
 3DTE,ASP\_232,3.87,0.14,-0.07,0  
 3F5D,GLU\_176,4.01,0.07,-0.56,0  
 3RFY,ASP\_391,3.26,0.07,-0.61,0  
 2Q99,ASP\_70,3.11,0.14,-0.83,0  
 1DZF,TYR\_208,10,0,0,0  
 2YXO,LYS\_116,10.08,-0.42,0,0  
 4EKU,GLU\_119,4.29,0.86,-1.07,0  
 4FH3,GLU\_333,4.94,0.44,0,0  
 1R15,ARG\_47,12.43,-0.07,0,0  
 1PNE,CYS\_127,9.58,-2.27,0,2.85  
 3GYW,TYR\_75,10,0,0,0  
 1LTU,TYR\_262,10.58,0.58,0,0  
 2B3M,TYR\_19,9.56,0.29,-0.73,0  
 1FQI,LYS\_397,10.5,0,0,0  
 3FHF,LYS\_32,10.08,-0.42,0,0  
 3M66,HIS\_345,7.44,1.08,0,-0.14  
 2VAN,ARG\_152,11.52,-0.98,0,0  
 1AK1,LYS\_81,10.5,0,0,0  
 3M7G,GLU\_54,4.57,0.07,0,0  
 2X4G,ARG\_166,12.69,-1.69,0,1.88  
 3JZC,GLU\_268,10.5,0,0,0  
 2IXM,GLU\_141,2.46,1.6,-0.8,-2.84  
 1FHL,HIS\_81,4.95,1.74,2.25,-5.55  
 3BQW,GLU\_157,4.5,0,0,0  
 3BQW,TYR\_253,12.01,0.21,-0.64,2.44  
 2OBI,CYS\_37,10.8,-0.22,0,2.02  
 3LH5,HIS\_566,4.81,0.45,0,-2.14  
 2AD1,HIS\_98,6.53,0.03,0,0  
 1WRU,GLU\_111,4.12,0.42,-0.8,0  
 1R53,GLU\_232,4.03,0.28,-0.75,0  
 2J8A,LYS\_320,10.5,0,0,0  
 3C6B,LYS\_203,10.5,0,0,0  
 2H14,GLU\_151,4.92,0.42,0,0  
 1PSW,ARG\_80,12.5,0,0,0  
 2C2Y,LYS\_102,10.5,0,0,0  
 1DVO,LYS\_42,10.5,0,0,0  
 1N81,GLU\_135,3.75,0.39,-1.14,0  
 4F8A,HIS\_579,4.02,0,0,-2.48  
 1MTZ,ASP\_80,3.75,0,-0.05,0  
 2PLQ,LYS\_36,10.5,0,0,0  
 1NWA,GLU\_136,3.84,0.14,-0.8,0  
 1LZL,GLU\_146,4.0,28,-0.79,0  
 2O4D,ASP\_109,3.42,0,-0.38,0  
 2IQT,HIS\_96,6.34,0.05,0,-0.21  
 3QKY,TYR\_112,12.38,0.58,0,1.8  
 3IU5,TYR\_126,10.55,0.07,-0.8,1.28  
 3BCH,TYR\_156,9.85,0,-0.15,0  
 3U2R,GLU\_34,4.57,0.07,0,0  
 2ZQ5,ARG\_256,11.8,-0.7,0,0  
 4DVD,LYS\_17,10.5,0,0,0  
 3IU5,GLU\_70,4.71,0.21,0,0  
 2IN0,TYR\_79,12.62,0.22,2.4  
 3ERF,TYR\_92,10.07,0.07,0,0  
 2P52,TYR\_104,10.14,0.14,0,0  
 1YLN,LYS\_177,10.29,-0.21,0,0  
 3BQE,ASP\_223,3.41,0.28,-0.67,0  
 3KT9,GLU\_50,3.48,0.98,-2,0  
 1X1E,GLU\_53,4.27,0.57,-0.8,0  
 3BWT,LYS\_857,10.29,-0.21,0,0  
 2OPJ,ARG\_142,12.43,-0.07,0,0  
 1ANU,GLU\_126,4.16,0.56,-0.9,0  
 3BQU,HIS\_91,4.28,0,0,-2.22  
 1UW7,CYS\_73,9,0,0,0  
 1EV8,ASP\_110,1.81,0.91,-2.9,0  
 3MIX,HIS\_480,5.06,0.8,0,-2.24  
 2G9D,TYR\_206,10.54,0.54,0,0  
 1D2K,TYR\_50,12.99,0.21,0.38,2.4  
 2PGE,LYS\_150,10.15,-0.35,0,0  
 3CN5,TYR\_145,11.17,1.17,0,0  
 2QV2,ASP\_149,3.73,0.63,-0.7,0  
 2Z0M,HIS\_302,5.71,1.6,0.42,-2.81  
 1Q5Z,HIS\_611,7.16,0.8,0,-0.14  
 3GYW,TYR\_49,10,0,0,0  
 1O5T,ASP\_322,3.66,0.28,-0.42,0  
 2Q13,GLU\_216,4.78,0.28,0,0  
 1YOY,CYS\_65,9,-0.07,0,0.07  
 1EDG,LYS\_114,10.43,-0.07,0,0  
 3RHE,LYS\_59,10.36,-0.14,0,0  
 3J5N,ARG\_173,12.5,0,0,0  
 1AK1,ASP\_278,3.72,0.35,-0.43,0  
 2XHC,ARG\_183,12.15,-0.35,0,0  
 3OBS,GLU\_5,3.72,0.28,-1.05,0  
 1RHS,GLU\_143,4.57,0.07,0,0  
 2IDC,ASP\_133,3.73,0.28,-0.35,0  
 2OBS,TYR\_125,10.07,0.07,0,0  
 3GMS,ARG\_175,11.89,-0.61,0,0  
 4H4J,GLU\_176,3.67,0.56,-1.39,0  
 1QQL,CYS\_17,4.58,-5.96,0,1.55  
 3VHJ,ASP\_125,3.45,0.35,-0.7,0  
 3CS1,GLU\_131,4.29,1.22,-0.8,-0.63  
 3MTT,GLU\_493,4.57,0.07,0,0  
 3BPP,TYR\_44,12.43,0.58,0,1.84  
 3HKX,ASP\_229,2.66,1.12,-2.26,0  
 1T07,TYR\_79,13.22,0.21,0.1,2.91  
 3ASA,GLU\_157,4.57,0.07,0,0  
 3LPZ,GLU\_142,2.87,0.77,-2.4,0  
 3R2E,LYS\_95,10.43,-0.07,0,0  
 1WXQ,GLU\_240,3.95,0.21,-0.76,0  
 3V46,TYR\_342,10,0,0,0  
 2R57,CYS\_263,8.54,-0.46,0,0  
 3J5N,LYS\_265,10.29,-0.21,0,0  
 2IDC,GLU\_142,2.87,0.77,-2.4,0  
 3LJC,GLU\_201,4.64,0.14,0,0  
 2B61,ASP\_343,1.91,0.49,-2.37,0  
 3TOW,HIS\_196,7.77,1.42,0,-0.14  
 3K8U,TYR\_6,10.07,0.07,0,0  
 3DHN,GLU\_132,4.5,0,0,0  
 1NAF,ASP\_171,2.92,0,-0.88,0  
 1JKS,ASP\_103,3.43,0.35,-0.72,0  
 3B21,GLU\_196,2.97,0.63,-2.16,0  
 1XKR,ASP\_55,3.3,0.63,-1.13,0  
 1U53,LYS\_76,10.5,0,0,0  
 2FZ4,CYS\_112,10.84,-0.88,2.06,0.67  
 1WPA,TYR\_467,12.39,0.0,-0.2,39  
 3GEC,ASP\_432,3.22,0.56,-1.14,0  
 1NWA,ASP\_59,2.41,0.7,-2.09,0  
 1R9W,GLU\_338,4.74,0.28,-0.04,0  
 2F4Q,ARG\_227,12.08,-0.42,0,0  
 2O4D,CYS\_73,8.5,-0.5,0,0  
 3DB9,GLU\_204,3.99,0.56,-1.07,0  
 1DCF,GLU\_15,4.5,0,0,0  
 1N81,ARG\_34,11.34,-1.16,0,0  
 1RSS,GLU\_57,4.5,0,0,0  
 2CXA,HIS\_128,5.21,0,0,-1.29  
 3RVC,ARG\_88,12.43,-0.07,0,0  
 4DBX,GLU\_184,2.45,0.35,-2.4,0  
 3NJM,ASP\_91,5.21,1.61,-0.2,0  
 1RWZ,ASP\_72,4.11,0.35,-0.04,0  
 1TXJ,ASP\_140,3.1,0.63,-1.33,0  
 1VSM,ASP\_82,2.68,0.49,-1.62,0  
 1BN6,ASP\_291,3.21,0.21,-0.8,0  
 2EFK,ASP\_286,3.38,0.49,-0.91,0  
 2O8P,GLU\_32,3.91,0.21,-0.8,0  
 3TMO,ASP\_256,3.7,0,-0.1,0  
 1L2F,ARG\_104,12.5,0,0,0  
 2Q13,LYS\_172,10.36,-0.14,0,0  
 2FBQ,LYS\_128,10.29,-0.21,0,0  
 4EVF,GLU\_242,10.5,0,0,0  
 3V4G,CYS\_68,8.6,-0.68,0,0.28  
 1R15,LYS\_267,10.5,0,0,0  
 1SNT,GLU\_153,4.71,0.21,0,0  
 1RHS,ARG\_229,11.8,-0.7,0,0  
 1X9G,LYS\_182,10.43,-0.07,0,0  
 2GZQ,HIS\_130,7.88,2.46,2.97,-4.05  
 1ZBS,CYS\_89,7.82,-1.4,0,0.21  
 1M5I,ARG\_213,11.66,-0.84,0,0  
 1Q2Y,ASP\_140,4.01,0.21,0,0  
 3T8R,LYS\_121,10.15,-0.35,0,0  
 1H09,HIS\_132,6.5,0,0,0  
 1FQI,LYS\_398,10.43,-0.07,0,0  
 3LH5,ARG\_663,11.94,-0.56,0,0  
 2X5Y,HIS\_807,3.39,0.17,0,-3.28  
 3BZT,LYS\_287,10.29,-0.21,0,0  
 1SFE,ARG\_129,12.43,-0.07,0,0

1QZN,LYS\_119,10.43,-0.07,0,0  
1SJ8,GLU\_567,5.01,0.56,-0.05,0  
1YW5,ASP\_36,3.82,0.07,-0.05,0  
4F8A,ASP\_566,3.64,0.28,-0.44,0  
2CE6,LYS\_77,10.36,-0.14,0,0  
2JKF,TYR\_55,10.56,0,0.56  
1JT9,ARG\_33,11.8,-0.7,0,0  
2BAA,ASP\_32,0.84,0.28,-3.24,0  
1JSX,ASP\_194,3.8,0,0,0  
2D7U,ARG\_96,10.36,-2.14,0,0  
3ETV,ASP\_68,3.45,0.49,-0.84,0  
3NR5,TYR\_48,9.9,0.07,-0.17,0  
3CBN,CYS\_58,11.51,-0.49,2.13,0.86  
2A4D,ASP\_114,3.8,0,0,0  
1W7B,LYS\_49,10.5,0,0,0  
1LFP,LYS\_72,10.01,-0.49,0,0  
2IXM,HIS\_237,6.65,0.29,-0.14  
2DVK,HIS\_66,6.36,0,0,-0.14  
3M70,ASP\_229,3.77,0,-0.03,0  
1EYH,GLU\_42,4.03,0.14,-0.61,0  
2CN1,HIS\_243,6.36,0,0,-0.14  
2OGQ,ARG\_516,11.94,-0.56,0,0  
1MTZ,GLU\_71,3.98,0.28,-0.8,0  
2PLQ,ARG\_241,12.29,-0.21,0,0  
1WNH,GLU\_154,3.97,1.07,-1.6,0  
1XKR,ARG\_200,11.94,-0.56,0,0  
4GA2,HIS\_63,4.79,0.95,0,-2.66  
2YX0,ASP\_106,3.04,0.77,-1.53,0  
3ANJ,LYS\_194,10.5,0,0,0  
3F6F,TYR\_44,10.13,0.93,-0.8,0  
4DIU,TYR\_43,13.33,0.41,0.52,2.4  
3Q9P,ASP\_100,3.3,0.21,-0.71,0  
1SQH,ARG\_245,11.94,-0.56,0,0  
2H01,GLU\_64,5.41,0.91,0,0  
3GMS,HIS\_9,7.23,0.8,0,-0.07  
3LJC,GLU\_126,4.5,0,0,0  
3CGW,TYR\_74,10.73,0,0,0.73  
2DFL,ARG\_83,12.36,-0.14,0,0  
1NRI,LYS\_137,10.43,-0.07,0,0  
3ANJ,HIS\_219,1.92,0,0,-4.58  
2C2Y,ASP\_72,3.82,0.21,-0.19,0  
2IN0,HIS\_41,6.29,0,0,-0.21  
3H04,HIS\_59,6.29,0,0,-0.21  
3LJC,GLU\_194,4.57,0.07,0,0  
1KCM,LYS\_235,10.29,-0.21,0,0  
1MJS,ASP\_407,3.93,0.14,-0.01,0  
4F85,GLU\_89,3.93,2.03,-0.8,-1.8  
1MD6,GLU\_33,4.64,0.14,0,0  
3KEY,GLU\_450,3.17,0.29,-0.42,-1.2  
1NWA,ARG\_105,12.29,-0.21,0,0  
2HRZ,ARG\_1,12.5,0,0,0  
4ETX,ASP\_310,2.46,0.21,-1.56,0  
2B2H,TYR\_327,10,0,0,0  
4DNU,HIS\_26,4.32,4.12,0,-6.3  
1SI7,ARG\_116,11.8,-0.7,0,0  
1DTO,ASP\_13,3.9,0.14,-0.04,0  
2AH5,GLU\_186,4.5,0,0,0  
1R3F,ASP\_27,3.25,0.07,-0.62,0  
2QDJ,LYS\_164,10.29,-0.21,0,0  
1OIS,TYR\_240,9.49,0.07,-0.58,0  
3M7D,ARG\_250,11.15,-3.0,1.64  
3IVF,GLU\_386,4.5,0,0,0  
1TLV,LYS\_245,10.29,-0.21,0,0  
3BQW,ASP\_183,2.16,0.63,-2.26,0  
1V6T,ARG\_2,11.87,-0.63,0,0  
3EIZ,LYS\_164,10.29,-0.21,0,0  
2YLF,TYR\_134,13.5,0,0,3.5  
4AE7,GLU\_75,4.5,0,0,0  
2QDJ,LYS\_136,9.73,-0.77,0,0  
2GEN,ARG\_120,12.5,0,0,0  
1TXJ,ASP\_16,2.98,0.63,-1.46,0  
1ZBS,ASP\_108,3.89,0.14,-0.05,0  
1HF8,LYS\_231,10.43,-0.07,0,0  
3QAV,GLU\_47,4.5,0,0,0  
2Y2T,LYS\_49,10.36,-0.14,0,0  
1X04,ARG\_80,12.08,-0.42,0,0  
3COU,GLU\_70,3.0,95,-2.45,0  
1AIL,ASP\_39,3.29,0.35,-0.86,0  
3TRE,HIS\_93,6.42,0.06,0,-0.14  
2FZP,ARG\_265,11.31,-1.19,0,0  
3B4D,HIS\_193,7.23,0.8,0,-0.07  
4FH3,CYS\_159,11.05,0,0,2.05  
1OXZ,LYS\_174,10.22,-0.28,0,0  
2YWJ,GLU\_33,3.66,0.14,-0.98,0  
2X5Y,LYS\_758,10.29,-0.21,0,0  
3ONT,ARG\_133,12.08,-0.42,0,0  
1TJE,ASP\_168,4.08,0.28,0,0  
3GW3,LYS\_104,10.5,0,0,0  
3GS9,GLU\_137,4.92,0.42,0,0  
1RAJ,HIS\_80,2.92,0.74,-1.73,-2.59  
2H2W,ASP\_202,3.8,0,0,0  
3HQX,GLU\_56,4.7,0.6,-0.4,0  
3M70,ASP\_175,3.07,0.56,-1.29,0  
2X4J,ASP\_120,4.08,0.28,0,0  
3L0D,ARG\_77,12.05,-0.45,0,0  
1Q42,TYR\_24,8.52,0.21,-1.69,0  
3V3T,ARG\_167,11.73,-0.77,0,0  
2BT8,CYS\_222,8.49,-0.89,0,0.38  
3GEC,ASP\_405,2.75,0.49,-1.55,0  
1RIS,HIS\_144,4.76,1.6,2.01,-5.35  
2B6P,TYR\_219,13.28,0.28,0.6,2.4  
3EJC,LYS\_47,10.5,0,0,0  
2GZR,GLU\_230,3.52,0.63,-1.61,0  
3P28,CYS\_240,7.19,-1.82,0,0  
3DSH,LYS\_243,10.29,-0.21,0,0  
3DHN,ARG\_106,12.46,-1.84,0,1.8  
4FZR,ASP\_352,1.82,0.42,-2.4,0  
4DBX,LYS\_70,10.29,-0.21,0,0  
1WPA,LYS\_506,10.43,-0.07,0,0  
200K,LYS\_111,10.36,-0.14,0,0  
2JKF,GLU\_147,4.12,0.21,-0.59,0  
1RIG,TYR\_8,11.42,1.56,-0.14,0  
3JSN,GLU\_46,3.11,1.26,-2.4,-0.25  
2I6I,ASP\_38,3.44,0.35,-0.71,0  
1BKB,ASP\_98,2.36,0.84,-2.28,0  
2HRZ,GLU\_167,1.64,2.74,-3.2,-2.4  
2XJ4,ARG\_225,11.87,-0.63,0,0  
3I4T,GLU\_104,4.64,0.14,0,0  
3C6B,TYR\_126,8.54,1.3,0,-2.76  
3ILC,TYR\_173,10.02,0.82,-0.8,0  
3UPD,HIS\_280,4.98,0.8,0,-2.32  
2O8I,ASP\_136,4.01,0.21,0,0  
2R2Y,CYS\_88,9,0,0,0  
1PGV,GLU\_301,4.42,0.42,-0.5,0  
1OXZ,GLU\_220,4.14,0.28,-0.64,0  
2Z0W,ARG\_23,12.43,-0.07,0,0  
1YLN,ASP\_80,3.29,0.28,-0.79,0  
4DNU,GLU\_271,4.5,0,0,0  
3RJX,HIS\_235,2.75,0,0,-3.75  
4D8L,TYR\_156,11.58,1.52,-0.1,0.16  
1DZF,LYS\_161,9.94,-0.56,0,0  
3ONT,ASP\_105,3.32,0.07,-0.56,0  
3RLE,GLU\_187,4.57,0.07,0,0  
1RWZ,ASP\_134,1.63,0.84,-3.01,0  
2ZTY,TYR\_122,10,0,0,0  
1OTM,GLU\_241,4.57,0.07,0,0  
2XMZ,GLU\_203,4.81,0.63,-0.32,0  
3CJW,GLU\_189,3.07,2.39,-1.42,-2.4  
3HUE,ARG\_49,12.15,-0.35,0,0  
3BCH,TYR\_204,11.71,0.07,-0.44,2.07  
2H14,CYS\_134,12.08,-0.67,0.33,3.42  
1F09,GLU\_354,3.59,0.21,-1.12,0  
1PSW,ASP\_329,3.31,0.35,-0.84,0  
3LJN,ARG\_34,12.15,-0.35,0,0  
1OIS,LYS\_320,10.43,-0.07,0,0  
2FC3,LYS\_117,10.29,-0.21,0,0  
1ES9,GLU\_150,4.53,0.21,-0.18,0  
3LJN,ASP\_63,3.84,0.14,-0.1,0  
1X04,GLU\_94,4.09,0.84,-1.25,0  
3RLN,GLU\_595,4.57,0.07,0,0  
2X5Y,ASP\_883,3.91,0.21,-0.1,0  
3MTT,GLU\_593,4.05,0.35,-0.8,0  
1R3D,GLU\_149,3.65,0.21,-1.06,0  
1NFN,ASP\_154,2.83,0.63,-1.6,0  
1OLR,TYR\_161,11.27,0.77,-0.18,0.68  
1V43,LYS\_20,10.08,-0.42,0,0  
2OYZ,ASP\_72,3.49,0.49,-0.8,0  
2WB8,TYR\_747,12.41,1.73,-1.1,1.78  
3BA1,ARG\_175,12.5,0,0,0  
3LD1,GLU\_222,4.43,0.07,-0.14,0  
3F6F,HIS\_57,6.5,0,0,0  
2B78,ASP\_43,3.79,0.28,-0.29,0  
1NRI,ARG\_17,12.5,0,0,0  
1LPL,TYR\_168,10.07,0.07,0,0  
2IN0,GLU\_99,4.5,0,0,0  
1SUU,CYS\_552,9.39,-1.35,0,1.73  
3HUE,GLU\_83,4.5,0,0,0  
1OXZ,GLU\_172,4.27,0.14,-0.37,0  
3JZ9,GLU\_425,2.09,1.19,-3.6,0  
3V55,TYR\_407,12.65,0.77,-0.52,2.4  
2R2Y,GLU\_119,4.06,0.35,-0.79,0  
3F6F,ASP\_81,2.51,0.42,-1.71,0  
3H5T,TYR\_53,10,0,0,0  
1W24,HIS\_124,6.36,0,0,-0.14  
3BPV,ARG\_24,12.5,0,0,0  
2V4U,ASP\_496,3.18,0.21,-0.83,0  
1DCF,GLU\_64,4.78,0.28,0,0  
1OOX,LYS\_87,10.5,0,0,0  
2QVT,ASP\_108,3.43,0.42,-0.79,0  
1Q42,GLU\_119,4.1,0.28,-0.68,0  
1Q46,TYR\_113,12.04,0.09,1.94  
1S7K,HIS\_54,6.46,0.03,0,-0.07  
2F9F,GLU\_98,2.43,1.39,-1.06,-2.4  
2APL,ARG\_74,12.61,-0.47,0,0.58  
1O17,LYS\_42,10.5,0,0,0  
2PWQ,LYS\_69,10.43,-0.07,0,0  
3HVM,LYS\_233,10.36,-0.14,0,0  
1O59,LYS\_326,10.01,-0.49,0,0  
1HF8,ARG\_206,11.99,-0.61,0,0.1  
3JZN,LYS\_89,10.43,-0.07,0,0  
1WPA,LYS\_485,10.43,-0.07,0,0  
1NFN,GLU\_50,4.99,0.56,-0.07,0  
2A6B,HIS\_56,4.31,0.02,0,-2.21  
1EYH,GLU\_55,3.98,0.28,-0.8,0  
3ULX,ARG\_107,12.5,0,0,0  
1T3Y,GLU\_84,4.57,0.07,0,0  
3LMF,ARG\_47,12.08,-0.42,0,0  
3G9T,ARG\_286,11.66,-0.84,0,0  
1SIG,ASP\_160,4.08,0.28,0,0  
1RL0,GLU\_116,2.9,0.42,-2.02,0  
2ROS,ARG\_60,11.87,-0.63,0,0  
1YLN,HIS\_106,6.43,0,0,-0.07  
2POL,TYR\_82,12.45,0.55,0.65,1.25  
3LJC,GLU\_210,4.44,0.28,-0.34,0  
1O9G,HIS\_183,6.36,0,0,-0.14  
2VC8,ARG\_24,12.29,-0.21,0,0  
3GMS,ASP\_313,3.87,0.07,0,0  
2W1R,TYR\_67,10,0,0,0  
1P6F,HIS\_176,5.36,0.8,0,-1.94  
3EJG,ASP\_100,3.77,0,-0.03,0  
1SQW,TYR\_46,10.4,0.4,0,0  
1LTU,LYS\_205,10.36,-0.14,0,0  
3QYB,LYS\_945,10.5,0,0,0  
3TRE,ASP\_78,2.3,0.91,-2.41,0  
200K,ASP\_116,2.93,0.35,-1.22,0  
1ZP2,ASP\_105,3.98,0.28,-0.1,0  
2QOP,GLU\_136,4.5,0,0,0  
1BYI,TYR\_68,9.11,0.73,-1.62,0  
1OIS,LYS\_204,10.43,-0.07,0,0  
3BQW,LYS\_242,10.43,-0.07,0,0  
2PP6,ARG\_66,12.43,-0.07,0,0  
1MIX,TYR\_395,9.95,0,-0.05,0  
1AKO,GLU\_45,4.5,0,0,0  
3HVM,GLU\_21,4.38,0,-0.12,0  
3ILC,TYR\_22,13.41,0.21,0.8,2.4  
1Z3X,ARG\_115,11.94,-0.56,0,0  
200K,HIS\_59,5.12,0.05,0,-1.43  
1P6F,ARG\_50,12.15,-0.35,0,0  
2PGE,ARG\_227,11.8,-0.7,0,0  
1R53,ARG\_285,12.5,0,0,0  
1JT9,ASP\_98,2.03,1.05,-2.82,0  
3I47,CYS\_133,9.35,0,0,0.35  
3FFM,GLU\_136,4.64,0.14,0,0  
1OLR,ASP\_179,3.86,0.14,-0.08,0  
1I60,LYS\_194,10.29,-0.21,0,0  
2NRR,CYS\_449,10.19,-0.19,0,1.38  
2CXA,HIS\_9,6.43,0,0,-0.07  
1R53,CYS\_234,8.63,-0.37,0,0  
4E8B,GLU\_149,4.64,0.14,0,0  
3EUR,CYS\_43,8.23,-1.5,0,0.73  
2QV2,ASP\_92,3.13,0.63,-1.3,0  
3PBH,HIS\_145,3.29,0.85,-0.98,-3.08  
1P4X,ASP\_59,2.92,0.56,-1.44,0  
4D8L,ASP\_227,3.35,0.35,-0.8,0  
1AKI,ARG\_310,12.29,-0.21,0,0  
3N2T,GLU\_252,3.26,0.35,-1.59,0  
1NJ4,LYS\_64,10.29,-0.21,0,0  
1SJ8,CYS\_732,6.42,-4.82,0.91,1.33  
3UV9,TYR\_364,13.55,0.35,0.8,2.4  
3LE4,HIS\_343,7.78,1.49,0,-0.21  
2XJ4,GLU\_65,3.84,0,-0.66,0  
3LH5,TYR\_520,9.86,0.07,-0.8,0.59  
2QHT,ARG\_22,12.5,0,0,0  
2H85,HIS\_14,7.55,1.26,0,-0.21  
1UXO,GLU\_158,4.85,0.35,0,0  
2WB8,ARG\_772,11.94,-0.56,0,0  
2FZP,LYS\_278,10.15,-0.35,0,0  
1NWA,GLU\_55,2.88,0.78,-2.4,0  
3M16,LYS\_269,10.01,-0.49,0,0  
2GLU,GLU\_69,4.5,0,0,0  
1SNT,TYR\_20,8.61,0.21,-1.6,0  
1WXQ,LYS\_391,10.36,-0.14,0,0  
3N2T,ASP\_235,2.69,0.77,-1.89,0  
3JZN,LYS\_398,9.94,-0.56,0,0  
2EJX,ASP\_77,2.82,0.77,-1.75,0  
3CN5,ARG\_190,12.01,-0.49,0,0  
1UOH,ARG\_41,12.77,-1.53,0,1.8  
1UW7,LYS\_81,10.5,0,0,0  
1LTU,CYS\_52,9.43,-0.45,0,0.88  
1ZYL,GLU\_151,3.67,2.33,-0.76,-2.4  
1YTQ,GLU\_24,4.54,0.21,-0.17,0  
2X5Y,LYS\_727,10.08,-0.42,0,0  
1O9G,HIS\_73,2.64,0,0,-3.86  
3GA2,HIS\_122,3.17,0,0,-3.33  
3TOW,LYS\_170,10.29,-0.21,0,0  
1X9G,ARG\_179,11.87,-0.63,0,0

3GEC,HIS\_430,6.36,0,0,-0.14  
2OJQ,GLU\_491,3.98,0.28,-0.8,0  
2FC3,GLU\_13,4.5,0,0,0  
2X4G,ARG\_195,12.22,-0.28,0,0  
3IL3,ARG\_315,11.66,-0.84,0,0  
2QZQ,GLU\_139,2.86,0.28,-1.92,0  
2APL,ARG\_37,11.59,-0.91,0,0  
1UOH,HIS\_119,6.99,0.71,0,-0.21  
1SI7,ARG\_147,11.5,-1.33,0,0.33  
3HYQ,GLU\_169,3.55,0.42,-1.37,0  
3LE4,TYR\_333,9.41,0.21,-0.8,0  
2BAA,ARG\_13,12.36,-0.14,0,0  
1R3F,LYS\_207,10.43,-0.07,0,0  
3IL3,ASP\_150,2.91,0.7,-1.59,0  
3LJC,LYS\_146,10.43,-0.07,0,0  
2G5X,TYR\_99,10,0,0,0  
3S0A,ASP\_37,3.54,0.21,-0.47,0  
2P65,ASP\_71,2.9,0.28,-1.18,0  
1SQW,ARG\_38,11.66,-0.84,0,0  
3KEY,LYS\_329,10.5,0,0,0  
3UAH,ASP\_177,3.28,0.28,-0.8,0  
2IF4,GLU\_259,4.5,0,0,0  
2E0T,ARG\_206,11.94,-0.56,0,0  
1TR9,ARG\_192,12.29,-0.21,0,0  
2Z61,LYS\_56,10.5,0,0,0  
2BLL,TYR\_423,13.34,0.14,0.8,2.4  
1OIS,LYS\_227,10.29,-0.21,0,0  
3P2F,GLU\_131,4.28,0.52,-0.74,0  
1PBV,ASP\_161,3.21,0.21,-0.8,0  
3CE7,ARG\_50,12.29,-0.21,0,0  
2RFA,TYR\_162,10.93,0.37,0,0.56  
2YT4,ASP\_636,3.93,0.14,-0.01,0  
1FKM,LYS\_283,10.43,-0.07,0,0  
1J33,ASP\_297,3.48,0.28,-0.6,0  
2ZOM,ARG\_104,12.29,-0.21,0,0  
1OGL,ARG\_116,12.36,-0.14,0,0  
2QHT,ARG\_64,11.87,-0.63,0,0  
1BYI,ARG\_32,12.22,-0.28,0,0  
1NIJ,ARG\_120,12.15,-0.35,0,0  
3F53,TYR\_62,10,0,0,0  
1N4,ARG\_248,11.73,-0.77,0,0  
3I4T,ASP\_66,3.94,0.14,0,0  
1Q5Z,LYS\_615,10.29,-0.21,0,0  
1UOH,GLU\_201,4.78,0.28,0,0  
3M16,TYR\_126,11.37,2.44,-1.11,0.04  
3BPV,ARG\_133,12.5,0,0,0  
2BLL,ARG\_404,12.29,-0.42,0,0  
1J33,ARG\_199,11.94,-0.56,0,0  
4DIU,GLU\_124,4.5,0,0,0  
1XAW,LYS\_497,10.22,-0.28,0,0  
1YB2,ASP\_153,3.8,0.07,-0.07,0  
2G5X,LYS\_39,10.5,0,0,0  
2D7U,TYR\_101,11.91,0.07,-0.56,2.4  
3FTT,ASP\_30,3.87,0.07,0,0  
2E3C,ARG\_257,12.01,-0.49,0,0  
2WB3,ARG\_332,11.52,-0.98,0,0  
2QK1,LYS\_444,10.22,-0.28,0,0  
1P2F,TYR\_123,11.97,0.99,-0.96,1.94  
2CYG,ARG\_72,11.66,-0.84,0,0  
1AKO,LYS\_70,10.22,-0.28,0,0  
2IQT,GLU\_285,3.38,0.28,-1.4,0  
2PP6,ARG\_63,12.5,0,0,0  
2AXO,GLU\_264,4.5,0,0,0  
2FPN,GLU\_153,4.5,0,0,0  
1EDG,HIS\_85,8.25,2.6,2.69,-3.54  
1G8P,ARG\_117,12.5,0,0,0  
3O48,GLU\_78,4.84,0.54,-0.2,0  
2RIK,ASP\_252,3.42,0.49,-0.87,0  
3EGN,TYR\_438,13.78,0.07,0.73,2.98  
1NAR,TYR\_190,12.38,1.6,-0.8,1.58  
1TLV,LYS\_110,10.5,0,0,0  
4F85,TYR\_59,12.26,2.22,0,0.04  
1YM5,ASP\_273,3.27,0.14,-0.67,0  
1M5I,GLU\_152,4.83,0.35,-0.02,0  
1HF8,GLU\_255,4.5,0,0,0  
2OBI,LYS\_164,10.22,-0.28,0,0  
3K8J,ARG\_272,12.5,0,0,0  
1R5Q,ASP\_29,3.39,0.14,-0.56,0  
2XMZ,ARG\_171,11.87,-0.63,0,0  
3EYE,ASP\_38,3.07,0.56,-1.29,0  
2A6B,LYS\_193,10.5,0,0,0  
3EIZ,ASP\_160,2.91,0.14,-1.03,0  
3BCH,HIS\_24,6.44,0.01,0,-0.07  
1SUU,LYS\_527,10.5,0,0,0  
4DIU,ARG\_140,12.29,-0.21,0,0  
3K8U,GLU\_56,4.64,0.14,0,0  
1P4X,ASP\_66,3.86,0.14,-0.08,0  
3GEC,LYS\_532,10.5,0,0,0  
3B7X,TYR\_64,10.54,0,-0.23,0.77  
1X04,GLU\_131,3.88,0.07,-0.69,0  
1Z3X,TYR\_136,10,0,0,0  
1YIB,ARG\_241,12.5,0,0,0  
3EZ7,HIS\_282,6.36,0,0,-0.14  
3BCH,TYR\_37,10.15,0.21,-0.06,0  
3M3P,GLU\_213,3.27,0.35,-1.58,0  
1KCM,GLU\_211,2.42,0.91,-2.99,0  
1X04,LYS\_127,10.08,-0.42,0,0  
3H5T,LYS\_18,10.22,-0.28,0,0  
1RZ2,ARG\_116,11.73,-0.77,0,0  
1BN6,HIS\_65,7.16,0.8,0,-0.14  
1PBV,ASP\_137,4.01,0.21,0,0  
1ZP2,ASP\_44,3.97,0.35,-0.18,0  
1V6T,LYS\_201,10.43,-0.07,0,0  
1WXF,TYR\_85,10.99,0,0.99  
3MTT,LYS\_447,10.5,0,0,0  
1MTZ,GLU\_242,3.18,0.42,-1.74,0  
3C6B,LYS\_178,10.08,-0.42,0,0  
1PGV,ASP\_343,3.49,0.49,-0.8,0  
3GG6,ARG\_39,12.22,-0.28,0,0  
2P52,HIS\_107,7.51,1.08,0,-0.07  
2FZ4,HIS\_44,6.22,0,0,-0.28  
3CE7,LYS\_43,10.29,-0.21,0,0  
1LFP,TYR\_181,10.79,1.19,0,-0.4  
1EDG,TYR\_293,9.85,0.14,-0.29,0  
1RL0,ARG\_53,11.29,-1.21,0,0  
3EVN,HIS\_258,6.43,0,0,-0.07  
1EQ6,LYS\_180,10.5,0,0,0  
1W24,GLU\_123,4.78,0.28,0,0  
2E0T,GLU\_107,4.5,0,0,0  
2BQQ,ASP\_108,1.71,0.42,-2.51,0  
3F1X,ASP\_141,3.55,0.63,-0.87,0  
2CL3,TYR\_226,10.07,0.07,0,0  
3GS3,ASP\_199,2.76,0.07,-1.1,0  
2X4G,ASP\_306,3.06,0.49,-1.23,0  
2OEW,TYR\_294,12.06,0,0.2,0.6  
1KCM,LYS\_153,10.29,-0.21,0,0  
1RKA,GLU\_267,3.47,0.35,-1.38,0  
3HZQ,LYS\_45,10.5,0,0,0  
3LJN,CYS\_271,7.88,-2.37,0,1.25  
3GS3,CYS\_127,11.16,-0.17,0,2.33  
1XKR,LYS\_132,10.5,0,0,0  
2FG1,LYS\_19,9.66,-0.84,0,0  
3BB7,HIS\_49,6.5,0,0,0  
3H13,TYR\_305,12.94,0,0.04,2.9  
2CVB,LYS\_65,10.43,-0.07,0,0  
1GQE,ASP\_231,3.37,0.14,-0.57,0  
2IDC,GLU\_142,3.84,0.49,-1.15,0  
1MTZ,ASP\_146,3.13,0.28,-0.95,0  
2Q99,LYS\_27,10.5,0,0,0  
3G9G,ASP\_243,3.27,0.35,-0.88,0  
1TWU,HIS\_76,6.43,0,0,-0.07  
2EJB,GLU\_136,4.57,0.07,0,0  
2O8P,LYS\_201,10.5,0,0,0  
3RRQ,ARG\_139,12.01,-0.49,0,0  
2HXB,ARG\_16,11.87,-0.63,0,0  
1MML,LYS\_264,10.15,-0.35,0,0  
3CBN,ARG\_126,12.15,-0.35,0,0  
3CGW,TYR\_137,9.63,0,-0.38,0  
3RAZ,CYS\_133,7.72,-1.35,0,0.07  
2EFK,CYS\_145,9.07,0,0,0.07  
2R51,GLU\_62,4.23,0.42,-0.69,0  
3CZC,LYS\_3,10.36,-0.14,0,0  
3U4K,ASP\_76,3.99,0.35,-0.16,0  
4EZB,ARG\_232,12.5,0,0,0  
2ATR,LYS\_11,10.36,-0.14,0,0  
3I47,CYS\_121,11.56,-0.42,0,2.98  
1JKS,ASP\_11,4.01,0.21,0,0  
3A0X,GLU\_605,4.56,0.14,-0.08,0  
1I60,LYS\_61,9.73,-0.77,0,0  
3OAT,ASP\_45,3.89,0.21,-0.12,0  
1ZBM,GLU\_208,4.05,0.35,-0.8,0  
3VJ8,ARG\_133,11.24,-1.26,0,0  
2OJQ,ASP\_560,3.94,0.14,0,0  
4DBL,ASP\_133,3.8,0,0,0  
2G55,GLU\_11,4.5,0,0,0  
3GT0,LYS\_72,10.5,0,0,0  
1TR9,HIS\_173,7.19,0.83,0,-0.14  
3F5D,LYS\_177,10.36,-0.14,0,0  
1M5I,GLU\_202,4.64,0.14,0,0  
1HF8,ARG\_243,13.06,-0.77,0,1.33  
3CAN,CYS\_31,9.04,-0.03,0,0.07  
1PNE,TYR\_24,10.19,0.19,0,0  
3CIV,GLU\_186,2.04,3.27,-4.58,-1.17  
3M7D,ARG\_20,11.66,-0.84,0,0  
1ATO,ASP\_347,3.7,0.49,-0.59,0  
3GT0,GLU\_217,4.4,0.14,-0.24,0  
1O0X,LYS\_200,10.36,-0.14,0,0  
3CCY,ARG\_121,11.8,-0.7,0,0  
3DTE,ASP\_55,3.89,0.14,-0.05,0  
3I4T,HIS\_139,6.5,0,0,0  
3IBT,CYS\_98,9.17,-3.78,0,3.96  
1NWA,ARG\_162,11.87,-0.63,0,0  
1JSX,ARG\_101,11.94,-0.56,0,0  
4ETX,ARG\_360,12.43,-0.07,0,0  
2QVT,LYS\_143,10.29,-0.21,0,0  
3I47,LYS\_238,9.52,-0.98,0,0  
1NAR,GLU\_207,4.64,0.14,0,0  
2QEV,ASP\_49,2.44,0.7,-2.05,0  
1UXO,TYR\_157,10,0,0,0  
2BCF,TYR\_111,8.47,0.35,-1.88,0  
2ZCX,ASP\_166,3.99,0.28,-0.09,0  
3LJI,ARG\_199,11.94,-0.56,0,0  
1TP6,HIS\_121,6.43,0,0,-0.07  
1I60,HIS\_230,1.78,0,0,-4.72  
3IDW,GLU\_29,3.91,0.21,-0.8,0  
3F5D,LYS\_108,10.5,0,0,0  
3RE9,GLU\_107,2.85,0.35,-2,0  
3M66,ASP\_239,2.26,0.28,-1.82,0  
2BLL,ARG\_535,7.58,-2.7,0,-2.22  
1AIL,ARG\_44,12.22,-0.28,0,0  
1V8E,ARG\_122,12.15,-0.35,0,0  
2XKZ,TYR\_215,10.69,0.14,0,0.55  
4EKU,HIS\_103,4.24,0.8,0,-3.06  
3MIX,GLU\_623,4.5,0,0,0  
2OEW,GLU\_34,4.6,0.35,-0.25,0  
3PBH,ASP\_254,3.8,0.14,-0.14,0  
3L3P,GLU\_484,4.5,0,0,0  
2V81,ASP\_167,3.82,0.14,-0.12,0  
4EZB,TYR\_221,9.55,0.07,-0.52,0  
3E7P,CYS\_255,11.45,0,0.2,4.5  
1U7U,TYR\_323,11.9,1.41,0,0.49  
1T95,LYS\_84,10.43,-0.07,0,0  
2Q13,TYR\_262,10.8,0,-0.05,0.85  
2OKT,TYR\_121,10.24,0.77,-0.53,0  
3HUE,CYS\_66,10.64,-0.01,0.47,1.18  
1JT9,ASP\_95,4.13,0.42,-0.09,0  
2DG7,ARG\_14,12.29,-0.21,0,0  
2Z84,CYS\_23,8.99,-0.01,0,0  
1O59,ARG\_75,12.5,0,0,0  
1UOH,LYS\_149,10.43,-0.07,0,0  
2D2S,ASP\_568,3.8,0.07,-0.07,0  
3PU6,GLU\_11,4.12,0.42,-0.8,0  
2Q13,TYR\_378,10.86,0,0,0.86  
3R2B,LYS\_108,10.5,0,0,0  
3H9W,HIS\_107,6.36,0,0,-0.14  
1PSW,TYR\_214,12.2,0,0,2.2  
3U0V,LYS\_153,10.22,-0.28,0,0  
2PGX,LYS\_238,10.5,0,0,0  
1ZBM,GLU\_51,2.81,0.7,-2.4,0  
3BQE,GLU\_358,3.89,0.14,-0.75,0  
2HXB,LYS\_62,10.15,-0.35,0,0  
1WYC,ASP\_323,3.94,0.14,0,0  
1R16,ARG\_280,8.52,-2.52,0,-1.46  
3GE9,HIS\_96,4.53,0.82,0,-2.79  
1G8P,GLU\_71,5.06,0.56,0,0  
2CXC,ARG\_97,12.5,0,0,0  
1T95,ASP\_202,2.18,0.35,-1.98,0  
1LZL,ASP\_73,4.42,0.7,-0.08,0  
2YX0,GLU\_336,4.57,0.07,0,0  
2X5Y,LYS\_836,10.36,-0.14,0,0  
3M66,LYS\_327,10.22,-0.28,0,0  
3FH,GLU\_174,3.73,0.21,-0.98,0  
2AD1,HIS\_113,5.27,0,0,-1.23  
3RVC,ARG\_118,12.15,-0.35,0,0  
4FCU,GLU\_152,3.25,0.35,-1.6,0  
1OGL,GLU\_237,4.3,0.14,-0.34,0  
1QZN,TYR\_95,12.03,0.46,-1.76,3.34  
2H85,GLU\_326,4.43,0.35,-0.42,0  
1T3Y,GLU\_121,4.57,0.07,0,0  
3H6Q,ASP\_62,4.08,0.28,0,0  
2WB3,GLU\_289,4.5,0,0,0  
3EVN,LYS\_138,10.22,-0.28,0,0  
3GMS,HIS\_300,6.43,0,0,-0.07  
1GPP,CYS\_1,7.86,-0.19,-1.93,0.98  
2IN0,GLU\_4,4.25,0,-0.25,0  
3OBS,TYR\_63,10.01,0,-0.75,0.76  
4F85,ASP\_190,4.06,0.28,-0.02,0  
3FK5,LYS\_71,10.29,-0.21,0,0  
3L7N,GLU\_204,4.36,0.07,-0.21,0  
3UV9,HIS\_312,6.5,0,0,0  
1WRU,ARG\_24,12.65,-3.23,0,3.38  
3Q1C,TYR\_151,10,0,0,0  
2P52,ARG\_172,9.79,-1.48,0,-1.23  
3RNV,ASP\_420,3.42,0.35,-0.73,0  
3H9W,ASP\_96,2.59,0.91,-2.12,0  
1YM5,GLU\_136,3.72,0.14,-0.92,0  
1NRI,CYS\_225,8.55,-0.6,0,0.14  
3EVP,LYS\_199,10.5,0,0,0  
2G2D,GLU\_41,2.31,0.21,-2.4,0  
2R51,TYR\_128,10.38,1.52,-1.14,0  
1OXZ,ASP\_269,3.52,0.14,-0.42,0  
2GEN,GLU\_80,3.53,0.21,-1.18,0  
3GFP,LYS\_478,10.5,0,0,0  
3Q2C,GLU\_31,4.5,0,0,0  
2FD5,LYS\_65,10.5,0,0,0  
3JZN,GLU\_90,1.06,2.34,-3.34,-2.44



1E5S,LYS\_177,10.43,-0.07,0,0  
3FNI,ASP\_37,2.77,0.56,-1.59,0  
3TMO,GLU\_297,3.7,0.77,-1.57,0  
1MTZ,LYS\_92,10.43,-0.07,0,0  
3H6Q,TYR\_27,10.03,0.03,0,0  
4FZR,CYS\_54,9.1,-0.23,0,0.33  
4GA2,LYS\_25,10.36,-0.14,0,0  
2VAN,ARG\_283,11.47,-1.03,0,0  
1SJB,ASP\_514,3.31,0.07,-0.56,0  
1EV8,ASP\_20,2.7,0.91,-2.01,0  
1K9S,LYS\_115,10.5,0,0,0  
2ZCO,TYR\_284,13.27,0.07,0.8,2.4  
1UCH,LYS\_108,10.36,-0.14,0,0  
3P51,ARG\_22,12.22,-0.28,0,0  
1XKR,TYR\_121,12.71,2.71,0,0  
1DOV,ASP\_242,2.75,0.56,-1.61,0  
3DHN,GLU\_213,3.46,0.35,-1.38,0  
3KEY,LYS\_391,10.29,-0.21,0,0  
1XAW,ASP\_461,3.73,0.42,-0.49,0  
1UJ8,ASP\_32,3.94,0.14,0,0  
3K8J,ARG\_89,12.5,0,0,0  
3M3P,HIS\_182,6.5,0,0,0  
1Q8B,GLU\_70,4.64,0.14,0,0  
2Q34,TYR\_175,13.35,0.28,-0.07,3.13  
1QQE,TYR\_201,9.95,0.53,-0.58,0  
3BQE,LYS\_253,10.43,-0.07,0,0  
2NMU,ARG\_125,13.55,-1.35,0,2.4  
3IVF,ASP\_222,4.06,0.28,-0.02,0  
1TR9,TYR\_178,13.67,0.35,-0.19,3.51  
3PM2,LYS\_71,10.43,-0.07,0,0  
1TR9,ARG\_148,11.87,-0.63,0,0  
3P28,GLU\_67,4.06,0.35,-0.79,0  
1HUF,ARG\_104,11.66,-0.84,0,0  
3ETU,GLU\_190,4.5,0,0,0  
2B02,CYS\_459,5.8,-5.26,0,2.06  
2YWX,LYS\_48,10.15,-0.35,0,0  
4AM1,ARG\_208,11.9,-3.0,2.4  
3HVV,ARG\_305,12.43,-0.07,0,0  
3BWT,GLU\_825,4.57,0.07,0,0  
3GMS,TYR\_66,11.19,1.19,0,0  
2YWH,LYS\_100,10.5,0,0,0  
2B3M,LYS\_25,10.29,-0.21,0,0  
2IDC,GLU\_32,4.57,0.07,0,0  
1XKR,ARG\_111,12.01,-0.49,0,0  
2E3I,GLU\_112,3.91,0.21,-0.8,0  
1HUF,ASP\_72,1.59,0.77,-2.97,0  
4EVF,GLU\_20,2.8,0.7,-2.4,0  
3L7N,LYS\_152,10.01,-0.49,0,0  
2H14,TYR\_243,10,0,0,0  
1YW5,ASP\_97,3.58,0.07,-0.3,0  
1R5Q,TYR\_25,13.41,0.21,0.8,2.4  
3OKQ,ASP\_640,3.9,0.14,-0.04,0  
2QZQ,LYS\_150,10.5,0,0,0  
1DOV,ARG\_126,12.01,-0.49,0,0  
2BV9,HIS\_170,1.96,0.75,0,-5.29  
2V81,GLU\_113,3.26,0.35,-1.58,0  
3M16,GLU\_241,4.26,0.46,-0.7,0  
3M70,CYS\_93,10.09,0.57,0.52  
2YYO,HIS\_160,6.51,0.01,0,0  
2F4Q,ARG\_97,12.89,-1.23,0,1.62  
3GOZ,GLU\_70,3.98,0.28,-0.8,0  
3JV1,LYS\_128,10.01,-0.49,0,0  
3GS9,TYR\_286,9.89,0.6,-0.36,-0.35  
3M7G,GLU\_165,3.98,0.28,-0.8,0  
2W0G,ARG\_167,12.5,0,0,0  
2F9F,GLU\_3,4.5,0,0,0  
4E6S,ARG\_29,12.22,-0.28,0,0  
1OLR,ARG\_213,12.08,-0.42,0,0  
4DBX,LYS\_269,10.5,0,0,0  
1GQE,ARG\_213,12.08,-0.42,0,0  
2HRZ,ASP\_246,3.049,-1.28,0  
1DOV,LYS\_216,10.5,0,0,0  
4DNU,ARG\_173,12.29,-0.21,0,0  
2X4G,TYR\_122,12.73,1.8,0,0.93  
2E0T,HIS\_185,7.41,0.98,0,-0.07  
1YW5,LYS\_116,10.5,0,0,0  
2W0G,ASP\_177,3.33,0.28,-0.75,0  
3CGW,ARG\_264,11.94,-0.56,0,0  
1IAP,ARG\_181,12.5,0,0,0  
2NSN,HIS\_33,7.01,0.58,0,-0.07  
3FHF,LYS\_204,10.15,-0.35,0,0  
1OI7,HIS\_224,6.43,0.14,0,-0.21  
2J8A,GLU\_352,4.64,0.14,0,0  
3GMS,TYR\_54,10.31,0.31,0,0  
3KB5,ARG\_309,12.36,-0.14,0,0  
1XTD,LYS\_61,10.5,0,0,0  
3ASA,ARG\_27,12.08,-0.42,0,0  
1G5Z,LYS\_60,10.5,0,0,0  
2H2Z,LYS\_61,10.43,-0.07,0,0  
1KCM,ASP\_146,2.27,0.7,-2.24,0  
1R1S,LYS\_248,10.29,-0.21,0,0  
2H85,GLU\_266,4.73,0.42,-0.19,0  
2BV9,HIS\_286,6.88,0.45,0,-0.07  
3CN5,ASP\_240,3.89,0.14,-0.05,0  
4AM1,TYR\_304,12.37,0.07,0.2,3  
1YTD,LYS\_366,10.5,0,0,0  
3CAN,ASP\_52,3.32,0.35,-0.83,0  
2IDC,LYS\_41,10.43,-0.07,0,0  
2PLQ,LYS\_113,10.5,0,0,0  
1SQH,GLU\_111,4.23,0.42,-0.69,0  
1QZN,ASP\_12,2.66,0.84,-1.98,0  
1ZCE,GLU\_78,4.78,0.28,0,0  
3DHN,LYS\_90,10.43,-0.07,0,0  
1QQH,TYR\_165,10,0,0,0  
1SUU,LYS\_659,10.5,0,0,0  
3RRQ,TYR\_68,9.34,0.14,-0.8,0  
1SIG,ASP\_332,3.84,0.14,-0.1,0  
1HUF,HIS\_9,7.02,0.8,0,-0.28  
1X8F,GLU\_76,4.27,0.21,-0.44,0  
1SQH,LYS\_194,10.01,-0.49,0,0  
2YLF,HIS\_232,6.44,0.01,0,-0.07  
2I88,LYS\_366,10.36,-0.14,0,0  
3MIX,LYS\_491,10.5,0,0,0  
1LZL,GLU\_104,5.29,0.79,0,0  
4FZN,LYS\_77,10.15,-0.35,0,0  
1U53,ASP\_87,4.01,0.35,-0.14,0  
1TXD,CYS\_967,10.91,0,0,1.91  
3HVV,ASP\_313,3.42,0.42,-0.8,0  
3LD1,CYS\_234,9.21,-0.38,0,0.59  
1VJG,LYS\_40,10.43,-0.07,0,0  
1O59,ARG\_161,12.22,-0.28,0,0  
1X04,GLU\_81,4.5,0,0,0  
1ZP2,ARG\_62,11.32,-1.18,0,0  
2QDJ,TYR\_225,8.85,0,-1.15,0  
2H01,ARG\_142,12.5,0,0,0  
2HNG,GLU\_10,4.05,0.35,-0.8,0  
2PGE,TYR\_178,11.3,0.35,0,0.95  
2X4L,ASP\_233,3.92,0.14,-0.02,0  
3CE7,GLU\_46,4.64,0.14,0,0  
3CIV,GLU\_106,4.57,0.07,0,0  
3B79,TYR\_114,9.28,0.43,-1.15,0  
2V4U,CYS\_313,8.22,-0.78,0,0  
3CX5,LYS\_147,10.29,-0.21,0,0  
1GVP,GLU\_5,3.98,0.28,-0.8,0  
2D7J,LYS\_92,10.5,0,0,0  
1SQW,GLU\_49,4.64,0.14,0,0  
2P65,ARG\_41,12.43,-0.07,0,0  
2BCF,ARG\_59,11.94,-0.56,0,0  
1X6J,ARG\_18,12.36,-0.14,0,0  
2JEO,ARG\_165,11.68,-2.29,0,1.47  
1TXJ,ARG\_41,11.73,-0.77,0,0  
4FZR,ARG\_191,12.22,-0.28,0,0  
3ERF,ARG\_50,12.15,-0.35,0,0  
2Z14,TYR\_38,10,0,0,0  
1R29,ASP\_75,3.02,0.42,-1.2,0  
3PP8,ARG\_167,12.08,-0.42,0,0  
2P52,ARG\_287,12.29,-0.21,0,0  
1Q8B,TYR\_15,10,0,0,0  
3DB9,CYS\_158,8.59,-0.97,0,0.56  
2EDM,CYS\_172,8.27,-0.8,0,0.07  
2XHC,LYS\_351,9.87,-0.63,0,0  
1H09,LYS\_308,10.29,-0.21,0,0  
2H85,LYS\_12,10.5,0,0,0  
1YR6,LYS\_225,10.43,-0.07,0,0  
3OOP,GLU\_114,4.57,0.07,0,0  
2YLF,HIS\_159,7.18,1.03,0,-0.35  
2D7U,GLU\_153,4.57,0.07,0,0  
3DZ1,ARG\_209,11.66,-0.84,0,0  
2O4D,GLU\_145,4.5,0,0,0  
2Y2T,ASP\_85,1.94,0.84,-2.7,0  
1MD6,LYS\_73,10.5,0,0,0  
3G9G,LYS\_69,10.43,-0.07,0,0  
1TD6,ARG\_26,12.36,-0.14,0,0  
2C2Y,TYR\_49,10,0,0,0  
3U0V,HIS\_132,10.15,5.2,3.17,-4.72  
3ETU,HIS\_328,5.08,1.84,0,-3.27  
1QQE,LYS\_162,10.5,0,0,0  
1BYI,HIS\_83,6.35,0.13,0,-0.28  
1SIG,LYS\_343,10.29,-0.21,0,0  
2BLL,GLU\_411,4.71,0.21,0,0  
3MEW,ASP\_266,2.76,0.49,-1.53,0  
2PIM,GLU\_77,3.43,0.07,-1.14,0  
3ETV,GLU\_57,4.85,0.35,0,0  
3F6M,ASP\_128,4.08,0.28,0,0  
2VAN,LYS\_331,10.01,-0.49,0,0  
2RGY,LYS\_340,10.5,0,0,0  
2X5Y,TYR\_889,13.86,0.66,0.8,2.4  
1GPP,GLU\_144,4.71,0.21,0,0  
1R7J,LYS\_42,10.36,-0.14,0,0  
1ZBP,GLU\_201,4.5,0,0,0  
2B02,LYS\_417,10.43,-0.07,0,0  
1V43,LYS\_9,10.29,-0.21,0,0  
4EVF,ASP\_19,3.15,0.35,-1,0  
3S0A,ASP\_87,2.55,0.35,-1.6,0  
2X4J,HIS\_31,7.71,1.35,0,-0.14  
1WXF,TYR\_237,13.8,0.6,0.8,2.4  
3HVV,ARG\_323,12.15,-0.35,0,0  
2PWQ,LYS\_145,10.43,-0.07,0,0  
2EJB,GLU\_65,4.57,0.07,0,0  
2RH3,LYS\_110,10.36,-0.14,0,0  
3F1X,LYS\_234,10.5,0,0,0  
3P51,GLU\_87,2.79,0.84,-2.55,0  
1AM2,ARG\_17,12.01,-0.49,0,0  
3ADO,TYR\_151,10.48,1.56,-1.08,0  
3NBI,HIS\_158,6.32,0.03,0,-0.21  
2Q98,LYS\_42,10.36,-0.14,0,0  
1NAR,TYR\_216,11.06,1.77,-0.8,0.09  
3CX5,ASP\_4,1.8,0.56,-2.57,0  
1X7F,GLU\_267,4.21,0.49,-0.78,0  
2O85,ARG\_18,12.5,0,0,0  
1PGV,ARG\_380,12.01,-0.49,0,0  
2AGB,ASP\_217,3.34,0.35,-0.81,0  
3DHN,HIS\_211,7.22,0.86,0,-0.14  
1O9G,GLU\_136,4.26,0.35,-0.59,0  
1R16,TYR\_304,11.72,1.49,-1.7,1.93  
2NRR,ARG\_489,12.01,-0.49,0,0  
3UX2,CYS\_155,9.13,-0.01,0,0.14  
3A7L,GLU\_46,4.5,0,0,0  
3JZ9,GLU\_528,4.5,0,0,0  
3JV1,GLU\_63,3.47,0.49,-1.52,0  
1AD6,GLU\_559,4.78,0.28,0,0  
1JKS,GLU\_94,1.09,1.04,-2.05,-2.4  
2O8I,GLU\_5,4.5,0,0,0  
1XAW,TYR\_493,10.02,0.07,-0.05,0  
2IRM,TYR\_177,13.1,0.28,0.42,2.4  
2JKF,CYS\_37,9.66,0,0,0.66  
1ANU,TYR\_110,10.69,0,0,0.69  
2H2Z,GLU\_290,3.04,1.83,-1.14,-2.16  
3M70,TYR\_137,12.32,0.66,0,1.66  
1PDB,GLU\_154,4.5,0,0,0  
1JT9,HIS\_19,4.66,1.6,-0.21,-3.23  
3B21,ASP\_178,2.74,0.14,-1.2,0  
4E8B,GLU\_225,3.02,0.28,-1.76,0  
3O16,GLU\_111,4.57,0.07,0,0  
2Z0M,GLU\_89,1.85,0.54,-1.02,-2.17  
3FTT,GLU\_5,3.19,0.14,-1.45,0  
1Q46,ARG\_87,11.94,-0.56,0,0  
3AUF,ASP\_82,0.81,0.49,-3.48,0  
2H14,GLU\_279,1.51,1.33,-4.31,0  
2O0K,GLU\_227,4.5,0,0,0  
2H30,GLU\_162,4.56,0.21,-0.15,0  
3GV0,LYS\_271,10.5,0,0,0  
1NAF,ASP\_274,3.39,0.07,-0.48,0  
3AUF,ARG\_65,12.5,0,0,0  
1JYH,TYR\_111,10.14,0,0,0.14  
2EFK,GLU\_223,11.46,-1.04,0,0  
3P28,ASP\_228,3.93,0.28,-0.15,0  
1XTZ,LYS\_195,9.66,-0.84,0,0  
3ON1,ASP\_88,2.33,0.35,-1.82,0  
1ZBP,GLU\_157,1.14,3.84,-2.4,-4.8  
3EVN,LYS\_310,10.36,-0.14,0,0  
1SUU,GLU\_575,3.71,0.35,-1.14,0  
1U3Y,ARG\_255,11.94,-0.56,0,0  
1EV8,ASP\_122,3.94,0.21,-0.07,0  
3PBH,LYS\_39,10.36,-0.14,0,0  
1L2F,GLU\_211,4.28,0.35,-0.57,0  
3ON1,GLU\_23,3.86,0.42,-1.06,0  
2W0Z,LYS\_472,10.29,-0.21,0,0  
3CRM,HIS\_299,6.29,0,0,-0.21  
3UPD,LYS\_208,10.5,0,0,0  
2NSN,GLU\_110,4.5,0,0,0  
1CBY,GLU\_152,4.71,0.21,0,0  
2AZP,ARG\_314,12.15,-0.35,0,0  
3C9C,LYS\_62,10.5,0,0,0  
1MHN,GLU\_104,5.13,0.63,0,0  
4EZB,ASP\_37,2.99,0.42,-1.23,0  
1OXZ,ASP\_204,3.92,0.21,-0.09,0  
1ZBP,GLU\_98,4.55,0,0,0  
1FQI,TYR\_410,9.55,0.07,-0.52,0  
3PZ9,HIS\_48,1.74,1.46,0,-6.21  
3M9A,GLU\_34,4.5,0,0,0  
3LOD,LYS\_92,10.29,-0.21,0,0  
3CX5,CYS\_150,9.29,-0.13,0,0.42  
1T07,ASP\_62,3.26,0.7,-1.23,0  
2OBI,ASP\_7,3.87,0.07,0,0  
2B61,ASP\_76,2.19,0.98,-2.58,0  
2BQQ,ARG\_59,11.24,-1.26,0,0  
2BDV,GLU\_143,3.02,0.28,-1.76,0  
1WPA,LYS\_512,10.22,-0.28,0,0  
3HKX,HIS\_122,6.5,0,0,0  
2AH5,HIS\_23,6.49,0.06,0,-0.07  
1ZYL,GLU\_253,3.66,0.35,-1.19,0  
2HXB,ASP\_44,3.63,0.28,-0.45,0  
3LJC,GLU\_41,4.5,0,0,0  
2V4U,GLU\_423,5.07,0.57,0,0  
3HUE,LYS\_312,10.22,-0.28,0,0

2B3M,ARG\_98,11.38,-1.12,0,0  
2EA9,TYR\_86,10,0,0,0  
1YB2,GLU\_198,4.64,0.14,0,0  
1L2F,ARG\_153,12.22,-0.28,0,0  
3LPZ,TYR\_139,9.65,0.68,0,-1.03  
2PGE,ASP\_13,1.05,0.84,-3.59,0  
2OOK,LYS\_63,10.08,-0.42,0,0  
3GW3,ARG\_238,12.36,-0.14,0,0  
2OKT,HIS\_263,7.16,0.8,0,-0.14  
3CS1,LYS\_56,10.22,-0.28,0,0  
2CWC,HIS\_159,1.71,0.08,-0.61,-4.26  
3CIV,GLU\_295,4.12,0.56,-0.94,0  
1XKR,ASP\_143,3.13,0.28,-0.95,0  
3M66,LYS\_295,10.43,-0.07,0,0  
2J8A,LYS\_269,10.43,-0.07,0,0  
2WB8,GLU\_728,4.19,0.35,-0.66,0  
1SQH,GLU\_196,2.76,1.46,-0.8,-2.4  
2NMU,ASP\_91,2.88,1.05,-1.96,0  
3G9G,TYR\_118,10.4,0.4,0,0  
3ERF,ARG\_215,11.8,-0.7,0,0  
3EUR,LYS\_81,10.5,0,0,0  
4DIU,GLU\_193,2.1,0.49,-2.06,-0.84  
1O17,TYR\_30,9.74,0.86,-1.6,0.47  
2BAA,ARG\_130,12.01,-0.49,0,0  
2DG7,ASP\_50,2.4,0.91,-2.3,0  
2Q13,ARG\_339,12.22,-0.28,0,0  
3UPD,TYR\_107,13.07,0.96,-0.29,2.4  
3V55,GLU\_653,3.45,0.28,-1.33,0  
2GSX,ASP\_105,3.34,0.28,-0.74,0  
3GW3,CYS\_59,12.25,-0.25,1.76,1.74  
1OIS,GLU\_312,2.69,0.98,-2.79,0  
2PWQ,GLU\_33,4.99,0.49,0,0  
1X7F,CYS\_197,9.29,-0.25,-1.18,1.72  
3TIR,ASP\_179,3.5,0.28,-0.58,0  
3JRT,ASP\_112,2.34,0.49,-1.95,0  
3ANJ,HIS\_114,9.71,1.6,3.75,-2.14  
1XWM,LYS\_15,10.43,-0.07,0,0  
2YX0,LYS\_341,10.5,0,0,0  
1JT9,GLU\_197,4.49,0.14,-0.15,0  
1X91,LYS\_130,10.43,-0.07,0,0  
2PWQ,CYS\_87,7.36,-1.78,0,0.14  
4FD6,LYS\_123,10.5,0,0,0  
1WNH,GLU\_73,3.98,0.28,-0.8,0  
3V75,ARG\_12,12.01,-0.49,0,0  
3RE9,LYS\_134,10.22,-0.28,0,0  
2E3C,ASP\_313,3.4,0.35,-0.75,0  
2P5D,TYR\_6,12.65,0.07,0.18,2.4  
1FQI,ARG\_318,12.08,-0.42,0,0  
3RJZ,LYS\_205,10.29,-0.21,0,0  
1XFK,HIS\_27,7.07,0.92,0,-0.35  
1OIS,GLU\_216,4.4,0.7,-0.8,0  
1WPA,ASP\_451,3.4,0.35,-0.75,0  
1DIO,HIS\_130,6.44,0.01,0,-0.07  
1EV8,ASP\_253,3.42,0.28,-0.66,0  
2OEW,ARG\_322,12.29,-0.21,0,0  
3DHN,HIS\_222,6.47,0.25,0,-0.28  
2CWC,LYS\_33,10.22,-0.28,0,0  
3RLN,ARG\_638,12.15,-0.35,0,0  
1W24,ASP\_107,3.8,0,0,0  
2AD1,LYS\_186,10.5,0,0,0  
2DFL,HIS\_215,5.47,1.47,0.03,-2.53  
2QOPLY,LYS\_53,10.5,0,0,0  
2YYO,HIS\_21,7.14,0.64,0,0  
2BLL,ARG\_424,12.22,-0.28,0,0  
1C44,GLU\_23,4.47,0.77,-0.8,0  
2WB8,GLU\_466,2.83,0.72,-0.8,-1.59  
2QHT,GLU\_15,4.71,0.21,0,0  
1PGV,LYS\_265,10.15,-0.35,0,0  
3COC,GLU\_329,4.57,0.07,0,0  
1S1Y,ASP\_26,2.98,0.7,-1.52,0  
4DEZ,TYR\_110,10.67,0.84,0,-0.17  
2H30,GLU\_74,1.43,0.93,-1.6,-2.4  
1D2S,ARG\_636,11.33,-1.9,0.0,7.3  
3E2Z,LYS\_67,10.5,0,0,0  
1FKM,HIS\_371,5.33,0.96,0,-2.13  
2P5D,LYS\_122,10.5,0,0,0  
2V4X,TYR\_66,9.49,0.29,-0.8,0  
4FD6,TYR\_85,10.92,0.07,0,0.85  
4E8B,GLU\_75,0.76,1.64,-2.98,-2.4  
3E2Z,ARG\_134,12.24,-2.11,0,1.85  
1AKO,LYS\_121,10.36,-0.14,0,0  
1Q46,LYS\_169,10.29,-0.21,0,0  
3EVP,LYS\_184,10.5,0,0,0  
2G3A,TYR\_110,10.81,0.81,0,0  
2VGY,CYS\_63,9.66,-0.14,0,0.8  
1SQW,TYR\_109,10,0,0,0  
2GQV,ARG\_76,12.5,0,0,0  
3V55,ASP\_595,3.74,0,-0.06,0  
2V81,GLU\_46,3.86,0.7,-1.34,0  
3QAV,LYS\_41,10.5,0,0,0  
2QOP,GLU\_150,4.78,0.28,0,0  
1SBX,GLU\_108,4.64,0.14,0,0  
3PM2,ASP\_158,3.67,0,-0.13,0  
2G5X,LYS\_155,10.5,0,0,0  
3CRM,HIS\_62,3.19,0.01,0,-3.32  
1IDK,LYS\_122,10.43,-0.07,0,0  
4EUG,HIS\_181,4.56,0,0,-1.94  
4EZB,TYR\_31,10.56,0.07,-0.05,0.54  
2D7U,GLU\_328,4.16,0.56,-0.9,0  
3LPZ,TYR\_168,13.97,0.34,-0.1,3.74  
3K9I,TYR\_60,10,0,0,0  
3CCY,ASP\_145,1.21,0.28,-2.87,0  
3V46,GLU\_281,4.12,0.42,-0.8,0  
2IF4,HIS\_125,3.99,0.26,0,-2.77  
1Q42,GLU\_65,3.91,0.21,-0.8,0  
2EYI,GLU\_81,3.66,0.21,-1.05,0  
3BWT,ARG\_629,13.6,-1.66,0,2.76  
3IBT,TYR\_13,12.39,0.21,-0.02,2.2  
1TJE,LYS\_169,10.36,-0.14,0,0  
1MJS,ARG\_287,12.43,-0.07,0,0  
2JHY,ARG\_134,11.45,-1.05,0,0  
3M7G,GLU\_263,4.28,0.21,-0.43,0  
3HQX,HIS\_53,6.5,0,0,0  
3F6M,ARG\_84,12.15,-0.35,0,0  
100X,HIS\_82,4.0,0.15,0.11,-2.77  
2AH5,CYS\_58,8.13,-0.87,0,0  
3LQE,ASP\_321,3.94,0.14,0,0  
3UAH,HIS\_414,7.6,1.63,3.7,-4.23  
3OOP,ARG\_80,12.01,-0.49,0,0  
3V55,CYS\_464,4.5,-3.6,-1.69,0.79  
3A4C,GLU\_457,4.59,0.21,-0.12,0  
2OBI,TYR\_63,12.88,0.14,0.34,2.4  
3BPP,TYR\_146,10.89,0.89,0,0  
3H13,GLU\_242,4.57,0.07,0,0  
1RZ2,ARG\_108,11.8,-0.7,0,0  
1U53,ARG\_125,11.94,-0.56,0,0  
4DNU,LYS\_296,10.5,0,0,0  
2EFK,LYS\_114,10.29,-0.21,0,0  
3V46,ASP\_309,3.85,0.14,-0.08,0  
2H2Z,TYR\_209,10.6,1.4,-0.8,0  
3UAH,ARG\_210,12.36,-0.14,0,0  
1J33,GLU\_242,4.5,0,0,0  
2EHG,LYS\_31,10.15,-0.35,0,0  
2QV2,TYR\_78,7.94,0.31,0,-2.37  
3ETV,TYR\_286,10,0,0,0  
3M70,LYS\_210,9.94,-0.56,0,0  
1WRU,TYR\_243,11.57,0.07,0,1.5  
1JYH,TYR\_74,10,0,0,0  
1X8F,ARG\_70,12.15,-0.35,0,0  
3IVF,TYR\_70,10.67,0,0,0.67  
1WLY,ARG\_32,11.73,-0.77,0,0  
3JZN,GLU\_107,4.5,0,0,0  
3ETU,GLU\_223,4.16,0.14,-0.48,0  
1F09,GLU\_149,4.0,4.9,-0.99,0  
1JKS,LYS\_249,10.29,-0.21,0,0  
3M16,ARG\_248,13.18,-1.45,0,2.13  
2OOK,GLU\_72,4.36,0.28,-0.42,0  
3CGW,ARG\_104,11.52,-0.98,0,0  
3COU,ARG\_42,12.36,-0.14,0,0  
3C38,ASP\_245,3.87,0.07,0,0  
4DBX,ASP\_256,2.61,0.28,-1.47,0  
3E2Z,ASP\_208,3.01,0.14,-0.93,0  
2FL4,GLU\_30,4.5,0,0,0  
4E8B,HIS\_79,4.01,0,0,-2.49  
3BRQ,ARG\_158,12.08,-0.42,0,0  
3RNV,LYS\_371,10.29,-0.21,0,0  
4FH3,TYR\_265,10,0,0,0  
1XDZ,LYS\_223,10.5,0,0,0  
3L3P,HIS\_282,6.49,0.27,0,-0.28  
2V81,ASP\_30,3.84,0.14,-0.1,0  
3M84,ARG\_984,12.01,-0.49,0,0  
1AM2,GLU\_12,4.5,0,0,0  
2QHT,ARG\_112,12.22,-0.28,0,0  
2YLF,LYS\_135,10.5,0,0,0  
1T3Y,ARG\_11,12.08,-0.42,0,0  
3I4T,ASP\_256,3.41,0.35,-0.73,0  
3RRQ,ARG\_96,12.43,-0.07,0,0  
2BDV,ARG\_206,12.5,0,0,0  
3G9T,GLU\_111,1.61,0.56,-3.45,0  
1XDZ,HIS\_95,7.2,0.91,0,-0.21  
1YR6,GLU\_231,3.48,0.56,-1.58,0  
3BA1,LYS\_124,10.29,-0.21,0,0  
3EJG,LYS\_160,10.43,-0.07,0,0  
2B2H,TYR\_351,10.73,0.73,0,0  
2AZL,ASP\_222,3.8,0,0,0  
3KB5,GLU\_323,4.57,0.07,0,0  
1RSS,ARG\_72,11.8,-0.7,0,0  
1XWM,ARG\_79,11.87,-0.63,0,0  
1OTM,LYS\_142,10.08,-0.42,0,0  
2YWJ,ASP\_134,3.52,0.28,-0.56,0  
1F09,ARG\_376,12.36,-0.14,0,0  
4ETX,GLU\_213,4.51,0.28,-0.27,0  
1NAR,LYS\_152,10.15,-0.35,0,0  
3A4C,ARG\_471,12.36,-0.14,0,0  
1Z3X,GLU\_20,4.64,0.14,0,0  
2G7O,CYS\_73,9.04,-0.03,0,0.07  
2RGY,GLU\_194,3.56,0.28,-1.22,0  
1XAW,LYS\_488,10.29,-0.21,0,0  
3H5T,ASP\_313,3.55,0.56,-0.81,0  
1ZKZ,LYS\_38,10.29,-0.21,0,0  
2QHT,TYR\_122,10,0,0,0  
3N2T,LYS\_294,10.5,0,0,0  
1PVT,GLU\_7,2.17,0.62,-1.18,-1.76  
1YLN,ASP\_183,3.22,0.49,-1.07,0  
3M70,LYS\_275,10.43,-0.07,0,0  
1R9W,GLU\_256,4.5,0,0,0  
3CQ1,ARG\_65,11.73,-0.77,0,0  
2HNG,GLU\_25,4.5,0,0,0  
1TLV,GLU\_135,4.71,0.21,0,0  
2OKT,GLU\_59,5.62,2,-1.9,1.02  
2NRR,TYR\_375,10,0,0,0  
1D2K,ASP\_324,3.28,0.28,-0.8,0  
3CBN,LYS\_149,10.29,-0.21,0,0  
2R57,GLU\_183,4.57,0.07,0,0  
1O17,LYS\_227,9.52,-0.98,0,0  
1YWS,LYS\_104,10.5,0,0,0  
2H14,ASP\_333,3.23,0.28,-0.85,0  
2XJ4,TYR\_224,12.47,1.31,0,1.16  
2AHE,GLU\_30,4.64,0.14,0,0  
3C38,ARG\_91,12.15,-0.35,0,0  
3SMD,LYS\_115,10.36,-0.14,0,0  
3F6M,ARG\_2\_12,0.1,-0.49,0,0  
1WPA,ASP\_479,3.96,0.28,-0.12,0  
2OPJ,ARG\_22,10.5,-3.24,0,1.25  
1P4X,GLU\_106,4.57,0.07,0,0  
3FFM,LYS\_48,10.08,-0.42,0,0  
1KCM,LYS\_163,9.94,-0.56,0,0  
1PVT,LYS\_144,10.5,0,0,0  
2DFL,ASP\_67,3.74,0.21,-0.27,0  
1X1E,TYR\_239,10.37,0,0,0.37  
3LJI,ASP\_224,2.99,0.42,-1.23,0  
1P2F,LYS\_100,10.15,-0.35,0,0  
2V1L,ARG\_92,12.29,-0.21,0,0  
1Q42,LYS\_118,11.87,-0.63,0,0  
2A4D,ARG\_121,12.08,-0.42,0,0  
1RSS,ARG\_76,11.87,-0.63,0,0  
2XWS,ARG\_47,12.15,-0.35,0,0  
1YWS,ARG\_96,12.22,-0.28,0,0  
1YTO,LYS\_119,9.87,-0.63,0,0  
1XAW,ARG\_483,12.22,-0.28,0,0  
3DZ1,TYR\_140,12.06,0.89,-0.34,1.52  
1AKO,HIS\_62,6.36,0,0,-0.14  
1W7B,ARG\_168,11.73,-0.77,0,0  
3EVN,HIS\_177,1.86,0,0,-4.64  
3EX9,HIS\_126,5.55,4.4,0,-5.35  
2QHT,ARG\_100,12.5,0,0,0  
1X8F,LYS\_259,10.5,0,0,0  
2QK0,TYR\_81,8.15,0.14,-1.99,0  
2CIU,HIS\_170,6.5,0,0,0  
3V46,TYR\_264,10.6,0.6,0,0  
3RFY,TYR\_343,11.32,0,0,1.32  
2BLL,GLU\_481,4.64,0.14,0,0  
1RKA,GLU\_29,3.1,0.28,-1.68,0  
3PM2,GLU\_17,4.46,0.07,-0.11,0  
4EKU,TYR\_238,10.21,0.21,0,0  
4DVD,LYS\_168,10.5,0,0,0  
3F5D,ASP\_78,3.74,0.07,-0.13,0  
2OEW,HIS\_162,4.82,0,0,-1.68  
3CJW,LYS\_340,10.5,0,0,0  
1TLV,ASP\_65,4.01,0.21,0,0  
2YWX,ARG\_38,12.29,-0.21,0,0  
1ZP2,ASP\_19,4.01,0.21,0,0  
1R3F,GLU\_189,2.55,0.7,-2.65,0  
2E0T,TYR\_170,13.27,0.07,0.8,2.4  
2ZTY,ARG\_79,11.66,-0.84,0,0  
2H80,LYS\_319,10.29,-0.21,0,0  
1N81,GLU\_129,0.24,3.78,-3.24,-4.8  
1L2F,GLU\_253,2.95,0.42,-1.97,0  
3M70,GLU\_25,3.98,0.28,-0.8,0  
3F7M,TYR\_129,10.24,0.24,0,0  
1DUN,LYS\_119,10.5,0,0,0  
2QV2,TYR\_64,10,0,0,0  
1SUU,LYS\_781,10.5,0,0,0  
2V1L,LYS\_15,10.5,0,0,0  
1GXN,TYR\_404,12.83,0.21,0.22,2.4  
4FCU,HIS\_72,6.36,0,0,-0.14  
3KB5,LYS\_462,10.5,0,0,0  
1WLY,LYS\_144,10.15,-0.35,0,0  
2DOA,ARG\_17,11.94,-0.56,0,0  
1SFE,LYS\_126,10.5,0,0,0  
3ASA,ARG\_81,10.25,-2.25,0,0  
1RWZ,TYR\_219,10,0,0,0  
3ZRI,ARG\_54,11.59,-0.91,0,0  
2H2Z,ASP\_56,3.28,0.28,-0.8,0  
3K1H,GLU\_119,4.5,0,0,0  
1PVT,ARG\_66,12.08,-0.42,0,0

4GA2, TYR\_132, 9.65, 0.07, -0.42, 0  
 1PDB, GLU\_150, 4.57, 0.07, 0, 0  
 3C6B, ASP\_42, 3.19, 0, -0.61, 0  
 2P52, GLU\_195, 3.18, 0.21, -1.53, 0  
 2Q13, GLU\_162, 4.72, 0.35, -0.13, 0  
 2B0J, LYS\_34, 10.36, -0.14, 0, 0  
 2GEN, ASP\_177, 3.87, 0.07, 0, 0  
 2JEO, GLU\_197, 4.71, 0.21, 0, 0  
 2D0A, LYS\_300, 10.5, 0, 0, 0  
 2X4J, TYR\_111, 10.0, 0, 0, 0  
 1JKS, TYR\_12, 13.11, 0.21, 0.5, 2.4  
 3QKY, TYR\_76, 10.11, 0, -0.06, 0.17  
 3T57, ARG\_322, 13.49, -1.41, 0.2, 4  
 1QQH, LYS\_125, 10.29, -0.21, 0, 0  
 1O3X, LYS\_195, 10.5, 0, 0, 0  
 2AHE, ASP\_120, 3.25, 0.21, -0.75, 0  
 3RRQ, ARG\_148, 12.43, -0.07, 0, 0  
 1O9G, GLU\_38, 1.32, 1.19, -4.37, 0  
 2XHC, GLU\_80, 2.67, 1.73, -1.67, -1.89  
 3CBN, ARG\_31, 12.36, -0.14, 0, 0  
 1AK1, ARG\_33, 12.15, -0.35, 0, 0  
 2X4L, ASP\_280, 3.42, 0.21, -0.59, 0  
 3M7D, GLU\_17, 4.5, 0, 0, 0  
 2WOZ, ASP\_516, 4.21, 0.63, -0.22, 0  
 2H2W, GLU\_215, 4.16, 0.14, -0.48, 0  
 2OPJ, ARG\_126, 13.83, -1.07, 0.2, 4  
 3Q1C, TYR\_86, 12.22, 0.2, 2.22  
 1SQW, ASP\_29, 4.01, 0.21, 0, 0  
 2D0A, TYR\_162, 11, 1, 0, 0  
 1RAJ, HIS\_423, 5.36, 1.6, 2.05, -4.79  
 2IF4, GLU\_45, 4.34, 0.28, -0.44, 0  
 3LD1, GLU\_157, 5.4, 0.9, 0, 0  
 2P52, ARG\_280, 11.73, -0.77, 0, 0  
 2RGY, GLU\_110, 3.79, 0.73, -1.44, 0  
 1M5I, GLU\_225, 3.98, 0.28, -0.8, 0  
 3M70, HIS\_76, 2.27, 1.39, -2.23, -3.39  
 3M70, TYR\_143, 11.48, 0.49, -0.01, 1  
 3LPZ, ASP\_49, 3.84, 0.07, -0.03, 0  
 3AU3, LYS\_398, 10.5, 0, 0, 0  
 3K9I, TYR\_90, 10.0, 0, 0, 0  
 3EUR, TYR\_24, 9.64, 0.07, -0.43, 0  
 1R15, ARG\_84, 11.84, -0.66, 0, 0  
 2D0A, HIS\_19, 6.36, 0, -0.14  
 350A, LYS\_114, 10.22, -0.28, 0, 0  
 3OBS, ARG\_50, 12.08, -0.42, 0, 0  
 2C13, LYS\_56, 10.43, -0.07, 0, 0  
 3V55, TYR\_569, 12.04, 0.07, 0.1, 9.7  
 2YT4, HIS\_600, 6.6, 0.17, 0, -0.07  
 3M3P, GLU\_102, 4.57, 0.07, 0, 0  
 1OXZ, GLU\_173, 4.5, 0, 0, 0  
 1FQI, ASP\_366, 2.1, 0.7, -2.4, 0  
 3DZ1, ARG\_123, 11.8, -0.7, 0, 0  
 1TLV, GLU\_253, 4.5, 0, 0, 0  
 2GZR, TYR\_190, 9.98, 0, -0.02, 0  
 2F9F, LYS\_148, 10.36, -0.14, 0, 0  
 2WB8, GLU\_531, 2.11, 0.43, -1.8, -1.03  
 2DG7, ASP\_85, 3.99, 0.21, -0.02, 0  
 1YB2, LYS\_219, 10.29, -0.21, 0, 0  
 3GE9, GLU\_207, 3.96, 1.45, -1.99, 0  
 2JEO, LYS\_42, 10.22, -0.28, 0, 0  
 3IOO, HIS\_156, 2.36, 0, -4.14  
 2H30, GLU\_103, 2.87, 1.25, -2.88, 0  
 1WLY, GLU\_86, 3.23, 0.86, -2.12, 0  
 4F85, ASP\_107, 2.44, 0.56, -1.92, 0  
 2RGY, GLU\_202, 4.71, 0.21, 0, 0  
 1WP5, LYS\_186, 10.15, -0.35, 0, 0  
 1RZ2, ARG\_43, 11.73, -0.77, 0, 0  
 3M70, GLU\_244, 3.71, 0.35, -1.14, 0  
 1OTM, ASP\_195, 4.15, 0.35, 0, 0  
 1IDK, TYR\_97, 12.03, 0, 0, 2.03  
 3IL3, ASP\_30, 4.15, 0.35, 0, 0  
 1ZBM, GLU\_223, 3.84, 0.14, -0.8, 0  
 2NYC, GLU\_228, 3.66, 0.28, -1.12, 0  
 2Q99, ARG\_355, 11.24, -1.26, 0, 0  
 1T6L, LYS\_18, 10.5, 0, 0, 0  
 3V75, ARG\_17, 11.1, -1.4, 0, 0  
 1E55, ASP\_194, 3.67, 0.07, -0.2, 0  
 3EVN, GLU\_66, 4.5, 0, 0, 0  
 2D2S, LYS\_598, 10.5, 0, 0, 0  
 1PSW, ARG\_196, 13.44, -0.47, 0.1, 4.1  
 1TR9, GLU\_312, 3.58, 0.07, -0.99, 0  
 2B61, GLU\_129, 4.05, 0.35, -0.8, 0  
 1IDK, ASP\_201, 3.73, 0.07, -0.14, 0  
 3M7G, ARG\_245, 12.08, -0.42, 0, 0  
 3EZ7, LYS\_117, 10.01, -0.49, 0, 0  
 3DZ1, ARG\_290, 11.8, -0.7, 0, 0  
 3LJN, LYS\_257, 10.36, -0.14, 0, 0  
 3E0H, ASP\_145, 3.33, 0, -0.47, 0  
 1UOH, GLU\_87, 3.95, 0.14, -0.69, 0  
 1P6F, TYR\_122, 11.59, 0, -0.1, 1.69  
 1P6F, GLU\_183, 4.57, 0.07, 0, 0  
 1J79, ARG\_126, 11.94, -0.56, 0, 0  
 2GZQ, LYS\_163, 10.43, -0.07, 0, 0  
 3EUR, GLU\_78, 4.57, 0.07, 0, 0  
 4E9E, TYR\_485, 10.76, 0, 0, 0.76  
 3D9H, LYS\_90, 10.5, 0, 0, 0  
 1LN4, LYS\_59, 10.08, -0.42, 0, 0  
 1C3K, TYR\_89, 10, 0, 0, 0  
 3JRT, CYS\_61, 11.4, 0, 0, 2.4  
 3M70, GLU\_96, 3.89, 0.46, -1.07, 0  
 3ZSL, GLU\_205, 3.32, 0.42, -1.6, 0  
 2J8A, HIS\_280, 6.49, 0.06, 0, -0.07  
 3GE9, GLU\_37, 3.54, 0.77, -1.74, 0  
 3GE9, ASP\_28, 1.89, 0.56, -2.47, 0  
 3T57, GLU\_320, 4.5, 0, 0, 0  
 2E3C, ASP\_318, 2.55, 0.7, -1.95, 0  
 1HUJ, LYS\_82, 10.5, 0, 0, 0  
 1WXQ, TYR\_143, 9.34, 0.14, -0.8, 0  
 1X8F, ASP\_153, 4.01, 0.35, -0.14, 0  
 1EV8, LYS\_158, 10.5, 0, 0, 0  
 1G5Z, LYS\_177, 10.22, -0.28, 0, 0  
 2YX0, LYS\_130, 10.5, 0, 0, 0  
 3PZ9, ARG\_111, 13.26, -1.64, 0.2, 4  
 3H04, ASP\_256, 3.72, 0, -0.08, 0  
 3EZ7, GLU\_332, 4.28, 0.07, -0.29, 0  
 1Z3X, HIS\_69, 6.39, 0.01, -0.12, 0  
 2YT4, GLU\_540, 4.62, 0.28, -0.16, 0  
 2HP7, LYS\_49, 10.5, 0, 0, 0  
 2A0J, LYS\_123, 10.22, -0.28, 0, 0  
 2OJQ, ARG\_606, 12.29, -0.21, 0, 0  
 3BB7, TYR\_56, 10.07, 0.07, 0, 0  
 1M5I, GLU\_135, 4.49, 0, -0.01, 0  
 2G55, ARG\_133, 12.8, -2.1, 0.2, 4  
 1XAW, ARG\_468, 12.22, -0.28, 0, 0  
 3CX2, CYS\_239, 10.19, 0, 0.1, 1.9  
 2ZQ5, HIS\_85, 2.19, 0.02, -1.33, -3  
 2VAN, ARG\_326, 12.5, 0, 0, 0  
 2DFL, ASP\_248, 3.05, 0.42, -1.17, 0  
 3G9G, HIS\_159, 6.43, 0, -0.07  
 2X4L, LYS\_159, 10.5, 0, 0, 0  
 1J33, GLU\_61, 3.84, 0.14, -0.8, 0  
 2D59, TYR\_44, 10.98, 0.14, -0.8, 1.64  
 3A4C, GLU\_455, 4.5, 0, 0, 0  
 2OSA, CYS\_268, 8.7, -0.37, 0.0, 0.07  
 1V8E, ASP\_154, 2.21, 0.28, -1.87, 0  
 1X9G, ARG\_66, 12.5, 0, 0, 0  
 3IBT, GLU\_152, 5.46, 0.96, 0, 0  
 1RZ2, TYR\_167, 12.9, 0, 0, 2.9  
 2NMU, ARG\_108, 11.52, -0.98, 0, 0  
 2NRK, GLU\_59, 4.64, 0.14, 0, 0  
 1NAF, LYS\_195, 10.5, 0, 0, 0  
 1SQH, TYR\_36, 10.64, 0.64, 0, 0  
 2YT4, ASP\_579, 3.87, 0.07, 0, 0  
 3CGW, ARG\_166, 11.94, -0.56, 0, 0  
 1QYI, GLU\_195, 5.25, 0.75, 0, 0  
 1R53, ARG\_9, 11.66, -0.84, 0, 0  
 1M5I, GLU\_201, 4.71, 0.21, 0, 0  
 3ONH, CYS\_537, 8.77, -0.23, 0, 0  
 2CXV, GLU\_108, 4.5, 0, 0, 0  
 3IL3, ASP\_21, 2.16, 0.28, -1.92, 0  
 2R4Q, HIS\_184, 6.5, 0, 0, 0  
 2ROS, ASP\_51, 4.72, 0.42, -0.82, 1.33  
 2Z84, CYS\_212, 11.59, 0.105, 1.54  
 1QQE, ARG\_114, 12.43, -0.07, 0, 0  
 3Q1C, ARG\_170, 12.08, -0.42, 0, 0  
 1WRU, ARG\_155, 13, -1.19, 0.1, 6.9  
 1DUP, ASP\_135, 3.94, 0.14, 0, 0  
 3CAN, GLU\_164, 4.5, 0, 0, 0  
 1QQE, ASP\_289, 3.92, 0.21, -0.09, 0  
 1M5I, LYS\_139, 10.5, 0, 0, 0  
 1U7U, HIS\_211, 6.5, 0, 0, 0  
 3DHN, LYS\_40, 10.5, 0, 0, 0  
 1P6F, GLU\_55, 4.02, 0.56, -1.04, 0  
 3LJN, LYS\_205, 10.29, -0.21, 0, 0  
 3EX9, GLU\_93, 4, 0.28, -0.79, 0  
 2FB6, ASP\_14, 3.58, 0.14, -0.36, 0  
 1V43, GLU\_205, 6.42, 1.96, -2.54, 2.51  
 3OBS, LYS\_10, 10.5, 0, 0, 0  
 1BN6, CYS\_72, 10.61, 0, 0, 1.61  
 2D7J, GLU\_176, 4.64, 0.14, 0, 0  
 2XHC, TYR\_286, 10.3, 0.3, 0, 0  
 2A6B, GLU\_16, 3.91, 0.21, -0.8, 0  
 2Q99, LYS\_99, 10.29, -0.21, 0, 0  
 3QKY, ARG\_229, 11.31, -1.19, 0, 0  
 2QV2, ASP\_184, 3.39, 0.35, -0.76, 0  
 3HYQ, HIS\_32, 6.43, 0, -0.07  
 2CXA, GLU\_139, 4.57, 0.07, 0, 0  
 4AF2, LYS\_46, 10.36, -0.14, 0, 0  
 3HKX, GLU\_107, 3.94, 0.49, -1.05, 0  
 3FTT, ASP\_59, 3.94, 0.14, 0, 0  
 1QQE, LYS\_88, 10.29, -0.21, 0, 0  
 3IOC, TYR\_309, 11.81, 0.44, 0.1, 3.7  
 4DNU, ARG\_212, 11.8, -0.7, 0, 0  
 2EFK, LYS\_140, 10.22, -0.28, 0, 0  
 3EZ7, GLU\_94, 4.36, 0.21, -0.35, 0  
 2BT8, ASP\_249, 2.06, 0.56, -2.3, 0  
 3V4G, GLU\_119, 4.57, 0.07, 0, 0  
 3K8J, LYS\_176, 9.94, -0.56, 0, 0  
 2PWQ, ASP\_119, 4.01, 0.21, 0, 0  
 2V4U, LYS\_331, 10.43, -0.07, 0, 0  
 1JT9, ARG\_91, 11.87, -0.63, 0, 0  
 1YTQ, ASP\_169, 4.22, 0.42, 0, 0  
 3FXH, TYR\_49, 9.9, 0, -0.1, 0  
 3R1X, LYS\_343, 10.08, -0.42, 0, 0  
 2G5X, TYR\_187, 9.85, 0, -0.15, 0  
 1X1U, ARG\_119, 12.5, 0, 0, 0  
 1LTU, GLU\_207, 5.66, 2.12, -0.96, 0  
 2C2Y, ASP\_90, 3.87, 0.07, 0, 0  
 2CBE, ASP\_101, 3.26, 0.35, -0.89, 0  
 4H86, HIS\_175, 7.31, 1.02, 0, -0.21  
 2FBQ, ASP\_214, 4.22, 0.42, 0, 0  
 1F2V, TYR\_14, 9.78, 0, -0.22, 0  
 2OBS, GLU\_119, 4.64, 0.42, -0.28, 0  
 2ZCO, CYS\_130, 11.23, -0.11, 0.19, 2.15  
 2D59, ARG\_135, 12.29, -0.21, 0, 0  
 3HOX, GLU\_31, 4.71, 0.21, 0, 0  
 3PP8, ASP\_35, 2.23, 0.7, -2.27, 0  
 2CVB, ARG\_63, 11.87, -0.63, 0, 0  
 3CRM, CYS\_31, 9.96, -0.23, 0.1, 1.18  
 1GVP, GLU\_40, 4.5, 0, 0, 0  
 1RAJ, LYS\_383, 10.5, 0, 0, 0  
 1ILW, TYR\_149, 13.34, 0.14, 0.8, 2.4  
 3CZC, HIS\_59, 6.5, 0, 0, 0  
 1QQE, GLU\_122, 4.1, 0.81, -1.21, 0  
 1WXQ, ARG\_352, 11.87, -0.63, 0, 0  
 2BDD, GLU\_139, 4.71, 0.21, 0, 0  
 2YWK, GLU\_18, 3.4, 0.91, -2.01, 0  
 3U2R, ASP\_26, 3.94, 0.21, -0.07, 0  
 3AU3, ASP\_651, 3.37, 0.07, -0.51, 0  
 2Q98, HIS\_173, 6.5, 0, 0, 0  
 1UJ8, ASP\_34, 2.9, 0.77, -1.67, 0  
 3BZT, TYR\_345, 10.41, 0, 0, 0.41  
 3F6M, GLU\_81, 3.62, 0.56, -1.44, 0  
 1ILW, TYR\_149, 13.34, 0.14, 0.8, 2.4  
 3T5B, LYS\_354, 9.87, -0.63, 0, 0  
 3B7X, TYR\_61, 13.34, 0.14, 0.8, 2.4  
 2ATR, GLU\_107, 4.5, 0, 0, 0  
 3PP8, ARG\_192, 13.92, -1.56, 0.2, 9.8  
 1U7U, HIS\_320, 6.79, 0.29, 0, 0  
 2IQT, ARG\_56, 11.45, -1.05, 0, 0  
 4FH3, CYS\_75, 8.34, -1.27, 0.0, 6.1  
 3HVM, HIS\_54, 6.22, 0, -0.28  
 1S1Y, ARG\_95, 12.99, -1.91, 0.2, 4  
 1GPP, TYR\_420, 10, 0, 0, 0  
 3M16, ARG\_188, 7.86, -1.88, 0, -2.76  
 3OIP, HIS\_12, 6.4, 0.04, 0, -0.14  
 4DIU, ARG\_32, 12.08, -0.42, 0, 0  
 2APL, HIS\_146, 6.5, 0, 0, 0  
 3FXH, GLU\_12, 2.52, 1.55, -3.52, 0  
 1AK1, ARG\_240, 11.94, -0.56, 0, 0  
 3E7P, ASP\_43, 2.79, 0.35, -1.37, 0  
 3DHN, ARG\_176, 12.29, -0.21, 0, 0  
 3IBT, ARG\_183, 11.66, -0.84, 0, 0  
 2RIK, ASP\_225, 3.35, 0.35, -0.8, 0  
 3G9G, LYS\_44, 10.43, -0.07, 0, 0  
 1T95, GLU\_103, 4.5, 0, 0, 0  
 1YDL, GLU\_55, 4.5, 0, 0, 0  
 3U2R, ARG\_27, 12.08, -0.42, 0, 0  
 3BQE, ARG\_217, 12.15, -0.35, 0, 0  
 2OEW, LYS\_269, 10.29, -0.21, 0, 0  
 3FTT, LYS\_183, 10.5, 0, 0, 0  
 1L2F, GLU\_22, 3.75, 0.21, -0.96, 0  
 2NMU, HIS\_137, 6.43, 0, 0, -0.07  
 3RKV, GLU\_327, 4.92, 0.42, 0, 0  
 3RFY, GLU\_178, 4.57, 0.07, 0, 0  
 3IL3, LYS\_24, 10.5, 0, 0, 0  
 3RE9, TYR\_111, 9.27, 0.07, -0.8, 0  
 3EUR, GLU\_97, 4.08, 0.56, -0.98, 0  
 1HF8, TYR\_44, 10, 0, 0, 0  
 3CNU, GLU\_39, 3.25, 0.7, -1.95, 0  
 3DHN, LYS\_153, 10.43, -0.07, 0, 0  
 2XJ4, GLU\_256, 3.53, 0.79, -1.76, 0  
 3ODJ, HIS\_39, 6.22, 0, -0.28  
 2H2Z, CYS\_22, 9.33, -0.17, 0.0, 5  
 2GAU, ARG\_199, 12.43, -0.07, 0, 0  
 3VJ8, HIS\_347, 7.09, 0.8, 0, -0.21  
 4AM1, GLU\_8, 4.5, 0, 0, 0  
 2QV2, GLU\_12, 4.05, 0.35, -0.8, 0  
 1YOY, LYS\_30, 10.22, -0.28, 0, 0  
 4FCU, ASP\_171, 2.62, 0.28, -1.46, 0  
 1L3K, ARG\_53, 12.5, 0, 0, 0  
 2CN1, LYS\_27, 10.5, 0, 0, 0  
 2IF4, TYR\_208, 11.77, 0.21, -0.49, 2.05  
 2Q34, LYS\_234, 10.43, -0.07, 0, 0  
 2OKT, GLU\_233, 3.84, 0.14, -0.8, 0  
 1WLY, LYS\_9, 10.29, -0.21, 0, 0

2HRZ,ARG\_209,10.62,-1.88,0,0  
 3V3T,GLU\_237,4.5,0,0,0  
 1GXN,ARG\_353,12.08,-0.42,0,0  
 3JZ9,LYS\_370,10.22,-0.28,0,0  
 15J8,LYS\_540,10.29,-0.21,0,0  
 1WXQ,CYS\_55,6.82,-2.25,0,0.07  
 2D8N,LYS\_194,8.79,-0.77,0,-0.94  
 4DBX,TYR\_252,11.05,0.96,-0.8,0.89  
 3GOZ,HIS\_8,6.5,0,0,0  
 4DVD,ASP\_11,3.57,0.42,-0.66,0  
 1QZN,LYS\_60,10.5,0,0,0  
 1RWZ,ASP\_70,2.62,0.63,-1.81,0  
 2IRM,ARG\_40,11.73,-0.77,0,0  
 1RSS,GLU\_90,4.57,0.07,0,0  
 1OLR,LYS\_76,10.08,-0.42,0,0  
 3JZ9,LYS\_491,9.94,-0.56,0,0  
 2YWJ,GLU\_16,4.71,0.21,0,0  
 3UC9,HIS\_31,6.5,0,0,0  
 3OA7,ARG\_566,12.08,-0.42,0,0  
 2ROS,LYS\_162,10.5,0,0,0  
 3CAX,LYS\_420,10.43,-0.07,0,0  
 3FRR,TYR\_64,10.12,0.0,0.12  
 3HXK,HIS\_28,4.88,0,-1.62  
 200K,GLU\_33,4.71,0.21,0,0  
 1W7B,ASP\_200,3.39,0.35,-0.76,0  
 1XTZ,LYS\_72,10.36,-0.14,0,0  
 1ZCE,ASP\_147,3.74,0.07,-0.13,0  
 4E8B,ARG\_223,12.29,-0.21,0,0  
 2ZOM,ARG\_70,12.36,-0.14,0,0  
 3O16,ARG\_16,11.73,-0.77,0,0  
 3IOO,ASP\_192,3.87,0.07,0,0  
 2AZP,ARG\_54,11.45,-1.05,0,0  
 1ZP2,ARG\_49,12.29,-0.21,0,0  
 3PM2,LYS\_86,10.43,-0.07,0,0  
 2BDD,GLU\_61,4.78,0.28,0,0  
 3F7M,ARG\_168,11.8,-0.7,0,0  
 2C13,HIS\_235,2.82,0.35,0,-4.03  
 2AXO,ASP\_124,2.64,0.42,-1.59,0  
 1Q46,LYS\_79,10.5,0,0,0  
 2V5B,LYS\_60,10.43,-0.07,0,0  
 2EDM,ASP\_177,2.86,0.35,-1.29,0  
 3F1X,GLU\_77,4.5,0,0,0  
 3CZC,LYS\_71,10.36,-0.14,0,0  
 1JKS,ASP\_238,3.73,0,-0.07,0  
 2FGG,ARG\_63,11.94,-0.56,0,0  
 3I4T,LYS\_51,10.22,-0.28,0,0  
 1WYC,ASP\_248,3.8,0,0,0  
 3FTT,GLU\_48,4.64,0.14,0,0  
 2E3S,HIS\_509,6.29,0,0,-0.21  
 3JZN,GLU\_145,4.12,1.84,-2.21,0  
 4F8A,HIS\_601,7.23,0.8,0,-0.07  
 3EYE,HIS\_79,6.43,0,0,-0.07  
 1XTD,CYS\_49,7.72,-1.44,0,0.16  
 3EVP,HIS\_235,6.43,0,0,-0.07  
 2YXO,ASP\_161,3.21,0.21,-0.8,0  
 2B2H,LYS\_173,10.15,-0.35,0,0  
 1ZBM,GLU\_36,3.62,0.49,-1.37,0  
 3BB7,TYR\_291,10.96,3.28,-0.55,-1.77  
 2CXY,GLU\_107,4.5,0,0,0  
 3GYW,LYS\_70,10.29,-0.21,0,0  
 3GS9,ASP\_131,2.41,0.98,-2.37,0  
 1QQE,ASP\_290,2.89,0.14,-1.05,0  
 2X4L,TYR\_328,11.79,0.83,0,0.96  
 2POY,ASP\_35,3.55,0.42,-0.67,0  
 3FNI,ARG\_111,12.43,-0.07,0,0  
 1QYI,GLU\_233,4.5,0,0,0  
 3DZ1,GLU\_253,3.82,3.56,-1.84,-2.4  
 3V55,LYS\_582,10.29,-0.21,0,0  
 2EEY,GLU\_114,4.55,1.14,-1.09,0  
 2D0A,CYS\_291,9.41,-0.93,0,1.34  
 1JKS,GLU\_109,4.5,0,0,0  
 3GW3,TYR\_202,12.67,2.7,-0.26,0.23  
 1W7B,GLU\_142,2.45,0.35,-2.4,0  
 3QYB,LYS\_888,10.5,0,0,0  
 2B0A,ASP\_173,3.19,0.07,-0.68,0  
 2P4D,GLU\_164,4.39,0.35,-0.46,0  
 1PGV,ARG\_248,12.36,-0.14,0,0  
 1RZ2,ASP\_127,2.58,0.7,-1.91,0  
 4FZR,GLU\_99,4.5,0,0,0  
 1J8B,LYS\_66,10.29,-0.21,0,0  
 2O8P,ARG\_53,11.05,-1.45,0,0  
 1QZN,ASP\_100,3.73,0,-0.07,0  
 2I6I,LYS\_26,10.5,0,0,0  
 3CRM,HIS\_217,6.36,0,0,-0.14  
 3U0V,LYS\_195,10.5,0,0,0  
 1P4X,GLU\_29,4.64,0.14,0,0  
 3COU,ARG\_129,12.08,-0.42,0,0  
 2H2Z,LYS\_102,10.5,0,0,0  
 1IDK,TYR\_211,11.37,0.98,0.1,0.29  
 2FGG,CYS\_11,8.97,-0.03,0,0  
 1X1E,ARG\_3,11.59,-0.91,0,0  
 1F09,GLU\_211,7.97,2.7,-0.99,1.76  
 4EUG,GLU\_14,4.19,0.49,-0.8,0  
 1ZBM,ASP\_125,3.71,0.28,-0.37,0  
 3LUN,TYR\_245,12.26,0.54,0.1,72  
 3AUF,ASP\_201,3.77,0.07,-0.1,0  
 2D8N,LYS\_97,10.36,-0.14,0,0  
 1IAP,ARG\_111,11.73,-0.77,0,0  
 3BWT,LYS\_634,10.43,-0.07,0,0  
 3GS3,GLU\_66,4.82,0.56,-0.24,0  
 1YTQ,LYS\_107,10.29,-0.21,0,0  
 3ODJ,TYR\_125,13.32,0.87,0.05,2.4  
 2YWK,ASP\_9,3.5,0.35,-0.65,0  
 1QQE,ARG\_50,12.15,-0.35,0,0  
 1O6D,LYS\_10,9.87,-0.63,0,0  
 1S17,ARG\_92,12.01,-0.49,0,0  
 3US6,LYS\_72,10.5,0,0,0  
 1R9W,ASP\_342,4.01,0.21,0,0  
 2YLF,ARG\_222,11.8,-0.7,0,0  
 3LMF,ASP\_44,3.64,0.21,-0.38,0  
 1X9G,TYR\_8,11.94,0.28,-0.74,2.4  
 2IIA,ARG\_73,12.29,-0.21,0,0  
 2FC3,GLU\_38,4.64,0.14,0,0  
 1K95,GLU\_143,3.63,0.84,-1.72,0  
 3GW3,CYS\_35,12.13,0.0,3.13  
 2CW4,ARG\_46,12.29,-0.21,0,0  
 2FBQ,HIS\_162,7.41,0.91,0,0  
 3CCY,ARG\_13,11.94,-0.56,0,0  
 1PSW,ARG\_105,11.52,-0.98,0,0  
 1AD6,ASP\_511,2.08,0.49,-2.21,0  
 1WYC,ARG\_387,12.01,-0.49,0,0  
 1W7B,LYS\_157,10.29,-0.21,0,0  
 1LZL,ASP\_47,3.75,0.07,-0.12,0  
 3GV0,ASP\_201,3.3,0.35,-0.85,0  
 3PP8,ASP\_307,3.93,0.42,-0.29,0  
 2V4U,GLU\_476,5.02,2.17,-1.65,0  
 3M7D,ASP\_336,3.8,0,0,0  
 2FZ4,GLU\_207,4.64,0.14,0,0  
 1O6D,GLU\_33,4.05,0.35,-0.8,0  
 3GA2,LYS\_186,10.29,-0.21,0,0  
 3JRT,ASP\_131,3.8,0,0,0  
 2Q13,LYS\_63,10.15,-0.35,0,0  
 1NWA,ARG\_93,12.89,-1.66,0.2,05  
 1RHS,LYS\_13,10.36,-0.14,0,0  
 2C2Y,ASP\_114,3.01,0.35,-1.14,0  
 2F8H,ARG\_166,12.57,-1.78,0,1.85  
 1BK8,GLU\_36,4.5,0,0,0  
 4AM1,LYS\_289,9.52,-0.98,0,0  
 1PSW,CYS\_243,10.61,0,0,1.61  
 3HNX,ARG\_63,11.87,-0.63,0,0  
 1R15,TYR\_226,10.4,0.07,-0.8,1.13  
 3K8U,GLU\_130,3.55,0.65,-1.6,0  
 3QYB,LYS\_888,10.5,0,0,0  
 2FC3,GLU\_93,4.64,0.14,0,0  
 2HP7,CYS\_214,11.13,-0.07,0.2,2  
 3HVM,HIS\_227,11.15,0.39,-2,-3.73  
 1AM2,HIS\_144,6.22,0,0,-0.28  
 1BKR,TYR\_98,10.86,1.66,-0.8,0  
 3P51,ARG\_130,11.87,-0.63,0,0  
 3GT0,TYR\_180,10,0,0,0  
 3JZN,ARG\_201,12.29,-0.21,0,0  
 4AF2,GLU\_74,3.94,0.21,-0.77,0  
 2F8H,ASP\_305,3.93,0.28,-0.15,0  
 2H30,LYS\_120,10.5,0,0,0  
 4EKU,CYS\_298,8.71,-0.43,0.14  
 3GOZ,GLU\_99,2.33,0.35,-2.53,0  
 1X7F,ARG\_333,12.08,-0.42,0,0  
 1BKR,LYS\_43,10.43,-0.07,0,0  
 1O0X,GLU\_249,4.23,0.21,-0.48,0  
 3CQ1,ASP\_20,2.4,0.7,-2.1,0  
 2VAN,LYS\_262,10.43,-0.07,0,0  
 3M7D,HIS\_373,6.5,0,0,0  
 1R53,LYS\_162,10.43,-0.07,0,0  
 3EVN,GLU\_22,4.17,0.28,-0.6,0  
 4H86,GLU\_38,4.28,0.07,-0.29,0  
 1O59,HIS\_244,6.74,0.59,0,-0.35  
 1YOY,GLU\_102,4.32,0,-0.18,0  
 2EFK,LYS\_173,10.22,-0.28,0,0  
 3VJ8,LYS\_115,10.29,-0.21,0,0  
 1ZHV,ASP\_75,3.94,0.14,0,0  
 3UPD,GLU\_303,3.59,0.56,-1.47,0  
 2YXO,GLU\_152,5.82,4.4,-3.08,0  
 3V55,CYS\_439,9.78,-0.34,0.1,12  
 3OIP,LYS\_13,10.5,0,0,0  
 1IAP,ASP\_182,3.07,0.63,-1.37,0  
 1JSX,LYS\_21,9.94,-0.56,0,0  
 1R3D,HIS\_150,6.5,0,0,0  
 3I4T,CYS\_247,11.38,0,0.2,38  
 2R6Y,TYR\_100,12.05,2.05,0,0  
 3V3T,ASP\_88,3.93,0.14,-0.01,0  
 1PZC,ASP\_94,3.69,0.07,-0.18,0  
 3BCH,ARG\_102,11.94,-0.56,0,0  
 3ADO,GLU\_271,4.5,0,0,0  
 200K,GLU\_303,4.61,0.14,-0.03,0  
 1NAR,ARG\_138,2.88,0.84,-2.46,0  
 3CCY,ASP\_104,3.19,0.42,-1.03,0  
 3CIV,CYS\_243,8.49,-0.51,0,0  
 2GZR,ASP\_179,3.29,0.91,-1.41,0  
 4ESS,ARG\_5,12.01,-0.49,0,0  
 2DG7,GLU\_144,4.5,0,0,0  
 2E3C,ARG\_356,11.8,-0.7,0,0  
 3ONT,ASP\_18,3.99,0.21,-0.02,0  
 3V75,ARG\_70,11.31,-1.19,0,0  
 1WYC,ARG\_328,12.34,-1.61,0.1,45  
 1LZL,ASP\_43,4.03,0.28,-0.05,0  
 1X7F,GLU\_131,3.84,0.14,-0.8,0  
 1LZL,LYS\_123,10.22,-0.28,0,0  
 3DB9,ARG\_179,12.08,-0.42,0,0  
 2BDV,GLU\_104,3.78,2.41,-4.32,1.19  
 3GOZ,TYR\_35,10,0,0,0  
 3FXH,ASP\_68,3.66,0,-0.14,0  
 3MTT,GLU\_436,4.07,0,-0.43,0  
 2OKT,TYR\_9,13.42,0.22,0.8,2.4  
 3BQW,LYS\_349,10.29,-0.21,0,0  
 3M9A,TYR\_25,10,0,0,0  
 2H8O,ARG\_69,11.66,-0.84,0,0  
 2BQQ,LYS\_54,10.5,0,0,0  
 2XMZ,GLU\_161,4.5,0,0,0  
 1JKS,LYS\_33,9.94,-0.56,0,0  
 2RH3,ARG\_179,12.22,-0.28,0,0  
 1O0X,TYR\_105,9.27,0.07,-0.8,0  
 3JTD,LYS\_116,10.15,-0.35,0,0  
 3H9W,ARG\_95,12.29,-0.21,0,0  
 1O59,HIS\_0,6.57,0.07,0,0  
 3ERF,GLU\_207,4.47,0.14,-0.17,0  
 1IDK,TYR\_149,8.89,0.08,-1.19,0  
 2B78,ARG\_16,11.66,-0.84,0,0  
 1Q8B,HIS\_83,7.02,0.8,0,-0.28  
 2YWK,ARG\_74,12.29,-0.21,0,0  
 2EYI,GLU\_53,4.5,0,0,0  
 3N0K,TYR\_132,10,0,0,0  
 2PLQ,ASP\_311,3.21,0.28,-0.87,0  
 1ES9,HIS\_79,4.16,0.01,1.41,-3.76  
 2APL,CYS\_295,6.45,0.02,0,-0.07  
 3OOP,ASP\_11,3.93,0.21,-0.08,0  
 1X91,ARG\_44,12.29,-0.21,0,0  
 2ZQ5,HIS\_121,1.33,0.66,-1.79,-4.04  
 3M66,LYS\_246,10.36,-0.14,0,0  
 2FBQ,HIS\_91,6.36,0,0,-0.14  
 1LFFL,LYS\_58,10.22,-0.28,0,0  
 3I47,ASP\_5,3.34,0.35,-0.81,0  
 1Z3X,LYS\_21,10.5,0,0,0  
 1G8P,ARG\_343,12.29,-0.21,0,0  
 3MIX,ARG\_533,12.15,-0.35,0,0  
 2DG7,ASP\_26,3.78,0.14,-0.16,0  
 2APL,CYS\_46,8.91,-0.16,0.0,07  
 2GZR,ASP\_96,3.73,0.07,-0.14,0  
 2PLQ,LYS\_205,10.43,-0.07,0,0  
 3CIV,ASP\_100,2.4,0.77,-2.16,0  
 3ULX,GLU\_9,4.99,0.49,0,0  
 1WP5,GLU\_122,4.61,0.21,-0.1,0  
 3AU3,ARG\_527,12.5,0,0,0  
 3CS1,CYS\_74,9.82,-1.39,0.2,21  
 3BPV,ASP\_82,3.34,0.98,-1.44,0  
 2Q12,LYS\_191,10.08,-0.42,0,0  
 1MUF,TYR\_281,10,0,0,0  
 1TWU,LYS\_97,10.15,-0.35,0,0  
 2A1V,ARG\_67,12.01,0.21,0,0  
 3FXH,GLU\_87,2.56,0.35,-2.29,0  
 1O6D,GLU\_52,4.69,0.63,-0.44,0  
 1H4U,ARG\_403,12.36,-0.14,0,0  
 3ANJ,LYS\_370,10.36,-0.14,0,0  
 2JEO,LYS\_204,10.36,-0.14,0,0  
 3DTE,ASP\_59,2.21,0.63,-2.22,0  
 2PIM,ASP\_123,3.91,0.14,-0.03,0  
 4FZR,GLU\_180,4.09,0.28,-0.69,0  
 3EUR,GLU\_45,4.5,0,0,0  
 1SJV,LYS\_142,10.36,-0.14,0,0  
 2A1V,ARG\_58,12.29,-0.21,0,0  
 2A1V,ARG\_67,12.01,-0.49,0,0  
 3ZRI,LYS\_145,10.5,0,0,0  
 4EUG,HIS\_180,3.77,1.18,0,-3.9  
 2B61,LYS\_255,10.5,0,0,0  
 3T5B,LYS\_53,10.43,-0.07,0,0  
 3GS3,ASP\_146,3.82,0.07,-0.05,0  
 3M7G,TYR\_177,9.78,0.07,-0.29,0  
 1WP5,LYS\_222,10.5,0,0,0  
 1PDB,GLU\_143,4.64,0.14,0,0  
 1NKD,GLU\_41,4.71,0.21,0,0  
 2FZ4,TYR\_183,10,0,0,0  
 3LH5,HIS\_759,6.5,0,0,0  
 1S17,ARG\_59,12.22,-0.28,0,0  
 1U7U,LYS\_187,10.36,-0.14,0,0  
 2EYI,ARG\_187,12.08,-0.42,0,0  
 3ETU,GLU\_67,4.5,0,0,0  
 2RIS,CYS\_59,11.32,0.82,1.5



3FS3,LYS\_233,10.5,0,0,0  
3M66,ASP\_335,3.28,0.28,-0.8,0  
157K,ARG\_14,11.73,-0.77,0,0  
1YG2,LYS\_99,10.5,0,0,0  
2RIK,GLU\_41,4.38,0.21,-0.33,0  
3ETV,LYS\_249,10.5,0,0,0  
2ZCO,TYR\_154,12.4,0,0.27,2.14  
1ES9,ARG\_93,12.22,-0.28,0,0  
2Q34,GLU\_163,3.86,0.21,-0.85,0  
2ZOM,ARG\_238,12.5,0,0,0  
1T3Y,ASP\_116,3.13,0.42,-1.09,0  
1YOK,GLU\_39,3.32,0.42,-1.6,0  
3GMS,ASP\_30,3.84,0.21,-0.17,0  
2A4D,GLU\_135,3.66,0.28,-1.12,0  
1NRI,ASP\_253,3.26,0,-0.54,0  
1PSW,ARG\_27,12.08,-0.42,0,0  
2H2W,ASP\_97,3.91,0.14,-0.03,0  
2H85,CYS\_290,8.34,-0.66,0,0  
1SI7,ARG\_186,12.5,0,0,0  
1X7F,ASP\_126,2.66,0.42,-1.56,0  
2FZPHIS\_251,6.08,0,0,-0.42  
1QQL,GLU\_36,3.97,0.42,-0.95,0  
4E8B,LYS\_91,10.36,-0.14,0,0  
3BJV,GLU\_49,4.5,0,0,0  
3H5T,GLU\_39,4.0,28,-0.78,0  
1H09,LYS\_207,10.22,-0.28,0,0  
3UPD,GLU\_148,2.53,1.92,-1.47,-2.43  
2FPN,GLU\_160,4.34,0.49,-0.65,0  
2EEY,LYS\_14,10.36,-0.14,0,0  
4FZN,ARG\_94,12.43,-0.07,0,0  
1FO9,LYS\_332,10.5,0,0,0  
1X04,GLU\_160,4.37,0.21,-0.34,0  
2G3A,ASP\_19,3.27,0.35,-0.88,0  
1OST,GLU\_414,4.12,0.42,-0.8,0  
3C6B,LYS\_270,10.5,0,0,0  
1X9G,CYS\_17,11.46,-0.23,0,2.69  
2P52,GLU\_221,3.92,0.21,-0.79,0  
1AK1,TYR\_165,11.27,1.27,0,0  
1MML,ARG\_159,12.01,-0.49,0,0  
1QQE,ASP\_246,3.94,0.14,0,0  
1GSZ,GLU\_61,4.57,0.21,-0.14,0  
2FZP,GLU\_315,3.98,0.28,-0.8,0  
3Q1C,LYS\_309,10.5,0,0,0  
1WP5,ASP\_309,2.36,0.42,-1.86,0  
2D7U,LYS\_109,10.01,-0.49,0,0  
2P0Y,LYS\_282,10.36,-0.14,0,0  
3ONH,ARG\_484,11.45,-1.05,0,0  
1DZF,GLU\_172,3.91,0.21,-0.8,0  
2FC3,ARG\_25,12.29,-0.21,0,0  
2DVK,ASP\_153,2.58,0.28,-1.5,0  
3DSH,LYS\_441,10.5,0,0,0  
1ZBP,ARG\_146,14,-1.36,0,2.85  
3LD1,HIS\_352,4.91,0.13,0,-1.72  
2C2Y,ASP\_7,2.84,0.35,-1.32,0  
3K8U,LYS\_7,10.08,-0.42,0,0  
1CBY,LYS\_140,10.43,-0.07,0,0  
1P2F,LYS\_29,10.5,0,0,0  
2B3M,GLU\_35,4.5,0,0,0  
1X1E,CYS\_218,11.69,0,2.69  
2ZQ5,ASP\_28,2.52,0.56,-1.84,0  
2AH5,LYS\_61,10.5,0,0,0  
2Q12,LYS\_158,10.5,0,0,0  
2B78,ARG\_248,12.29,-0.21,0,0  
3NR5,LYS\_100,10.43,-0.07,0,0  
4EVF,GLU\_10,4.57,0.07,0,0  
2EEY,TYR\_157,10,0,0,0  
3P28,GLU\_42,3.71,0.35,-1.14,0  
1RHS,LYS\_135,10.43,-0.07,0,0  
2IQT,LYS\_94,10.5,0,0,0  
3JSN,GLU\_106,4.53,0.28,-0.25,0  
4ECC,ARG\_18,12.12,-3.56,0.3.18  
3M7G,GLU\_8,3.32,0.42,-1.6,0  
2JEO,TYR\_115,10.66,0.66,0,0  
1K9S,GLU\_71,3.73,0.28,-1.04,0  
4EZB,GLU\_200,3.46,0.56,-1.6,0  
3A4C,CYS\_491,9.61,-0.03,0,0.64  
3I4T,GLU\_21,4.5,0,0,0  
2D8N,ASP\_61,2.87,0.35,-1.28,0  
3CAN,LYS\_180,10.5,0,0,0  
2XHC,ASP\_75,3.04,0.63,-1.39,0  
3GEC,ARG\_272,12.22,-0.28,0,0  
2INO,HIS\_439,8.3,1.6,1.83,-1.63  
3FRR,TYR\_128,10.04,0.34,-0.3,0  
3OBS,LYS\_90,10.5,0,0,0  
2E3C,ASP\_386,3.94,0.56,-0.42,0  
3ERF,GLU\_123,4.78,0.28,0,0  
3HNX,ASP\_82,1.66,0.91,-3.06,0  
157K,ARG\_146,12.01,-0.49,0,0  
1NRI,GLU\_177,4.64,0.14,0,0  
1D2K,ARG\_39,12.63,-2.27,0,2.4  
3L3P,LYS\_496,10.5,0,0,0  
2YLF,ARG\_75,12.29,-0.21,0,0  
1ZBS,GLU\_48,3.6,0.28,-1.18,0  
2E3S,ARG\_574,11.87,-0.63,0,0  
3RLN,LYS\_696,10.22,-0.28,0,0  
2D2S,ASP\_544,3.53,0.49,-0.76,0  
3OOP,GLU\_35,2.45,0.35,-2.4,0  
3PU6,TYR\_82,9.69,0.07,-0.38,0  
1WXQ,GLU\_230,4.5,0,0,0  
2YT4,GLU\_594,4.5,0,0,0  
3K8J,LYS\_200,10.5,0,0,0  
1O9G,GLU\_141,4.79,0.42,-0.13,0  
2EEY,CYS\_76,9.1,-0.04,0,0.14  
3HFH,GLU\_110,4.5,0,0,0  
2OPJ,ARG\_49,12.01,-0.49,0,0  
4AM1,LYS\_24,10.36,-0.14,0,0  
3G6S,GLU\_259,4.64,0.14,0,0  
3H5T,CYS\_247,11.03,-0.03,0.11,1.95  
2XHC,TYR\_172,10.18,0.21,-2.17,2.15  
2OPJ,ARG\_190,11.94,-0.56,0,0  
2EEY,ASP\_71,4.05,0.28,-0.03,0  
1WRU,ASP\_131,1.4,0.77,-3.16,0  
3O7K,ARG\_49,11.94,-0.56,0,0  
3IVF,ASP\_125,3.71,0.07,-0.16,0  
2G7O,GLU\_111,4.78,0.28,0,0  
2HRZ,LYS\_336,10.43,-0.07,0,0  
1XFK,LYS\_216,10.5,0,0,0  
2RIS,CYS\_181,9.18,-1.03,0,1.21  
3HKX,ASP\_258,3.57,0.77,-1,0  
1SBX,ASP\_156,3.74,0.49,-0.55,0  
2A0J,HIS\_41,6.43,0,0,-0.07  
1P2F,LYS\_142,10.5,0,0,0  
2D59,ARG\_36,12.43,-0.07,0,0  
3NOK,GLU\_81,4.5,0,0,0  
1Q5Z,ASP\_568,3.42,0.42,-0.8,0  
2CXV,GLU\_28,4.5,0,0,0  
3FWU,ARG\_16,12.15,-0.35,0,0  
2G9D,ARG\_103,12.15,-0.35,0,0  
3BA1,LYS\_89,10.43,-0.07,0,0  
2W2S,GLU\_126,4.5,0,0,0  
2A6B,ASP\_109,2.92,0.28,-1.16,0  
2J8A,ASP\_265,3.67,0.21,-0.34,0  
1WP5,ARG\_298,12.29,-0.21,0,0  
3H13,TYR\_322,10,0,0,0  
3OA7,GLU\_434,4.57,0.07,0,0  
1ZCE,ASP\_102,3.26,0.07,-0.62,0  
2W0Z,TYR\_571,9.88,0.14,-1.05,0.8  
2YXO,GLU\_99,4.5,0,0,0  
1MTZ,LYS\_257,10.43,-0.07,0,0  
1P1L,LYS\_57,10.01,-0.49,0,0  
1WLY,TYR\_46,10,0,0,0  
2FXT,ASP\_410,3.87,0.07,0,0  
1BN6,GLU\_296,4.51,0.07,-0.06,0  
2NRR,ARG\_478,11.52,-0.98,0,0  
2H85,GLU\_233,3.64,0.39,-1.25,0  
3AUF,ARG\_23,11.8,-0.7,0,0  
3GOZ,GLU\_16,4.5,0,0,0  
1ZKZ,LYS\_64,10.5,0,0,0  
3CXS,GLU\_37,4.5,0,0,0  
1AT0,GLU\_297,3.91,0.21,-0.8,0  
4AM1,ARG\_202,11.67,-1,0,0.17  
2PGE,ARG\_71,12.5,0,0,0  
1XTD,GLU\_128,3.61,0.35,-1.24,0  
1BN6,ASP\_42,3.67,0.14,-0.27,0  
2V81,ARG\_188,12.08,-0.42,0,0  
3RE9,LYS\_120,10.29,-0.21,0,0  
3M7D,ARG\_83,12.81,-1.64,0,1.95  
1P4X,GLU\_207,3.84,0.14,-0.8,0  
3UC9,GLU\_133,4.5,0,0,0  
1IAP,GLU\_50,3.49,0.28,-1.29,0  
2EA9,TYR\_104,9.9,0,-0.1,0  
2EJB,ARG\_109,12.15,-0.35,0,0  
1WLY,GLU\_20,3.77,0.07,-0.8,0  
2B3M,TYR\_112,9.34,0.44,-1.1,0  
3F6M,ARG\_80,11.87,-0.63,0,0  
2NRK,GLU\_170,3.91,0.21,-0.8,0  
1Z9L,HIS\_4,6.4,0.11,0,-0.21  
3BA1,LYS\_132,10.29,-0.21,0,0  
3ERF,HIS\_134,6.5,0,0,0  
1ZBS,LYS\_18,10.5,0,0,0  
2B78,GLU\_172,4.5,0,0,0  
1U53,ASP\_33,1.25,0.91,-3.45,0  
2EYI,GLU\_235,3.9,0.14,-0.74,0  
3ASA,GLU\_267,4.64,0.14,0,0  
1SIG,HIS\_331,6.5,0,0,0  
1MML,LYS\_267,10.43,-0.07,0,0  
1GSZ,LYS\_110,10.22,-0.28,0,0  
1QQL,TYR\_22,10.07,0.07,0,0  
3M66,LYS\_196,10.29,-0.21,0,0  
4EVF,ARG\_78,12.01,-3.61,0,3.12  
1XDZ,GLU\_46,4.5,0,0,0  
3EVP,GLU\_61,4.1,1.25,-1.65,0  
1ZKZ,TYR\_35,11.85,0,0,1.85  
3CAN,ARG\_47,12.08,-0.42,0,0  
2XJ4,ARG\_50,11.8,-0.7,0,0  
4GA2,CYS\_105,9.16,0,0,0.16  
4H4J,ASP\_38,4.01,0.21,0,0  
3TMO,ASP\_209,3.86,0.35,-0.29,0  
1I60,TYR\_252,11.55,0.89,-1.03,1.69  
2ZCO,LYS\_283,10.29,-0.21,0,0  
3EJG,LYS\_129,10.5,0,0,0  
3L7N,ASP\_151,3.59,0,-0.21,0  
3E0H,LYS\_118,10.29,-0.21,0,0  
2Z14,TYR\_84,9.24,0.43,-1.19,0  
1WYQ,GLU\_139,4.57,0.07,0,0  
2WHT,GLU\_74,4.5,0,0,0  
3I0C,ASP\_259,3.5,0.77,-1.06,0  
2NMO,CYS\_45,10.09,0,1.09  
2WZ9,ASP\_101,1.54,0.63,-2.89,0  
2RIK,LYS\_99,10.01,-0.49,0,0  
2O8I,HIS\_41,11.19,4.2,2.58,-2.09  
1GPP,ASP\_12,1.97,0.42,-2.25,0  
3UOV,ASP\_95,3.55,0.56,-0.81,0  
1W7B,LYS\_169,10.43,-0.07,0,0  
1NJ4,LYS\_294,10.5,0,0,0  
2FB6,GLU\_79,3.78,0.42,-1.14,0  
3QKY,TYR\_56,9.32,0,-0.68,0  
3AU3,ARG\_554,12.22,-0.28,0,0  
3M16,LYS\_194,10.36,-0.14,0,0  
3LH5,TYR\_722,8.32,1.11,-2.91,0.12  
1AKO,ARG\_77,11.59,-0.91,0,0  
3EIZ,ASP\_98,4.81,0.77,-1.87,2.11  
3FRR,ARG\_109,11.44,-1.06,0,0  
3LQE,ARG\_437,12.29,-0.21,0,0  
2XHC,GLU\_142,4.49,0,-0.01,0  
1PDB,GLU\_104,4.61,0.14,-0.03,0  
1UAJ,HIS\_72,6.5,0.14,0,-0.14  
3G53,LYS\_84,9.94,-0.56,0,0  
2CXC,GLU\_111,4.5,0,0,0  
3UC9,ASP\_28,3.87,0.14,-0.07,0  
1R29,ARG\_24,12.15,-0.35,0,0  
1HUF,ARG\_10,12.08,-0.42,0,0  
1LN4,GLU\_64,4.64,0.14,0,0  
2P0Y,TYR\_32,11.66,0.73,-0.8,1.73  
2FBQ,ARG\_59,9.86,-2.09,0,-0.55  
1NAF,LYS\_198,10.5,0,0,0  
3H9W,HIS\_98,7.16,0.8,0,-0.14  
1YM5,GLU\_131,4.71,0.21,0,0  
3HKX,ASP\_82,3.94,0.14,0,0  
2R0S,ARG\_86,12.36,-0.14,0,0  
3UAH,TYR\_424,10,0,0,0  
3U2R,ARG\_99,12.5,0,0,0  
3IV4,LYS\_73,10.43,-0.07,0,0  
2GKG,GLU\_101,2.59,0.49,-2.4,0  
2OJQ,GLU\_565,3.98,0.07,-0.59,0  
3R05,ARG\_86,11.94,-0.56,0,0  
2E0T,ARG\_84,12.22,-0.28,0,0  
1RZ2,ASP\_89,4.01,0.21,0,0  
3G9G,ASP\_212,3.94,0.21,-0.07,0  
1PSW,ARG\_146,12.22,-0.28,0,0  
3E5T,LYS\_220,9.73,-0.77,0,0  
2GZR,ARG\_206,12.36,-0.14,0,0  
1P4X,LYS\_200,10.36,-0.14,0,0  
2EJX,LYS\_51,10.36,-0.14,0,0  
1V43,CYS\_49,5.06,-2.72,-2.28,1.05  
2AZL,LYS\_127,10.36,-0.14,0,0  
2XJ4,HIS\_123,2.7,0.83,0,-4.63  
1FO9,GLU\_249,4.27,0.14,-0.37,0  
3DTE,ARG\_77,10.75,-1.75,0,0  
3JSN,ASP\_226,3.94,0.14,0,0  
2D2S,ASP\_630,3.87,0.07,0,0  
3L3P,GLU\_314,4.71,0.21,0,0  
3EVZ,HIS\_193,7.24,0.95,0,-0.21  
2ZTA,LYS\_106,10.29,-0.21,0,0  
2ZOM,ARG\_209,12.43,-0.07,0,0  
2EDM,ASP\_47,3.3,0.56,-1.06,0  
2P52,ARG\_210,10.94,-1.56,0,0  
3M7D,ARG\_276,12.5,0,0,0  
2IQT,ASP\_89,3.31,0.35,-0.84,0  
1YTD,TYR\_214,10.32,0.28,-0.14,0.19  
1SJV,ARG\_6,11.8,-0.7,0,0  
1J74,LYS\_129,10.5,0,0,0  
2F4Q,GLU\_11,4.73,0.23,0,0  
3FXH,ARG\_108,12.5,0,0,0  
2E3C,ARG\_226,12.15,-0.35,0,0  
4GA2,GLU\_41,4.5,0.28,-0.28,0  
3DTE,ARG\_32,11.48,-1.02,0,0  
1O17,LYS\_112,10.5,0,0,0  
2Q5X,GLU\_803,4.58,0.08,0,0  
1ZHV,GLU\_76,4.5,0,0,0  
1SJV,ASP\_60,3.93,0.21,-0.08,0  
1TR9,HIS\_260,6.43,0,0,-0.07  
3FK5,LYS\_39,10.43,-0.07,0,0  
1XDZ,GLU\_196,4.19,0.49,-0.8,0  
1W7B,ARG\_309,12.22,-0.28,0,0  
1XTD,LYS\_58,10.5,0,0,0

2Q34,GLU\_47,2.38,0.28,-2.4,0  
 2JEO,HIS\_153,4.81,0.8,0,-2.49  
 1UAJ,GLU\_188,4.5,0,0,0  
 3BA1,GLU\_19,3.39,0.49,-1.6,0  
 2DFL,TYR\_33,10.0,0,0,0  
 1T95,GLU\_168,3.6,0.77,-1.67,0  
 3Q1C,TYR\_292,8.38,0.43,-2.04,0  
 2I88,LYS\_395,10.5,0,0,0  
 1YOK,ARG\_117,12.29,-0.21,0,0  
 2CWY,GLU\_66,4.19,0.49,-0.8,0  
 2B0A,TYR\_96,10.0,0,0,0  
 2H01,GLU\_114,3.88,0.28,-0.9,0  
 1V6T,TYR\_235,13.49,0.07,0.8,2.62  
 1NWA,GLU\_127,1.79,0.94,-1.6,-2.05  
 3BWT,TYR\_760,10.0,0,0,0  
 2B78,LYS\_13,10.15,-0.35,0,0  
 2YWJ,LYS\_56,10.5,0,0,0  
 1GXN,LYS\_490,10.22,-0.28,0,0  
 1SUU,LYS\_669,9.87,-0.63,0,0  
 2WB8,GLU\_604,1.83,1.33,-1.6,-2.4  
 3JSN,GLU\_65,3.84,0.14,-0.8,0  
 1RAJ,HIS\_398,6.43,0,0,-0.07  
 3HVM,TYR\_189,11.43,3.21,-1.77,0  
 3LE4,HIS\_321,6.44,0.08,0,-0.14  
 3ADO,GLU\_278,4.64,0.14,0,0  
 3H8Y,LYS\_29,10.29,-0.21,0,0  
 1XEU,ARG\_204,11.66,-0.84,0,0  
 2G9D,CYS\_328,6.55,-2.51,0,0,07  
 2B3M,TYR\_136,10.0,0,0,0  
 1PVT,HIS\_192,5.87,0,0,-0.63  
 1DCF,CYS\_43,10.36,0,0,1.36  
 1UOH,GLU\_57,4.64,0.14,0,0  
 1ES9,ARG\_29,12.29,-0.21,0,0  
 2CBE,GLU\_69,2.54,0.44,-2.4,0  
 3FFM,ASP\_97,2.3,0.49,-1.99,0  
 1AKO,GLU\_139,4.64,0.14,0,0  
 2H30,HIS\_102,6.5,0,0,0  
 2X5Y,ASP\_823,3.49,0.49,-0.8,0  
 3GEC,TYR\_318,9.32,0,-0.68,0  
 1RKA,LYS\_289,10.5,0,0,0  
 3C38,GLU\_257,3.98,0.63,-1.15,0  
 2FZ4,LYS\_46,10.5,0,0,0  
 1WNH,GLU\_86,4.13,0.28,-0.65,0  
 1UCH,ASP\_218,3.8,0,0,0  
 3FFM,GLU\_69,4.71,0.21,0,0  
 3HVM,GLU\_263,3.54,0,-0.96,0  
 3N2T,ARG\_232,11.87,-0.63,0,0  
 2F8H,ASP\_85,3.17,0.49,-1.12,0  
 2OYZ,GLU\_92,4.57,0.07,0,0  
 2VAN,GLU\_186,4.57,0.07,0,0  
 3IBT,GLU\_169,1.77,0.81,-2.1,-1.45  
 3HXK,ARG\_180,12.08,-0.42,0,0  
 1YLN,GLU\_221,4.5,0,0,0  
 3M16,GLU\_10,4.18,0.14,-0.46,0  
 2FM9,ASP\_130,1.58,0.84,-3.07,0  
 1DZF,LYS\_197,10.22,-0.28,0,0  
 2HNG,ARG\_83,12.15,-0.35,0,0  
 3IRA,GLU\_150,4.57,0.07,0,0  
 1WLY,LYS\_142,10.5,0,0,0  
 2CXA,ARG\_204,11.44,-1.06,0,0  
 4FD6,ARG\_143,12.08,-0.42,0,0  
 2CXV,GLU\_9,4.78,0.28,0,0  
 3P51,GLU\_69,4.57,0.07,0,0  
 1TD6,GLU\_113,4.57,0.07,0,0  
 3H13,LYS\_460,10.36,-0.14,0,0  
 2X5Y,GLU\_895,4.5,0,0,0  
 2X5Y,HIS\_735,6.43,0,0,-0.07  
 2RJD,ARG\_461,12.22,-0.28,0,0  
 2G3A,ARG\_18,12.5,0,0,0  
 2OEW,GLU\_62,4.5,0,0,0  
 3DB9,ARG\_20,11.73,-1.43,0,0.66  
 3BJV,TYR\_58,11.31,1.1,-0.8,1.01  
 3IOC,GLU\_107,4.2,0,-0.3,0  
 1PZC,TYR\_74,9.39,0.46,-1.07,0  
 3FRR,CYS\_136,7.45,-2.29,0,0.74  
 2GEN,TYR\_43,10.07,0.07,0,0  
 3A2Z,ARG\_65,13.39,-2.66,0,3.55  
 1AT0,ARG\_272,12.5,0,0,0  
 2E35,HIS\_422,3.6,0,0,-2.9  
 2IRM,LYS\_112,10.5,0,0,0  
 2RIS,GLU\_27,4.5,0,0,0  
 2GEN,ASP\_122,3.88,0.14,-0.06,0  
 3CS1,GLU\_45,4.45,0.07,-0.12,0  
 1TXJ,LYS\_92,10.5,0,0,0  
 3ZRI,ARG\_112,13.56,-2.06,0,3.12  
 2DVK,GLU\_161,4.5,0,0,0  
 2GKG,TYR\_102,9.0,14,-1.9,0.76  
 1TLV,TYR\_64,11.51,0,0,1.51  
 4ECC,LYS\_153,10.43,-0.07,0,0  
 1CBY,LYS\_94,10.08,-0.42,0,0  
 3RNV,GLU\_438,4.05,0.35,-0.8,0  
 3N0K,GLU\_117,4.71,0.21,0,0  
 1MIX,TYR\_377,10.67,0.07,-0.77,1.37  
 1MUF,ARG\_249,10.71,-1.79,0,0  
 1YDL,LYS\_71,9.94,-0.56,0,0  
 3V46,ASP\_237,3.95,0.21,-0.06,0  
 3FHF,ASP\_64,3.28,0.28,-0.8,0  
 3U0V,HIS\_204,11.52,3.61,1.41,0  
 1FO9,LYS\_256,10.22,-0.28,0,0  
 2FM9,LYS\_89,9.94,-0.56,0,0  
 1SNT,ARG\_283,12.15,-0.35,0,0  
 2AXO,ASP\_72,3.23,0.7,-1.27,0  
 2IIA,ARG\_68,12.29,-0.21,0,0  
 3JV1,GLU\_217,4.63,0.21,-0.08,0  
 2EFK,ASP\_220,3.49,0.49,-0.8,0  
 3HYQ,HIS\_101,6.5,0,0,0  
 2IF4,GLU\_163,3.66,0.56,-1.4,0  
 1Q2Y,GLU\_26,3.89,0.91,-1.51,0  
 2AXO,ASP\_136,3.89,0.14,-0.05,0  
 3GFP,TYR\_420,11.08,1.64,-0.56,0  
 3RKV,CYS\_252,9.18,-0.3,0.048  
 2RGY,GLU\_158,3.77,0.07,-0.8,0  
 2EYH,HIS\_6,6.43,0,0,-0.07  
 2B78,TYR\_183,12.01,2.11,-0.19,0.09  
 3IPZ,LYS\_130,10.43,-0.07,0,0  
 3M7G,ARG\_76,13.41,-1.54,0,2.45  
 3RJZ,LYS\_177,9.94,-0.56,0,0  
 3ONT,TYR\_57,9.68,0,-0.32,0  
 1GQE,ASP\_71,3.38,0.42,-0.84,0  
 1TD6,ASP\_272,3.78,0,-0.02,0  
 2CL3,LYS\_169,10.08,-0.42,0,0  
 1NJ4,ARG\_243,11.73,-0.77,0,0  
 2EYI,LYS\_162,10.5,0,0,0  
 3ADO,CYS\_94,11,-1.6,0.54,3.06  
 1SQW,GLU\_22,4.5,0,0,0  
 3BQW,ARG\_343,12.29,-0.21,0,0  
 1R16,ASP\_139,1.85,0.49,-2.44,0  
 3F6F,GLU\_143,3.98,0.28,-0.8,0  
 3GMS,TYR\_330,13.6,0.4,0.8,2.4  
 3L7N,ARG\_35,12.5,0,0,0  
 3KT2,ARG\_41,12.5,0,0,0  
 2QDJ,LYS\_143,10.01,-0.49,0,0  
 2WZ9,ARG\_99,11.8,-0.7,0,0  
 4H4J,ASP\_195,3.12,0.49,-1.17,0  
 3FHF,LYS\_77,10.29,-0.21,0,0  
 1OIS,CYS\_232,10.1,0,0,1.1  
 3LJC,TYR\_228,12.68,0,0,28.24  
 3NBI,HIS\_66,6.43,0,0,-0.07  
 3P51,GLU\_15,3.63,0.14,-1.01,0  
 2DFL,TYR\_247,10.0,0,0,0  
 3OOP,ARG\_122,12.15,-0.35,0,0  
 3G9T,LYS\_201,10.43,-0.07,0,0  
 3EUR,ARG\_83,12.01,-0.49,0,0  
 1AKO,GLU\_166,4.5,0,0,0  
 2FBQ,TYR\_129,9.27,0.07,-0.8,0  
 4EVF,GLU\_105,3.51,0.42,-1.41,0  
 2G3A,GLU\_134,4.23,0.35,-0.62,0  
 3AU3,LYS\_581,10.43,-0.07,0,0  
 3EIZ,ASP\_112,3.21,0.42,-1.01,0  
 4DND,GLU\_30,4.5,0,0,0  
 3V3T,ASP\_301,3.92,0.28,-0.16,0  
 2F9F,LYS\_37,10.43,-0.07,0,0  
 2RFA,ASP\_57,2.9,0.28,-1.19,0  
 1EW4,CYS\_32,9.5,0,0,0.5  
 4DBX,ARG\_163,12.29,-0.21,0,0  
 3F5D,TYR\_184,10.0,0,0,0  
 4EZB,ASP\_270,3.87,0.07,0,0  
 3LH5,LYS\_660,10.22,-0.28,0,0  
 3OOP,LYS\_60,10.22,-0.28,0,0  
 1RLO,LYS\_92,10.01,-0.49,0,0  
 2Z61,GLU\_174,4.57,0.07,0,0  
 2G9D,LYS\_256,10.5,0,0,0  
 3RHE,ASP\_110,2.32,0.98,-2.46,0  
 2RFA,LYS\_263,10.43,-0.07,0,0  
 2OJQ,LYS\_654,10.36,-0.14,0,0  
 1Q46,GLU\_167,4.18,0.35,-0.67,0  
 1W24,CYS\_36,9.97,-2.31,0.02,3.25  
 3KV0,TYR\_164,10.02,0,0,0.02  
 2Z84,GLU\_103,2.87,1.32,-2.95,0  
 2CBE,ASP\_52,3.31,0.14,-0.64,0  
 3ZRI,ARG\_123,12.01,-0.49,0,0  
 1AT0,LYS\_273,10.15,-0.35,0,0  
 2BV9,LYS\_80,10.29,-0.21,0,0  
 1MUF,ARG\_152,12.36,-0.14,0,0  
 3CE7,GLU\_62,4.78,0.28,0,0  
 3E0H,ARG\_23,12.22,-0.28,0,0  
 1OXZ,ASP\_247,3.94,0.14,0,0  
 2X4G,ARG\_116,12.5,0,0,0  
 3IBT,ARG\_87,12.5,0,0,0  
 3MEW,GLU\_221,4.64,0.14,0,0  
 3V55,LYS\_516,10.22,-0.28,0,0  
 2CXV,LYS\_6,10.43,-0.07,0,0  
 2BQQ,TYR\_125,12.86,0.21,-0.65,3.29  
 3TRE,HIS\_4,7.23,0.8,0,-0.07  
 3O16,LYS\_223,10.5,0,0,0  
 1WP5,LYS\_76,10.5,0,0,0  
 3AU3,CYS\_483,8.7,-0.18,-1.77,1.65  
 2HXB,ASP\_5,2.52,0.49,-1.77,0  
 3L7N,ASP\_104,3.52,0.42,-0.7,0  
 2AHE,GLU\_239,3.08,0.56,-1.98,0  
 2VAN,ASP\_314,4.01,0.21,0,0  
 3PAC,GLU\_9,4.68,0.89,-0.71,0  
 3G59,ARG\_169,12.22,-0.28,0,0  
 4DIU,GLU\_242,3.63,0.42,-1.29,0  
 2YT4,LYS\_562,10.5,0,0,0  
 2PWQ,LYS\_73,10.29,-0.21,0,0  
 3FWU,CYS\_105,9.07,0,0,0.07  
 1NIJ,GLU\_72,4.5,0,0,0  
 3LJI,ARG\_140,12.22,-0.28,0,0  
 2G2D,LYS\_115,10.43,-0.07,0,0  
 3PAC,LYS\_117,10.01,-0.49,0,0  
 2A6B,HIS\_116,6.95,0.73,0,-0.28  
 2XCB,GLU\_34,4.24,0.28,-0.54,0  
 3GT0,LYS\_111,10.15,-0.35,0,0  
 3VHJ,ASP\_134,1.98,0.49,-2.3,0  
 3HVM,GLU\_306,4.57,0.07,0,0  
 3VJ8,GLU\_116,5.49,0.35,0,0.64  
 3G65,TYR\_83,12.33,0.36,-0.09,2.06  
 1R15,ARG\_239,12.43,-0.07,0,0  
 1S17,LYS\_212,10.29,-0.21,0,0  
 3US6,HIS\_77,6.43,0,0,-0.07  
 1PBV,LYS\_70,10.5,0,0,0  
 4FH3,TYR\_348,10.0,0,0,0  
 1OST,ASP\_454,3.72,0,-0.08,0  
 1BKR,TYR\_61,10.0,0,0,0  
 2B0J,ASP\_126,4.0,21,-0.01,0  
 2QDJ,GLU\_237,3.58,0.7,-1.62,0  
 1FHL,TYR\_57,9.09,1.21,-0.8,-1.32  
 1RLO,CYS\_220,8.01,-0.99,0,0  
 3M9A,TYR\_69,10.07,0.07,0,0  
 3ETV,GLU\_295,4.92,0.42,0,0  
 2Q34,GLU\_236,3.29,2.17,-3.38,0  
 1O59,TYR\_181,13.92,2.22,0,1.7  
 2E3C,TYR\_384,10.5,0,0,0  
 3PAC,CYS\_110,9.72,0,0,0.72  
 1Q2Y,GLU\_41,4.57,0.07,0,0  
 2YT4,LYS\_501,10.5,0,0,0  
 2QHT,GLU\_6,3.41,0.51,-1.6,0  
 1MJS,TYR\_297,9.46,0,-0.54,0  
 1R6Y,LYS\_94,4.5,0,0,0  
 2GEN,HIS\_45,6.43,0,0,-0.07  
 4F85,CYS\_162,9.04,-0.17,0,0.21  
 3AU3,ASP\_434,3.52,0,-0.28,0  
 3TMO,GLU\_290,3.32,0.42,-1.6,0  
 2AD1,LYS\_219,10.5,0,0,0  
 1U3Y,LYS\_334,10.5,0,0,0  
 2F9F,LYS\_42,10.36,-0.14,0,0  
 3H04,ARG\_253,12.5,0,0,0  
 1AT0,TYR\_401,12.21,0.01,1.2,1.1  
 4EKU,GLU\_340,3.76,0.61,-1.35,0  
 1W7B,ARG\_179,10.16,-2.34,0,0  
 1K95,ARG\_95,12.22,-0.28,0,0  
 3VHJ,HIS\_126,6.32,0.03,0,-0.21  
 3CBN,ASP\_121,3.53,0.07,-0.34,0  
 1UCH,LYS\_121,10.5,0,0,0  
 3CIV,ARG\_108,12.29,-0.21,0,0  
 2FZ4,TYR\_209,11.25,0.16,0,1.09  
 4E88,LYS\_127,10.15,-0.35,0,0  
 3HVM,LYS\_246,10.5,0,0,0  
 4ACJ,LYS\_735,10.15,-0.35,0,0  
 3BQE,LYS\_315,10.29,-0.21,0,0  
 4EZB,ARG\_34,11.87,-0.63,0,0  
 3PAC,GLU\_183,4.1,0.21,-0.61,0  
 1KN3,TYR\_81,10.0,0,0,0  
 2NYC,TYR\_239,10.29,0,0,0.29  
 2BLL,GLU\_561,2.55,0.48,-2.43,0  
 3UC9,LYS\_41,10.5,0,0,0  
 1SJ8,ARG\_741,12.08,-0.42,0,0  
 3LD1,CYS\_357,9.57,-0.22,0,0.79  
 2R57,LYS\_289,10.5,0,0,0  
 1X91,GLU\_87,4.5,0,0,0  
 1Q2Y,LYS\_62,10.43,-0.07,0,0  
 3OKQ,GLU\_604,4.64,0.14,0,0  
 3GV0,ARG\_155,13.71,-1.48,0,2.68  
 2EHG,GLU\_123,3.25,0.49,-1.74,0  
 3AU3,HIS\_462,7.09,0.8,0,-0.21  
 2R57,LYS\_340,10.5,0,0,0  
 3RLE,TYR\_17,10.22,0.07,-1.22,1.37  
 1A8Q,LYS\_210,10.5,0,0,0  
 1T3J,GLU\_727,4.78,0.28,0,0  
 3B7X,TYR\_116,13.12,0.21,0.51,2.4  
 1FHL,TYR\_77,11.99,3.74,-0.8,-0.94  
 1SIG,ARG\_423,12.36,-0.14,0,0  
 2XJ4,ARG\_176,11.94,-0.56,0,0  
 1RKA,ARG\_307,11.94,-0.56,0,0  
 2IF4,HIS\_90,6.5,0,0,0

2APL,ARG\_13,11.8,-0.7,0,0  
 1BGF,CYS\_108,10.5,-0.8,0.99,1.31  
 2OPJ,ARG\_86,12.22,-0.28,0,0  
 1TXJ,GLU\_12,4.78,0.28,0,0  
 1WJG,CYS\_131,8.07,-0.94,0,0  
 2G3A,ASP\_45,2.23,0.28,-1.85,0  
 2A6B,GLU\_179,4.5,0,0,0  
 2R57,LYS\_315,10.43,-0.07,0,0  
 2WZ9,LYS\_126,10.5,0,0,0  
 1UW7,GLU\_68,4.19,0.49,-0.8,0  
 2FD4,ARG\_536,12.29,-0.21,0,0  
 2FZ4,ARG\_31,12.5,0,0,0  
 2D7U,LYS\_290,10.5,0,0,0  
 2OKT,ASP\_38,1.87,1.05,-2.99,0  
 1GVP,TYR\_41,10,0,0,0  
 3C6B,GLU\_67,4.71,0.21,0,0  
 3A7L,GLU\_6,4.5,0,0,0  
 2HXB,TYR\_81,9.27,0.07,-0.8,0  
 3HST,LYS\_327,10.5,0,0,0  
 2HRZ,GLU\_316,2.31,1.5,-3.69,0  
 3D9H,GLU\_213,3.98,0.28,-0.8,0  
 3ASA,ASP\_258,2.24,0.56,-2.12,0  
 2Z61,TYR\_322,12.03,0.07,0,1.96  
 1Ri6,GLU\_114,4.47,0.35,-0.38,0  
 2H85,ARG\_135,12.22,-0.28,0,0  
 2IF4,LYS\_101,10.22,-0.28,0,0  
 2OPJ,ARG\_28,12.22,-0.28,0,0  
 1XTZ,ASP\_239,3.8,0.49,-0.49,0  
 1WJG,ASP\_44,3.87,0.07,0,0  
 3GW3,ASP\_346,3.19,0.56,-1.17,0  
 2XJ4,GLU\_152,2.29,0.35,-2.56,0  
 1P4X,ARG\_84,12.43,-0.07,0,0  
 3CRM,ASP\_69,0.82,0.56,-3.54,0  
 2H01,LYS\_170,10.5,0,0,0  
 1JKS,TYR\_240,11.44,0.0,1.44  
 1NJ4,GLU\_354,4.5,0,0,0  
 3UX2,GLU\_58,3.34,0.42,-1.58,0  
 1P4X,GLU\_48,4.29,0,-0.21,0  
 3F1X,CYS\_92,9.26,0.19,0,0.07  
 3RLE,GLU\_64,3.22,0.84,-2.12,0  
 1BGF,HIS\_81,6.5,0,0,0  
 4EF5,ARG\_178,11.66,-0.84,0,0  
 2Z61,ARG\_66,12.08,-0.42,0,0  
 2IXM,ARG\_200,12.22,-0.28,0,0  
 2OPJ,GLU\_82,4.3,0.14,-0.34,0  
 2Z61,LYS\_291,10.29,-0.21,0,0  
 1WYC,GLU\_168,6.05,1.55,0,0  
 1WLY,LYS\_229,10.22,-0.28,0,0  
 3A2Z,ASP\_29,2.2,0.35,-1.95,0  
 2X4L,ASP\_201,4.22,0.42,0,0  
 1H4U,HIS\_429,7.07,0.57,0,0  
 3FTT,GLU\_24,3.85,0.28,-0.93,0  
 1ILW,GLU\_168,4.85,0.35,0,0  
 3GE9,GLU\_151,4.71,0.21,0,0  
 1JYH,ASP\_145,2.1,0.7,-2.4,0  
 1OTM,ASP\_79,3.17,0.21,-0.84,0  
 1DZF,LYS\_166,10.5,0,0,0  
 3CIV,GLU\_282,6.96,2.52,-0.06,0  
 3F5D,ASP\_31,2.25,0.77,-2.32,0  
 3VJ8,GLU\_165,5.29,0.53,-0.8,1.06  
 1MTZ,LYS\_221,10.29,-0.21,0,0  
 2H85,LYS\_307,9.94,-0.56,0,0  
 3CSR,ARG\_111,12.15,-0.35,0,0  
 2OGQ,ASP\_537,1.52,0.77,-3.05,0  
 1JSX,LYS\_10,10.29,-0.21,0,0  
 1O59,HIS\_324,4.53,0.6,0,-2.58  
 1WXF,TYR\_37,10,0,0,0  
 3US6,ARG\_55,11.8,-0.7,0,0  
 2F4Q,ARG\_214,11.8,-0.7,0,0  
 3M7G,LYS\_134,10.43,-0.07,0,0  
 1O0X,GLU\_179,4.05,0.35,-0.8,0  
 2OSA,ASP\_322,3.87,0.63,-0.56,0  
 3QKY,GLU\_178,1.48,1.18,-1.8,-2.4  
 1V43,ARG\_56,12.08,-0.42,0,0  
 2YYO,GLU\_156,3.94,0.21,-0.77,0  
 2ZQ5,HIS\_212,6.44,3.6,2.07,-5.73  
 2AD1,ASP\_24,3.75,0.07,-0.12,0  
 1GPP,ARG\_417,12.08,-0.42,0,0  
 2H2W,LYS\_169,10.5,0,0,0  
 3KB5,HIS\_442,6.5,0,0,0  
 1O9G,ASP\_86,4.08,0.28,0,0  
 2CWY,GLU\_6,4.05,0.07,-0.52,0  
 3N2T,ARG\_120,12.01,-0.49,0,0  
 3JSN,HIS\_40,6.43,0,0,-0.07  
 3CAX,TYR\_284,13.87,1.42,0.05,2.4  
 1YOY,GLU\_158,4.5,0,0,0  
 3TMO,LYS\_216,10.22,-0.28,0,0  
 2EYI,HIS\_44,1.18,0.52,-2.25,-3.59  
 2H2W,GLU\_195,4.83,0.48,-0.01,-0.14  
 2I88,HIS\_440,6.29,0,0,-0.21  
 1JT9,CYS\_239,8.47,-2.37,0.08,1.76  
 1ZP2,ASP\_192,2.94,0.21,-1.07,0  
 2G5X,TYR\_92,9.97,0,-0.03,0  
 3H04,ASP\_204,3.79,0,-0.01,0  
 2IN0,LYS\_74,10.43,-0.07,0,0  
 1SI7,ARG\_210,12.39,-2.51,0,2.4  
 1WP5,GLU\_93,2.6,1.22,-0.77,-2.36  
 3K8J,ARG\_173,12.05,-0.76,0,0.31  
 3QYB,LYS\_896,10.5,0,0,0  
 1ATO,GLU\_350,4.5,0,0,0  
 1OGL,LYS\_207,10.5,0,0,0  
 1YG2,LYS\_34,10.5,0,0,0  
 3GG6,HIS\_175,6.71,0.28,0,-0.07  
 2VAN,GLU\_154,4.5,0.42,-0.42,0  
 1JKS,LYS\_69,10.43,-0.07,0,0  
 3CX5,TYR\_84,10,0,0,0  
 1T95,ARG\_17,12.15,-0.35,0,0  
 2OPJ,HIS\_274,6.43,0,0,-0.07  
 3PBH,LYS\_158,10.5,0,0,0  
 3IOC,ARG\_81,11.17,-1.33,0,0  
 2AZL,ASP\_62,3.49,0.07,-0.38,0  
 2J8A,ASP\_309,3.63,0.21,-0.38,0  
 1YR6,TYR\_142,9.72,0.55,-0.83,0  
 2J8A,LYS\_339,10.22,-0.28,0,0  
 3KV0,ASP\_174,3.8,0.07,-0.07,0  
 2GYZ,ARG\_40,11.59,-0.91,0,0  
 1H09,ASP\_157,1.72,0.63,-2.7,0  
 1IAP,ASP\_156,2.97,0.56,-1.39,0  
 2CE6,ARG\_25,11.8,-0.7,0,0  
 2CXA,ASP\_138,3.34,0.07,-0.53,0  
 3BQE,ARG\_199,11.87,-0.63,0,0  
 2ZCO,LYS\_64,10.43,-0.07,0,0  
 1WPA,LYS\_444,10.5,0,0,0  
 1MTZ,TYR\_81,11.29,0.09,0,1.2  
 1WYC,ASP\_172,3.05,0.49,-1.24,0  
 2D8N,ARG\_43,12.29,-0.21,0,0  
 3G9T,HIS\_112,6.22,0,0,-0.28  
 3LMF,GLU\_42,3.26,0.77,-2.01,0  
 3F53,HIS\_182,6.31,0.02,0,-0.21  
 2QVO,ASP\_89,3.41,0.28,-0.67,0  
 4DBX,TYR\_88,9.62,0,-0.38,0  
 3BJV,CYS\_135,9,0,0,0  
 2H2Z,LYS\_269,10.15,-0.35,0,0  
 2X4J,HIS\_125,6.58,0.22,0,-0.14  
 3KT9,GLU\_102,4.5,0,0,0  
 2OPJ,ARG\_211,11.59,-0.91,0,0  
 1ZYL,TYR\_328,10,0,0,0  
 2X4J,ASP\_127,3.74,0.21,-0.27,0  
 1UJ8,ASP\_56,3.9,0.14,-0.04,0  
 3M66,GLU\_154,4.5,0,0,0  
 3O16,LYS\_47,10.43,-0.07,0,0  
 1LFP,ARG\_37,11.73,-0.77,0,0  
 1SQW,LYS\_72,10.5,0,0,0  
 3FHF,GLU\_117,4.33,0.35,-0.52,0  
 3LJN,LYS\_262,10.43,-0.07,0,0  
 2ZCO,TYR\_200,13.41,0.21,0.8,2.4  
 1D2K,LYS\_204,10.01,-0.49,0,0  
 1D2K,ARG\_349,11.8,-0.7,0,0  
 1LZL,ARG\_313,12.15,-0.35,0,0  
 3LJN,LYS\_167,10.08,-0.42,0,0  
 2VGM,LYS\_7,10.5,0,0,0  
 4EVF,ARG\_289,11.52,-0.98,0,0  
 2FXT,ASP\_405,3.53,0.63,-0.9,0  
 3EVZ,LYS\_75,10.29,-0.21,0,0  
 3T5B,ASP\_147,3.56,0.21,-0.45,0  
 1QQE,GLU\_52,4.49,0.35,-0.36,0  
 2FM9,CYS\_197,9,0,0,0  
 2NRK,LYS\_24,10.5,0,0,0  
 3IBT,GLU\_260,3.98,0.28,-0.8,0  
 1O17,GLU\_109,4.58,0.42,-0.34,0  
 2RIS,TYR\_201,13.41,0.21,0.8,2.4  
 2O85,HIS\_22,6.86,0.57,0,-0.21  
 2O8I,LYS\_38,10.5,0,0,0  
 2FD5,GLU\_22,4.71,0.21,0,0  
 3AUF,TYR\_89,13.29,1.44,-0.56,2.41  
 1OLR,GLU\_18,4.85,1.15,-0.8,0  
 2Q5X,ASP\_772,2,1.12,-2.91,0  
 3F6F,ASP\_2,3.29,1.19,-1.7,0  
 2P52,ARG\_171,12.08,-0.42,0,0  
 2FZ4,ARG\_55,11.66,-0.84,0,0  
 1SIG,CYS\_132,9.53,-0.22,0,0.75  
 2RGY,ASP\_157,2.87,0.07,-1,0  
 3E0H,TYR\_39,11.19,1.78,-0.59,0  
 3EZ7,ARG\_184,12.08,-0.42,0,0  
 2OSA,ARG\_348,11.9,-0.6,0,0  
 3HVM,LYS\_74,10.01,-0.49,0,0  
 1SNT,TYR\_27,10.66,0.67,-0.01,0  
 1O0X,GLU\_78,4.84,0.57,-1.06,0.83  
 2FC3,ARG\_31,12.36,-0.14,0,0  
 2APL,TYR\_131,13.16,0.35,0.41,2.4  
 1R2Z,GLU\_157,4.64,0.14,0,0  
 2FGG,ARG\_25,12.01,-0.49,0,0  
 1YTQ,LYS\_67,10.5,0,0,0  
 1SFE,ASP\_20,3.28,0.28,-0.8,0  
 1UOH,LYS\_162,10.43,-0.07,0,0  
 1V43,HIS\_98,7.12,0.62,0,0  
 1X04,LYS\_53,10.36,-0.14,0,0  
 2V81,ASP\_148,3.32,0.07,-0.55,0  
 2OPJ,CYS\_159,9.05,-0.02,0,0.07  
 2X5Y,LYS\_729,10.36,-0.14,0,0  
 3CN5,ARG\_187,12.29,-0.21,0,0  
 3GMS,ARG\_40,8.58,-3.92,0,0  
 3HYQ,ARG\_50,12.22,-0.28,0,0  
 2Q98,GLU\_35,4.71,0.21,0,0  
 2O8PHIS\_54,6.5,0,0,0  
 1KN3,LYS\_157,9.87,-0.63,0,0  
 2CIU,LYS\_149,10.5,0,0,0  
 2P4D,LYS\_62,10.43,-0.07,0,0  
 2Q98,ARG\_89,11.94,-0.56,0,0  
 1X04,GLU\_35,4.32,0.49,-0.67,0  
 3P28,ARG\_25,12.08,-0.42,0,0  
 1GQE,HIS\_253,6.36,0,0,-0.14  
 1NJ4,TYR\_222,10.07,0.07,0,0  
 3L3P,LYS\_479,10.01,-0.49,0,0  
 3ETU,GLU\_136,4.5,0,0,0  
 3TOW,TYR\_176,12.74,0.07,0.27,2.4  
 1U53,LYS\_92,10.36,-0.14,0,0  
 3FHF,ARG\_148,12.22,-0.28,0,0  
 1O59,LYS\_318,10.5,0,0,0  
 1WLY,GLU\_310,4.37,0.21,-0.34,0  
 2Q99,ASP\_160,3.21,0.14,-0.73,0  
 3M66,LYS\_233,10.36,-0.14,0,0  
 1XKR,GLU\_199,4.5,0,0,0  
 3UV9,LYS\_475,10.29,-0.21,0,0  
 1Z9L,ASP\_62,3.82,0.14,-0.12,0  
 3QAV,TYR\_82,13.48,0.28,0.8,2.4  
 2ATR,LYS\_6,10.43,-0.07,0,0  
 1D7O,GLU\_2,4.5,0,0,0  
 3LQE,LYS\_351,9.8,-0.7,0,0  
 1JKS,TYR\_234,10.94,0.94,0,0  
 1RWZ,LYS\_53,10.43,-0.07,0,0  
 3T57,CYS\_127,5.61,-2.32,-1.3,0.23  
 2O85,GLU\_113,4.5,0,0,0  
 3BWT,HIS\_885,6.43,0,0,-0.07  
 1TLV,GLU\_251,4.78,0.28,0,0  
 2G9D,ARG\_247,11.8,-0.7,0,0  
 4F85,CYS\_232,8.26,-1.47,0,0.74  
 1P2F,LYS\_17,10.29,-0.21,0,0  
 4FZN,TYR\_9,11.37,1.13,-0.8,1.04  
 2R4Q,ASP\_224,3.43,0.35,-0.72,0  
 3GS9,TYR\_52,10,0,0,0  
 3CN5,LYS\_138,10.29,-0.21,0,0  
 2OJQ,GLU\_682,4.5,0,0,0  
 1OLR,ASP\_109,3.2,0.49,-1.08,0  
 4DVD,HIS\_73,4.63,0.8,0,-2.67  
 1YTD,ARG\_282,11.8,-0.7,0,0  
 2GKG,ASP\_108,2.68,0.35,-1.48,0  
 4HDE,LYS\_191,10.29,-0.21,0,0  
 2B3M,TYR\_40,10.14,0.14,0,0  
 2JEO,ARG\_168,11.94,-0.56,0,0  
 1NJ4,ARG\_287,11.59,-0.91,0,0  
 3V55,LYS\_481,10.5,0,0,0  
 4H86,LYS\_8,10.5,0,0,0  
 3PBH,LYS\_50,10.5,0,0,0  
 2C13,LYS\_250,10.43,-0.07,0,0  
 2FGG,HIS\_85,6.5,0,0,0  
 2HRZ,GLU\_78,3.97,0.21,-0.74,0  
 3IRA,GLU\_29,4.42,0.42,-0.5,0  
 3OIP,HIS\_45,6.36,0,0,-0.14  
 3EYE,LYS\_81,10.22,-0.28,0,0  
 3RLE,HIS\_18,9.15,4.28,1.76,-3.39  
 2Q12,ARG\_238,12.29,-0.21,0,0  
 3HUE,LYS\_171,9.94,-0.56,0,0  
 3RLN,ARG\_721,10.8,-1.7,0,0  
 2RIK,GLU\_211,4.64,0.14,0,0  
 3ILC,ASP\_133,3.83,0.14,-0.11,0  
 2H85,LYS\_173,10.5,0,0,0  
 2X4L,GLU\_303,3.16,0.49,-1.83,0  
 2V4U,GLU\_510,4.56,2.67,-1.5,-1.11  
 1NIJ,TYR\_258,11.39,1.45,-0.06,0  
 2H85,ASP\_132,3.92,0.14,-0.02,0  
 3MEW,TYR\_183,9.62,0.42,-0.8,0  
 1Q46,ARG\_6,11.38,-1.12,0,0  
 1P4X,ASP\_122,3.37,0.63,-1.06,0  
 2RIK,GLU\_111,3.89,0.35,-0.96,0  
 4EKU,GLU\_24,4.5,0,0,0  
 2YWJ,ASP\_11,3.91,0.14,-0.03,0  
 3E7P,GLU\_112,4.5,0,0,0  
 3JRT,GLU\_124,4.5,0,0,0  
 2V5B,GLU\_189,4.12,0.42,-0.8,0  
 3I47,GLU\_156,4.5,0,0,0  
 1JSX,LYS\_187,10.43,-0.07,0,0  
 1O6D,LYS\_20,10.5,0,0,0  
 2POL,ARG\_65,11.94,-0.56,0,0  
 2D7J,LYS\_123,10.22,-0.28,0,0  
 3ZTA,HIS\_29,6.5,0,0,0

3LH5,LYS\_749,10.08,-0.42,0,0  
 4FZR,HIS\_325,6.9,0.4,0,0  
 1OIS,GLU\_267,3.88,0.77,-1.38,0  
 3LD1,HIS\_355,4.61,1.1,0,-2.99  
 2D7U,GLU\_236,4.68,0.42,-0.06,0  
 2POY,ASP\_220,3.87,0.07,0,0  
 3CX2,TYR\_213,10.06,0.07,-0.01,0  
 2CXA,LYS\_167,10.5,0,0,0  
 1P6F,ASP\_66,4.08,0.28,0,0  
 3ZSL,LYS\_199,10.08,-0.42,0,0  
 1HF8,ARG\_157,12.01,-0.49,0,0  
 2B61,TYR\_243,10,0,0,0  
 3IVF,TYR\_378,12.27,1.3,0.48,0.49  
 1Z9L,CYS\_121,8.82,-0.72,0,0.54  
 3OKQ,ASP\_625,3.32,0.35,-0.83,0  
 2CWC,ARG\_204,12.08,-0.42,0,0  
 1KCM,GLU\_138,4.48,0.14,-0.16,0  
 1YW5,ASP\_135,0.46,0.84,-4.18,0  
 3NBI,ARG\_133,11.73,-0.77,0,0  
 1YM5,GLU\_76,0.67,0.97,-2.4,-2.4  
 2XHC,ARG\_37,12.01,-0.49,0,0  
 3TIR,ARG\_170,11.8,-0.7,0,0  
 3HUE,LYS\_318,10.43,-0.07,0,0  
 1MIX,HIS\_250,6.71,0.28,0,-0.07  
 3E7P,GLU\_204,3.92,0.28,-0.86,0  
 3M7G,LYS\_184,9.94,-0.56,0,0  
 2H2Z,GLU\_288,1.94,1.19,-1.84,-1.91  
 3I47,LYS\_24,10.5,0,0,0  
 3HUE,LYS\_41,10.5,0,0,0  
 1R53,LYS\_270,10.15,-0.35,0,0  
 1YW5,GLU\_64,3.56,0.21,-1.15,0  
 1A8Q,GLU\_243,4.19,0.35,-0.66,0  
 1XIP,ARG\_68,11.59,-0.91,0,0  
 3RKV,ARG\_282,10.6,-1.9,0,0  
 1KW4,ASP\_34,3.88,0.14,-0.06,0  
 3P2F,HIS\_159,6.4,0.04,0,-0.14  
 1PDB,LYS\_63,10.29,-0.21,0,0  
 2OYZ,GLU\_69,3.55,0.21,-1.16,0  
 3U2A,ASP\_35,2.78,0.56,-1.58,0  
 3AU3,HIS\_598,4.09,0.58,0,-2.99  
 3P29,TYR\_220,9.7,0,-0.3,0  
 3OA7,TYR\_548,10,0,0,0  
 2XMZ,HIS\_51,1.38,0.98,0,-6.1  
 2WOZ,TYR\_468,9.27,0.05,-0.91,0.13  
 4EUG,GLU\_13,4.5,0,0,0  
 1X7F,LYS\_109,9.94,-0.56,0,0  
 2X5Y,GLU\_763,4.4,0.14,-0.24,0  
 2F19,CYS\_39,11.11,0,0,2.11  
 2D59,CYS\_132,6.6,-4.05,0.1,1.55  
 1XIP,ASP\_146,4.15,0.35,0,0  
 1YB2,ASP\_235,3.48,0.42,-0.74,0  
 2XHC,TYR\_215,10,0,0,0  
 1XTD,GLU\_81,4.17,0.07,-0.4,0  
 3OA7,TYR\_517,10,0,0,0  
 2V1L,TYR\_76,13.27,0.07,0.8,2.4  
 1OTM,ASP\_222,2.91,0.21,-1.1,0  
 1YTD,LYS\_223,10.15,-0.35,0,0  
 1WXQ,TYR\_140,10.07,0.07,0,0  
 1F2V,GLU\_3,4.5,0,0,0  
 3O7K,GLU\_110,4.64,0.14,0,0  
 1P1L,LYS\_26,10.22,-0.28,0,0  
 1UCH,ARG\_134,12.45,-1.93,0,1.88  
 2ZCX,ARG\_67,11.26,-1.24,0,0  
 3ETV,LYS\_137,10.5,0,0,0  
 3ASA,GLU\_53,4.5,0,0,0  
 2BOJ,TYR\_228,10.6,0,0,0.6  
 2D8N,LYS\_131,10.43,-0.07,0,0  
 2Z14,TYR\_105,11.64,0,0,1.64  
 3CO1,LYS\_122,9.8,-0.7,0,0  
 3HZQ,LYS\_29,10.22,-0.28,0,0  
 3CRM,GLU\_78,2.74,0.42,-2.18,0  
 1XAW,LYS\_504,10.43,-0.07,0,0  
 1OGL,GLU\_110,4.71,0.21,0,0  
 3E0H,GLU\_130,0.68,0.98,-2.4,-2.4  
 3LJC,HIS\_109,6.43,0,0,-0.07  
 2FL7,TYR\_90,11.95,2.75,-0.8,0  
 3VJ8,TYR\_105,10.14,0.14,0,0  
 3LPZ,ARG\_318,12.22,-0.28,0,0  
 2RGY,GLU\_131,4.22,0.21,-0.49,0  
 1JYH,LYS\_128,10.01,-0.49,0,0  
 2AHE,GLU\_97,4.5,0,0,0  
 3GA2,LYS\_8,10.5,0,0,0  
 1L2F,GLU\_128,3.84,0.14,-0.8,0  
 3G9T,LYS\_246,10.36,-0.14,0,0  
 2Q34,GLU\_104,4.05,0.28,-0.73,0  
 1PBM,LYS\_102,10.43,-0.07,0,0  
 4DND,GLU\_58,3.83,0.35,-1.02,0  
 1DTO,GLU\_39,3.55,0.94,-0.76,-1.13  
 2R51,GLU\_13,4.94,0.35,0.09,0  
 2R0S,TYR\_133,9.92,0,-0.08,0  
 3N2T,GLU\_94,3.88,0.49,-1.11,0  
 2AH5,GLU\_82,3.39,0.49,-1.6,0  
 3ZRI,ASP\_154,3.94,0.14,0,0  
 1ZHV,LYS\_6,10.29,-0.21,0,0  
 3ZXY,LYS\_206,10.43,-0.07,0,0  
 2B61,TYR\_335,9.27,0.07,-0.8,0  
 2PGE,TYR\_9,13.39,0.21,0.78,2.4  
 4FLE,LYS\_154,12.36,-0.14,0,0  
 2FPN,GLU\_33,3.85,0.07,-0.72,0  
 2CN1,GLU\_93,4.5,0,0,0  
 2Z0M,ASP\_249,2.72,0.63,-1.71,0  
 2R2Y,GLU\_70,1.91,0.28,-2.87,0  
 3F6F,LYS\_86,10.5,0,0,0  
 1H09,TYR\_231,10.22,0.22,0,0  
 2IQT,LYS\_125,10.5,0,0,0  
 2G5X,ARG\_195,12.08,-0.42,0,0  
 3IVF,ASP\_221,3.32,0.42,-0.9,0  
 2AD1,GLU\_204,1.36,0.77,-1.51,-2.4  
 3H13,HIS\_302,4.27,1.12,0,-3.35  
 1E5S,CYS\_223,8.58,-2.33,0,1.91  
 1PNE,ASP\_80,3.76,0.21,-0.25,0  
 1BGF,ARG\_85,12.22,-0.28,0,0  
 2QEV,GLU\_28,3.9,0.21,-0.81,0  
 4F85,GLU\_84,1.62,0.7,-3.58,0  
 1TP6,HIS\_11,6.36,0,0,-0.14  
 1LTU,TYR\_36,11.01,1.81,-0.8,0  
 2ILR,GLU\_463,4.5,0,0,0  
 1O5J,ARG\_36,12.22,-0.28,0,0  
 1QQE,LYS\_242,10.43,-0.07,0,0  
 3PZ9,ARG\_387,11.31,-1.19,0,0  
 2GYZ,GLU\_25,3.91,0.28,-0.87,0  
 1QQE,ASP\_264,3.15,0.49,-1.14,0  
 3MTT,TYR\_460,10,0,0,0  
 2DFL,HIS\_279,6.43,0,0,-0.07  
 2XMZ,LYS\_5,10.29,-0.21,0,0  
 1MTZ,GLU\_70,3.8,0.49,-1.19,0  
 3TIR,ARG\_194,12.01,-0.49,0,0  
 2V5B,GLU\_105,3.46,0.49,-1.53,0  
 2DG7,ARG\_105,13.4,-1.5,0.2,4  
 2WOZ,LYS\_576,10.36,-0.14,0,0  
 2B78,ARG\_140,12.01,-0.49,0,0  
 3IOO,CYS\_111,8.68,-0.32,0,0  
 2WB8,HIS\_647,1.6,1.6,0,-6.5  
 2IKM,GLU\_72,4.43,0,-0.07,0  
 2FBI,LYS\_136,10.43,-0.07,0,0  
 3V55,GLU\_368,4.54,0.84,-0.8,0  
 1R7J,TYR\_57,9.35,0.07,-0.72,0  
 1TJE,TYR\_103,11.46,0.13,-0.3,1.62  
 1BKR,ASP\_88,3.67,0,-0.13,0  
 1R7J,ARG\_77,12.08,-0.42,0,0  
 2POY,HIS\_141,6.34,0.12,0,-0.28  
 3GW3,ARG\_50,11.42,-1.08,0,0  
 1G8P,HIS\_325,1.08,1.82,-1.92,-5.33  
 1PZC,GLU\_51,4.5,0,0,0  
 1X7F,GLU\_298,4.57,0.07,0,0  
 1KN3,LYS\_113,10.29,-0.21,0,0  
 1D2K,TYR\_354,10.97,0.97,0,0  
 2YXO,ARG\_238,9.57,-2.93,0,0  
 1BKB,ASP\_130,3.93,0.14,-0.01,0  
 4ACJ,LYS\_652,10.29,-0.21,0,0  
 1X7F,ASP\_274,2.73,0.35,-1.42,0  
 3JSN,LYS\_184,10.5,0,0,0  
 2XMZ,LYS\_262,10.5,0,0,0  
 3RHE,ARG\_115,11.99,-1.05,0.0,54  
 3UAH,TYR\_170,12.66,1.07,-1.28,2.86  
 1LZL,GLU\_268,4.64,0.14,0,0  
 1TJE,ARG\_191,11.94,-0.56,0,0  
 1DOV,TYR\_237,10,0,0,0  
 3M66,ARG\_374,12.29,-0.21,0,0  
 3CSR,LYS\_88,10.36,-0.14,0,0  
 3FKS,LYS\_243,10.5,0,0,0  
 2EA9,LYS\_54,10.22,-0.28,0,0  
 2IF4,ARG\_175,11.66,-0.84,0,0  
 1V6T,GLU\_22,4.57,0.07,0,0  
 3M9A,GLU\_48,4.64,0.14,0,0  
 3G9T,ARG\_187,11.87,-0.63,0,0  
 1EYH,ASP\_113,2.59,1.26,-2.48,0  
 3C6B,LYS\_258,10.5,0,0,0  
 3FK5,ARG\_53,12.01,-0.49,0,0  
 1L2F,GLU\_132,4.71,0.21,0,0  
 2V5B,GLU\_108,3.84,0.28,-0.95,0  
 3V55,LYS\_524,10.22,-0.28,0,0  
 4AF2,ASP\_139,2.49,0.98,-2.29,0  
 3IRA,LYS\_168,10.5,0,0,0  
 2XJ4,CYS\_104,9.01,-0.09,0.0,1  
 2ZCO,GLU\_31,4.11,0.35,-0.74,0  
 2VAN,LYS\_206,10.22,-0.28,0,0  
 2GZR,ASP\_220,4.09,0.42,-0.13,0  
 4EKU,TYR\_90,12.23,1.9,-0.8,1.13  
 1GPP,CYS\_416,6.17,-0.88,-2.4,0.45  
 4DNU,ASP\_367,2.45,0.84,-2.18,0  
 2CWC,ARG\_153,12.01,-0.49,0,0  
 1X8F,CYS\_166,12.8,0,0.08,3.72  
 4DVD,HIS\_78,6.5,0,0,0  
 4EVF,LYS\_128,10.5,0,0,0  
 3MEW,ASP\_223,3.49,0.49,-0.8,0  
 3CAX,GLU\_159,4.42,0.07,-0.15,0  
 2WB8,GLU\_694,3.53,0.49,-1.46,0  
 3R2E,ARG\_114,11.8,-0.7,0,0  
 2W2S,CYS\_178,8.69,-0.38,0,0.07  
 1SUU,GLU\_761,3.67,0.21,-1.04,0  
 1DUP,ARG\_104,12.08,-0.42,0,0  
 3QKY,TYR\_230,11.07,0.36,-0.8,1.51  
 1GQE,TYR\_27,13.34,0.14,0.8,2.4  
 2YYO,LYS\_130,10.5,0,0,0  
 2EFK,HIS\_17,6.54,0.04,0,0  
 1OOX,LYS\_34,10.29,-0.21,0,0  
 3JSN,GLU\_158,4.64,0.14,0,0  
 3H9W,ARG\_91,11.59,-0.91,0,0  
 1P6F,TYR\_32,10,0,0,0  
 1Q46,CYS\_97,11.27,0.15,0.77  
 1PDB,ARG\_28,12.15,-0.35,0,0  
 1Y2Q,GLU\_28,4.22,0.28,-0.56,0  
 3F6F,ASP\_209,3.99,0.42,-0.23,0  
 1W7B,GLU\_139,1.47,2.18,-1.86,-3.35  
 2EFK,ARG\_278,12.5,0,0,0  
 2Q12,ARG\_72,12.5,0,0,0  
 3DB9,HIS\_252,1.85,0.13,0,-4.78  
 2FM9,ASP\_53,3.83,0.14,-0.11,0  
 2EJB,HIS\_134,6.49,0.2,0,-0.21  
 2O4D,GLU\_122,2.89,0.84,-2.45,0  
 1WNH,TYR\_8,10,0,0,0  
 3GA2,GLU\_107,4.5,0,0,0  
 1DUP,ARG\_116,12.22,-0.28,0,0  
 2BDV,ARG\_41,12.01,-0.49,0,0  
 2X4L,LYS\_265,10.29,-0.21,0,0  
 4EZB,GLU\_149,4.03,0.14,-0.61,0  
 2CIU,GLU\_117,4.5,0,0,0  
 2PGE,ARG\_284,12.5,0,0,0  
 3RKV,LYS\_319,10.43,-0.07,0,0  
 1TD6,TYR\_239,10.57,1.04,0,-0.47  
 1SQH,ARG\_216,12.29,-0.21,0,0  
 1PZC,LYS\_106,10.5,0,0,0  
 3UAH,TYR\_170,12.66,1.07,-1.28,2.86  
 2A4D,ASP\_113,2.94,0.7,-1.55,0  
 1XTZ,ARG\_223,12.5,0,0,0  
 2E3C,TYR\_446,8.33,0.13,-0.22,-1.58  
 1YB2,GLU\_41,4.71,0.21,0,0  
 2O0K,LYS\_23,10.5,0,0,0  
 1PSW,LYS\_47,12.01,-0.49,0,0  
 2JEO,ASP\_150,3.92,0.42,-0.3,0  
 3GV0,ARG\_196,12.01,-0.49,0,0  
 3RHE,ASP\_88,3.93,0.21,-0.08,0  
 1MJS,TYR\_237,11.85,0.0,1.85  
 3GV0,GLU\_299,4.32,3.02,-0.8,-2.4  
 1ANU,LYS\_62,10.5,0,0,0  
 3F53,ARG\_68,12.29,-0.21,0,0  
 3B4D,GLU\_189,4.19,0.49,-0.8,0  
 2Q13,LYS\_6,10.5,0,0,0  
 3EJC,GLU\_70,4.32,0.63,-0.81,0  
 2IDC,TYR\_111,11.11,1.11,0,0  
 2Q98,LYS\_191,7.47,-1.6,0.0,07  
 2CVB,GLU\_119,1.28,2.54,-3.98,-1.79  
 4GCO,ASP\_198,3.98,0.28,-0.1,0  
 2R4Q,ASP\_269,3.14,0.14,-0.8,0  
 1R29,ARG\_28,12.43,-0.07,0,0  
 4FCU,HIS\_182,2.09,0.2,0,-4.61  
 1SUU,GLU\_761,3.67,0.21,-1.04,0  
 4DEZ,ARG\_127,12.08,-0.42,0,0  
 2EHG,ARG\_94,12.08,-0.42,0,0  
 3LJN,LYS\_153,10.36,-0.14,0,0  
 4ECC,CYS\_191,8.52,-0.55,0.0,07  
 3GV0,ASP\_300,2.94,0.35,-1.21,0  
 3B21,GLU\_183,4.5,0,0,0  
 3HYQ,ASP\_108,2.27,1.05,-2.58,0  
 1LZL,GLU\_53,4.71,0.21,0,0  
 2GS5,ARG\_5,12.5,0,0,0  
 3IL3,ARG\_4,11.8,-0.7,0,0  
 1YTO,LYS\_75,10.43,-0.07,0,0  
 2OKT,LYS\_288,10.22,-0.28,0,0  
 2NRK,GLU\_80,3.62,0.42,-1.3,0  
 3FHF,ARG\_169,11.8,-0.7,0,0  
 1GPP,LYS\_152,10.43,-0.07,0,0  
 3P51,TYR\_65,11.87,0.32,0,1.55  
 2OSA,HIS\_277,7.26,0.9,0,-0.14  
 3RKV,LYS\_285,10.22,-0.28,0,0  
 4EUG,HIS\_73,1.39,0.23,-1.14,-4.2  
 2FG1,GLU\_47,3.06,0.56,-2,0  
 2A0J,ARG\_51,12.15,-0.35,0,0  
 2XJ4,ARG\_56,12.01,-0.49,0,0  
 1V6T,ASP\_41,1.66,0.77,-2.91,0  
 2GM,ASP\_98,4.01,0.21,0,0  
 1GXN,ARG\_604,12.01,-0.49,0,0  
 1TD6,HIS\_11,4.83,0.43,0.24,-2.34  
 3P2F,ARG\_155,12.5,0,0,0  
 3RNV,CYS\_446,6.66,-2.42,0,0.07



2OEW,GLU\_293,4.57,0.07,0  
 4DVD,ASP\_124,3.59,0.35,-0.56,0  
 4DEZ,LYS\_148,10.08,-0.42,0,0  
 2QVO,LYS\_58,10.5,0,0,0  
 2EOT,HIS\_172,6.5,0,0,0  
 1UOH,HIS\_45,3.14,1.14,0.55,-5.06  
 3V55,HIS\_503,6.5,0,0,0  
 1BKB,ARG\_131,11.8,-0.7,0,0  
 1OST,LYS\_412,10.5,0,0,0  
 2ZOM,ARG\_263,11.87,-0.63,0,0  
 2XWS,GLU\_19,4.55,0.21,-0.16,0  
 1O6D,HIS\_114,6.46,0.03,0,-0.07  
 3PU6,ARG\_138,12.22,-0.28,0,0  
 2FM9,LYS\_135,10.43,-0.07,0,0  
 3I0C,TYR\_255,10.47,0,-0.08,0.54  
 3EVP,TYR\_113,10,0,0,0  
 3IVF,ASP\_233,3.11,0.14,-0.83,0  
 2WZ9,ASP\_98,1.86,0.56,-2.5,0  
 1FHL,ASP\_318,2.07,0.77,-2.51,0  
 2F19,ARG\_108,12.01,-0.49,0,0  
 1G5Z,GLU\_63,4.09,0.28,-0.69,0  
 3NR5,GLU\_132,4.5,0,0,0  
 3J5N,GLU\_167,6.72,2.68,-0.62,0.16  
 2YWJ,ASP\_34,1.92,0.56,-2.44,0  
 2VAN,TYR\_296,12.53,0.15,2.38  
 2HXB,LYS\_157,10.29,-0.21,0,0  
 2D0A,ARG\_38,11.8,-0.7,0,0  
 1R7J,GLU\_53,4.05,0.35,-0.8,0  
 2HXB,GLU\_53,4.5,0,0,0  
 2JEO,ASP\_161,3.65,0,-0.15,0  
 3LD1,ARG\_153,11.38,-1.12,0,0  
 3ONH,ASP\_488,3.25,0.77,-1.32,0  
 2F8H,ARG\_227,11.94,-0.56,0,0  
 1Q46,ASP\_93,2.25,0.28,-1.83,0  
 2IJB,LYS\_44,10.5,0,0,0  
 3C6B,ARG\_226,12.5,0,0,0  
 3CGW,GLU\_19,4.85,0.35,0,0  
 3LMF,ASP\_92,3.64,0.14,-0.3,0  
 2QHT,GLU\_181,4.19,0.49,-0.8,0  
 3RE9,GLU\_186,4.53,0.14,-0.11,0  
 3CCY,GLU\_10,4.5,0,0,0  
 1YM5,ARG\_74,12.43,-0.07,0,0  
 3CS1,LYS\_23,10.5,0,0,0  
 4ECC,LYS\_100,10.5,0,0,0  
 2D0A,ASP\_14,3.47,0.35,-0.68,0  
 2W1R,GLU\_103,4.57,0.07,0,0  
 1IDK,HIS\_247,3.42,0.87,0.96,-4.9  
 3V55,LYS\_644,10.43,-0.07,0,0  
 2O8P,GLU\_140,2.45,0.35,-2.4,0  
 1BYI,GLU\_94,3.51,0.35,-1.35,0  
 2F4Q,ASP\_59,3.28,0.63,-1.15,0  
 1WOU,LYS\_40,10.5,0,0,0  
 3CXS,GLU\_156,4.5,0.42,-0.42,0  
 3KV0,ARG\_93,11.45,-1.05,0,0  
 3ETU,LYS\_125,10.5,0,0,0  
 3F6F,TYR\_114,10.83,1.63,-0.8,0  
 3CCY,TYR\_9,10,0,0,0  
 1WYC,ARG\_251,11.94,-0.56,0,0  
 3IL3,ARG\_291,11.8,-0.7,0,0  
 1SBX,ASP\_133,3.87,0.07,0,0  
 3OA7,HIS\_8,6.5,0,0,0  
 2Q12,GLU\_69,4.57,0.07,0,0  
 2ILR,GLU\_276,4.5,0,0,0  
 1BN6,TYR\_57,10.09,0.75,-0.35,-0.32  
 2J8A,ASP\_286,1.04,0.91,-3.67,0  
 2DFL,LYS\_74,10.36,-0.14,0,0  
 1NKD,CYS\_54,9.07,0,0,0.07  
 3RRQ,ARG\_94,11.45,-1.05,0,0  
 1WXQ,TYR\_268,10.07,0.07,0,0  
 2V81,GLU\_92,3.47,0.21,-1.23,0  
 2RIK,LYS\_186,10.15,-0.35,0,0  
 2Q99,ASP\_211,3.49,0.49,-0.8,0  
 3V1Q,LYS\_662,10.5,0,0,0  
 1O17,HIS\_86,7.12,0.76,0,-0.14  
 3V4G,GLU\_64,4.16,0.35,-0.69,0  
 1T07,ARG\_63,11.94,-0.56,0,0  
 3CIV,CYS\_91,13.33,-0.67,1.16,3.85  
 1V43,TYR\_231,12.33,0.89,0.8,0.65  
 2YT4,LYS\_567,10.08,-0.42,0,0  
 2H01,HIS\_76,6.55,2.2,3.13,-5.28  
 3IBT,HIS\_126,4.69,0,0,-1.81  
 3LMO,GLU\_95,4.58,0.21,-0.13,0  
 1WLJ,GLU\_204,5.01,0.21,0.3,0  
 1RZ2,LYS\_152,10.36,-0.14,0,0  
 4DNU,ARG\_209,12.29,-0.21,0,0  
 3COC,ARG\_328,12.08,-0.42,0,0  
 3IDW,ASP\_38,3.86,0.14,-0.08,0  
 2D7U,ASP\_289,3.6,0.91,-1.11,0  
 2CW4,ARG\_101,11.94,-0.56,0,0  
 2B78,LYS\_15,10.36,-0.14,0,0  
 1L2F,LYS\_129,9.87,-0.63,0,0  
 3GOZ,TYR\_218,10,0,0,0  
 2GZR,ASP\_62,0.81,0.77,-3.77,0  
 2VGM,LYS\_271,10.5,0,0,0  
 3A2Z,GLU\_164,3.39,0.49,-1.6,0  
 2O0K,TYR\_323,11.13,1.13,0,0  
 1V8E,ARG\_120,12.5,0,0,0  
 2FG1,LYS\_140,10.29,-0.21,0,0  
 2A1V,GLU\_70,4.64,0.14,0,0  
 2CXJ,GLU\_29,4.64,0.14,0,0  
 1H09,TYR\_41,9.22,0.07,-1.03,0.18  
 2IQT,LYS\_194,9.73,-0.77,0,0  
 3U0V,HIS\_175,6.65,2.58,1.62,-4.06  
 1P4X,GLU\_213,4.5,0,0,0  
 1YTD,HIS\_364,7.13,0.63,0,0  
 2DG7,HIS\_23,6.76,0.26,0,0  
 1ZBM,ARG\_68,12.01,-0.49,0,0  
 2Q12,LYS\_160,10.15,-0.35,0,0  
 3EUR,TYR\_115,10.48,0.5,-0.87,0.86  
 3FK5,ARG\_35,11.66,-0.84,0,0  
 2OPJ,ARG\_215,11.94,-0.56,0,0  
 3HYQ,ARG\_105,12.08,-0.42,0,0  
 3CRM,ASP\_307,3.35,0.07,-0.52,0  
 1R5Q,ASP\_87,3.09,0.49,-1.2,0  
 3HVM,TYR\_228,10.28,0.0,0.28  
 3GVO,ASP\_126,0.87,1.05,-3.98,0  
 1V43,GLU\_247,4.64,0.14,0,0  
 3GA2,HIS\_227,6.36,0,0,-0.14  
 1E55,ASP\_81,1.49,0.91,-3.22,0  
 3H13,ASP\_452,3.35,0.35,-0.8,0  
 1NIJ,ASP\_265,3.87,0.07,0,0  
 1YTO,CYS\_66,8.66,-0.34,0,0  
 2V81,GLU\_71,4.1,0.49,-0.89,0  
 2V4X,ARG\_129,11.94,-0.56,0,0  
 2H85,GLU\_3,3.94,0.21,-0.77,0  
 2E3C,ARG\_310,11.8,-0.7,0,0  
 1MML,LYS\_274,10.29,-0.21,0,0  
 1QQE,LYS\_69,10.43,-0.07,0,0  
 3FTT,ASP\_99,3.02,0.42,-1.2,0  
 1SQH,GLU\_280,4.64,0.14,0,0  
 1V43,LYS\_116,10.5,0,0,0  
 1Y0K,LYS\_148,10.29,-0.21,0,0  
 3EVZ,TYR\_71,10,0,0,0  
 1VJG,ASP\_153,3.27,0.21,-0.74,0  
 2H01,HIS\_132,3.39,0.4,0,-3.51  
 2D8N,LYS\_5,10.43,-0.07,0,0  
 1UOH,GLU\_171,4.5,0,0,0  
 2CN1,ARG\_17,12.43,-0.07,0,0  
 1F09,ARG\_419,13.55,-0.27,0,1.32  
 1PDB,ASP\_94,3.43,0.21,-0.58,0  
 3F6F,ASP\_80,3.27,0.49,-1.02,0  
 1F2V,ARG\_16,12.36,-0.14,0,0  
 2H2W,GLU\_159,4.5,0,0,0  
 1T95,GLU\_24,3.57,0.49,-1.42,0  
 1MTZ,GLU\_87,3.61,0.71,-1.6,0  
 2IRM,CYS\_21,2.48,-5.35,-1.94,0.77  
 2X4L,LYS\_102,10.5,0,0,0  
 2PPN,GLU\_107,3.98,0.28,-0.8,0  
 3LJC,ASP\_85,3.46,0.35,-0.69,0  
 3IRA,ARG\_140,11.59,-0.91,0,0  
 1ZYL,LYS\_238,10.43,-0.07,0,0  
 3RAZ,ARG\_110,12.01,-0.49,0,0  
 3R2E,GLU\_78,3.47,0.56,-1.59,0  
 4ANN,TYR\_205,10.14,0.14,0,0  
 1SNT,ARG\_41,12.15,-0.35,0,0  
 4DIU,LYS\_139,10.5,0,0,0  
 2DFL,ARG\_320,10.88,-1.62,0,0  
 2AHE,ARG\_40,12.1,-1.98,0,1.58  
 3QAV,LYS\_123,10.36,-0.14,0,0  
 1NIJ,HIS\_215,6.86,0.43,0,-0.07  
 2EJX,TYR\_64,10,0,0,0  
 3MEW,ASP\_258,2.12,0.63,-2.3,0  
 1DOV,GLU\_95,4.05,0.28,-0.73,0  
 3I4T,ASP\_93,3.54,0.07,-0.33,0  
 1V43,ARG\_307,12.15,-0.35,0,0  
 3CN5,TYR\_53,10.07,0.07,0,0  
 1FKM,LYS\_263,10.29,-0.21,0,0  
 2Q34,LYS\_178,10.43,-0.07,0,0  
 2B61,TYR\_266,10.95,1.91,-0.25,-0.71  
 1X91,ARG\_69,12.22,-0.28,0,0  
 2AZL,GLU\_247,4.85,0.35,0,0  
 4EF5,TYR\_182,13.41,0.21,0.8,2.4  
 1AHL,ARG\_35,11.87,-0.63,0,0  
 3EZ7,TYR\_59,10.93,0,0,0.93  
 3VJ8,CYS\_70,10.67,-0.01,0,1.68  
 3JRT,LYS\_63,10.43,-0.07,0,0  
 3BQE,ASP\_357,3.2,0.49,-1.09,0  
 1Q2Y,GLU\_21,4.58,0.14,-0.06,0  
 1V6T,LYS\_246,10.36,-0.14,0,0  
 1T95,ARG\_98,12.29,-0.21,0,0  
 3M3P,ASP\_105,3.04,0.07,-0.83,0  
 3OKQ,GLU\_638,4.05,0.35,-0.8,0  
 1QQI,HIS\_102,6.51,0.29,0,-0.28  
 1MJS,ARG\_372,12.08,-0.42,0,0  
 2HXB,LYS\_168,9.94,-0.56,0,0  
 3IPZ,GLU\_76,4.5,0,0,0  
 2O8P,TYR\_67,8.8,0.07,-1.27,0  
 2EEY,GLU\_42,4.19,0.49,-0.8,0  
 2FXT,GLU\_267,4.44,0,-0.06,0  
 1SJJ,GLU\_12,2.84,0.56,-2.22,0  
 3A7L,GLU\_111,3.13,0.63,-2,0  
 1BN6,ASP\_84,2.97,0.56,-1.39,0  
 2A1V,GLU\_25,4.19,0.49,-0.8,0  
 3A2Z,TYR\_47,9.34,0.14,-0.8,0  
 2GZQ,ARG\_89,12.38,-1.38,0,1.26  
 1KN3,ARG\_49,13.96,-0.48,0,1.94  
 4F85,ARG\_286,12.22,-0.28,0,0  
 2V4U,ASP\_418,3.57,0.35,-0.58,0  
 3G53,GLU\_143,4.5,0,0,0  
 2A6B,GLU\_43,4.5,0,0,0  
 3HVM,CYS\_158,6.15,-3.87,-1.48,2.49  
 3BB7,TYR\_180,10.26,0,-0.18,0.43  
 2O8PLYS\_100,10.5,0,0,0  
 3Q1C,HIS\_240,6.43,0,0,-0.07  
 3NR5,ARG\_157,11.58,-0.92,0,0  
 2BV9,ASP\_140,4.01,0.28,-0.07,0  
 3B79,TYR\_15,10,0,0,0  
 2PGX,ARG\_114,11.36,-1.14,0,0  
 2NYC,ARG\_288,12.08,-0.42,0,0  
 2Q07,TYR\_441,10.27,0,0,0.27  
 4DEZ,ARG\_95,12.22,-0.28,0,0  
 3DHN,ASP\_180,3.48,0.56,-0.89,0  
 3FK5,ARG\_220,11.73,-0.77,0,0  
 3OOP,TYR\_4,10,0,0,0  
 2F4Q,ARG\_313,12.5,0,0,0  
 2PIM,ARG\_109,12.01,-0.49,0,0  
 1AD6,ASP\_507,3.56,0.14,-0.38,0  
 2OSA,LYS\_280,10.5,0,0,0  
 3KT9,ASP\_37,2.37,0.56,-1.99,0  
 2A1V,ASP\_30,3.87,0.07,0,0  
 3Q6L,LYS\_22,10.36,-0.14,0,0  
 1SBX,TYR\_191,12.14,0.09,2.04  
 1WXQ,TYR\_64,9.67,0.21,-0.54,0  
 3CIV,HIS\_183,3.86,0.76,-3.39  
 3PU6,ASP\_75,2.11,0.7,-2.38,0  
 3IU5,ASP\_107,3.51,0.14,-0.43,0  
 3BPP,GLU\_218,4.5,0,0,0  
 4E9E,LYS\_514,10.36,-0.14,0,0  
 3N2T,GLU\_199,4.64,0.14,0,0  
 1Z3X,HIS\_211,3.79,1.17,0,-3.88  
 1IDK,ASP\_255,2.91,0.35,-1.24,0  
 2FG1,GLU\_147,4.5,0,0,0  
 2CVB,ASP\_141,2.82,0.63,-1.61,0  
 1J7G,GLU\_58,4.5,0,0,0  
 1R5Q,GLU\_59,3.82,0.21,-0.89,0  
 2OJQ,GLU\_387,4.78,0.28,0,0  
 4FCU,ARG\_243,12.08,-0.42,0,0  
 3CXS,LYS\_115,10.22,-0.28,0,0  
 2W2S,TYR\_138,10.43,1.07,-0.64,0  
 3CAX,HIS\_400,5.95,1.1,0.07,-1.72  
 3O16,GLU\_20,4.5,0,0,0  
 1SQH,GLU\_264,2.31,1.91,-1.6,-2.5  
 3CGW,GLU\_139,4.71,0.21,0,0  
 4GA2,GLU\_57,4.5,0,0,0  
 3CCY,ASP\_36,1.6,0.35,-2.55,0  
 3UV9,CYS\_486,0.71,-8.43,0,0.14  
 1J74,GLU\_121,3.69,0.63,-1.44,0  
 1OXZ,CYS\_256,9.47,-0.05,0.52  
 3T8R,GLU\_72,4.5,0,0,0  
 2V5B,GLU\_98,4.57,0.07,0,0  
 1TR9,TYR\_83,11.27,0,0,1.27  
 3CIV,GLU\_41,4.64,0.14,0,0  
 3ONH,LYS\_523,9.94,-0.56,0,0  
 2N15,LYS\_59,10.5,0,0,0  
 2B6P,GLU\_232,3.39,0.7,-1.81,0  
 2AZP,TYR\_139,11.14,0,0,1.14  
 1R5S,ARG\_79,11.94,-0.56,0,0  
 3ZXY,ASP\_52,3.08,0.35,-1.07,0  
 4AF2,TYR\_118,11.26,1.45,-0.19,0  
 3L7N,ASP\_47,1.91,0.56,-2.45,0  
 2Q5X,LYS\_841,10.5,0,0,0  
 3M70,HIS\_150,6.43,0,0,-0.07  
 3CS1,GLU\_111,4.78,0.28,0,0  
 1MN3,GLU\_429,4.03,0.28,-0.75,0  
 1T6L,ARG\_137,12.08,-0.42,0,0  
 1DFZ,GLU\_160,2.72,0.49,-2.26,0  
 3H04,ARG\_263,12.29,-0.21,0,0  
 3CAN,ASP\_111,2.25,0.28,-1.84,0  
 3UAH,ASP\_195,3.58,0.42,-0.64,0  
 2B78,GLU\_151,3.99,1.07,-1.58,0  
 2H2Z,ASP\_248,4.02,0.35,-0.13,0  
 2O8PLYS\_100,10.5,0,0,0  
 2CN1,ASP\_236,2.9,0.7,-1.6,0  
 1DZF,LYS\_56,10.5,0,0,0  
 1T95,ASP\_218,3.75,0,-0.05,0  
 1NIJ,ASP\_223,3.2,0.14,-0.74,0

2H85,ASP\_78,2.75,0.28,-1.33,0  
 2NRK,LYS\_95,10.5,0,0,0  
 2E3C,GLU\_332,4.97,0.49,-0.02,0  
 4E5S,ARG\_71,11.94,-0.56,0,0  
 3G9T,ARG\_30,11.8,-0.7,0,0  
 3G59,TYR\_149,10.67,0.07,-0.82,1.42  
 2QOP,LYS\_80,10.5,0,0,0  
 4DIU,ASP\_175,3.8,0,0,0  
 1DOV,GLU\_197,4.37,0,-0.13,0  
 3BB7,TYR\_51,10.49,0.49,0,0  
 1P1L,LYS\_91,10.5,0,0,0  
 2APL,GLU\_22,4.64,0.14,0,0  
 3M3P,GLU\_200,4.5,0,0,0  
 2VAN,LYS\_120,10.5,0,0,0  
 3H5T,GLU\_207,4.5,0,0,0  
 1TR9,TYR\_223,12.13,0,0,2.13  
 3GW3,GLU\_293,4.57,0.07,0,0  
 2AD1,GLU\_69,4.71,0.21,0,0  
 1CBY,ARG\_212,12.01,-0.49,0,0  
 1BKR,HIS\_44,5.38,1.14,0,-2.26  
 4EF5,ARG\_180,11.87,-0.63,0,0  
 1BN6,HIS\_50,1.67,0.84,0.78,-6.45  
 1KCM,ASP\_160,1.42,1.26,-3.65,0  
 2IF4,GLU\_203,4.71,0.21,0,0  
 3OOP,GLU\_101,4.64,0.14,0,0  
 1EV8,LYS\_140,10.5,0,0,0  
 1ILW,CYS\_126,11.41,-0.23,0,2.64  
 2G55,ARG\_179,11.17,-1.33,0,0  
 2D7U,ASP\_158,2.61,0.7,-1.89,0  
 3EJC,LYS\_65,10.29,-0.21,0,0  
 2YX0,LYS\_247,10.43,-0.07,0,0  
 1X6J,ARG\_41,11.87,-0.63,0,0  
 1R29,CYS\_121,8.99,-0.08,0,0.07  
 2BV9,HIS\_290,7.37,1.01,0,-0.14  
 4H4J,GLU\_86,4.5,0,0,0  
 2PGX,TYR\_134,10.06,0.46,-0.4,0  
 3TIR,GLU\_99,3.61,0.35,-1.24,0  
 3SMD,ASP\_141,3.72,0.21,-0.29,0  
 3COU,LYS\_113,10.22,-0.28,0,0  
 2WOZ,ASP\_397,4.01,0.21,0,0  
 1ANU,ASP\_121,2.39,1.05,-2.46,0  
 2G9D,ASP\_274,3.55,0.21,-0.46,0  
 1YOY,ASP\_154,3.75,0,-0.05,0  
 3JV1,ASP\_62,3.49,0.21,-0.52,0  
 1XAW,LYS\_444,10.43,-0.07,0,0  
 2ZCX,ASP\_160,2.8,0.84,-1.83,0  
 1L3K,GLU\_118,3.91,0.21,-1.89,0  
 3OIP,LYS\_129,10.43,-0.07,0,0  
 3H13,LYS\_473,10.43,-0.07,0,0  
 3VJ8,GLU\_167,3.98,0.28,-0.8,0  
 1ZP2,GLU\_120,4.34,0.07,-0.23,0  
 1WYC,HIS\_31,6.36,0,0,-0.14  
 1BKB,LYS\_37,10.36,-0.14,0,0  
 4FCU,LYS\_38,10.36,-0.14,0,0  
 2Q13,GLU\_131,4.64,0.14,0,0  
 2R4Q,GLU\_221,2.51,0.49,-2.48,0  
 2Y2T,LYS\_78,10.43,-0.07,0,0  
 2OOK,LYS\_153,10.29,-0.21,0,0  
 1K95,TYR\_55,10,0,0,0  
 2D7U,GLU\_311,4.71,0.21,0,0  
 1HF8,HIS\_41,6.36,0,0,-0.14  
 3VJ8,ASP\_108,3.94,0.14,0,0  
 3CCY,ARG\_60,11.94,-0.56,0,0  
 2CXA,ARG\_2,12.43,-0.07,0,0  
 3LOD,GLU\_91,4.33,0.21,-0.38,0  
 1I60,ARG\_34,13.42,-1.48,0,2.4  
 2OBI,CYS\_107,9,0,0,0  
 1U3Y,GLU\_284,3.36,0.42,-1.56,0  
 4FCU,GLU\_101,7.79,2.04,0,1.25  
 2G5X,GLU\_131,3.56,0.21,-1.15,0  
 1XTD,GLU\_91,4.19,0.49,-0.8,0  
 3JZN,ASP\_303,3.8,0,0,0  
 4GCO,ARG\_195,12.08,-0.42,0,0  
 1R5S,GLU\_123,4.19,1.27,-1.58,0  
 2EFK,LYS\_56,10.5,0,0,0  
 3UC9,GLU\_171,4.03,0.28,-0.75,0  
 3VJ8,LYS\_315,10.5,0,0,0  
 3TIR,ARG\_58,12.08,-0.42,0,0  
 1EDG,ARG\_217,9.88,-2.62,0,0  
 1IAP,TYR\_100,13.21,0,0.03,3.18  
 3E7P,GLU\_136,4.12,0.42,-0.8,0  
 2FZ4,TYR\_97,7.99,0.14,-2.15,0  
 3ILC,GLU\_92,3.98,0.28,-0.8,0  
 2FL7,LYS\_202,10.5,0,0,0  
 3T5B,LYS\_2,10.43,-0.07,0,0  
 3DHN,LYS\_139,10.36,-0.14,0,0  
 3BA1,GLU\_247,3.6,0.35,-1.25,0  
 4DEZ,LYS\_43,10.5,0,0,0  
 1KCM,ASP\_52,2.86,0.42,-1.36,0  
 3EJC,HIS\_133,6.78,0.42,0,-0.14  
 1S17,ASP\_26,1.08,0.98,-3.7,0  
 1J5X,GLU\_115,4.5,0,0,0  
 3FK5,ARG\_203,11.8,-0.7,0,0  
 1ZHV,ASP\_117,3.83,0.07,-0.04,0  
 2WOZ,LYS\_471,10.5,0,0,0  
 2B0A,TYR\_163,9.87,0.14,-0.27,0  
 3QAV,GLU\_104,1.41,0.7,-1.43,-2.36  
 2Z14,LYS\_40,10.36,-0.14,0,0  
 1T95,ARG\_130,12.29,-0.21,0,0  
 1L2F,LYS\_57,10.15,-0.35,0,0  
 1J74,GLU\_39,4.57,0.07,0,0  
 2Z84,TYR\_135,13.62,0.42,0.8,2.4  
 3QYB,LYS\_904,10.22,-0.28,0,0  
 2QK1,ARG\_519,11.8,-0.7,0,0  
 2V4U,GLU\_493,3.91,0.21,-0.8,0  
 2R57,ARG\_374,12.01,-0.49,0,0  
 2H2Z,TYR\_239,11.31,1.31,0,0  
 1PGV,ASP\_223,3.0,49,-1.29,0  
 2D7J,ARG\_144,12.22,-0.28,0,0  
 2C2Y,CYS\_57,6.97,-3.71,0,1.68  
 2D0A,CYS\_227,8.43,-1.24,0,0.67  
 3V55,HIS\_540,6.5,0,0,0  
 2FGG,ASP\_67,2.58,0.56,-1.78,0  
 2IF4,LYS\_272,9.87,-0.63,0,0  
 3BQW,ASP\_280,2.72,0.28,-1.36,0  
 1C3K,ARG\_20,11.94,-0.56,0,0  
 3NR5,CYS\_41,6.99,-2.01,0,0  
 2ILR,TYR\_396,9.72,0,-0.28,0  
 3I4T,TYR\_49,11.16,1.14,0,0.02  
 1V8E,LYS\_73,9.66,-0.84,0,0  
 4AF2,ASP\_76,3.77,0,-0.03,0  
 1X1E,GLU\_161,4.57,0.07,0,0  
 1RAJ,HIS\_199,7.4,0.97,0,-0.07  
 2CXA,ARG\_21,12.22,-0.28,0,0  
 2FGG,ASP\_79,4.04,0.28,-0.04,0  
 1LTU,LYS\_82,10.43,-0.07,0,0  
 1R29,LYS\_66,10.5,0,0,0  
 1DZF,ASP\_74,3.93,0.14,-0.01,0  
 3N2T,ARG\_270,12.82,-2.0,2.32  
 4ECC,GLU\_25,4.64,0.14,0,0  
 2WOZ,ASP\_474,3.75,0.49,-0.54,0  
 1Q8B,HIS\_14,6.43,0,0,-0.07  
 2PLQ,ASP\_11,1.96,0.7,-2.54,0  
 3F6M,LYS\_106,10.5,0,0,0  
 3HUE,TYR\_183,10,0,0,0  
 1WP5,TYR\_166,10,0,0,0  
 4FH3,ASP\_148,0.92,1.12,-4,0  
 3LMO,ARG\_7,12.01,-0.49,0,0  
 3AUF,ASP\_58,3.28,0.42,-0.94,0  
 3GW3,HIS\_339,2.07,0,-1.72,-2.71  
 1MUF,GLU\_176,4.5,0,0,0  
 3LPZ,ARG\_165,12.15,-0.35,0,0  
 3HNX,ASP\_61,3.13,0.35,-1.02,0  
 3GE9,CYS\_43,9.07,0,0,0.07  
 2B3M,ASP\_120,3.11,0.49,-1.18,0  
 3BQW,GLU\_185,4.31,0.35,-0.54,0  
 3PZ9,GLU\_384,3.88,0.14,-0.76,0  
 1NIJ,ASP\_136,3.16,0.35,-0.99,0  
 1LPL,LYS\_206,10.36,-0.14,0,0  
 3R1X,ARG\_195,10.26,-2.24,0,0  
 2GYZ,HIS\_21,6.5,0,0,0  
 4HDE,GLU\_109,4.5,0,0,0  
 3M3P,GLU\_157,4.71,0.21,0,0  
 2X4G,TYR\_208,10.21,0.21,0,0  
 3BPP,TYR\_25,13.11,0.28,0.43,2.4  
 2OPJ,ARG\_149,12.08,-0.42,0,0  
 4DVD,ARG\_58,11.68,-0.82,0,0  
 3P51,ARG\_145,11.45,-1.05,0,0  
 1K95,ASP\_69,2.8,0.91,-1.9,0  
 1ZBP,LYS\_29,10.43,-0.07,0,0  
 3TRE,LYS\_31,10.36,-0.14,0,0  
 3CXS,TYR\_165,10.58,0.58,0,0  
 3H5T,GLU\_163,3.18,0.28,-1.6,0  
 3J5N,ASP\_124,3.8,0,0,0  
 2AZL,ARG\_19,11.77,-0.73,0,0  
 3M16,GLU\_145,3.0,56,-2.06,0  
 1PV5,ARG\_34,11.8,-0.7,0,0  
 3V75,GLU\_85,4.71,0.21,0,0  
 3FHF,HIS\_-1,6.52,0.16,0,-0.14  
 2IDC,GLU\_105,2.55,1.25,-0.8,-2.4  
 3Q1C,ARG\_245,12.08,-0.42,0,0  
 2CXA,ARG\_218,12.5,0,0,0  
 3LQE,CYS\_451,2.63,-7.35,-2.4,3.38  
 2CE6,TYR\_41,9.42,0.28,-1.78,0.93  
 2IXM,GLU\_67,4.5,0,0,0  
 1LFP,HIS\_171,6.44,0.15,0,-0.21  
 1XIP,LYS\_126,10.43,-0.07,0,0  
 1S1J,GLU\_118,4.57,0.07,0,0  
 3MIX,GLU\_630,4.71,0.21,0,0  
 1GQE,LYS\_334,10.15,-0.35,0,0  
 1FHL,LYS\_280,10.43,-0.07,0,0  
 3RNV,LYS\_357,10.29,-0.21,0,0  
 2X4G,HIS\_43,6.4,0.04,0,-0.14  
 2JKF,HIS\_130,2.45,0.69,-0.39,-4.34  
 3RFY,TYR\_394,12.36,0.69,0,1.66  
 2IRM,GLU\_344,4.5,0,0,0  
 3C2E,GLU\_81,3.97,0.21,-0.74,0  
 3CN5,ARG\_225,8.5,-4,0,0  
 3PP8,GLU\_297,3.66,0.28,-1.12,0  
 1L2F,GLU\_296,4.62,0.21,-0.09,0  
 1MTZ,TYR\_243,13.65,0.07,0.54,3.04  
 3M16,HIS\_223,6.83,0.61,0,-0.28  
 3G6S,ASP\_63,3.49,0.35,-0.66,0  
 4FZR,HIS\_292,4.48,0.22,0,-2.24  
 1WXQ,GLU\_52,4.42,0,-0.08,0  
 2D0A,GLU\_21,4.57,0.07,0,0  
 3LPZ,HIS\_151,1.51,0,-1.61,-3.38  
 4EKU,GLU\_268,4.51,0.21,-0.2,0  
 2IF4,ASP\_148,3.15,0.35,-1,0  
 1MSI,LYS\_153,10.29,-0.21,0,0  
 4D8L,GLU\_117,4.64,0.14,0,0  
 2HRZ,HIS\_152,6.55,0.12,0,-0.07  
 3ALD,LYS\_272,10.5,0,0,0  
 3UAH,TYR\_290,13.48,0.39,0.69,2.4  
 2HNG,GLU\_34,4.5,0,0,0  
 2P52,ARG\_246,11.45,-1.05,0,0  
 2RIS,ASP\_28,2.79,0.21,-1.22,0  
 1QYI,LYS\_221,10.15,-0.35,0,0  
 2G2D,ASP\_56,2.44,0.49,-1.85,0  
 2F4Q,ASP\_163,4.05,0.28,-0.03,0  
 1J7G,LYS\_48,10.43,-0.07,0,0  
 2J8A,GLU\_277,4.64,0.14,0,0  
 2OPJ,ASP\_144,4.01,0.21,0,0  
 1SQH,ARG\_56,12.29,-0.21,0,0  
 1PVT,ASP\_50,4.22,0.42,0,0  
 2P5D,LYS\_100,10.01,-0.49,0,0  
 2XHC,LYS\_139,10.5,0,0,0  
 1MSI,TYR\_159,10,0,0,0  
 3EX9,TYR\_30,11.39,3.22,-0.42,-1.41  
 2ZTY,GLU\_99,4.64,0.14,0,0  
 2CVB,ASP\_75,2.18,0.7,-2.32,0  
 2Q99,LYS\_300,10.5,0,0,0  
 3Q6L,CYS\_2,7.12,-1.88,0,0  
 1R9W,ASP\_220,3.9,0.14,-0.04,0  
 2XMZ,GLU\_263,4.71,0.21,0,0  
 1RAJ,GLU\_382,3.55,0.07,-1.02,0  
 4EVF,ARG\_116,11.8,-0.7,0,0  
 1XIP,GLU\_114,4.71,0.21,0,0  
 3LOD,GLU\_58,4.57,0.07,0,0  
 2EYI,CYS\_180,10.12,-0.65,0,1.77  
 2R05,HIS\_54,7.18,0.96,0,-0.28  
 1HUF,GLU\_50,4.64,0.14,0,0  
 2XMZ,ASP\_59,4.01,0.21,0,0  
 3H5T,TYR\_340,10.88,0,0,0.88  
 2AXO,LYS\_195,10.43,-0.07,0,0  
 1G8P,GLU\_73,2.98,0.14,-1.66,0  
 2CL3,LYS\_29,10.15,-0.35,0,0  
 1MML,ASP\_216,3.87,0.07,0,0  
 3BB7,TYR\_245,10,0,0,0  
 3CS1,ASP\_68,3.52,0.14,-0.42,0  
 1F2V,CYS\_76,11.79,0.06,6.2,13  
 2BDD,LYS\_96,10.08,-0.42,0,0  
 2CBE,GLU\_234,3.84,0.14,-0.8,0  
 2RIK,ASP\_255,2.22,0.63,-2.21,0  
 3M7D,GLU\_129,4.53,3.2,-1.36,-1.82  
 2GAU,GLU\_117,4.12,0.14,-0.52,0  
 3MIT,TYR\_651,11.69,0,-0.1,1.79  
 3MXX,LYS\_558,10.5,0,0,0  
 3BWT,HIS\_849,6.43,0,0,-0.07  
 3GA2,TYR\_195,9.95,0.12,-0.17,0  
 1XIP,LYS\_5,10.5,0,0,0  
 3ERF,GLU\_142,4.26,0.35,-0.59,0  
 3ANJ,ARG\_356,11.59,-0.91,0,0  
 2O8P,TYR\_16,10,0,0,0  
 2EJX,ASP\_15,3.62,0.21,-0.39,0  
 1NAF,LYS\_295,10.43,-0.07,0,0  
 2HXB,TYR\_32,10.57,0.7,-1.13,1  
 4EUG,TYR\_93,11.4,1.4,0,0  
 2QVO,LYS\_52,9.87,-0.63,0,0  
 3K8J,GLU\_64,4.92,0.42,0,0  
 3DTE,ASP\_94,3.79,0,-0.01,0  
 2VGM,ASP\_75,3.2,0.35,-0.94,0  
 3UV9,LYS\_372,9.52,-0.98,0,0  
 2PLQ,TYR\_192,12.02,1.01,-1.09,2.11  
 1EV8,TYR\_242,8.9,0.49,-1.59,0  
 3LD1,ARG\_152,10.97,-1.53,0,0  
 3IVF,TYR\_71,10.53,0.07,-1.18,1.64  
 2R51,TYR\_284,12.62,0.14,0.08,2.4  
 1KW4,GLU\_43,4.5,0,0,0  
 3LJI,ARG\_267,11.8,-0.7,0,0  
 1FHL,LYS\_67,10.01,-0.49,0,0  
 1YM5,LYS\_201,10.29,-0.21,0,0  
 1MD6,ASP\_138,4.22,0.42,0,0  
 1R3F,GLU\_285,3.39,0.49,-1.6,0  
 1WPA,ARG\_459,12.15,-0.35,0,0  
 3I47,GLU\_9,4.35,0.21,-0.36,0

3E5T,HIS\_193,3.69,1.19,-0.28,-3.71  
3ODJ,LYS\_10,10.5,0,0,0  
2JHY,ARG\_152,11.52,-0.98,0,0  
2E3C,GLU\_207,4.57,0.07,0,0  
2YX0,LYS\_50,10.36,-0.14,0,0  
1SUU,LYS\_623,10.15,-0.35,0,0  
3L7N,ARG\_164,11.87,-0.63,0,0  
3BJV,LYS\_8,10.5,0,0,0  
3Q1C,LYS\_237,10.36,-0.14,0,0  
2C13,CYS\_83,9.66,-0.02,0.0,0.68  
1R5Q,ASP\_37,3.28,0.28,-0.8,0  
3CO1,CYS\_55,9.36,-0.89,0.19,1.06  
2CWY,LYS\_30,10.5,0,0,0  
2DVK,GLU\_74,4.07,0.35,-0.78,0  
1YG2,ARG\_76,11.8,-0.7,0,0  
2BAA,ASP\_141,3.16,0.21,-0.85,0  
1YM5,ASP\_191,3.8,0,0,0  
3RFF,ARG\_78,12.29,-0.21,0,0  
2QV2,HIS\_226,7.49,1.2,0,-0.21  
1CHD,ARG\_202,12.5,0,0,0  
1ZCU,GLU\_56,4.12,0.42,-0.8,0  
1DUP,GLU\_17,4.71,0.21,0,0  
3Z5L,HIS\_158,7.01,1.9,1.87,-3.26  
1EW4,ARG\_82,12.5,0,0,0  
2X4L,LYS\_220,9.59,-0.91,0,0  
3M70,LYS\_45,10.08,-0.42,0,0  
1WXQ,ASP\_315,3.41,0.28,-0.67,0  
1WLY,LYS\_224,10.43,-0.07,0,0  
3GS3,GLU\_99,3.88,0.49,-1.11,0  
1OST,ASP\_209,3.69,0.14,-0.25,0  
2OGQ,HIS\_538,6.5,0,0,0  
3ANJ,LYS\_135,10.36,-0.14,0,0  
200K,HIS\_293,9.41,4.44,1.45,-2.98  
2B6P,ARG\_5,12.29,-0.21,0,0  
3EVN,CYS\_117,8.81,-0.33,0.0,0.14  
1WP5,HIS\_81,6.93,0.57,0,-0.14  
3HST,ARG\_162,12.15,-0.35,0,0  
2H85,GLU\_145,4.69,0.28,-0.09,0  
1ZCE,CYS\_92,8.84,-0.21,0,0.05  
4DEZ,ASP\_84,3.81,0.21,-0.2,0  
1CBY,ARG\_25,12.5,0,0,0  
2ZCX,GLU\_204,4.5,0,0,0  
3U2R,TYR\_18,10.07,0.07,0,0  
3BA1,ARG\_260,12.43,-0.07,0,0  
3EVN,ARG\_38,12.5,0,0,0  
1P1L,ASP\_95,4.13,0.35,-0.02,0  
3SMD,GLU\_59,3.56,0.35,-1.28,0  
3CS1,GLU\_52,4.82,0.35,-0.03,0  
3CNU,GLU\_55,3.84,0.21,-0.87,0  
2H2W,ASP\_200,3.42,0.42,-0.8,0  
2F8H,ARG\_38,12.22,-0.28,0,0  
1DTO,ASP\_28,3.25,0.35,-0.9,0  
2OGQ,ARG\_507,12.5,0,0,0  
2CN1,TYR\_249,12.95,1.7,0,1.25  
1RLO,ASP\_219,2.62,0.42,-1.6,0  
1PBV,LYS\_71,10.29,-0.21,0,0  
3B4D,GLU\_186,4.64,0.14,0,0  
1KCM,ASP\_16,3.74,0,-0.06,0  
3GMS,TYR\_124,10.72,2.2,-0.84,-0.64  
3F5D,LYS\_192,10.29,-0.21,0,0  
3HVM,LYS\_129,10.36,-0.14,0,0  
1L2F,GLU\_120,4.57,0.14,-0.07,0  
1X04,TYR\_57,9.32,0.07,-0.75,0  
2G2D,GLU\_140,3.29,0.49,-1.7,0  
3NOK,ASP\_150,3.94,0.14,0,0  
3RLN,GLU\_607,3.63,0.28,-1.15,0  
3GE9,GLU\_138,4.57,0.07,0,0  
2QK1,LYS\_469,10.5,0,0,0  
2D0A,ASP\_130,3.94,0.14,0,0  
1YLN,ASP\_152,3.8,0,0,0  
2BLL,ARG\_601,12.43,-0.07,0,0  
1T07,GLU\_13,4.26,0.56,-0.8,0  
3LH5,HIS\_692,6.43,0,0,-0.07  
1NFN,ARG\_114,11.45,-1.05,0,0  
2CXY,GLU\_100,2.72,1,-2.78,0  
1R7J,LYS\_78,10.36,-0.14,0,0  
1R53,ASP\_61,3.8,0,0,0  
1AKO,GLU\_254,4.5,0,0,0  
1I60,ARG\_74,12.01,-0.49,0,0  
2Q34,ASP\_194,4.15,0.35,0,0  
3M7G,GLU\_13,4.5,0,0,0  
1DVO,TYR\_144,10.2,0,0.2,0  
3GS3,LYS\_22,10.5,0,0,0  
2FBQ,ARG\_75,12.08,-0.42,0,0  
2FXT,LYS\_307,9.87,-0.63,0,0  
1P6F,HIS\_15,5.31,0.4,0,-1.59  
4H86,ARG\_-6,12.5,0,0,0  
4DIU,GLU\_12,4.05,0.35,-0.8,0  
1XDZ,CYS\_74,11.22,-0.09,0.2,31  
2I6I,ASP\_47,2.56,0.56,-1.8,0  
1ILW,LYS\_43,10.43,-0.07,0,0  
2PGE,ASP\_92,3.64,0.07,-0.23,0  
2Q98,LYS\_115,9.87,-0.63,0,0  
3IVF,CYS\_236,9.66,-0.12,0.0,0.78  
4ACJ,TYR\_728,10.07,0.07,0,0  
2Q5X,ASP\_828,3.86,0.14,-0.08,0  
1CBY,ASP\_147,3.16,0.63,-1.26,0  
1SNT,CYS\_272,7.26,-0.41,-3.63,2.29  
1NIJ,ASP\_232,3.8,0,0,0  
2A0J,ARG\_130,11.31,-1.19,0,0  
3CBN,GLU\_82,3.75,0.35,-1.1,0  
1XWM,HIS\_153,6.43,0,0,-0.07  
1MIX,GLU\_252,2.86,0.21,-1.85,0  
2EFK,LYS\_150,10.29,-0.21,0,0  
3BCY,ASP\_41,4.0,0.21,-0.01,0  
2FBI,LYS\_82,10.22,-0.28,0,0  
4DEZ,GLU\_88,4.57,0.07,0,0  
3RFY,GLU\_379,5.71,1.21,0,0  
3HKX,ARG\_206,12.93,-1.82,0.2,25  
2B3M,LYS\_47,10.36,-0.14,0,0  
2F4Q,ASP\_306,2.76,0.35,-1.39,0  
1BYI,CYS\_20,10.1,-0.84,0.01,1.94  
3J5N,ARG\_270,12.15,-0.35,0,0  
1WNH,LYS\_134,10.15,-0.35,0,0  
2V4U,TYR\_554,10.03,0.54,-0.87,0.35  
2XHC,ARG\_326,12.15,-0.35,0,0  
3DHN,GLU\_152,2.8,0.56,-2.26,0  
2FG1,CYS\_25,7.67,-3.61,0.2,28  
3OKQ,GLU\_668,4.57,0.07,0,0  
3M70,TYR\_98,13.57,0.37,0.8,2.4  
3GFP,ASP\_442,2.63,0.98,-2.15,0  
1O0X,GLU\_88,3.73,0.28,-1.06,0  
3KEY,ARG\_374,12.08,-0.42,0,0  
3O16,ASP\_124,3.55,0.42,-0.67,0  
1NAF,GLU\_172,4.64,0.14,0,0  
3UPD,LYS\_263,10.5,0,0,0  
3BPP,TYR\_142,10,0,0,0  
2BQ,ASP\_81,3.76,0.07,-0.11,0  
3IOO,ARG\_112,11.87,-0.63,0,0  
2QVO,ASP\_75,3.77,0,-0.03,0  
1XDZ,GLU\_207,4.78,0.49,-0.21,0  
3M7G,TYR\_30,12.56,1.31,-0.09,1.34  
1EYH,GLU\_125,4.5,0,0,0  
1H09,ARG\_298,12.5,0,0,0  
2FM9,LYS\_147,10.5,0,0,0  
1ES9,HIS\_187,6.43,0,0,-0.07  
2G5X,TYR\_233,10.12,0,0,0.12  
2G55,TYR\_188,10,0,0,0  
1EV8,ARG\_234,11.45,-1.05,0,0  
1OST,GLU\_408,4.94,0.44,0,0  
1W7B,LYS\_47,10.29,-0.21,0,0  
2ATR,GLU\_97,4.5,0,0,0  
3FTT,ARG\_39,11.94,-0.56,0,0  
3COC,HIS\_349,6.36,0,0,-0.14  
3CIV,GLU\_263,4.43,0.21,-0.28,0  
2CXA,HIS\_82,6.5,0,0,0  
3QKY,ARG\_278,12.5,0,0,0  
2RH3,ARG\_156,11.52,-0.98,0,0  
3MIX,LYS\_498,10.43,-0.07,0,0  
1OLR,GLU\_205,7.2,3.02,-0.8,0.48  
2B78,GLU\_323,4.5,0,0,0  
3M7G,TYR\_149,9.31,1.42,-1.53,-0.58  
3PZ9,ASP\_337,3.4,0.42,-0.82,0  
4EKU,GLU\_172,4.64,0.14,0,0  
1OIS,LYS\_265,10.36,-0.14,0,0  
1XAW,LYS\_433,10.5,0,0,0  
3MIX,GLU\_378,4.57,0.28,-0.21,0  
1EYH,ASP\_66,2.57,0.42,-1.66,0  
3I0C,ARG\_187,11.91,-0.59,0,0  
2AHS,TYR\_103,11.74,0.07,0.1,67  
3LJC,LYS\_176,10.22,-0.28,0,0  
3RLE,ASP\_140,3.35,0.35,-0.8,0  
1ZBS,ARG\_259,12.15,-0.35,0,0  
1V43,ASP\_37,3.37,0.07,-0.5,0  
3FNI,GLU\_49,4.32,0.07,-0.25,0  
2AXO,ARG\_181,12.01,-0.49,0,0  
1WRU,ARG\_73,12.08,-0.42,0,0  
2EFK,HIS\_181,6.43,0,0,-0.07  
1MIX,GLU\_293,3.98,0.14,-0.66,0  
3EVN,GLU\_31,4.4,0,-0.1,0  
2CVB,HIS\_44,13.94,5.2,4.55,-2.31  
2X4L,ARG\_182,13.91,-0.99,0.2,4  
3BQW,ARG\_231,11.66,-0.84,0,0  
1KCM,ASP\_256,3.93,0.21,-0.08,0  
2B78,LYS\_277,10.43,-0.07,0,0  
2C13,ARG\_98,11.38,-1.12,0,0  
1DCF,TYR\_66,9.83,0,-0.17,0  
2G55,ASP\_4,3.16,0.14,-0.78,0  
2ZTY,LYS\_108,10.36,-0.14,0,0  
3O48,LYS\_117,10.29,-0.21,0,0  
3GS9,ARG\_123,12.01,-0.49,0,0  
2BV9,ARG\_33,12.48,-0.93,0,0.91  
1ZCU,ARG\_29,12.5,0,0,0  
1Y2Q,GLU\_143,3.76,0.14,-0.88,0  
3CAN,TYR\_99,10,0,0,0  
2Z0M,ARG\_247,12.08,-0.42,0,0  
2ZCO,LYS\_72,10.29,-0.21,0,0  
3HVM,GLU\_221,4.43,0.28,-0.35,0  
3JZ9,GLU\_347,4.64,0.14,0,0  
3AZZ,GLU\_196,4.38,0.21,-0.33,0  
2UJK,GLU\_64,4.57,0.07,0,0  
3Q6L,LYS\_121,10.43,-0.07,0,0  
2F19,GLU\_65,3.46,0.49,-1.53,0  
1WNH,HIS\_7,6.43,0,0,-0.07  
1O9G,TYR\_28,11.02,0.21,0,0.81  
3ZSL,ARG\_224,11.38,-1.12,0,0  
3R1X,TYR\_95,12.48,0,0.2,2.28  
1DUP,ASP\_11,2.34,0.63,-2.09,0  
2D7J,ARG\_121,12.15,-0.35,0,0  
1O0X,LYS\_17,10.15,-0.35,0,0  
3ERF,GLU\_172,4.5,0,0,0  
2FPN,LYS\_187,10.22,-0.28,0,0  
3CRM,ASP\_27,3.42,0.42,-0.8,0  
1ZCE,ARG\_89,11.94,-0.56,0,0  
3NR5,ASP\_60,3.62,0.21,-0.39,0  
3IBT,CYS\_209,7.37,-1.01,-2.28,1.66  
1SQH,GLU\_137,4.24,0.21,-0.47,0  
2EHG,LYS\_89,10.36,-0.14,0,0  
2ZCO,GLU\_139,3.22,1.12,-2.4,0  
3BQE,GLU\_312,4.88,0.69,-0.31,0  
3B4D,LYS\_207,9.94,-0.56,0,0  
4FCU,ASP\_91,3.94,0.14,0,0  
2GZR,LYS\_46,10.36,-0.14,0,0  
3H6Q,TYR\_157,10.22,0.73,-0.79,0.28  
3M3P,ASP\_48,3.98,0.21,-0.03,0  
1X9G,LYS\_12,10.29,-0.21,0,0  
1LZL,CYS\_102,11.9,-0.03,0.16,2.77  
2F8H,GLU\_93,4.5,0,0,0  
1C3K,LYS\_49,10.08,-0.42,0,0  
2ZCO,TYR\_260,13.13,0.07,0.66,2.4  
2ZCO,HIS\_12.8,6.8,1.6,2.4,-1.82  
3ZSL,ASP\_207,3.94,0.14,0,0  
3TIR,ARG\_97,12.5,0,0,0  
2VAN,ASP\_117,4.56,0.21,-0.15,0  
3JZ9,LYS\_362,10.5,0,0,0  
1RSS,ARG\_95,11.73,-0.77,0,0  
2G7O,ASP\_126,3.8,0,0,0  
2BT8,TYR\_180,11.27,0,-0.07,1.33  
3UC9,ASP\_91,2.41,0.84,-2.23,0  
1AMC,ASP\_91,3.94,0.14,0,0  
3O7K,GLU\_104,4.5,0,0,0  
4FLE,ASP\_58,3.93,0.21,-0.08,0  
1BKB,ASP\_57,0.78,0.7,-3.73,0  
2OJQ,ASP\_500,3.8,0.21,-0.21,0  
1FKM,ASP\_588,3.62,0,-0.18,0  
2ZQ5,GLU\_138,4.56,0.21,-0.15,0  
3T5B,GLU\_316,4.5,0,0,0  
1YR6,HIS\_240,3.51,0,0,-2.99  
3M9A,ARG\_74,12.29,-0.21,0,0  
1H4U,GLU\_542,3.44,2.71,-1.6,-2.17  
3NR5,CYS\_112,7.36,-1.64,0,0  
2VAN,ARG\_299,12.15,-0.35,0,0  
1DOV,LYS\_181,10.22,-0.28,0,0  
4H89,ASP\_36,3.18,0.56,-1.18,0  
3ONH,GLU\_501,2.99,0.7,-2.21,0  
4DNU,LYS\_175,10.22,-0.28,0,0  
1AK1,LYS\_162,10.29,-0.21,0,0  
3BQE,LYS\_260,10.22,-0.28,0,0  
2B0J,ASP\_287,3.94,0.14,0,0  
2B78,ASP\_358,3.74,0.49,-0.55,0  
2OBI,LYS\_125,10.43,-0.07,0,0  
2PGX,ASP\_91,3.11,0.49,-1.18,0  
1X7F,LYS\_171,10.43,-0.07,0,0  
3C38,ASP\_194,4.01,0.21,0,0  
3BCY,TYR\_123,14.0,8.0,8.2,4  
3IVF,ASP\_264,4.14,0.35,-0.01,0  
2W2S,TYR\_83,11.22,1.17,-0.38,0.43  
1QQH,LYS\_68,10.43,-0.07,0,0  
3UX2,GLU\_153,4.61,0.49,-0.38,0  
2R2Y,LYS\_103,10.5,0,0,0  
1FHL,LYS\_107,10.5,0,0,0  
3V1Q,ARG\_629,12.29,-0.21,0,0  
1UXO,ASP\_118,2.98,0.35,-1.18,0  
1L3K,ARG\_178,11.94,-0.56,0,0  
3GS3,LYS\_121,10.43,-0.07,0,0  
1UXO,ASP\_167,3.15,0.49,-1.84,0  
3RFY,ASP\_405,3.87,0.07,0,0  
2PGX,LYS\_46,10.01,-0.49,0,0  
2IXM,LYS\_40,10.29,-0.21,0,0  
2OSA,GLU\_449,4.61,0.36,-0.25,0  
1FHL,LYS\_228,10.5,0,0,0  
1U53,ASP\_4,3.8,0,0,0  
1JKS,LYS\_175,9.94,-0.56,0,0  
3EVN,LYS\_85,10.29,-0.21,0,0  
2JHY,HIS\_155,6.43,0,0,-0.07  
2DVK,HIS\_52,6.22,0,0,-0.28

109G,HIS\_207,6.36,0,0,-0.14  
15JY,GLU\_125,3.41,0.14,-1.22,0  
1AD6,LYS\_417,10.29,-0.21,0,0  
2ZTY,HIS\_40,3.52,0,0,-2.98  
3RFY,ASP\_114,3.87,0,0,0  
2OKT,GLU\_73,3.95,0.21,-0.76,0  
310C,ARG\_312,12.08,-0.42,0,0  
2D8N,LYS\_55,10.5,0,0,0  
1W7B,ARG\_295,13.52,-2.84,0,3.86  
2AZL,GLU\_187,4.71,0.21,0,0  
3FFM,LYS\_137,10.43,-0.07,0,0  
2JKF,GLU\_146,4.71,0.21,0,0  
1DZF,ARG\_167,12.29,-0.21,0,0  
3E5T,GLU\_175,4.71,0.21,0,0  
2QV2,ARG\_57,11.66,-0.84,0,0  
2CIU,LYS\_193,10.43,-0.07,0,0  
2H2Z,TYR\_126,11.66,1.17,-1.19,1.68  
2R0S,LYS\_78,9.87,-0.63,0,0  
2BQQ,ASP\_130,2.68,0.7,-1.82,0  
1Q46,LYS\_136,10.22,-0.28,0,0  
1Y2Q,CYS\_127,9.07,0,0,0.07  
4E8B,ARG\_238,12.01,-0.49,0,0  
2BAA,HIS\_206,7.34,1.05,0,-0.21  
3LQE,TYR\_250,10,0,0,0  
1GXN,LYS\_501,10.5,0,0,0  
1QQL,TYR\_74,12.71,0.07,0.24,2.4  
3EVN,HIS\_237,2.38,0,-1.27,-2.85  
3RHE,TYR\_11,12.18,0.86,-0.11,1.42  
2ZCO,LYS\_35,10.36,-0.14,0,0  
3G6S,ARG\_116,9.19,-2.8,0,-0.51  
1E59,HIS\_91,6.5,0,0,0  
2HRZ,ARG\_273,12.01,-0.49,0,0  
1MTZ,TYR\_19,9.41,0.21,-0.8,0  
1NIJ,CYS\_66,12.94,0.5,2.16,1.29  
3GFP,ARG\_463,12.01,-0.49,0,0  
1OST,TYR\_214,10,0,0,0  
3BCH,ARG\_80,12.87,-1.19,0,1.56  
3CZC,GLU\_43,3.19,0.35,-1.67,0  
1AKO,ARG\_216,12.01,-0.49,0,0  
2VGM,TYR\_113,10,0,0,0  
2FG1,LYS\_87,10.5,0,0,0  
1N81,ARG\_75,11.87,-0.63,0,0  
3BQW,LYS\_148,10.36,-0.14,0,0  
4ETX,CYS\_446,9.83,0,0,0.83  
2E3C,ARG\_290,12.01,-0.49,0,0  
3UPD,GLU\_89,4.47,0.07,-0.1,0  
1W24,LYS\_30,10.5,0,0,0  
1QYI,LYS\_33,10.22,-0.28,0,0  
3I47,CYS\_183,9,0,0,0  
3E27,HIS\_323,6.5,0,0,0  
3BPV,ARG\_124,12.22,-0.28,0,0  
2OEW,CYS\_231,9.78,0,0,0.78  
3FNI,HIS\_154,6.5,0,0,0  
4GCO,ARG\_252,12.43,-0.07,0,0  
1WRU,ARG\_158,10.11,-1.31,0,-1.08  
2QV2,ARG\_327,11.94,-0.56,0,0  
3IU5,LYS\_154,10.5,0,0,0  
1TP6,ARG\_70,12.5,0,0,0  
1PNE,GLU\_82,4.63,0.28,-0.15,0  
3G9T,LYS\_281,10.08,-0.42,0,0  
3CZC,GLU\_83,2.39,0.91,-3.02,0  
1A8Q,GLU\_270,4.14,0.07,-0.43,0  
3GS3,ASP\_171,2.76,0.56,-1.6,0  
3IL3,ASP\_147,3.5,0.84,-1.13,0  
1AK1,ASP\_42,3.19,0.42,-1.02,0  
3UC9,GLU\_124,4.5,0,0,0  
1WXQ,GLU\_380,4.19,0.49,-0.8,0  
1LTU,TYR\_155,12.11,3.1,-0.99,0  
1OGL,ARG\_37,12.01,-0.49,0,0  
1ZBM,GLU\_189,4.57,0.07,0,0  
3HVM,GLU\_140,0.53,2.99,-2.97,-3.98  
3T5B,ARG\_327,12.15,-0.35,0,0  
2X5Y,GLU\_811,4.57,0.07,0,0  
1RZ2,ASP\_101,2.23,0.77,-2.33,0  
3CZC,GLU\_63,3.76,0.21,-0.95,0  
4E8B,TYR\_210,13.1,0.07,0.7,2.34  
4FZN,ARG\_25,13.66,-1,0,2.16  
4FH3,ARG\_73,12.15,-0.35,0,0  
3ZRI,LYS\_146,10.5,0,0,0  
3U2A,LYS\_77,10.29,-0.21,0,0  
2P5D,LYS\_80,10.36,-0.14,0,0  
3EVP,ASP\_291,3.36,0.14,-0.58,0  
1YOY,HIS\_15,6.5,0,0,0  
1YTD,ARG\_260,11.66,-0.84,0,0  
3EIZ,LYS\_122,10.36,-0.14,0,0  
2FPN,TYR\_92,9.69,0.14,-0.45,0  
1O0X,GLU\_158,4.18,0.21,-0.53,0  
2YX0,LYS\_256,10.43,-0.07,0,0  
4E5S,GLU\_82,3.45,0.63,-1.68,0  
2QK1,LYS\_427,10.5,0,0,0  
3OOP,GLU\_76,4.5,0,0,0  
4E8B,LYS\_60,10.5,0,0,0  
1ZBM,GLU\_118,4.5,0.14,-0.14,0  
3BPP,ARG\_156,9.78,-3.71,0,0.99  
1O17,LYS\_285,10.5,0,0,0  
3I82,ARG\_15,12.43,-0.07,0,0  
2YX0,GLU\_113,3.2,0.84,-2.14,0  
2F9F,ASP\_154,3.48,0.14,-0.46,0  
1PSW,ARG\_303,12.15,-0.35,0,0  
1T95,GLU\_96,3.51,0.35,-1.34,0  
2AXO,LYS\_43,10.29,-0.21,0,0  
4DIU,HIS\_22,2.23,1.06,0,-5.32  
3H5T,ARG\_224,10.11,-4.16,0,1.76  
3RUX,TYR\_97,9.9,0,-0.1,0  
2OKT,GLU\_13,4.79,0.56,-0.27,0  
2D7U,GLU\_86,4.18,0.35,-0.67,0  
1ILW,GLU\_131,2.66,1.07,-2.91,0  
3F5D,TYR\_128,11.5,0,0,1.5  
2EYI,LYS\_84,10.5,0,0,0  
2P1W,GLU\_189,4.5,0,0,0  
1QZN,ARG\_152,11.87,-0.63,0,0  
2CVB,CYS\_42,2.62,-8.44,0,2.186  
1E5S,HIS\_76,6.29,0,0,-0.21  
2CL3,GLU\_55,2.1,0.8,-0.8,-2.4  
3UC9,CYS\_61,10,-0.07,0.56,0.51  
1YR6,TYR\_124,11.19,0,0,1.19  
2WB8,TYR\_688,12.29,3.36,-1.06,0  
3VJ8,LYS\_311,10.15,-0.35,0,0  
2ZQ5,ARG\_62,11.73,-0.77,0,0  
2WB8,LYS\_672,10.08,-0.42,0,0  
1S1G,ASP\_278,3.37,0.28,-0.71,0  
3RUX,CYS\_125,10.28,-2.1,0,3.37  
4ECC,GLU\_34,4.46,0.28,-0.32,0  
2FXT,GLU\_421,2.55,0.69,-0.24,-2.4  
2ZQ5,GLU\_298,2.59,0.49,-2.4,0  
3BQW,TYR\_328,12.48,0,0,2.49  
2V81,LYS\_59,10.43,-0.07,0,0  
3ELI,ASP\_115,3.41,0.63,-1.02,0  
3UPD,LYS\_47,10.36,-0.14,0,0  
1NJ4,TYR\_25,10.62,0.68,0,-0.06  
1MUF,LYS\_195,10.29,-0.21,0,0  
1HUF,GLU\_52,2.14,0.75,-3.11,0  
3GV0,ASP\_213,2.62,0.49,-1.67,0  
2F19,GLU\_57,4.5,0,0,0  
3NZL,LYS\_74,10.22,-0.28,0,0  
2G2D,HIS\_87,6.43,0,0,-0.07  
1RKA,HIS\_113,6.47,0.11,0,-0.14  
3LJI,GLU\_265,3.85,0.14,-0.79,0  
1X9G,GLU\_29,4.5,0,0,0  
1ZBS,CYS\_70,9.39,-0.62,0,1.01  
2AH5,HIS\_200,6.85,0.42,0,-0.07  
3B7X,ARG\_103,12.01,-0.49,0,0  
3R87,LYS\_29,10.43,-0.07,0,0  
1WXQ,GLU\_129,4.5,0,0,0  
1S17,ASP\_315,3.23,0.07,-0.64,0  
3BQW,TYR\_188,10.83,0.07,0,0.76  
2AXO,GLU\_260,4.85,0.35,0,0  
1NAR,GLU\_132,1.71,1.72,-0.8,-3.71  
1R3F,TYR\_312,10,0,0,0  
1O5J,GLU\_50,2.66,0.56,-2.4,0  
4F8A,CYS\_602,8.74,-0.26,0,0  
3C2E,CYS\_207,9.58,0,0,0.58  
3BPV,ARG\_117,12.08,-0.42,0,0  
3HVM,GLU\_255,4.65,0.28,-0.13,0  
2QHT,GLU\_107,5.31,0.81,0,0  
1Q8B,ASP\_86,3.76,0.42,-0.46,0  
3L7N,LYS\_75,10.5,0,0,0  
1O6D,ARG\_27,11.87,-0.63,0,0  
3DTE,ARG\_195,11.87,-0.63,0,0  
2WOZ,LYS\_518,10.5,0,0,0  
2W1R,ASP\_129,3.71,0,-0.09,0  
2YLF,GLU\_154,4.65,0.07,0.08,0  
3HNX,ARG\_8,11.52,-0.98,0,0  
1WRU,ASP\_144,3.87,0.07,0,0  
2C2Y,TYR\_152,10.45,0.21,-1.12,1.36  
1FOY,ARG\_312,11.94,-2.96,0,2.4  
1YOY,GLU\_108,4.5,0,0,0  
2RJD,GLU\_245,3.9,2.46,-3.06,0  
2V4U,HIS\_355,7.06,0.7,0,-0.14  
2WOZ,GLU\_523,4.78,0.28,0,0  
2BV9,HIS\_289,6.36,0,0,-0.14  
3LQE,LYS\_540,10.5,0,0,0  
2FZ4,TYR\_160,12.29,0.0,2.29  
1GPP,GLU\_121,4.5,0,0,0  
2D2S,LYS\_725,10.5,0,0,0  
1VJG,ASP\_24,0.65,0.98,-4.13,0  
1FHL,TYR\_325,13.27,0.18,-0.52,3.61  
2ATR,TYR\_99,10,0,0,0  
2V1L,ASP\_47,1.49,0.91,-3.22,0  
2BV9,LYS\_249,10.01,-0.49,0,0  
2AHE,GLU\_153,4.05,0.35,-0.8,0  
3H5T,TYR\_286,11.64,0,0,1.64  
1ZBS,HIS\_88,6.5,0,0,0  
3JV1,ARG\_117,13.01,-1.25,0,1.76  
3H6Q,GLU\_138,4.64,0.28,-0.14,0  
3HVV,ARG\_229,11.59,-0.91,0,0  
3Q6L,LYS\_97,10.5,0,0,0  
3M16,TYR\_217,10.3,0.23,-0.35,0.41  
2F4Q,ASP\_185,2.24,0.42,-1.98,0  
2AZP,HIS\_-1,6.36,0,0,-0.14  
2R51,TYR\_183,9.32,1.38,-2.06,0  
2R57,GLU\_187,4.5,0,0,0  
2AXO,GLU\_99,4.71,0.21,0,0  
1F2V,ARG\_89,8.81,-1.29,0,-2.4  
3O7K,GLU\_57,4.57,0.07,0,0  
1TUL,GLU\_20,4.5,0,0,0  
1QSZ,GLU\_597,3.93,0.14,-0.71,0  
2G3A,ASP\_10,3.67,0.35,-0.48,0  
1MN3,GLU\_408,4.12,0.21,-0.59,0  
3COC,GLU\_341,3.57,0.14,-1.07,0  
2FZ4,GLU\_200,5.68,1.21,-0.03,0  
1A8Q,GLU\_248,4.5,0,0,0  
3M7D,ARG\_148,12.55,-2.84,0,2.89  
2AXO,ASP\_81,3.14,0.49,-1.15,0  
2QEV,LYS\_107,10.5,0,0,0  
2EHG,CYS\_10,7.4,-1.82,0,0.22  
1SQH,ARG\_246,12.22,-0.28,0,0  
3QKY,TYR\_45,9.49,0.68,0,-1.19  
1UXO,HIS\_18,3.45,0,0,-3.05  
2RJD,LYS\_298,10.29,-0.21,0,0  
2QDJ,LYS\_236,10.15,-0.35,0,0  
1MD6,ASP\_50,2.34,0.35,-1.82,0  
3NR5,GLU\_74,3.98,0.35,-0.87,0  
2QVO,GLU\_24,4.67,0.7,-0.53,0  
3BWT,ARG\_872,12.22,-0.28,0,0  
2FXT,LYS\_380,10.15,-0.35,0,0  
3H9W,GLU\_70,4.64,0.14,0,0  
2FD5,ARG\_126,12.22,-0.28,0,0  
2G3A,LYS\_91,10.29,-0.21,0,0  
3Q1C,HIS\_255,6.43,0,0,-0.07  
2D59,ARG\_65,12.15,-0.35,0,0  
2Z61,LYS\_343,10.43,-0.07,0,0  
2FXT,ASP\_361,4.08,0.28,0,0  
1D20,LYS\_174,3.69,0.35,-1.14,0  
3LJN,GLU\_147,4.5,0,0,0  
4GA2,ASP\_43,3.87,0.07,0,0  
2D2S,LYS\_746,10.5,0,0,0  
3GYW,TYR\_62,10,0,0,0  
3NR5,LYS\_35,10.15,-0.35,0,0  
3M7G,TYR\_107,9.59,1.47,-1.11,-0.76  
3F6F,GLU\_43,3.71,0.35,-1.14,0  
3N0K,HIS\_93,6.42,0.06,0,-0.14  
1NAR,GLU\_168,3.84,0.49,-1.15,0  
1RI6,GLU\_215,4.49,0.07,-0.08,0  
1BN6,TYR\_25,9.82,0,-0.18,0  
1LFP,GLU\_178,3.69,0.35,-1.17,0  
3U2A,GLU\_117,4.13,0.35,-0.72,0  
2CL3,GLU\_200,3.91,0.21,-0.8,0  
1OTM,LYS\_209,10.5,0,0,0  
2E3H,LYS\_280,10.43,-0.07,0,0  
1ZP2,GLU\_24,4.5,0,0,0  
3RLN,ASP\_619,3.85,0.07,-0.02,0  
3IRA,HIS\_58,6.5,0,0,0  
2QHT,GLU\_98,3.97,0.21,-0.74,0  
3LD1,GLU\_318,4.5,0,0,0  
2AXO,HIS\_265,6.5,0,0,0  
2A4D,LYS\_100,10.5,0,0,0  
3DTE,ARG\_150,11.94,-0.56,0,0  
2G5S,ASP\_176,3.7,0.35,-0.45,0  
1YW5,GLU\_159,0.7,2.27,-2.57,-3.5  
3U2R,ASP\_67,3.87,0.07,0,0  
2P5D,GLU\_70,3.46,0.07,-1.11,0  
2HRZ,CYS\_190,6.99,-4.76,0,2.75  
3ADO,CYS\_252,9,0,0,0  
1WXF,LYS\_138,10.22,-0.28,0,0  
3PM2,LYS\_169,10.29,-0.21,0,0  
3IOO,LYS\_151,10.29,-0.21,0,0  
3JRT,TYR\_116,10,0,0,0  
3EOD,ARG\_76,12.01,-0.49,0,0  
3UV9,ASP\_302,1.68,0.28,-2.4,0  
3JV1,GLU\_54,4.57,0.07,0,0  
3LQE,GLU\_494,4.41,0.56,-0.65,0  
1J8B,ASP\_56,3.87,0.07,0,0  
2W0G,GLU\_272,4.71,0.21,0,0  
4FD6,GLU\_24,3.66,0.28,-1.12,0  
1S17,ARG\_269,11.87,-0.63,0,0  
1O17,GLU\_97,4.64,0.14,0,0  
1NJ4,LYS\_325,10.5,0,0,0  
1ZP2,GLU\_193,4.5,0,0,0  
2RIK,ASP\_110,4.15,0.35,0,0  
1A8Q,GLU\_71,4.5,0,0,0  
2IKR,HIS\_533,6.43,0,0,-0.07  
1NFN,TYR\_74,9.95,0.07,-0.5,0.38  
2G7O,GLU\_116,4.5,0,0,0  
3PP8,ASP\_235,2.8,0.63,-1.63,0  
1QYI,GLU\_244,6.57,2.18,0,-0.11



2QZQ,ASP\_80,3.6,0,-0.2,0  
 1EV8,HIS\_73,6.5,0,0,0  
 1FKM,ASP\_614,2.37,0.49,-1.92,0  
 3CJW,GLU\_393,4.38,0.42,-0.54,0  
 3FTT,ASP\_187,3.8,0,0,0  
 3RJX,GLU\_144,4.51,0.21,-0.2,0  
 2Z84,ARG\_123,12.15,-0.35,0,0  
 3M7D,ASP\_121,3.84,0.28,-0.24,0  
 3IU5,CYS\_50,8.8,-0.73,0,0.53  
 3RLE,LYS\_159,9.87,-0.63,0,0  
 3FWU,CYS\_59,9.17,0,0,0.17  
 1MTZ,TYR\_106,12.93,2.93,0,0  
 2EEY,GLU\_39,3.84,0.14,-0.8,0  
 1DVO,GLU\_159,3.68,0.35,-1.17,0  
 3GS3,GLU\_81,4.3,0.21,-0.41,0  
 3LH5,ARG\_715,12.01,-0.49,0,0  
 2OKT,LYS\_266,10.29,-0.21,0,0  
 1X7F,GLU\_12,3.52,0.7,-1.68,0  
 4FH3,LYS\_243,10.36,-0.14,0,0  
 1R3D,GLU\_216,3.81,0.28,-0.97,0  
 1QYI,LYS\_346,10.5,0,0,0  
 2VGY,CYS\_79,9.32,-0.21,0,0.53  
 1WPA,ASP\_465,3.93,0.14,-0.01,0  
 2A6B,GLU\_196,4.5,0,0,0  
 1BKB,GLU\_112,3.77,0.35,-1.08,0  
 1PGV,GLU\_375,4.5,0,0,0  
 2XHC,ARG\_107,12.15,-0.35,0,0  
 3I47,GLU\_226,4.5,0,0,0  
 3B21,LYS\_25,10.5,0,0,0  
 3E5T,GLU\_111,4.64,0.14,0,0  
 3US6,GLU\_131,4.53,0.21,-0.18,0  
 3CJW,LYS\_301,10.01,-0.49,0,0  
 2C2Y,CYS\_190,7.15,-2.08,0,0.23  
 2F4Q,ASP\_197,4.08,0.28,0,0  
 2GZQ,ASP\_68,4.15,0.35,0,0  
 1UJ8,LYS\_63,10.5,0,0,0  
 1BN6,CYS\_187,10.02,-0.21,-0.5,1.73  
 2DFL,LYS\_205,10.29,-0.21,0,0  
 2GZR,TYR\_51,11.91,1.91,0,0  
 4ANN,GLU\_185,2.27,0.56,-2.78,0  
 3KT9,GLU\_23,4.5,0,0,0  
 2Q13,ARG\_149,12.43,-0.07,0,0  
 3ZTA,GLU\_84,4.85,0.35,0,0  
 1AKO,ARG\_142,12.15,-0.35,0,0  
 3IBT,HIS\_165,5.33,1.6,1.45,-4.22  
 2FG1,LYS\_105,10.15,-0.35,0,0  
 1NKD,ASP\_48,2.95,0.56,-1.41,0  
 1XEU,ASP\_49,1.43,1.19,-3.56,0  
 3ASA,LYS\_105,10.5,0,0,0  
 3IPZ,ASP\_93,4.01,0.21,0,0  
 3EVZ,ASP\_150,3.09,0.49,-1.19,0  
 1V43,GLU\_160,2.99,0.49,-2,0  
 2B2H,GLU\_297,5.57,3.74,-2.9,0.23  
 2CN1,LYS\_72,10.5,0,0,0  
 3K8J,CYS\_144,10.8,0,1.8  
 3LPZ,TYR\_285,9.88,0.31,-0.42,0  
 1X04,GLU\_176,4.24,0.35,-0.61,0  
 3RLN,LYS\_713,10.29,-0.21,0,0  
 3LJN,LYS\_298,9.66,-0.84,0,0  
 1TJE,ASP\_209,2.65,0.42,-1.57,0  
 4E8B,GLU\_196,4.5,0,0,0  
 4F85,GLU\_194,1.13,0.98,-4.35,0  
 1QQH,TYR\_160,13.86,0.68,0.78,2.4  
 3N2T,LYS\_219,10.43,-0.07,0,0  
 3F53,TYR\_49,10.04,0.07,-0.03,0  
 2VGY,ASP\_66,3.61,0.42,-0.61,0  
 3P51,TYR\_124,10.84,0.05,0,0.79  
 3F1X,GLU\_19,3.55,0.28,-1.23,0  
 2E3H,LYS\_224,10.43,-0.07,0,0  
 2BLL,TYR\_378,9.75,0,-0.25,0  
 2VAN,ASP\_92,3.54,0,-0.26,0  
 3HKX,TYR\_135,11.13,0,0,1.13  
 1PVT,ARG\_35,12.08,-0.42,0,0  
 3EYE,ASP\_132,2.06,0.7,-2.45,0  
 1TLV,TYR\_265,9.35,0.65,-1.3,0  
 3T8R,ARG\_56,12.29,-0.21,0,0  
 1GQE,ARG\_200,11.87,-0.63,0,0  
 3A7L,LYS\_103,10.08,-0.42,0,0  
 3BCH,TYR\_202,11.22,1.22,0,0  
 2CWC,TYR\_83,10.65,2.87,-0.2,-2.02  
 3CAN,HIS\_37,6.36,0,0,-0.14  
 2J8A,TYR\_300,11.46,0.97,0,0.49  
 1GXN,LYS\_348,10.43,-0.07,0,0  
 1LZL,TYR\_33,11.79,1.9,-0.11,0  
 2B0A,ARG\_99,12.15,-0.35,0,0  
 3HYQ,TYR\_99,12.45,0,0.15,2.3  
 2X4L,ASP\_113,3.87,0.07,0,0  
 3EVN,ASP\_314,3.05,0.28,-1.03,0  
 3LJC,ARG\_164,12.01,-0.49,0,0  
 2EHG,TYR\_26,12.45,0.1,0.26,2.09  
 2A6B,LYS\_23,10.5,0,0,0  
 2BAA,ARG\_240,12.5,0,0,0  
 3BQW,LYS\_178,10.43,-0.07,0,0  
 3UX2,GLU\_34,4.71,0.21,0,0  
 3R2E,TYR\_18,10,0,0,0  
 2EFK,GLU\_112,3.3,0.28,-1.48,0  
 4E5S,LYS\_150,10.5,0,0,0  
 3A7L,ASP\_56,3.03,0.07,-0.84,0  
 2G7O,GLU\_127,4.71,0.21,0,0  
 2XHC,ARG\_86,12.36,-0.14,0,0  
 2PLQ,TYR\_151,10.06,0,-0.38,0.44  
 1A8Q,HIS\_59,6.5,0,0,0  
 3I4T,ARG\_141,12.29,-0.21,0,0  
 1P4X,LYS\_55,10.08,-0.42,0,0  
 3RVC,GLU\_159,1.74,1.24,-1.82,-2.18  
 1TUL,ARG\_108,12.22,-0.28,0,0  
 3GG6,LYS\_133,10.5,0,0,0  
 1R53,TYR\_13,9.29,0.14,-0.85,0  
 2VGM,ASP\_225,3.8,0,0,0  
 3FK5,GLU\_81,3.95,0.42,-0.97,0  
 2Q99,ARG\_327,11.84,-0.81,0,0.15  
 2I88,TYR\_445,13.41,0.95,0.246  
 3RFF,GLU\_30,4.08,0.28,-0.7,0  
 4FZN,TYR\_54,11.53,1.53,0,0  
 3TOW,ASP\_77,2.54,0.56,-1.82,0  
 3BA1,LYS\_22,10.29,-0.21,0,0  
 3T5B,ASP\_387,2.61,0.91,-2.1,0  
 1PV5,GLU\_141,3.42,0.7,-1.78,0  
 2CN1,CYS\_23,9.07,0,0,0.07  
 3FRR,LYS\_127,9.94,-0.56,0,0  
 4EKU,ARG\_93,13.13,-2.35,0.299  
 3FHF,LYS\_60,10.43,-0.07,0,0  
 1J8B,GLU\_67,4.5,0,0,0  
 1IAP,GLU\_190,0.53,1.33,-2.4,-2.9  
 2GZR,TYR\_132,10.11,0,0,0.11  
 3ZRI,CYS\_28,9.08,-0.13,0,0.21  
 1R53,ARG\_62,12.5,0,0,0  
 2PWQ,GLU\_17,3.6,0.35,-1.24,0  
 1C3K,HIS\_57,6.44,0.01,0,-0.07  
 3CAX,ARG\_383,9.3,-1.62,0,-1.58  
 3G9G,GLU\_236,3.12,0.56,-1.94,0  
 4H4J,ASP\_49,3.79,0,-0.01,0  
 1QYI,TYR\_295,10.21,0.21,0,0  
 3J29,TYR\_532,10.03,0.14,-0.11,0  
 1ZCU,ASP\_224,1.66,0.77,-2.91,0  
 4FCU,GLU\_195,4.61,0.35,-0.24,0  
 2ZCX,GLU\_43,4.71,0.21,0,0  
 3MIX,ASP\_357,2.94,0.28,-1.14,0  
 1T6L,ASP\_98,3.83,0.07,-0.04,0  
 2V5B,TYR\_87,10.07,0.07,0,0  
 2V1L,ASP\_141,3.61,0.21,-0.4,0  
 1YB2,ASP\_57,3,0.21,-1.01,0  
 2CW4,ASP\_79,3.72,0.35,-0.43,0  
 3A0X,ARG\_648,12.15,-0.35,0,0  
 3H5T,HIS\_254,6.5,0,0,0  
 3I0O,ASP\_182,2.77,0.35,-1.39,0  
 3IL3,ASP\_27,3.87,0.07,0,0  
 3B21,LYS\_209,9.52,-0.98,0,0  
 2OJQ,ARG\_496,12.43,-0.07,0,0  
 1WNH,TYR\_146,10,0,0,0  
 1WXF,CYS\_201,9.21,0,0,0.21  
 2P65,ASP\_28,3.69,0,-0.11,0  
 1UOH,TYR\_138,10.04,0,0,0.04  
 3G6S,CYS\_114,7.56,-1.44,0,0  
 3HKX,ARG\_280,12.5,0,0,0  
 2B78,ASP\_271,2.41,0.49,-1.88,0  
 1ZHV,ASP\_60,2.78,0.49,-1.51,0  
 3PBH,ARG\_8,13.65,-1.25,0.24  
 2OYZ,GLU\_34,3.96,0.21,-0.75,0  
 2B3M,GLU\_13,4.5,0,0,0  
 1GPP,GLU\_80,1.75,0.79,-2.1,-1.44  
 2P1W,ARG\_65,11.94,-0.56,0,0  
 3K8J,TYR\_101,10.34,1.31,-0.97,0  
 1MML,LYS\_102,10.5,0,0,0  
 2I88,ASP\_509,2.84,0.21,-1.17,0  
 1EQ6,ASP\_99,2.58,0.56,-1.77,0  
 1PBV,LYS\_77,10.08,-0.42,0,0  
 1MTZ,GLU\_172,4.31,0.21,-0.4,0  
 1XIP,ASP\_69,4.02,0.35,-0.13,0  
 1XTZ,HIS\_264,6.5,0,0,0  
 1Ri6,HIS\_211,6.93,0.5,0,-0.07  
 2CN1,CYS\_63,6.75,-2.86,0,0.6  
 2H01,GLU\_47,3.68,1.18,-1.99,0  
 3FHF,HIS\_-4,6.5,0,0,0  
 1AD6,TYR\_529,11.97,0,0.09,1.88  
 3RJZ,ARG\_126,11.66,-0.84,0,0  
 2B78,ASP\_189,3.62,0.28,-0.46,0  
 1S7K,ARG\_135,11.8,-0.7,0,0  
 3L3P,GLU\_398,4.5,0,0,0  
 1ZBM,ARG\_222,12.29,-0.21,0,0  
 1SIG,TYR\_143,10.61,0.61,0,0  
 3QYB,HIS\_978,4.28,0.79,-3.01  
 3M7D,ARG\_241,12.43,-0.07,0,0  
 208I,HIS\_17,7.1,0.6,0,0  
 3PP8,ARG\_89,12.16,-0.34,0,0  
 2G3A,ARG\_90,11.73,-0.77,0,0  
 1OLR,ARG\_75,12.08,-0.42,0,0  
 3HUE,GLU\_189,4.08,0.77,-1.19,0  
 1X6J,ARG\_83,11.1,-1.4,0,0  
 3F53,TYR\_191,10.07,0.07,0,0  
 2H8O,ARG\_246,12.15,-0.35,0,0  
 3CXS,GLU\_175,4.5,0,0,0  
 1WYC,HIS\_373,6.43,0,0,-0.07  
 1R29,ARG\_26,13.48,-1.6,0.2,58  
 2RIS,GLU\_10,4.5,0,0,0  
 1OXZ,ARG\_214,11.94,-0.56,0,0  
 1PVT,LYS\_110,10.5,0,0,0  
 1ZBP,GLU\_99,4.5,0,0,0  
 3KT9,LYS\_53,10.5,0,0,0  
 1GPP,GLU\_22,4.5,0,0,0  
 2CN1,LYS\_51,10.5,0,0,0  
 1XIP,GLU\_85,4.64,0.14,0,0  
 1WNH,LYS\_217,10.43,-0.07,0,0  
 1WPA,GLU\_470,3.6,0.28,-1.17,0  
 1WLY,TYR\_275,9.27,0.07,-0.8,0  
 1L3K,ASP\_123,3.87,0.14,-0.07,0  
 3F6M,ARG\_144,11.8,-0.7,0,0  
 2CXV,ARG\_22,12.36,-0.14,0,0  
 3A2Z,LYS\_177,10.22,-0.28,0,0  
 2IXM,ARG\_69,12.36,-0.14,0,0  
 1YR6,CYS\_242,8.69,-0.38,0,0.07  
 3KT9,CYS\_40,8.85,-0.52,0,0.37  
 1ZBM,TYR\_67,10.5,1.1,-0.6,0  
 3ANJ,LYS\_16,10.5,0,0,0  
 4E6S,HIS\_9,7.09,0.8,0,-0.21  
 1LTU,HIS\_138,6.1,1.6,3.48,-5.48  
 3E7P,CYS\_201,8.32,-1.29,0,0.61  
 200K,ARG\_104,12.5,0,0,0  
 1TUL,ARG\_54,12.22,-0.28,0,0  
 1OGL,GLU\_250,4.02,0.14,-0.62,0  
 1TD6,GLU\_39,4.5,0,0,0  
 4F3J,ASP\_203,2.3,0.56,-2.07,0  
 1PVT,GLU\_179,4.71,0.21,0,0  
 2Q0K,ARG\_104,12.5,0,0,0  
 1QQE,GLU\_288,4.02,0.63,-1.11,0  
 1ZBS,ASP\_221,3.49,0.49,-0.8,0  
 2V5B,TYR\_224,11.67,0.76,0,0.91  
 1XWM,ASP\_115,3.39,0.35,-0.76,0  
 4FLE,TYR\_160,12.6,2.47,-0.8,0.93  
 2V1L,TYR\_82,10,0,0,0  
 1EDG,HIS\_176,6.75,0.32,0,-0.07  
 2P52,GLU\_201,2.31,0.21,-2.4,0  
 1P6F,LYS\_52,10.43,-0.07,0,0  
 2FD4,LYS\_453,10.29,-0.21,0,0  
 2Z84,ARG\_49,11.66,-0.84,0,0  
 2QK1,LYS\_531,10.5,0,0,0  
 1LN4,HIS\_43,6.5,0,0,0  
 1E5S,CYS\_98,9.12,-1.75,-0.05,1.93  
 3M3P,GLU\_230,3.39,0.49,-1.6,0  
 4HDE,CYS\_69,2.51,-6.17,-0.6,0.28  
 2DIU,GLU\_235,4.71,0.21,0,0  
 4HD7,GLU\_81,4.48,0.07,-0.09,0  
 3F53,ASP\_119,3.06,0.07,-0.81,0  
 1KCM,GLU\_248,4.69,0.19,0,0  
 1SNT,TYR\_91,9.91,0,-0.09,0  
 3HNX,TYR\_3,11.36,1.36,0,0  
 3LPZ,ARG\_11,12.01,-0.49,0,0  
 4AM1,GLU\_173,3.02,0.49,-1.97,0  
 2E0T,TYR\_70,12.56,0.16,2.4  
 1YTD,ARG\_142,12.15,-0.35,0,0  
 2B0J,GLU\_125,4.71,0.21,0,0  
 3IRA,GLU\_165,4.71,0.21,0,0  
 3OOP,GLU\_110,4.5,0,0,0  
 3TOW,ASP\_74,2.33,0.49,-1.95,0  
 2QHT,TYR\_63,8.59,0.21,-1.62,0  
 3G53,ASP\_114,2.09,0.7,-2.41,0  
 2Q99,LYS\_193,10.22,-0.28,0,0  
 3RUX,LYS\_116,10.5,0,0,0  
 2GEN,HIS\_21,6.43,0,0,-0.07  
 2OKT,GLU\_315,4.5,0,0,0  
 3M7D,GLU\_375,5.17,0.67,0,0  
 3H04,HIS\_234,6.29,0,0,-0.21  
 3BQW,ARG\_224,12.36,-0.14,0,0  
 3IU5,GLU\_133,4.08,0.35,-0.77,0  
 3CJW,ARG\_246,12.15,-0.35,0,0  
 2OKT,GLU\_315,4.5,0,0,0  
 1J74,ASP\_38,4.22,0.42,0,0  
 3RKV,GLU\_277,4.57,0.07,0,0  
 3BZT,ARG\_338,12.5,0,0,0  
 2B0A,ARG\_138,11.87,-0.63,0,0  
 3ZTA,ASP\_64,3.45,0.35,-0.7,0  
 220M,ARG\_77,13.65,-1.02,0.2,17  
 2R0S,LYS\_174,10.22,-0.28,0,0  
 1P2F,LYS\_163,10.5,0,0,0  
 1SIG,ARG\_157,12.15,-0.35,0,0  
 1P1L,LYS\_25,10.5,0,0,0

3R87,HIS\_51,6.29,0,0,-0.21  
3M7D,ARG\_144,11.58,-3.93,0,3,01  
3EZ7,HIS\_138,6.5,0,0,0  
1SFE,GLU\_30,3.61,0.71,-1.6,0  
2FBI,GLU\_17,3.78,0.28,-1,0  
1J85,LYS\_61,10.43,-0.07,0,0  
2V4U,HIS\_330,7.45,1.09,0,-0.14  
3MTT,TYR\_505,11.4,0,0,1.4  
1NJ4,LYS\_6,10.43,-0.07,0,0  
2GAU,GLU\_27,4.57,0.07,0,0  
3CXS,GLU\_106,3.22,0.49,-1.77,0  
1AKO,ASP\_208,3.64,0.35,-0.52,0  
2IF4,TYR\_202,10.98,0.78,-0.8,1  
3SMD,TYR\_139,11.56,1.56,0,0  
1NIJ,ASP\_52,3.54,0.07,-0.33,0  
2GAU,ARG\_183,12.15,-0.35,0,0  
1X91,ASP\_57,3.3,0.35,-0.85,0  
4ACJ,GLU\_732,4.22,0.21,-0.49,0  
2WB3,ASP\_291,3.68,0.49,-0.61,0  
3J5N,GLU\_271,4.4,0,-0.1,0  
3H6Q,TYR\_64,10.13,0.49,-0.64,0.28  
1PSW,ARG\_70,12.29,-0.21,0,0  
3IVF,ARG\_303,11.94,-0.56,0,0  
4GCO,TYR\_214,10.14,0.14,0,0  
3M16,LYS\_274,10.5,0,0,0  
3SMD,GLU\_53,4.19,0.49,-0.8,0  
1WXF,ARG\_25,12.08,-0.42,0,0  
1RSQ,ARG\_97,12.29,-0.21,0,0  
3M3P,GLU\_138,9.86,3.66,1.23,0.47  
3BJV,GLU\_9,4.72,0.35,-0.13,0  
1ZCU,CYS\_130,9,0,0,0  
2ZTY,ASP\_51,3.94,0.14,0,0  
1A8Q,ARG\_266,12.5,0,0,0  
3HVV,TYR\_175,10.69,0,0,0.69  
2OGQ,TYR\_453,12.95,0.28,-0.8,3.47  
3ERF,HIS\_114,7.28,0.78,0,0  
1D2K,LYS\_199,10.5,0,0,0  
4FZR,ARG\_349,12.43,-0.07,0,0  
2AXO,TYR\_204,10.21,0.21,0,0  
2B61,ASP\_205,4.07,0.35,-0.08,0  
2PPN,TYR\_80,12.19,0.14,-0.35,2.4  
3O16,ASP\_112,3.22,0.14,-0.72,0  
4ECC,GLU\_64,4.57,0.07,0,0  
3GEC,CYS\_312,6.75,-0.96,-2.4,1.1  
4ECC,GLU\_141,4.78,0.28,0,0  
4ETX,GLU\_394,4.26,0,-0.24,0  
1QQH,TYR\_179,12.5,0.07,0.33,2.1  
1NIJ,GLU\_308,4.57,0.07,0,0  
3ASA,ASP\_339,2.63,0.7,-1.87,0  
3EVN,GLU\_245,4.17,0.28,-0.61,0  
1UOH,CYS\_48,11.32,0,0,2.32  
2FB6,GLU\_72,3.92,1.01,-1.59,0  
1WPA,TYR\_432,9.62,0.42,-0.8,0  
3LQE,TYR\_370,10.35,0.07,0,0.28  
4H4J,HIS\_148,6.44,0.08,0,-0.14  
2YT4,ASP\_549,3.83,0.07,-0.04,0  
3LJC,LYS\_143,10.29,-0.21,0,0  
4AE7,CYS\_218,10.13,-0.77,0,1.91  
2RFA,GLU\_71,4.5,0,0,0  
1NJ4,CYS\_115,9.94,-0.05,-1.71,2.7  
2Z14,ARG\_35,12.08,-0.42,0,0  
1PGV,ARG\_232,12.36,-0.14,0,0  
1AKO,LYS\_255,10.43,-0.07,0,0  
2X4G,TYR\_15,13.99,0.29,0.8,2.9  
1YG2,HIS\_37,6.29,0,-0.21  
2QZQ,LYS\_142,10.43,-0.07,0,0  
1DOV,ASP\_172,2.84,0.07,-1.03,0  
1LFP,GLU\_146,4.5,0,0,0  
1FKM,ARG\_343,12.15,-0.35,0,0  
3ONT,CYS\_122,8.5,-0.5,0,0  
2EHG,GLU\_61,4.8,0.3,0,0  
3HKX,ARG\_93,12.01,-0.49,0,0  
2O8P,CYS\_59,10.15,-0.21,0,1.36  
3GS9,TYR\_189,9.11,0.14,-1.03,0  
3N2T,GLU\_127,8.25,4.01,-0.3,0.04  
2X5Y,TYR\_793,9.63,0,-0.37,0  
3P28,LYS\_114,10.22,-0.28,0,0  
4EVF,LYS\_246,9.35,-0.14,0,-1.01  
2FL7,LYS\_120,10.36,-0.14,0,0  
3SMD,LYS\_113,10.5,0,0,0  
3FK5,ARG\_210,12.22,-0.28,0,0  
3F6F,LYS\_189,10.36,-0.14,0,0  
3CRM,ARG\_63,12.29,-0.21,0,0  
1J8B,GLU\_26,4.17,0.35,-0.68,0  
2YYO,ASP\_39,3.77,0,-0.03,0  
2FBI,TYR\_91,10.36,0,0,0.36  
3MIX,GLU\_398,4.71,0.21,0,0  
4DIU,TYR\_119,13.34,0.14,0.8,2.4  
1J85,TYR\_51,10.06,0.14,-0.08,0  
3RUX,LYS\_219,10.5,0,0,0  
3A2Z,LYS\_142,10.08,-0.42,0,0  
4GCO,LYS\_149,10.36,-0.14,0,0  
2RFA,HIS\_257,7.53,1.09,-0.07  
2OGQ,LYS\_556,10.01,-0.49,0,0  
1P4X,TYR\_42,13.94,0.97,0.58,2.4  
1VJG,GLU\_26,3.99,0.14,-0.65,0  
2R2Y,LYS\_83,10.43,-0.07,0,0  
2RFA,GLU\_104,3.81,0.49,-1.18,0  
2QOP,GLU\_118,4.71,0.21,0,0  
1ZBM,GLU\_134,3.84,0.14,-0.8,0  
3OKQ,GLU\_644,4.5,0,0,0  
1WJG,ASP\_79,4.06,0.77,-0.51,0  
3COC,ASP\_307,3.19,0.07,-0.68,0  
1PBV,ARG\_145,11.24,-1.26,0,0  
1D2K,LYS\_422,10.36,-0.14,0,0  
3F7M,ASP\_266,2.96,0.35,-1.19,0  
2XJ4,LYS\_62,10.01,-0.49,0,0  
3G9T,ARG\_205,11.73,-0.77,0,0  
2A6B,LYS\_74,10.15,-0.35,0,0  
2WOZ,LYS\_460,10.43,-0.07,0,0  
1ZCE,GLU\_128,4.5,0,0,0  
3HUE,LYS\_80,10.5,0,0,0  
3PM2,LYS\_94,10.43,-0.07,0,0  
1AM2,TYR\_178,10.07,0.07,0,0  
3GV0,ARG\_234,11.94,-0.56,0,0  
3M7G,ASP\_160,3.68,0,-0.12,0  
3P2F,ARG\_58,11.94,-0.56,0,0  
3NBI,GLU\_204,4.57,0.07,0,0  
1EV8,GLU\_58,6.02,2.32,-0.8,0  
3U0V,ASP\_140,2.93,0.49,-1.36,0  
3LMO,GLU\_63,3.89,0.07,-0.68,0  
1O5J,LYS\_63,10.5,0,0,0  
3ERF,GLU\_121,2.28,1.25,-1.44,-2.02  
1YTQ,ASP\_82,2.98,0.42,-1.24,0  
2R2Y,ASP\_79,3.1,0.49,-1.19,0  
2FL7,HIS\_114,7.02,0.8,0,-0.28  
2AZL,LYS\_93,10.01,-0.49,0,0  
1NAR,ASP\_272,3.75,0.07,-0.12,0  
3M66,HIS\_314,6.75,0.53,0,-0.28  
4H4J,TYR\_69,8.75,1.25,-1.9,-0.6  
2E3I,CYS\_111,8.41,-0.66,0.07  
3T57,ARG\_271,12.08,-0.42,0,0  
2IQT,ASP\_202,3.17,0.28,-0.91,0  
2F4Q,ARG\_24,12.5,0,0,0  
3BPV,ARG\_79,11.8,-0.7,0,0  
2Z84,GLU\_132,3.91,0.21,-0.8,0  
1YR6,GLU\_234,3.39,0.49,-1.6,0  
1ILW,HIS\_54,1.92,1.26,-1.7,-4.16  
1YR6,TYR\_97,12.22,0.91,0,1.31  
2ZQ5,LYS\_226,10.01,-0.49,0,0  
2F4Q,ARG\_41,11.45,-1.05,0,0  
1ZNL,ASP\_15,3.53,0.49,-0.76,0  
2Z9M,LYS\_200,10.29,-0.21,0,0  
3RFY,ASP\_197,3.94,0.14,0,0  
1TR9,GLU\_73,4.5,0,0,0  
3RFY,HIS\_172,7.4,0.97,0,-0.07  
1YTQ,GLU\_77,4.57,0.07,0,0  
3JRT,CYS\_48,7.84,-1.3,0,0.14  
2X5Y,TYR\_886,9.62,0.58,-1.06,0.1  
4DBL,ARG\_92,12.29,-0.21,0,0  
4E9E,LYS\_518,10.43,-0.07,0,0  
2V5B,TYR\_103,11.27,0,0,1.27  
3LJC,LYS\_48,10.29,-0.21,0,0  
2FBQ,LYS\_151,10.5,0,0,0  
1C3K,LYS\_126,10.5,0,0,0  
3IVF,ARG\_358,12.36,-0.14,0,0  
1BKR,LYS\_53,10.29,-0.21,0,0  
2D2S,ASP\_742,3.22,0.35,-0.93,0  
1YM5,LYS\_143,10.5,0,0,0  
1JSX,TYR\_63,10,0,0,0  
1KCM,TYR\_24,12.82,0.14,0.28,2.4  
1GQE,TYR\_296,10.9,0,0,0.9  
2EJB,LYS\_19,10.36,-0.14,0,0  
2YYO,TYR\_88,13.83,0.07,0.19,3.57  
2AD1,TYR\_141,10.03,0.07,-0.04,0  
2XUO,GLU\_165,3.39,0.49,-1.6,0  
1LTU,ASP\_3,3.09,0.56,-1.27,0  
2VGM,GLU\_302,4.2,0.49,-0.79,0  
2CYG,HIS\_291,7.49,1.61,2.4,-3.02  
2B02,GLU\_390,3.09,0.56,-1.97,0  
3PBH,ASP\_60,3.06,0.07,-0.81,0  
1YB2,CYS\_86,8.49,-1.28,0,0.77  
1BN6,GLU\_225,4.42,0,-0.08,0  
1MIX,LYS\_284,10.29,-0.21,0,0  
3CJW,TYR\_312,11.21,1.26,-0.05,0  
3ETV,HIS\_128,0.16,0.94,-2.12,-5.16  
3CCY,ARG\_185,12.29,-0.21,0,0  
4H4J,ASP\_220,3.8,0,0,0  
3GMS,ARG\_57,11.66,-0.84,0,0  
2QVO,TYR\_46,10,0,0,0  
3BA1,ASP\_237,3.9,0.42,-0.32,0  
3ETU,ARG\_208,11.94,-0.56,0,0  
3U4K,CYS\_178,9,0,0,0  
1O9G,LYS\_225,10.5,0,0,0  
1NAR,HIS\_130,0.67,0,-0.24,-5.59  
3N2T,LYS\_259,10.43,-0.07,0,0  
1RI5,HIS\_127,6.36,0,0,-0.14  
4ESS,ARG\_39,12.15,-0.35,0,0  
2F8H,ASP\_335,2.73,0.28,-1.34,0  
3US6,LYS\_58,10.5,0,0,0  
2P65,GLU\_30,3.46,0.28,-1.33,0  
2Z0W,ARG\_12,12.5,0,0,0  
3US6,ASP\_59,3.8,0.07,-0.07,0  
2H01,ASP\_152,3.49,0.49,-0.8,0  
1YLN,GLU\_72,4.78,0.28,0,0  
3IRA,ARG\_84,12.01,-0.49,0,0  
3M7G,ASP\_20,12.08,-0.42,0,0  
1SUU,ARG\_681,12.36,-0.14,0,0  
1GXN,LYS\_521,10.08,-0.42,0,0  
3QAV,LYS\_137,10.5,0,0,0  
3IRA,ARG\_101,12.08,-0.42,0,0  
2QRX,ASP\_18,3.87,0.07,0,0  
2APL,ARG\_97,12.36,-0.14,0,0  
2IQT,GLU\_185,4.5,0,0,0  
1K95,HIS\_105,6.97,0.75,0,-0.28  
1KW4,LYS\_53,10.5,0,0,0  
2RIK,LYS\_234,9.52,-0.98,0,0  
2E3C,TYR\_308,10,0,0,0  
1XIP,ARG\_189,12.5,0,0,0  
2QDJ,CYS\_102,10.35,-0.06,0,1.41  
1PVT,CYS\_78,9.05,-1.12,0,1.16  
1SQW,ARG\_154,12.36,-0.14,0,0  
3VHJ,GLU\_163,3.98,0.28,-0.8,0  
1Q46,TYR\_32,10.07,0.07,0,0  
3S0A,LYS\_109,10.22,-0.28,0,0  
2Q13,GLU\_28,4.64,0.14,0,0  
2D7J,LYS\_120,10.15,-0.35,0,0  
1XFK,ARG\_94,12.29,-0.21,0,0  
2ZCO,HIS\_79,6.43,0,0,-0.07  
3EAZ,GLU\_108,3.68,0.35,-1.17,0  
2OKT,TYR\_333,10.46,0,0,0.46  
3L3P,GLU\_519,4.22,0.21,-0.49,0  
2R51,ASP\_68,4.12,0.63,-0.31,0  
2A1V,HIS\_75,6.36,0,0,-0.42  
1PVT,HIS\_123,6.38,2.52,2.4,-5.04  
2FPN,LYS\_62,10.43,-0.07,0,0  
3GYW,TYR\_277,9.65,0,-0.35,0  
2Q99,LYS\_28,10.43,-0.07,0,0  
1I60,LYS\_94,10.5,0,0,0  
3NBI,GLU\_150,2.11,1.12,-3.51,0  
3VJ8,LYS\_138,10.15,-0.35,0,0  
3GE9,GLU\_74,3.95,0.21,-0.76,0  
1EQ6,HIS\_107,6.38,1.6,1.81,-3.53  
1P1L,GLU\_92,3.83,0.42,-1.09,0  
3EVP,ASP\_68,4.12,0.63,-0.31,0  
2CVB,ARG\_186,12.01,-0.49,0,0  
3GS9,TYR\_57,10.08,0.07,-0.47,0.48  
1KW4,ASP\_10,3.8,0.28,-0.28,0  
2H01,GLU\_60,4.55,0.28,-0.23,0  
3R2E,ASP\_45,3.81,0.07,-0.06,0  
3EZ7,GLU\_189,4.5,0,0,0  
1SIG,GLU\_154,4.7,0.21,-0.01,0  
3OBS,ARG\_64,12.36,-0.14,0,0  
3MYI,HIS\_974,6.75,0.32,0,-0.07  
1AK1,GLU\_94,0.79,0.47,-1.78,-2.4  
3V46,ARG\_300,12.15,-0.35,0,0  
3VHJ,ARG\_135,12.01,-0.49,0,0  
2JHY,HIS\_131,6.5,0,0,0  
3CQ1,CYS\_54,9,0,0,0  
4DNU,ARG\_99,10.84,-3.06,0,1.4  
3CXS,HIS\_107,6.5,0.07,0,-0.07  
1R53,CYS\_23,9.82,-1.04,0,1.86  
2P4D,HIS\_74,7.3,1.01,0,-0.21  
3HYQ,ARG\_172,11.38,-1.12,0,0  
1NRI,LYS\_124,10.5,0,0,0  
3GW3,ARG\_193,12.01,-0.49,0,0  
3IVF,ARG\_220,13.38,-0.69,0,1.57  
2FGG,GLU\_58,4.35,0.49,-0.64,0  
1WRU,GLU\_311,4.71,0.21,0,0  
2OEW,ASP\_302,3.97,0.21,-0.04,0  
3LD1,LYS\_214,10.08,-0.42,0,0  
1Q5Z,HIS\_595,7.2,0.91,0,-0.21  
2RIS,ASP\_105,0.56,0.98,-4.23,0  
1XTZ,CYS\_125,13.04,-0.24,3.25,1.03  
1WOU,TYR\_68,13.78,0.58,0.8,2.4  
1S17,HIS\_117,6.4,0.18,0,-0.28  
1JSX,GLU\_67,4.57,0.07,0,0  
4ACJ,LYS\_649,10.22,-0.28,0,0  
3OA7,HIS\_570,6.43,0,0,-0.07  
3M7G,GLU\_255,3.79,0.07,-0.78,0  
3ADO,LYS\_279,10.43,-0.07,0,0  
1ZBS,ARG\_128,12.29,-0.21,0,0  
2FC3,LYS\_84,10.5,0,0,0  
3E7P,HIS\_235,7.09,0.8,0,-0.21  
2FC3,CYS\_70,10.08,-0.16,0,1.24

1IDK, TYR\_179, 13.64, 3.64, 0, 0  
3I4T, CYS\_26, 9.29, -0.17, 0, 0.46  
3F53, HIS\_120, 7.3, 1.15, 0, -0.35  
4E5S, HIS\_146, 7.08, 1.66, 1.78, -2.86  
1V8E, ARG\_201, 12.36, -0.14, 0, 0  
2VGM, ASP\_285, 3.94, 0.14, 0, 0  
2Q07, LYS\_394, 10.5, 0, 0, 0  
1G5Z, LYS\_80, 10.43, -0.07, 0, 0  
1O9G, ARG\_217, 12.08, -0.42, 0, 0  
1V6T, CYS\_221, 10.68, -1.01, -0.61, 3.3  
1O9G, LYS\_121, 10.36, -0.14, 0, 0  
1GXN, LYS\_467, 10.08, -0.42, 0, 0  
1C3K, TYR\_90, 10, 0, 0, 0  
3EZ7, TYR\_101, 10, 0, 0, 0  
3O16, ARG\_83, 12.5, 0, 0, 0  
1V8E, LYS\_184, 10.5, 0, 0, 0  
3HXK, ASP\_43, 1.89, 0.49, -2.4, 0  
3UC9, LYS\_9, 10.01, -0.49, 0, 0  
2PGX, LYS\_213, 10.5, 0, 0, 0  
1P4X, ASP\_88, 2.89, 0.56, -1.47, 0  
1R2Z, GLU\_66, 4.57, 0.07, 0, 0  
2IXM, ARG\_187, 13.31, -0.89, 0, 1.7  
2GKG, TYR\_63, 9.99, 0.07, -0.08, 0  
3MEW, ASP\_153, 3.37, 0.14, -0.57, 0  
1UXO, ASP\_30, 2.78, 0.56, -1.58, 0  
2QRX, CYS\_69, 9.8, -0.46, 0, 1.26  
3GMS, ARG\_267, 11.8, -0.7, 0, 0  
1R6Y, ASP\_91, 3.56, 0.56, -0.8, 0  
1V43, LYS\_278, 10.5, 0, 0, 0  
2OJQ, ASP\_693, 3.84, 0.14, -0.1, 0  
3BPP, TYR\_209, 10, 0, 0, 0  
3BA1, GLU\_87, 4.57, 0.07, 0, 0  
2P0Y, ARG\_165, 11.94, -0.56, 0, 0  
1XDZ, ARG\_227, 11.24, -1.26, 0, 0  
1UW7, LYS\_92, 10.5, 0, 0, 0  
1ZCE, ASP\_87, 4.64, 0.84, 0, 0  
3BQW, GLU\_246, 4.5, 0, 0, 0  
2F8H, HIS\_340, 5.67, 0.152, -2.35  
1DZF, ARG\_169, 12.5, 0, 0, 0  
1UAJ, ARG\_68, 11.73, -0.77, 0, 0  
1OOX, LYS\_20, 10.01, -0.49, 0, 0  
1KCM, ARG\_220, 11.94, -0.56, 0, 0  
2HP7, ASP\_168, 3.79, 0.07, -0.08, 0  
2G5X, ARG\_76, 12.01, -0.49, 0, 0  
3U2R, GLU\_32, 3.97, 0.13, -0.66, 0  
4ACJ, GLU\_788, 4.57, 0.07, 0, 0  
3H9W, CYS\_82, 7.69, -1.45, 0, 0.14  
4FCU, TYR\_163, 10, 0, 0, 0  
1ZBM, GLU\_49, 4.08, 0, -0.42, 0  
3GOZ, HIS\_238, 6.36, 0, -0.14  
2HXB, GLU\_46, 4.5, 0, 0, 0  
2A0J, HIS\_12, 6.94, 1.07, 1.56, -2.19  
2FBQ, GLU\_131, 4.08, 0.35, -0.77, 0  
3KV0, HIS\_101, 6.22, 0, 0, -0.28  
1SUU, ASP\_788, 3.87, 0.07, 0, 0  
1L2F, GLU\_66, 4.57, 0.07, 0, 0  
3IDW, LYS\_63, 10.5, 0, 0, 0  
1WOU, ASP\_45, 3.62, 0, -0.18, 0  
3P2F, ARG\_104, 12.05, -1.85, 0, 1.41  
2RIS, GLU\_200, 4.68, 0.35, -0.17, 0  
1RKA, ARG\_53, 12.88, -1.99, 0, 2.37  
1Q5Z, HIS\_612, 3.84, 0.79, 0, -3.45  
1YM5, ASP\_61, 2.7, 0.49, -1.59, 0  
3JV1, GLU\_59, 3.18, 0.28, -1.6, 0  
3A0X, TYR\_619, 12.35, 0.02, 2.33  
2OGQ, LYS\_474, 10.5, 0, 0, 0  
2H85, ASP\_16, 3.59, 0.56, -0.77, 0  
1KCM, GLU\_33, 4.64, 0.14, 0, 0  
2PGE, ARG\_10, 12.5, 0, 0, 0  
3ETV, HIS\_340, 5.19, 2.0, -3.31  
2GEN, GLU\_9, 4.5, 0, 0, 0  
2IXM, LYS\_197, 10.43, -0.07, 0, 0  
1UW7, CYS\_23, 9.21, 0, 0, 0.21  
3PP8, ARG\_185, 12.36, -0.14, 0, 0  
3L3P, ASP\_503, 2.98, 0.21, -1.03, 0  
2VAN, TYR\_266, 10.4, 0.4, 0, 0  
2FBI, LYS\_85, 10.5, 0, 0, 0  
1WRU, ARG\_72, 12.22, -0.28, 0, 0  
2YWK, TYR\_65, 10, 0, 0, 0  
3CGW, TYR\_252, 12.36, 2.36, 0, 0  
3VJ8, ARG\_110, 12.15, -0.35, 0, 0  
3BCH, TYR\_47, 9.77, 0, -0.23, 0  
4FZN, ASP\_65, 3.72, 0.07, -0.15, 0  
4FH3, ARG\_137, 12.22, -0.28, 0, 0  
1FO9, TYR\_184, 10, 0, 0, 0  
2QVO, LYS\_79, 10.5, 0, 0, 0  
4EVF, ASP\_271, 2.07, 0.42, -2.14, 0  
3VJ8, GLU\_193, 3.75, 1.59, -2.33, 0  
1X1E, LYS\_4, 9.87, -0.63, 0, 0  
2H14, GLU\_258, 3.91, 0.21, -0.8, 0  
2BT8, ASP\_170, 3.94, 0.14, 0, 0  
3CGW, LYS\_213, 10.29, -0.21, 0, 0  
3RE9, CYS\_220, 1.06, -7.21, -0.94, 0.21  
1GXN, ARG\_610, 11.8, -0.7, 0, 0  
1H09, LYS\_87, 10.29, -0.21, 0, 0  
1ANU, ASP\_123, 3.87, 0.07, 0, 0  
3V75, ARG\_48, 12.08, -0.42, 0, 0  
1RWZ, LYS\_139, 10.19, -0.56, 0, 0.25  
2W0G, LYS\_268, 10.5, 0, 0, 0  
1SQW, TYR\_134, 11.15, 0.7, 0, 0.45  
3H6Q, ARG\_127, 11.31, -1.19, 0, 0  
3QAV, HIS\_44, 6.77, 0.41, 0, -0.14  
2NMU, ARG\_38, 12.15, -0.35, 0, 0  
2ZCO, TYR\_208, 11.98, 1.98, 0, 0  
2O4D, LYS\_118, 10.22, -0.28, 0, 0  
2R4Q, GLU\_237, 4.5, 0, 0, 0  
2YX0, TYR\_33, 11.26, 1.26, 0, 0  
3K8J, ARG\_248, 12.29, -0.21, 0, 0  
3ZSL, GLU\_230, 4.12, 0.42, -0.8, 0  
3V3T, HIS\_45, 6.31, 0.02, 0, -0.21  
3ONT, ARG\_140, 12.22, -0.28, 0, 0  
1IDK, LYS\_148, 9.94, -0.56, 0, 0  
4FCU, ASP\_44, 3.7, 0.7, -0.8, 0  
2BV9, LYS\_96, 10.5, 0, 0, 0  
4EF5, HIS\_157, 6.5, 0, 0, 0  
1Q42, ARG\_137, 12.08, -0.42, 0, 0  
1X6J, ARG\_15, 11.66, 0.84, 0, 0  
4E9E, GLU\_572, 4.57, 0.07, 0, 0  
2R2Y, HIS\_120, 4.27, 0.28, 0, -2.51  
2CWY, GLU\_19, 4.44, 0.28, -0.34, 0  
1NUJ, ARG\_22, 12.29, -0.21, 0, 0  
2AHE, ARG\_206, 11.97, -1.13, 0, 0.6  
1NAR, LYS\_49, 10.29, -0.21, 0, 0  
2JEO, ASP\_215, 3.8, 0, 0, 0  
3BWT, ASP\_574, 3.57, 0, -0.23, 0  
2XMX, GLU\_151, 4.18, 0.42, -0.36, -0.38  
2EJX, LYS\_58, 10.5, 0, 0, 0  
4AM1, LYS\_40, 10.01, -0.49, 0, 0  
1P4X, TYR\_3, 13.51, 0.97, 0.14, 2.4  
3M66, ASP\_395, 2.96, 0.14, -0.98, 0  
1MIX, TYR\_216, 9.43, 1.39, -0.35, -1.61  
1NRI, ARG\_246, 12.22, -0.28, 0, 0  
2P0Y, ARG\_246, 11.8, -0.7, 0, 0  
1ANU, ASP\_57, 2.53, 0.98, -2.25, 0  
1TJE, HIS\_195, 7.23, 0.73, 0, 0  
3N2T, LYS\_98, 10.22, -0.28, 0, 0  
1F2V, ARG\_40, 11.25, -1.25, 0, 0  
1O5T, LYS\_349, 10.5, 0, 0, 0  
1BN6, GLU\_194, 3.97, 0.21, -0.74, 0  
3P29, LYS\_68, 10.43, -0.07, 0, 0  
3RAZ, ASP\_83, 2.02, 0.91, -2.7, 0  
3L7N, LYS\_41, 10.5, 0, 0, 0  
2ZOM, ASP\_241, 3.5, 0.07, -0.37, 0  
1WOU, LYS\_98, 10.22, -0.28, 0, 0  
4AE7, LYS\_139, 10.22, -0.28, 0, 0  
3Q1C, ARG\_120, 11.94, -0.56, 0, 0  
2PGE, TYR\_337, 9.9, 1.29, -0.11, -1.29  
2Q98, HIS\_195, 6.43, 0, 0, -0.07  
1FKM, ASP\_340, 2.4, 0.56, -1.96, 0  
4H4J, LYS\_166, 10.43, -0.07, 0, 0  
3B21, ASP\_182, 3.7, 0, -0.1, 0  
2ZTY, GLU\_121, 4.71, 0.21, 0, 0  
3L7N, TYR\_116, 10.93, 0.7, -0.06, 0.29  
1G8PLYS\_239, 10.01, -0.49, 0, 0  
3EVZ, GLU\_86, 7.82, 3.88, -0.56, 0  
1FHL, ASP\_167, 3.21, 0.21, -0.8, 0  
4FZR, GLU\_316, 3.34, 2.44, -1.53, -2.06  
4ECC, ASP\_159, 3.81, 0.07, -0.06, 0  
2WB8, GLU\_535, 5.53, 3.43, -1.33, -1.07  
3UAH, ARG\_455, 12.64, -0.94, 0, 1.08  
3M70, LYS\_30, 10.5, 0, 0, 0  
2OJQ, ARG\_446, 11.66, -0.84, 0, 0  
1XDZ, LYS\_47, 10.29, -0.21, 0, 0  
1R3F, CYS\_58, 9.71, -1.26, 0, 1.97  
4GA2, TYR\_11, 10.07, 0.07, 0, 0  
3HXK, ASP\_269, 3.29, 0.56, -1.07, 0  
1QYI, GLU\_45, 4.57, 0.07, 0, 0  
3ELI, GLU\_130, 4.99, 0.49, 0, 0  
1XTZ, CYS\_75, 11.16, 0, 0, 2.16  
2GEN, ASP\_24, 3.04, 0.07, -0.83, 0  
3DSH, ASP\_442, 3.19, 0.42, -1.03, 0  
2PGX, CYS\_111, 10.08, 0, 1, 0.08  
2FPN, GLU\_46, 4.5, 0, 0, 0  
1NKD, ARG\_16, 12.01, -0.49, 0, 0  
1SI7, ASP\_5, 3.75, 0.07, -0.12, 0  
2FZP, GLU\_263, 4.5, 0, 0, 0  
3ADO, GLU\_246, 4.61, 0.14, -0.03, 0  
1V6T, ARG\_206, 12.36, -0.14, 0, 0  
2WZ9, CYS\_46, 1.66, -5.56, -2.0, 2.22  
3IL3, GLU\_47, 4.5, 0, 0, 0  
3E7P, LYS\_212, 10.5, 0, 0, 0  
3MIX, ASP\_676, 2.91, 0.49, -1.38, 0  
3CX5, GLU\_76, 4.64, 0.14, 0, 0  
2BQQ, ASP\_117, 3.78, 0.07, -0.09, 0  
4ECC, HIS\_92, 8.13, 1.77, 0, -0.14  
2P52, HIS\_190, 0.52, 0, -2.23, -3.75  
3M7G, ARG\_206, 11.8, -0.7, 0, 0  
1YR6, ARG\_179, 12.22, -0.28, 0, 0  
3EVP, GLU\_192, 4.57, 0.07, 0, 0  
4FH3, GLU\_128, 3.54, 0.21, -1.16, 0  
1O5J, TYR\_92, 10.07, 0.07, 0, 0  
4HDE, LYS\_82, 10.5, 0, 0, 0  
3GFP, GLU\_368, 4.28, 0.42, -0.64, 0  
1QQH, TYR\_139, 12.89, 0.07, -0.89, 3.7  
3EJC, GLU\_93, 3.91, 0.21, -0.8, 0  
1UW7, LYS\_36, 10.5, 0, 0, 0  
1VJG, ARG\_53, 12.22, -0.28, 0, 0  
1V8E, GLU\_109, 3.61, 0.21, -1.09, 0  
1MN3, ASP\_444, 3.99, 0.21, -0.02, 0  
3T57, HIS\_180, 8.9, 1.83, 3.46, -2.9  
2V81, HIS\_24, 6.36, 0, 0, -0.14  
3TMO, ARG\_331, 12.5, 0, 0, 0  
3BCY, TYR\_153, 12.16, 2.16, 0, 0  
2FZ4, LYS\_100, 10.5, 0, 0, 0  
2XJ4, LYS\_13, 10.36, -0.14, 0, 0  
2WOZ, ASP\_458, 2.2, 0.77, -2.37, 0  
1YB2, GLU\_213, 4.57, 0.07, 0, 0  
1R15, ARG\_188, 11.94, -0.56, 0, 0  
2BLL, TYR\_436, 10.36, 2.47, -1.47, -0.63  
1EYH, LYS\_149, 10.5, 0, 0, 0  
3GOZ, ASP\_156, 3.7, 0, -0.1, 0  
1UAJ, ASP\_119, 2.27, 0.63, -2.17, 0  
3ASA, CYS\_68, 5.44, -3.63, 0, 0.07  
1YIB, ASP\_191, 3.64, 0, -0.16, 0  
2FPN, LYS\_146, 10.29, -0.21, 0, 0  
3CJW, ASP\_330, 3.13, 0.35, -1.01, 0  
4DBX, LYS\_65, 10.29, -0.21, 0, 0  
3ERF, GLU\_85, 4.57, 0.33, -0.26, 0  
2POL, CYS\_149, 9.63, -0.38, -1.08, 2.08  
2QHT, ARG\_49, 11.87, -0.63, 0, 0  
1NJ4, LYS\_184, 10.5, 0, 0, 0  
3IV4, TYR\_45, 10, 0, 0, 0  
4DIU, GLU\_218, 2.59, 0.49, -2.4, 0  
2XMX, TYR\_181, 10.43, -0.07, 0, 0  
3CE7, GLU\_51, 4.57, 0.07, 0, 0  
3COC, LYS\_312, 10.5, 0, 0, 0  
1SNT, ASP\_169, 1.87, 1.05, -2.97, 0  
2C13, LYS\_195, 10.5, 0, 0, 0  
1SJ8, GLU\_599, 4.06, 0.91, -1.35, 0  
3ULX, CYS\_33, 8.76, -0.28, 0, 0.04  
1AD6, ARG\_500, 12.29, -0.21, 0, 0  
1R3F, ARG\_307, 12.15, -0.35, 0, 0  
1GPP, GLU\_156, 4.08, 0.28, -0.7, 0  
1L3K, HIS\_120, 6.22, 0, 0, -0.28  
1DUP, ARG\_13, 11.66, -0.84, 0, 0  
2QK1, HIS\_465, 12.76, 4.13, 5.27, -3.14  
3BQW, LYS\_168, 9.94, -0.56, 0, 0  
3GE9, TYR\_44, 10, 0, 0, 0  
1FQI, ARG\_382, 12.15, -0.35, 0, 0  
3T57, GLU\_294, 3.93, 0.07, -0.64, 0  
3PBH, HIS\_190, 11.12, 1.88, 3.22, -0.49  
3LJN, GLU\_183, 4.5, 0, 0, 0  
2Q34, HIS\_51, 6.43, 0, 0, -0.07  
2BDV, ARG\_47, 11.66, -0.84, 0, 0  
2X4J, ASP\_49, 2.25, 0.42, -1.97, 0  
3JZN, LYS\_335, 10.36, -0.14, 0, 0  
1J8B, GLU\_63, 4.64, 0.14, 0, 0  
2Q12, ARG\_46, 12.5, 0, 0, 0  
1IDK, GLU\_95, 4.47, 0.07, -0.1, 0  
1QYI, HIS\_41, 7.32, 0.96, 0, -0.14  
3A0X, GLU\_697, 4.64, 0.14, 0, 0  
2C13, GLU\_263, 2.28, 0.56, -2.77, 0  
3L7N, TYR\_101, 10.72, 0.72, 0, 0  
2Q99, LYS\_264, 10.5, 0, 0, 0  
1G8P, CYS\_153, 10.83, 0, 0, 1.83  
1NJ4, TYR\_20, 9.38, 0.25, -0.87, 0  
1DOV, LYS\_155, 10.43, -0.07, 0, 0  
3HVW, TYR\_216, 10, 0, 0, 0  
3G53, LYS\_197, 10.5, 0, 0, 0  
3QAV, ASP\_198, 3.94, 0.14, 0, 0  
1PV5, TYR\_111, 12.24, 0.19, -0.08, 2.12  
3V55, ASP\_701, 3.09, 0.21, -0.91, 0  
1LZL, LYS\_219, 9.59, -0.91, 0, 0  
1NRI, GLU\_38, 4.16, 0.21, -0.55, 0  
2B6P, ARG\_241, 12.43, -0.07, 0, 0  
1XDZ, GLU\_178, 4.5, 0, 0, 0  
2D0A, TYR\_4, 13.26, 0.14, 0.72, 2.4  
1ZCU, HIS\_150, 6.8, 0.3, 0, 0  
3TIR, ARG\_86, 12.5, 0, 0, 0  
1GQE, ARG\_343, 11.73, -0.77, 0, 0  
1R29, ARG\_67, 11.94, -0.56, 0, 0  
1PZC, GLU\_1, 4.5, 0, 0, 0  
1XTZ, TYR\_245, 13.85, 0.85, 0, 3  
1XDZ, HIS\_54, 1.01, 0.09, -1.63, -3.95  
2OKT, ASP\_201, 2.61, 0.42, -1.61, 0  
4DBX, HIS\_254, 8.03, 1.66, 2.09, -2.22

2PLQ, TYR\_67, 13.19, 1.18, -0.87, 2.89  
 4H86, CYS\_120, 9.86, -0.97, 1.29, 0.53  
 3M9A, LYS\_95, 10.29, -0.21, 0, 0  
 1XWM, GLU\_56, 4.92, 0.42, 0, 0  
 3A2Z, GLU\_125, 4.71, 0.21, 0, 0  
 3EVZ, ASP\_113, 2.66, 0.77, -1.91, 0  
 2Q5X, HIS\_862, 6.43, 0, 0, -0.07  
 1YTD, ARG\_141, 12.5, 0, 0, 0  
 1EQ6, GLU\_102, 4.48, 0.07, -0.09, 0  
 2B78, LYS\_312, 10.36, -0.14, 0, 0  
 1DOV, CYS\_228, 8.59, -0.62, 0, 0.21  
 2Q99, CYS\_364, 9.72, 0, 0, 0.72  
 3PAC, GLU\_175, 4.28, 0.21, -0.43, 0  
 3R87, LYS\_59, 10.5, 0, 0, 0  
 3BQW, ASP\_268, 2.85, 0.84, -1.8, 0  
 1WLJ, LYS\_304, 10.5, 0, 0, 0  
 1SQW, HIS\_165, 7.09, 1.6, 1.79, -2.8  
 3M70, ASP\_84, 3.08, 0.49, -1.21, 0  
 3EVP, HIS\_239, 6.43, 0, 0, -0.07  
 1WNH, GLU\_60, 1.8, 1.41, -4.1, 0  
 3M66, ARG\_318, 11.87, -0.63, 0, 0  
 1TLV, TYR\_201, 7.97, 0.9, -0.53, -2.4  
 1BK8, LYS\_18, 10.5, 0, 0, 0  
 1YB2, HIS\_33, 6.43, 0, 0, -0.07  
 1YR6, LYS\_29, 10.36, -0.14, 0, 0  
 3P2F, LYS\_41, 10.22, -0.28, 0, 0  
 3K8U, LYS\_60, 10.29, -0.21, 0, 0  
 2Z61, LYS\_4, 10.5, 0, 0, 0  
 3GE9, GLU\_3, 4.5, 0, 0, 0  
 2E3S, ASP\_444, 3.7, 0.21, -0.31, 0  
 3V1Q, LYS\_576, 10.43, -0.07, 0, 0  
 3IVF, TYR\_377, 11.8, 0, 0, 1.8  
 2PIM, ARG\_9, 11.66, -0.84, 0, 0  
 3CE7, ARG\_53, 12.29, -0.21, 0, 0  
 4D8L, GLU\_276, 3.69, 0.21, -1.02, 0  
 2BAA, ASP\_51, 3.58, 0.07, -0.29, 0  
 1PDB, TYR\_177, 12.94, 0.07, 0.56, 2.31  
 1X7F, GLU\_284, 3.84, 0.14, -0.8, 0  
 1FKM, ASP\_408, 1.86, 0.77, -2.71, 0  
 3RE9, GLU\_191, 4.64, 0.14, 0, 0  
 2YT4, TYR\_553, 11.97, 1.97, 0, 0  
 1YOK, ARG\_29, 11.8, -0.7, 0, 0  
 2AD1, HIS\_293, 6.5, 0, 0, 0  
 2PP6, GLU\_35, 3.75, 0.35, -1.09, 0  
 3CX2, ASP\_214, 2.28, 0.49, -2.01, 0  
 3TRE, ASP\_66, 3.45, 0.42, -0.77, 0  
 1DCF, LYS\_75, 9.66, -0.84, 0, 0  
 1ZKZ, ARG\_14, 11.73, -0.77, 0, 0  
 2AXO, HIS\_79, 1.61, 0.01, 0, -4.9  
 2H8O, LYS\_286, 10.5, 0, 0, 0  
 1R53, GLU\_206, 4.68, 0.21, -0.03, 0  
 1WP5, LYS\_127, 10.5, 0, 0, 0  
 1GVP, LYS\_24, 10.5, 0, 0, 0  
 1AT0, ARG\_377, 11.94, -0.56, 0, 0  
 3UX2, ARG\_48, 11.8, -0.7, 0, 0  
 2CIU, GLU\_210, 4.71, 0.21, 0, 0  
 3ASA, ASP\_211, 4.08, 0.42, -0.14, 0  
 2EJX, GLU\_424, 1.13, 0.21, -0.58, 0  
 3Q1C, GLU\_71, 3.46, 0.63, -1.67, 0  
 2BAA, GLU\_67, 2.71, 2.25, -0.8, -3.24  
 2AZL, LYS\_261, 10.01, -0.49, 0, 0  
 2V5B, LYS\_198, 10.22, -0.28, 0, 0  
 1NFN, GLU\_131, 3.81, 0.07, -0.76, 0  
 3LMF, ASP\_8, 3.87, 0.07, 0, 0  
 2CI3, HIS\_254, 5.53, 1.82, 0, -2.79  
 1YB2, TYR\_15, 10.07, 0.32, -0.93, 0.68  
 2D2S, LYS\_669, 10.36, -0.14, 0, 0  
 4ETX, ASP\_209, 2.38, 0.42, -1.83, 0  
 1T9S, ASP\_154, 3.77, 0, -0.03, 0  
 3HQX, ASP\_97, 3.94, 0.14, 0, 0  
 3T8R, ASP\_128, 2.98, 0.14, -0.96, 0  
 3V7S, GLU\_163, 4.5, 0, 0, 0  
 1YDL, LYS\_31, 10.43, -0.07, 0, 0  
 2FB6, GLU\_63, 4.64, 0.14, 0, 0  
 2R2Y, CYS\_121, 9.62, -0.12, 0, 0.74  
 2YYO, LYS\_127, 9.87, -0.63, 0, 0  
 1CBY, HIS\_227, 6.5, 0, 0, 0  
 3ETV, GLU\_266, 3.67, 0.5, -0.8, -0.53  
 1YLN, GLU\_224, 4.5, 0, 0, 0  
 1O0X, LYS\_40, 10.43, -0.07, 0, 0  
 3BQW, ASP\_198, 4.02, 0.35, -0.13, 0  
 1WOU, ASP\_83, 3.77, 0.14, -0.17, 0  
 2FPN, ASP\_136, 3.44, 0.35, -0.71, 0  
 2JHY, GLU\_87, 4.57, 0.07, 0, 0  
 3MTT, GLU\_507, 3.55, 0.14, -1.09, 0  
 1BN6, TYR\_98, 11.36, 0.07, 0, 1.29  
 2AZP, HIS\_124, 6.29, 0, -0.21  
 3IAT, GLU\_64, 4.43, 0.07, -0.14, 0  
 3ASA, LYS\_21, 10.5, 0, 0, 0  
 3ZTA, GLU\_139, 4.02, 0.21, -0.69, 0  
 2FZP, GLU\_303, 3.72, 0.14, -0.92, 0  
 3CQ1, ARG\_4, 12.5, 0, 0, 0  
 1N81, ASP\_69, 2.43, 0.77, -2.14, 0  
 1TXJ, LYS\_170, 10.5, 0, 0, 0  
 1PBV, GLU\_104, 4.1, 0.07, -0.47, 0  
 1SIG, LYS\_257, 10.22, -0.28, 0, 0  
 1TLV, GLU\_271, 4.78, 0.28, 0, 0  
 3IL3, HIS\_178, 4.32, 0.68, 0, -2.86  
 2B02, HIS\_401, 6.15, 0, 0, -0.35  
 3ONH, GLU\_516, 3.52, 0.42, -1.4, 0  
 2FD5, ARG\_173, 12.01, -0.49, 0, 0  
 1XDZ, HIS\_199, 6.22, 0, 0, -0.28  
 1XFK, HIS\_67, 6.43, 0, 0, -0.07  
 3FXH, GLU\_66, 4.85, 0.35, 0, 0  
 1SBX, ARG\_152, 12.36, -0.14, 0, 0  
 2FBI, LYS\_137, 10.5, 0, 0, 0  
 4EKU, ARG\_68, 11.87, -0.63, 0, 0  
 2GAU, TYR\_90, 11.93, 0.14, 0, 1.79  
 4EKU, HIS\_192, 6.5, 0, 0, 0  
 3DZ1, ASP\_98, 3.8, 0.14, -0.14, 0  
 1DTO, LYS\_52, 10.5, 0, 0, 0  
 3IDW, ASP\_4, 2.93, 0.35, -1.21, 0  
 2CN1, GLU\_211, 4.5, 0, 0, 0  
 2E0T, LYS\_147, 10.36, -0.14, 0, 0  
 2B02, LYS\_419, 10.08, -0.42, 0, 0  
 3GV0, GLU\_231, 4.5, 0, 0, 0  
 3L7N, CYS\_91, 4.92, -7.34, 0.14, 3.13  
 3V4G, GLU\_36, 4.78, 0.28, 0, 0  
 1TR9, HIS\_37, 7.23, 0.8, 0, -0.07  
 3IL3, ARG\_217, 12.01, -0.49, 0, 0  
 1UCH, HIS\_102, 0.72, 0.54, 0, -6.31  
 1FHL, ASP\_239, 3.8, 0, 0, 0  
 3ZTA, LYS\_15, 10.29, -0.21, 0, 0  
 1OIS, ASP\_269, 3.44, 0.21, -0.57, 0  
 1X04, ARG\_100, 12.01, -0.49, 0, 0  
 2FM9, TYR\_123, 12.28, 2.28, 0, 0  
 1JSX, ARG\_123, 12.15, -0.35, 0, 0  
 4GA2, GLU\_119, 4.35, 0.14, -0.29, 0  
 1R9W, LYS\_219, 10.5, 0, 0, 0  
 3O16, ARG\_119, 13.11, -1.65, 0, 2.26  
 3LH5, LYS\_577, 10.5, 0, 0, 0  
 3JV1, ASP\_180, 3.71, 0, -0.09, 0  
 1A8Q, ASP\_141, 3.87, 0.14, -0.07, 0  
 1SQW, GLU\_104, 4.57, 0.07, 0, 0  
 1WYC, ARG\_187, 12.01, -0.49, 0, 0  
 3QAV, LYS\_134, 10.36, -0.14, 0, 0  
 4FH3, HIS\_224, 2.91, 0.18, 0, -3.77  
 1BN6, GLU\_262, 3.37, 0.42, -1.55, 0  
 2H2W, HIS\_170, 2.34, 0.97, 0, -5.12  
 3HVW, ARG\_227, 11.87, -0.63, 0, 0  
 3M7G, TYR\_268, 10.67, 0.21, -1.01, 1.46  
 1E5S, ARG\_31, 11.73, -0.77, 0, 0  
 3HVW, ASP\_228, 3.26, 0.35, -0.89, 0  
 4EKU, ASP\_139, 3.44, 0.28, -0.64, 0  
 3AUF, ARG\_176, 12.08, -0.42, 0, 0  
 2OOK, CYS\_113, 9.91, 0, 0, 0.91  
 1QYI, TYR\_207, 10.83, 0.91, 0, -0.08  
 1J33, HIS\_276, 5.71, 1.61, 1.54, -3.94  
 2JKF, GLU\_77, 3.73, 1.87, -2.63, 0  
 4E6S, ARG\_31, 12.15, -0.35, 0, 0  
 3OAT, HIS\_50, 6.6, 0.1, 0, 0  
 1UAJ, ARG\_39, 12.29, -0.21, 0, 0  
 2B0J, LYS\_335, 10.36, -0.14, 0, 0  
 1PBV, GLU\_94, 4.03, 0.14, -0.61, 0  
 1XWM, ARG\_106, 11.94, -0.56, 0, 0  
 4FH3, TYR\_370, 9.69, 0, -0.31, 0  
 3GMS, ARG\_87, 13.48, -0.8, 0, 1.78  
 1XDZ, ARG\_20, 12.01, -0.49, 0, 0  
 1L3K, ARG\_140, 12.5, 0, 0, 0  
 1WNH, ASP\_121, 3.27, 0.28, -0.81, 0  
 1WP5, CYS\_65, 10.55, 0, 1.55  
 2DVK, ARG\_179, 11.94, -0.56, 0, 0  
 2GQV, CYS\_47, 9.07, 0, 0, 0.07  
 3C2E, LYS\_94, 10.36, -0.14, 0, 0  
 2CN1, TYR\_82, 11.37, 0.31, -0.16, 1.23  
 1DOV, LYS\_193, 10.43, -0.07, 0, 0  
 2XHC, LYS\_188, 10.5, 0, 0, 0  
 1DOV, LYS\_199, 10.5, 0, 0, 0  
 2H8S, CYS\_292, 6.86, -3.6, 0, 1.46  
 4D8L, GLU\_142, 4.0, 0.14, -0.64, 0  
 3HVM, LYS\_2, 10.22, -0.28, 0, 0  
 2P52, ARG\_193, 11.45, -1.39, 0.34  
 2VAN, ASP\_170, 2.45, 0.63, -1.98, 0  
 1L3K, ARG\_122, 12.08, -0.42, 0, 0  
 3I82, CYS\_201, 9.99, -0.31, 0, 1.3  
 2R4Q, ARG\_245, 12.15, -0.35, 0, 0  
 1EYH, LYS\_69, 10.5, 0, 0, 0  
 2GKG, LYS\_71, 10.5, 0, 0, 0  
 1LPL, TYR\_200, 8.25, 0.14, -1.89, 0  
 4EZB, ARG\_143, 11.73, -0.77, 0, 0  
 2CXC, TYR\_74, 10.24, 0, 0.24, 0  
 1KN3, CYS\_168, 9.06, -2.11, 0, 2.17  
 3BQE, GLU\_301, 3.34, 0.69, -1.85, 0  
 3BZT, TYR\_316, 10, 0, 0, 0  
 1PDB, LYS\_178, 10.36, -0.14, 0, 0  
 2DFL, ASP\_301, 3.55, 0.21, -0.46, 0  
 1SIG, ASP\_213, 3.51, 0.07, -0.36, 0  
 2RFA, TYR\_115, 10, 0, 0, 0  
 3KEY, GLU\_341, 4.57, 0.07, 0, 0  
 1W7B, LYS\_249, 10.5, 0, 0, 0  
 1T3J, ASP\_703, 3.85, 0.07, -0.02, 0  
 3PP8, GLU\_153, 4.5, 0, 0, 0  
 4HDE, LYS\_170, 10.22, -0.28, 0, 0  
 1ZBS, HIS\_247, 6.43, 0, 0, -0.07  
 2Q5X, LYS\_753, 10.5, 0, 0, 0  
 2OEW, CYS\_40, 8.84, -0.3, 0, 0.14  
 1XEU, GLU\_101, 4.06, 0.42, -0.86, 0  
 3LJC, GLU\_185, 4.34, 0.21, -0.37, 0  
 2PWQ, LYS\_130, 10.08, -0.42, 0, 0  
 1EVB, ARG\_35, 12.29, -0.21, 0, 0  
 4E8B, HIS\_172, 6.29, 0, 0, -0.21  
 2HRZ, ARG\_27, 12.01, -0.49, 0, 0  
 2QOP, HIS\_95, 5.05, 0, 0, -1.45  
 1KN3, ASP\_59, 3.33, 0.63, -1.1, 0  
 2FL7, ARG\_92, 13.55, -1.35, 0, 2.4  
 3COC, ASP\_340, 2.76, 0.7, -1.74, 0  
 2XMZ, LYS\_202, 10.43, -0.07, 0, 0  
 3H04, GLU\_58, 4.24, 0, -0.26, 0  
 1L3K, LYS\_113, 10.5, 0, 0, 0  
 2QVT, HIS\_115, 6.5, 0, 0, 0  
 2DG7, ARG\_36, 12.08, -0.42, 0, 0  
 2FG1, LYS\_33, 10.43, -0.07, 0, 0  
 1ZKZ, GLU\_18, 4.57, 0.07, 0, 0  
 3UAH, ASP\_203, 4.17, 0.21, 0.16, 0  
 3ETV, LYS\_298, 10.43, -0.07, 0, 0  
 2QVT, HIS\_110, 6.43, 0, 0, -0.07  
 3M3P, GLU\_243, 4.24, 0.07, -0.33, 0  
 2V81, ARG\_201, 12.29, -0.21, 0, 0  
 1X7F, HIS\_213, 2.73, 0, -3.77  
 1NRI, GLU\_180, 4.5, 0, 0, 0  
 3BQW, ASP\_53, 3.28, 0.28, -0.8, 0  
 2A1V, GLU\_124, 3.18, 0.91, -2.23, 0  
 4DIU, ASP\_227, 2.35, 0.42, -1.88, 0  
 3MIX, LYS\_520, 10.36, -0.14, 0, 0  
 3C5V, GLU\_51, 3.22, 0.42, -1.7, 0  
 2RIK, GLU\_228, 4.44, 0.28, -0.34, 0  
 3Q1C, ARG\_69, 12.5, 0, 0, 0  
 2WB3, LYS\_272, 10.5, 0, 0, 0  
 3B7X, GLU\_66, 2.9, 0.91, -2.51, 0  
 1OIS, ARG\_263, 11.8, -0.7, 0, 0  
 3UX2, CYS\_107, 9, 0, 0, 0  
 2WB8, LYS\_455, 10.15, -0.35, 0, 0  
 3U2R, HIS\_124, 7.19, 0.76, 0, -0.07  
 2W0G, GLU\_261, 3.88, 0.07, -0.69, 0  
 3EJG, ASP\_10, 3.87, 0.07, 0, 0  
 1PV5, GLU\_180, 4.5, 0, 0, 0  
 2E3S, HIS\_430, 5.26, 0.8, 0, -2.04  
 1L2F, GLU\_78, 4.64, 0.14, 0, 0  
 2B0J, GLU\_102, 4.12, 0.07, -0.45, 0  
 2PGE, LYS\_17, 10.43, -0.07, 0, 0  
 1V43, TYR\_78, 10.8, 0, 0, 0.8  
 2RIK, TYR\_235, 11.5, 0, 0, 1.5  
 1UW7, LYS\_58, 10.01, -0.49, 0, 0  
 3RJK, HIS\_127, 1.61, 0, -2.4, -2.49  
 3JSN, LYS\_298, 10.5, 0, 0, 0  
 3DHN, TYR\_145, 9.86, 0.45, -0.36, -0.22  
 1ES9, GLU\_90, 2.52, 0.42, -2.4, 0  
 3LOR, TYR\_114, 9.67, 1.32, -1.65, 0  
 3L0D, ARG\_132, 11.59, -0.91, 0, 0  
 2D7U, ASP\_165, 4.03, -0.15, 0, 0  
 2G3A, TYR\_113, 13.52, 0.52, 0.6, 2.4  
 1MML, HIS\_77, 6.74, 0.24, 0, 0  
 2Q34, ASP\_224, 3.73, 0, -0.07, 0  
 2VGM, GLU\_226, 5.56, 0.77, -0.92, 1.23  
 1O5T, ARG\_134, 11.05, -1.45, 0, 0  
 3GW3, CYS\_65, 10.18, -0.46, 0, 1.64  
 2DVK, ARG\_79, 12.08, -0.42, 0, 0  
 3BB7, ASP\_68, 3.62, 0, -0.18, 0  
 2AH5, LYS\_164, 10.5, 0, 0, 0  
 2JKF, ASP\_145, 3.13, 0.49, -1.16, 0  
 3NR5, ASP\_117, 3.37, 0.49, -0.93, 0  
 3COU, ARG\_38, 12.08, -0.42, 0, 0  
 1UAJ, LYS\_75, 10.43, -0.07, 0, 0  
 2D0A, ARG\_47, 12.14, -0.36, 0, 0  
 3G9G, GLU\_65, 3.84, 0.14, -0.8, 0  
 4EVF, ASP\_241, 3.29, 0.21, 0, -0.72  
 1U53, LYS\_178, 10.29, -0.21, 0, 0  
 2W2S, GLU\_147, 4.5, 0, 0, 0  
 2V81, LYS\_139, 10.5, 0, 0, 0  
 1WP5, TYR\_25, 10, 0, 0, 0  
 2BAA, ASP\_77, 3.35, 0.35, -0.8, 0  
 2R0S, ASP\_218, 2.29, 0.63, -2.15, 0  
 2X5Y, HIS\_828, 4.69, 0, 0, -1.81  
 3EVN, ARG\_317, 11.87, -0.63, 0, 0  
 3GV0, GLU\_307, 3.84, 0.14, -0.8, 0  
 3JV1, ARG\_58, 12.5, 0, 0, 0



3I4T,ARG\_186,11.73,-0.77,0,0  
2A0J,GLU\_85,4.71,0.21,0,0  
3T5B,ASP\_388,3.67,0,-0.13,0  
2OBS,GLU\_80,4.92,0.42,0,0  
1UCH,ARG\_47,12.01,-0.49,0,0  
1UOH,LYS\_153,10.5,0,0,0  
2P1W,ARG\_237,12.08,-0.42,0,0  
3ETU,GLU\_227,4.57,0.07,0,0  
1O1T,ASP\_103,3.9,0.21,-0.11,0  
1QYI,LYS\_144,10.15,-0.35,0,0  
1QZN,ARG\_77,12.36,-0.14,0,0  
2OSA,ASP\_269,2,0.56,-2.35,0  
2V5B,ASP\_86,3.8,0,0,0  
1ZBS,GLU\_250,3.51,0.49,-1.48,0  
3U2R,ARG\_53,11.87,-0.63,0,0  
3BZT,GLU\_299,4.64,0.14,0,0  
1G8P,ARG\_326,11.92,-2.54,0,1.96  
1PSW,ARG\_77,11.87,-0.63,0,0  
1CHD,ARG\_219,12.15,-0.35,0,0  
1YDL,CYS\_12,8.26,-0.74,0,0  
2GZQ,GLU\_23,3.77,0.07,-0.8,0  
1O59,CYS\_143,10.41,-0.02,0,1.43  
4AM1,LYS\_146,10.29,-0.21,0,0  
3F6F,ARG\_67,12.19,-2.53,0,2.22  
1S17,ARG\_199,10.15,-2.35,0,0  
1W7B,GLU\_247,4.4,0.7,-0.8,0  
2YX0,LYS\_126,10.29,-0.21,0,0  
2WOZ,ARG\_297,12.5,0,0,0  
1QYI,ASP\_43,3.37,0.28,-0.71,0  
1WYC,HIS\_180,4.96,1.6,2.14,-5.27  
1NAF,GLU\_279,4.65,0.21,-0.06,0  
2R4Q,ARG\_240,14,-0.9,0,2.4  
1E59,CYS\_55,8.88,-0.12,0,0  
2WB8,ASP\_504,3.87,0.07,0,0  
1UX0,LYS\_101,10.15,-0.35,0,0  
2R51,TYR\_78,10.62,0,0,0.62  
3Q1C,ARG\_354,11.59,-0.91,0,0  
2BCF,ARG\_251,12.08,-0.42,0,0  
1J74,ASP\_37,3.21,0.21,-0.8,0  
3M70,GLU\_183,3.84,0.14,-0.8,0  
1PZC,TYR\_64,9.73,0.07,-0.34,0  
2XWS,LYS\_92,9.59,-0.91,0,0  
1SQW,TYR\_128,10,0,0,0  
2HRZ,TYR\_112,11.84,0,0,1.84  
1TR9,LYS\_125,10.5,0,0,0  
3UX2,LYS\_113,10.5,0,0,0  
3D9H,HIS\_41,2.99,1.21,0,-4.72  
2Q5X,ARG\_817,12.29,-0.21,0,0  
3CAX,HIS\_179,10.2,3.48,5.86,-5.64  
3D9H,LYS\_184,10.43,-0.07,0,0  
3I0C,LYS\_124,10.43,-0.07,0,0  
3GE9,ASP\_137,3.89,0.14,-0.05,0  
3V46,LYS\_371,10.29,-0.21,0,0  
3I4T,HIS\_238,6.43,0,0,-0.07  
3C6B,LYS\_47,10.5,0,0,0  
3I0C,TYR\_206,10.47,0.47,0,0  
3A0X,GLU\_696,4.5,0.07,-0.07,0  
3LD1,LYS\_52,10.5,0,0,0  
1L2F,ARG\_144,12.36,-0.14,0,0  
3IVF,GLU\_346,4.57,0.07,0,0  
1R2Z,ASP\_199,3.33,0.14,-0.61,0  
3EZ7,GLU\_350,4.19,0.21,-0.52,0  
3RLE,TYR\_198,10,0,0,0  
1Z9L,ASP\_77,3.87,0.07,0,0  
4HDE,LYS\_138,10.22,-0.28,0,0  
2EJX,ARG\_86,11.94,-0.56,0,0  
3JV1,ASP\_151,2.99,0.49,-1.29,0  
2RIK,HIS\_247,6.5,0,0,0  
3HZQ,LYS\_6,10.5,0,0,0  
3H04,GLU\_257,4.47,0.14,-0.17,0  
3EVZ,LYS\_101,9.87,-0.63,0,0  
2GEN,ARG\_76,12.5,0,0,0  
2F19,GLU\_116,4.71,0.21,0,0  
3CBN,ASP\_138,2.92,0.42,-1.3,0  
3CJW,GLU\_297,3.17,0.35,-1.68,0  
3Q6L,ARG\_127,12.37,-2.31,0,2.17  
3A0X,GLU\_664,4.64,0.14,0,0  
1A8Q,ASP\_133,3.86,0.07,-0.01,0  
2RIK,LYS\_202,10.36,-0.14,0,0  
2B78,ARG\_280,11.59,-0.91,0,0  
3ODJ,ASP\_32,3.61,0,-0.19,0  
1PDB,LYS\_108,9.94,-0.56,0,0  
3K8U,ARG\_126,12.5,0,0,0  
1R15,GLU\_285,2.98,1.72,-0.84,-2.4  
1RH5,LYS\_236,10.5,0,0,0  
2CYG,TYR\_329,10,0,0,0  
1Y0K,ARG\_181,11.56,-0.94,0,0  
3RKV,GLU\_295,4.64,0.14,0,0  
2PLQ,LYS\_21,10.29,-0.21,0,0  
3FWU,LYS\_75,10.29,-0.21,0,0  
3ETU,LYS\_222,10.5,0,0,0  
2B61,ARG\_184,13.34,-1.56,0,2.4  
3LJI,ASP\_90,3.87,0.07,0,0  
3ADO,ARG\_185,11.94,-0.56,0,0  
3GA2,ARG\_183,12.43,-0.07,0,0  
3A7L,LYS\_8,10.43,-0.07,0,0  
1ZBS,ASP\_126,2.15,0.63,-2.28,0  
1PBV,GLU\_156,3.82,0.35,-1.03,0  
2Q5X,LYS\_801,10.36,-0.14,0,0  
3F7M,CYS\_177,6.98,-5.35,-0.13,3.45  
1D2K,LYS\_177,10.01,-0.49,0,0  
3OA7,HIS\_562,6.44,0.01,0,-0.07  
4H86,LYS\_156,10.43,-0.07,0,0  
4F85,TYR\_185,13.01,0.87,0,2.15  
3U2A,ARG\_38,12.15,-0.35,0,0  
3FNI,TYR\_133,10.07,0.14,-0.19,0.13  
3BPP,TYR\_36,10,0,0,0  
2WB8,HIS\_778,5.15,0.099,-2.34  
3JRT,TYR\_31,10,0,0,0  
3EVP,GLU\_290,4.5,0,0,0  
4EF5,GLU\_296,4.5,0,0,0  
3F6F,GLU\_75,4.71,0.21,0,0  
1HF8,HIS\_83,3.81,1.6,0.87,-5.16  
3EGN,GLU\_402,3.47,0.14,-1.16,0  
1OGL,LYS\_63,10.36,-0.14,0,0  
1F2Y,TYR\_4,10,0,0,0  
1T95,ASP\_76,3,0.28,-1.08,0  
1QYI,TYR\_305,9.51,0.34,-0.83,0  
3CAX,ASP\_344,3.07,0.42,-1.14,0  
1L2H,ARG\_4,12.36,-0.14,0,0  
2W2S,GLU\_108,4.39,0.42,-0.53,0  
3Q9P,ARG\_96,12.08,-0.42,0,0  
3N0K,HIS\_107,6.22,0,0,-0.28  
1YLN,ARG\_155,12.01,-0.49,0,0  
3G9T,HIS\_233,1.46,0.33,-0.07,-5.3  
3ULX,ARG\_126,12.43,-0.07,0,0  
1SJ8,ARG\_765,12.43,-0.07,0,0  
2P52,GLU\_225,4.5,0,0,0  
3VHJ,ARG\_148,11.94,-0.56,0,0  
1O0X,ARG\_148,11.8,-0.7,0,0  
3SMD,LYS\_80,10.08,-0.42,0,0  
1R2Z,ARG\_141,12.08,-0.42,0,0  
3BPP,LYS\_194,10.22,-0.28,0,0  
1VJG,LYS\_115,9.94,-0.56,0,0  
3P28,LYS\_92,10.36,-0.14,0,0  
3B7H,TYR\_73,13.34,0.35,0.59,2.4  
3UX2,LYS\_103,10.43,-0.07,0,0  
1YG2,LYS\_46,10.5,0,0,0  
3KVO,GLU\_72,3.93,0.21,-0.78,0  
1O6D,GLU\_74,4.05,0.35,-0.8,0  
1YTQ,LYS\_100,10.5,0,0,0  
1J33,ARG\_116,11.73,-0.77,0,0  
2HXB,LYS\_139,10.29,-0.21,0,0  
3GFP,ASP\_375,3.95,0.21,-0.06,0  
3R2E,ASP\_46,2.98,0.21,-1.03,0  
3C38,ARG\_171,11.17,-1.33,0,0  
3HUE,ARG\_316,12.29,-0.21,0,0  
2RH3,ARG\_133,12.01,-0.49,0,0  
3IV4,TYR\_52,10.75,0,-0.15,0.91  
1TJE,HIS\_13,6.43,0,0,-0.07  
2JKF,GLU\_113,4.71,0.21,0,0  
3UC9,ARG\_80,11.03,-1.47,0,0  
3UC9,TYR\_5,10,0,0,0  
1JT9,CYS\_118,9.14,-0.35,0,0.49  
3GS3,CYS\_34,9.62,0,0,0.62  
1TR9,ASP\_38,2.17,0.49,-2.12,0  
3A4C,ARG\_465,11.87,-0.63,0,0  
2D7U,ASP\_90,3.71,0.14,-0.22,0  
1O9G,ARG\_132,11.8,-0.7,0,0  
3IPZ,GLU\_82,4.64,0.14,0,0  
4FZT,ARG\_242,12.08,-0.42,0,0  
3LH5,TYR\_755,9.77,0,-0.23,0  
1Q5Z,ASP\_647,1.23,0.63,-3.2,0  
2XWS,CYS\_59,8.88,-0.13,0,0  
2GZR,TYR\_67,11.76,1.31,0.05,0.4  
1JYH,ASP\_105,2.96,0.35,-1.19,0  
3F7M,TYR\_299,9.96,0.07,-0.11,0  
2BV9,ARG\_52,11.87,-0.63,0,0  
3LJI,GLU\_293,4.85,0.35,0,0  
3P2F,ARG\_139,11.73,-0.77,0,0  
1TD6,ASP\_38,1.11,0.84,-3.53,0  
2PLQ,TYR\_284,10,0,0,0  
1SNT,ARG\_243,12.07,-4.93,0,4.5  
2OGQ,LYS\_480,10.08,-0.42,0,0  
3CAX,ASP\_296,3.11,0.07,-0.76,0  
3C38,HIS\_154,4.6,0.28,0,-2.18  
1YB2,LYS\_17,10.43,-0.07,0,0  
1YTQ,ARG\_89,12.08,-0.42,0,0  
3BA1,ARG\_154,12.29,-0.21,0,0  
3HKX,HIS\_20,7.04,0.82,0,-0.28  
3LPZ,GLU\_141,4.64,0.14,0,0  
3C6B,TYR\_39,11.96,0.37,-0.23,1.81  
3CAX,GLU\_465,4.64,0.14,0,0  
1GXN,HIS\_513,2.36,1,0,-5.13  
1T3Y,GLU\_103,4.02,0.21,-0.69,0  
2D59,LYS\_103,10.5,0,0,0  
3RNV,ASP\_370,3.54,0.42,-0.68,0  
1WPA,ASP\_437,3.97,0.35,-0.18,0  
3M16,LYS\_48,10.36,-0.14,0,0  
1PVT,GLU\_172,4.94,0.56,-0.12,0  
2FPN,LYS\_26,10.43,-0.07,0,0  
4FH3,TYR\_324,10,0,0,0  
1Q8B,CYS\_19,8.74,-0.26,0,0  
3GFP,ASP\_467,3.2,0.28,-0.88,0  
3N0K,ASP\_114,3.4,0.07,-0.47,0  
1JSX,GLU\_157,4.5,0,0,0  
3UPD,HIS\_17,6.32,1.16,0.51,-1.86  
3N0K,ASP\_82,3.42,0.42,-0.8,0  
1PDB,TYR\_156,11.26,0.64,0,0.62  
1NKD,HIS\_46,6.54,0.04,0,0  
2AZP,ARG\_132,12.29,-0.21,0,0  
2CWC,ARG\_243,11.31,-1.19,0,0  
3F53,LYS\_45,10.43,-0.07,0,0  
1GQE,GLU\_16,4.38,0.21,-0.33,0  
2R51,HIS\_63,6.74,0.31,0,-0.07  
2E0T,HIS\_138,6.29,0,0,-0.21  
4FH3,ARG\_340,12.29,-0.21,0,0  
3LJI,CYS\_56,9.94,-0.21,0,1.16  
2RFA,GLU\_176,3.35,0.28,-1.43,0  
3EZ7,ASP\_72,3.94,0.14,0,0  
2ZQ5,GLU\_15,3.45,0.28,-1.33,0  
3FNI,LYS\_125,10.5,0,0,0  
1YR6,TYR\_181,9.79,0,-0.21,0  
1RAJ,GLU\_226,4.79,0.35,-0.06,0  
3AU3,HIS\_652,6.36,0,0,-0.14  
3CJW,GLU\_311,4.97,1.65,-3.58,2.4  
2HNG,LYS\_8,10.08,-0.42,0,0  
1YM5,GLU\_40,4.81,0.56,-0.25,0  
2YWJ,ARG\_146,12.15,-0.35,0,0  
1ZBM,GLU\_204,4.57,0.07,0,0  
2E3H,CYS\_242,9.68,0,0,0.68  
3O48,ARG\_108,12.36,-0.14,0,0  
2OBI,GLU\_158,4.12,0.21,-0.59,0  
1WOU,GLU\_20,4.54,0.07,-0.03,0  
1UX0,ARG\_12,12.5,0,0,0  
4E9E,TYR\_540,12.88,1.61,-0.8,2.07  
2Z61,ASP\_153,3.8,0.07,-0.07,0  
2I6I,LYS\_56,10.36,-0.14,0,0  
3I0E,ASP\_410,3.51,0.07,-0.36,0  
3CCY,GLU\_97,3.98,0.28,-0.8,0  
2QRX,ASP\_8,4.08,0.28,0,0  
3OBS,HIS\_102,7.36,1.07,0,-0.21  
3GV0,ARG\_179,11.87,-0.63,0,0  
3F7M,ARG\_222,11.87,-0.63,0,0  
1RWZ,CYS\_202,10.45,-0.17,-0.25,1.86  
3CCY,GLU\_97,3.98,0.28,-0.8,0  
3DSH,GLU\_354,4.57,0.07,0,0  
2VGM,LYS\_82,10.08,-0.42,0,0  
3RFF,HIS\_60,7.19,0.83,0,-0.14  
1X04,ASP\_169,3.97,0.28,-0.11,0  
2IQT,GLU\_247,3.96,0.21,-0.75,0  
1X1E,TYR\_224,10,0,0,0  
1R3D,HIS\_166,6.73,0.3,0,-0.07  
4FZR,ARG\_210,11.81,-0.91,0,0.22  
1WOU,GLU\_50,3.49,0.53,-1.54,0  
3JV1,TYR\_189,12.07,0.07,-0.32,2.32  
1H4U,GLU\_523,4.5,0,0,0  
1V43,GLU\_292,1.11,1.35,-1.9,-2.83  
4HDE,LYS\_31,10.5,0,0,0  
2AHE,ASP\_228,3.66,0.07,-0.21,0  
1X91,LYS\_10,9.87,-0.63,0,0  
2QDJ,GLU\_170,4.35,0.07,-0.22,0  
3GW3,ARG\_179,12.29,-0.21,0,0  
2V5B,ARG\_162,11.66,-0.84,0,0  
2VGY,ASP\_69,1.39,0.98,-3.4,0  
1Y0K,GLU\_113,4.14,0.21,-0.57,0  
1GQE,ARG\_22,11.52,-0.98,0,0  
2CXV,TYR\_95,9.69,0.07,-0.38,0  
1DTO,ASP\_25,3.52,0.14,-0.42,0  
2IRM,TYR\_339,11.32,0.14,0,1.18  
3RLN,LYS\_695,10.5,0,0,0  
2YLF,ASP\_212,4.01,0.21,0,0  
2RH3,HIS\_183,5.31,0.35,0,-1.54  
2CW4,ARG\_114,12.08,-0.42,0,0  
2FBQ,ARG\_127,12.5,0,0,0  
4EKU,GLU\_88,4.46,0.99,-1.03,0  
2GZR,LYS\_262,10.5,0,0,0  
1LTU,ARG\_233,11.87,-0.63,0,0  
4FZR,HIS\_29,7.13,0.7,0,-0.07  
3A2Z,ARG\_64,11.47,-2.46,0,1.43  
2FZP,GLU\_292,4.36,0.66,-0.8,0  
4ANN,CYS\_160,9.87,-0.04,0,0.91  
3GG6,CYS\_100,9.76,0,0,0.76  
2FD5,ASP\_169,3.2,0.42,-1.02,0  
1DOV,CYS\_116,9,0,0,0  
1KN3,LYS\_182,10.5,0,0,0

2OJQ,CYS\_524,8.94,-0.06,0,0  
 3ADO,GLU\_157,0.37,1.24,-3.82,-1.56  
 2HZH,HIS\_163,0.09,0.2,-1.38,-5.23  
 3PZ9,ASP\_154,2.65,0.7,-1.84,0  
 2AZL,LYS\_238,10.15,-0.35,0,0  
 1NIJ,ARG\_69,11.86,-0.64,0,0  
 1MUF,GLU\_329,3.06,0.35,-1.8,0  
 1G8P,GLU\_115,3.73,0.35,-1.12,0  
 3COU,GLU\_169,3.66,0.28,-1.13,0  
 2JEO,LYS\_76,10.29,-0.21,0,0  
 2IF4,HIS\_252,4.65,1.05,0,-2.9  
 1X9G,ASP\_122,3.77,0.07,-0.1,0  
 1XTZ,TYR\_67,10.71,0,-0.5,1.21  
 2CWC,CYS\_64,10.04,-0.04,0,1.08  
 2O4D,TYR\_50,10,0,0,0  
 3ZSL,GLU\_193,4.14,0.35,-0.71,0  
 3IDW,TYR\_22,12.21,0.21,-0.4,2.4  
 2QHT,ASP\_135,4.07,0.56,-0.29,0  
 3T5B,TYR\_274,11.42,1.63,-0.2,-0.01  
 2DFL,TYR\_220,12.33,0.14,-0.14,2.33  
 1ZYL,ARG\_284,10.09,-2.98,0,0.58  
 3TRE,LYS\_97,10.43,-0.07,0,0  
 3COU,HIS\_21,5.06,0.81,0,-2.26  
 1XWM,LYS\_85,10.5,0,0,0  
 1QQE,CYS\_164,12.03,0.11,1.73,1.18  
 3ERF,ASP\_79,1.87,0.42,-2.35,0  
 4EVF,HIS\_92,4.41,0,-2.09  
 1RI6,GLU\_126,4.13,0.28,-0.65,0  
 3M7D,ARG\_102,10.9,-3.76,0,2.17  
 3CRM,ARG\_276,11.87,-0.63,0,0  
 1NRI,ASP\_121,3.97,0.21,-0.04,0  
 1XTZ,LYS\_90,10.22,-0.28,0,0  
 3GMS,TYR\_190,10,0,0,0  
 1GVP,GLU\_30,3.6,0.42,-1.32,0  
 2OGQ,GLU\_575,3.05,0.35,-1.8,0  
 1R29,ARG\_40,12.5,0,0,0  
 3K8J,GLU\_271,4.5,0,0,0  
 3ASA,GLU\_296,4.5,0,0,0  
 2QRX,LYS\_44,10.43,-0.07,0,0  
 1GQE,TYR\_187,8.91,0.8,-0.1,-1.79  
 3K8J,ASP\_259,3.39,0.21,-0.62,0  
 2ROS,ASP\_277,3.94,0.21,-0.07,0  
 4ETX,ASP\_434,3.06,0.35,-1.1,0  
 3ODJ,HIS\_169,4.56,0,0,-1.94  
 1RKA,ASP\_83,2.03,0.49,-2.26,0  
 3RNV,ARG\_445,12.15,-0.35,0,0  
 2ZCO,ASP\_56,2.6,0.56,-1.75,0  
 3EVP,ASP\_179,3.72,0.7,-0.78,0  
 2E3C,LYS\_192,10.29,-0.21,0,0  
 1SI7,ASP\_250,3.43,0.35,-0.72,0  
 4AF2,ASP\_-3,3.9,0.14,-0.04,0  
 3PU6,CYS\_102,7.81,-1.66,0,0.46  
 1SUU,LYS\_734,10.5,0,0,0  
 1JSX,ASP\_146,2.46,0.21,-1.55,0  
 2W1R,ASP\_80,4.08,0.28,0,0  
 2XMZ,GLU\_264,4.78,0.28,0,0  
 1WPA,ASP\_516,2.55,0.42,-1.67,0  
 3NBI,GLU\_199,4.5,0,0,0  
 1J85,GLU\_68,4.5,0,0,0  
 2HP7,ARG\_152,12.15,-0.35,0,0  
 2QKO,GLU\_67,4.5,0,0,0  
 1EDG,LYS\_317,10.29,-0.21,0,0  
 3HO4,GLU\_3,4.5,0,0,0  
 1KN3,ARG\_82,13,-0.7,0,1.2  
 1RI6,ARG\_243,12.5,0,0,0  
 3JZN,ASP\_390,3.07,0.35,-1.08,0  
 1WXQ,HIS\_341,6.36,0,0,-0.14  
 2CXC,LYS\_108,10.36,-0.14,0,0  
 2B0J,GLU\_59,4.4,0.42,-0.52,0  
 3EVN,LYS\_82,10.36,-0.14,0,0  
 3M7D,ARG\_206,12.01,-0.49,0,0  
 3T5B,ASP\_44,2.98,0.35,-1.17,0  
 1LFP,LYS\_145,10.5,0,0,0  
 1O5T,ASP\_382,3.67,0.07,-0.2,0  
 4ECC,LYS\_144,10.43,-0.07,0,0  
 1DCF,GLU\_99,4.57,0.07,0,0  
 3CS1,LYS\_55,10.43,-0.07,0,0  
 1AKO,GLU\_46,3.74,0.28,-1.04,0  
 1WP5,ARG\_19,11.73,-0.77,0,0  
 1PVT,TYR\_13,10.07,0.07,0,0  
 3C6B,TYR\_278,10.66,2.12,-1.46,0  
 2W0G,LYS\_240,10.01,-0.49,0,0  
 1S7K,GLU\_18,3.91,0.56,-1.15,0  
 2H85,GLU\_191,4.5,0,0,0  
 1QQE,GLU\_250,4.14,0.14,-0.5,0  
 2XHC,LYS\_132,10.5,0,0,0  
 3UPD,LYS\_213,10.5,0,0,0  
 1WYC,ARG\_33,12.5,0,0,0  
 3KVO,ASP\_29,3.33,0.35,-0.82,0  
 1NAR,TYR\_116,12.2,1.22,0,0.98  
 4DBX,TYR\_190,10,0,0,0  
 1WP5,GLU\_293,3.96,0.56,-1.1,0  
 3E5T,LYS\_71,10.5,0,0,0  
 3JZ9,ASP\_480,2.22,0.35,-1.93,0  
 3BQE,GLU\_335,4.57,0.07,0,0  
 1YOY,GLU\_16,1.86,0.56,-3.2,0  
 1OGL,LYS\_216,10.08,-0.42,0,0  
 2ILR,HIS\_317,7.23,0.8,0,-0.07  
 3RFY,TYR\_265,10.81,0.76,-0.09,0.15  
 3JRT,LYS\_29,10.08,-0.42,0,0  
 2Q98,HIS\_30,3.84,0.08,0,-2.74  
 3M7G,GLU\_217,2.09,1.53,-1.87,-2.07  
 1MTZ,LYS\_151,10.08,-0.42,0,0  
 3LMF,LYS\_72,10.5,0,0,0  
 2XWS,ASP\_110,2.81,0.35,-1.34,0  
 4DVD,ARG\_179,11.87,-0.63,0,0  
 3BQW,LYS\_26,10.43,-0.07,0,0  
 2I88,ASP\_410,3.25,0.42,-0.97,0  
 3I47,GLU\_255,4.6,0.21,-0.11,0  
 3LH5,LYS\_737,10.43,-0.07,0,0  
 3HVM,LYS\_178,10.29,-0.21,0,0  
 2HRZ,GLU\_297,4.78,0.28,0,0  
 2OEW,LYS\_207,10.36,-0.14,0,0  
 2EDM,ARG\_51,12.36,-0.14,0,0  
 3DTE,ARG\_149,12.08,-0.42,0,0  
 1SUU,GLU\_598,2.55,0.84,-2.79,0  
 1WRU,TYR\_207,9.99,0.36,-1.06,0.7  
 3EVP,TYR\_197,11.07,0,0,1.07  
 2B0J,LYS\_161,10.36,-0.14,0,0  
 3HO4,GLU\_152,4.57,0.07,0,0  
 2X4L,GLU\_247,4.21,0.89,-1.18,0  
 3OIF,LYS\_77,10.5,0,0,0  
 2B0J,GLU\_137,3.98,0.28,-0.8,0  
 1PBV,ASP\_225,2.88,0.56,-1.48,0  
 1MUF,GLU\_135,4.5,0,0,0  
 3RE9,TYR\_124,10.07,0.07,0,0  
 1U7U,GLU\_335,4.53,0.35,-0.32,0  
 1Y0K,TYR\_164,10.95,0.59,-0.7,1.06  
 2E3C,LYS\_311,10.29,-0.21,0,0  
 4ECC,LYS\_138,10.5,0,0,0  
 2G5X,ASP\_77,2.52,0.42,-1.71,0  
 1P1L,GLU\_61,3.91,0.21,-0.8,0  
 1MTZ,GLU\_256,4.49,0.42,-0.43,0  
 1XDZ,ARG\_210,13.47,-1.1,0,2.07  
 3GS9,ASP\_76,3.94,0.14,0,0  
 1L2F,ARG\_160,12.5,0,0,0  
 1SIG,ARG\_374,12.5,0,0,0  
 3BPV,LYS\_106,10.15,-0.35,0,0  
 2GEN,ASP\_91,1.74,0.49,-2.55,0  
 3RHE,LYS\_13,10.5,0,0,0  
 3RFF,ASP\_94,2.95,0.28,-1.13,0  
 1OIS,LYS\_144,9.94,-0.56,0,0  
 2BAA,ASP\_209,1.52,0.98,-3.26,0  
 3GV0,ARG\_187,11.94,-0.56,0,0  
 3ELI,GLU\_104,4.79,0.42,-0.13,0  
 1SI7,GLU\_145,3.32,0.42,-1.6,0  
 1ZHV,HIS\_135,6.51,0.01,0,0  
 1YW5,GLU\_98,3.12,0.28,-1.66,0  
 3NR5,HIS\_24,7.54,1.18,0,-0.14  
 3QKY,ARG\_145,12.08,-0.42,0,0  
 3FHF,GLU\_192,4.79,0.96,-1.18,0.52  
 1SBX,GLU\_159,4.57,0.07,0,0  
 3GFP,ASP\_470,3.74,0,-0.06,0  
 1ZBS,TYR\_66,8.16,1.67,-1.35,-2.16  
 2ZCO,HIS\_207,6.43,0,0,-0.07  
 1PZC,ASP\_29,2.37,0.7,-2.12,0  
 3LJC,GLU\_243,4.71,0.21,0,0  
 1ZYL,ARG\_197,10.32,-2.18,0,0  
 3CAX,LYS\_239,10.15,-0.35,0,0  
 1GPP,ARG\_172,10.92,-1.58,0,0  
 1SUU,GLU\_732,4.35,0.21,-0.36,0  
 2IQT,ARG\_261,12.18,-0.32,0,0  
 2O8I,LYS\_152,10.5,0,0,0  
 2QEV,ARG\_17,12.01,-0.49,0,0  
 1IDK,LYS\_47,9.94,-0.56,0,0  
 3IVF,TYR\_216,9.63,1.48,-0.28,-1.57  
 3A2Z,GLU\_92,4.64,0.21,-0.07,0  
 4ESS,ASP\_81,4.01,0.21,0,0  
 3RFY,ASP\_300,3.72,0.14,-0.22,0  
 3V75,ARG\_144,11.94,-0.56,0,0  
 3RFY,LYS\_116,10.5,0,0,0  
 2W1R,LYS\_118,10.29,-0.21,0,0  
 1P6F,GLU\_117,3.75,0.35,-1.1,0  
 1DZF,GLU\_81,4.96,1.26,-0.8,0  
 3K1H,LYS\_131,9.94,-0.56,0,0  
 4FLE,GLU\_47,4.78,0.28,0,0  
 1XTD,ASP\_147,3.79,0.35,-0.36,0  
 4F85,GLU\_239,2.3,0.38,-1.05,-1.53  
 1FQJ,GLU\_348,4.7,0.35,-0.15,0  
 3P51,ARG\_52,13.06,-3.19,0,3.75  
 1IAP,GLU\_212,4.5,0,0,0  
 1XDZ,GLU\_26,3.78,0.28,-1,0  
 2FL7,ARG\_169,12.15,-0.35,0,0  
 3TRE,GLU\_80,4.64,0.14,0,0  
 1U3Y,LYS\_343,10.43,-0.07,0,0  
 1O59,LYS\_168,9.87,-0.63,0,0  
 2BCF,ARG\_109,11.73,-0.77,0,0  
 3C38,ARG\_95,11.66,-0.84,0,0  
 3UPD,GLU\_309,4.5,0,0,0  
 1P2F,TYR\_204,11.71,0.28,-0.94,2.37  
 2FM9,LYS\_118,10.43,-0.07,0,0  
 3GEC,ARG\_522,12.36,-0.14,0,0  
 1GPP,ARG\_33,12.36,-0.14,0,0  
 3UAH,TYR\_255,7.45,0.65,-0.8,-2.4  
 1WP5,LYS\_220,9.38,-1.12,0,0  
 3IOC,LYS\_82,9.94,-0.56,0,0  
 1GXN,TYR\_526,11.21,0.35,-0.78,1.63  
 3EOD,ARG\_99,12.29,-0.21,0,0  
 1RI5,LYS\_195,10.29,-0.21,0,0  
 2YWJ,LYS\_174,10.29,-0.21,0,0  
 3C0C,GLU\_318,3.86,0.21,-0.84,0  
 3UV9,ASP\_386,3.14,0.56,-1.22,0  
 1PVT,GLU\_55,4.03,0.42,-0.88,0  
 1RWZ,ASP\_157,2.39,0.7,-2.1,0  
 3CAX,ASP\_249,3.44,0.42,-0.78,0  
 1UXO,HIS\_164,6.72,1.62,6.68,-4.06  
 3N2T,ASP\_12,3.69,0.07,-0.18,0  
 2X5Y,LYS\_816,10.29,-0.21,0,0  
 2BQQ,LYS\_53,9.73,-0.77,0,0  
 2IXM,TYR\_151,12.96,3.31,-1.6,1.25  
 2B6P,GLU\_134,4.53,3.21,-3.18,0  
 4E8B,GLU\_101,3.84,0.14,-0.8,0  
 2VGM,ASP\_296,4.47,0.7,-0.03,0  
 2B3M,GLU\_70,4.45,0.07,-0.12,0  
 2F4Q,TYR\_225,13.29,1.25,0.68,1.37  
 1JB3,TYR\_44,10.14,0.14,0,0  
 3CQ1,GLU\_94,3.53,0.28,-1.25,0  
 3CQ1,TYR\_34,9.8,0.14,-0.34,0  
 2HZZ,GLU\_178,4.5,0,0,0  
 3ONH,ASP\_496,3.8,0,0,0  
 2P5D,LYS\_114,10.5,0,0,0  
 2B0J,ASP\_56,3.26,0.07,-0.61,0  
 3BB7,CYS\_249,9.06,-2.75,0,2.81  
 3ZSL,LYS\_139,10.36,-0.14,0,0  
 2QDJ,GLU\_322,3.43,0.28,-1.35,0  
 3RJZ,GLU\_174,4.64,0.14,0,0  
 2Q98,TYR\_169,11.94,0,0,1.94  
 1DUP,ASP\_107,3.94,0.14,0,0  
 1ZBM,GLU\_253,4.69,0.49,-0.3,0  
 2B8T,TYR\_289,9.61,0.07,-0.46,0  
 2RFA,LYS\_209,10.15,-0.35,0,0  
 1LZL,ARG\_30,11.66,-0.84,0,0  
 2IF4,LYS\_274,9.8,-0.7,0,0  
 4AF2,GLU\_152,1.48,1.05,-4.07,0  
 1F2V,GLU\_24,4.57,0.07,0,0  
 3ZSL,LYS\_139,10.36,-0.14,0,0  
 3M7D,ARG\_245,12.43,-0.07,0,0  
 3I82,LYS\_167,10.29,-0.21,0,0  
 3GG6,GLU\_53,4.57,0.07,0,0  
 2QDJ,GLU\_137,4.5,0,0,0  
 4F85,HIS\_189,6.43,0,0,-0.07  
 2HXB,LYS\_57,10.36,-0.14,0,0  
 3F5D,ARG\_183,11.94,-0.56,0,0  
 3FK5,LYS\_159,10.43,-0.07,0,0  
 2IXM,HIS\_155,2.29,0.68,0,-4.89  
 1GPP,GLU\_36,4.5,0,0,0  
 2WB8,LYS\_759,10.15,-0.35,0,0  
 3FP7,GLU\_84,4.58,0.21,-0.13,0  
 2A4D,ARG\_157,12.08,-0.42,0,0  
 4FZN,ASP\_190,3.31,0.42,-0.91,0  
 3HVM,LYS\_184,10.5,0,0,0  
 3HUE,ASP\_9,3.94,0.14,0,0  
 1RLO,ARG\_237,11.73,-0.77,0,0  
 2V81,LYS\_69,10.43,-0.07,0,0  
 1KW4,LYS\_70,10.22,-0.28,0,0  
 3GV0,GLU\_227,4.11,1.03,-0.84,-0.58  
 4F3J,GLU\_200,3.99,0.07,-0.58,0  
 2G5X,GLU\_22,3.84,0.14,-0.8,0  
 1YM5,LYS\_246,10.5,0,0,0  
 3PU6,LYS\_48,10.43,-0.07,0,0  
 1YW5,LYS\_87,10.29,-0.21,0,0  
 3CAX,ARG\_430,12.5,0,0,0  
 3FHF,LYS\_103,9.52,-0.98,0,0  
 2G9D,ARG\_173,12.15,-0.35,0,0  
 2E0T,HIS\_151,2.49,0.42,-0.42  
 1J33,ARG\_32,11,-2.33,0,0.84  
 1BYI,TYR\_36,11.22,1.61,-0.39,0  
 1WPA,TYR\_474,11.31,0,0,1.31  
 3G9G,GLU\_77,4.5,0,0,0  
 3RHE,LYS\_122,10.36,-0.14,0,0  
 2CXA,GLU\_100,4.5,0,0,0  
 3ETU,CYS\_257,11.31,-0.22,0,2.53  
 1ZYL,LYS\_315,10.36,-0.14,0,0  
 1VSM,HIS\_93,3.37,0,0,-3.13  
 3A7L,LYS\_105,10.43,-0.07,0,0  
 2QDJ,CYS\_283,9,0,0,0

1P6F,CYS\_27,7.78,-1.36,0,0.14  
1GQE,LYS\_74,10.5,0,0,0  
2AZP,ARG\_173,12.01,-0.49,0,0  
3R1X,GLU\_257,3.04,0.98,-2.44,0  
3GYW,ARG\_105,12.15,-0.35,0,0  
2D0A,ARG\_283,12.08,-0.42,0,0  
1R15,ASP\_129,3.18,0.21,-0.83,0  
2R0S,ASP\_184,3.54,0.56,-0.82,0  
3JZ9,GLU\_386,3.46,0.14,-1.18,0  
2YWJ,GLU\_36,4.6,0.14,-0.04,0  
1ZP2,CYS\_100,8.86,-0.21,0,0.07  
2B2H,TYR\_377,10,0,0,0  
1F2V,ARG\_52,12.08,-0.42,0,0  
2RH3,ASP\_100,2.98,0.49,-1.31,0  
1YOY,TYR\_119,13.15,0.21,0.54,2.4  
3BPP,LYS\_178,10.5,0,0,0  
1RS5,ARG\_115,12.29,-0.21,0,0  
4ECC,GLU\_147,4.01,1.19,-1.68,0  
2GEN,ASP\_33,3.41,0.49,-0.88,0  
2P65,GLU\_169,4.78,0.28,0,0  
2Q98,LYS\_142,10.36,-0.14,0,0  
4GCO,ASP\_173,3.69,0.49,-0.6,0  
3V46,ARG\_377,12.15,-0.35,0,0  
3U56,ARG\_7,11.94,-0.56,0,0  
1LTU,GLU\_109,4.16,0.07,-0.41,0  
1NAF,ASP\_269,3.9,0.21,-0.11,0  
2Q34,ARG\_88,11.94,-0.56,0,0  
2OYZ,LYS\_14,10.5,0,0,0  
2QEV,ASP\_53,2.94,0.77,-1.64,0  
3FK5,CYS\_219,9.19,-0.48,0,0.67  
1DZF,TYR\_112,9.96,0,-0.04,0  
1ZP2,ASP\_31,3.76,0,-0.04,0  
3MIX,GLU\_621,4.49,0.42,-0.43,0  
2JHY,LYS\_133,10,0,0,0  
2PLQ,LYS\_93,10.43,-0.07,0,0  
1PGV,ASP\_234,3.19,0.84,-1.45,0  
3CNU,GLU\_52,3.42,0.35,-1.43,0  
1EDG,LYS\_142,10.29,-0.21,0,0  
3V4G,GLU\_28,3.43,0.51,-1.58,0  
3M1T,ASP\_575,3.06,0.42,-1.16,0  
3MEW,ARG\_209,11.87,-0.63,0,0  
2OSA,LYS\_325,10.22,-0.28,0,0  
3RVC,GLU\_196,4.5,0,0,0  
3LPZ,TYR\_171,9.98,0.26,-0.28,0  
3ETV,GLU\_20,4.64,0.14,0,0  
2CWC,TYR\_87,11.4,0.07,0.133  
3EOH,GLU\_30,2.98,0.35,-1.87,0  
2Z14,ARG\_70,11.66,-0.84,0,0  
3E5T,LYS\_207,10.5,0,0,0  
1M1X,ASP\_397,3.85,0.07,-0.02,0  
3EVZ,ARG\_132,12.36,-0.14,0,0  
2F4Q,GLU\_315,4.57,0.07,0,0  
3QAV,TYR\_148,13.1,0.28,0.42,2.4  
3GW3,ASP\_355,3.86,0.14,-0.08,0  
3J5N,GLU\_41,2.66,0.56,-2.4,0  
2C13,ASP\_209,3.43,0.21,-0.58,0  
2G55,ARG\_102,12.5,0,0,0  
1PBV,LYS\_64,10.29,-0.21,0,0  
4FZN,GLU\_90,5.73,0.98,-0.33,0.57  
3R1V,GLU\_274,4.5,0,0,0  
3JZN,ARG\_436,12.88,-1.51,0.189  
3TOW,ASP\_118,3.22,0.28,-0.86,0  
3FTT,GLU\_10,4.5,0,0,0  
1YW5,ASP\_65,4.01,0.21,0,0  
3N2T,ASP\_193,3.18,0.42,-1.05,0  
3O7K,LYS\_12,10.5,0,0,0  
1KCM,TYR\_18,12.86,2.8,0.06  
1EDG,LYS\_248,10.29,-0.21,0,0  
1R10,GLU\_106,3.16,0.49,-1.83,0  
1O17,GLU\_199,3.06,0.56,-2,0  
1R3D,HIS\_211,4.13,0,0,-2.37  
3BQE,ASP\_265,1.59,0.42,-2.63,0  
3FHF,HIS\_-2,6.5,0,0,0  
1IAP,LYS\_94,10.5,0,0,0  
1ZP2,CYS\_172,9.45,-0.71,-1.01,2.18  
2FZP,TYR\_272,10.49,0.65,-0.17,0  
3S0A,GLU\_78,4.46,0,-0.04,0  
2FPN,ASP\_19,3.68,0.7,-0.82,0  
4E6S,GLU\_19,3.49,0.14,-1.15,0  
2OBI,HIS\_15,6.09,0.01,0,-0.42  
1X04,LYS\_149,10.08,-0.42,0,0  
2FB6,LYS\_37,10.5,0,0,0  
3FTT,ARG\_182,12.22,-0.28,0,0  
3H13,ARG\_338,12.5,0,0,0  
1O1S,ASP\_233,2.22,0.35,-1.93,0  
1GXN,GLU\_527,1.32,2.11,-2.62,-2.67  
1SNT,TYR\_151,9.85,0.42,-0.57,0  
1BY1,ARG\_51,11.38,-1.12,0,0  
2RH3,GLU\_197,3.06,0.77,-2.2,0  
2AD1,CYS\_124,10.31,-0.91,1.48,0.73  
2DG7,LYS\_51,9.8,-0.7,0,0  
2Z61,LYS\_45,10.43,-0.07,0,0  
1UAJ,ASP\_231,3.6,0,-0.21,0  
3ERF,TYR\_68,10,0,0,0  
1FQ1,LYS\_352,10.5,0,0,0  
1R5Q,GLU\_94,3.98,0.28,-0.8,0  
2CBE,LYS\_252,10.08,-0.42,0,0  
2H14,ARG\_181,12.43,-0.07,0,0  
2AH5,ASP\_62,3.41,0.42,-0.81,0  
3I4T,ASP\_257,3.67,0,-0.13,0  
1R6Y,LYS\_26,10.29,-0.21,0,0  
3DSH,LYS\_358,10.15,-0.35,0,0  
3F6F,CYS\_127,5.9,-3.63,0.2,2.3  
1RWZ,ASP\_150,2.65,0.28,-1.43,0  
1J8B,ARG\_82,12.08,-0.42,0,0  
4EVF,GLU\_147,4.57,0.07,0,0  
3BA1,LYS\_145,10.08,-0.42,0,0  
2R57,GLU\_182,4.5,0,0,0  
2FG1,TYR\_86,10,0,0,0  
3M70,CYS\_122,9.49,0,0,0.49  
1X04,TYR\_148,10,0,0,0  
1VJG,GLU\_102,3.58,0.14,-1.06,0  
3L0D,ASP\_105,3.94,0.14,0,0  
3O16,ASP\_143,3.48,0.49,-0.81,0  
2A6B,TYR\_163,11.67,0.07,0.1,6  
3HQX,ASP\_32,2.02,0.49,-2.27,0  
3E7P,GLU\_162,3.98,0.28,-0.8,0  
2H14,HIS\_178,0.38,0.21,-1.51,-4.81  
1DUP,HIS\_78,6.43,0,0,-0.07  
2RJD,LYS\_307,10.5,0,0,0  
1G5Z,GLU\_171,4.13,0.7,-1.07,0  
3RE9,ARG\_233,11.45,-1.05,0,0  
2QDJ,TYR\_239,13.17,0.61,0.43,2.13  
1TLV,LYS\_257,10.5,0,0,0  
3U0V,ARG\_11,12.08,-0.42,0,0  
3G9G,ARG\_26,12.08,-0.42,0,0  
4FH3,ARG\_323,12.36,-0.14,0,0  
1X04,ARG\_221,11.8,-0.7,0,0  
2Z0W,ARG\_67,12.5,0,0,0  
1ES9,HIS\_188,6.36,0,0,-0.14  
1XTD,ASP\_53,3.94,0.14,0,0  
1PGV,GLU\_225,4.19,0.35,-0.66,0  
3LH5,LYS\_733,10.22,-0.28,0,0  
3N2T,HIS\_80,6.09,0.8,1.65,-2.86  
4AE7,LYS\_213,10.08,-0.42,0,0  
4ETX,ARG\_273,12.36,-0.14,0,0  
2D2S,ARG\_753,12.5,0,0,0  
1MML,LYS\_152,10.15,-0.35,0,0  
1MUF,ARG\_258,12.36,-0.14,0,0  
1JKS,HIS\_80,6.22,0,0,-0.28  
3B21,HIS\_68,1.91,0.57,0,-5.16  
3DZ1,ARG\_263,11.67,-3.23,0,2.4  
4H86,LYS\_79,10.29,-0.21,0,0  
3COC,TYR\_359,10,0,0,0  
1V43,ASP\_333,3.91,0.14,-0.03,0  
1O17,ASP\_277,3.73,0,-0.07,0  
3F1X,HIS\_194,4.74,0,0,-1.76  
1YLN,ASP\_192,0.71,1.26,-4.35,0  
3M66,ARG\_245,12.15,-0.35,0,0  
4FH3,LYS\_98,10.29,-0.21,0,0  
3UC9,LYS\_51,10.5,0,0,0  
3GYW,GLU\_118,4.64,0.14,0,0  
2DFL,HIS\_125,0.6,1.19,-1.68,-5.4  
3GV0,GLU\_145,4.64,0.14,0,0  
3FFM,TYR\_44,11.01,0.07,0,0.94  
2B0J,GLU\_168,4.5,0,0,0  
1C44,LYS\_58,10.5,0,0,0  
3U2R,TYR\_25,10,0,0,0  
1EDG,HIS\_123,1.82,0.82,-1.94,-3.56  
1SQH,LYS\_290,10.15,-0.35,0,0  
2CIU,GLU\_143,4.1,0.21,-0.61,0  
3COU,ARG\_54,12.22,-0.28,0,0  
2NRK,LYS\_33,10.5,0,0,0  
2AH5,HIS\_123,6.56,0.06,0,0  
3MIX,ARG\_373,12.22,-0.28,0,0  
3ANJ,ASP\_328,4.08,0.28,0,0  
2POY,LYS\_31,10.29,-0.21,0,0  
4EKU,LYS\_188,10.15,-0.35,0,0  
1T95,ASP\_77,2.6,0.35,-1.55,0  
2DG7,GLU\_165,4.5,0,0,0  
1TP6,ARG\_25,12.36,-0.14,0,0  
3EYE,LYS\_122,10.29,-0.21,0,0  
1P4X,TYR\_203,9.79,0,-0.21,0  
3I4T,HIS\_33,6.36,0,0,-0.14  
2B61,ASP\_58,3.52,0.07,-0.35,0  
1V5M,ARG\_74,12.01,-0.49,0,0  
1J33,ARG\_320,12.08,-0.42,0,0  
3IVF,GLU\_126,3.71,0.42,-1.21,0  
3CEF,CYS\_57,8.57,-0.43,0,0  
2YT4,GLU\_652,4.1,0.28,-0.69,0  
2G2D,ARG\_141,11.87,-0.63,0,0  
3E7P,LYS\_88,10.29,-0.21,0,0  
1X1E,LYS\_58,10.36,-0.14,0,0  
1XNU,TYR\_69,10,0,0,0  
1ANW,ARG\_139,12.08,-0.42,0,0  
3GV0,LYS\_302,10.43,-0.07,0,0  
3FHF,TYR\_155,11.82,0,0,1.82  
2H2W,TYR\_136,10.62,0.07,0.55  
2AZL,GLU\_281,4.5,0.21,-0.21,0  
3ADO,ARG\_31,12.29,-0.21,0,0  
3LJN,GLU\_150,4.28,0.14,-0.36,0  
2WB8,LYS\_658,10.36,-0.14,0,0  
1TXJ,LYS\_122,10.5,0,0,0  
2P52,CYS\_179,8.84,-0.23,0,0.07  
1U7U,ARG\_339,12.08,-0.42,0,0  
2XWS,TYR\_17,9.57,0.6,-1.03,0  
3LJC,ARG\_132,12.15,-0.35,0,0  
2BAA,LYS\_152,10.43,-0.07,0,0  
1U3Y,ASP\_254,3.06,0.7,-1.44,0  
3M7G,GLU\_21,4.64,0.14,0,0  
3CRM,LYS\_267,10.5,0,0,0  
2APL,ASP\_47,3.96,0.21,-0.05,0  
3K8U,HIS\_28,6.43,0,0,-0.07  
1NKD,CYS\_40,9,0,0,0  
2EEY,TYR\_41,9.79,0,-0.21,0  
2JHY,GLU\_164,4.5,0,0,0  
1D2K,LYS\_221,10.15,-0.35,0,0  
3C6B,TYR\_175,12.48,0.38,-0.3,2.4  
3H6Q,GLU\_167,4.64,0.14,0,0  
1TWU,HIS\_44,6.43,0,0,-0.07  
3IVF,ASP\_53,2.95,0.42,-1.27,0  
1YM5,LYS\_188,10.5,0,0,0  
3E7P,GLU\_215,4.5,0,0,0  
1AKO,GLU\_249,3.84,0.14,-0.8,0  
1RHS,GLU\_77,3.68,0.35,-1.17,0  
2EJX,LYS\_87,10.15,-0.35,0,0  
2EJX,LYS\_135,10.5,0,0,0  
3F5D,GLU\_60,2.79,0.63,-2.34,0  
2F9F,ASP\_40,3.53,0.35,-0.62,0  
3CRM,GLU\_72,3.57,0.35,-1.28,0  
2BDD,LYS\_134,10.43,-0.07,0,0  
2I6I,GLU\_43,4.64,0.14,0,0  
3FHF,TYR\_172,10.61,2.63,-1.97,-0.05  
2EUR,ARG\_16,12.15,-0.35,0,0  
1H4U,LYS\_614,10.5,0,0,0  
2R51,LYS\_264,10.5,0,0,0  
3A4C,HIS\_553,6.5,0,0,0  
2QRX,HIS\_91,7.11,0.61,0,0  
2YWK,ARG\_22,11.94,-0.56,0,0  
1Z3X,GLU\_36,4.05,0.35,-0.8,0  
1ZKZ,LYS\_71,10.5,0,0,0  
2GZR,LYS\_153,10.15,-0.35,0,0  
3EYE,LYS\_48,10.5,0,0,0  
1MML,ARG\_173,11.31,-1.19,0,0  
2IF4,LYS\_191,10.29,-0.21,0,0  
3EUR,LYS\_101,9.94,-0.56,0,0  
3PZ9,HIS\_228,6.51,2.14,2.4,-4.52  
1KCM,LYS\_156,10.43,-0.07,0,0  
1O3X,ARG\_260,12.22,-0.28,0,0  
3UC9,HIS\_102,6.5,0,0,0  
3M66,LYS\_389,10.22,-0.28,0,0  
1WOU,LYS\_86,9.94,-0.56,0,0  
3OAJ,LYS\_507,10.29,-0.21,0,0  
3NBI,LYS\_125,10.5,0,0,0  
2AH5,ARG\_44,11.87,-0.63,0,0  
2CXC,CYS\_29,10.68,-0.06,0.55,1.19  
1XKR,LYS\_8,10.22,-0.28,0,0  
1WUJ,LYS\_28,10.43,-0.07,0,0  
1VJG,CYS\_151,10.12,0,0,1.12  
2GZQ,ARG\_154,12.01,-0.49,0,0  
2B61,ASP\_277,1.77,0.7,-2.74,0  
3Q1C,GLU\_379,3.11,0.35,-1.74,0  
1R2Z,GLU\_173,3.5,0.56,-1.56,0  
1S1G,ARG\_129,12.01,-0.49,0,0  
1WP5,GLU\_306,4.57,0.07,0,0  
4EKU,ASP\_32,3.88,0.14,-0.06,0  
3M16,LYS\_13,9.94,-0.56,0,0  
3JRT,CYS\_143,7.89,-1.51,0,0.4  
4ACJ,GLU\_721,3.24,1.14,-2.4,0  
1T6L,ARG\_16,11.87,-0.63,0,0  
2P5D,TYR\_47,11.13,1.18,-0.05,0  
3GA2,TYR\_147,10.02,0.07,-0.91,0.86  
2P65,LYS\_94,10.22,-0.28,0,0  
2YLF,ASP\_158,4.09,0.49,-0.2,0  
2IXM,CYS\_165,12.38,-0.12,1.36,2.14  
3ZXY,HIS\_15,6.5,0,0,0  
3H04,LYS\_5,10.5,0,0,0  
3UAH,GLU\_501,4.57,0.07,0,0  
1LTU,LYS\_239,10.43,-0.07,0,0  
3LJI,ARG\_275,12.08,-0.42,0,0  
1WXF,LYS\_144,10.29,-0.21,0,0  
3HUE,LYS\_35,7.11,0.82,0,-0.21  
2WB8,GLU\_776,4.87,0.49,-0.12,0  
3CGW,LYS\_115,10.43,-0.07,0,0  
3ZSL,ARG\_168,12.5,0,0,0  
1X9G,ARG\_40,11.5,-1.45,0,0.45

1X7F,LYS\_118,10.43,-0.07,0  
4GCO,ARG\_256,11.73,-0.77,0,0  
3GE9,ARG\_83,11.94,-0.56,0,0  
3ANJ,LYS\_26,10.15,-0.35,0,0  
1N81,GLU\_61,4.5,0,0,0  
1J8B,ARG\_53,12.22,-0.28,0,0  
2D8N,LYS\_150,10.08,-0.42,0,0  
3V55,TYR\_657,10,0,0,0  
3CAX,ASP\_292,2.8,0.77,-1.77,0  
2ZOM,TYR\_91,11.1,0,-0.27,1.37  
1Q2Y,CYS\_72,10.95,0,-0.47,2.42  
1FKM,ARG\_499,13.99,-2.0,3.49  
3V4G,ARG\_83,12.15,-0.35,0,0  
3M3P,HIS\_170,2.2,0.02,0,-4.32  
3ERF,ASP\_167,2.81,1.19,-2.18,0  
3EVP,LYS\_271,10.43,-0.07,0,0  
3OAT,ARG\_452,12.36,-0.14,0,0  
3M3P,HIS\_246,6.43,0,0,-0.07  
3BPV,LYS\_125,10.5,0,0,0  
3G6S,ARG\_5,12.15,-0.35,0,0  
1SIG,ARG\_218,12.36,-0.14,0,0  
3BQW,GLU\_181,4.71,0.21,0,0  
3BCH,HIS\_169,6.36,0,0,-0.14  
1QQE,ASP\_3,3.35,0.49,-0.94,0  
1WRU,GLU\_280,3.56,0.49,-1.42,0  
1NAR,GLU\_56,3.05,0.5,-1.95,0  
1OTM,HIS\_219,6.39,0.03,0,-0.14  
3A0X,ASP\_638,3.11,0.7,-1.39,0  
2OKT,ARG\_287,12.5,0,0,0  
2P6S,ARG\_10,12.15,-0.35,0,0  
1KCM,ASP\_243,2.25,0.49,-2.05,0  
1Q8B,GLU\_46,4.5,0,0,0  
4EVF,ARG\_89,12.5,0,0,0  
1Y2Q,GLU\_142,3.94,0.14,-0.7,0  
2EA9,CYS\_82,8.33,-0.82,0,0.14  
2VGM,ASP\_78,3.8,0,0,0  
3QKY,ARG\_251,12.43,-0.07,0,0  
2PWQ,HIS\_133,6.47,0.04,0,-0.07  
2BAA,TYR\_84,13.19,3.88,-0.8,0.11  
3UPD,LYS\_153,10.29,-0.21,0,0  
3CCY,GLU\_184,3.94,0.21,-0.77,0  
3V5S,GLU\_531,3.57,0.42,-1.35,0  
2IQT,HIS\_134,7.22,0.86,0,-0.14  
3IOO,CYS\_191,6.09,-3.05,0,0.14  
2P1W,LYS\_160,9.73,-0.77,0,0  
1RI6,ASP\_115,3.27,0.21,-0.74,0  
1XAW,GLU\_472,4.44,0.14,-0.2,0  
2H2W,GLU\_18,2.45,0.35,-2.4,0  
2QEV,ASP\_5,2.78,0.35,-1.36,0  
2P52,CYS\_121,9.55,0,0,0.55  
2H14,ASP\_242,2.09,0.49,-2.2,0  
1ANU,ARG\_72,12.5,0,0,0  
2ZOM,ARG\_160,10.73,-1.77,0,0  
1SIG,ARG\_422,11.24,-1.26,0,0  
3E0H,HIS\_40,6.53,0.03,0,0  
3B7X,TYR\_118,10.7,0.67,0,0.03  
2ILR,LYS\_468,10.43,-0.07,0,0  
1R22,ASP\_144,1.54,0.7,-2.96,0  
2G9D,GLU\_251,4.71,0.21,0,0  
3K9I,ASP\_72,2.78,0.28,-1.3,0  
1SNT,ASP\_144,3.31,0.14,-0.62,0  
1SFE,ASP\_82,3.65,0.14,-0.29,0  
3LJC,ARG\_38,12.15,-0.35,0,0  
2DFL,ARG\_294,12.01,-0.49,0,0  
3LJI,TYR\_176,10,0,0,0  
1DOV,LYS\_105,10.5,0,0,0  
1NIJ,TYR\_280,10.71,0,0,0.71  
2B0A,ASP\_114,4.78,0.07,-0.09,0  
2D7U,ARG\_244,12.08,-0.42,0,0  
3HNX,ASP\_45,2.44,0.28,-1.65,0  
2P0L,ASP\_233,3.45,0.42,-0.77,0  
2IDC,HIS\_53,7.17,0.67,0,0  
2CVB,GLU\_33,3.78,0.21,-0.92,0  
1LPL,GLU\_176,3.71,0.28,-1.07,0  
2OEW,GLU\_86,4.78,0.28,0,0  
4DIU,ARG\_190,11.8,-0.7,0,0  
3I4T,ASP\_261,3.87,0.21,-0.14,0  
1X91,GLU\_76,4.64,0.14,0,0  
1WYC,ARG\_51,12.15,-0.35,0,0  
1PSW,CYS\_41,9.39,0,0,0.39  
3GMS,TYR\_100,13.16,0.03,2.83  
3A2Z,ARG\_91,12.08,-0.42,0,0  
2VGM,GLU\_343,4.32,0.21,-0.39,0  
1QQL,GLU\_104,4.5,0,0,0  
1RL0,GLU\_119,3.74,0.21,-0.97,0  
1SQU,ARG\_278,12.08,-0.42,0,0  
2FZP,CYS\_238,10.2,0,0,1.2  
1EDG,ASP\_234,3.74,0.07,-0.13,0  
3EVN,TYR\_104,10,0,0,0  
2VAN,GLU\_249,4.5,0,0,0  
1PSW,GLU\_133,4.07,0.56,-0.99,0  
3IL3,ARG\_42,9.88,-2.62,0,0  
4GA2,TYR\_48,10,0,0,0  
3R87,ASP\_125,3.4,0.28,-0.68,0  
2Q12,GLU\_155,3.76,0.49,-1.24,0  
2ZQ5,GLU\_156,4.05,0.21,-0.67,0  
2ZQZ,ARG\_93,11.73,-0.77,0,0  
1WXF,LYS\_173,10.08,-0.42,0,0  
1MN3,ASP\_422,3.83,0.14,-0.11,0  
1KCM,HIS\_60,6.36,0,0,-0.14  
2FL4,GLU\_132,1.87,0.42,-3.05,0  
2EDM,ARG\_103,12.5,0,0,0  
3F6F,GLU\_126,4.5,0,0,0  
1N81,TYR\_168,10,0,0,0  
3FHF,ASP\_161,3.8,0,0,0  
3CCY,HIS\_154,6.5,0,0,0  
2V4U,GLU\_322,4.57,0.07,0,0  
2W0G,ARG\_231,11.8,-0.7,0,0  
2ILR,GLU\_474,3.82,0.07,-0.75,0  
3HKX,ASP\_40,3.39,0.42,-0.83,0  
2D0A,ARG\_278,12.08,-0.42,0,0  
1TJE,ASP\_109,3.94,0.21,-0.07,0  
1LZL,HIS\_141,6.43,0,0,-0.07  
2CN1,LYS\_73,10.29,-0.21,0,0  
1JSX,ARG\_160,11.59,-0.91,0,0  
2CBE,HIS\_15,7.17,0.95,0,-0.28  
3GV0,GLU\_92,4.42,0.49,-0.57,0  
2Z14,TYR\_98,9.27,0.07,-0.8,0  
1MML,GLU\_201,2.65,0.84,-2.69,0  
4F85,GLU\_132,4.28,1.35,-1.57,0  
3LQE,ARG\_476,12.29,-0.21,0,0  
1DZF,ARG\_52,12.08,-0.42,0,0  
1ZYL,ARG\_26,12.29,-0.21,0,0  
1Z3X,CYS\_175,9.07,0,0,0.07  
2EFK,LYS\_132,10.5,0,0,0  
3GMS,LYS\_29,10.5,0,0,0  
1J74,GLU\_139,4.64,0.14,0,0  
1QQH,ASP\_147,3.99,0.42,-0.22,0  
3ZRI,HIS\_-6,6.5,0,0,0  
3FHF,HIS\_133,8.18,5.2,1.25,-4.77  
3V5S,LYS\_513,10.43,-0.07,0,0  
3N2T,ASP\_133,1.59,1.05,-3.25,0  
3ANJ,TYR\_334,11.15,0,0,1.15  
3US6,GLU\_122,2.66,0.56,-2.4,0  
3RNV,TYR\_337,13.2,0.07,0.73,2.4  
3I47,LYS\_249,10.36,-0.14,0,0  
3A2Z,GLU\_37,4.92,0.14,0.28,0  
3GOZ,LYS\_266,9.87,-0.63,0,0  
3H04,GLU\_227,3.24,2.01,-0.87,-2.4  
3G9T,ARG\_126,12.01,-0.49,0,0  
3HVW,ARG\_317,12.08,-0.42,0,0  
1J8S,GLU\_10,3.17,0.49,-1.82,0  
2RIK,HIS\_223,6.29,0,0,-0.21  
1OTM,GLU\_167,4.54,0.35,-0.31,0  
1C44,ASP\_5,3.2,0.14,-0.74,0  
1AT0,ARG\_369,12.22,-0.28,0,0  
1XAW,LYS\_512,10.22,-0.28,0,0  
3PU6,GLU\_43,3.93,0.56,-1.14,0  
2C13,LYS\_280,10.22,-0.28,0,0  
3T5B,GLU\_139,4.64,0.14,0,0  
2A0J,GLU\_107,4.5,0,0,0  
1HF8,GLU\_220,4.5,0,0,0  
1HF8,LYS\_38,10.29,-0.21,0,0  
4E8B,GLU\_157,3.9,0.28,-0.88,0  
2C13,LYS\_280,10.22,-0.28,0,0  
3T5B,GLU\_139,4.64,0.14,0,0  
2A0J,GLU\_107,4.5,0,0,0  
1HF8,GLU\_220,4.5,0,0,0  
1HF8,LYS\_38,10.29,-0.21,0,0  
4E8B,GLU\_157,3.9,0.28,-0.88,0  
1ZBP,GLU\_96,4.57,0.07,0,0  
2Q5X,ARG\_778,12.22,-0.28,0,0  
2OOK,ARG\_154,11.73,-0.77,0,0  
4DEZ,GLU\_18,3.9,0.35,-0.95,0  
2FZ4,TYR\_202,7.09,0.8,0,-0.21  
1F2V,TYR\_6,9.71,0.07,-0.36,0  
2NKK,ARG\_96,11.87,-0.63,0,0  
1C44,ASP\_66,3.41,0.07,-0.46,0  
2H30,ASP\_149,3.52,0.21,-0.49,0  
1JYH,TYR\_123,10,0,0,0  
1ZP2,GLU\_21,4.5,0,0,0  
3FRR,LYS\_134,10.5,0,0,0  
1QQL,HIS\_93,6.79,0.57,0,-0.28  
2XHC,ARG\_251,11.94,-0.56,0,0  
3FHF,CYS\_44,6.58,-3.61,-2.23,3.41  
2NMU,GLU\_70,3.96,0.21,-0.75,0  
2CIU,GLU\_165,4.5,0,0,0  
3CGW,LYS\_61,10.5,0,0,0  
2FBQ,GLU\_156,2.77,0.98,-2.72,0  
3C38,GLU\_139,4.32,0.49,-0.67,0  
3T57,ASP\_129,3.01,0.7,-1.5,0  
3A7L,TYR\_9,12.13,0.54,-0.4,1.99  
1UOH,LYS\_23,10.43,-0.07,0,0  
4EZB,ARG\_23,11.87,-0.63,0,0  
2R57,ARG\_250,12.06,-2.16,0,1.72  
1O9G,ASP\_15,1.01,0.63,-3.42,0  
3CSV,LYS\_206,10.5,0,0,0  
2OPJ,GLU\_83,4.41,0,-0.09,0  
2AD1,CYS\_169,10.43,-0.12,0,1.55  
1OIS,GLU\_225,4.05,0.35,-0.8,0  
3GEC,HIS\_395,1.87,0,0,-4.63  
2OEW,ARG\_41,12.08,-0.42,0,0  
2OSA,TYR\_443,10,0,0,0  
3KV0,GLU\_46,3.91,0.21,-0.8,0  
1SUU,CYS\_665,11.32,0,0,2.32  
3L0D,GLU\_26,4.57,0.07,0,0  
1YMS,LYS\_58,9.8,-0.7,0,0  
3H6Q,GLU\_99,4.57,0.07,0,0  
3CIV,GLU\_218,4.92,0.42,0,0  
2F9F,GLU\_124,4.14,0.14,-0.5,0  
3BQW,LYS\_164,9.94,-0.56,0,0  
2GYZ,ARG\_22,12.22,-0.28,0,0  
2YWK,GLU\_61,4.01,0.49,-0.98,0  
3BZT,TYR\_324,10.07,0.07,0,0  
4E9E,HIS\_454,6.7,0.34,0,-0.14  
2CXA,ARG\_76,12.5,0,0,0  
3FHF,LYS\_39,9.94,-0.56,0,0  
3RLE,GLU\_208,2.31,0.21,-2.4,0  
1GBP,ARG\_224,12.22,-0.28,0,0  
3BZT,LYS\_296,10.36,-0.14,0,0  
2POY,ASP\_115,3.25,0.35,-0.89,0  
3G6G,ARG\_147,12.15,-0.35,0,0  
2F4Q,LYS\_174,10.5,0,0,0  
3HUE,LYS\_267,10.5,0,0,0  
1RIS,TYR\_61,12.16,0.45,0,1.71  
2PGX,GLU\_186,3.76,0.63,-1.36,0  
3LJC,GLU\_10,4.78,0.42,-0.14,0  
3QKY,TYR\_81,12.11,0.02,0,1.89  
1MHN,ARG\_120,12.5,0,0,0  
3B4D,LYS\_243,10.43,-0.07,0,0  
2Q07,ARG\_400,12.01,-0.49,0,0  
3IVF,LYS\_320,10.5,0,0,0  
1DCF,GLU\_42,2.93,0.42,-1.99,0  
1W24,ASP\_154,3.21,0.42,-1.01,0  
3M7D,HIS\_246,4.58,1.27,0,-3.19  
2IRM,GLU\_97,3.45,0.14,-1.19,0  
3G6S,LYS\_27,10.36,-0.14,0,0  
3DB9,ASP\_25,3.71,0.07,-0.16,0  
3LD1,LYS\_257,9.87,-0.63,0,0  
1X6J,ASP\_51,2.47,0.63,-1.96,0  
1YLN,GLU\_138,4.37,0.21,-0.34,0  
3I47,ASP\_12,3.58,0.28,-0.5,0  
3J1V,LYS\_224,10.43,-0.07,0,0  
1EW4,LYS\_65,10.5,0,0,0  
2G9D,HIS\_147,6.55,0.19,0,-0.14  
3VJ8,GLU\_156,2.73,0.63,-2.4,0  
3HVW,CYS\_263,10.17,-0.1,0,1.27  
2IDC,TYR\_112,10.07,0.07,0,0  
3LMF,GLU\_115,4.57,0.07,0,0  
3V46,LYS\_236,10.5,0,0,0  
2A1V,ARG\_45,12.01,-0.49,0,0  
3KV0,GLU\_182,4.26,0.56,-0.8,0  
3COU,ARG\_105,12.15,-0.35,0,0  
1ILW,GLU\_4,4.22,0.14,-0.41,0  
3CO1,GLU\_70,2.68,0.35,-2.17,0  
2BQQ,ARG\_111,12.22,-0.28,0,0  
1CBY,LYS\_115,9.94,-0.56,0,0  
1WOU,GLU\_107,4.64,0.14,0,0  
2Q98,ARG\_177,13.45,-1.45,0,2.4  
1O9G,TYR\_64,11.85,1.05,-0.48,1.28  
3IL3,HIS\_85,6.5,0,0,0  
1SQH,GLU\_244,4.52,0.28,-0.26,0  
4H86,ARG\_141,12.84,-2.02,0,2.36  
3C38,GLU\_107,3.83,0.35,-1.02,0  
1SUU,LYS\_662,10.29,-0.21,0,0  
2IF4,ARG\_245,12.22,-0.28,0,0  
3IBT,GLU\_249,3.48,1.09,-2.12,0  
1QQL,GLU\_81,4.76,0.56,-0.3,0  
2ZCO,HIS\_151,6.43,0,0,-0.07  
1J8S,TYR\_7,13.03,0.07,0.56,2.4  
2CN1,ARG\_52,10.77,-1.73,0,0  
1RSS,LYS\_70,10.43,-0.07,0,0  
1IAP,GLU\_121,4.71,0.21,0,0  
1T9S,GLU\_179,3.48,0.42,-1.44,0  
3N2T,ARG\_17,10.17,-1.96,0,-0.37  
3PM2,LYS\_13,9.8,-0.7,0,0  
2RIS,GLU\_65,4.5,0,0,0  
1L2F,GLU\_221,3.68,0.35,-1.17,0  
2QRX,ASP\_177,3.87,0.07,0,0  
3RHE,LYS\_17,10.5,0,0,0  
1SBX,LYS\_162,9.87,-0.63,0,0  
2RFA,ARG\_190,11.73,-0.77,0,0  
2A6B,ASP\_24,3.94,0.21,-0.07,0  
3IOC,CYS\_284,10.95,0,-0.52,2.47  
1UJ8,GLU\_62,4.5,0,0,0  
3CAX,GLU\_353,4.5,0,0,0  
1WXQ,ASP\_151,3.46,0,-0.34,0  
3P2F,CYS\_177,9.81,-0.76,0,1.57  
1XKR,LYS\_48,10.36,-0.14,0,0  
3LJI,LYS\_45,10.29,-0.21,0,0  
2WB8,ARG\_723,11.45,-1.05,0,0  
1O17,GLU\_131,2.87,0.35,-1.98,0



2RH3,ASP\_122,3.73,0.49,-0.56,0  
 2ZCO,ASP\_147,3.99,0.21,-0.02,0  
 350A,GLU\_13,3.47,0.49,-1.52,0  
 3EVZ,GLU\_114,3.47,0.07,-1.1,0  
 3BCH,ARG\_128,12.08,-0.42,0,0  
 1BKR,ASP\_52,2.94,0.14,-1.01,0  
 1QQE,GLU\_142,4.53,0.14,-0.11,0  
 1QQH,HIS\_108,6.73,0.3,0,-0.07  
 2B0J,HIS\_120,5.96,4.67,0.06,-5.27  
 3C6B,GLU\_6,4.05,0.35,-0.8,0  
 2B0J,LYS\_188,10.5,0,0,0  
 2FPN,TYR\_50,11,1,0,0  
 2YWK,ASP\_44,1.68,1.19,-3.31,0  
 2E3S,ASP\_545,3.8,0,0,0  
 1HF8,LYS\_252,10.5,0,0,0  
 1ZCE,HIS\_54,6.36,0,0,-0.14  
 2I6I,ARG\_150,11.94,0.56,0,0  
 1WOU,LYS\_104,10.43,-0.07,0,0  
 2HXB,LYS\_141,10.43,-0.07,0,0  
 2OSA,LYS\_362,10.29,-0.21,0,0  
 1WXQ,HIS\_107,2.46,0.88,0,-4.93  
 1SQH,ASP\_58,3.23,0.84,-1.42,0  
 3LMF,ASP\_16,3.93,0.21,-0.08,0  
 4GCO,ARG\_216,11.42,-1.77,0,0.69  
 1T3Y,LYS\_130,10.5,0,0,0  
 1RAJ,ASP\_349,3.69,0.42,-0.54,0  
 3BB7,TYR\_343,10,0,0,0  
 3VJ8,ASP\_253,3.8,0.07,-0.07,0  
 1L3K,TYR\_167,10,0,0,0  
 2BLL,ARG\_497,11.88,-0.62,0,0  
 2Q13,HIS\_180,6.82,0.39,0,-0.07  
 1O6D,LYS\_121,10.29,-0.21,0,0  
 1Q8B,LYS\_33,10.36,-0.14,0,0  
 2P4D,TYR\_54,11.93,0,0,1.93  
 2FG1,GLU\_133,3.42,0.07,-1.15,0  
 1PDB,TYR\_162,10.14,0.14,0,0  
 2VAN,HIS\_285,7.13,0.91,0,-0.28  
 1IDK,TYR\_252,10.1,0.1,0,0  
 3IRA,ARG\_35,12.08,-0.42,0,0  
 3QAV,GLU\_34,4.12,0.42,-0.8,0  
 2YYO,CYS\_101,9.25,-0.44,0,0.69  
 2B78,LYS\_56,10.5,0,0,0  
 1O9G,ASP\_50,3.57,0.07,-0.3,0  
 2QV2,ASP\_254,3.13,0.35,-1.02,0  
 3GFP,ARG\_429,12.01,-0.49,0,0  
 3B21,ASP\_38,3.64,0.14,-0.31,0.02  
 2DFL,LYS\_63,9.94,-0.56,0,0  
 2GZQ,HIS\_157,6.5,0,0,0  
 2QOP,ARG\_131,12.22,-0.28,0,0  
 4DIU,ASP\_178,3.83,0.28,-0.25,0  
 2W1R,GLU\_161,2.67,0.84,-2.67,0  
 1HF8,LYS\_226,10.5,0,0,0  
 3T57,ASP\_204,3.11,0.56,-1.25,0  
 2B2H,ARG\_370,13.24,-1.66,0,2.4  
 3FXH,HIS\_5,7.25,1.17,0,-0.42  
 2CN1,TYR\_135,12.56,0.16,2.4  
 2VAN,ARG\_112,12.36,-0.14,0,0  
 4DIU,TYR\_104,12.29,0.63,0,1.66  
 1KN3,ARG\_76,11.73,-0.77,0,0  
 3CRM,ARG\_253,11.8,-0.7,0,0  
 3RKV,GLU\_273,3.11,0.21,-1.6,0  
 3HVM,GLU\_71,4.64,0.14,0,0  
 3ZXY,ARG\_267,12.5,0,0,0  
 1TD6,HIS\_33,6.43,0,0,-0.07  
 1BK8,LYS\_78,10.36,-0.14,0,0  
 3RLN,TYR\_704,11.55,0,-0.2,1.75  
 3JZN,ARG\_236,12.01,-0.49,0,0  
 1PZC,ARG\_114,11.38,-1.12,0,0  
 2G5X,GLU\_191,4.78,0.28,0,0  
 2VGM,TYR\_219,12.13,0.14,0.03,1.96  
 4DEZ,GLU\_236,4.57,0.07,0,0  
 3LPZ,CYS\_183,11.95,0,0,2.95  
 3LPZ,TYR\_190,11.56,1.57,-0.01,0  
 3DZ1,ARG\_251,12.01,-0.49,0,0  
 2D59,GLU\_122,4.71,0.21,0,0  
 3BPP,LYS\_81,10.43,-0.07,0,0  
 1BGF,LYS\_75,10.5,0,0,0  
 2P0L,LYS\_198,10.5,0,0,0  
 1QOE,ARG\_10,12.08,-0.42,0,0  
 1NJ4,GLU\_33,4.11,0.14,-0.53,0  
 1ZHV,ASP\_30,3.79,0.07,-0.08,0  
 1DTO,LYS\_45,10.43,-0.07,0,0  
 2I6I,TYR\_110,10.67,0.67,0,0  
 2E3I,ARG\_59,12.15,-0.35,0,0  
 1XTZ,ARG\_56,11.66,-0.84,0,0  
 1OXZ,LYS\_195,10.5,0,0,0  
 3ZXY,ARG\_213,12.01,-0.49,0,0  
 4ESS,GLU\_98,4.57,0.07,0,0  
 4FD6,ARG\_94,11.73,-0.77,0,0  
 1WXF,TYR\_147,13.54,0.55,0.59,2.4  
 1YW5,TYR\_24,10,0,0,0  
 1L2F,ARG\_232,13.66,-1.24,0,2.4  
 3C5V,GLU\_374,4.57,0.07,0,0  
 4AM1,ARG\_280,12.82,-2.08,0,2.4  
 3C5V,LYS\_236,10.22,-0.28,0,0  
 3ADO,ASP\_100,3.72,0,-0.08,0  
 1ILW,GLU\_25,4.57,0.07,0,0  
 3M66,ARG\_282,12.36,-0.14,0,0  
 2FZ4,GLU\_170,3.69,0.35,-1.16,0  
 2X4J,GLU\_37,4.57,0.07,0,0  
 3G9T,LYS\_213,10.5,0,0,0  
 3GEC,ASP\_248,3.87,0.49,-0.42,0  
 1Z9L,LYS\_45,10.36,-0.14,0,0  
 3PM2,ASP\_101,3.14,0.14,-0.8,0  
 3UAH,LYS\_253,10.43,-0.07,0,0  
 2BLL,TYR\_477,9.55,0.07,-0.8,0.28  
 3C2E,LYS\_136,10.43,-0.07,0,0  
 4ANN,GLU\_105,4.71,0.21,0,0  
 2KH5,HIS\_249,6.85,4.56,0,-4.21  
 2OKT,ASP\_177,2.83,0.42,-1.38,0  
 1ZBM,GLU\_32,4.64,0.14,0,0  
 1WOU,GLU\_73,4.57,0.07,0,0  
 1TLW,ARG\_124,13.92,-0.98,0,2.4  
 3Q1C,ASP\_335,3.87,0.07,0,0  
 2CE6,ARG\_63,11.31,-1.19,0,0  
 4ETX,ASP\_177,3.24,0.28,-0.84,0  
 1KCM,ARG\_253,12.5,0,0,0  
 3IVF,LYS\_268,10.5,0,0,0  
 1JKS,ARG\_63,13.03,-1.15,0,1.68  
 3RKV,LYS\_329,10.43,-0.07,0,0  
 3JSN,LYS\_211,10.5,0,0,0  
 3M66,ARG\_226,11.17,-1.33,0,0  
 2R4Q,GLU\_202,4.5,0,0,0  
 4E8B,ARG\_123,12.22,-0.28,0,0  
 1ZBP,LYS\_102,10.43,-0.07,0,0  
 3PBH,ARG\_202,11.77,-3.99,0,3.26  
 2B78,HIS\_221,6.43,0,0,-0.07  
 1LTU,ASP\_23,2.09,0.63,-2.34,0  
 3CJW,TYR\_177,10,0,0,0  
 1OXZ,GLU\_302,5.34,0.84,0,0  
 2ILR,CYS\_328,10.28,-0.62,0,1.89  
 2B78,TYR\_39,10,0,0,0  
 2E3C,LYS\_228,10.43,-0.07,0,0  
 4FZR,ARG\_322,12.08,-0.42,0,0  
 3GE9,HIS\_98,6.5,0,0,0  
 2ZCO,HIS\_263,7.21,0.85,0,-0.14  
 1QZN,LYS\_29,10.43,-0.07,0,0  
 2P4D,ARG\_29,12.01,-0.49,0,0  
 1YR6,ARG\_61,12.29,-0.21,0,0  
 2XMZ,LYS\_136,10.5,0,0,0  
 3ZSL,LYS\_210,10.22,-0.28,0,0  
 4ECC,GLU\_37,3.74,0.42,-1.18,0  
 4E6S,LYS\_45,10.5,0,0,0  
 3QKY,TYR\_171,10.62,0.5,-0.48,0.6  
 3LJI,LYS\_168,10.5,0,0,0  
 3ELI,GLU\_7,4.43,0.21,-0.28,0  
 1OST,LYS\_374,10.36,-0.14,0,0  
 2C13,GLU\_100,2.63,2.94,-2.4,-2.41  
 2FB6,ARG\_95,12.01,-0.49,0,0  
 2WZ9,GLU\_78,4.5,0,0,0  
 3U56,ASP\_65,3.86,0.21,-0.15,0  
 2BQQ,ARG\_63,12.29,-0.21,0,0  
 3QAV,LYS\_204,10.29,-0.21,0,0  
 1UXO,ASP\_153,3.34,0.07,-0.53,0  
 1OXZ,LYS\_32,4.5,0,0,0  
 3F5D,ASP\_16,2,0.77,-2.58,0  
 3BA1,GLU\_88,4.15,0.21,-0.56,0  
 2V81,GLU\_37,7.83,3.52,0,-0.19  
 2POL,TYR\_179,12.76,2.46,0,0.3  
 3MIX,GLU\_612,4.5,0,0,0  
 3E27,LYS\_9,10.5,0,0,0  
 3BWT,LYS\_744,10.08,-0.42,0,0  
 3RKV,LYS\_292,10.29,-0.21,0,0  
 1J85,TYR\_142,10.07,0.07,0,0  
 1FO9,ARG\_295,11.76,-2.84,0,2.1  
 2P5D,LYS\_37,10.5,0,0,0  
 1X1E,TYR\_144,12.62,2.69,-0.07,0  
 2PWQ,ASP\_122,0.97,0.63,-3.46,0  
 1XIP,ASP\_264,3.21,0.21,-0.8,0  
 1Q46,ARG\_54,12.5,0,0,0  
 3OKQ,GLU\_560,4.48,0.21,-0.23,0  
 2CVB,TYR\_26,11.08,0,0,1.08  
 3UAH,GLU\_469,4.57,0.07,0,0  
 1R29,CYS\_53,9.83,0,0,0.83  
 3CAX,LYS\_147,10.36,-0.14,0,0  
 3BB7,TYR\_199,10.4,1.37,-0.97,0  
 2B78,LYS\_86,10.43,-0.07,0,0  
 2Q13,CYS\_368,8.95,-0.12,0,0.07  
 1S17,GLU\_86,4.24,0.54,-0.8,0  
 2QV2,ARG\_263,11.94,-0.56,0,0  
 3QAV,GLU\_43,4.07,0.35,-0.78,0  
 2PPN,LYS\_47,10.43,-0.07,0,0  
 2CYG,CYS\_32,11.74,-0.92,0.25,3.41  
 2H01,LYS\_53,10.43,-0.07,0,0  
 3IVF,CYS\_29,10.11,-0.22,0,1.34  
 1W24,ASP\_109,2.65,0.63,-1.78,0  
 2Z61,ARG\_285,12.69,-2.21,0,2.4  
 4FLE,GLU\_119,4.15,0.21,-0.56,0  
 2FZP,LYS\_230,10.29,-0.21,0,0  
 3M9A,TYR\_7,10,0,0,0  
 2AH5,HIS\_138,6.43,0,0,-0.07  
 1UXO,ASP\_52,3.9,0.14,-0.04,0  
 3FHF,CYS\_42,11.67,0,0,2.67  
 2OOK,HIS\_191,6.36,0,0,-0.14  
 3RJK,GLU\_187,3.47,0.35,-1.38,0  
 1R53,ASP\_194,2.6,0.56,-1.76,0  
 4EKU,LYS\_35,10.5,0,0,0  
 2OOK,GLU\_2,4.5,0,0,0  
 3EJG,LYS\_147,9.73,-0.77,0,0  
 3AUF,ASP\_40,3.8,0,0,0  
 1X7F,HIS\_183,4.53,0.63,-2.6  
 1PV5,GLU\_6,4.5,0,0,0  
 3IV4,ASP\_95,3.8,0,0,0  
 1AM2,LYS\_150,10.5,0,0,0  
 2PGX,GLU\_205,4.5,0,0,0  
 1UAJ,LYS\_27,10.08,-0.42,0,0  
 2ZOM,LYS\_122,10.29,-0.21,0,0  
 1TJE,HIS\_16,7.23,0.8,0,-0.07  
 3P28,ARG\_194,12.22,-0.28,0,0  
 3P51,GLU\_57,4.78,0.28,0,0  
 2BLL,GLU\_521,4.6,0.14,-0.04,0  
 3GMS,HIS\_157,2.67,1.18,-1.2,-3.81  
 3GG6,GLU\_86,3.48,0.28,-1.3,0  
 2CIU,HIS\_169,7.96,1.6,0,-0.14  
 2B0J,LYS\_240,10.43,-0.07,0,0  
 1V43,GLU\_168,3.65,1.44,-2.19,-0.1  
 3GW3,TYR\_236,9.66,0.48,-0.82,0  
 2EYI,ASP\_210,3.24,0.28,-0.84,0  
 3FHF,LYS\_16,10.29,-0.21,0,0  
 1O59,LYS\_87,10.15,-0.35,0,0  
 2D0A,ARG\_281,11.8,-0.7,0,0  
 3T57,ARG\_246,12.36,-0.14,0,0  
 2FBQ,GLU\_183,4.92,0.42,0,0  
 3R87,ASP\_50,3.97,0.21,-0.04,0  
 2ATR,GLU\_13,3.87,0.28,-0.91,0  
 2IRM,ASP\_56,1.97,0.7,-2.53,0  
 3EVZ,TYR\_43,10,0,0,0  
 3PAC,ASP\_21,3.28,0.28,-0.8,0  
 2R2Y,CYS\_60,8.81,-0.41,0,0.22  
 3L7N,ASP\_230,1.31,0.56,-3.05,0  
 1YOY,LYS\_56,10.5,0,0,0  
 3CGW,GLU\_179,4.33,0.35,-0.52,0  
 3CJW,CYS\_343,9,0,0,0  
 4AM1,LYS\_216,10.08,-0.42,0,0  
 3RVC,GLU\_172,3.45,0,-1.05,0  
 1R15,GLU\_277,2.61,0.56,-2.45,0  
 3FK5,HIS\_50,6.5,0,0,0  
 2WB3,GLU\_260,4.5,0,0,0  
 1QQE,ASP\_74,3.21,0.56,-1.16,0  
 4ETX,GLU\_445,3.84,0.14,-0.8,0  
 3G59,GLU\_280,4.5,0,0,0  
 2G9D,ARG\_255,12.15,-0.35,0,0  
 1T6L,GLU\_36,4.5,0,0,0  
 3DZ1,GLU\_127,4.5,0,0,0  
 1G8P,ARG\_328,12.5,0,0,0  
 3I00,TYR\_200,10.06,0.07,-0.01,0  
 2D25,GLU\_608,4.78,0.28,0,0  
 3IVF,LYS\_29,10.11,-0.22,0,1.34  
 2CL3,ARG\_150,12.49,-2.21,0,2.2  
 3CAX,HIS\_301,4.83,0,0,-1.67  
 3UX2,LYS\_52,9.8,-0.7,0,0  
 2R51,HIS\_27,3.48,0,0,-3.02  
 3CIV,ASP\_256,3.61,0,-0.19,0  
 2XWS,GLU\_30,4.05,0.35,-0.8,0  
 1MN3,CYS\_442,9.07,0,0,0.07  
 1T6L,TYR\_20,11.93,2.73,-0.8,0  
 1AK1,GLU\_174,4.64,0.14,0,0  
 1X1E,TYR\_129,10.35,0.59,-1.47,1.22  
 1WXQ,GLU\_239,5.34,1.09,-0.8,0.55  
 2BQQ,ASP\_86,3.48,0.28,-0.8,0  
 1ES9,HIS\_209,6.43,0,0,-0.07  
 1TP6,TYR\_5,10.05,0.21,-0.16,0  
 3GS3,GLU\_193,4.5,0,0,0  
 1NWA,TYR\_44,12.14,0.18,0,1.95  
 2AZP,HIS\_170,4.25,0.95,0,-3.2  
 3EGN,ASP\_15,3.89,0.56,-1.17,0  
 3DZ1,LYS\_151,10.5,0,0,0  
 3PU6,TYR\_97,9.48,0.28,-0.8,0  
 3M7G,ARG\_252,12.29,-0.21,0,0  
 1WRU,LYS\_106,9.87,-0.63,0,0  
 1Q5Z,GLU\_543,1.39,0.49,-1.56,-2.03  
 2CXV,GLU\_15,3.89,0.56,-1.17,0  
 2C13,GLU\_85,4.47,0.35,-0.38,0  
 1W24,TYR\_129,10.2,0.18,-0.06,0.08  
 1YTD,HIS\_334,2.75,0,-1.38,-2.37  
 3K8J,TYR\_217,13.15,0.78,0.28,2.09

1ZBP,LYS\_227,10.36,-0.14,0,0  
1160,GLU\_12,4.64,0.14,0,0  
1ZP2,GLU\_143,4.78,0.28,0,0  
2G55,ASP\_99,3.08,0.35,-1.07,0  
3ASA,GLU\_29,3.98,0.28,-0.8,0  
1WXQ,GLU\_137,4.57,0.07,0,0  
4DND,TYR\_25,11.19,0.14,-0.54,1.58  
2VGM,GLU\_40,4.64,0.14,0,0  
3MEW,TYR\_154,11.24,0.19,-0.81,1.87  
1X8F,TYR\_41,11.78,2.83,-1.05,0  
3DSH,GLU\_270,4.05,0.28,-0.73,0  
3RJX,LYS\_330,10.5,0,0,0  
1YW5,GLU\_149,3.79,0.49,-1.2,0  
1YOK,ARG\_132,12.08,-0.42,0,0  
1AKO,ARG\_173,12.15,-0.35,0,0  
3TOW,HIS\_198,6.36,0,0,-0.14  
3G53,GLU\_222,2.75,1.45,-0.8,-2.4  
3TOW,GLU\_103,4.5,0,0,0  
1AD6,LYS\_530,10.22,-0.28,0,0  
3HYQ,ARG\_174,11.73,-0.77,0,0  
3CN5,HIS\_193,6.5,0,0,0  
3KT9,ARG\_16,11.73,-0.77,0,0  
1X91,TYR\_75,10.7,1.5,-0.8,0  
3IV4,ARG\_47,12.15,-0.35,0,0  
2IQT,GLU\_191,4.25,0.07,-0.32,0  
3CIV,HIS\_223,5,0,0,-1.5  
2EYI,ARG\_156,12.08,-0.42,0,0  
1VJG,GLU\_166,4.05,0.35,-0.8,0  
1J33,GLU\_224,4.26,0.56,-0.8,0  
3O16,GLU\_218,3.82,0.42,-1.1,0  
2GEN,TYR\_57,10.75,0.82,-0.07,0  
2Q5X,GLU\_852,3.58,0.21,-1.13,0  
3IBT,ASP\_64,3.51,0.14,-0.43,0  
1MML,ASP\_124,3.47,0.14,-0.48,0  
1SI7,LYS\_120,10.29,-0.21,0,0  
1XFK,CYS\_319,12.03,0,0,3.03  
1AK1,HIS\_116,1.39,0,0,-5.11  
1O3X,ARG\_255,12.5,0,0,0  
4GA2,ASP\_111,2.39,0.56,-1.97,0  
2OGQ,TYR\_562,11.84,0.65,-0.8,1.99  
4FCU,LYS\_119,9.8,-0.7,0,0  
2VGY,ASP\_34,3.39,0.14,-0.55,0  
3M7G,ARG\_135,11.8,-0.7,0,0  
1WYC,ARG\_376,12.22,-0.28,0,0  
2YWX,ARG\_111,12.29,-0.21,0,0  
1DCF,ASP\_125,3.92,0.28,-0.16,0  
2VC8,HIS\_42,6.69,0.75,-0.56  
1N81,GLU\_90,4.41,0.14,-0.23,0  
1BKB,GLU\_16,3.49,0.14,-1.15,0  
3ZR1,HIS\_40,2.99,0.12,0,-3.62  
3PZ9,ARG\_374,12.17,-1.53,0,1.2  
2IIA,ASP\_42,3.05,0.35,-1.09,0  
1X91,LYS\_100,10.43,-0.07,0,0  
1L2F,GLU\_7,4.5,0,0,0  
1MUF,TYR\_305,11.37,1.37,0,0  
1MTZ,GLU\_147,4.35,0.35,-0.5,0  
3JZN,GLU\_238,5.4,0,0,0  
3K8U,TYR\_29,10.15,0.15,0,0  
4FZR,ARG\_71,12.29,-0.21,0,0  
1PV5,LYS\_148,10.36,-0.14,0,0  
3OA7,GLU\_19,4.5,0,0,0  
3GW3,HIS\_360,6.68,0.25,0,-0.07  
3OIP,ARG\_86,12.15,-0.35,0,0  
2VC8,CYS\_14,9,0,0,0  
2BT8,ARG\_226,11.52,-0.98,0,0  
3F1X,HIS\_28,6.84,0.41,0,-0.07  
4DIU,GLU\_168,4.78,0.28,0,0  
1IAP,ASP\_98,3.77,0.07,-0.1,0  
2RFA,HIS\_153,7.23,1.08,0,-0.35  
1G5Z,LYS\_47,10.36,-0.14,0,0  
4DEZ,ASP\_181,3.43,0.35,-0.72,0  
1H4U,LYS\_476,10.5,0,0,0  
2G3A,LYS\_34,10.36,-0.14,0,0  
1FO9,ARG\_296,12.29,-0.21,0,0  
4E8B,LYS\_65,10.29,-0.21,0,0  
2QK0,LYS\_88,10.15,-0.35,0,0  
2H2W,CYS\_291,12.09,0.17,1.43,1.49  
1SQH,ARG\_262,11.73,-0.77,0,0  
1YG2,LYS\_23,10.43,-0.07,0,0  
3EUR,ASP\_118,1.93,0.98,-2.86,0  
3O7K,ASP\_13,3.73,0.07,-0.14,0  
2DFL,ASP\_201,1.86,0.77,-2.7,0  
4EZB,GLU\_91,4.5,0,0,0  
3GA2,ARG\_220,11.87,-0.63,0,0  
2BDV,HIS\_162,6.5,0,0,0  
2V81,ASP\_178,4.04,0.28,-0.04,0  
2F8H,ARG\_248,11.39,-1.11,0,0  
3M7G,ASP\_239,2.48,0.56,-1.88,0  
4HDE,ASP\_102,3.5,0.56,-0.86,0  
1SQW,LYS\_50,10.22,-0.28,0,0  
2WB3,LYS\_309,10.5,0,0,0  
3RJZ,TYR\_103,9.27,0.07,-0.8,0  
3RFF,LYS\_55,10.43,-0.07,0,0  
1ESS,ARG\_171,11.73,-0.77,0,0  
2AZL,GLU\_241,4.64,0.14,0,0  
3A2Z,ASP\_121,3.19,0.35,-0.96,0  
2AXO,GLU\_62,3.76,0.07,-0.8,0  
2YYO,ASP\_76,4.08,0.28,0,0  
4FH3,GLU\_64,4.92,0.42,0,0  
3KB5,GLU\_443,3.84,0.14,-0.8,0  
3PZ9,TYR\_370,13.41,0.21,0.8,2.4  
3MIX,ASP\_366,3.79,0,-0.01,0  
1X9G,CYS\_34,10.84,-0.17,0.2,0.1  
1X04,ASP\_145,3.67,0.35,-0.48,0  
2C2Y,GLU\_84,3.66,0.7,-1.54,0  
2JHY,LYS\_98,10.22,-0.28,0,0  
350A,LYS\_7,9.8,-0.7,0,0  
2Q99,LYS\_225,10.15,-0.35,0,0  
1P4X,GLU\_211,4.45,0.14,-0.19,0  
4EKU,LYS\_295,10.5,0,0,0  
1160,LYS\_114,10.5,0,0,0  
2H8O,ARG\_244,12.15,-0.35,0,0  
1G8P,GLU\_132,4.85,0.35,0,0  
2I6I,ASP\_75,1.7,0.35,-2.45,0  
3OIP,ARG\_116,12.36,-0.14,0,0  
1ZBM,ARG\_196,11.94,-0.56,0,0  
1FO9,ARG\_165,12.15,-0.35,0,0  
2F4Q,ARG\_94,13.61,-1.29,0.2,4  
3B79,LYS\_2,10.5,0,0,0  
1X8F,GLU\_98,4.64,0.14,0,0  
1FKM,ASP\_464,3.71,0,-0.09,0  
1PSW,LYS\_301,10.43,-0.07,0,0  
2QK1,GLU\_397,4.81,1.11,-0.8,0  
3IL3,ARG\_294,13.27,-1.26,0.2,0.3  
2P52,ARG\_264,11.59,-0.91,0,0  
1S7K,ARG\_64,12.01,-0.49,0,0  
1O59,GLU\_142,4.5,0,0,0  
3EAZ,TYR\_133,10.21,0.21,0,0  
1YTD,LYS\_279,10.29,-0.21,0,0  
1EQ6,ASP\_167,3.73,0.14,-0.21,0  
3IBT,ARG\_46,11.94,-0.56,0,0  
2XHC,LYS\_95,10.43,-0.07,0,0  
2VGM,ASP\_295,3.61,0.07,-0.97,0  
3FRR,ARG\_12,11.8,-0.7,0,0  
1PVT,GLU\_113,4.5,0,0,0  
1XDZ,GLU\_119,4.57,0.07,0,0  
3L3P,ASP\_332,3.73,0,-0.07,0  
2PGE,ARG\_311,11.52,-0.98,0,0  
3ZSL,LYS\_233,10.43,-0.07,0,0  
1SUU,LYS\_744,10.15,-0.35,0,0  
3I47,GLU\_167,3.98,0.28,-0.8,0  
3BPP,TYR\_38,11.95,0,0,1.95  
2BDV,GLU\_176,4.12,0.42,-0.8,0  
3UC9,GLU\_127,4.29,0.42,-0.63,0  
2F19,ASP\_67,3.8,0,0,0  
2O8I,GLU\_16,4.05,0.35,-0.8,0  
3SMD,LYS\_86,10.29,-0.21,0,0  
2D25,ASP\_706,4.06,0.35,-0.09,0  
2OEW,HIS\_61,6.43,0,0,-0.07  
2QZQ,LYS\_44,10.22,-0.28,0,0  
2G5X,ARG\_21,13.3,-3.07,0.3,86  
3JZ9,ARG\_418,12.5,0,0,0  
1EW4,ARG\_106,11.8,-0.7,0,0  
2WOZ,GLU\_411,4.5,0,0,0  
2V4X,TYR\_29,10,0,0,0  
3OA7,HIS\_530,6.36,0,0,-0.14  
1AIL,HIS\_17,6.43,0,0,-0.07  
3RVC,GLU\_96,2.66,0.56,-2.4,0  
4DBX,ASP\_19,3.94,0.14,0,0  
2FPN,HIS\_186,6.59,0.3,0,-0.21  
4DBL,ARG\_8,10.82,-1.68,0,0  
3D9H,ARG\_143,12.01,-0.49,0,0  
2ZQ5,TYR\_370,11.18,0.21,-0.52,1.49  
1TUL,ASP\_82,3.28,0.28,-0.8,0  
1RSS,ASP\_45,3.81,0.14,-0.13,0  
3F7M,LYS\_184,10.43,-0.07,0,0  
1PGV,GLU\_233,4.57,0.07,0,0  
4ANN,TYR\_74,8.33,0.87,-1.12,-1.42  
1MTZ,LYS\_291,10.29,-0.21,0,0  
1Z9L,GLU\_108,4.71,0.21,0,0  
2E3H,ARG\_261,11.38,-1.12,0,0  
1QZN,ASP\_141,3.87,0.07,0,0  
2WOZ,GLU\_513,1.54,2.05,-3.19,-1.82  
2W0G,TYR\_189,13.48,0.28,0.8,2.4  
2DVK,GLU\_98,4.05,0.21,-0.66,0  
4H89,ASP\_15,2.65,0.84,-1.99,0  
2YX0,TYR\_210,10.56,1.33,-0.77,0  
2Q34,GLU\_248,3.47,0.14,-1.17,0  
1A8Q,HIS\_219,2.83,0.1,56,-5.23  
1O5J,HIS\_73,3.51,0.88,0,-3.87  
3M16,GLU\_91,4.5,0,0,0  
1PGV,ARG\_315,11.94,-0.56,0,0  
2I88,LYS\_426,10.5,0,0,0  
2V5B,ARG\_139,12.36,-0.14,0,0  
2WOZ,ASP\_372,2.29,0.49,-1.99,0  
3JZ9,LYS\_350,10.15,-0.35,0,0  
2XHC,GLU\_146,3.9,0.28,-0.88,0  
3D5H,HIS\_364,6.5,0,0,0  
1SI7,ASP\_142,3.61,0,-0.19,0  
1X7F,ARG\_243,11.21,-1.29,0,0  
1FKM,TYR\_365,11.79,0.07,-0.68,2.4  
1R16,GLU\_13,4.64,0.14,0,0  
3LJN,GLU\_101,4.05,0.21,-0.66,0  
3ETV,TYR\_123,8.48,0.28,-0.1,-1.7  
4D8L,GLU\_158,2.32,0.32,-1.26,-1.23  
1UCH,ASP\_177,2.54,0.49,-1.75,0  
1GQE,ASP\_68,3.97,0.28,-0.11,0  
1V43,ARG\_263,12.22,-0.28,0,0  
2QK0,LYS\_43,10.43,-0.07,0,0  
3CAX,ASP\_342,1.24,1.05,-3.61,0  
1X91,LYS\_133,10.29,-0.21,0,0  
4GA2,ARG\_84,12.22,-0.28,0,0  
1WOU,LYS\_78,10.36,-0.14,0,0  
2WB3,ASP\_377,3.7,0.14,-0.24,0  
1TJE,LYS\_63,10.29,-0.21,0,0  
1G8P,ARG\_208,11.66,-0.84,0,0  
2EDM,ASP\_89,3.94,0.14,0,0  
1W24,ASP\_47,4.11,0.42,-0.12,0  
1H4U,GLU\_424,4.36,0.21,-0.35,0  
1160,LYS\_118,10.22,-0.28,0,0  
3N2T,HIS\_43,6.87,0.65,0,-0.28  
2ZTY,ASP\_64,2.33,1.05,-2.61,0  
1FO9,GLU\_282,3.5,0.49,-1.49,0  
3H9W,ARG\_110,12.15,-0.35,0,0  
1KCM,ASP\_51,3.72,0,-0.08,0  
2QEV,HIS\_70,4.27,0.94,0,-3.16  
1A8Q,ASP\_221,3.12,0.63,-1.31,0  
1WPA,TYR\_517,13.27,0.28,0.64,2.35  
2YX0,ASP\_206,2.48,0.84,-2.16,0  
3RHE,TYR\_22,10.14,0.14,0,0  
3K8U,LYS\_69,9.8,-0.7,0,0  
1FHL,LYS\_70,10.36,-0.14,0,0  
2E3C,GLU\_218,4.5,0,0,0  
3MIX,TYR\_660,12.16,0.03,-0.32,2.45  
2OEW,GLU\_356,4.57,0.07,0,0  
1TJE,LYS\_197,10.36,-0.14,0,0  
1T3J,ARG\_716,12.5,0,0,0  
1DOV,LYS\_238,10.36,-0.14,0,0  
1W24,GLU\_143,4.49,0,-0.01,0  
2QVO,LYS\_85,10.22,-0.28,0,0  
1RAJ,GLU\_93,4.57,0.07,0,0  
3H5T,ARG\_150,11.73,-0.77,0,0  
3BWT,LYS\_807,10.43,-0.07,0,0  
1UW7,TYR\_31,10.86,0.86,0,0  
4DVD,GLU\_33,1.9,0.35,-2.95,0  
1R3F,LYS\_190,10.5,0,0,0  
1SUU,TYR\_526,11.18,1.18,0,0  
2RIS,GLU\_147,2.62,1.39,-3.27,0  
3M3P,CYS\_89,4.36,-4.99,-2.21,2.56  
3IDW,ARG\_67,11.87,-0.63,0,0  
2R57,GLU\_300,3.77,0.21,-0.94,0  
1UW7,HIS\_48,6.43,0,0,-0.07  
2FG1,TYR\_153,8.42,0.31,-1.89,0  
1J8B,GLU\_86,4.57,0.07,0,0  
2AHE,LYS\_90,10.43,-0.07,0,0  
2BDV,GLU\_172,3.42,0,-1.08,0  
2QK1,HIS\_468,6.36,0,0,-0.14  
3VHJ,LYS\_164,10.5,0,0,0  
3HYQ,GLU\_77,3.31,0.21,-1.4,0  
1QYI,LYS\_114,9.59,-0.91,0,0  
3CNU,ARG\_92,12.08,-0.42,0,0  
4AE7,GLU\_210,4.49,0.35,-0.37,0  
2W1R,LYS\_163,10.29,-0.21,0,0  
2R57,ASP\_341,3.87,0.07,0,0  
2QK0,ASP\_73,1.47,0.56,-2.89,0  
3BQE,LYS\_328,9.94,-0.56,0,0  
1ZHV,HIS\_134,6.43,0,0,-0.07  
2G3A,ASP\_7,3.52,0.07,-0.35,0  
3DZ1,ARG\_181,13.2,-1.57,0.2,27  
3A0X,LYS\_652,10.15,-0.35,0,0  
2D0A,LYS\_64,10.29,-0.21,0,0  
2BQQ,GLU\_123,4.29,0.21,-0.42,0  
2OEW,ASP\_210,0.95,0.35,-1.86,-1.34  
1AM2,GLU\_65,3.15,0.84,-2.18,0  
2NSN,ASP\_48,4.08,0.28,0,0  
1BKR,ARG\_32,12.15,-0.35,0,0  
1UCH,HIS\_175,4.97,0.93,-0.06,-2.41  
3JZN,ASP\_395,3.35,0.35,-0.8,0  
1V43,ASP\_365,1.04,0.7,-3.47,0  
2VAN,TYR\_250,11,0,0,1  
3TIR,ASP\_166,3.34,0.07,-0.53,0  
3BPP,GLU\_49,0.64,0.81,-2.26,-2.4  
3G9T,ASP\_159,2.59,0.63,-1.84,0  
3MIX,GLU\_407,4.18,0.7,-1.02,0  
2P0Y,GLU\_222,5.09,0.59,0,0  
1DTO,GLU\_20,4.57,0.07,0,0

3IO0,ASP\_270,3.85,0.07,-0.02,0  
2OJQ,LYS\_553,10.36,-0.14,0,0  
1T95,ARG\_121,12.5,0,0,0  
2YX0,LYS\_22,10.5,0,0,0  
2YWJ,LYS\_20,10.5,0,0,0  
1BKB,GLU\_103,4.5,0,0,0  
1WXF,GLU\_66,3.39,0.49,-1.6,0  
2BOA,HIS\_136,10.61,4.69,3.54,-4.13  
2GAU,GLU\_104,4.44,0.49,-0.55,0  
3HVV,ARG\_231,12.15,-0.35,0,0  
1ZP2,LYS\_88,10.08,-0.42,0,0  
3PBH,ASP\_69,3.88,0.21,-0.13,0  
3ZTA,LYS\_65,9.94,-0.56,0,0  
1WPA,ARG\_418,12.5,0,0,0  
2EYI,HIS\_186,4.92,1.14,0,-2.72  
3UV9,HIS\_461,6.5,0,0,0  
2PSD,GLU\_88,3.14,0.28,-1.63,0  
3LQE,HIS\_242,7.87,4.7,2.4,-5.73  
2ZOM,ARG\_216,12.22,-0.28,0,0  
3PZF,ARG\_172,12.08,-0.42,0,0  
3MIX,TYR\_350,10,0,0,0  
3C2E,ARG\_151,12.08,-0.42,0,0  
1T3Y,LYS\_110,10.5,0,0,0  
2E3S,TYR\_576,12.43,2.43,0,0  
1TR9,GLU\_12,4.5,0,0,0  
1Z3X,ARG\_60,12.53,-1.53,0,1.56  
1E5S,HIS\_138,6.35,0.13,0,-0.28  
1ILW,LYS\_39,10.08,-0.42,0,0  
1L3K,ASP\_42,3.19,0.07,-0.68,0  
1FKM,HIS\_442,6.43,0,0,-0.07  
1Y0K,ASP\_153,3.17,0.42,-1.05,0  
2CXY,CYS\_53,9.28,-0.09,0,0.37  
3G9G,ARG\_141,11.38,-1.12,0,0  
3V46,HIS\_381,6.5,0,0,0  
4FZR,GLU\_78,4.12,0.42,-0.8,0  
1JB3,GLU\_11,4.61,0.91,-0.8,0  
3UX2,GLU\_57,3.6,0.63,-1.53,0  
2VAN,GLU\_123,4.34,0,-0.16,0  
2BOJ,TYR\_200,13.91,2.96,-0.03,0.98  
3G9T,GLU\_5,3.91,0.42,-1.01,0  
2PSD,TYR\_56,10.14,0,14,0,0  
3IPZ,GLU\_131,3.28,0.77,-1.99,0  
3RNV,TYR\_345,10.1,0.22,-0.12,0  
3GA2,LYS\_25,9.94,-0.56,0,0  
1XWM,ASP\_47,3.87,0.35,-0.28,0  
3DTE,HIS\_63,6.6,0.24,0,-0.14  
2BV9,LYS\_216,10.08,-0.42,0,0  
2V5B,TYR\_102,10.24,0,0,0.24  
3TOW,LYS\_87,10.43,-0.07,0,0  
2JKF,GLU\_66,4.5,0,0,0  
3QKY,TYR\_87,9.6,0.07,-0.47,0  
3ANJ,ASP\_145,3.36,0.42,-0.86,0  
3DZ1,ASP\_34,1.7,0.42,-2.52,0  
1O0X,CYS\_234,10.37,-0.76,0,2.13  
2D2S,GLU\_542,4.57,0.07,0,0  
3CS1,LYS\_153,10.08,-0.42,0,0  
3CAX,LYS\_275,11.13,-0.84,0,1.47  
3CGW,GLU\_182,4.5,0,0,0  
2ZCO,ARG\_246,13.02,-1.16,0,1.68  
2H2W,GLU\_212,4.0,0.21,-0.71,0  
1YW5,LYS\_105,10.5,0,0,0  
3HVV,ASP\_300,3.87,0.07,0,0  
4AF2,ASP\_124,2.89,0.42,-1.33,0  
2FG1,ASP\_154,3.71,0.28,-0.37,0  
2Z84,HIS\_137,2.37,0,0,-4.13  
1TD6,HIS\_243,4.45,0,0,-2.05  
2O4D,GLU\_93,0.52,1.09,-2.67,-2.4  
2NMU,ARG\_55,12.01,-0.49,0,0  
3IBT,HIS\_20,6.5,0,0,0  
2GEN,ARG\_32,11.87,-0.63,0,0  
2I6I,ARG\_31,10.7,-1.8,0,0  
1Q46,GLU\_142,3.95,0.21,-0.76,0  
3ADO,ARG\_40,12.5,0,0,0  
157K,ASP\_17,2.02,0.49,-2.26,0  
1NAR,ASP\_155,3.92,0.14,-0.02,0  
350A,LYS\_42,10.29,-0.21,0,0  
1UOH,ARG\_118,11.52,-0.98,0,0  
3ADO,LYS\_139,10.5,0,0,0  
1IDK,LYS\_335,10.29,-0.21,0,0  
1DIO,GLU\_118,4.22,0.35,-0.63,0  
1Y2Q,LYS\_106,10.15,-0.35,0,0  
3NBI,TYR\_201,11.77,0,0,1.77  
3T57,ARG\_315,12.08,-0.42,0,0  
1LFP,ARG\_108,11.38,-1.12,0,0  
2P4D,TYR\_63,9.67,0.47,-0.8,0  
2JFK,ASP\_92,3.51,0.35,-0.64,0  
4DIU,TYR\_204,10,0,0,0  
3CQ1,ARG\_70,12.5,0,0,0  
2H30,GLU\_79,4.09,0.77,-1.18,0  
1H4U,HIS\_436,6.43,0,0,-0.07  
1SJ8,LYS\_613,10.29,-0.21,0,0  
1ZCE,GLU\_57,4.5,0,0,0  
2NRR,LYS\_443,10.5,0,0,0  
3EVZ,LYS\_207,10.43,-0.07,0,0  
3HUE,ASP\_259,2.89,0.42,-1.33,0  
1EV8,GLU\_245,3.73,0.42,-1.19,0  
1DOV,TYR\_148,9.27,0.07,-0.8,0  
2JKF,ASP\_92,3.51,0.35,-0.64,0  
4DND,ASP\_104,3.21,0.35,-0.94,0  
2VAN,LYS\_141,10.43,-0.07,0,0  
1U7U,LYS\_378,10.36,-0.14,0,0  
2QDJ,TYR\_173,10.74,1.02,-0.8,0.52  
4DNU,CYS\_37,9.94,-0.93,0,1.87  
2O0K,ASP\_69,3.1,0.28,-0.98,0  
2PLQ,LYS\_314,10.36,-0.14,0,0  
3HYQ,LYS\_56,10.5,0,0,0  
3ZTA,ARG\_42,12.01,-0.49,0,0  
3EAZ,LYS\_169,10.29,-0.21,0,0  
3T5B,TYR\_32,11.54,2.53,-0.7,-0.28  
4ETX,LYS\_329,10.36,-0.14,0,0  
1UW7,ASP\_60,3.65,0.42,-0.56,0  
3DB9,LYS\_213,10.5,0,0,0  
2H30,ARG\_154,11.66,-0.84,0,0  
3IU5,LYS\_61,10.43,-0.07,0,0  
1PSW,ARG\_281,13.36,-1.49,0,2.35  
3V55,GLU\_451,4.0,0.28,-0.78,0  
4EVF,GLU\_191,4.5,0,0,0  
4DIU,LYS\_215,10.29,-0.21,0,0  
4HDE,ASP\_149,4.07,0.28,-0.01,0  
1X04,GLU\_173,4.5,0,0,0  
2R51,HIS\_223,6.43,0,0,-0.07  
4GA2,ARG\_2,12.5,0,0,0  
2OGQ,ASP\_588,3.47,0.14,-0.47,0  
2FD4,LYS\_464,10.29,-0.21,0,0  
1WP5,LYS\_233,10.22,-0.28,0,0  
2CXA,CYS\_187,10.95,0.28,1.67  
3M7G,ARG\_112,11.94,-0.56,0,0  
2BLI,GLU\_571,4.12,0.42,-0.8,0  
3H13,HIS\_396,6.43,0,0,-0.07  
3RFF,ASP\_75,3.93,0.14,-0.01,0  
1P4X,GLU\_102,4.57,0.07,0,0  
3LJC,ASP\_160,3.94,0.14,0,0  
1PDB,ASP\_152,3.13,0.49,-1.16,0  
2EOT,ARG\_203,12.5,0,0,0  
2R51,HIS\_204,8.37,2.08,0,-0.21  
1SNT,LYS\_9,10.36,-0.14,0,0  
2A0J,GLU\_36,2.81,0.67,-0.8,-1.56  
1W24,TYR\_139,9.83,0,-0.17,0  
3MEW,LYS\_217,10.22,-0.28,0,0  
3CX5,CYS\_113,9,0,0,0  
2FZP,TYR\_196,10.45,0.07,0,0.39  
1HF8,LYS\_28,10.36,-0.14,0,0  
3HFH,LYS\_124,10.01,-0.49,0,0  
1T95,ARG\_70,12.22,-0.28,0,0  
2AHE,LYS\_62,9.59,-0.91,0,0  
2E3S,GLU\_373,4.22,0.14,-0.42,0  
2IDC,ASP\_37,4.21,0.49,-0.08,0  
3FK5,ARG\_135,13.12,-0.42,0,1.04  
1XWM,GLU\_161,4.5,0,0,0  
3P28,LYS\_83,10.36,-0.14,0,0  
3PP8,ASP\_40,4.08,0.28,0,0  
3IOC,GLU\_174,4.64,0.14,0,0  
1TXJ,LYS\_105,10.5,0,0,0  
1LTU,TYR\_181,11.5,1.5,0,0  
1WOU,ARG\_17,12.43,-0.07,0,0  
2IF4,LYS\_244,10.43,-0.07,0,0  
2D59,TYR\_93,12.35,0.38,0,1.97  
1W24,CYS\_15,7.83,-1.6,0,0.43  
1D2K,CYS\_108,9.13,-1.49,0.12,1.49  
1OLR,ARG\_220,12.08,-0.42,0,0  
3CSR,ASP\_112,3.8,0,0,0  
3M7D,GLU\_19,1.95,2.06,-2.7,-1.91  
4E6S,GLU\_78,4.57,0.07,0,0  
1PGV,GLU\_240,4.57,0.07,0,0  
1O0X,LYS\_92,10.01,-0.49,0,0  
3CGW,ARG\_99,11.81,-3.1,0,2.41  
1SNT,CYS\_352,11.15,-1.51,0,3.65  
1XKR,GLU\_155,4.34,0.07,-0.23,0  
2X5Y,ARG\_871,12.01,-0.49,0,0  
1QQH,ASP\_206,3.05,0.42,-1.18,0  
2FXT,GLU\_247,4.5,0,0,0  
3IL3,ASP\_233,3.44,0.49,-0.85,0  
1RIS,TYR\_194,8.6,0.81,-0.8,-1.41  
1UJ8,HIS\_5,6.43,0,0,-0.07  
1UJ8,ASP\_74,3.24,0.21,-0.77,0  
1ZCU,LYS\_201,10.43,-0.07,0,0  
3GFP,LYS\_305,10.43,-0.07,0,0  
1QZN,GLU\_8,4.71,0.21,0,0  
2HP7,LYS\_153,10.43,-0.07,0,0  
1R53,ASP\_166,3.68,0.7,-0.82,0  
3BB7,LYS\_114,10.5,0,0,0  
3HQX,ASP\_7,3.4,0.35,-0.75,0  
350A,GLU\_93,2.93,0.49,-2.06,0  
3AU3,GLU\_484,3.57,0.42,-1.35,0  
1UCH,GLU\_124,4.26,0.56,-0.8,0  
1O9G,LYS\_95,10.43,-0.07,0,0  
1QYI,HIS\_379,6.43,0.14,-0.21  
3BJV,TYR\_153,11.89,0,0,1.89  
2XHC,ARG\_126,12.5,0,0,0  
2BDV,LYS\_87,10.36,-0.14,0,0  
1UOH,GLU\_21,4.5,0,0,0  
1EV8,LYS\_229,10.43,-0.07,0,0  
1Q2Y,ASP\_14,3.38,0.42,-0.84,0  
3DB9,ARG\_189,11.94,-0.56,0,0  
3EJG,GLU\_135,4.29,0,-0.21,0  
1V8E,LYS\_140,10.5,0,0,0  
4H86,GLU\_29,4.57,0.07,0,0  
1MJS,GLU\_266,4.5,0,0,0  
2AZP,ARG\_291,11.59,-0.91,0,0  
2C2Y,ASP\_42,3.72,0.14,-0.22,0  
1SNT,HIS\_297,5.75,2.92,2.05,-5.72  
1RSQ,ARG\_69,12.43,-0.07,0,0  
2R51,LYS\_91,10.5,0,0,0  
2IDC,TYR\_22,9.63,2.22,-0.36,-2.23  
3RJX,TYR\_315,9.5,2.83,-1.48,-1.84  
2HNG,GLU\_90,4.57,0.07,0,0  
3EGN,LYS\_494,10.5,0,0,0  
2CXA,TYR\_210,10.57,0,0,0.57  
1ZBP,LYS\_232,10.15,-0.35,0,0  
2PGX,LYS\_51,10.5,0,0,0  
3COU,GLU\_11,4.02,0.35,-0.83,0  
2BT8,ASP\_176,3.73,0.42,-0.49,0  
1EYH,ASP\_138,3.73,0.07,-0.14,0  
1YLN,LYS\_67,10.22,-0.28,0,0  
2IDC,ASP\_154,2.84,0.98,-1.94,0  
1NFN,LYS\_95,10.5,0,0,0  
1SIG,TYR\_394,9.66,0.21,-0.55,0  
3IBT,TYR\_142,9.41,0,-0.59,0  
3M16,TYR\_52,12.15,0.96,-1.02,2.21  
4GCO,ARG\_183,13.36,-1.54,0,2.4  
1PBV,GLU\_120,4.5,0,0,0  
2QV2,ARG\_278,12.15,-0.35,0,0  
1RKA,GLU\_300,3.57,0.42,-1.35,0  
1PGV,ARG\_385,12.08,-0.42,0,0  
4EZB,ARG\_150,12.01,-0.49,0,0  
3RJZ,LYS\_218,10.36,-0.14,0,0  
2EFK,TYR\_53,10,0,0,0  
3RFY,ASP\_367,4.01,0.21,0,0  
2QHT,GLU\_108,4.5,0,0,0  
3ETV,GLU\_287,4.5,0,0,0  
2CXC,ARG\_144,12.08,-0.42,0,0  
1T3Y,HIS\_47,6.5,0,0,0  
3P51,ARG\_51,12.08,-0.42,0,0  
2B02,TYR\_456,11.55,0,-0.04,1.59  
4FZR,ARG\_378,11.8,-0.7,0,0  
2YX0,GLU\_137,4.5,0,0,0  
1DUPTYR\_23,10,0,0,0  
2D7U,GLU\_28,3.91,0.21,-0.8,0  
1LFP,ARG\_136,12.29,-0.21,0,0  
2AHE,TYR\_244,11.13,1.13,0,0  
3TMO,ARG\_244,12.15,-0.35,0,0  
3L3P,GLU\_129,4.57,0.07,0,0  
2AXO,ASP\_159,3.44,0.28,-0.64,0  
3C5V,LYS\_338,10.29,-0.21,0,0  
3RLN,CYS\_737,7.6,-0.55,-2.4,1.55  
3F7M,ARG\_230,11.94,-0.56,0,0  
1RSS,GLU\_129,4.57,0.07,0,0  
1XWM,TYR\_213,12.4,0.64,-0.75,2.51  
1RHS,HIS\_120,3.71,1.56,0,-4.35  
3OKQ,GLU\_611,4.57,0.07,0,0  
3EX9,GLU\_154,4.57,0.07,0,0  
1OIS,ARG\_294,12.43,-0.07,0,0  
3FK5,ARG\_149,12.29,-0.21,0,0  
3EYE,ARG\_234,11.87,-0.63,0,0  
4H4J,HIS\_44,6.43,0,0,-0.07  
3HVM,LYS\_123,10.08,-0.42,0,0  
1C3K,LYS\_60,10.22,-0.28,0,0  
2AHE,GLU\_92,3.61,1.32,-0.63,-1.58  
1V43,LYS\_353,10.29,-0.21,0,0  
2AH5,HIS\_144,6.36,0,0,-0.14  
2R51,LYS\_186,10.29,-0.21,0,0  
1LN4,GLU\_98,3.48,0.42,-1.44,0  
2D7J,HIS\_155,6.29,0,-0.21  
3M70,GLU\_152,4.5,0,0,0  
1YR6,GLU\_172,4.77,0.28,-0.01,0  
2FM9,LYS\_151,10.5,0,0,0  
2I88,ARG\_409,11.38,-1.12,0,0  
3NR5,GLU\_19,4.78,0.28,0,0  
2Q07,LYS\_284,10.5,0,0,0  
2X4L,GLU\_222,4.09,0.7,-1.11,0  
35MD,GLU\_65,5.76,1.13,-0.8,0.93  
1O5T,HIS\_129,2.45,0,-4.05  
1QQE,ARG\_110,12.29,-0.21,0,0  
2D0A,ARG\_308,12.15,-0.35,0,0  
1P1L,ARG\_17,12.15,-0.35,0,0  
2WB8,LYS\_664,10.5,0,0,0

2FPN,ASP\_58,3.88,0.56,-0.48,0  
 3GEC,ARG\_266,12.43,-0.07,0,0  
 3UX2,GLU\_74,4.57,0.07,0,0  
 2QHT,TYR\_13,11.61,1.9,-0.07,-0.21  
 2B61,ASP\_236,3.52,0.14,-0.42,0  
 2PGX,ASP\_28,3.69,0.63,-0.74,0  
 3BPP,LYS\_229,10.5,0,0,0  
 1YDL,HIS\_2,6.43,0,0,-0.07  
 1SQW,LYS\_62,10.43,-0.07,0,0  
 4EKU,CYS\_44,8.23,-0.67,-0.75,0.65  
 3H6Q,GLU\_168,4.5,0,0,0  
 1DOV,GLU\_158,3.98,0.28,-0.8,0  
 2ZOM,ARG\_175,11.51,-0.47,0,-0.52  
 3L3P,GLU\_446,0.98,0.97,-2.09,-2.4  
 1R6Y,ASP\_58,4.22,0.42,0,0  
 3US6,ARG\_8,11.8,-0.7,0,0  
 2EFK,ARG\_113,11.45,-1.05,0,0  
 1D2K,LYS\_97,10.36,-0.14,0,0  
 1R5Q,LYS\_38,10.5,0,0,0  
 3MTT,LYS\_589,10.5,0,0,0  
 1TUL,TYR\_81,10.01,0,0,0.01  
 1VSM,ARG\_137,12.01,-0.49,0,0  
 2POL,LYS\_171,10.5,0,0,0  
 2FBQ,ASP\_73,3.38,0.42,-0.84,0  
 2B2H,HIS\_134,4.02,1.69,0,-4.17  
 3QKY,ARG\_30,12.5,0,0,0  
 1TLV,ASP\_99,4.03,0.42,-0.19,0  
 2YLF,ARG\_197,12.22,-0.28,0,0  
 2Q99,GLU\_90,1.78,1.28,-1.6,-2.4  
 2A6B,ASP\_59,3.87,0.14,-0.07,0  
 1DOV,ARG\_194,11.94,-0.56,0,0  
 1ZBP,GLU\_193,5.15,0.28,0.36,0  
 2AD1,GLU\_210,4.45,0.28,-0.33,0  
 3V55,GLU\_588,4.5,0,0,0  
 2IQT,LYS\_31,10.36,-0.14,0,0  
 1OIS,GLU\_288,4.22,0.14,-0.42,0  
 3V3T,HIS\_137,4.14,1.23,0,-3.59  
 1FHL,GLU\_18,4.5,0,0,0  
 2D7U,GLU\_30,3.84,0.14,-0.8,0  
 3FHF,LYS\_21,10.29,-0.21,0,0  
 1XWM,ARG\_188,12.22,-0.28,0,0  
 2AHE,ARG\_219,11.45,-1.05,0,0  
 3PP8,ASP\_218,2.91,0.14,-1.03,0  
 3HUE,HIS\_47,3.61,0.8,0,-3.69  
 3LJI,LYS\_202,10.5,0,0,0  
 1QZN,ARG\_102,11.73,-0.77,0,0  
 3HVM,CYS\_98,9.78,-0.53,0,1.31  
 3CAX,HIS\_123,2.92,0,0,-3.58  
 4AM1,CYS\_23,5.23,-3.98,0,0.21  
 1MN3,CYS\_432,9.07,0,0,0.07  
 1UJ8,HIS\_7,6.83,0.4,0,-0.07  
 3F53,ARG\_105,12.15,-0.35,0,0  
 2HXB,TYR\_56,10,0,0,0  
 3IOO,LYS\_163,10.29,-0.21,0,0  
 1WXQ,ARG\_156,12.22,-0.28,0,0  
 3P51,TYR\_91,10.92,1.72,-0.8,0  
 1T3Y,GLU\_40,3.44,0.7,-1.76,0  
 3CGW,GLU\_273,4.64,0.14,0,0  
 1R6Y,HIS\_16,7.12,0.83,0,-0.21  
 1SQH,GLU\_265,4.5,0,0,0  
 2RFA,ARG\_180,11.8,-0.7,0,0  
 2IRM,CYS\_93,8.8,-0.2,0,0  
 3KEY,HIS\_435,6.43,0,0,-0.07  
 2GYZ,GLU\_76,4.15,0.14,-0.49,0  
 1ZP2,HIS\_147,6.5,0,0,0  
 3T5B,GLU\_179,3.91,0.21,-0.8,0  
 3GT0,GLU\_141,4.5,0,0,0  
 1RWZ,ARG\_155,11.94,-0.56,0,0  
 2B6P,HIS\_172,1.67,0.98,0,-5.81  
 2V5B,HIS\_96,1.66,0.97,-1.62,-4.19  
 1LFP,ARG\_114,12.15,-0.35,0,0  
 3GS9,GLU\_316,4.5,0,0,0  
 2W1R,GLU\_114,4.57,0.07,0,0  
 2X4L,ASP\_173,3.87,0.07,0,0  
 4DBX,ASP\_179,3.89,0.14,-0.05,0  
 3LJN,LYS\_195,10.5,0,0,0  
 1ZHV,ARG\_58,12.36,-0.14,0,0  
 3L7N,TYR\_129,10.35,0.07,0,0.28  
 1J74,ARG\_123,11.31,-1.19,0,0  
 2D7U,TYR\_155,10.14,0.14,0,0  
 3CAX,LYS\_272,9.8,-0.7,0,0  
 2ZTY,GLU\_5,4.5,0,0,0  
 1RAJ,ASP\_406,3.29,0.42,-0.93,0  
 4F85,HIS\_86,7.44,0.094,0  
 1X91,CYS\_136,11.03,0,0,2.03  
 1IAP,ARG\_191,11.94,-0.56,0,0  
 1X9G,ASP\_174,2.0,7,-2.5,0  
 2EJB,ARG\_37,12.36,-0.14,0,0  
 1LFP,LYS\_217,10.5,0,0,0  
 2D2S,GLU\_617,4.85,0.35,0,0  
 3ASA,ARG\_369,10.85,-3.58,0,1.93  
 3OIP,GLU\_25,4.54,0.35,-0.31,0  
 3UX2,CYS\_99,9.03,-0.04,0,0.07  
 3L7N,LYS\_110,10.22,-0.28,0,0  
 2D7U,ARG\_273,12.5,0,0,0  
 2P0L,GLU\_232,3.42,0.28,-1.36,0  
 1TR9,LYS\_309,10.29,-0.21,0,0  
 3EUR,LYS\_80,10.01,-0.49,0,0  
 1O0X,TYR\_65,8.83,0.08,-1.26,0  
 2CL3,TYR\_202,10.85,0,0,0.85  
 1FO9,LYS\_248,10.5,0,0,0  
 1A8Q,ASP\_229,3.25,0.28,-0.83,0  
 1YB2,GLU\_226,3.66,0.21,-1.05,0  
 2XMZ,ASP\_251,3.85,0.07,-0.02,0  
 2FL4,ARG\_120,12.01,-0.49,0,0  
 2X4L,ASP\_300,3.87,0.07,0,0  
 3CJW,ARG\_371,13.96,-0.77,0,2.23  
 3ANJ,LYS\_3,10.5,0,0,0  
 1FKM,GLU\_475,4.5,0,0,0  
 3HVM,LYS\_212,10.43,-0.07,0,0  
 1FQI,GLU\_345,5.0,35,0.15,0  
 2H85,HIS\_18,6.5,0,0,0  
 2B0J,LYS\_105,10.5,0,0,0  
 2ZQ5,ASP\_14,3.76,0,-0.04,0  
 2FM9,HIS\_243,6.5,0,0,0  
 3H04,CYS\_217,7.73,-2.36,0.55,0.53  
 1Q42,TYR\_38,7.66,0.75,-0.82,-2.28  
 1R6Y,HIS\_38,7.09,0.8,0,-0.21  
 2X4J,TYR\_83,11.84,1.84,0,0  
 3VHJ,ASP\_27,2.53,0.35,-1.62,0  
 3HVM,LYS\_179,10.5,0,0,0  
 2ZTY,ASP\_32,3.46,0.42,-0.76,0  
 3BJV,GLU\_124,4.71,0.21,0,0  
 2EFK,ARG\_196,12.5,0,0,0  
 3EYE,GLU\_97,4.19,0.49,-0.8,0  
 3OOP,GLU\_104,4.57,0.07,0,0  
 2CN1,TYR\_48,10,0,0,0  
 1O3X,LYS\_206,10.5,0,0,0  
 4H86,CYS\_31,6.85,-2.15,0,0  
 2RIK,GLU\_161,3.01,0.35,-1.84,0  
 1NJ4,ARG\_198,11.55,-0.95,0,0  
 1AIL,ASP\_2,3.78,0.07,-0.09,0  
 3JRT,HIS\_42,6.43,0,0,-0.07  
 1CHD,GLU\_213,4.19,0.49,-0.8,0  
 2H2W,LYS\_13,10.5,0,0,0  
 1YOY,LYS\_125,10.22,-0.28,0,0  
 3CGW,GLU\_23,4.01,0.28,-0.77,0  
 3K1H,GLU\_65,3.94,0.49,-1.05,0  
 4DBX,ASP\_175,3.3,0.42,-0.92,0  
 3ULX,ARG\_34,12.15,-0.35,0,0  
 3N2T,LYS\_255,10.15,-0.35,0,0  
 1QQE,TYR\_47,11.58,0.07,-0.02,1.54  
 2BDV,LYS\_75,10.22,-0.28,0,0  
 2EA9,TYR\_108,13.27,0.07,0.8,2.4  
 3V3T,GLU\_82,4.5,0,0,0  
 1JSX,HIS\_19,6.5,0,0,0  
 4EKU,LYS\_225,10.5,0,0,0  
 1YR6,LYS\_40,10.36,-0.14,0,0  
 3E0H,ASP\_126,3.94,0.21,-0.07,0  
 3E7P,HIS\_236,6.5,0,0,0  
 3BQE,HIS\_337,3.33,0,0,-3.17  
 2NSN,TYR\_97,10,0,0,0  
 3UC9,ARG\_93,12.01,-0.49,0,0  
 3IBT,LYS\_115,10.22,-0.28,0,0  
 2IF4,ASP\_212,3.78,0.07,-0.09,0  
 2D8N,TYR\_86,10.85,0.85,0,0  
 3CS1,GLU\_138,4.5,0,0,0  
 3RLE,GLU\_15,4.64,0.14,0,0  
 3MTT,ARG\_559,12.29,-0.21,0,0  
 3FRR,ARG\_164,12.08,-0.42,0,0  
 3ETU,LYS\_195,10.15,-0.35,0,0  
 3NR5,LYS\_40,10.5,0,0,0  
 3K8J,ASP\_134,3.35,0.35,-0.8,0  
 1QZN,ASP\_168,3.33,0.21,-0.67,0  
 3H13,GLU\_277,4.22,0.21,-0.49,0  
 2VGM,HIS\_325,5.21,2.23,0.28,-3.8  
 1MUF,GLU\_212,6.01,3.75,-3.11,0.87  
 1T6L,ASP\_106,2.25,0.49,-2.04,0  
 1ZHV,ARG\_39,11.73,-0.77,0,0  
 2AD1,HIS\_176,1.1,0.61,0,-6.01  
 2W1R,LYS\_60,10.36,-0.14,0,0  
 1O59,GLU\_99,1.77,2.15,-2.4,-2.47  
 4AM1,HIS\_262,4.1,0,0,-2.4  
 1O59,ARG\_337,8.64,-2.85,0,-1.01  
 3OIP,LYS\_222,10.5,0,0,0  
 1RWZ,GLU\_159,4.27,0.07,-0.3,0  
 2G5X,TYR\_210,9.25,0.22,-0.97,0  
 2OJQ,LYS\_473,10.5,0,0,0  
 4DIU,HIS\_234,3.06,0,0,-3.44  
 1AD6,HIS\_555,6.22,0,0,-0.28  
 3EJG,LYS\_96,10.5,0,0,0  
 3IBT,GLU\_184,4.15,0.88,-1.22,0  
 2O8P,ASP\_28,3.26,0.28,-0.82,0  
 2NRK,ARG\_72,12.36,-0.14,0,0  
 3EUR,LYS\_66,10.43,-0.07,0,0  
 2EFK,GLU\_156,4.14,0.21,-0.57,0  
 2FBI,ARG\_115,12.22,-0.28,0,0  
 3ODJ,ARG\_52,10.89,-1.61,0,0  
 3ETV,ARG\_279,11.55,-1.06,0,0.11  
 3CX2,HIS\_210,6.36,0,0,-0.14  
 3F6F,LYS\_20,10.5,0,0,0  
 3R87,LYS\_43,10.29,-0.21,0,0  
 4DBX,ASP\_42,4.15,0.35,0,0  
 3BQW,GLU\_167,4.5,0,0,0  
 1QQI,LYS\_100,10.43,-0.07,0,0  
 2YT4,GLU\_596,4.42,0.14,-0.22,0  
 3EVZ,GLU\_100,3.35,0.7,-1.85,0  
 1RKA,GLU\_203,4.11,0.14,-0.53,0  
 2G9D,ASP\_145,4.08,0.28,0,0  
 3RFY,ARG\_230,12.5,0,0,0  
 3T5B,ASP\_157,2.97,0.42,-1.25,0  
 3GG6,GLU\_109,3.42,0.42,-1.5,0  
 2H2Z,ASP\_92,2.54,0.49,-1.76,0  
 2H85,ARG\_90,13.73,-0.66,0,1.89  
 1ZP2,TYR\_182,10.52,0.02,0,0.5  
 3VJ8,ARG\_52,12.01,-0.49,0,0  
 1J33,ARG\_72,12.22,-0.28,0,0  
 1XIP,ARG\_153,12.5,0,0,0  
 2B3M,ASP\_139,3.77,0.21,-0.24,0  
 2BDV,HIS\_145,7.16,1.01,0,-0.35  
 3P28,HIS\_121,2.03,0,0,-4.47  
 2G55,GLU\_66,3.88,0.49,-1.11,0  
 2QEV,GLU\_1,3.98,0.28,-0.8,0  
 1D2K,TYR\_342,9.38,0.48,-1.1,0  
 1T3Y,ASP\_97,2.68,0.56,-1.68,0  
 1R16,GLU\_206,4.92,0.56,-0.14,0  
 1TR9,ARG\_313,11.8,-0.7,0,0  
 3DHN,GLU\_30,4.71,0.21,0,0  
 1X91,GLU\_3,4.57,0.07,0,0  
 4H4J,LYS\_184,10.29,-0.21,0,0  
 1X9G,LYS\_53,10.01,-0.49,0,0  
 3BWT,TYR\_603,10.86,0,0,0.86  
 3OBS,TYR\_42,10,0,0,0  
 3BQW,ASP\_112,2.89,0.63,-1.54,0  
 1UAJ,LYS\_45,10.5,0,0,0  
 3UAH,ASP\_217,2.95,0.56,-1.4,0  
 1Q46,ASP\_76,2.98,0.7,-1.52,0  
 2NMU,ASP\_51,2.61,0.42,-1.61,0  
 3V55,ASP\_716,3.28,0.28,-0.8,0  
 3ADO,GLU\_205,4.59,0.77,-0.68,0  
 3KT9,GLU\_32,4.48,0.07,-0.09,0  
 3ETU,GLU\_332,3.84,0.14,-0.8,0  
 2R0S,GLU\_309,4.03,0.14,-0.61,0  
 2R0S,TYR\_38,13.4,0.27,0.73,2.4  
 1X04,ASP\_107,3.94,0.14,0,0  
 3GEC,LYS\_485,10.5,0,0,0  
 2ZCX,ARG\_62,12.5,0,0,0  
 1YTQ,ARG\_159,12.5,0,0,0  
 1SNT,HIS\_300,6.15,0,0,-0.35  
 1YTD,ASP\_68,2.69,0.07,-1.18,0  
 2EHG,LYS\_91,10.22,-0.28,0,0  
 4DIU,CYS\_115,8.47,-2.88,0.3,2.04  
 2B2H,GLU\_387,4.64,0.14,0,0  
 1L2F,ARG\_117,12.08,-0.42,0,0  
 1D2K,LYS\_403,10.5,0,0,0  
 1LN4,GLU\_31,4.5,0,0,0  
 1QQL,GLU\_87,5.23,0.77,-0.04,0  
 1F2Y,GLU\_34,3.41,0.42,-1.51,0  
 1ZHV,GLU\_113,4.5,0,0,0  
 1H4U,GLU\_521,4.57,0.07,0,0  
 1WPA,GLU\_473,3.55,0.14,-1.1,0  
 3K8U,TYR\_77,11.69,0,0,1.69  
 2I88,LYS\_406,10.29,-0.21,0,0  
 2PGX,GLU\_76,0.59,0.82,-2.4,-2.33  
 3H04,ASP\_267,3.89,0.14,-0.05,0  
 3Q1C,ASP\_256,3.28,0.21,-0.73,0  
 3O7K,GLU\_50,4.71,0.21,0,0  
 2VAN,ARG\_328,11.94,-0.56,0,0  
 1ZYC,ARG\_144,11.52,-3.5,0,2.52  
 2FC3,GLU\_108,4.51,0.49,-0.48,0  
 4EZB,TYR\_279,13.04,0.56,-0.37,2.85  
 2D59,LYS\_88,10.5,0,0,0  
 2Q07,LYS\_355,10.5,0,0,0  
 3PP8,ARG\_227,11.54,-0.96,0,0  
 1O17,HIS\_140,6.36,0,0,-0.14  
 3OIP,TYR\_209,10,0,0,0  
 2FZP,ASP\_298,3.54,0.14,-0.39,0  
 3KV0,GLU\_17,3.47,0.21,-1.24,0  
 3IOC,ARG\_279,12.08,-0.42,0,0  
 2B78,LYS\_308,10.36,-0.14,0,0  
 2FZ4,HIS\_203,6.5,0,0,0  
 3EVZ,LYS\_231,9.94,-0.56,0,0  
 2FL4,ASP\_11,3.6,0.07,-0.27,0  
 2EDM,LYS\_145,10.15,-0.35,0,0  
 3LJI,LYS\_103,10.43,-0.07,0,0  
 3IPZ,GLU\_121,4.64,0.14,0,0



1IDK,TYR\_343,10,0,0,0  
1R53,GLU\_302,4.74,0.24,0,0  
2EJB,TYR\_130,10,0,0,0  
1AT0,GLU\_364,3.9,0.42,-1.02,0  
3M66,LYS\_267,10.5,0,0,0  
1O9G,ASP\_244,3.69,0.14,-0.25,0  
1O0X,GLU\_93,3.86,0.49,-1.13,0  
1Z3X,ARG\_209,12.29,-0.21,0,0  
2VGY,TYR\_52,10,0,0,0  
2PGX,HIS\_176,6.43,0,0,-0.07  
3UAH,TYR\_379,13.07,2,0,01,1.05  
2G5X,CYS\_115,9.9,0,0,0.9  
1R5Q,HIS\_91,7.71,1.35,0,-0.14  
2OEW,ASP\_316,3.92,0.14,-0.02,0  
3NOK,ARG\_124,12.15,-0.35,0,0  
3T8R,ARG\_106,12.29,-0.21,0,0  
1O5J,GLU\_91,3.71,0.35,-1.14,0  
1JT9,GLU\_10,4.4,0.14,-0.24,0  
1NAR,TYR\_178,10.38,0.38,0,0  
1DZF,CYS\_83,7.4,-2.26,0.19,0.47  
1JSX,GLU\_118,3.94,0.07,-0.63,0  
3E5T,ARG\_198,12.22,-0.28,0,0  
1QQE,GLU\_75,4.28,0,-0.22,0  
3CAX,ASP\_279,3.84,0.14,-0.1,0  
1BKB,GLU\_13,4.64,0.14,0,0  
2D2S,GLU\_626,4.64,0.14,0,0  
2CIU,LYS\_211,10.5,0,0,0  
2PLQ,GLU\_173,2.99,0.36,-1.87,0  
2E3C,LYS\_331,10.15,-0.35,0,0  
2ATR,ASP\_127,4.01,0.21,0,0  
2CN1,LYS\_95,9.52,-0.98,0,0  
1YTD,LYS\_320,10.08,-0.42,0,0  
1L2F,LYS\_95,10.5,0,0,0  
1DUP,ASP\_61,2.27,0.49,-2.02,0  
1X8F,GLU\_161,4.64,0.14,0,0  
1L3K,GLU\_114,4.08,0.56,-0.98,0  
3MIX,ASP\_551,2.62,0.49,-1.67,0  
3PP8,ARG\_169,12.01,-0.49,0,0  
1LPL,GLU\_223,4.64,0.14,0,0  
1UAJ,GLU\_18,4.78,0.28,0,0  
2DG7,ASP\_169,1.93,0.35,-2.43,0  
3UV9,LYS\_319,10.22,-0.28,0,0  
1DZF,GLU\_67,4.5,0,0,0  
1V43,GLU\_134,4.64,0.14,0,0  
2BAA,HIS\_17,8.22,1.93,0,-0.21  
2ZCX,CYS\_116,10.68,0,0,1.68  
2JHY,LYS\_113,10.22,-0.28,0,0  
2FBI,GLU\_118,4.64,0.14,0,0  
1MML,ASP\_209,3.5,0,-0.3,0  
1YTD,ASP\_9,3.59,0,-0.21,0  
2P1W,GLU\_215,4.44,0.35,-0.41,0  
2WOZ,ASP\_294,3.87,0.07,0,0  
3UX2,HIS\_112,6.74,0.32,0,-0.07  
2CN1,ARG\_71,11.45,-1.05,0,0  
2Z61,ASP\_64,3.063,-1.43,0  
1OLR,CYS\_206,7.34,-4.79,0,3.13  
1O9G,GLU\_109,3.61,0.63,-1.52,0  
3K8J,ARG\_167,12.43,-0.07,0,0  
1AD6,GLU\_465,4.05,0.35,-0.8,0  
3ETV,GLU\_130,1.74,0.44,-0.8,-2.4  
3RLN,GLU\_643,3.68,0.63,-1.45,0  
2Q13,GLU\_220,4.5,0,0,0  
3HQX,CYS\_104,12.85,0.4,2.4,1.05  
1S17,LYS\_251,10.01,-0.49,0,0  
3RKV,GLU\_232,4.57,0.07,0,0  
2PLQ,LYS\_181,10.01,-0.49,0,0  
3E5T,HIS\_214,4.69,0.2,0,-2.01  
2WOZ,GLU\_531,4.64,0.14,0,0  
3PAC,ASP\_146,3.46,0.91,-1.25,0  
3QKY,ARG\_261,12.01,-0.49,0,0  
3UC9,HIS\_109,6.87,0.58,0,-0.21  
3PU6,ASP\_78,2.41,0.42,-1.81,0  
1YTD,ASP\_232,1.35,0.77,-3.23,0  
2EJB,LYS\_172,10.5,0,0,0  
3DZ1,CYS\_163,9.81,-0.8,-0.51,2.12  
1O5T,TYR\_420,11.93,1.09,-1.56,2.4  
1R6Y,GLU\_64,5.29,1.59,-0.8,0  
3EYE,ARG\_139,12.22,-0.28,0,0  
3UPD,LYS\_88,10.5,0,0,0  
1AK1,GLU\_272,5.23,1.06,-0.1,-0.22  
1AM2,ARG\_181,11.8,-0.7,0,0  
2Q98,TYR\_185,11.04,0.8,-0.22,0.46  
3OIP,LYS\_50,10.29,-0.21,0,0  
2NRK,GLU\_17,4.57,0.07,0,0  
3FFM,ASP\_132,2.89,0.7,-1.6,0  
3K8J,GLU\_264,4.64,0.14,0,0  
3BPP,LYS\_195,10.22,-0.28,0,0  
3NR5,ASP\_95,3.74,0.14,-0.2,0  
3JRT,ARG\_86,12.05,-0.84,0,0.39  
2YWX,GLU\_41,3.84,0.7,-1.36,0  
3D9H,GLU\_42,3.81,0.21,-0.9,0  
1OTM,GLU\_74,2.67,0.49,-2.32,0  
1SIG,ARG\_363,12.43,-0.07,0,0  
3A7L,GLU\_113,4.57,0.07,0,0  
3GMS,LYS\_298,10.5,0,0,0  
2AHE,CYS\_100,8.27,-0.73,0,0  
2P0L,TYR\_210,10.26,0.14,-0.37,0.49  
3ZXY,ASP\_243,2.36,0.35,-1.79,0  
2B61,TYR\_80,10.27,0.51,-0.24,0  
1EQ6,CYS\_195,9.79,0,-0.13,0.92  
2CN1,LYS\_193,10.36,-0.14,0,0  
2H30,LYS\_111,10.36,-0.14,0,0  
3ZTA,ASP\_24,3.05,0.14,-0.89,0  
2FB6,LYS\_6,10.01,-0.49,0,0  
1V8E,ARG\_183,11.8,-0.7,0,0  
3K8J,LYS\_69,10.5,0,0,0  
3BCH,TYR\_139,10,0,0,0  
4HDE,LYS\_112,10.29,-0.21,0,0  
2Q99,LYS\_113,10.5,0,0,0  
1UAJ,CYS\_35,10.03,0,0,1.03  
1X04,ASP\_186,4.01,0.21,0,0  
3M70,GLU\_259,3.34,0.7,-1.86,0  
2D7U,GLU\_266,4.21,0.28,-0.57,0  
3MIX,TYR\_399,10.41,0.81,-0.82,0.42  
1GPP,ASP\_430,3.83,0.07,-0.04,0  
3ILC,ARG\_6,12.08,-0.42,0,0  
2QRX,TYR\_165,10,0,0,0  
2AZL,ASP\_102,3.7,0.14,-0.24,0  
4H89,LYS\_136,10.5,0,0,0  
3CX2,HIS\_257,7.16,0.8,0,-0.14  
4AM1,LYS\_33,10.29,-0.21,0,0  
2FC3,ASP\_106,3.94,0.21,-0.07,0  
3RNV,GLU\_449,3.88,0.07,-0.69,0  
2QEV,HIS\_124,6.5,0,0,0  
3MIX,ASP\_593,3.87,0.14,-0.07,0  
2OEW,LYS\_11,10.5,0,0,0  
2B3M,ASP\_69,2.63,0.42,-1.58,0  
3GW3,GLU\_97,4.5,0,0,0  
1XTD,TYR\_29,10.07,0.07,0,0  
3G9B,LYS\_63,10.43,-0.07,0,0  
3P51,GLU\_143,4.45,0.14,-0.19,0  
2E3H,TYR\_262,10.49,0.14,-1.93,2.29  
3LJI,HIS\_77,0.74,0,-2.4,-3.36  
1DCF,TYR\_133,10,0,0,0  
1BKB,GLU\_111,3.91,0.21,-0.8,0  
2JHY,LYS\_186,10.5,0,0,0  
2GZQ,LYS\_39,9.94,-0.56,0,0  
4EKU,GLU\_34,4.64,0.14,0,0  
3LQE,GLU\_456,2.59,1.09,-3.01,0  
1YMS,CYS\_173,10.51,-0.06,-0.44,2.01  
3JV1,HIS\_181,6.5,0.07,0,-0.07  
2OGQ,ASP\_416,1.66,0.63,-2.77,0  
3CO1,TYR\_32,10.86,1.57,-0.71,0  
1XIP,GLU\_236,3.99,0.14,-0.65,0  
2B61,HIS\_268,2.76,0.08,0,-3.82  
3R87,CYS\_112,9.18,-0.17,0,0.35  
3H13,TYR\_464,10.07,0.07,0,0  
1ZKZ,GLU\_33,3.52,0.98,-1.96,0  
1S17,LYS\_213,10.5,0,0,0  
2BLL,ARG\_418,12.15,-0.35,0,0  
3FK5,ARG\_163,12.01,-0.49,0,0  
1O9G,ARG\_5,11.87,-0.63,0,0  
3SMD,GLU\_31,4.5,0,0,0  
1NRI,ASP\_25,3.27,0.42,-0.94,0  
2EAG,ARG\_26,11.59,-0.91,0,0  
1O17,ASP\_274,3.35,0.35,-0.8,0  
1QY1,LYS\_333,10.15,-0.35,0,0  
1FKM,ASP\_438,1.72,0.7,-2.78,0  
1SJJ,ARG\_150,11.8,-0.7,0,0  
3H5T,ARG\_174,12.29,-0.21,0,0  
3IL3,GLU\_205,4.57,0.07,0,0  
1RHS,ARG\_44,12.29,-0.21,0,0  
3OOP,ARG\_2,12.5,0,0,0  
2AZP,ARG\_5,11.59,-0.91,0,0  
2H14,LYS\_291,10.5,0,0,0  
3BQE,ASP\_285,2.43,0.28,-0.86,-0.79  
3QAV,ASP\_31,3.58,0.21,-0.43,0  
1AK1,HIS\_70,6.53,0.1,0,-0.07  
3NZL,HIS\_8.6,15,0,0,-0.35  
1P1L,GLU\_99,4.64,0.14,0,0  
1N81,ASP\_171,3.8,0,0,0  
3ONH,GLU\_467,4.5,0,0,0  
1AD6,TYR\_403,13.34,0.14,0.8,2.4  
1YOY,ASP\_115,2.33,0.49,-1.96,0  
2H85,GLU\_339,4.34,0.21,-0.37,0  
2OOK,TYR\_87,11.81,0.07,-0.67,2.4  
4DEZ,ASP\_120,3.2,0.42,-1.02,0  
3O16,TYR\_231,11.89,0,0,1.89  
3M70,LYS\_207,10.43,-0.07,0,0  
2H85,LYS\_334,10.5,0,0,0  
1O0X,ASP\_230,2.53,0.42,-1.68,0  
3LPZ,LYS\_260,10.5,0,0,0  
2XHC,TYR\_113,11.2,0.21,-1.4,2.4  
1YTD,ASP\_132,3.39,0.14,-0.55,0  
3P28,HIS\_91,4.87,0.35,0,-1.98  
3JSN,ARG\_99,12.01,-0.49,0,0  
1VSM,LYS\_129,10.15,-0.35,0,0  
3UV9,ARG\_325,12.29,-0.21,0,0  
3ODJ,ARG\_129,11.38,-1.12,0,0  
3V55,GLU\_696,4.5,0,0,0  
1PZ3,ASP\_47,4.15,0.35,0,0  
3FTT,HIS\_119,6.36,0,0,-0.14  
2GEN,HIS\_44,6.5,0,0,0  
2V4U,HIS\_439,6.52,0.23,0,-0.21  
2YX0,HIS\_342,6.5,0,0,0  
3EAZ,LYS\_76,10.5,0,0,0  
2D7U,ARG\_34,9.21,-4.03,0.74  
1ILW,ARG\_62,12.01,-0.49,0,0  
3BB7,TYR\_208,9.61,0.73,-1.82,0.69  
1V43,TYR\_70,13.28,0.07,0,3.21  
2BDD,GLU\_42,4.64,0.14,0,0  
2XSY,GLU\_808,3.24,2.82,-3.51,-0.57  
2HRZ,HIS\_4,6.5,0,0,0  
2YLF,ARG\_81,11.8,-0.7,0,0  
2EHG,ARG\_141,12.5,0,0,0  
1XFK,HIS\_185,6.9,0.47,0,-0.07  
1SJB,GLU\_759,4.38,0.21,-0.33,0  
3AUF,ARG\_91,12.01,-0.49,0,0  
4DIU,GLU\_109,3.66,0.21,-1.05,0  
2FL4,TYR\_86,13.27,0.07,0.8,2.4  
2D0A,LYS\_50,10.15,-0.35,0,0  
2IF4,LYS\_104,10.29,-0.21,0,0  
3ASA,CYS\_148,9,-1.9,0,1.9  
2Q12,GLU\_27,3.25,0.35,-1.6,0  
1GQE,ASP\_79,3.92,0.21,-0.09,0  
2XMZ,GLU\_217,2.98,0.35,-1.87,0  
2Q13,ARG\_275,12.08,-0.42,0,0  
1VSM,ASP\_174,3.93,0.14,-0.01,0  
4ETX,TYR\_204,10.67,0.67,0,0  
3DZ1,ARG\_190,12.12,-0.89,0,0.51  
3AU3,ASP\_512,3.15,0.77,-1.42,0  
2IDC,ASP\_52,3.77,0.14,-0.17,0  
2FZ4,TYR\_179,12.96,1.31,-0.04,1.69  
3E27,ARG\_96,12.01,-0.49,0,0  
1QQE,LYS\_271,10.5,0,0,0  
4FH3,CYS\_105,7.7,-2.53,0,1.23  
1R3F,GLU\_211,3.74,0.28,-1.04,0  
3OIP,ASP\_23,3.25,0.42,-0.97,0  
3IBT,GLU\_207,4.24,0.42,-0.68,0  
3E27,ARG\_96,12.01,-0.49,0,0  
2NRK,TYR\_77,13.62,0.75,0.47,2.4  
3L3P,ASP\_384,3.64,0.28,-0.44,0  
1OLR,TYR\_37,10,0,0,0  
1T07,LYS\_64,10.5,0,0,0  
2E3C,LYS\_336,10.36,-0.14,0,0  
1YB2,ASP\_126,3.76,0,-0.04,0  
1IDK,TYR\_34,11.48,0,0,1.48  
3U56,HIS\_79,6.43,0,0,-0.07  
2QOP,HIS\_15,6.66,0.16,0,0  
2I6I,GLU\_20,3.39,0.63,-1.74,0  
2B61,LYS\_137,10.29,-0.21,0,0  
2V4U,LYS\_417,10.15,-0.35,0,0  
3U2R,ARG\_68,12.43,-0.07,0,0  
3FXH,HIS\_25,6.43,0,0,-0.07  
3BCH,ASP\_31,2.94,0.35,-1.22,0  
1ZBS,GLU\_40,4.1,0.49,-0.89,0  
1U3Y,GLU\_293,3.98,0.42,-0.94,0  
3ERF,CYS\_206,8.22,-0.78,0,0  
1LTU,HIS\_126,6.36,0,0,-0.14  
3I4T,ARG\_18,12.5,0,0,0  
2WB3,LYS\_385,10.5,0,0,0  
1FHL,TYR\_22,10.65,1.55,-0.9,0  
2QK1,LYS\_549,9.8,-0.7,0,0  
1WYC,ASP\_72,3.94,0.14,0,0  
2DVK,ARG\_30,12.43,-0.07,0,0  
2EFK,GLU\_12,3.04,0.28,-1.74,0  
1EV8,ARG\_225,11.59,-0.91,0,0  
2A4D,LYS\_205,10.5,0,0,0  
2OB5,ASP\_12,3.14,0.14,-0.8,0  
2QZQ,ARG\_116,12.43,-0.07,0,0  
3IDW,ARG\_21,12.01,-0.49,0,0  
3I47,TYR\_149,9.78,0.14,-0.36,0  
4DIU,LYS\_156,10.22,-0.28,0,0  
2YWX,LYS\_75,10.22,-0.28,0,0  
1R15,LYS\_115,10.5,0,0,0  
1YMS,LYS\_243,9.94,-0.56,0,0  
2QV2,HIS\_185,4.05,0.01,0,-2.46  
4F8A,TYR\_684,10,0,0,0  
4DVD,GLU\_109,4.5,0,0,0  
1G5Z,ASP\_124,3.2,0.42,-1.02,0  
2C2Y,ARG\_202,11.73,-0.77,0,0  
2P52,LYS\_232,10.29,-0.21,0,0  
1Z9L,LYS\_19,10.5,0,0,0  
2YWX,LYS\_126,10.5,0,0,0  
2XMZ,GLU\_126,4.78,0.28,0,0  
3CBN,ARG\_100,11.94,-0.56,0,0



3GOZ,ASP\_149,3.62,0.49,-0.66,0  
3E7P,ARG\_159,11.45,-1.05,0,0  
3GA2,LYS\_149,10.36,-0.14,0,0  
2P52,LYS\_162,10.08,-0.42,0,0  
1SN7,ARG\_83,12.08,-0.42,0,0  
3U2R,GLU\_138,3.98,0.28,-0.8,0  
3M7D,ARG\_93,12.22,-0.28,0,0  
4EZB,GLU\_50,4.5,0,0,0  
1P6F,TYR\_37,8.65,0.48,-1.83,0  
2E3I,GLU\_62,3.73,0.98,-1.74,0  
1P2F,ASP\_177,3.87,0.07,0,0  
1WXQ,ARG\_377,12.01,-0.49,0,0  
3M7G,GLU\_213,4.23,0.35,-0.62,0  
3IU5,ARG\_66,12.15,-0.35,0,0  
2WZ9,LYS\_96,10.5,0,0,0  
3FNI,CYS\_57,10.42,-0.01,0,1.43  
2H2Z,HIS\_64,6.36,0,0,-0.14  
2VGM,GLU\_361,4.5,0,0,0  
4FLE,GLU\_168,3.35,0.35,-1.5,0  
2WOZ,HIS\_440,4.69,4.11,0,-5.91  
2H85,GLU\_228,4.21,0.42,-0.71,0  
3LPZ,ASP\_116,2.61,0.35,-1.54,0  
3CS1,GLU\_160,4.05,0.35,-0.8,0  
1YTD,ASP\_302,4.01,0.21,0,0  
2QHT,GLU\_54,4.07,0.14,-0.57,0  
1GPP,TYR\_154,11.48,0.07,-0.41,1.82  
1V6T,ASP\_134,2.02,0.63,-2.41,0  
1SNT,LYS\_370,10.5,0,0,0  
1U3Y,GLU\_341,4.57,0.07,0,0  
3DZ1,LYS\_70,10.29,-0.21,0,0  
3L7N,LYS\_79,10.22,-0.28,0,0  
3OIP,ASP\_102,3.07,0.7,-1.42,0  
2OJQ,ASP\_591,4.15,0.35,0,0  
2IRM,ASP\_36,3.87,0.07,0,0  
3BZT,LYS\_321,10.15,-0.35,0,0  
2IN0,ARG\_43,11.94,-0.56,0,0  
3EVN,ASP\_79,4.17,0.42,-0.05,0  
3CAN,LYS\_116,10.22,-0.28,0,0  
3KB5,LYS\_317,10.5,0,0,0  
1Y2Q,GLU\_69,4.64,0.14,0,0  
1EDG,ARG\_172,11.19,-2.05,0,0.74  
2Q13,ARG\_154,12.5,0,0,0  
2F8H,ARG\_244,11.94,-0.56,0,0  
3GEC,TYR\_335,9.38,0.07,-0.69,0  
1160,LYS\_265,10.36,-0.14,0,0  
2Z61,LYS\_59,10.08,-0.42,0,0  
1OST,ARG\_388,11.94,-0.56,0,0  
2QVT,ASP\_140,3.67,0.07,-0.19,0  
3V55,LYS\_702,10.36,-0.14,0,0  
2O4D,ARG\_41,13.51,-1.39,0,2.4  
2NYC,ARG\_264,11.8,-0.7,0,0  
2R0S,GLU\_305,4.19,0.28,-0.59,0  
2P4D,LYS\_51,10.22,-0.28,0,0  
3JRT,HIS\_105,6.29,0,0,-0.21  
3LJN,LYS\_66,10.29,-0.21,0,0  
1LZL,GLU\_10,3.83,0.49,-1.16,0  
2H2Z,TYR\_237,10.14,0.14,0,0  
3F53,ASP\_80,3.37,0.28,-0.71,0  
3KEY,TYR\_337,13.14,0,-0.05,3.19  
2BOA,LYS\_67,9.73,-0.77,0,0  
4DBX,ASP\_174,3.03,0.14,-0.91,0  
1D7O,TYR\_87,9.03,0.14,-1.11,0  
4D8L,TYR\_239,13.4,0.07,0.68,2.66  
2ZTY,ARG\_13,12.22,-0.28,0,0  
2ZCX,ARG\_128,12.15,-0.35,0,0  
4ACJ,TYR\_769,10.07,0.07,0,0  
2IQT,ARG\_153,12.29,-0.21,0,0  
3C2E,LYS\_292,10.22,-0.28,0,0  
1UCH,CYS\_95,2.68,-5.95,-1.87,1.49  
2D7U,HIS\_331,6.36,0,0,-0.14  
1GQE,ARG\_60,12.22,-0.28,0,0  
2FL4,HIS\_145,6.29,0,0,-0.21  
1R5S,ASP\_140,2.68,0.56,-1.68,0  
3CNU,LYS\_109,10.43,-0.07,0,0  
3RLE,ASP\_148,1.49,0.84,-3.15,0  
3O16,ASP\_94,2.18,0.42,-2.04,0  
3IU5,TYR\_60,9.92,0,-0.08,0  
2WB8,HIS\_746,2,0.54,-2.09,-2.95  
1R3F,TYR\_199,10.07,0.07,0,0  
3M70,LYS\_117,10.43,-0.07,0,0  
3GYW,TYR\_53,12.67,0,0.37,2.29  
2YWJ,ARG\_106,12.22,-0.28,0,0  
3FK5,GLU\_172,4.5,0,0,0  
1X8F,ARG\_168,10.28,-1.73,0,-0.49  
3CSR,LYS\_120,10.22,-0.28,0,0  
1S17,HIS\_82,6.5,0,0,0  
3CCY,LYS\_122,10.43,-0.07,0,0  
2FBQ,LYS\_21,10.36,-0.14,0,0  
3R2E,GLU\_8,4.5,0,0,0  
2R0S,ASP\_299,1.82,0.42,-2.4,0  
2PGX,ASP\_201,2.66,0.14,-1.28,0  
3SMD,LYS\_132,10.29,-0.21,0,0  
4FD6,LYS\_215,10.36,-0.14,0,0  
3IVF,ASP\_110,3.15,0.07,-0.72,0  
2P4D,LYS\_128,10.22,-0.28,0,0  
1TUL,LYS\_94,10.5,0,0,0  
1R1S,ARG\_64,12.36,-0.14,0,0  
3OBS,CYS\_73,8.49,-1.6,0,1.09  
3LOD,HIS\_116,6.5,0,0,0  
1YTQ,ARG\_190,11.52,-0.98,0,0  
1ZP2,CYS\_82,11.8,0,0,2.8  
2EA9,GLU\_74,3.92,0.21,-0.79,0  
2G9D,TYR\_164,8.04,0.07,-2.02,0  
1X04,GLU\_166,3.91,0.21,-0.8,0  
4GA2,CYS\_141,8.59,-0.48,0,0.07  
2Q13,LYS\_119,10.5,0,0,0  
1X04,LYS\_205,10.5,0,0,0  
3ZTA,GLU\_143,4.73,0.28,-0.05,0  
1R1S,ARG\_183,12.82,-2,0,2.32  
3SMD,GLU\_69,3.87,0.17,-0.8,0  
2Z61,ASP\_112,3.67,0.14,-0.27,0  
1XKR,GLU\_35,3.84,0.14,-0.8,0  
3IL3,GLU\_41,4.64,0.14,0,0  
2X4G,GLU\_230,4.05,0.35,-0.8,0  
4EZB,HIS\_87,7.23,0.87,0,-0.14  
1JYH,ASP\_56,3.8,0,0,0  
2W2S,GLU\_48,4.5,0,0,0  
1160,LYS\_138,10.5,0,0,0  
3RE9,GLU\_199,4.5,0,0,0  
3GS9,ASP\_4,4.01,0.21,0,0  
3RLN,LYS\_621,9.94,-0.56,0,0  
1PSW,CYS\_186,11.63,-0.4,0.3,0.03  
3BB7,GLU\_72,4.5,0,0,0  
4AF2,GLU\_156,3.98,0.28,-0.8,0  
1RAJ,HIS\_320,6.43,0,0,-0.07  
3ERF,LYS\_149,10.5,0,0,0  
3PP8,ARG\_266,11.94,-0.56,0,0  
1EYH,HIS\_15,6.5,0,0,0  
3B7X,GLU\_45,4.71,0.21,0,0  
2OKT,GLU\_174,0.85,0.72,-0.89,-3.48  
3HYQ,GLU\_87,3.2,1.5,-0.8,-2.85  
2FG1,TYR\_5,13.55,0.35,0.8,2.4  
2BLL,LYS\_382,10.36,-0.14,0,0  
1NWA,ARG\_147,11.52,-0.98,0,0  
3JSN,GLU\_51,4.22,0.77,-1.05,0  
1KN3,ARG\_26,11.94,-0.56,0,0  
2R0S,ASP\_67,3.3,0.35,-0.85,0  
3RRQ,TYR\_121,10.03,0.95,-0.08,-0.84  
1WNH,GLU\_191,3.91,0.14,-0.73,0  
2R0S,LYS\_57,10.5,0,0,0  
2X4L,GLU\_277,3.74,0.21,-0.97,0  
1H4U,ASP\_511,2.24,0.91,-2.47,0  
2PP6,GLU\_73,4.5,0.28,-0.28,0  
2B3M,LYS\_27,10.22,-0.28,0,0  
3DZ1,HIS\_168,2.99,0.45,-0.17,-3.8  
2G9D,TYR\_260,9.58,0.19,-0.61,0  
3EUR,GLU\_89,3.92,0.49,-1.07,0  
2YT4,GLU\_534,4.5,0,0,0  
2Q98,HIS\_180,6.5,0,0,0  
1OIS,TYR\_170,10.9,0.21,-2.2,2.88  
4HDE,LYS\_107,10.08,-0.42,0,0  
3AU3,CYS\_607,9.78,-0.33,0,1.11  
3I0C,LYS\_75,10.15,-0.35,0,0  
2W2S,ARG\_87,12.08,-0.42,0,0  
3GW3,GLU\_167,3.35,0.91,-2.06,0  
3BZT,CYS\_269,9.12,-1.73,0,1.85  
1XEU,GLU\_221,4.57,0.07,0,0  
1SIG,HIS\_180,8.05,1.6,2.53,-2.58  
2O4D,GLU\_66,2.45,0.35,-2.4,0  
1ZYL,ARG\_305,11.94,-0.56,0,0  
2CXA,LYS\_83,10.5,0,0,0  
3ANJ,GLU\_83,1.82,1.86,-2.14,-2.4  
2GZQ,CYS\_187,10.55,-0.21,0,1.76  
2YX0,ARG\_265,12.15,-0.35,0,0  
2CXA,GLU\_17,3.84,0.14,-0.8,0  
2D0A,HIS\_78,6.43,0,0,-0.07  
3HNX,HIS\_0,7.31,0.88,0,-0.07  
3UPD,ARG\_8,11.73,-0.77,0,0  
3PZ9,TYR\_366,10.99,0,0.99  
3EOD,HIS\_72,6.43,0,0,-0.07  
2D7U,GLU\_216,4.54,0.3,0,-0.26  
2B6P,ASP\_150,0.41,1.12,-4.5,0  
2BQQ,ASP\_134,4.48,0.7,-0.02,0  
1UAJ,LYS\_206,10.29,-0.21,0,0  
2F9F,LYS\_130,10.5,0,0,0  
1DUPL,LYS\_8,10.43,-0.07,0,0  
3P2F,TYR\_22,11.33,1.18,-1.07,1.22  
3CGW,GLU\_242,4.64,0.14,0,0  
1F09,ARG\_179,12.08,-0.42,0,0  
1XFK,ARG\_24,11.52,-0.98,0,0  
4DNU,GLU\_345,3.65,0.35,-1.2,0  
3LQE,ASP\_313,2.04,0.49,-2.25,0  
1CHD,LYS\_340,10.22,-0.28,0,0  
2Q13,GLU\_14,3.84,0.14,-0.8,0  
1PV5,GLU\_21,3.95,0.14,-0.69,0  
1YR6,ARG\_117,12.22,-0.28,0,0  
4DBX,GLU\_129,4.19,0.49,-0.8,0  
1AT0,GLU\_277,4.19,0.21,-0.52,0  
3RLE,GLU\_78,4.5,0,0,0  
3G9G,ASP\_178,1.89,0.49,-2.4,0  
2Q34,HIS\_220,6.5,0,0,0  
2E3C,GLU\_337,4.45,0.35,-0.4,0  
2ILR,LYS\_491,10.5,0,0,0  
2B3M,ARG\_41,12.29,-0.21,0,0  
1IAP,GLU\_132,4.51,0.07,-0.06,0  
2CL3,TYR\_24,10,0,0,0  
4EKU,LYS\_216,10.5,0,0,0  
2A6B,GLU\_161,4.5,0,0,0  
3DSH,ARG\_353,11.59,-0.91,0,0  
3I4T,GLU\_201,2.27,1.12,-3.34,0  
2CWC,TYR\_220,13.48,0.28,0.8,2.4  
2HRZ,HIS\_227,0.22,0,-1.47,-4.81  
1OSJ,GLU\_98,4.78,0.28,0,0  
3EVZ,GLU\_115,4.49,0.07,-0.08,0  
1RHS,GLU\_172,4.5,0,0,0  
2CXA,LYS\_183,10.5,0,0,0  
1OLR,HIS\_188,4.18,0,0,-2.32  
1R9W,HIS\_306,6.43,0,0,-0.07  
2E3I,LYS\_123,10.5,0,0,0  
3EVZ,LYS\_229,10.29,-0.21,0,0  
1ZBP,ARG\_222,11.73,-0.77,0,0  
2QK1,ASP\_457,3.12,0.35,-1.03,0  
3OKQ,HIS\_630,6.43,0,0,-0.07  
1F09,ARG\_387,11.52,-0.98,0,0  
3H8Y,ARG\_38,12.22,-0.28,0,0  
2P1W,GLU\_205,4.38,0.21,-0.33,0  
2XMZ,GLU\_8,4.71,0.21,0,0  
1J79,ASP\_113,3.02,0.35,-1.12,0  
3OBS,LYS\_14,10.5,0,0,0  
3C6B,TYR\_38,10.09,0.09,0,0  
2C2Y,ASP\_196,3.51,0.21,-0.5,0  
2CVB,HIS\_132,10.3,2.3,3.86,-3.56  
2YX0,ASP\_220,2.7,0.49,-1.58,0  
3IU5,GLU\_64,6.0,0.14,0,0  
2IQT,LYS\_145,10.36,-0.14,0,0  
3V55,GLU\_568,4.5,0,0,0  
2Z61,ASP\_114,2.56,0.7,-1.94,0  
3LH5,ARG\_645,9.99,-2.51,0,0  
4E8B,ARG\_30,11.38,-1.12,0,0  
1517,ASP\_100,3.43,0.63,-1.0  
3A7L,HIS\_13,4.26,0,0,-2.24  
2CBE,LYS\_225,10.36,-0.14,0,0  
4F8A,ASP\_675,3.63,0.14,-0.32,0  
1PV5,GLU\_55,4.71,0.21,0,0  
1O9G,ARG\_74,11.38,-1.12,0,0  
2OKT,GLU\_134,4.57,0.07,0,0  
2EEY,GLU\_148,4.11,0.35,-0.74,0  
2OB5,TYR\_110,10.33,0.33,0,0  
3MTT,HIS\_450,6.62,0.19,0,-0.07  
2C2Y,HIS\_245,6.36,0,0,-0.14  
4GCO,ARG\_205,12.29,-0.21,0,0  
1E59,HIS\_195,5.65,0.8,0,-1.65  
1KCM,HIS\_226,1.03,0,-0.39,-5.08  
1XTZ,ARG\_83,12.36,-0.14,0,0  
3LOD,CYS\_62,10,-0.44,0,1.44  
3ASA,TYR\_71,10,0,0,0  
2IF4,ASP\_247,3.87,0.07,0,0  
1TUL,LYS\_36,10.5,0,0,0  
3CNU,GLU\_44,4.67,0.14,0.03,0  
2ZTY,TYR\_31,11.28,0.07,-0.01,1.22  
2OEW,TYR\_29,13.12,0.21,0.51,2.4  
1C3K,ASP\_66,2.94,0.14,-1,0  
2W2S,LYS\_60,10.43,-0.07,0,0  
3P8B,LYS\_32,10.29,-0.21,0,0  
1DVO,TYR\_161,9.94,0,-0.06,0  
1NFN,ARG\_119,11.66,-0.84,0,0  
2EJX,ASP\_100,3.15,0.63,-1.28,0  
3VJ8,ARG\_148,12.08,-0.42,0,0  
2BLL,CYS\_420,11.12,-0.15,0.2,2.27  
3GYW,ASP\_275,3.99,0.21,-0.02,0  
2CXC,LYS\_59,10.5,0,0,0  
1RKA,ARG\_131,11.73,-0.77,0,0  
2BQQ,ARG\_102,11.94,-0.56,0,0  
3BCY,HIS\_108,6.43,0,0,-0.07  
2AXO,LYS\_196,10.29,-0.21,0,0  
2P1W,ARG\_148,12.29,-0.21,0,0  
3H5T,GLU\_257,3.84,0.14,-0.8,0  
3GYW,TYR\_79,10.04,0.39,0,-0.35  
3GW3,CYS\_66,7.84,-1.63,0,0.47  
1GPP,ARG\_94,12.22,-0.28,0,0  
1N81,LYS\_147,10.5,0,0,0  
2GZR,ASP\_59,3.21,0.21,-0.8,0  
3HVM,HIS\_130,6.22,0,0,-0.28  
4HDE,LYS\_56,10.43,-0.07,0,0  
2CXC,ASP\_112,3.87,0.07,0,0  
3CAX,LYS\_206,10.22,-0.28,0,0

2QDJ,ARG\_320,12.01,-0.49,0,0  
 3RFF,ARG\_155,11.94,-0.56,0,0  
 4E5S,GLU\_141,3.88,0.21,-0.83,0  
 2V4U,ARG\_479,12.36,-0.14,0,0  
 3P28,HIS\_188,6.62,0.26,-0.14  
 2OPJ,ARG\_288,12.29,-0.21,0,0  
 2FG1,GLU\_48,3.91,0.21,-0.8,0  
 2BDD,LYS\_79,10.5,0,0,0  
 1YLN,CYS\_56,9.61,0,0,0.61  
 3V55,GLU\_437,3.48,0.21,-1.23,0  
 2CIU,ARG\_152,11.52,-0.98,0,0  
 2EDM,ASP\_196,3.39,0.49,-0.9,0  
 2P4D,GLU\_131,4.5,0,0,0  
 1F2V,ARG\_29,11.73,-0.77,0,0  
 1J33,ARG\_207,12.43,-0.07,0,0  
 3ASA,ASP\_341,3.58,0.07,-0.29,0  
 2HP7,ARG\_94,12.36,-0.14,0,0  
 3M3P,ASP\_40,2.98,0.42,-1.24,0  
 2J8A,LYS\_273,10.43,-0.07,0,0  
 1YR6,CYS\_244,9.93,0.79,0.14  
 4FCU,ARG\_170,12.43,-0.07,0,0  
 3AU3,GLU\_422,4.5,0,0,0  
 1HUF,ASP\_22,3.43,0.49,-0.86,0  
 3IL3,TYR\_87,10,0,0,0  
 3COU,HIS\_109,1.26,0,-1.53,-3.71  
 1OXZ,TYR\_253,13.41,0.21,0.8,2.4  
 1J33,GLU\_196,4.5,0,0,0  
 1F09,ARG\_117,12.43,-0.07,0,0  
 1WXQ,LYS\_114,10.43,-0.07,0,0  
 1R53,GLU\_64,4.57,0.07,0,0  
 1KCM,ARG\_245,11.87,-0.63,0,0  
 1PVT,HIS\_92,5.5,0.88,0,-1.88  
 3D9H,HIS\_69,6.43,0,0,-0.07  
 4H89,HIS\_155,6.29,0,0,-0.21  
 1TR9,CYS\_267,10.84,0,0,1.84  
 1XIP,LYS\_195,10.01,-0.49,0,0  
 2OKT,LYS\_261,10.29,-0.21,0,0  
 1W7B,LYS\_310,10.15,-0.35,0,0  
 3JZN,TYR\_278,13.44,0.81,0.23,2.4  
 4DEZ,GLU\_85,4.5,0,0,0  
 1YTD,ASP\_70,3.03,0.49,-1.27,0  
 1QQE,GLU\_128,0.96,0.89,-2.03,-2.4  
 1AD6,ARG\_467,12.08,-0.42,0,0  
 3CX2,LYS\_244,10.5,0,0,0  
 3RLE,GLU\_110,4.52,0.14,-0.12,0  
 3ADO,ARG\_314,11.87,-0.63,0,0  
 3CAX,GLU\_268,4.71,0.21,0,0  
 3G9G,GLU\_20,4.05,0.35,-0.8,0  
 3M7G,GLU\_190,4.5,0,0,0  
 3FRR,CYS\_125,8.98,-0.99,0.26,0.7  
 1D2K,LYS\_358,10.29,-0.21,0,0  
 1H09,ASP\_234,2.04,0.98,-2.75,0  
 3K1H,ASP\_68,2.21,0.49,-2.09,0  
 1RWZ,ARG\_26,11.17,-1.33,0,0  
 3C38,GLU\_228,2.1,1.12,-3.52,0  
 3IDW,LYS\_2,10.5,0,0,0  
 1WRU,ARG\_265,13.55,-1.6,0.2,6.5  
 3MEW,GLU\_231,4.5,0,0,0  
 3IVF,LYS\_274,10.5,0,0,0  
 3ERF,ARG\_219,13.91,-0.99,0.2,4  
 3V46,LYS\_368,10.5,0,0,0  
 1NRI,CYS\_254,7.63,-1.45,0,0.07  
 3G9T,ASP\_182,3.8,0,0,0  
 3L0D,TYR\_124,11.99,1.99,0,0  
 3B4D,ARG\_172,11.8,-0.7,0,0  
 2VGM,LYS\_293,10.36,-0.14,0,0  
 3RVC,LYS\_175,10.15,-0.35,0,0  
 3FNI,GLU\_153,4.5,0,0,0  
 2Q98,ARG\_16,12.43,-0.07,0,0  
 3ULX,TYR\_137,8.4,1.25,-0.45,-2.4  
 3RE9,GLU\_243,4.39,0.21,-0.32,0  
 1X8F,GLU\_278,4.5,0,0,0  
 2FZ4,GLU\_163,3.3,0.63,-1.83,0  
 3H13,TYR\_360,11.71,1.65,-1.35,1.42  
 1GQE,GLU\_94,4.5,0,0,0  
 1SIG,GLU\_124,4.55,1.07,-1.03,0  
 2Z61,ASP\_141,3.07,0.21,-0.94,0  
 3L3P,GLU\_476,3.95,0.35,-0.91,0  
 1G5Z,GLU\_132,4.57,0.07,0,0  
 2OJQ,ASP\_376,4.12,0.42,-0.1,0  
 1LN4,HIS\_44,6.36,0,0,-0.14  
 1WLY,GLU\_73,3.95,0.21,-0.76,0  
 2V1L,LYS\_7,10.5,0,0,0  
 1WPS,LYS\_50,10.01,-0.49,0,0  
 1TXJ,ASP\_28,3.71,0,-0.09,0  
 1XWM,TYR\_137,11.43,1.71,-0.28,0  
 3MIX,LYS\_620,10.43,-0.07,0,0  
 3RFY,LYS\_248,10.15,-0.35,0,0  
 3KEY,ARG\_454,13.82,-0.31,0,1.62  
 2HRZ,ASP\_115,2.35,0.7,-2.15,0  
 3PU6,ARG\_80,12.5,0,0,0  
 3G9G,ARG\_205,11.73,-0.77,0,0  
 3H5T,ASP\_46,3.35,0.35,-0.8,0  
 1M5I,GLU\_211,4.71,0.21,0,0  
 3BB7,TYR\_264,11.96,0,-0.27,2.23  
 1D2K,ASP\_152,3.91,0.14,-0.03,0  
 4H4J,ASP\_59,3.86,0.07,-0.01,0  
 1WYC,ARG\_274,8.96,-1.14,0,-2.4  
 2IXM,GLU\_75,4.57,0.07,0,0  
 1F2V,GLU\_79,4.31,0.28,-0.47,0  
 3EVZ,TYR\_119,11,0,-0.4,1.41  
 1RAJ,ARG\_402,12.01,-0.49,0,0  
 3K8U,GLU\_64,4.5,0,0,0  
 2O0K,GLU\_109,3.25,0.35,-1.6,0  
 2V4U,LYS\_309,10.36,-0.14,0,0  
 2X4L,LYS\_281,10.15,-0.35,0,0  
 2RJD,HIS\_398,3.86,0.09,0,-2.73  
 2J8A,GLU\_282,4.71,0.21,0,0  
 3I47,ASP\_41,3.94,0.14,0,0  
 2E3H,ASP\_235,3.2,0.28,-0.88,0  
 3FHF,ARG\_152,12.36,-0.14,0,0  
 3GFP,ARG\_423,9.21,-3.29,0,0  
 3DZ1,ARG\_94,11.59,-0.91,0,0  
 2VGM,GLU\_261,3.01,0.56,-2.05,0  
 3M66,GLU\_304,4.22,0.42,-0.7,0  
 1PBV,GLU\_165,3.86,0.07,-0.71,0  
 1X04,LYS\_155,10.5,0,0,0  
 3OKQ,LYS\_619,10.43,-0.07,0,0  
 4D8L,HIS\_152,1.5,0.36,0,-5.36  
 1KW4,LYS\_55,10.5,0,0,0  
 3IRA,GLU\_157,3.91,0.21,-0.8,0  
 2CX4,GLU\_70,3.78,0.42,-1.14,0  
 3OKQ,ASP\_671,3.64,0.21,-0.36,0  
 2A4D,GLU\_97,4.09,0.14,-0.55,0  
 1Q42,ASP\_159,3.54,0.28,-0.54,0  
 3B21,ARG\_210,12.22,-0.28,0,0  
 2FL4,LYS\_101,10.15,-0.35,0,0  
 2ZQ5,HIS\_153,6.45,0.23,0,-0.28  
 3ASA,HIS\_163,6.98,0.76,0,-0.28  
 3H13,TYR\_276,11.69,2.49,-0.8,0  
 2C2Y,GLU\_183,0.82,1.05,-2.34,-2.4  
 2IXM,LYS\_194,10.01,-0.49,0,0  
 3FFM,LYS\_24,10.36,-0.14,0,0  
 2EHG,GLU\_33,3.78,0.35,-1.08,0  
 1P6F,ARG\_56,12.5,0,0,0  
 2NRR,GLU\_349,5.25,0.77,-0.02,0  
 1DUP,HIS\_58,6.39,0.17,0,-0.28  
 2EJB,ARG\_178,12.29,-0.21,0,0  
 4EKU,GLU\_36,4.05,0.35,-0.8,0  
 2IXM,GLU\_234,4.16,0,-0.34,0  
 1FKM,LYS\_320,10.43,-0.07,0,0  
 2OKT,LYS\_252,10.29,-0.21,0,0  
 2CIU,ASP\_163,1.43,0.98,-3.36,0  
 1CBY,HIS\_59,5.44,0.85,0,-1.91  
 2XHC,LYS\_130,10.5,0,0,0  
 2EEY,LYS\_43,10.22,-0.28,0,0  
 2RGY,ARG\_116,11.8,-0.7,0,0  
 3M9A,ARG\_77,12.5,0,0,0  
 3IVF,LYS\_334,10.5,0,0,0  
 2H8O,ARG\_63,11.24,-1.26,0,0  
 3A4C,CYS\_453,5.29,-3.71,0,0  
 3ZSL,LYS\_227,10.43,-0.07,0,0  
 1WYC,ARG\_293,11.52,-0.98,0,0  
 1IAP,GLU\_176,4.54,0.14,-0.1,0  
 2BDV,ASP\_2,9.17,-1.09,-2.03,3.3  
 3O48,ARG\_77,12.15,-0.35,0,0  
 1L3K,LYS\_87,10.08,-0.42,0,0  
 1XTD,CYS\_43,9,0,0,0  
 2E3C,GLU\_340,3.63,0.21,-1.08,0  
 2FM9,ASP\_161,3.94,0.14,0,0  
 1LN4,GLU\_90,4.71,0.21,0,0  
 3HUE,ARG\_304,12.5,0,0,0  
 1PZC,TYR\_82,10.38,0.38,0,0  
 3F5D,ASP\_73,4.04,0.28,-0.04,0  
 3P2F,GLU\_101,5.38,2.83,-1.65,-0.3  
 3JSN,LYS\_248,9.94,-0.56,0,0  
 3COC,TYR\_315,10,0,0,0  
 3EJC,ARG\_118,12.15,-0.35,0,0  
 3GW3,ARG\_184,11.94,-0.56,0,0  
 1LZL,GLU\_96,4.57,0.07,0,0  
 1SJ8,LYS\_533,10.36,-0.14,0,0  
 2AZP,GLU\_146,4.33,0.63,-0.8,0  
 1RWZ,ASP\_146,3.35,0.35,-0.8,0  
 3CCY,LYS\_127,10.29,-0.21,0,0  
 1RKA,LYS\_269,10.22,-0.28,0,0  
 3RJX,LYS\_159,10.36,-0.14,0,0  
 1PVT,ASP\_206,3.86,0.07,-0.01,0  
 1QYI,GLU\_355,4.57,0.07,0,0  
 1WYC,HIS\_108,7.37,2.91,1.76,-3.8  
 2YX0,LYS\_120,10.29,-0.21,0,0  
 2WB8,ARG\_779,12.01,-0.49,0,0  
 2IQT,ARG\_251,12.08,-0.42,0,0  
 2ZCX,ARG\_91,12.01,-0.49,0,0  
 3C38,ASP\_216,3.84,0.21,-0.17,0  
 2G9D,HIS\_19,6.5,0,0,0  
 1DOV,ARG\_137,12.01,-0.49,0,0  
 3GE9,ARG\_193,13.27,-1.63,0.2,4  
 3GG6,TYR\_145,10,0,0,0  
 3ONT,TYR\_8,10,0,0,0  
 3I4T,LYS\_269,10.5,0,0,0  
 1UAJ,GLU\_130,4.05,0.35,-0.8,0  
 3V1Q,GLU\_543,4.43,0.21,-0.28,0  
 2R51,GLU\_177,3.98,0.28,-0.8,0  
 1V43,GLU\_16,4.53,0.14,-0.11,0  
 2V5B,ARG\_99,11.87,-0.63,0,0  
 2PP6,LYS\_50,10.29,-0.21,0,0  
 2FBQ,ARG\_139,11.87,-0.63,0,0  
 1G5Z,GLU\_140,3.67,0.42,-1.25,0  
 2E0T,GLU\_177,3.32,0.35,-1.53,0  
 2GKG,CYS\_66,9.16,0,-1.06,1.22  
 1R3D,CYS\_43,9.94,0,0,0.94  
 1XFK,TYR\_301,13.27,0.69,0.18,2.4  
 3OBS,LYS\_16,10.5,0,0,0  
 4FZN,ARG\_176,11.59,-0.91,0,0  
 1W7B,GLU\_66,4.5,0,0,0  
 1ZHV,GLU\_129,4.5,0,0,0  
 2E3C,ASP\_292,4.01,0.21,0,0  
 2F9F,GLU\_56,3.03,0.35,-1.82,0  
 3CRM,GLU\_275,4.5,0,0,0  
 3GW3,ASP\_117,1.36,0.42,-2.87,0  
 2Q34,ARG\_211,11.59,-0.91,0,0  
 1YW5,HIS\_106,4.11,0,0,-2.39  
 3RKV,LYS\_229,10.5,0,0,0  
 2A0J,GLU\_27,4.43,0.07,-0.14,0  
 2AXO,CYS\_234,9.63,-0.85,0,1.48  
 1EDG,LYS\_363,10.01,-0.49,0,0  
 3M7G,GLU\_15,2.82,0.56,-2.24,0  
 2I88,LYS\_510,10.15,-0.35,0,0  
 3IL3,GLU\_148,4.18,0.14,-0.46,0  
 2JEO,HIS\_98,6.5,0,0,0  
 3V55,CYS\_667,8.36,-0.72,0,0.07  
 3U2R,ARG\_91,11.45,-1.05,0,0  
 2VGM,LYS\_238,10.43,-0.07,0,0  
 2OBI,LYS\_136,13.41,0.21,0.8,2.4  
 3I0O,ARG\_172,12.5,0,0,0  
 1NFN,GLU\_66,2.38,0.28,-2.4,0  
 4FLE,ARG\_95,11.87,-0.63,0,0  
 1L2F,ASP\_241,3.19,0.49,-1.1,0  
 1Q5Z,GLU\_620,4.04,0.21,-0.67,0  
 1S1G,GLU\_620,4.04,0.21,0,0  
 2B2H,GLU\_183,4.14,0.07,-0.43,0  
 3TOW,TYR\_189,12.48,0.2,0.05,2.22  
 1JYH,GLU\_82,4.5,0,0,0  
 1X91,ARG\_63,12.29,-0.21,0,0  
 3JZN,TYR\_387,8.34,0.14,-1.8,0  
 3F5D,ASP\_127,3.42,0.42,-0.8,0  
 4EKU,GLU\_69,3.39,0.42,-1.53,0  
 4HDE,LYS\_141,10.29,-0.21,0,0  
 2AXO,LYS\_231,10.22,-0.28,0,0  
 3OOP,ASP\_124,2.11,0.28,-1.97,0  
 2W1R,ASP\_68,3.8,0.14,-0.14,0  
 3CSV,GLU\_295,4.57,0.07,0,0  
 2A0J,ASP\_16,3.64,0.49,-0.65,0  
 1YTQ,GLU\_42,4.5,0,0,0  
 1NRI,ASP\_40,3.77,0,-0.03,0  
 1G8P,ARG\_253,11.66,-0.84,0,0  
 3AU3,HIS\_672,6.5,0,0,0  
 2HRZ,GLU\_330,4.12,0.42,-0.8,0  
 1DUN,ASP\_72,3.56,0.07,-0.31,0  
 1TUL,LYS\_58,10.15,-0.35,0,0  
 3BQE,LYS\_355,10.5,0,0,0  
 1CBY,ASP\_151,4.01,0.21,0,0  
 2GEN,ASP\_8,3.27,0.21,-0.74,0  
 2QDJ,ARG\_167,12.15,-0.35,0,0  
 3UAH,TYR\_385,10.85,0.85,0,0  
 3BCH,TYR\_39,10,0,0,0  
 3BA1,ARG\_28,11.94,-0.56,0,0  
 4DVD,ARG\_84,11.31,-1.19,0,0  
 3PU6,GLU\_122,4.57,0.07,0,0  
 1V6T,ARG\_50,12.01,-0.49,0,0  
 3IRA,GLU\_82,4.57,0.07,0,0  
 2RFA,GLU\_108,4.07,0.28,-0.71,0  
 3U4K,TYR\_155,9.21,0.82,-0.44,-1.17  
 1WRU,LYS\_53,10.36,-0.14,0,0  
 1GXN,LYS\_418,10.29,-0.21,0,0  
 3CRM,GLU\_211,4.64,0.14,0,0  
 3LJI,TYR\_33,10,0,0,0  
 2CBE,LYS\_9,10.36,-0.14,0,0  
 2OEW,HIS\_320,7.51,1.08,0,-0.07  
 1PSW,GLU\_53,4.29,0.14,-0.35,0  
 2ZCU,LYS\_75,10.08,-0.42,0,0  
 1PCU,ASP\_38,3.89,0.49,-0.4,0  
 1W24,LYS\_43,10.29,-0.21,0,0  
 4ECC,ASP\_39,3.87,0.07,0,0  
 2QRX,LYS\_15,10.5,0,0,0  
 1JSX,HIS\_152,7.53,1.17,0,-0.14



2Z84,GLU\_168,3.25,0.7,-1.94,0  
 3FK5,LYS\_239,10.29,-0.21,0,0  
 4FD6,TYR\_19,10.07,0.07,0,0  
 2XHC,LYS\_32,10.43,-0.07,0,0  
 1KCM,GLU\_6,1.82,1.56,-0.8,-3.44  
 3P28,GLU\_63,4.0,2.1,-0.71,0  
 2B61,TYR\_282,12.98,0.14,0.44,2.4  
 2E3C,GLU\_360,4.05,0.35,-0.8,0  
 2Z84,CYS\_101,10.32,-0.98,0.51,1.79  
 4E8B,GLU\_10,4.64,0.14,0,0  
 1L3K,GLU\_66,4.5,0,0,0  
 3LH5,GLU\_746,4.5,0,0,0  
 1TXJ,ASP\_130,3.92,0.14,-0.02,0  
 4FCU,GLU\_217,3.17,0.98,-2.32,0  
 2P1W,ASP\_60,2.07,0.28,-2.01,0  
 2FL7,ARG\_21,12.5,0,0,0  
 1O9G,ARG\_135,11.94,-0.56,0,0  
 3JSN,GLU\_264,4.5,0,0,0  
 1E59,LYS\_10,9.66,-0.84,0,0  
 3B7H,GLU\_14,4.5,0.14,-0.14,0  
 1T07,ASP\_78,3.8,0,0,0  
 2B61,HIS\_337,5.14,1.6,2.45,-5.41  
 1R53,LYS\_73,10.5,0,0,0  
 3M16,GLU\_317,3.8,0.76,-2.4,0.94  
 4EKU,GLU\_142,4.64,0.14,0,0  
 3OIP,ARG\_15,11.38,-1.12,0,0  
 2GEN,ASP\_149,3.73,0,-0.07,0  
 3E7P,ARG\_138,11.94,-0.91,0,0.35  
 2FD5,GLU\_129,4.64,0.14,0,0  
 2ZCO,LYS\_231,10.5,0,0,0  
 3CX5,CYS\_157,9.07,0,0,0.07  
 1TR9,TYR\_305,13.27,0.67,0.2,2.4  
 2JKF,ASP\_45,4.03,0.49,-0.26,0  
 3BJV,GLU\_87,4.38,0,-0.12,0  
 3I4T,ASP\_84,1.82,0.77,-2.75,0  
 3RE9,TYR\_214,11.04,0.07,-0.68,1.65  
 1J33,HIS\_110,6.6,0.31,0,-0.21  
 1TLV,HIS\_189,6.86,0.5,0,-0.14  
 4EZB,GLU\_239,5.15,0.65,0,0  
 2WOZ,GLU\_323,3.98,0.28,-0.8,0  
 2INO,GLU\_411,4.63,0.14,-0.01,0  
 4FH3,ASP\_253,2.99,0.56,-1.38,0  
 2YT4,ARG\_522,12.01,-0.49,0,0  
 3A7L,GLU\_94,3.75,0.21,-0.96,0  
 2D7U,GLU\_330,3.48,0.35,-1.37,0  
 1UCH,HIS\_112,6.29,0,0,-0.21  
 3CSV,TYR\_285,9.95,0,-0.05,0  
 2FI9,LYS\_94,10.5,0,0,0  
 2B78,LYS\_343,10.29,-0.21,0,0  
 2C13,LYS\_119,10.43,-0.07,0,0  
 2JEO,TYR\_205,9.48,0.07,-0.6,0  
 4AM1,CYS\_127,9.58,-0.78,-2.3,3.6  
 2ZOM,ASP\_126,2.79,0.63,-1.63,0  
 1WNH,CYS\_20,10.16,0,0,1.16  
 1L3K,ASP\_139,1.17,0.42,-3.04,0  
 1O9G,ARG\_150,12.22,-0.28,0,0  
 4DVD,ARG\_43,12.43,-0.07,0,0  
 1WYC,ARG\_12,10.32,-2.3,0.0,12  
 1WNH,LYS\_97,10.5,0,0,0  
 4D8L,HIS\_116,6.53,0.17,0,-0.14  
 3F5D,LYS\_92,9.87,-0.63,0,0  
 1RAJ,ASP\_71,2.04,0.98,-2.74,0  
 4EVF,LYS\_194,9.87,-0.63,0,0  
 1G5Z,GLU\_173,4.99,0.49,0,0  
 2IRM,HIS\_336,6.39,0.16,0,-0.28  
 3G9B,LYS\_149,10.5,0,0,0  
 3F1X,HIS\_202,6.43,0,0,-0.07  
 2FXT,HIS\_292,4.37,0,0,-2.13  
 1A8Q,ASP\_129,3.74,0,-0.06,0  
 1DCF,ARG\_130,12.5,0,0,0  
 2A4D,GLU\_93,4.57,0.07,0,0  
 3RUX,GLU\_66,4.64,0.14,0,0  
 3U56,ARG\_114,12.01,-0.49,0,0  
 1Z9L,HIS\_86,6.36,0,0,-0.14  
 1N81,GLU\_26,4.58,0.28,-0.2,0  
 3L7N,HIS\_107,6.43,0,0,-0.07  
 1YLN,CYS\_158,10.53,-0.17,0,1.7  
 1JKS,ASP\_259,2.95,0.84,-1.69,0  
 1YLN,ARG\_227,11.73,-0.77,0,0  
 2FZP,ASP\_222,2.35,0.28,-1.73,0  
 3BWT,LYS\_698,10.29,-0.21,0,0  
 3NBI,LYS\_130,10.15,-0.35,0,0  
 3IVF,GLU\_132,4.1,0,-0.4,0  
 3GW3,TYR\_311,13.41,0.21,0.8,2.4  
 2RJD,GLU\_311,4.74,0.49,-0.25,0  
 1O5J,LYS\_20,10.29,-0.21,0,0  
 2PGE,TYR\_287,10.46,0.51,-0.05,0  
 2OJQ,LYS\_374,10.22,-0.28,0,0  
 1PZC,HIS\_6,6.43,0,0,-0.07  
 1YTD,LYS\_32,10.5,0,0,0  
 4FZN,TYR\_24,12.44,1.06,-0.19,1.57  
 1TXJ,GLU\_103,4.57,0.07,0,0  
 1H09,LYS\_203,9.87,-0.63,0,0  
 3ETU,LYS\_69,10.22,-0.28,0,0  
 1WLJ,ARG\_102,10.11,-3.1,0,0.71  
 2X4G,ASP\_249,3.24,0.21,-0.77,0  
 1YM5,TYR\_279,11.67,0,-0.08,1.74  
 1X7F,TYR\_150,9.7,1.04,-1.34,0  
 3I4T,ASP\_154,3.25,0.42,-0.97,0  
 3BB7,TYR\_331,8.75,0.58,-1.84,0.01  
 2ZCO,TYR\_10,13.07,0.12,0.55,2.4  
 1JT9,HIS\_96,7.41,1.05,0,-0.14  
 2V4U,LYS\_344,10.36,-0.14,0,0  
 3FXH,GLU\_109,2.08,0.42,-2.84,0  
 1CHD,TYR\_295,10,0,0,0  
 3DZ1,LYS\_185,10.5,0,0,0  
 1OIS,HIS\_338,6.18,0.03,0,-0.35  
 3EJG,CYS\_141,10.31,0,0,1.31  
 3FK5,ARG\_93,11.57,-1.09,0.16  
 4DNU,ARG\_146,12.08,-0.42,0,0  
 1JYH,LYS\_62,10.5,0,0,0  
 3T57,LYS\_163,10.29,-0.21,0,0  
 1VSM,HIS\_142,4.99,1.34,0,-2.85  
 1MTZ,ASP\_120,3.8,0,0,0  
 2HP7,GLU\_221,4.64,0.14,0,0  
 3JZN,GLU\_337,4.5,0,0,0  
 3EVP,CYS\_228,10.32,-1.44,-0.09,2.85  
 3BQE,ARG\_354,12.08,-0.42,0,0  
 1Z3X,ARG\_94,12.36,-0.14,0,0  
 2VGY,TYR\_68,10,0,0,0  
 4FH3,TYR\_220,11.25,1.35,-0.1,0  
 1S17,TYR\_304,10.76,1.17,-0.41,0  
 3RAZ,ASP\_30,1.85,0.7,-2.66,0  
 2FBQ,ARG\_29,12.01,-0.49,0,0  
 2QZQ,LYS\_112,10.43,-0.07,0,0  
 3O48,TYR\_88,10,0,0,0  
 3CAX,LYS\_468,10.36,-0.14,0,0  
 2IQT,GLU\_122,4.57,0.07,0,0  
 3NR5,ARG\_73,12.22,-0.28,0,0  
 3GW3,GLU\_27,3.98,0.28,-0.8,0  
 1PBV,GLU\_241,4.8,0.35,-0.05,0  
 3BCY,GLU\_32,5.05,0.56,-0.01,0  
 3A0X,GLU\_623,4.3,0.28,-0.48,0  
 1V6T,LYS\_228,10.15,-0.35,0,0  
 2CBE,LYS\_113,10.5,0,0,0  
 3ZSL,TYR\_118,10,0,0,0  
 2Z84,GLU\_10,4.5,0,0,0  
 2BCF,CYS\_100,8.41,-0.59,0,0  
 1Q46,LYS\_117,10.08,-0.42,0,0  
 3A4C,HIS\_510,4.8,0.96,0,-2.66  
 3FS3,TYR\_276,9.34,0.28,-1.23,0.29  
 1J33,ARG\_80,12.01,-0.49,0,0  
 3M7D,LYS\_347,10.15,-0.35,0,0  
 3JRT,LYS\_73,10.22,-0.28,0,0  
 3H6Q,LYS\_34,9.94,-0.56,0,0  
 3F6F,ARG\_37,12.01,-0.49,0,0  
 2Q13,GLU\_252,5.06,0.21,0.35,0  
 1G5Z,LYS\_138,10.36,-0.14,0,0  
 1L2F,LYS\_335,10.5,0,0,0  
 3COU,GLU\_76,4.57,0.87,-0.8,0  
 3EJG,ARG\_85,12.15,-0.35,0,0  
 2DOA,TYR\_213,9.22,0.07,-0.85,0  
 1O9G,CYS\_59,12.24,-0.92,1.75,2.41  
 1TLV,ARG\_272,12.08,-0.42,0,0  
 1MML,GLU\_117,3.32,0.28,-1.46,0  
 2IRM,LYS\_152,10.5,0,0,0  
 4AM1,HIS\_185,6.5,0,0,0  
 1QVI,GLU\_353,4.71,0.21,0,0  
 1JSX,LYS\_206,10.15,-0.35,0,0  
 3HUE,CYS\_231,10.19,0,0,1.19  
 3A4C,HIS\_525,6.43,0,0,-0.07  
 1NAR,LYS\_115,10.29,-0.21,0,0  
 1SFE,ARG\_92,12.15,-0.35,0,0  
 3DZ1,ASP\_287,3.29,0.14,-0.65,0  
 3G9T,ASP\_27,3.21,0.35,-0.94,0  
 1T6L,TYR\_103,10.94,0,-0.52,1.46  
 3V75,ASP\_232,3.28,0.63,-1.14,0  
 1JYH,GLU\_46,0.29,1.39,-3.2,-2.4  
 3H13,GLU\_263,0.57,2.09,-3.61,-2.4  
 1I60,HIS\_146,6.36,0,0,-0.14  
 3KEY,LYS\_402,9.73,-0.77,0,0  
 4E9E,LYS\_458,10.36,-0.14,0,0  
 1DCF,HIS\_29,6.5,0,0,0  
 2Q13,CYS\_183,8.72,-0.28,0,0  
 3L3P,GLU\_307,4.78,0.28,0,0  
 1C3K,ASP\_76,2.85,0.21,-1.16,0  
 3T57,LYS\_133,10.5,0,0,0  
 2XHC,LYS\_108,10.08,-0.42,0,0  
 2J8A,GLU\_322,4.68,0.63,-0.45,0  
 1TUL,CYS\_73,8.72,-1.29,0,1.01  
 2O8P,LYS\_150,9.8,-0.7,0,0  
 1Z3X,ARG\_181,12.08,-0.42,0,0  
 1TWU,GLU\_24,4.5,0,0,0  
 2GAU,TYR\_180,13.41,0.21,0.8,2.4  
 1WLJ,TYR\_243,11.97,2.37,-0.4,0  
 4E6S,HIS\_70,6.43,0,0,-0.07  
 1SOH,ASP\_23,3.94,0.14,0,0  
 1XDZ,CYS\_159,12.37,0,0,3.37  
 3TRE,GLU\_28,4.64,0.14,0,0  
 3F1X,GLU\_255,3.76,0.28,-1.02,0  
 1VSM,ARG\_161,12.22,-0.28,0,0  
 2G3A,LYS\_135,10.22,-0.28,0,0  
 2GEN,TYR\_137,9.74,0,-0.47,0.21  
 2E3S,GLU\_400,3.87,0.14,-0.77,0  
 2DFL,ASP\_193,4.08,0.28,0,0  
 1R53,GLU\_160,4.5,0,0,0  
 3ETU,ASP\_300,4.08,0.28,0,0  
 1AT0,ARG\_387,12.22,-0.28,0,0  
 2PGE,TYR\_300,9.76,0.94,-0.32,-0.86  
 1T6L,ARG\_208,11.8,-0.7,0,0  
 1MUJ,LYS\_286,10.43,-0.07,0,0  
 2ZCO,ARG\_224,11.87,-0.63,0,0  
 1SNT,ASP\_345,1.4,0.63,-3.03,0  
 4FZR,ARG\_91,11.24,-1.26,0,0  
 1X9G,GLU\_70,4.07,0.07,-0.5,0  
 1NFN,GLU\_77,4.57,0.07,0,0  
 3JRT,GLU\_137,4.5,0,0,0  
 3ZXY,ASP\_201,3.59,0.21,-0.42,0  
 2CL3,CYS\_144,8.11,-1.28,0,0.39  
 2E3S,ARG\_520,11.66,-0.84,0,0  
 3OKQ,ASP\_578,3.93,0.21,-0.08,0  
 2OEW,LYS\_19,10.5,0,0,0  
 1ZP2,LYS\_110,10.5,0,0,0  
 1BN6,TYR\_90,10.38,1.24,-0.86,0  
 2P4D,ASP\_79,2.5,0.28,-1.58,0  
 3LPZ,TYR\_25,10.01,0,0,0.01  
 4DIU,GLU\_153,4.71,0.21,0,0  
 3DSH,LYS\_402,9.94,-0.56,0,0  
 3I47,LYS\_222,10.5,0,0,0  
 3UAH,ARG\_418,13.07,-0.42,0,0.99  
 3IV4,TYR\_3,10,0,0,0  
 1XDZ,GLU\_238,4.78,0.28,0,0  
 3TMO,ARG\_227,11.17,-1.33,0,0  
 2POY,ASP\_114,2.5,0.77,-2.07,0  
 3M16,CYS\_174,11.44,-0.36,0.28  
 4E8B,GLU\_165,3.76,0.14,-0.88,0  
 2RIS,HIS\_104,7.24,0.81,0,-0.07  
 3GG6,HIS\_99,6.36,0,0,-0.14  
 4H4J,GLU\_68,3.94,3.33,-1.54,-2.35  
 3PP8,GLU\_261,3.74,0.21,-0.96,0  
 1WXQ,LYS\_152,10.5,0,0,0  
 1ZBM,LYS\_95,10.29,-0.21,0,0  
 2YYO,TYR\_80,13.23,0.56,0.27,2.4  
 2G2D,HIS\_130,2.18,0.53,-1.95,-2.9  
 3ILC,ARG\_165,12.15,-0.35,0,0  
 3T57,GLU\_261,3.74,0.21,-0.96,0  
 3FTT,ASP\_166,3.14,0.56,-1.22,0  
 2X4L,LYS\_124,10.29,-0.21,0,0  
 1OGL,TYR\_245,9.16,0.14,-0.98,0  
 1SNT,CYS\_332,8.08,-2.44,0,1.52  
 2FC3,TYR\_20,9.46,0.27,-1.1,0.3  
 4H4J,LYS\_167,10.5,0,0,0  
 1WRU,CYS\_96,9.04,-0.03,0,0.07  
 2POL,HIS\_50,1.52,0,0,-4.98  
 3JRT,ASP\_165,3.2,0.35,-0.95,0  
 1FQI,TYR\_337,12.04,0,0,2.04  
 3HKX,ASP\_94,3.35,0.42,-0.87,0  
 3T57,GLU\_259,3.31,0.35,-1.84,0  
 2I6I,LYS\_57,10.08,-0.42,0,0  
 2EYI,TYR\_215,9.72,0,-0.28,0  
 3V3T,GLU\_132,4.33,0,-0.17,0  
 2Z14,GLU\_94,4.71,0.21,0,0  
 1YOK,ARG\_105,12.36,-0.14,0,0  
 1G8P,CYS\_78,3.33,-6.51,0.85  
 1VJG,ARG\_193,12.5,0,0,0  
 3JZ9,HIS\_496,6.5,0,0,0  
 2VGM,GLU\_23,3.96,0.49,-1.03,0  
 2QRX,ARG\_167,12.01,-0.49,0,0  
 2E3C,LYS\_245,10.43,-0.07,0,0  
 2HRZ,HIS\_229,4.78,3.6,0,-5.32  
 3ETV,LYS\_102,10.29,-0.21,0,0  
 1O5T,ARG\_321,12.03,-1.88,0,1.41  
 3A7L,TYR\_96,9.98,0.61,-1.53,0.9  
 1WYC,ARG\_50,12.15,-0.35,0,0  
 1Y2Q,GLU\_24,1.02,0.85,-1.93,-2.4  
 3YKQ,ASP\_556,11.94,-0.56,0,0  
 1NWA,ASP\_133,3.72,0.07,-0.15,0  
 1OIS,LYS\_304,10.29,-0.21,0,0  
 3NZL,HIS\_19,6.36,0,0,-0.14  
 2B61,TYR\_56,11.34,0.07,-0.2,1.47  
 1WRU,GLU\_151,3.25,0.42,-1.67,0  
 2IF4,LYS\_289,10.43,-0.07,0,0  
 1Q2Y,LYS\_25,10.08,-0.42,0,0  
 2YX0,GLU\_191,3.84,0.14,-0.8,0  
 1GVP,CYS\_33,8.82,-0.63,0,0.45  
 2CBE,ASP\_85,3.87,0.07,0,0

3ADO,ARG\_298,12.08,-0.42,0,0  
3ODJ,TYR\_120,10,0,0,0  
3LJN,ARG\_106,11.31,-1.19,0,0  
1MIX,ARG\_207,11.73,-0.77,0,0  
3DHN,TYR\_85,10,0,0,0  
3RJX,LYS\_297,10.5,0,0,0  
2C13,ARG\_31,11.87,-0.63,0,0  
2V4U,ASP\_350,3.26,0.28,-0.82,0  
3PM2,LYS\_152,10.29,-0.21,0,0  
3G9G,ASP\_102,3.45,0.49,-0.84,0  
4DEZ,HIS\_99,5.22,0.25,0,-1.53  
3IVF,GLU\_237,4.43,0.42,-0.49,0  
1YR6,ASP\_184,4.43,0.63,0,0  
2XWS,HIS\_10,6.36,0,0,-0.14  
3LJN,LYS\_104,10.5,0,0,0  
3BWT,HIS\_795,6.36,0,0,-0.14  
2J8A,LYS\_299,10.45,0.07,0,0  
4EKU,HIS\_106,4.97,1.6,0.73,-3.86  
3ZTA,GLU\_57,4.37,0.21,-0.34,0  
3L3P,ARG\_508,12.08,-0.42,0,0  
4D8L,ARG\_98,11.24,-1.26,0,0  
2AZL,ARG\_259,12.5,0,0,0  
2ZOM,LYS\_151,10.29,-0.21,0,0  
2AZL,GLU\_21,4.47,0.14,-0.17,0  
1VSM,LYS\_119,9.24,-1.26,0,0  
2FGG,ASP\_21,3.92,0.28,-0.16,0  
1O5J,GLU\_76,4.5,0,0,0  
1DVQ,TYR\_149,11.46,0,0,1.46  
3PM2,HIS\_131,4.55,0.48,0,-2.43  
2O8PHIS\_163,6.36,0,0,-0.14  
3M3P,ARG\_47,12.43,-0.07,0,0  
3G9T,HIS\_268,5.55,1.6,2.26,-4.81  
3V1Q,ARG\_535,11.59,-0.91,0,0  
2O8P,GLU\_42,4.12,0.42,-0.8,0  
1GPP,GLU\_103,3.53,0.63,-1.6,0  
3CSR,LYS\_156,10.36,-0.14,0,0  
3N2T,ASP\_34,3.14,0.14,-0.8,0  
2FZP,LYS\_283,10.29,-0.21,0,0  
4FCU,GLU\_253,4.71,0.21,0,0  
2RIS,TYR\_57,10,0,0,0  
1YG2,TYR\_129,10.01,0.01,0,0  
3TMO,HIS\_282,6.43,0,0,-0.07  
2E3H,ASP\_247,1.87,0.56,-2.49,0  
1YR6,GLU\_52,3.99,0.83,-1.6,0.26  
1GQE,ARG\_117,12.01,-0.49,0,0  
3E7P,ARG\_26,12.26,-2.44,0.2,2  
1QYI,ARG\_17,13.18,-1.42,0.2,1  
1PSW,ARG\_134,11.59,-0.91,0,0  
2D7U,TYR\_52,10.39,0.07,0,0.32  
1NUJ,ARG\_213,12.29,-0.21,0,0  
1X8F,GLU\_29,1.2,0.49,-1.6,-2.19  
2IXM,ASP\_229,4.01,0.21,0,0  
1SUU,LYS\_668,10.43,-0.07,0,0  
2CVB,GLU\_162,4.21,0.28,-0.57,0  
1AM2,HIS\_197,6.57,1.6,1.05,-2.58  
3O48,GLU\_32,1.65,0.7,-3.55,0  
4DNU,ASP\_326,3.43,0.28,-0.65,0  
3HUE,LYS\_45,10.43,-0.07,0,0  
2X4L,GLU\_88,4.64,0.14,0,0  
1JKS,HIS\_272,6.88,0.8,0,-0.42  
3HUE,GLU\_239,5.66,0.75,-0.23,0.65  
1GSZ,LYS\_120,10.29,-0.21,0,0  
3PP8,LYS\_121,10.5,0,0,0  
1XEU,TYR\_246,10.15,0.07,0,0.08  
3UAH,ASP\_261,2.82,0.63,-1.61,0  
2D7U,ASP\_215,2.81,0.49,-1.48,0  
1XWM,LYS\_211,10.5,0,0,0  
1RZ2,ARG\_133,11.52,-0.98,0,0  
2Q13,GLU\_27,4.53,0.83,-0.8,0  
4H89,GLU\_117,4.06,0.14,-0.58,0  
3HNX,GLU\_86,4.64,0.14,0,0  
2R57,HIS\_345,6.54,0.04,0,0  
1X7F,LYS\_140,10.29,-0.21,0,0  
3EYE,ARG\_93,11.73,-0.77,0,0  
1R16,ARG\_66,11.73,-0.77,0,0  
2B61,LYS\_21,10.5,0,0,0  
1AT0,CYS\_400,6.86,-3.63,0,1.48  
1KCM,LYS\_68,10.36,-0.14,0,0  
3ZXY,ASP\_100,1.44,0.35,-2.71,0  
1Z3X,ASP\_97,2.77,0.49,-1.52,0  
3ADO,CYS\_305,8.94,-0.13,0,0.07  
2DFL,LYS\_200,10.5,0,0,0  
1SUY,GLU\_53,4.25,0.07,-0.32,0  
1MTZ,HIS\_271,4.21,1.6,2.54,-6.42  
2JHY,TYR\_156,9.58,0.14,-0.56,0  
1BN6,GLU\_132,4.0,0.63,-1.13,0  
3D9H,ARG\_53,11.87,-0.63,0,0  
3FHF,LYS\_11,10.08,-0.42,0,0  
2GEN,ARG\_107,11.94,-0.56,0,0  
3FHF,LYS\_5,10.5,0,0,0  
2WOZ,GLU\_377,4.5,0,0,0  
1X9G,GLU\_22,3.91,0.21,-0.8,0  
1SNT,ASP\_58,3.92,0.14,-0.02,0  
2H01,HIS\_156,6.36,0,0,-0.14  
3MEW,ASP\_139,2.98,0.28,-1.1,0  
2B2H,GLU\_375,4.92,0.42,0,0  
1X1P,LYS\_246,10.15,-0.35,0,0  
3PAC,ASP\_92,3.94,0.14,0,0  
3F1X,GLU\_85,4.05,0.35,-0.8,0  
2OGQ,LYS\_492,10.01,-0.49,0,0  
2GEN,ARG\_170,12.08,-0.42,0,0  
1QYI,TYR\_302,13.4,0.42,0.58,2.4  
2B61,GLU\_330,4.05,0.35,-0.8,0  
1HUF,GLU\_36,4.01,0.21,-0.7,0  
4EUG,HIS\_108,4.99,1.22,0,-2.73  
1OIS,LYS\_286,10.22,-0.28,0,0  
3O16,LYS\_77,10.29,-0.21,0,0  
3BZT,TYR\_271,13.34,0.14,0.8,2.4  
1WPA,LYS\_504,10.43,-0.07,0,0  
2R2Y,LYS\_97,10.08,-0.42,0,0  
1QQL,ARG\_13,11.66,-0.84,0,0  
3RLN,GLU\_660,4.5,0,0,0  
3GOZ,ASP\_28,2.48,0.63,-1.95,0  
3M7G,ASP\_182,2.03,0.77,-2.54,0  
3RKV,HIS\_307,7.35,1.2,0,-0.35  
2D25,LYS\_685,10.5,0,0,0  
3GS9,CYS\_281,9.34,0,0,0.34  
2GS5,ARG\_180,13.46,-1.44,0,2.4  
2QDJ,GLU\_323,3.84,0.14,-0.8,0  
2QDJ,GLU\_79,4.28,0.21,-0.43,0  
1AM2,TYR\_163,11.21,1.12,0,0.09  
2EJX,GLU\_49,4.57,0.07,0,0  
4GCO,LYS\_212,8.5,-0.28,0,-1.72  
1RLO,LYS\_157,10.08,-0.42,0,0  
2R0S,ASP\_204,2.27,0.77,-2.3,0  
2ZQ5,ASP\_308,2.9,0.28,-1.18,0  
3H5T,LYS\_191,10.29,-0.21,0,0  
3ILC,TYR\_15,13.0,0.21,0.39,2.4  
2IQT,ARG\_232,10.67,-1.83,0,0  
1AT0,ASP\_318,3.08,0.63,-1.35,0  
3GS3,LYS\_218,10.5,0,0,0  
2FZP,GLU\_248,4.57,0.07,0,0  
2JHY,ARG\_117,12.15,-0.35,0,0  
1V6T,LYS\_137,10.5,0,0,0  
1QYI,ARG\_370,12.01,-0.49,0,0  
1ILW,GLU\_80,4.27,0.35,-0.58,0  
1OTM,LYS\_131,10.5,0,0,0  
2R0S,LYS\_201,10.5,0,0,0  
1YTD,HIS\_144,6.29,0,0,-0.21  
3UOV,GLU\_108,1.3,0.8,-1.6,-2.4  
3RLE,TYR\_72,10.17,0.19,-0.02,0  
2ORW,ASP\_235,3.8,0,0,0  
3DHN,GLU\_63,3.91,0.21,-0.8,0  
3T57,GLU\_266,3.57,0.49,-1.42,0  
1W7B,ARG\_245,11.94,-0.56,0,0  
1PBV,ASP\_236,3.77,0.14,-0.17,0  
1WP5,HIS\_68,6.43,0,0,-0.07  
3T8R,ARG\_81,11.73,-0.77,0,0  
2CXC,GLU\_11,2.31,0.56,-2.74,0  
2V1L,ASP\_118,3.87,0.07,0,0  
4FLE,TYR\_111,10,0,0,0  
3DB9,HIS\_256,3.76,0,0,-2.74  
1T3Y,ASP\_123,3.72,0,-0.08,0  
1R9W,CYS\_276,4.43,-4.72,0,0.14  
3UV1,ARG\_93,12.22,-0.28,0,0  
1YW5,GLU\_44,4.5,0,0,0  
1PGV,ARG\_253,12.01,-0.49,0,0  
3PP8,GLU\_135,3.36,0.21,-1.35,0  
1R29,LYS\_123,10.5,0,0,0  
1UOH,GLU\_54,4.57,0.07,0,0  
1TXJ,ASP\_73,3.56,0.56,-0.8,0  
4DEZ,ARG\_64,12.5,0,0,0  
1NRI,HIS\_134,6.5,0,0,0  
2CWY,ARG\_63,11.8,-0.7,0,0  
1YOK,GLU\_48,3.25,0.63,-1.88,0  
3EGN,GLU\_403,4.48,0.14,-0.16,0  
1S17,GLU\_264,4.5,0,0,0  
1KN3,GLU\_19,3.94,0.21,-0.77,0  
3ZSL,ASP\_241,3.99,0.21,-0.02,0  
3CRM,ARG\_219,12.01,-0.49,0,0  
2YT4,TYR\_609,9.25,0,-0.74,0  
2XHC,ASP\_47,3.55,0.07,-0.32,0  
1XDZ,LYS\_219,10.5,0,0,0  
2XWS,TYR\_63,10.07,0.07,0,0  
3VJ8,HIS\_101,6.99,0.7,0,-0.21  
3P2F,ARG\_95,12.22,-0.28,0,0  
3ADO,ARG\_254,12.08,-0.42,0,0  
1R3F,ASP\_185,1.75,0.42,-2.47,0  
4DBX,LYS\_158,10.29,-0.21,0,0  
3GV0,ARG\_139,12.36,-2.54,0,2.4  
1N81,TYR\_51,10,0,0,0  
3V75,ARG\_242,12.15,-0.35,0,0  
2IRM,GLU\_101,4.28,0.42,-0.64,0  
3ERF,HIS\_58,4.17,0,0,-2.33  
4H89,HIS\_167,6.36,0,0,-0.14  
2D0A,GLU\_148,4.57,0.07,0,0  
2X5Y,ASP\_865,3.035,-1.15,0  
3JV1,GLU\_161,3.77,0.07,-0.8,0  
1YW5,TYR\_39,10,0,0,0  
3ADO,ASP\_191,3.84,0.07,-0.03,0  
1P2F,LYS\_21,10.29,-0.21,0,0  
1X7F,GLU\_232,3.67,0.28,-1.11,0  
3Q1C,GLU\_263,3.97,0.07,-0.6,0  
3RNV,TYR\_396,13.27,0.07,0.8,2.4  
3ADO,HIS\_90,2.01,0.8,0,-5.29  
1QYI,LYS\_2,10.22,-0.28,0,0  
4FZr,ARG\_95,12.29,-0.21,0,0  
2JKF,ASP\_49,3.51,0.42,-0.7,0  
3FXH,HIS\_80,6.87,0.44,0,-0.07  
2C13,GLU\_84,4.03,0.14,-0.61,0  
2GEN,ASP\_98,3.16,0.21,-0.85,0  
2IRM,ARG\_347,12.22,-0.28,0,0  
3FXH,LYS\_54,10.43,-0.07,0,0  
3M70,TYR\_103,13.34,0.14,0.8,2.4  
3M7D,GLU\_256,4.71,0.21,0,0  
2V4U,TYR\_314,9.68,1.08,-1.4,0  
1SBX,GLU\_118,4.5,0,0,0

3RLE,ASP\_171,2.76,0.56,-1.6,0  
 3A4C,LYS\_482,10.5,0,0,0  
 2QDJ,LYS\_65,10.29,-0.21,0,0  
 2IDC,ASP\_102,3.21,0.21,-0.8,0  
 1P6F,GLU\_112,4.57,0.07,0,0  
 2WB8,TYR\_736,13.41,1.31,0,2.1  
 3M66,HIS\_338,6.36,0,0,-0.14  
 1U3Y,ASP\_318,3.2,0.49,-1.09,0  
 1L2F,GLU\_301,4.57,0.07,0,0  
 3V1Q,LYS\_577,10.29,-0.21,0,0  
 2A0J,ARG\_69,12.36,-0.14,0,0  
 2XHC,TYR\_255,10,0,0,0  
 2EFK,GLU\_240,2.45,0.35,-2.4,0  
 2Q13,TYR\_36,10,0,0,0  
 3COU,ASP\_150,1.95,0.63,-2.48,0  
 3GG6,ARG\_77,12.15,-0.35,0,0  
 2R51,LYS\_192,10.29,-0.21,0,0  
 3BA1,LYS\_177,10.5,0,0,0  
 4ETX,TYR\_208,10,0,0,0  
 1T3Y,TYR\_45,11.39,1.39,0,0  
 3FRR,ARG\_147,12.5,0,0,0  
 2NSN,HIS\_19,0.72,0.08,-0.28  
 1D7O,GLU\_48,4.23,0.14,-0.41,0  
 2B78,HIS\_90,6.5,0,0,0  
 3ELI,GLU\_123,4.5,0,0,0  
 2IDC,ARG\_104,11.59,-0.91,0,0  
 3HVM,LYS\_239,10.43,-0.07,0,0  
 1YTD,ASP\_264,3.07,0.7,-1.43,0  
 3E7P,ASP\_13,3.67,0,-0.13,0  
 3IBT,ASP\_200,3.97,0.21,-0.04,0  
 4FD6,HIS\_211,6.5,0,0,0  
 3CRM,TYR\_263,10,0,0,0  
 2ZCX,GLU\_161,4.17,0.07,-0.4,0  
 3H04,ARG\_130,13.76,-1.14,0,2.4  
 3EYE,LYS\_94,10.43,-0.07,0,0  
 3ILC,LYS\_20,10.29,-0.21,0,0  
 2H2W,HIS\_133,6.93,0.43,0,0  
 3DTE,TYR\_205,9.36,0,-0.64,0  
 2IRM,ARG\_330,11.94,-0.56,0,0  
 2GQV,GLU\_60,2.94,0.84,-2.4,0  
 3F1X,TYR\_70,10,0,0,0  
 1RHS,TYR\_36,12.59,1.18,-1.65,3.07  
 3CJW,HIS\_333,6.5,0,0,0  
 3PBH,ARG\_85,12.43,-0.07,0,0  
 1BKR,TYR\_103,10,0,0,0  
 3M3P,LYS\_196,10.5,0,0,0  
 2R0S,LYS\_172,10.36,-0.14,0,0  
 2CL3,ASP\_133,3.13,0.56,-1.22,0  
 1A8Q,ARG\_113,11.8,-0.7,0,0  
 4EKU,GLU\_315,4.5,0,0,0  
 3O16,TYR\_29,11.49,3.09,-1.6,0  
 3IVF,LYS\_254,10.43,-0.07,0,0  
 1X91,ASP\_93,2.37,0.42,-1.85,0  
 3TIR,ASP\_24,3.98,0.28,-0.1,0  
 3MIX,GLU\_664,4.05,0.35,-0.8,0  
 4E8B,ASP\_202,3.79,0,-0.01,0  
 3FHF,ARG\_97,11.22,-1.28,0,0  
 2AXO,ARG\_123,11.69,-0.81,0,0  
 3C2E,ARG\_15,11.94,-0.56,0,0  
 4DIU,LYS\_212,9.94,-0.56,0,0  
 3IVF,LYS\_66,10.15,-0.35,0,0  
 2OYZ,LYS\_55,10.08,-0.42,0,0  
 3D9H,ASP\_192,3.3,0.56,-1.06,0  
 3O48,GLU\_105,4.37,0.07,-0.2,0  
 1ZKZ,GLU\_106,4.64,0.14,0,0  
 3NOK,HIS\_18,5.45,0.8,0,-1.85  
 1SQW,LYS\_75,10.5,0,0,0  
 2BCF,ARG\_185,11.8,-0.7,0,0  
 2H2W,GLU\_123,3.19,0.84,-2.15,0  
 4H86,HIS\_66,0.55,0.51,-1.5,-4.96  
 2IRM,ASP\_249,3.05,0.42,-1.17,0  
 3O16,LYS\_23,10.43,-0.07,0,0  
 4DBX,GLU\_26,4.01,0.21,-0.7,0  
 2V81,GLU\_20,3.23,0.28,-1.55,0  
 4DNU,ARG\_234,12.7,-2.04,0,2.24  
 1NJ4,LYS\_306,9.73,-0.77,0,0  
 2VGY,ARG\_80,11.45,-1.05,0,0  
 3EOD,ASP\_24,2.55,0.35,-1.6,0  
 1X8F,ASP\_10,2.86,0.28,-1.21,0  
 3HYQ,ARG\_181,12.29,-0.21,0,0  
 2HRZ,GLU\_270,3.85,0.14,-0.79,0  
 3LD1,LYS\_244,10.43,-0.07,0,0  
 3FXH,TYR\_57,9.41,0.07,-0.66,0  
 3GS3,ASP\_206,2.57,0.42,-1.65,0  
 2CVB,ARG\_27,12.22,-0.28,0,0  
 3DSH,GLU\_293,4.33,0.07,-0.24,0  
 3I4T,ASP\_235,4.1,0.35,-0.05,0  
 1YM5,GLU\_240,4.04,0.49,-0.94,0  
 2ZQ5,CYS\_210,8.65,-0.7,0,0.35  
 2H8O,ARG\_177,11.94,-0.56,0,0  
 3A0X,ARG\_643,11.94,-0.56,0,0  
 1WNN,GLU\_18,4.09,2.64,-1.18,-1.87  
 3I0C,ARG\_199,11.8,-0.7,0,0  
 3ASA,CYS\_227,10.41,0,0,1.41  
 3NJM,CYS\_34,9,0,0,0  
 1F2V,GLU\_126,4.29,0,-0.21,0  
 2D7U,TYR\_190,10,0,0,0  
 1RZ2,TYR\_110,13.03,0.66,0.2,38  
 1T3Y,GLU\_122,4.46,0.07,-0.11,0  
 2R51,LYS\_182,10.15,-0.35,0,0  
 2RJD,TYR\_211,13.94,0.74,0.8,2.4  
 2FD4,LYS\_546,10.5,0,0,0  
 1NIJ,HIS\_187,6.43,0,0,-0.07  
 1X9G,ARG\_43,11.66,-0.84,0,0  
 2BDD,HIS\_22,6.98,0.55,0,-0.07  
 200K,ASP\_115,3.63,0.63,-0.8,0  
 1YB2,ASP\_133,3.18,0.35,-0.97,0  
 3U2A,GLU\_84,4.3,0.07,-0.27,0  
 3FFM,ARG\_18,11.17,-1.33,0,0  
 4F3J,ASP\_126,1.65,0.56,-2.71,0  
 1X7F,HIS\_172,7.23,0.8,0,-0.07  
 3LH5,LYS\_763,10.5,0,0,0  
 4EVF,ASP\_163,4.15,0.35,0,0  
 3SMD,LYS\_8,10.36,-0.14,0,0  
 3O48,TYR\_18,10,0,0,0  
 1GQE,ASP\_208,2.57,0.63,-1.85,0  
 1JYH,TYR\_52,13.94,0.74,0.8,2.4  
 1P6F,GLU\_21,4.5,0,0,0  
 3PZ9,HIS\_302,1.43,1.6,0,-6.67  
 1J33,GLU\_329,1.7,0.49,-3.29,0  
 4F8A,LYS\_640,10.5,0,0,0  
 2QK1,LYS\_410,9.94,-0.56,0,0  
 3RNV,LYS\_393,10.29,-0.21,0,0  
 4ANN,TYR\_112,7.87,0.39,-0.77,-1.76  
 3JRT,GLU\_121,3.54,0.21,-1.17,0  
 2B02,CYS\_380,8.7,-0.68,0.38  
 3HUE,ARG\_46,12.15,-0.35,0,0  
 3R87,ASP\_75,2.71,0.84,-1.93,0  
 3BCH,GLU\_69,2.87,0.28,-1.91,0  
 1WOU,ASP\_79,3.12,0.49,-1.17,0  
 2GZR,TYR\_204,10.56,0.61,-0.05,0  
 2PLQ,ARG\_324,11.73,-0.77,0,0  
 2XWS,ARG\_27,12.15,-0.35,0,0  
 3CS1,LYS\_47,10.29,-0.21,0,0  
 1WXF,ARG\_105,12.29,-0.21,0,0  
 3CAX,HIS\_207,8.86,3.24,16,-5.01  
 3M7G,ARG\_249,12.01,-0.49,0,0  
 3PZ9,LYS\_120,10.08,-0.42,0,0  
 3M3P,HIS\_19,5,0.8,0,-2.3  
 1DVQ,ASP\_184,3.56,0.42,-0.67,0  
 3BWT,GLU\_736,4.5,0,0,0  
 1O6D,LYS\_91,10.29,-0.21,0,0  
 2R0S,ASP\_114,3.93,0.14,-0.01,0  
 2ZOM,ARG\_303,11.65,-3.25,0,2.4  
 3EVZ,ARG\_126,11.38,-1.12,0,0  
 3RFY,TYR\_433,11.74,0,0,1.74  
 1AIL,LYS\_41,9.8,-0.7,0,0  
 2CL3,GLU\_51,4.64,0.14,0,0  
 3GE9,ARG\_87,12.5,0,0,0  
 3O48,GLU\_23,2.22,0.49,-2.77,0  
 3UPD,GLU\_307,4.71,0.21,0,0  
 3M7G,GLU\_89,4.5,0,0,0  
 1G8P,ARG\_187,11.87,-0.63,0,0  
 3Q9P,LYS\_171,10.5,0,0,0  
 3ZSL,ASP\_154,3.36,0.7,-1.14,0  
 2G5X,LYS\_100,9.87,-0.63,0,0  
 3NR5,CYS\_156,10.6,-0.55,0,2.14  
 2G5X,ARG\_184,12.08,-0.42,0,0  
 1R9W,ARG\_330,12.15,-0.35,0,0  
 2OKT,GLU\_69,3.91,0.21,-0.8,0  
 2G3A,LYS\_15,10.29,-0.21,0,0  
 3RLN,HIS\_755,1.47,0,-2.28,-2.75  
 2GEN,ARG\_34,11.87,-0.63,0,0  
 3I4T,LYS\_168,10.5,0,0,0  
 3IPZ,ASP\_116,1.23,0.49,-3.07,0  
 3C38,LYS\_163,10.15,-0.35,0,0  
 1RZ2,TYR\_110,13.03,0.66,0.2,38  
 1TD6,LYS\_271,10.01,-0.49,0,0  
 3EVN,GLU\_170,4.5,0,0,0  
 1RZ2,HIS\_247,1.29,0,0,-5.21  
 1PGV,ASP\_235,0.3,0.77,-4.27,0  
 3EVZ,ARG\_37,11.8,-0.7,0,0  
 3H13,ARG\_435,11.66,-0.84,0,0  
 3FFM,HIS\_27,6.43,0,0,-0.07  
 3E27,LYS\_73,9.52,-0.98,0,0  
 2OBI,HIS\_114,4.19,0.73,0,-3.04  
 1DUN,ASP\_33,4.22,0.42,0,0  
 2G2D,ARG\_32,11.52,-0.98,0,0  
 3ETV,ARG\_328,12.15,-0.35,0,0  
 1NAR,HIS\_75,6.72,0.36,0,-0.14  
 3R2E,ASP\_37,2.54,0.7,-1.95,0  
 1O3X,LYS\_198,10.43,-0.07,0,0  
 1SI7,TYR\_114,9.56,0.07,-1.68,1.17  
 4D8L,GLU\_14,4.45,0.07,-0.12,0  
 1AM2,ASP\_20,1.89,0.49,-2.4,0  
 3V55,LYS\_709,10.29,-0.21,0,0  
 3UAH,ARG\_500,12.43,-0.07,0,0  
 3JZN,CYS\_324,5.77,-3.66,0.04,0.38  
 1R3F,ARG\_212,12.5,0,0,0  
 2IF4,GLU\_260,3.89,0.07,-0.68,0  
 1TXD,LYS\_949,10.43,-0.07,0,0  
 1RZ2,ASP\_64,3.94,0.14,0,0  
 1L3K,GLU\_28,3.34,0.28,-1.44,0  
 2Q99,LYS\_181,10.5,0,0,0  
 4F8A,ASP\_616,2.94,0.21,-1.06,0  
 3V1Q,LYS\_640,10.5,0,0,0  
 3AD0,LYS\_287,10.15,-0.35,0,0  
 1WRU,ASP\_202,3.81,0.14,-0.13,0  
 2QK1,HIS\_314,7.35,0.92,0,-0.07  
 1QVI,GLU\_368,3.13,0.35,-1.72,0  
 3DHN,ARG\_171,12.22,-0.28,0,0  
 3UV9,GLU\_395,0.62,0.92,-2.4,-2.4  
 1NWA,LYS\_123,10.5,0,0,0  
 3EOH,HIS\_156,6.43,0,0,-0.07  
 2OGQ,TYR\_510,6.77,0.24,-0.8,-2.68  
 3ELI,GLU\_96,3.88,0.28,-0.89,0  
 2EYI,ASP\_192,3.55,0.42,-0.67,0  
 3F6M,GLU\_151,3.91,0.21,-0.8,0  
 1WPA,ARG\_468,12.15,-0.35,0,0  
 1RI6,ASP\_71,2.67,0.42,-1.55,0  
 3BCY,ASP\_65,3.57,0.84,-1.07,0  
 3EYE,LYS\_116,10.08,-0.42,0,0  
 2IF4,LYS\_162,10.22,-0.28,0,0  
 3O48,GLU\_15,4.3,0.28,-0.48,0  
 1PSW,ASP\_253,3.18,0.35,-0.96,0  
 4AE7,TYR\_70,10,0,0,0  
 2H2Z,TYR\_154,10,0,0,0  
 3IL3,TYR\_271,13.9,0.7,0.8,2.4  
 2Q13,LYS\_375,10.5,0,0,0  
 2GZR,HIS\_287,5.12,0,0,-1.38  
 3ANJ,TYR\_278,7.52,0.9,-1.72,-1.66  
 3C2E,TYR\_167,10.42,0.42,0,0  
 2YT4,ARG\_527,12.5,0,0,0  
 2A6B,ARG\_80,11.24,-1.26,0,0  
 2Q5X,ARG\_800,11.52,-0.98,0,0  
 3GW3,TYR\_164,11.65,1.65,0,0  
 1RAJ,GLU\_337,3.91,0.21,-0.8,0  
 2Q34,LYS\_228,10.36,-0.14,0,0  
 3E5T,ARG\_125,12.5,0,0,0  
 1DVO,LYS\_95,10.5,0,0,0  
 3HQX,LYS\_36,10.22,-0.28,0,0  
 3EX9,ARG\_139,11.94,-0.56,0,0  
 1XTZ,HIS\_259,6.43,0,0,-0.07  
 1Q2Y,LYS\_125,10.22,-0.28,0,0  
 3M7D,ASP\_6,2.97,0.49,-1.32,0  
 2CE6,CYS\_42,9,0,0,0  
 2AZL,GLU\_269,4.57,0.07,0,0  
 4ETX,GLU\_418,1.53,0.42,-3.39,0  
 2B0J,TYR\_218,10.07,0.07,0,0  
 3ETV,LYS\_207,10.29,-0.21,0,0  
 1YW5,HIS\_20,6.43,0,0,-0.07  
 1BN6,ARG\_265,11.8,-0.7,0,0  
 2WB3,LYS\_288,10.5,0,0,0  
 2QDJ,ARG\_73,12.29,-0.21,0,0  
 1J79,TYR\_74,9.23,0,-0.77,0  
 3LH5,GLU\_568,4.5,0.28,-0.28,0  
 3EVZ,TYR\_58,10.93,1.01,-0.08,0  
 3HQX,GLU\_98,4.64,0.14,0,0  
 1BN6,ASP\_209,4.23,0.49,-0.06,0  
 1UAJ,ARG\_92,12.01,-0.49,0,0  
 3DHN,GLU\_60,3.83,0.49,-1.16,0  
 1X7F,ASP\_254,3.64,0,-0.16,0  
 2W0G,GLU\_200,4.26,0.07,-0.31,0  
 2Q12,ARG\_171,11.73,-0.77,0,0  
 1QQL,TYR\_64,9.67,0.07,-0.4,0  
 3EAZ,GLU\_93,4.81,0.35,-0.04,0  
 1Z3X,TYR\_64,10.61,0.82,-0.21,0  
 2B61,TYR\_249,8.15,0.12,-0.1,-1.87  
 2BV9,HIS\_287,6.36,0,0,-0.14  
 1AK1,HIS\_262,2.46,0.12,0,-4.16  
 3K1H,LYS\_60,10.5,0,0,0  
 3CGW,GLU\_269,4.5,0,0,0  
 3CX2,ASP\_228,3.86,0.21,-0.15,0  
 1WXQ,ASP\_361,3.73,0.21,-0.27,0  
 1F2V,GLU\_178,4.64,0.14,0,0  
 3DTE,TYR\_234,12.32,0.07,-0.15,2.4  
 1N81,LYS\_173,10.43,-0.07,0,0  
 2ZCO,LYS\_16,10.5,0,0,0  
 4AM1,TYR\_211,10.54,0.74,-0.2,0  
 2GZR,HIS\_264,6.43,0,0,-0.07  
 2AHE,ASP\_28,1.44,0.7,-3.06,0  
 3GEC,TYR\_264,10.53,0.98,-0.45,0  
 2Q07,LYS\_286,10.08,-0.42,0,0  
 3M70,LYS\_26,10.22,-0.28,0,0  
 2EYI,HIS\_156,7.27,0.91,0,-0.14  
 4ETX,ASP\_271,3.92,0.14,-0.02,0

3G9T,LYS\_39,10.5,0,0,0  
4E6S,ARG\_75,12.08,-0.42,0,0  
1XIP,ASP\_244,3.28,0.28,-0.8,0  
3LJI,ARG\_285,11.45,-1.05,0,0  
2A6B,ASP\_73,1,0.42,-3.22,0  
3F7M,ARG\_122,11.94,-0.56,0,0  
2Q5X,ARG\_834,12.22,-0.28,0,0  
3EVZ,GLU\_188,4.17,0,-0.33,0  
3AU3,HIS\_668,4.63,0.82,0,-2.69  
3KB5,ARG\_278,12.22,-0.28,0,0  
2P52,GLU\_282,0.79,0.76,-0.92,-3.55  
1A8Q,GLU\_99,2.44,4.5,-2.4,-4.16  
3V3T,HIS\_51,6.88,0.59,0,-0.21  
2R0S,TYR\_247,13.2,0.8,0.2,4  
1R2Z,LYS\_249,10.08,-0.42,0,0  
3QYB,LYS\_917,10.29,-0.21,0,0  
2B61,TYR\_24,10.07,0,0,0.07  
2X5Y,GLU\_852,2.37,0.49,-2.62,0  
2W2S,ASP\_30,2.6,0,-1.2,0  
1A8Q,ARG\_86,11.94,-0.56,0,0  
2BT8,ASP\_215,3.78,0.07,-0.09,0  
1JYH,LYS\_155,10.22,-0.28,0,0  
3QAV,ARG\_101,13.51,-1.35,0.2,36  
1FQI,ASP\_286,1.82,0.42,-2.4,0  
1SQH,GLU\_160,3.04,0.21,-1.67,0  
3VJ8,CYS\_303,10.76,0,0,1.76  
3V55,TYR\_367,10.93,0.33,-0.38,0.99  
3GE9,ARG\_129,12.08,-0.42,0,0  
2DFL,ARG\_66,12.5,0,0,0  
1VSM,LYS\_166,10.43,-0.07,0,0  
3EOD,TYR\_125,10.48,0,0,0.48  
3HZQ,GLU\_4,4.5,0,0,0  
2F4Q,ARG\_78,12.15,-0.35,0,0  
1QQI,GLU\_62,4.5,0,0,0  
2WB3,LYS\_336,10.01,-0.49,0,0  
1X04,TYR\_203,11.69,0.21,0,1.48  
3LJC,ARG\_125,12.5,0,0,0  
2H01,ASP\_145,3.71,0.07,-0.16,0  
1SUU,LYS\_787,10.5,0,0,0  
2BDD,TYR\_130,13.27,0.07,0.8,2.4  
2Q98,GLU\_143,4.5,0,0,0  
1LPL,LYS\_183,10.36,-0.14,0,0  
2C2Y,GLU\_250,4.5,0,0,0  
1R7J,LYS\_84,10.5,0,0,0  
1PVT,LYS\_191,10.22,-0.28,0,0  
1NWA,ASP\_64,2.08,0.42,-2.13,0  
3V3T,ARG\_252,12.22,-0.28,0,0  
1X8F,GLU\_223,4.78,0.28,0,0  
1TUL,TYR\_57,8.49,0.14,-2.06,0.41  
3I47,LYS\_160,10.43,-0.07,0,0  
1HF8,HIS\_84,3.97,0,-2.53  
2ZQ5,TYR\_313,13.41,0.21,0.8,2.4  
1TR9,GLU\_247,3.94,0.63,-1.19,0  
2APL,GLU\_83,4.64,0.14,0,0  
1ZCU,ASP\_44,3.63,0,-0.17,0  
2ZCO,TYR\_248,10.64,2.59,-0.42,-1.52  
1SUU,ASP\_679,3.85,0.21,-0.16,0  
2YX0,ASP\_327,2.99,0.42,-1.23,0  
4FLE,HIS\_31,6.38,0.02,0,-0.14  
2D0A,TYR\_104,10.34,1.14,-0.8,0  
3HVM,LYS\_48,10.5,0,0,0  
3C38,LYS\_240,10.29,-0.21,0,0  
2R2Y,ASP\_53,3.58,0.07,-0.29,0  
3LH5,ARG\_752,12.29,-0.21,0,0  
3Q6L,GLU\_55,4.56,0.14,-0.08,0  
1V43,ASP\_120,2.83,0.63,-1.6,0  
3N0K,HIS\_89,7.42,1.05,0,-0.14  
1LPL,CYS\_203,8.73,-0.41,0,0.14  
3E5T,GLU\_185,2.86,0.28,-1.92,0  
2IIA,TYR\_60,9.27,0.14,-0.87,0  
1O5T,ARG\_300,12.15,-0.35,0,0  
1O6D,LYS\_16,10.5,0,0,0  
1ANU,CYS\_33,10.93,-0.11,0,2.04  
3T57,GLU\_289,4.5,0,0,0  
4FZR,GLU\_304,4.59,0.09,0,0  
3NR5,CYS\_34,9.67,-0.1,0,0.77  
3G6S,ARG\_56,12.36,-0.14,0,0  
3I4T,LYS\_73,10.29,-0.21,0,0  
3ADO,ASP\_219,3.67,0.07,-0.2,0  
3V1Q,GLU\_666,4.5,0,0,0  
2HXB,ASP\_49,2.55,0.35,-1.6,0  
3VJ8,TYR\_304,12.65,0.87,-0.01,1.79  
3COU,CYS\_23,10.48,-0.22,0,1.7  
2GZR,HIS\_238,2.53,0.08,0,-4.05  
1F2V,ASP\_9,3.12,0.42,-1.1,0  
3JV1,ARG\_83,11.38,-1.12,0,0  
1DUN,GLU\_15,3.52,0.35,-1.33,0  
1ES9,HIS\_180,6.85,0.43,0,-0.07  
3A2Z,ASP\_77,2.48,0.07,-0.16,-1.23  
1ZBS,GLU\_144,2.63,0.59,-2.46,0  
3DZ1,LYS\_55,9.59,-0.91,0,0  
1MTZ,LYS\_139,10.43,-0.07,0,0  
2I88,GLU\_394,4.55,0.14,-0.09,0  
3UX2,ARG\_106,12.43,-0.07,0,0  
1O17,ARG\_236,11.94,-0.56,0,0  
2CWC,TYR\_294,9.74,0.14,-0.65,0.26  
3ERF,ASP\_78,3.87,0.07,0,0  
1E5S,LYS\_197,10.5,0,0,0  
1NIJ,LYS\_254,10.22,-0.28,0,0  
3CSR,CYS\_36,10.45,0,0,1.45  
2B6P,ARG\_156,12.5,0,0,0  
1OIS,GLU\_246,4.5,0,0,0  
3JZN,GLU\_131,2.45,0.35,-2.4,0  
1V6T,LYS\_216,10.29,-0.21,0,0  
2GYZ,ARG\_38,12.5,0,0,0  
1QQL,TYR\_97,13.54,2.05,0,1.49  
4FLE,TYR\_7,10.32,1.86,-1.54,0  
3M16,GLU\_156,4.05,0.35,-0.8,0  
3B7H,LYS\_2,10.22,-0.28,0,0  
2H30,LYS\_55,10.5,0,0,0  
2RIK,LYS\_184,10.29,-0.21,0,0  
3B4D,ARG\_248,11.87,-0.63,0,0  
3EJG,ARG\_99,12.36,-0.14,0,0  
1O0X,LYS\_253,10.29,-0.21,0,0  
1YLN,HIS\_113,6.4,0.04,0,-0.14  
3EZ7,GLU\_354,4.4,0.14,-0.24,0  
1ZYL,GLU\_319,4.5,0,0,0  
3C6B,ARG\_232,11.87,-0.63,0,0  
3H5T,HIS\_117,6.5,0,0,0  
2B2H,TYR\_129,13.98,4.08,-0.1,0  
2GS5,ASP\_31,3.82,0.07,-0.05,0  
2I88,LYS\_420,10.5,0,0,0  
2QHT,ASP\_160,3.79,0,-0.01,0  
2PPN,GLU\_60,2.92,0.63,-2.21,0  
1SJV,TYR\_139,9.74,0.07,-0.33,0  
2YX0,HIS\_292,6.95,0.8,0,-0.35  
1LTU,ARG\_114,12.29,-0.21,0,0  
1J85,CYS\_22,11.09,0,0,2.09  
2YLF,TYR\_196,12.53,0.93,0,1.6  
2YLF,LYS\_142,10.43,-0.07,0,0  
2APL,GLU\_85,4.12,0.42,-0.8,0  
1F2V,TYR\_181,10.1,0.14,-0.04,0  
3HNX,HIS\_88,7.09,0.8,0,-0.21  
1MML,GLU\_123,4.01,0.28,-0.77,0  
1JT9,GLU\_261,4.58,0.21,-0.13,0  
1YR6,ASP\_195,3.8,0,0,0  
1Z3X,TYR\_165,13.5,3.5,0,0  
2GAU,GLU\_184,3.65,0.14,-0.99,0  
2QVT,TYR\_38,10.03,0.07,-0.04,0  
3EGN,GLU\_462,3.94,0.63,-1.19,0  
3JZN,TYR\_365,11.64,3.33,-0.37,-1.32  
3KB5,GLU\_399,4.5,0,0,0  
1P2F,LYS\_149,9.94,-0.56,0,0  
2CXC,ASP\_77,2.67,0.42,-1.55,0  
3CGW,GLU\_83,4.25,0.42,-0.67,0  
1UJ8,TYR\_27,11.67,0.07,0,1.6  
2RIK,HIS\_112,6.5,0,0,0  
2GAU,CYS\_96,7.37,-0.2,-1.45,0.01  
2WZ9,LYS\_79,10.29,-0.21,0,0  
3GT0,LYS\_24,10.29,-0.21,0,0  
2AH5,LYS\_41,10.43,-0.07,0,0  
2CWC,ARG\_106,12.5,0,0,0  
2RJD,ARG\_321,12.08,-0.42,0,0  
1WOU,ARG\_85,11.38,-1.12,0,0  
1NRI,GLU\_238,4.57,0.07,0,0  
1O59,LYS\_2,10.43,-0.07,0,0  
2I88,LYS\_369,10.5,0,0,0  
2BLL,ARG\_355,11.66,-0.84,0,0  
3EJG,TYR\_106,10.81,2.5,-1.88,0.2  
3N0K,ASP\_52,4.12,0.49,-0.17,0  
1CBY,LYS\_208,10.5,0,0,0  
1E5S,ARG\_30,11.59,-0.91,0,0  
2OYZ,ASP\_85,4.01,0.21,0,0  
2O8I,ARG\_99,12.29,-0.21,0,0  
2FI9,GLU\_64,4.78,0.28,0,0  
4DIU,ARG\_16,11.73,-0.77,0,0  
2B2H,GLU\_85,4.78,0.28,0,0  
2D0A,LYS\_206,10.15,-0.35,0,0  
2G2D,ARG\_133,11.71,-0.79,0,0  
2VGM,TYR\_255,10,0,0,0  
2NYC,ARG\_263,12.29,-0.21,0,0  
2QVO,GLU\_16,4.07,0.14,-0.57,0  
1E5S,TYR\_222,10,0,0,0  
1TLV,ASP\_91,3.64,0,-0.16,0  
4DNU,GLU\_189,4.78,0.28,0,0  
2XMZ,LYS\_79,10.15,-0.35,0,0  
2O0K,ARG\_86,12.74,-1.89,0,2.13  
3EUR,LYS\_63,10.5,0,0,0  
3CIV,ASP\_74,3.94,0.14,0,0  
3CJW,ASP\_290,3.21,0.21,-0.8,0  
3C2E,TYR\_135,9.73,0.35,-0.64,0.03  
3RNV,LYS\_362,10.5,0,0,0  
2W0G,HIS\_180,7.23,0.8,0,-0.07