Delving Deep into the Structural Aspects of A Furin Cleavage Site Inserted into the Spike Protein of SARS-CoV-2: Supplementary materials

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List of Tables

Supplementary materials

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
MODEL	A_ARG_34	NH1	A_GLU_191	OE2	2.674
MODEL	A_ARG_44	NH1	A_ASP_40	OD1	2.695
MODEL	A_ARG_44	NH1	A_ASP_40	OD2	3.232
MODEL	A_ARG_44	NH2	A_ASP_40	OD1	3.625
MODEL	A_ARG_44	NH2	A_ASP_40	OD2	2.635
MODEL	A_ARG_78	NH1	A_ASP_138	OD2	2.688
MODEL	A_ARG_102	NH1	A_GLU_96	OE1	3.329
MODEL	A_LYS_195	NZ	A_ASP_53	OD1	2.683
MODEL	A_LYS_195	NZ	A_ASP_53	OD2	2.722
MODEL	A_LYS_206	NZ	A_GLU_224	OE1	2.749
MODEL	A_LYS_206	NZ	A_GLU_224	OE2	2.697
MODEL	A_ARG_214	NH1	A_ASP_215	OD1	2.721
MODEL	A_ARG_214	NH1	A_ASP_215	OD2	3.669
MODEL	A_ARG_273	NH2	A_ASP_290	OD1	2.616
MODEL	A_ARG_273	NH2	A_ASP_290	OD2	3.058
MODEL	A_LYS_278	NZ	A_ASP_287	OD2	3.755
MODEL	A_LYS_310	NZ	A_ASP_663	OD1	2.628
MODEL	A_LYS_310	NZ	A_ASP_663	OD2	2.667
MODEL	A_ARG_319	NH1	B_ASP_737	OD2	2.735
MODEL	A_ARG_319	NH1	B_ASP_745	OD1	3.587
MODEL	A_ARG_319	NH2	B_ASP_737	OD2	3.982
MODEL	A_ARG_328	NH1	A_ASP_578	OD2	3.263
MODEL	A_ARG_328	NH2	A_ASP_578	OD2	3.964
MODEL	A_ARG_355	NH2	A_ASP_398	OD1	3.101
MODEL	A_ARG_355	NH2	A_ASP_398	OD2	2.632
MODEL	A_LYS_356	NZ	A_GLU_340	OE1	2.636
MODEL	A_ARG_403	NH1	A_GLU_406	OE2	3.089
MODEL	A_LYS_458	NZ	A_GLU_471	OE1	2.430
MODEL	A_ARG_466	NH1	A_ASP_467	OD1	3.188
MODEL	A_ARG_466	NH1	A_ASP_467	OD2	2.659
MODEL	A_ARG_509	NH1	A_ASP_442	OD1	2.803
MODEL	A_ARG_509	NH1	A_ASP_442	OD2	3.407
MODEL	A_LYS_537	NZ	A_GLU_324	OE1	2.730
MODEL	A_LYS_537	NZ	A_GLU_324	OE2	2.652
MODEL	A_LYS_557	NZ	A_ASP_568	OD1	2.715
MODEL	A_LYS_557	NZ	A_ASP_568	OD2	2.782
MODEL	A_LYS_557	NZ	A_ASP_574	OD1	2.869
MODEL	A_LYS_557	NZ	A_ASP_574	OD2	2.649
MODEL	A_ARG_567	NH1	A_ASP_571	OD1	2.606
MODEL	A_ARG_567	NH2	A_ASP_571	OD1	2.720
MODEL	A_LYS_733	NZ	A_ASP_775	OD1	3.202
MODEL	A_LYS_733	NZ	A_ASP_775	OD2	2.601
MODEL	A_LYS_790	NZ	C_GLU_702	OE1	2.623
MODEL	A_LYS_790	NZ	C_GLU_702	OE2	2.744
MODEL	A_LYS_811	NZ	A_ASP_820	OD2	2.461
MODEL	A_ARG_815	NH1	A_ASP_820	OD1	2.649
MODEL	A_LYS_986	NZ	A_GLU_748	OE2	2.597
MODEL	A_ARG_995	NH1	B_ASP_994	OD1	3.497
MODEL	A_ARG_995	NH1	B_ASP_994	OD2	2.691
MODEL	A_ARG_995	NH2	B_ASP_994	OD1	2.657
MODEL	A_ARG_995	NH2	B_ASP_994	OD2	3.473
MODEL	A_ARG_1019	NH1	A_GLU_773	OE1	2.777
MODEL	A_ARG_1019	NH2	A_GLU_780	OE1	3.073
MODEL	A_ARG_1019	NH2	A_GLU_780	OE2	3.823
MODEL	A_LYS_1028	NZ	A_GLU_725	OE1	2.878
MODEL	A_LYS_1028	NZ	A_GLU_725	OE2	2.589
MODEL	A_ARG_1039	NH1	A_GLU_1031	OE1	2.697

MODEL	A_ARG_1039	NH1	A_GLU_1031	OE2	3.642
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE1	3.621
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE2	2.620
MODEL	A_HIS_1064	NE2	A_GLU_725	OE1	2.720
MODEL	A_HIS_1083	ND1	A_ASP_1084	OD1	3.726
MODEL	A_HIS_1083	NE2	A_ASP_1084	OD1	2.954
MODEL	A_HIS_1083	NE2	A_ASP_1084	OD2	3.064
MODEL	A_LYS_1086	NZ	A_ASP_1084	OD2	2.860
MODEL	B_ARG_34	NH1	B_GLU_191	OE2	2.594
MODEL	B_ARG_78	NH2	B_ASP_80	OD1	3.853
MODEL	B_ARG_78	NH2	B_ASP_80	OD2	3.115
MODEL	B_LYS_195	NZ	B_ASP_53	OD1	2.671
MODEL	B_LYS_195	NZ	B_ASP_53	OD2	2.656
MODEL	B_LYS_206	NZ	B_GLU_224	OE1	3.459
MODEL	B_LYS_206	NZ	B_GLU_224	OE2	2.611
MODEL	B_ARG_273	NH2	B_ASP_290	OD1	2.633
MODEL	B_ARG_273	NH2	B_ASP_290	OD2	3.259
MODEL	B_LYS_278	NZ	B_ASP_287	OD2	2.604
MODEL	B_LYS_310	NZ	B_ASP_663	OD1	2.691
MODEL	B_LYS_310	NZ	B_ASP_663	OD2	2.615
MODEL	B_ARG_319	NH1	C_ASP_745	OD1	2.606
MODEL	B_ARG_319	NH1	C_ASP_745	OD2	3.565
MODEL	B_ARG_319	NH2	C_ASP_745	OD1	3.325
MODEL	B_ARG_319	NH2	C_ASP_745	OD2	2.636
MODEL	B_ARG_328	NH1	B_ASP_578	OD2	3.286
MODEL	B_ARG_328	NH2	B_ASP_578	OD1	3.906
MODEL	B_ARG_328	NH2	B_ASP_578	OD2	2.659
MODEL	B_ARG_355	NH2	B_ASP_398	OD2	2.596
MODEL	B_ARG_403	NH1	B_GLU_406	OE2	2.630
MODEL	B_ARG_403	NH2	B_GLU_406	OE2	3.754
MODEL	B_ARG_408	NH1	B_ASP_405	OD1	2.895
MODEL	B_ARG_408	NH1	B_ASP_405	OD2	2.755
MODEL	B_ARG_408	NH2	B_ASP_405	OD2	3.887
MODEL	B_ARG_454	NH1	B_ASP_467	OD2	2.590
MODEL	B_LYS_462	NZ	B_GLU_465	OE2	3.504
MODEL	B_ARG_509	NH1	B_ASP_442	OD1	2.673
MODEL	B_ARG_509	NH1	B_ASP_442	OD2	3.881
MODEL	B_LYS_528	NZ	B_ASP_389	OD2	2.658
MODEL	B_LYS_535	NZ	B_GLU_554	OE2	2.577
MODEL	B_LYS_537	NZ	B_GLU_324	OE1	2.634
MODEL	B_LYS_537	NZ	B_GLU_324	OE2	2.706
MODEL	B_LYS_557	NZ	B_ASP_586	OD1	2.689
MODEL	B_LYS_557	NZ	B_ASP_586	OD2	2.627
MODEL	B_ARG_567	NH1	B_ASP_571	OD1	2.826
MODEL	B_ARG_567	NH1	B_ASP_571	OD2	2.786
MODEL	B_ARG_567	NH2	B_ASP_571	OD1	3.551
MODEL	B_HIS_625	ND1	B_ASP_627	OD2	3.516
MODEL	B_HIS_625	NE2	B_ASP_627	OD2	3.967
MODEL	B_ARG_646	NH1	B_ASP_614	OD2	2.839
MODEL	B_LYS_733	NZ	B_ASP_775	OD1	3.016
MODEL	B_LYS_733	NZ	B_ASP_775	OD2	2.582
MODEL	B_LYS_776	NZ	B_GLU_780	OE1	2.710
MODEL	B_LYS_776	NZ	B_GLU_780	OE2	2.672
MODEL	B_LYS_790	NZ	A_GLU_702	OE1	2.570
MODEL	B_LYS_790	NZ	A_GLU_702	OE2	3.570
MODEL	B_ARG_815	NH1	B_ASP_820	OD1	2.696
MODEL	B_ARG_815	NH2	B_ASP_867	OD1	2.920
MODEL	B_ARG_815	NH2	B_GLU_868	OE2	3.311

MODEL	B_LYS_854	NZ	A_ASP_614	OD1	3.487
MODEL	B_ARG_983	NH2	B_ASP_979	OD1	2.614
MODEL	B_ARG_983	NH2	B_ASP_979	OD2	3.538
MODEL	B_LYS_986	NZ	C_ASP_427	OD2	3.985
MODEL	B_ARG_995	NH1	C_ASP_994	OD1	2.636
MODEL	B_ARG_995	NH1	C_ASP_994	OD2	3.371
MODEL	B_ARG_995	NH2	C_ASP_994	OD1	3.182
MODEL	B_ARG_995	NH2	C_ASP_994	OD2	2.637
MODEL	B_ARG_1019	NH1	B_GLU_773	OE1	3.284
MODEL	B_ARG_1019	NH1	B_GLU_773	OE2	2.600
MODEL	B_LYS_1028	NZ	B_GLU_725	OE1	2.732
MODEL	B_LYS_1028	NZ	B_GLU_725	OE2	2.670
MODEL	B_ARG_1039	NH1	B_GLU_1031	OE1	2.669
MODEL	B_ARG_1039	NH1	B_GLU_1031	OE2	3.057
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE1	2.711
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE2	3.989
MODEL	B_LYS_1045	NZ	B_ASP_1041	OD1	2.637
MODEL	B_HIS_1064	NE2	B_GLU_725	OE2	2.768
MODEL	B_LYS_1086	NZ	B_ASP_1084	OD2	2.620
MODEL	C_LYS_97	NZ	C_GLU_96	OE2	2.761
MODEL	C_LYS_97	NZ	C_ASP_253	OD1	2.693
MODEL	C_LYS_97	NZ	C_ASP_253	OD2	2.866
MODEL	C_LYS_113	NZ	B_GLU_471	OE2	2.679
MODEL	C_LYS_129	NZ	C_GLU_169	OE1	2.582
MODEL	C_LYS_129	NZ	C_GLU_169	OE2	2.463
MODEL	C_LYS_150	NZ	C_GLU_154	OE1	2.608
MODEL	C_LYS_150	NZ	C_GLU_154	OE2	2.752
MODEL	C_ARG_158	NH2	C_GLU_154	OE2	3.189
MODEL	C_LYS_187	NZ	C_GLU_180	OE2	2.873
MODEL	C_LYS_202	NZ	C_ASP_228	OD2	2.762
MODEL	C_ARG_246	NH1	C_GLU_156	OE1	2.756
MODEL	C_ARG_246	NH1	C_GLU_156	OE2	3.170
MODEL	C_ARG_246	NH2	C_GLU_156	OE1	3.528
MODEL	C_ARG_246	NH2	C_GLU_156	OE2	2.612
MODEL	C_ARG_273	NH1	C_ASP_290	OD1	2.966
MODEL	C_ARG_273	NH1	C_ASP_290	OD2	3.840
MODEL	C_ARG_273	NH2	C_ASP_290	OD1	2.966
MODEL	C_ARG_273	NH2	C_ASP_290	OD2	2.552
MODEL	C_LYS_310	NZ	C_ASP_663	OD1	3.129
MODEL	C_ARG_319	NH1	A_ASP_745	OD1	3.819
MODEL	C_ARG_328	NH1	C_ASP_578	OD2	2.598
MODEL	C_ARG_328	NH2	C_ASP_578	OD1	3.708
MODEL	C_ARG_328	NH2	C_ASP_578	OD2	2.801
MODEL	C_ARG_355	NH2	C_ASP_398	OD1	3.407
MODEL	C_ARG_355	NH2	C_ASP_398	OD2	2.579
MODEL	C_LYS_356	NZ	C_GLU_340	OE1	2.568
MODEL	C_ARG_403	NH1	C_GLU_406	OE1	3.581
MODEL	C_ARG_403	NH1	C_GLU_406	OE2	2.672
MODEL	C_ARG_403	NH2	C_GLU_406	OE2	2.658
MODEL	C_LYS_458	NZ	A_ASP_389	OD2	3.696
MODEL	C_LYS_462	NZ	C_GLU_465	OE1	2.614
MODEL	C_LYS_462	NZ	C_GLU_465	OE2	2.647
MODEL	C_ARG_509	NH1	C_ASP_442	OD1	2.578
MODEL	C_LYS_528	NZ	C_ASP_389	OD1	3.189
MODEL	C_LYS_528	NZ	C_ASP_389	OD2	3.148
MODEL	C_LYS_535	NZ	C_GLU_554	OE1	2.654
MODEL	C_LYS_535	NZ	C_GLU_554	OE2	2.723
MODEL	C_LYS_537	NZ	C_GLU_324	OE2	2.535

MODEL	C_LYS_557	NZ	C_ASP_568	OD1	2.816
MODEL	C_LYS_557	NZ	C_ASP_568	OD2	2.819
MODEL	C_LYS_557	NZ	C_ASP_574	OD1	3.661
MODEL	C_LYS_557	NZ	C_ASP_574	OD2	2.584
MODEL	C_ARG_567	NH1	C_ASP_571	OD1	3.523
MODEL	C_ARG_567	NH1	C_ASP_571	OD2	2.610
MODEL	C_ARG_567	NH2	C_ASP_571	OD1	2.539
MODEL	C_ARG_567	NH2	C_ASP_571	OD2	3.300
MODEL	C_ARG_646	NH1	A_ASP_848	OD2	3.643
MODEL	C_ARG_646	NH2	A_ASP_848	OD1	3.695
MODEL	C_ARG_646	NH2	A_ASP_848	OD2	2.627
MODEL	C_LYS_733	NZ	C_ASP_775	OD1	3.066
MODEL	C_LYS_733	NZ	C_ASP_775	OD2	2.575
MODEL	C_LYS_811	NZ	C_ASP_820	OD2	3.817
MODEL	C_ARG_815	NH1	C_ASP_820	OD1	2.929
MODEL	C_ARG_815	NH1	C_ASP_820	OD2	2.916
MODEL	C_ARG_815	NH2	C_ASP_820	OD1	3.727
MODEL	C_ARG_847	NH1	B_GLU_619	OE1	3.034
MODEL	C_LYS_854	NZ	B_ASP_614	OD1	2.686
MODEL	C_LYS_986	NZ	C_GLU_748	OE1	2.531
MODEL	C_ARG_995	NH1	A_ASP_994	OD1	2.647
MODEL	C_ARG_995	NH1	A_ASP_994	OD2	3.498
MODEL	C_ARG_995	NH2	A_ASP_994	OD1	3.382
MODEL	C_ARG_995	NH2	A_ASP_994	OD2	2.636
MODEL	C_ARG_1019	NH1	B_GLU_1017	OE2	2.726
MODEL	C_ARG_1019	NH1	C_GLU_773	OE2	2.647
MODEL	C_ARG_1019	NH2	B_GLU_1017	OE2	3.415
MODEL	C_LYS_1028	NZ	C_GLU_725	OE1	2.678
MODEL	C_LYS_1028	NZ	C_GLU_725	OE2	2.787
MODEL	C_ARG_1039	NH1	C_GLU_1031	OE1	3.735
MODEL	C_ARG_1039	NH1	C_GLU_1031	OE2	2.669
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE1	3.509
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE2	2.596
MODEL	C_HIS_1064	NE2	C_GLU_725	OE1	2.774
MODEL	C_LYS_1086	NZ	C_ASP_1084	OD2	2.855

Table 1: Salt bridging networks within the PDB entries. In this table, the residue naming scheme is **Chain ID_residue name_residue number**.

Count	Residue A	Residue B
12	ARG995	ASP994
12	ARG1039	GLU1031
9	ARG567	ASP571
8	ARG328	ASP578
8	ARG273	ASP290
6	ARG403	GLU406
6	LYS733	ASP775
6	LYS1028	GLU725
6	ARG319	ASP745
5	LYS310	ASP663
5	ARG815	ASP820
5	ARG355	ASP398
5	ARG509	ASP442
5	LYS537	GLU324
4	LYS790	GLU702
4	LYS206	GLU224
4	ARG1019	GLU773
4	LYS557	ASP568
4	ARG246	GLU156
4	LYS557	ASP574
4	LYS195	ASP53
4	ARG44	ASP40
3	LYS1086	ASP1084
3	ARG408	ASP405
3	LYS528	ASP389
3	LYS462	GLU465
3	LYS535	GLU554
3	ARG646	ASP848
3	HIS1064	GLU725
3	HIS1083	ASP1084
2	ARG214	ASP215
2	ARG34	GLU191
2	ARG1019	GLU780
2	LYS150	GLU154
2	LYS811	ASP820
2	LYS854	ASP614
2	LYS986	GLU748
2	ARG466	ASP467
2	ARG319	ASP737
2	LYS278	ASP287
2	LYS557	ASP586
2	LYS97	ASP253
2	HIS625	ASP627
2	ARG1019	GLU1017
2	ARG78	ASP80
2	LYS356	GLU340
2	LYS129	GLU169
2	LYS776	GLU780
2	ARG983	ASP979
1	ARG78	ASP138
1	ARG102	GLU96
1	ARG158	GLU154
1	LYS458	ASP389
1	LYS187	GLU180
1	ARG815	GLU868
1	ARG646	ASP614
1	LYS202	ASP228

1	LYS458	GLU471
1	ARG454	ASP467
1	LYS986	ASP427
1	LYS97	GLU96
1	ARG815	ASP867
1	LYS113	GLU471
1	ARG847	GLU619
1	LYS1045	ASP1041

Table 2: Counting of salt bridges within the PDB entries in Table 1.

PDB	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH$(°)
MODEL.PDB	O, A_VAL_62	N, A_THR_29	H, A_THR_29	2.95	2.12	28.08
MODEL.PDB	O, A_SER_60	N, A_SER_31	H, A_SER_31	2.90	1.91	7.61
MODEL.PDB	O, A_PRO_217	NE, A_ARG_34	HE, A_ARG_34	2.69	1.82	24.55
MODEL.PDB	OE2, A_GLU_191	NH1, A_ARG_34	HH11, A_ARG_34	2.67	1.78	22.19
MODEL.PDB	O, C_PHE_562	NZ, A_LYS_41	HZ1, A_LYS_41	2.82	1.90	19.31
MODEL.PDB	O, C_PHE_565	N, A_PHE_43	H, A_PHE_43	2.86	1.91	16.15
MODEL.PDB	OD1, A_ASP_40	NH1, A_ARG_44	HH12, A_ARG_44	2.70	1.70	6.73
MODEL.PDB	OD2, A_ASP_40	NH2, A_ARG_44	HH22, A_ARG_44	2.63	1.66	12.76
MODEL.PDB	O, A_PHE_275	N, A_THR_51	H, A_THR_51	2.92	1.93	8.57
MODEL.PDB	OD1, A_ASP_53	N, A_LEU_54	H, A_LEU_54	2.69	1.75	17.28
MODEL.PDB	O, A_GLN_271	N, A_PHE_55	H, A_PHE_55	2.89	1.93	14.85
MODEL.PDB	O, A_SER_31	N, A_PHE_59	H, A_PHE_59	2.79	1.91	23.18
MODEL.PDB	OG, A_SER_31	N, A_SER_60	H, A_SER_60	2.95	2.05	22.69
MODEL.PDB	O, A_PRO_57	OG, A_SER_60	HG, A_SER_60	2.69	1.88	25.91
MODEL.PDB	O, A_THR_29	N, A_VAL_62	H, A_VAL_62	2.85	1.86	7.63
MODEL.PDB	O, A_VAL_267	N, A_THR_63	H, A_THR_63	2.96	2.07	22.96
MODEL.PDB	O, A_TYR_265	N, A_PHE_65	H, A_PHE_65	2.90	1.90	8.15
MODEL.PDB	O, A_THR_76	N, A_GLY_72	H, A_GLY_72	2.98	2.04	17.50
MODEL.PDB	OD2, A_ASP_138	NH1, A_ARG_78	HH11, A_ARG_78	2.69	1.82	24.44
MODEL.PDB	O, A_PHE_238	N, A_LEU_84	H, A_LEU_84	2.88	1.90	12.05
MODEL.PDB	O, A_THR_236	N, A_PHE_86	H, A_PHE_86	2.97	2.03	17.03
MODEL.PDB	O, A_PHE_194	N, A_VAL_90	H, A_VAL_90	2.96	2.00	13.46
MODEL.PDB	O, A_GLY_268	N, A_TYR_91	H, A_TYR_91	2.82	1.91	20.75
MODEL.PDB	OE1, A_GLU_191	OH, A_TYR_91	HH, A_TYR_91	2.70	1.78	13.73
MODEL.PDB	O, A_PHE_192	N, A_PHE_92	H, A_PHE_92	2.81	1.81	6.16
MODEL.PDB	O, A_TYR_266	N, A_ALA_93	H, A_ALA_93	2.95	1.97	12.98
MODEL.PDB	O, A_ALA_264	OG, A_SER_94	HG, A_SER_94	2.80	1.88	13.90
MODEL.PDB	O, A_GLU_96	N, A_ASN_99	H, A_ASN_99	2.80	1.94	25.08
MODEL.PDB	O, A_LEU_241	N, A_ARG_102	H, A_ARG_102	2.91	1.99	20.77
MODEL.PDB	O, A_ILE_119	N, A_TRP_104	H, A_TRP_104	2.92	1.96	15.26
MODEL.PDB	O, A_GLN_239	N, A_ILE_105	H, A_ILE_105	2.83	1.82	3.74
MODEL.PDB	OD1, A_ASP_111	N, A_SER_112	H, A_SER_112	2.90	2.03	25.00
MODEL.PDB	O, A_ASP_111	N, A_LYS_113	H, A_LYS_113	2.76	1.81	15.43
MODEL.PDB	OE1, A_GLU_132	N, A_GLN_115	H, A_GLN_115	2.79	1.92	24.34
MODEL.PDB	O, A_PHE_106	N, A_LEU_117	H, A_LEU_117	2.77	1.82	16.07
MODEL.PDB	O, A_TRP_104	N, A_ILE_119	H, A_ILE_119	2.95	2.01	18.10
MODEL.PDB	O, A_VAL_127	N, A_VAL_120	H, A_VAL_120	2.94	1.93	5.02
MODEL.PDB	O, A_ARG_102	N, A_ASN_121	H, A_ASN_121	2.84	1.83	3.77
MODEL.PDB	OD1, A_ASN_122	N, A_ASN_125	H, A_ASN_125	2.92	1.95	12.42
MODEL.PDB	O, A_SER_172	N, A_VAL_126	H, A_VAL_126	2.85	1.93	20.11
MODEL.PDB	O, A_VAL_120	N, A_VAL_127	H, A_VAL_127	2.83	1.82	5.12
MODEL.PDB	O, A_TYR_170	N, A_ILE_128	H, A_ILE_128	2.90	1.91	10.23
MODEL.PDB	O, A_ASN_164	N, A_GLU_132	H, A_GLU_132	2.83	1.85	11.69
MODEL.PDB	OD1, A_ASP_111	N, A_PHE_135	H, A_PHE_135	2.92	2.01	20.87
MODEL.PDB	O, A_GLU_156	N, A_GLY_142	H, A_GLY_142	2.74	1.80	16.62
MODEL.PDB	OD1, A_ASN_149	N, A_LYS_150	H, A_LYS_150	2.72	1.74	12.62
MODEL.PDB	O, A_LYS_150	N, A_MET_153	H, A_MET_153	2.92	2.00	19.68
MODEL.PDB	O, A_SER_155	N, A_PHE_157	H, A_PHE_157	2.94	2.05	22.37
MODEL.PDB	O, A_GLN_134	OG, A_SER_161	HG, A_SER_161	2.70	1.75	5.85
MODEL.PDB	O, A_GLU_132	OG, A_SER_162	HG, A_SER_162	2.74	1.92	25.70
MODEL.PDB	OE1, A_GLU_169	N, A_PHE_168	H, A_PHE_168	2.88	1.96	19.77
MODEL.PDB	OD1, A_ASP_178	N, A_GLU_180	H, A_GLU_180	2.81	1.87	16.86
MODEL.PDB	O, A_ASP_178	ND2, A_ASN_188	HD21, A_ASN_188	2.73	1.81	19.79
MODEL.PDB	O, A_THR_208	N, A_LEU_189	H, A_LEU_189	2.72	1.73	10.06
MODEL.PDB	O, A_SER_94	N, A_ARG_190	H, A_ARG_190	2.99	1.98	2.82
MODEL.PDB	O, A_LYS_206	N, A_GLU_191	H, A_GLU_191	2.92	1.91	3.51
MODEL.PDB	O, A_PHE_92	N, A_PHE_192	H, A_PHE_192	2.77	1.81	14.78

MODEL.PDB	O, A_TYR_204	N, A_VAL_193	H, A_VAL_193	2.82	1.83	8.26
MODEL.PDB	O, A_VAL_90	N, A_PHE_194	H, A_PHE_194	2.94	1.94	7.39
MODEL.PDB	OH, A_TYR_37	NZ, A_LYS_195	HZ2, A_LYS_195	2.76	1.80	13.93
MODEL.PDB	O, A_ILE_233	ND2, A_ASN_196	HD22, A_ASN_196	2.94	1.97	13.74
MODEL.PDB	O, A_TYR_200	N, A_ILE_197	H, A_ILE_197	2.86	1.86	6.00
MODEL.PDB	O, A_ILE_197	N, A_TYR_200	H, A_TYR_200	2.74	1.79	15.00
MODEL.PDB	OE2, C_GLU_516	OH, A_TYR_200	HH, A_TYR_200	2.56	1.75	25.87
MODEL.PDB	O, A_LEU_229	N, A_PHE_201	H, A_PHE_201	2.78	1.81	12.01
MODEL.PDB	O, A_LYS_195	N, A_LYS_202	H, A_LYS_202	2.92	1.99	18.19
MODEL.PDB	O, A_VAL_193	N, A_TYR_204	H, A_TYR_204	2.86	1.89	13.20
MODEL.PDB	O, A_GLU_224	N, A_SER_205	H, A_SER_205	2.85	1.87	12.48
MODEL.PDB	O, A_GLU_191	N, A_LYS_206	H, A_LYS_206	2.90	1.94	15.36
MODEL.PDB	OE2, A_GLU_224	NZ, A_LYS_206	HZ3, A_LYS_206	2.70	1.79	20.97
MODEL.PDB	O, A_LEU_189	N, A_THR_208	H, A_THR_208	2.79	1.81	9.89
MODEL.PDB	OD1, A_ASP_215	NE, A_ARG_214	HE, A_ARG_214	2.96	2.08	24.64
MODEL.PDB	OD1, A_ASP_215	NH1, A_ARG_214	HH11, A_ARG_214	2.72	1.80	19.02
MODEL.PDB	OE2, A_GLU_191	OG, A_SER_221	HG, A_SER_221	2.68	1.80	18.27
MODEL.PDB	O, A_ILE_203	N, A_LEU_226	H, A_LEU_226	2.83	1.83	4.53
MODEL.PDB	O, A_GLY_199	N, A_ILE_231	H, A_ILE_231	2.83	1.85	11.58
MODEL.PDB	O, A_GLY_199	N, A_GLY_232	H, A_GLY_232	2.86	1.87	10.07
MODEL.PDB	O, A_LEU_84	N, A_PHE_238	H, A_PHE_238	2.85	1.85	8.44
MODEL.PDB	O, A_ILE_105	N, A_GLN_239	H, A_GLN_239	2.91	1.97	16.96
MODEL.PDB	O, A_ASN_81	NE2, A_GLN_239	HE21, A_GLN_239	2.98	2.13	26.80
MODEL.PDB	O, A_GLY_103	N, A_LEU_241	H, A_LEU_241	2.77	1.79	10.99
MODEL.PDB	O, A_LEU_141	N, A_LEU_244	H, A_LEU_244	2.88	1.94	17.90
MODEL.PDB	O, A_GLY_75	NH2, A_ARG_246	HH22, A_ARG_246	2.87	2.00	25.70
MODEL.PDB	O, A_SER_247	OG1, A_THR_250	HG1, A_THR_250	2.77	1.95	25.64
MODEL.PDB	OG, A_SER_255	N, A_GLY_252	H, A_GLY_252	2.92	1.98	17.69
MODEL.PDB	O, A_PHE_65	N, A_TYR_265	H, A_TYR_265	2.93	1.95	10.39
MODEL.PDB	O, A_ALA_93	N, A_TYR_266	H, A_TYR_266	2.74	1.76	10.55
MODEL.PDB	O, A_THR_63	N, A_VAL_267	H, A_VAL_267	2.85	1.85	6.97
MODEL.PDB	O, A_TYR_91	N, A_GLY_268	H, A_GLY_268	2.83	1.82	2.64
MODEL.PDB	O, A_GLY_89	N, A_LEU_270	H, A_LEU_270	2.99	2.01	10.68
MODEL.PDB	O, A_PHE_55	N, A_GLN_271	H, A_GLN_271	2.81	1.85	14.88
MODEL.PDB	O, A_GLN_271	N, A_ARG_273	H, A_ARG_273	2.86	2.02	27.75
MODEL.PDB	OD1, A_ASP_290	NH2, A_ARG_273	HH21, A_ARG_273	2.62	1.69	18.86
MODEL.PDB	O, A_THR_51	N, A_PHE_275	H, A_PHE_275	2.91	1.94	13.07
MODEL.PDB	O, A_VAL_289	N, A_LEU_276	H, A_LEU_276	2.98	1.99	8.88
MODEL.PDB	O, A_HIS_49	N, A_LEU_277	H, A_LEU_277	2.78	1.78	1.92
MODEL.PDB	O, A_VAL_47	N, A_TYR_279	H, A_TYR_279	2.95	1.96	9.17
MODEL.PDB	O, A_THR_284	N, A_ASN_280	H, A_ASN_280	2.94	1.96	10.38
MODEL.PDB	O, A_ASN_280	N, A_GLY_283	H, A_GLY_283	2.96	2.01	17.01
MODEL.PDB	O, A_LYS_278	N, A_THR_286	H, A_THR_286	2.96	1.98	10.87
MODEL.PDB	OD1, A_ASN_280	OG1, A_THR_286	HG1, A_THR_286	2.71	1.94	29.85
MODEL.PDB	O, A_LEU_276	N, A_VAL_289	H, A_VAL_289	2.95	1.96	9.94
MODEL.PDB	O, A_THR_274	N, A_CYS_291	H, A_CYS_291	2.95	2.00	16.00
MODEL.PDB	OD2, A_ASP_294	N, A_LEU_296	H, A_LEU_296	2.82	1.92	22.27
MODEL.PDB	OD1, A_ASP_294	N, A_SER_297	H, A_SER_297	2.97	2.06	20.77
MODEL.PDB	O, A_LEU_296	N, A_LYS_300	H, A_LYS_300	2.92	1.94	10.34
MODEL.PDB	OG, A_SER_50	NZ, A_LYS_304	HZ3, A_LYS_304	2.91	1.95	14.53
MODEL.PDB	O, A_THR_307	OG, A_SER_305	HG, A_SER_305	2.80	1.88	13.53
MODEL.PDB	OG1, A_THR_602	N, A_VAL_308	H, A_VAL_308	2.97	1.99	10.38
MODEL.PDB	OD1, A_ASP_663	NZ, A_LYS_310	HZ2, A_LYS_310	2.63	1.74	22.20
MODEL.PDB	OE2, A_GLU_298	OG, A_SER_316	HG, A_SER_316	2.68	1.73	6.59
MODEL.PDB	O, A_GLY_593	N, A_PHE_318	H, A_PHE_318	2.98	2.06	20.51
MODEL.PDB	OD2, B_ASP_737	NH1, A_ARG_319	HH12, A_ARG_319	2.74	1.78	15.71
MODEL.PDB	O, A_SER_591	N, A_VAL_320	H, A_VAL_320	2.97	1.99	11.29
MODEL.PDB	O, A_CYS_538	N, A_THR_323	H, A_THR_323	2.93	1.95	10.24

MODEL.PDB	O, A_ASN_542	N, A_ARG_328	H, A_ARG_328	2.88	1.98	21.34
MODEL.PDB	OE1, A_GLN_580	N, A_PHE_329	H, A_PHE_329	2.81	1.82	9.80
MODEL.PDB	OD1, A_ASN_334	N, A_LEU_335	H, A_LEU_335	2.82	1.96	26.15
MODEL.PDB	O, A_CYS_336	N, A_PHE_338	H, A_PHE_338	2.97	2.14	29.13
MODEL.PDB	O, A_PHE_338	N, A_VAL_341	H, A_VAL_341	2.95	2.02	18.44
MODEL.PDB	O, A_PHE_338	N, A_PHE_342	H, A_PHE_342	2.98	2.01	12.39
MODEL.PDB	O, A_THR_345	NH2, A_ARG_346	HH21, A_ARG_346	2.80	1.86	17.05
MODEL.PDB	OD1, A_ASP_398	NE, A_ARG_355	HE, A_ARG_355	2.67	1.68	10.27
MODEL.PDB	OD2, A_ASP_398	NH2, A_ARG_355	HH21, A_ARG_355	2.63	1.83	29.83
MODEL.PDB	O, A_ALA_397	N, A_LYS_356	H, A_LYS_356	2.93	1.96	11.64
MODEL.PDB	O, A_VAL_395	N, A_ILE_358	H, A_ILE_358	2.71	1.71	4.67
MODEL.PDB	OD1, A_ASN_394	OG, A_SER_359	HG, A_SER_359	2.65	1.78	19.43
MODEL.PDB	O, A_ASN_334	N, A_VAL_362	H, A_VAL_362	2.75	1.76	9.36
MODEL.PDB	O, A_CYS_525	N, A_ALA_363	H, A_ALA_363	2.83	1.91	19.65
MODEL.PDB	O, A_SER_366	N, A_ASN_370	H, A_ASN_370	2.89	1.93	14.11
MODEL.PDB	O, A_ALA_435	N, A_SER_375	H, A_SER_375	2.89	1.98	21.38
MODEL.PDB	O, A_ALA_435	N, A_THR_376	H, A_THR_376	2.80	1.87	18.08
MODEL.PDB	O, A_SER_383	N, A_LYS_386	H, A_LYS_386	2.96	1.96	7.83
MODEL.PDB	OG, A_SER_383	NZ, A_LYS_386	HZ1, A_LYS_386	2.87	2.00	24.63
MODEL.PDB	O, A_VAL_524	N, A_PHE_392	H, A_PHE_392	2.75	1.76	8.61
MODEL.PDB	O, A_GLU_516	N, A_THR_393	H, A_THR_393	2.86	1.93	18.67
MODEL.PDB	O, A_ALA_520	OG1, A_THR_393	HG1, A_THR_393	2.79	2.02	29.69
MODEL.PDB	OE1, A_GLU_516	ND2, A_ASN_394	HD21, A_ASN_394	2.79	1.83	15.55
MODEL.PDB	O, A_SER_514	N, A_TYR_396	H, A_TYR_396	2.91	1.91	5.69
MODEL.PDB	O, A_LYS_356	N, A_ALA_397	H, A_ALA_397	2.88	1.87	3.73
MODEL.PDB	O, A_VAL_512	N, A_ASP_398	H, A_ASP_398	2.91	1.92	10.71
MODEL.PDB	O, A_ASN_354	N, A_SER_399	H, A_SER_399	2.78	1.82	14.47
MODEL.PDB	O, A_GLN_506	N, A_GLY_404	H, A_GLY_404	2.96	2.12	27.68
MODEL.PDB	O, A_GLU_406	N, A_GLN_409	H, A_GLN_409	2.88	2.02	26.07
MODEL.PDB	OD2, A_ASP_420	N, A_GLY_416	H, A_GLY_416	2.76	1.75	4.30
MODEL.PDB	O, A_GLY_416	N, A_ASP_420	H, A_ASP_420	2.89	1.90	9.12
MODEL.PDB	O, A_LYS_417	ND2, A_ASN_422	HD21, A_ASN_422	2.79	1.87	19.66
MODEL.PDB	O, A_ARG_454	ND2, A_ASN_422	HD22, A_ASN_422	2.96	2.03	19.30
MODEL.PDB	O, A_ILE_418	N, A_TYR_423	H, A_TYR_423	2.93	2.07	26.20
MODEL.PDB	OD1, A_ASP_428	N, A_PHE_429	H, A_PHE_429	2.69	1.82	24.27
MODEL.PDB	O, A_LYS_378	N, A_VAL_433	H, A_VAL_433	2.77	1.78	8.60
MODEL.PDB	O, A_VAL_511	N, A_ILE_434	H, A_ILE_434	2.87	1.88	7.98
MODEL.PDB	O, A_THR_376	N, A_ALA_435	H, A_ALA_435	2.87	1.87	5.43
MODEL.PDB	OE1, A_GLN_506	ND2, A_ASN_437	HD22, A_ASN_437	2.76	1.75	1.26
MODEL.PDB	O, A_PRO_507	N, A_SER_438	H, A_SER_438	2.93	1.99	17.33
MODEL.PDB	OD1, A_ASN_437	N, A_ASN_439	H, A_ASN_439	2.96	2.00	13.44
MODEL.PDB	O, A_ASN_437	ND2, A_ASN_440	HD22, A_ASN_440	2.94	1.98	14.12
MODEL.PDB	O, A_SER_438	N, A_ASP_442	H, A_ASP_442	2.86	1.86	8.06
MODEL.PDB	O, A_ASN_439	N, A_LYS_444	H, A_LYS_444	2.74	1.85	22.59
MODEL.PDB	O, A_SER_443	N, A_GLY_446	H, A_GLY_446	2.87	1.94	17.87
MODEL.PDB	OE1, A_GLN_498	ND2, A_ASN_448	HD21, A_ASN_448	2.95	2.09	25.72
MODEL.PDB	OG, A_SER_349	N, A_LEU_452	H, A_LEU_452	2.95	1.98	11.79
MODEL.PDB	O, A_GLN_493	N, A_TYR_453	H, A_TYR_453	2.93	1.92	5.92
MODEL.PDB	OD1, A_ASN_422	N, A_ARG_454	H, A_ARG_454	2.75	1.77	11.10
MODEL.PDB	O, A_PRO_491	N, A_LEU_455	H, A_LEU_455	2.93	1.93	7.72
MODEL.PDB	OE1, A_GLU_471	NZ, A_LYS_458	HZ1, A_LYS_458	2.43	1.55	23.29
MODEL.PDB	O, A_LEU_461	OG, A_SER_459	HG, A_SER_459	2.80	1.90	16.75
MODEL.PDB	OE2, A_GLU_465	ND2, A_ASN_460	HD21, A_ASN_460	2.81	1.80	4.71
MODEL.PDB	OD1, A_ASP_467	NE, A_ARG_466	HE, A_ARG_466	2.70	1.70	7.41
MODEL.PDB	OD2, A_ASP_467	NH1, A_ARG_466	HH11, A_ARG_466	2.66	1.80	25.17
MODEL.PDB	O, A_VAL_483	OH, A_TYR_473	HH, A_TYR_473	2.71	1.79	14.10
MODEL.PDB	O, A_TYR_473	N, A_GLY_476	H, A_GLY_476	2.92	1.98	17.30
MODEL.PDB	O, A_PRO_479	N, A_GLY_482	H, A_GLY_482	2.79	1.82	12.46

MODEL.PDB	O, A_GLY_482	N, A_GLY_485	H, A_GLY_485	2.91	2.09	29.03
MODEL.PDB	O, A_PHE_486	N, A_CYS_488	H, A_CYS_488	2.97	2.13	28.02
MODEL.PDB	O, A_TYR_453	N, A_GLN_493	H, A_GLN_493	2.99	1.99	6.69
MODEL.PDB	O, A_TYR_451	N, A_TYR_495	H, A_TYR_495	2.96	1.97	9.57
MODEL.PDB	O, A_ASN_501	OH, A_TYR_505	HH, A_TYR_505	2.88	2.04	24.22
MODEL.PDB	O, A_GLY_502	NE2, A_GLN_506	HE21, A_GLN_506	2.98	2.00	10.57
MODEL.PDB	O, A_ILE_402	N, A_TYR_508	H, A_TYR_508	2.82	1.83	8.87
MODEL.PDB	OD2, A_ASP_442	NE, A_ARG_509	HE, A_ARG_509	2.69	1.74	14.88
MODEL.PDB	OD1, A_ASP_442	NH1, A_ARG_509	HH11, A_ARG_509	2.80	1.80	3.45
MODEL.PDB	O, A_PHE_400	N, A_VAL_510	H, A_VAL_510	2.87	1.87	6.51
MODEL.PDB	O, A_ILE_434	N, A_VAL_511	H, A_VAL_511	2.81	1.80	5.23
MODEL.PDB	O, A_CYS_432	N, A_LEU_513	H, A_LEU_513	2.80	1.79	4.79
MODEL.PDB	O, A_TYR_396	N, A_SER_514	H, A_SER_514	2.93	1.94	9.36
MODEL.PDB	O, A_ASN_394	N, A_GLU_516	H, A_GLU_516	2.89	1.88	3.81
MODEL.PDB	O, A_THR_393	OG1, A_THR_523	HG1, A_THR_523	2.72	1.84	18.92
MODEL.PDB	O, A_LEU_552	N, A_ASN_536	H, A_ASN_536	2.75	1.74	3.68
MODEL.PDB	O, A_GLY_550	N, A_VAL_539	H, A_VAL_539	2.92	1.94	9.43
MODEL.PDB	O, A_GLY_548	N, A_PHE_541	H, A_PHE_541	2.91	1.91	3.70
MODEL.PDB	O, A_ILE_326	N, A_ASN_542	H, A_ASN_542	2.93	1.97	13.73
MODEL.PDB	O, A_LEU_546	N, A_PHE_543	H, A_PHE_543	2.77	1.83	17.00
MODEL.PDB	O, A_PHE_543	N, A_LEU_546	H, A_LEU_546	2.91	1.96	16.31
MODEL.PDB	O, A_THR_588	N, A_VAL_551	H, A_VAL_551	2.76	1.79	12.83
MODEL.PDB	OD2, A_ASP_574	NZ, A_LYS_557	HZ1, A_LYS_557	2.65	1.80	26.29
MODEL.PDB	OD1, A_ASP_568	NZ, A_LYS_557	HZ2, A_LYS_557	2.72	1.90	29.52
MODEL.PDB	O, A_PRO_330	NE2, A_GLN_564	HE22, A_GLN_564	2.94	2.08	25.95
MODEL.PDB	O, A_ALA_575	N, A_GLY_566	H, A_GLY_566	2.80	1.88	19.43
MODEL.PDB	O, B_PHE_43	N, A_ARG_567	H, A_ARG_567	2.91	1.92	8.97
MODEL.PDB	O, A_ILE_569	OG1, A_THR_572	HG1, A_THR_572	2.67	1.71	1.58
MODEL.PDB	O, A_LEU_585	N, A_VAL_576	H, A_VAL_576	2.85	1.87	11.61
MODEL.PDB	O, A_GLN_564	N, A_ARG_577	H, A_ARG_577	2.89	1.89	5.64
MODEL.PDB	O, A_GLN_563	NH2, A_ARG_577	HH21, A_ARG_577	2.74	1.89	25.87
MODEL.PDB	OE1, A_GLN_564	NH2, A_ARG_577	HH22, A_ARG_577	2.71	1.88	28.37
MODEL.PDB	O, A_PHE_329	NE2, A_GLN_580	HE22, A_GLN_580	2.80	1.86	17.32
MODEL.PDB	OD1, A_ASP_578	N, A_GLU_583	H, A_GLU_583	2.90	1.95	17.00
MODEL.PDB	O, A_VAL_576	N, A_LEU_585	H, A_LEU_585	2.84	1.87	12.06
MODEL.PDB	O, A_THR_553	N, A_ASP_586	H, A_ASP_586	2.92	1.94	11.42
MODEL.PDB	O, A_ASP_574	N, A_ILE_587	H, A_ILE_587	2.68	1.77	20.36
MODEL.PDB	O, A_SER_316	N, A_VAL_595	H, A_VAL_595	2.97	1.97	1.84
MODEL.PDB	O, A_TYR_313	N, A_VAL_597	H, A_VAL_597	2.95	1.98	13.96
MODEL.PDB	O, A_ALA_609	N, A_ILE_598	H, A_ILE_598	2.81	1.84	12.73
MODEL.PDB	O, A_VAL_308	N, A_THR_602	H, A_THR_602	2.89	1.96	18.79
MODEL.PDB	O, A_PRO_600	OG1, A_THR_604	HG1, A_THR_604	2.84	2.00	24.26
MODEL.PDB	OH, A_TYR_636	NE2, A_GLN_607	HE22, A_GLN_607	2.96	2.00	15.28
MODEL.PDB	O, A_ILE_651	N, A_VAL_610	H, A_VAL_610	2.87	1.88	9.58
MODEL.PDB	O, A_SER_596	N, A_LEU_611	H, A_LEU_611	2.77	1.79	10.81
MODEL.PDB	O, A_CYS_649	N, A_TYR_612	H, A_TYR_612	2.95	1.95	5.25
MODEL.PDB	OD2, A_ASP_627	NE2, A_GLN_628	HE21, A_GLN_628	2.77	1.86	20.74
MODEL.PDB	OG1, A_THR_632	OG1, A_THR_630	HG1, A_THR_630	2.93	2.01	13.87
MODEL.PDB	OE1, A_GLN_628	N, A_ARG_634	H, A_ARG_634	2.91	1.90	4.18
MODEL.PDB	O, A_SER_637	N, A_SER_640	H, A_SER_640	2.95	1.96	10.14
MODEL.PDB	O, A_GLY_648	OG1, A_THR_645	HG1, A_THR_645	2.61	1.70	14.29
MODEL.PDB	O, A_PHE_643	N, A_LEU_650	H, A_LEU_650	2.84	1.84	6.92
MODEL.PDB	O, A_VAL_610	N, A_ILE_651	H, A_ILE_651	2.81	1.82	9.29
MODEL.PDB	O, A_ASN_641	N, A_GLY_652	H, A_GLY_652	2.89	1.91	11.58
MODEL.PDB	O, A_ILE_692	N, A_GLU_654	H, A_GLU_654	2.86	1.86	5.94
MODEL.PDB	O, A_THR_696	OG, A_SER_659	HG, A_SER_659	2.72	1.91	26.75
MODEL.PDB	OD1, A_ASN_658	OH, A_TYR_660	HH, A_TYR_660	2.82	1.96	21.62
MODEL.PDB	OE2, A_GLU_661	N, A_CYS_662	H, A_CYS_662	2.68	1.71	13.40

MODEL.PDB	O, A_ILE_670	N, A_ILE_666	H, A_ILE_666	2.97	2.04	18.47
MODEL.PDB	O, B_PRO_863	N, A_ALA_668	H, A_ALA_668	2.78	1.79	9.02
MODEL.PDB	O, B_LEU_864	N, A_GLY_669	H, A_GLY_669	2.82	1.95	24.85
MODEL.PDB	OD2, A_ASP_663	OG, A_SER_673	HG, A_SER_673	2.68	1.81	20.07
MODEL.PDB	O, A_SER_680	NE2, A_GLN_675	HE21, A_GLN_675	2.84	1.86	12.29
MODEL.PDB	O, A_THR_604	NE, A_ARG_683	HE, A_ARG_683	2.90	1.95	15.53
MODEL.PDB	O, A_SER_691	N, A_ALA_688	H, A_ALA_688	2.92	2.02	21.69
MODEL.PDB	O, A_SER_689	NE2, A_GLN_690	HE21, A_GLN_690	2.81	1.89	20.34
MODEL.PDB	O, A_GLU_654	N, A_ALA_694	H, A_ALA_694	2.80	1.83	12.75
MODEL.PDB	O, A_GLU_661	OH, A_TYR_695	HH, A_TYR_695	2.62	1.68	9.06
MODEL.PDB	O, A_GLY_669	N, A_MET_697	H, A_MET_697	2.86	1.87	9.86
MODEL.PDB	O, A_TYR_660	N, A_SER_698	H, A_SER_698	2.75	1.74	2.22
MODEL.PDB	O, B_ASP_796	OH, A_TYR_707	HH, A_TYR_707	2.70	1.86	23.36
MODEL.PDB	OD1, A_ASN_710	OG, A_SER_708	HG, A_SER_708	2.64	1.84	27.39
MODEL.PDB	OD1, A_ASN_717	N, A_PHE_718	H, A_PHE_718	2.87	1.98	22.86
MODEL.PDB	OE1, A_GLN_926	N, A_ILE_720	H, A_ILE_720	2.86	1.86	8.42
MODEL.PDB	OD2, A_ASP_775	NZ, A_LYS_733	HZ3, A_LYS_733	2.60	1.62	11.48
MODEL.PDB	O, A_THR_859	N, A_SER_735	H, A_SER_735	2.98	2.00	11.48
MODEL.PDB	O, A_GLY_857	N, A_ASP_737	H, A_ASP_737	2.75	1.75	6.26
MODEL.PDB	OD1, A_ASP_737	N, A_THR_739	H, A_THR_739	2.98	2.15	28.75
MODEL.PDB	O, A_ASP_737	N, A_TYR_741	H, A_TYR_741	2.83	1.88	16.65
MODEL.PDB	O, A_CYS_738	N, A_ILE_742	H, A_ILE_742	2.96	1.96	5.81
MODEL.PDB	O, A_LEU_754	N, A_GLY_757	H, A_GLY_757	2.99	2.08	20.35
MODEL.PDB	O, A_CYS_760	N, A_ASN_764	H, A_ASN_764	2.99	2.00	9.92
MODEL.PDB	O, A_THR_761	N, A_ARG_765	H, A_ARG_765	2.94	1.97	13.53
MODEL.PDB	OG1, C_THR_961	NH2, A_ARG_765	HH22, A_ARG_765	2.95	1.98	13.10
MODEL.PDB	O, A_GLN_762	N, A_ALA_766	H, A_ALA_766	2.91	1.95	14.00
MODEL.PDB	O, A_ASN_764	N, A_THR_768	H, A_THR_768	2.87	1.89	11.48
MODEL.PDB	O, A_ASN_764	OG1, A_THR_768	HG1, A_THR_768	2.93	2.04	18.67
MODEL.PDB	O, A_ARG_765	N, A_GLY_769	H, A_GLY_769	2.83	1.85	11.62
MODEL.PDB	O, A_LEU_767	N, A_ALA_771	H, A_ALA_771	3.00	2.03	13.96
MODEL.PDB	O, A_THR_768	N, A_VAL_772	H, A_VAL_772	2.95	1.97	11.62
MODEL.PDB	O, A_GLU_773	N, A_ASN_777	H, A_ASN_777	2.90	1.96	17.54
MODEL.PDB	O, A_LYS_776	N, A_GLU_780	H, A_GLU_780	2.69	1.72	13.06
MODEL.PDB	O, A_ASN_777	N, A_VAL_781	H, A_VAL_781	2.92	1.93	8.95
MODEL.PDB	O, A_THR_778	N, A_PHE_782	H, A_PHE_782	2.97	2.03	17.12
MODEL.PDB	O, A_GLN_779	N, A_ALA_783	H, A_ALA_783	2.88	1.94	18.54
MODEL.PDB	O, C_ALA_701	N, A_ILE_788	H, A_ILE_788	2.77	1.84	18.31
MODEL.PDB	O, A_ASP_796	N, A_GLY_798	H, A_GLY_798	2.76	1.87	22.26
MODEL.PDB	OD1, A_ASN_928	N, A_ASN_801	H, A_ASN_801	2.77	1.78	8.53
MODEL.PDB	OD2, A_ASP_808	OG, A_SER_810	HG, A_SER_810	2.73	1.94	28.41
MODEL.PDB	O, A_PRO_809	NZ, A_LYS_814	HZ1, A_LYS_814	2.69	1.78	20.99
MODEL.PDB	OD1, A_ASP_820	NH1, A_ARG_815	HH11, A_ARG_815	2.65	1.73	19.61
MODEL.PDB	OE1, A_GLU_819	N, A_SER_816	H, A_SER_816	2.97	1.97	5.35
MODEL.PDB	OG, A_SER_816	N, A_GLU_819	H, A_GLU_819	2.89	1.90	8.71
MODEL.PDB	O, A_SER_816	N, A_ASP_820	H, A_ASP_820	2.88	1.89	8.63
MODEL.PDB	O, A_ILE_818	N, A_LEU_822	H, A_LEU_822	2.76	1.81	15.85
MODEL.PDB	O, A_GLU_819	N, A_PHE_823	H, A_PHE_823	2.96	1.97	8.29
MODEL.PDB	O, A_SER_939	NZ, A_LYS_825	HZ1, A_LYS_825	2.84	2.00	27.52
MODEL.PDB	O, A_THR_941	NZ, A_LYS_825	HZ3, A_LYS_825	2.82	1.84	9.65
MODEL.PDB	OD1, A_ASP_830	N, A_GLY_832	H, A_GLY_832	2.78	1.79	8.57
MODEL.PDB	O, C_ASP_614	NE, A_ARG_847	HE, A_ARG_847	2.97	2.12	27.07
MODEL.PDB	O, C_ASP_614	NH1, A_ARG_847	HH11, A_ARG_847	2.71	1.79	19.16
MODEL.PDB	O, A_ALA_846	NH2, A_ARG_847	HH21, A_ARG_847	2.88	1.89	8.74
MODEL.PDB	O, A_CYS_851	N, A_GLN_853	H, A_GLN_853	2.90	2.01	22.82
MODEL.PDB	O, A_THR_859	NZ, A_LYS_854	HZ2, A_LYS_854	2.82	1.97	27.00
MODEL.PDB	OG1, A_THR_734	NZ, A_LYS_854	HZ3, A_LYS_854	2.90	2.01	23.94
MODEL.PDB	O, A_SER_735	N, A_THR_859	H, A_THR_859	2.88	1.89	7.72

MODEL.PDB	OD2, C_ASP_614	OG1, A_THR_859	HG1, A_THR_859	2.83	1.95	19.70
MODEL.PDB	O, A_LYS_733	N, A_LEU_861	H, A_LEU_861	2.77	1.82	15.26
MODEL.PDB	OD1, A_ASP_775	N, A_LEU_864	H, A_LEU_864	2.74	1.75	8.23
MODEL.PDB	O, A_THR_866	N, A_ILE_870	H, A_ILE_870	2.78	1.79	9.38
MODEL.PDB	OE2, A_GLU_819	OG1, A_THR_874	HG1, A_THR_874	2.63	1.71	12.98
MODEL.PDB	O, A_ALA_871	N, A_SER_875	H, A_SER_875	2.96	1.96	8.90
MODEL.PDB	O, A_GLN_872	N, A_ALA_876	H, A_ALA_876	2.99	2.03	14.76
MODEL.PDB	O, A_TYR_873	N, A_LEU_877	H, A_LEU_877	2.94	1.94	8.91
MODEL.PDB	O, A_SER_875	N, A_ALA_879	H, A_ALA_879	2.85	1.87	12.06
MODEL.PDB	O, A_ALA_879	OG1, A_THR_883	HG1, A_THR_883	2.74	1.87	20.29
MODEL.PDB	O, A_GLY_880	N, A_SER_884	H, A_SER_884	2.74	1.84	21.59
MODEL.PDB	O, A_SER_884	OG1, A_THR_887	HG1, A_THR_887	2.69	1.84	22.55
MODEL.PDB	O, A_THR_881	NE2, A_GLN_901	HE22, A_GLN_901	2.83	1.89	17.61
MODEL.PDB	O, A_PHE_898	N, A_MET_902	H, A_MET_902	2.91	1.94	13.16
MODEL.PDB	O, A_ALA_899	N, A_ALA_903	H, A_ALA_903	2.87	1.89	10.99
MODEL.PDB	O, A_TYR_904	N, A_GLY_908	H, A_GLY_908	2.76	1.80	14.47
MODEL.PDB	O, A_ASN_907	N, A_GLY_910	H, A_GLY_910	2.96	2.02	16.87
MODEL.PDB	O, A_ASN_914	N, A_GLU_918	H, A_GLU_918	2.85	1.84	2.96
MODEL.PDB	O, A_LEU_922	N, A_GLN_926	H, A_GLN_926	2.88	1.89	7.46
MODEL.PDB	O, A_ILE_923	N, A_PHE_927	H, A_PHE_927	2.88	1.91	11.70
MODEL.PDB	O, A_ALA_924	N, A_ASN_928	H, A_ASN_928	2.89	1.90	9.51
MODEL.PDB	O, A_GLN_926	N, A_ALA_930	H, A_ALA_930	2.86	1.91	16.76
MODEL.PDB	O, A_PHE_927	N, A_ILE_931	H, A_ILE_931	2.94	1.95	8.80
MODEL.PDB	OD1, A_ASP_936	NE2, A_GLN_935	HE21, A_GLN_935	2.78	1.84	17.00
MODEL.PDB	O, A_LYS_933	N, A_SER_937	H, A_SER_937	2.83	1.86	13.30
MODEL.PDB	O, A_ILE_934	N, A_LEU_938	H, A_LEU_938	2.93	1.95	10.55
MODEL.PDB	O, A_GLN_935	N, A_SER_939	H, A_SER_939	2.87	1.95	18.79
MODEL.PDB	O, A_ALA_942	OG, A_SER_943	HG, A_SER_943	2.85	1.99	21.59
MODEL.PDB	O, A_LEU_945	N, A_GLN_949	H, A_GLN_949	2.94	1.98	14.33
MODEL.PDB	OD1, A_ASN_953	NE2, A_GLN_949	HE21, A_GLN_949	2.96	1.95	3.82
MODEL.PDB	O, A_GLY_946	N, A_ASP_950	H, A_ASP_950	2.94	1.97	13.52
MODEL.PDB	O, A_GLN_949	N, A_ASN_953	H, A_ASN_953	2.87	1.89	11.96
MODEL.PDB	O, A_ASP_950	N, A_GLN_954	H, A_GLN_954	2.87	1.87	8.29
MODEL.PDB	O, A_ASN_953	N, A_GLN_957	H, A_GLN_957	2.89	1.92	12.65
MODEL.PDB	O, A_GLN_954	N, A_ALA_958	H, A_ALA_958	2.93	1.97	14.97
MODEL.PDB	O, A_ALA_956	N, A_ASN_960	H, A_ASN_960	2.92	1.94	9.86
MODEL.PDB	O, A_GLN_957	N, A_THR_961	H, A_THR_961	2.91	1.93	11.06
MODEL.PDB	O, A_LEU_959	N, A_VAL_963	H, A_VAL_963	2.96	1.97	8.70
MODEL.PDB	O, A_ASN_960	N, A_LYS_964	H, A_LYS_964	2.96	2.00	13.66
MODEL.PDB	OE1, A_GLN_965	OG, A_SER_968	HG, A_SER_968	2.75	1.97	29.51
MODEL.PDB	O, B_GLN_755	N, A_PHE_970	H, A_PHE_970	2.80	1.82	10.56
MODEL.PDB	OE1, A_GLN_992	N, A_ILE_973	H, A_ILE_973	2.87	1.98	23.13
MODEL.PDB	O, C_THR_547	ND2, A_ASN_978	HD21, A_ASN_978	2.99	2.12	24.76
MODEL.PDB	O, A_ASN_978	N, A_SER_982	H, A_SER_982	2.83	1.91	20.13
MODEL.PDB	OE2, A_GLU_988	N, A_ASP_985	H, A_ASP_985	2.80	1.81	9.30
MODEL.PDB	OD2, A_ASP_985	N, A_LYS_986	H, A_LYS_986	2.76	1.82	17.86
MODEL.PDB	O, A_ASP_985	N, A_ALA_989	H, A_ALA_989	2.81	1.89	18.69
MODEL.PDB	O, A_ALA_989	N, A_ILE_993	H, A_ILE_993	2.88	1.90	11.01
MODEL.PDB	O, A_GLU_990	N, A_ASP_994	H, A_ASP_994	2.77	1.81	13.95
MODEL.PDB	O, A_GLY_971	NE, A_ARG_995	HE, A_ARG_995	2.85	2.01	27.94
MODEL.PDB	OD2, B_ASP_994	NH1, A_ARG_995	HH12, A_ARG_995	2.69	1.68	3.63
MODEL.PDB	OD1, B_ASP_994	NH2, A_ARG_995	HH22, A_ARG_995	2.66	1.65	4.49
MODEL.PDB	O, A_ILE_993	N, A_ILE_997	H, A_ILE_997	2.74	1.75	7.28
MODEL.PDB	O, A_ASP_994	OG1, A_THR_998	HG1, A_THR_998	2.80	2.00	27.57
MODEL.PDB	O, B_VAL_62	N, B_THR_29	H, B_THR_29	2.85	1.84	2.85
MODEL.PDB	O, B_SER_60	N, B_SER_31	H, B_SER_31	2.96	1.96	7.86
MODEL.PDB	O, B_GLY_219	NE, B_ARG_34	HE, B_ARG_34	2.92	2.08	27.78
MODEL.PDB	OE2, B_GLU_191	NH1, B_ARG_34	HH11, B_ARG_34	2.59	1.61	10.99

MODEL.PDB	O, B_GLY_219	NH2, B_ARG_34	HH21, B_ARG_34	2.89	1.99	22.37
MODEL.PDB	O, B_LEU_54	OH, B_TYR_37	HH, B_TYR_37	2.63	1.85	28.94
MODEL.PDB	O, A_PHE_565	N, B_PHE_43	H, B_PHE_43	2.96	2.00	13.42
MODEL.PDB	O, B_GLU_281	OG, B_SER_45	HG, B_SER_45	2.78	1.89	18.26
MODEL.PDB	O, B_LEU_277	N, B_HIS_49	H, B_HIS_49	2.95	1.96	9.78
MODEL.PDB	O, B_PHE_275	N, B_THR_51	H, B_THR_51	2.94	1.96	10.82
MODEL.PDB	OD1, B_ASP_53	N, B_LEU_54	H, B_LEU_54	2.71	1.77	18.19
MODEL.PDB	O, B_GLN_271	N, B_PHE_55	H, B_PHE_55	2.91	2.05	25.85
MODEL.PDB	O, B_PRO_57	OG, B_SER_60	HG, B_SER_60	2.69	1.91	29.81
MODEL.PDB	O, B_SER_60	N, B_VAL_62	H, B_VAL_62	2.95	2.08	25.32
MODEL.PDB	O, B_VAL_267	N, B_THR_63	H, B_THR_63	2.93	1.93	5.51
MODEL.PDB	O, B_TYR_265	N, B_PHE_65	H, B_PHE_65	2.89	1.94	15.91
MODEL.PDB	ND1, B_HIS_66	N, B_ALA_67	H, B_ALA_67	2.87	1.93	17.76
MODEL.PDB	O, B_ASN_74	N, B_THR_76	H, B_THR_76	2.88	1.98	22.22
MODEL.PDB	O, B_ALA_243	NH2, B_ARG_78	HH22, B_ARG_78	2.71	1.73	12.65
MODEL.PDB	O, B_THR_236	N, B_PHE_86	H, B_PHE_86	2.89	1.89	7.28
MODEL.PDB	O, B_GLY_268	N, B_TYR_91	H, B_TYR_91	2.82	1.89	18.99
MODEL.PDB	O, B_PHE_192	N, B_PHE_92	H, B_PHE_92	2.77	1.76	4.73
MODEL.PDB	O, B_TYR_266	N, B_ALA_93	H, B_ALA_93	2.95	1.99	14.28
MODEL.PDB	O, B_ALA_264	OG, B_SER_94	HG, B_SER_94	2.73	1.78	6.10
MODEL.PDB	OE1, B_GLU_96	N, B_LYS_97	H, B_LYS_97	2.71	1.74	12.03
MODEL.PDB	O, B_ASN_121	NE, B_ARG_102	HE, B_ARG_102	2.94	2.02	20.18
MODEL.PDB	O, B_ILE_119	N, B_TRP_104	H, B_TRP_104	2.90	1.94	14.54
MODEL.PDB	O, B_GLN_239	N, B_ILE_105	H, B_ILE_105	2.84	1.85	10.53
MODEL.PDB	O, B_LEU_117	N, B_PHE_106	H, B_PHE_106	2.95	1.96	9.18
MODEL.PDB	OG1, B_THR_114	OG1, B_THR_109	HG1, B_THR_109	2.95	2.04	16.45
MODEL.PDB	OD1, B_ASP_111	N, B_SER_112	H, B_SER_112	2.80	1.91	22.62
MODEL.PDB	OG1, B_THR_167	NE2, B_GLN_115	HE22, B_GLN_115	2.93	1.99	17.65
MODEL.PDB	O, B_PHE_106	N, B_LEU_117	H, B_LEU_117	2.76	1.82	16.86
MODEL.PDB	O, B_LYS_129	N, B_LEU_118	H, B_LEU_118	2.85	1.89	15.41
MODEL.PDB	O, B_VAL_127	N, B_VAL_120	H, B_VAL_120	2.94	1.94	7.20
MODEL.PDB	O, B_ARG_102	N, B_ASN_121	H, B_ASN_121	2.74	1.79	15.23
MODEL.PDB	O, B_ASN_125	N, B_ASN_122	H, B_ASN_122	2.81	1.85	13.44
MODEL.PDB	O, B_SER_172	N, B_VAL_126	H, B_VAL_126	2.86	1.89	11.70
MODEL.PDB	O, B_VAL_120	N, B_VAL_127	H, B_VAL_127	2.89	1.88	1.69
MODEL.PDB	O, B_TYR_170	N, B_ILE_128	H, B_ILE_128	2.88	1.89	9.86
MODEL.PDB	O, B_CYS_131	N, B_PHE_133	H, B_PHE_133	2.96	2.08	23.79
MODEL.PDB	O, B_SER_155	N, B_VAL_143	H, B_VAL_143	2.95	1.95	8.05
MODEL.PDB	O, B_TRP_152	N, B_SER_155	H, B_SER_155	2.96	2.07	22.62
MODEL.PDB	OE1, B_GLU_156	N, B_PHE_157	H, B_PHE_157	2.73	1.77	13.74
MODEL.PDB	O, B_GLN_134	OG, B_SER_161	HG, B_SER_161	2.81	2.01	27.77
MODEL.PDB	OE2, B_GLU_169	N, B_PHE_168	H, B_PHE_168	2.82	1.90	19.46
MODEL.PDB	O, B_ILE_128	N, B_TYR_170	H, B_TYR_170	2.87	1.89	12.37
MODEL.PDB	OD2, B_ASP_178	N, B_GLU_180	H, B_GLU_180	2.82	1.85	12.31
MODEL.PDB	O, B_PHE_186	N, B_GLN_183	H, B_GLN_183	2.79	1.95	27.57
MODEL.PDB	OD1, B_ASN_211	ND2, B_ASN_185	HD22, B_ASN_185	2.96	1.98	11.82
MODEL.PDB	O, B_SER_94	N, B_ARG_190	H, B_ARG_190	2.85	1.85	6.15
MODEL.PDB	O, B_PHE_92	N, B_PHE_192	H, B_PHE_192	2.74	1.73	1.77
MODEL.PDB	O, B_TYR_204	N, B_VAL_193	H, B_VAL_193	2.92	1.95	13.51
MODEL.PDB	O, B_VAL_90	N, B_PHE_194	H, B_PHE_194	2.95	1.95	6.38
MODEL.PDB	OD1, B_ASP_53	NZ, B_LYS_195	HZ1, B_LYS_195	2.67	1.77	21.61
MODEL.PDB	OH, B_TYR_37	NZ, B_LYS_195	HZ2, B_LYS_195	2.81	1.83	10.84
MODEL.PDB	O, B_TYR_200	N, B_ILE_197	H, B_ILE_197	2.79	1.79	4.25
MODEL.PDB	O, B_ILE_197	N, B_TYR_200	H, B_TYR_200	2.81	1.92	22.60
MODEL.PDB	O, B_LEU_229	N, B_PHE_201	H, B_PHE_201	2.85	1.93	19.52
MODEL.PDB	O, B_LYS_195	N, B_LYS_202	H, B_LYS_202	2.84	1.83	2.11
MODEL.PDB	O, B_VAL_227	N, B_ILE_203	H, B_ILE_203	2.97	1.97	4.39
MODEL.PDB	O, B_VAL_193	N, B_TYR_204	H, B_TYR_204	2.86	1.86	8.69

MODEL.PDB	O, B_GLU_224	N, B_SER_205	H, B_SER_205	2.74	1.80	17.11
MODEL.PDB	O, B_GLU_191	N, B_LYS_206	H, B_LYS_206	2.77	1.92	26.56
MODEL.PDB	OE2, B_GLU_224	NZ, B_LYS_206	HZ1, B_LYS_206	2.61	1.63	10.77
MODEL.PDB	ND1, B_HIS_207	N, B_THR_208	H, B_THR_208	2.91	2.09	29.09
MODEL.PDB	O, B_GLN_218	N, B_LEU_212	H, B_LEU_212	2.82	2.01	29.95
MODEL.PDB	O, B_VAL_36	N, B_LEU_223	H, B_LEU_223	2.83	1.84	8.38
MODEL.PDB	O, B_ILE_203	N, B_LEU_226	H, B_LEU_226	2.90	1.91	6.87
MODEL.PDB	O, B_PHE_201	N, B_LEU_229	H, B_LEU_229	2.81	1.86	16.98
MODEL.PDB	O, B_GLY_199	N, B_GLY_232	H, B_GLY_232	2.78	1.87	20.92
MODEL.PDB	O, B_GLY_107	N, B_THR_236	H, B_THR_236	2.99	2.03	14.29
MODEL.PDB	O, B_ASN_81	NE2, B_GLN_239	HE21, B_GLN_239	2.83	1.94	22.52
MODEL.PDB	O, B_GLY_103	N, B_LEU_241	H, B_LEU_241	2.91	2.08	28.14
MODEL.PDB	OE1, B_GLU_154	OG, B_SER_247	HG, B_SER_247	2.58	1.63	5.81
MODEL.PDB	O, B_ALA_260	N, B_ALA_262	H, B_ALA_262	2.85	1.99	25.54
MODEL.PDB	O, B_PHE_65	N, B_TYR_265	H, B_TYR_265	2.98	1.99	7.38
MODEL.PDB	O, B_ALA_93	N, B_TYR_266	H, B_TYR_266	2.74	1.74	7.02
MODEL.PDB	O, B_THR_63	N, B_VAL_267	H, B_VAL_267	2.96	1.99	13.04
MODEL.PDB	O, B_TYR_91	N, B_GLY_268	H, B_GLY_268	2.83	1.83	4.91
MODEL.PDB	O, B_PHE_55	N, B_GLN_271	H, B_GLN_271	2.85	1.93	19.01
MODEL.PDB	O, B_ASP_53	N, B_ARG_273	H, B_ARG_273	2.97	2.01	15.13
MODEL.PDB	OD2, B_ASP_290	NE, B_ARG_273	HE, B_ARG_273	2.67	1.80	24.19
MODEL.PDB	OD1, B_ASP_290	NH2, B_ARG_273	HH21, B_ARG_273	2.63	1.66	12.98
MODEL.PDB	O, B_THR_51	N, B_PHE_275	H, B_PHE_275	2.80	1.81	9.02
MODEL.PDB	O, B_VAL_289	N, B_LEU_276	H, B_LEU_276	2.95	2.00	17.03
MODEL.PDB	O, B_HIS_49	N, B_LEU_277	H, B_LEU_277	2.90	1.90	7.03
MODEL.PDB	OD2, B_ASP_287	NZ, B_LYS_278	HZ1, B_LYS_278	2.60	1.60	3.72
MODEL.PDB	O, B_THR_284	N, B_ASN_280	H, B_ASN_280	2.79	1.79	4.72
MODEL.PDB	OD1, B_ASN_280	N, B_GLU_281	H, B_GLU_281	2.98	2.13	26.69
MODEL.PDB	O, B_LEU_276	N, B_VAL_289	H, B_VAL_289	2.93	1.99	17.77
MODEL.PDB	OG, B_SER_50	NZ, B_LYS_304	HZ1, B_LYS_304	2.84	1.83	5.53
MODEL.PDB	O, B_THR_307	OG, B_SER_305	HG, B_SER_305	2.73	1.82	14.38
MODEL.PDB	OG1, B_THR_602	N, B_VAL_308	H, B_VAL_308	2.99	1.99	5.20
MODEL.PDB	OD2, B_ASP_663	NZ, B_LYS_310	HZ3, B_LYS_310	2.62	1.67	16.87
MODEL.PDB	O, B_THR_599	N, B_GLY_311	H, B_GLY_311	2.99	2.00	8.71
MODEL.PDB	O, B_GLY_593	N, B_PHE_318	H, B_PHE_318	2.81	1.82	8.98
MODEL.PDB	OE1, B_GLN_580	NE, B_ARG_328	HE, B_ARG_328	2.68	1.70	11.58
MODEL.PDB	O, B_CYS_336	N, B_PHE_338	H, B_PHE_338	2.77	1.88	22.83
MODEL.PDB	O, B_PHE_338	N, B_PHE_342	H, B_PHE_342	2.91	1.90	3.53
MODEL.PDB	O, B_SER_349	N, B_ALA_352	H, B_ALA_352	2.92	2.01	20.99
MODEL.PDB	OD2, B_ASP_398	NH2, B_ARG_355	HH21, B_ARG_355	2.60	1.63	13.35
MODEL.PDB	O, B_ALA_397	N, B_LYS_356	H, B_LYS_356	2.91	1.91	5.86
MODEL.PDB	O, B_VAL_395	N, B_ILE_358	H, B_ILE_358	2.73	1.74	9.85
MODEL.PDB	OG1, B_THR_523	OG, B_SER_359	HG, B_SER_359	2.73	1.79	9.26
MODEL.PDB	O, B_ASN_334	N, B_VAL_362	H, B_VAL_362	2.95	2.00	16.82
MODEL.PDB	O, B_CYS_525	N, B_ALA_363	H, B_ALA_363	2.82	1.88	17.11
MODEL.PDB	OD1, B_ASN_388	N, B_TYR_365	H, B_TYR_365	2.92	1.97	15.70
MODEL.PDB	OD1, B_ASP_364	N, B_SER_366	H, B_SER_366	2.85	1.92	18.58
MODEL.PDB	OD1, B_ASP_364	OG, B_SER_366	HG, B_SER_366	2.74	1.87	20.38
MODEL.PDB	O, B_TYR_365	N, B_TYR_369	H, B_TYR_369	2.94	2.07	25.38
MODEL.PDB	OG, B_SER_373	OG, B_SER_371	HG, B_SER_371	2.84	1.90	10.21
MODEL.PDB	OG1, B_THR_376	NZ, B_LYS_378	HZ3, B_LYS_378	2.86	1.89	13.06
MODEL.PDB	O, C_LEU_984	NZ, B_LYS_386	HZ3, B_LYS_386	2.72	1.89	28.40
MODEL.PDB	O, B_VAL_524	N, B_PHE_392	H, B_PHE_392	2.80	1.80	6.45
MODEL.PDB	OE2, B_GLU_516	OG1, B_THR_393	HG1, B_THR_393	2.60	1.68	12.70
MODEL.PDB	O, B_ILE_358	N, B_VAL_395	H, B_VAL_395	2.90	1.91	8.10
MODEL.PDB	O, B_SER_514	N, B_TYR_396	H, B_TYR_396	2.73	1.72	4.61
MODEL.PDB	O, B_LYS_356	N, B_ALA_397	H, B_ALA_397	2.91	1.97	16.65
MODEL.PDB	O, B_VAL_512	N, B_ASP_398	H, B_ASP_398	2.89	1.93	15.82

MODEL.PDB	O, B_ASN_354	N, B_SER_399	H, B_SER_399	2.81	1.83	10.30
MODEL.PDB	O, B_GLN_506	N, B_GLY_404	H, B_GLY_404	2.90	2.00	22.81
MODEL.PDB	O, B_PRO_412	NE2, B_GLN_414	HE21, B_GLN_414	2.98	1.98	7.33
MODEL.PDB	OD2, B_ASP_420	N, B_GLY_416	H, B_GLY_416	2.83	1.90	18.61
MODEL.PDB	O, B_GLY_416	N, B_ASP_420	H, B_ASP_420	2.74	1.73	0.82
MODEL.PDB	O, B_ILE_418	N, B_ASN_422	H, B_ASN_422	2.90	1.99	21.02
MODEL.PDB	O, B_LYS_417	ND2, B_ASN_422	HD21, B_ASN_422	2.95	2.04	21.43
MODEL.PDB	O, B_ARG_454	ND2, B_ASN_422	HD22, B_ASN_422	2.94	2.01	18.80
MODEL.PDB	O, B_ILE_418	N, B_TYR_423	H, B_TYR_423	2.79	1.84	15.89
MODEL.PDB	OD2, B_ASP_398	OH, B_TYR_423	HH, B_TYR_423	2.64	1.73	15.03
MODEL.PDB	OD1, B_ASN_460	NZ, B_LYS_424	HZ2, B_LYS_424	2.64	1.68	12.99
MODEL.PDB	OD1, B_ASP_428	N, B_PHE_429	H, B_PHE_429	2.76	1.87	23.57
MODEL.PDB	O, B_LYS_378	N, B_VAL_433	H, B_VAL_433	2.76	1.78	10.96
MODEL.PDB	O, B_ARG_509	N, B_TRP_436	H, B_TRP_436	2.96	2.00	14.46
MODEL.PDB	OE1, B_GLN_506	ND2, B_ASN_437	HD22, B_ASN_437	2.76	1.76	7.71
MODEL.PDB	OD2, B_ASP_442	OG, B_SER_438	HG, B_SER_438	2.68	1.74	9.15
MODEL.PDB	OD1, B_ASN_437	N, B_ASN_439	H, B_ASN_439	2.86	1.86	8.85
MODEL.PDB	O, B_SER_438	N, B_ASP_442	H, B_ASP_442	2.81	1.85	14.24
MODEL.PDB	O, B_ASN_439	OG, B_SER_443	HG, B_SER_443	3.00	2.04	2.32
MODEL.PDB	OD1, B_ASN_440	NZ, B_LYS_444	HZ1, B_LYS_444	2.69	1.88	29.21
MODEL.PDB	OD2, B_ASP_442	OH, B_TYR_451	HH, B_TYR_451	2.68	1.72	0.75
MODEL.PDB	OG, B_SER_349	N, B_LEU_452	H, B_LEU_452	2.95	2.13	29.55
MODEL.PDB	O, B_GLN_493	N, B_TYR_453	H, B_TYR_453	2.76	1.77	9.91
MODEL.PDB	OD1, B_ASN_422	N, B_ARG_454	H, B_ARG_454	2.70	1.76	16.69
MODEL.PDB	O, B_PRO_491	N, B_LEU_455	H, B_LEU_455	2.73	1.75	10.97
MODEL.PDB	OD1, B_ASP_420	ND2, B_ASN_460	HD21, B_ASN_460	2.68	1.79	21.99
MODEL.PDB	O, B_TYR_489	N, B_TYR_473	H, B_TYR_473	2.99	2.14	26.94
MODEL.PDB	O, B_SER_477	OG1, B_THR_478	HG1, B_THR_478	2.84	2.04	27.32
MODEL.PDB	O, B_GLY_485	N, B_CYS_488	H, B_CYS_488	2.86	1.86	5.52
MODEL.PDB	OD1, B_ASN_487	OH, B_TYR_489	HH, B_TYR_489	2.67	1.80	20.09
MODEL.PDB	O, B_TYR_453	N, B_GLN_493	H, B_GLN_493	2.76	1.86	21.87
MODEL.PDB	O, B_TYR_449	OG, B_SER_494	HG, B_SER_494	2.98	2.19	29.01
MODEL.PDB	O, B_TYR_451	N, B_TYR_495	H, B_TYR_495	2.79	1.78	4.96
MODEL.PDB	O, B_ASN_448	N, B_PHE_497	H, B_PHE_497	2.88	1.91	13.40
MODEL.PDB	O, B_ILE_402	N, B_TYR_508	H, B_TYR_508	2.70	1.70	5.53
MODEL.PDB	O, B_TRP_436	N, B_ARG_509	H, B_ARG_509	2.82	1.92	21.88
MODEL.PDB	OD1, B_ASP_442	NH1, B_ARG_509	HH11, B_ARG_509	2.67	1.81	24.93
MODEL.PDB	O, B_PHE_400	N, B_VAL_510	H, B_VAL_510	2.87	1.89	11.62
MODEL.PDB	O, B_ILE_434	N, B_VAL_511	H, B_VAL_511	2.87	1.94	17.81
MODEL.PDB	O, B_ASP_398	N, B_VAL_512	H, B_VAL_512	2.77	1.81	13.60
MODEL.PDB	O, B_CYS_432	N, B_LEU_513	H, B_LEU_513	2.82	1.86	14.37
MODEL.PDB	O, B_TYR_396	N, B_SER_514	H, B_SER_514	2.90	1.91	9.86
MODEL.PDB	O, B_PHE_392	N, B_THR_523	H, B_THR_523	2.96	2.03	19.55
MODEL.PDB	O, B_THR_393	OG1, B_THR_523	HG1, B_THR_523	2.62	1.71	16.03
MODEL.PDB	OD2, B_ASP_389	NZ, B_LYS_528	HZ3, B_LYS_528	2.66	1.77	22.25
MODEL.PDB	OD1, B_ASN_532	N, B_LEU_533	H, B_LEU_533	2.81	1.94	24.59
MODEL.PDB	OE2, B_GLU_554	NZ, B_LYS_535	HZ3, B_LYS_535	2.58	1.58	6.75
MODEL.PDB	O, B_LEU_552	N, B_ASN_536	H, B_ASN_536	2.81	1.82	7.48
MODEL.PDB	O, B_GLY_550	N, B_VAL_539	H, B_VAL_539	2.96	1.97	8.57
MODEL.PDB	O, B_GLY_548	N, B_PHE_541	H, B_PHE_541	2.79	1.80	9.02
MODEL.PDB	O, B_ILE_326	N, B_ASN_542	H, B_ASN_542	2.82	1.81	1.58
MODEL.PDB	O, B_LEU_546	N, B_PHE_543	H, B_PHE_543	2.76	1.87	23.13
MODEL.PDB	O, B_PHE_543	N, B_LEU_546	H, B_LEU_546	2.95	2.00	16.40
MODEL.PDB	O, B_THR_588	N, B_VAL_551	H, B_VAL_551	2.86	1.86	6.80
MODEL.PDB	O, B_ILE_584	OG, B_SER_555	HG, B_SER_555	2.72	1.91	26.62
MODEL.PDB	OD2, B_ASP_586	NZ, B_LYS_557	HZ3, B_LYS_557	2.63	1.78	26.14
MODEL.PDB	OE1, B_GLN_563	N, B_LEU_560	H, B_LEU_560	2.87	2.05	29.35
MODEL.PDB	O, B_ALA_575	N, B_GLY_566	H, B_GLY_566	2.80	1.81	8.86

MODEL.PDB	OD1, B_ASP_574	N, B_ASP_568	H, B_ASP_568	2.69	1.70	7.58
MODEL.PDB	O, B_GLN_563	NH2, B_ARG_577	HH21, B_ARG_577	2.68	1.83	26.18
MODEL.PDB	O, B_LEU_560	NH2, B_ARG_577	HH22, B_ARG_577	2.71	1.75	13.66
MODEL.PDB	O, B_GLU_583	N, B_ASP_578	H, B_ASP_578	2.85	1.88	12.76
MODEL.PDB	OD1, B_ASP_578	N, B_THR_581	H, B_THR_581	2.86	2.01	27.04
MODEL.PDB	OD1, B_ASP_578	N, B_LEU_582	H, B_LEU_582	2.73	1.90	28.03
MODEL.PDB	OE1, B_GLU_583	N, B_ILE_584	H, B_ILE_584	2.88	2.00	24.69
MODEL.PDB	O, B_THR_553	N, B_ASP_586	H, B_ASP_586	2.83	1.84	10.38
MODEL.PDB	O, B_ASP_574	N, B_ILE_587	H, B_ILE_587	2.76	1.75	4.59
MODEL.PDB	OE1, B_GLU_619	OG, B_SER_591	HG, B_SER_591	2.62	1.73	18.48
MODEL.PDB	O, B_SER_316	N, B_VAL_595	H, B_VAL_595	2.87	1.86	1.12
MODEL.PDB	O, B_LEU_611	N, B_SER_596	H, B_SER_596	2.93	1.92	2.05
MODEL.PDB	O, B_TYR_313	N, B_VAL_597	H, B_VAL_597	2.83	1.84	9.20
MODEL.PDB	O, B_ALA_609	N, B_ILE_598	H, B_ILE_598	2.78	1.78	4.93
MODEL.PDB	O, B_VAL_308	N, B_THR_602	H, B_THR_602	2.86	1.92	16.77
MODEL.PDB	O, B_ILE_598	N, B_ALA_609	H, B_ALA_609	2.97	1.97	2.92
MODEL.PDB	O, B_SER_596	N, B_LEU_611	H, B_LEU_611	2.72	1.73	8.98
MODEL.PDB	O, B_CYS_649	N, B_TYR_612	H, B_TYR_612	2.84	1.83	5.58
MODEL.PDB	O, B_ALA_647	N, B_ASP_614	H, B_ASP_614	2.90	1.92	11.84
MODEL.PDB	OD1, B_ASN_616	N, B_CYS_617	H, B_CYS_617	2.85	1.94	20.77
MODEL.PDB	ND1, B_HIS_625	N, B_ALA_626	H, B_ALA_626	2.86	1.92	17.37
MODEL.PDB	OG1, B_THR_632	NE, B_ARG_634	HE, B_ARG_634	2.87	1.95	20.06
MODEL.PDB	O, B_SER_637	OG1, B_THR_638	HG1, B_THR_638	2.58	1.66	13.61
MODEL.PDB	O, B_LEU_650	N, B_PHE_643	H, B_PHE_643	2.86	1.89	11.47
MODEL.PDB	OD2, B_ASP_614	NH1, B_ARG_646	HH12, B_ARG_646	2.84	1.93	20.79
MODEL.PDB	O, B_PHE_643	N, B_LEU_650	H, B_LEU_650	2.79	1.78	0.13
MODEL.PDB	O, B_VAL_610	N, B_ILE_651	H, B_ILE_651	2.82	1.81	2.67
MODEL.PDB	O, B_ILE_692	N, B_GLU_654	H, B_GLU_654	2.81	1.82	9.58
MODEL.PDB	OE2, B_GLU_654	N, B_HIS_655	H, B_HIS_655	2.78	1.90	23.29
MODEL.PDB	O, B_ALA_694	N, B_VAL_656	H, B_VAL_656	2.96	2.02	17.75
MODEL.PDB	O, B_THR_696	OG, B_SER_659	HG, B_SER_659	2.72	1.93	28.63
MODEL.PDB	OE1, B_GLU_661	N, B_CYS_662	H, B_CYS_662	2.86	2.05	29.83
MODEL.PDB	O, B_ILE_670	N, B_ILE_666	H, B_ILE_666	2.98	2.09	23.24
MODEL.PDB	O, C_PRO_863	N, B_ALA_668	H, B_ALA_668	2.82	1.84	9.55
MODEL.PDB	O, C_LEU_864	N, B_GLY_669	H, B_GLY_669	2.81	1.90	20.41
MODEL.PDB	O, B_ILE_664	N, B_ALA_672	H, B_ALA_672	2.81	1.85	14.70
MODEL.PDB	OH, B_TYR_695	N, B_SER_673	H, B_SER_673	2.96	2.09	24.82
MODEL.PDB	O, B_GLN_677	N, B_SER_680	H, B_SER_680	2.87	1.88	9.34
MODEL.PDB	O, B_VAL_687	NE, B_ARG_685	HE, B_ARG_685	2.86	1.99	25.09
MODEL.PDB	O, B_VAL_687	NH1, B_ARG_685	HH11, B_ARG_685	2.75	1.91	27.04
MODEL.PDB	O, B_SER_691	N, B_ALA_688	H, B_ALA_688	2.76	1.81	15.69
MODEL.PDB	O, B_ALA_688	N, B_SER_691	H, B_SER_691	2.95	2.09	26.04
MODEL.PDB	O, B_GLU_654	N, B_ALA_694	H, B_ALA_694	2.77	1.83	16.90
MODEL.PDB	O, B_GLY_669	N, B_MET_697	H, B_MET_697	2.77	1.77	5.38
MODEL.PDB	O, B_TYR_660	N, B_SER_698	H, B_SER_698	2.65	1.65	3.25
MODEL.PDB	OD1, B_ASN_710	OG, B_SER_708	HG, B_SER_708	2.65	1.81	23.38
MODEL.PDB	OD2, C_ASP_796	ND2, B_ASN_709	HD21, B_ASN_709	2.69	1.82	25.22
MODEL.PDB	OD1, B_ASN_717	N, B_PHE_718	H, B_PHE_718	2.92	2.03	23.25
MODEL.PDB	OE1, B_GLN_926	N, B_ILE_720	H, B_ILE_720	2.80	1.80	6.25
MODEL.PDB	N, B_MET_731	OG, B_SER_730	HG, B_SER_730	2.89	2.10	29.05
MODEL.PDB	OG1, B_THR_734	OG1, B_THR_732	HG1, B_THR_732	2.80	2.02	29.06
MODEL.PDB	OD2, B_ASP_775	NZ, B_LYS_733	HZ1, B_LYS_733	2.58	1.59	8.03
MODEL.PDB	O, B_THR_859	N, B_SER_735	H, B_SER_735	2.81	1.81	5.47
MODEL.PDB	O, B_GLY_857	N, B_ASP_737	H, B_ASP_737	2.79	1.84	16.33
MODEL.PDB	OD1, B_ASP_737	N, B_MET_740	H, B_MET_740	2.88	1.87	5.67
MODEL.PDB	O, B_CYS_738	N, B_ILE_742	H, B_ILE_742	2.74	1.74	8.23
MODEL.PDB	O, B_THR_739	N, B_CYS_743	H, B_CYS_743	2.86	1.93	19.00
MODEL.PDB	O, B_THR_747	OG, B_SER_750	HG, B_SER_750	2.98	2.08	16.33

MODEL.PDB	O, B_LEU_753	N, B_TYR_756	H, B_TYR_756	2.91	1.95	13.71
MODEL.PDB	O, B_SER_758	N, B_GLN_762	H, B_GLN_762	3.00	2.01	9.83
MODEL.PDB	O, B_CYS_760	N, B_ASN_764	H, B_ASN_764	2.89	1.90	7.19
MODEL.PDB	O, B_THR_761	N, B_ARG_765	H, B_ARG_765	2.98	2.02	14.57
MODEL.PDB	O, B_ASN_764	N, B_THR_768	H, B_THR_768	2.91	1.94	12.25
MODEL.PDB	O, B_ASN_764	OG1, B_THR_768	HG1, B_THR_768	2.97	2.06	15.36
MODEL.PDB	O, B_ARG_765	N, B_GLY_769	H, B_GLY_769	2.85	1.86	10.66
MODEL.PDB	O, B_ILE_770	N, B_GLN_774	H, B_GLN_774	2.93	2.01	20.08
MODEL.PDB	O, B_GLU_773	N, B_ASN_777	H, B_ASN_777	2.79	1.84	15.71
MODEL.PDB	O, B_LYS_776	N, B_GLU_780	H, B_GLU_780	2.79	1.84	16.37
MODEL.PDB	O, B_GLN_779	N, B_ALA_783	H, B_ALA_783	2.96	2.03	18.63
MODEL.PDB	O, B_VAL_781	NE2, B_GLN_784	HE21, B_GLN_784	2.85	1.91	17.39
MODEL.PDB	O, A_ALA_701	N, B_ILE_788	H, B_ILE_788	2.81	1.89	19.07
MODEL.PDB	OE1, A_GLU_702	NZ, B_LYS_790	HZ2, B_LYS_790	2.57	1.72	25.91
MODEL.PDB	OD1, B_ASP_796	N, B_GLY_798	H, B_GLY_798	2.97	2.03	17.56
MODEL.PDB	OD1, B_ASN_928	N, B_ASN_801	H, B_ASN_801	2.73	1.76	12.36
MODEL.PDB	OD1, B_ASN_801	NE2, B_GLN_804	HE21, B_GLN_804	2.93	1.97	14.52
MODEL.PDB	OD1, B_ASP_820	NE, B_ARG_815	HE, B_ARG_815	2.83	1.98	26.93
MODEL.PDB	OD1, B_ASP_820	NH1, B_ARG_815	HH11, B_ARG_815	2.70	1.79	20.55
MODEL.PDB	OD1, B_ASP_867	NH2, B_ARG_815	HH21, B_ARG_815	2.92	2.02	21.93
MODEL.PDB	OE1, B_GLU_819	N, B_SER_816	H, B_SER_816	2.89	1.89	5.29
MODEL.PDB	OG, B_SER_816	N, B_GLU_819	H, B_GLU_819	2.97	1.98	10.31
MODEL.PDB	O, B_SER_816	N, B_ASP_820	H, B_ASP_820	2.93	1.93	6.62
MODEL.PDB	O, B_ILE_818	N, B_LEU_822	H, B_LEU_822	2.86	1.89	13.69
MODEL.PDB	O, B_SER_939	NZ, B_LYS_825	HZ2, B_LYS_825	2.70	1.72	10.45
MODEL.PDB	OE1, B_GLN_949	N, B_THR_827	H, B_THR_827	2.83	1.82	3.45
MODEL.PDB	OD2, B_ASP_848	N, B_ARG_847	H, B_ARG_847	2.97	1.98	8.70
MODEL.PDB	O, B_LEU_849	N, B_CYS_851	H, B_CYS_851	2.78	1.85	18.62
MODEL.PDB	O, B_ASN_856	N, B_LEU_858	H, B_LEU_858	2.97	2.06	21.69
MODEL.PDB	O, B_SER_735	N, B_THR_859	H, B_THR_859	2.83	1.82	3.32
MODEL.PDB	OD2, A_ASP_614	OG1, B_THR_859	HG1, B_THR_859	2.98	2.16	26.02
MODEL.PDB	O, B_LYS_733	N, B_LEU_861	H, B_LEU_861	2.91	1.90	2.20
MODEL.PDB	OD1, B_ASP_775	N, B_LEU_864	H, B_LEU_864	2.75	1.76	9.72
MODEL.PDB	O, B_ILE_844	OG1, B_THR_866	HG1, B_THR_866	2.77	2.00	29.97
MODEL.PDB	O, B_THR_866	N, B_ILE_870	H, B_ILE_870	2.94	1.96	11.60
MODEL.PDB	O, B_ASP_867	N, B_ALA_871	H, B_ALA_871	2.79	1.85	16.87
MODEL.PDB	O, B_GLU_868	N, B_GLN_872	H, B_GLN_872	2.85	1.90	15.95
MODEL.PDB	O, B_ILE_870	N, B_THR_874	H, B_THR_874	2.91	1.96	16.23
MODEL.PDB	OE2, B_GLU_819	OG1, B_THR_874	HG1, B_THR_874	2.73	1.83	16.33
MODEL.PDB	O, B_ALA_871	N, B_SER_875	H, B_SER_875	2.83	1.83	7.32
MODEL.PDB	O, B_GLN_872	N, B_ALA_876	H, B_ALA_876	2.95	2.01	17.47
MODEL.PDB	O, B_TYR_873	N, B_LEU_877	H, B_LEU_877	2.99	1.99	5.57
MODEL.PDB	O, B_THR_874	N, B_LEU_878	H, B_LEU_878	2.90	1.95	15.92
MODEL.PDB	O, B_SER_875	N, B_ALA_879	H, B_ALA_879	2.80	1.80	8.47
MODEL.PDB	O, B_LEU_877	N, B_THR_881	H, B_THR_881	2.98	2.01	12.62
MODEL.PDB	O, B_THR_887	N, B_GLY_891	H, B_GLY_891	2.90	1.90	6.42
MODEL.PDB	O, B_THR_881	NE2, B_GLN_901	HE22, B_GLN_901	2.80	1.99	29.78
MODEL.PDB	O, B_PHE_898	N, B_MET_902	H, B_MET_902	2.89	1.91	12.26
MODEL.PDB	O, B_ALA_899	N, B_ALA_903	H, B_ALA_903	2.88	1.92	15.49
MODEL.PDB	O, B_MET_902	N, B_PHE_906	H, B_PHE_906	2.83	1.85	11.89
MODEL.PDB	O, B_TYR_904	N, B_GLY_908	H, B_GLY_908	2.77	1.81	15.60
MODEL.PDB	O, B_ASN_907	N, B_GLY_910	H, B_GLY_910	2.97	2.05	19.90
MODEL.PDB	O, B_ASN_914	N, B_GLU_918	H, B_GLU_918	2.92	1.91	2.07
MODEL.PDB	O, B_GLY_798	NE2, B_GLN_920	HE21, B_GLN_920	2.96	2.03	18.49
MODEL.PDB	O, B_GLN_920	N, B_ALA_924	H, B_ALA_924	2.88	1.88	6.38
MODEL.PDB	O, B_LEU_922	N, B_GLN_926	H, B_GLN_926	2.88	1.91	12.43
MODEL.PDB	O, B_ILE_923	N, B_PHE_927	H, B_PHE_927	2.99	2.01	10.10
MODEL.PDB	O, B_ALA_924	N, B_ASN_928	H, B_ASN_928	2.92	1.94	10.79

MODEL.PDB	O, B_GLN_926	N, B_ALA_930	H, B_ALA_930	2.95	2.01	18.22
MODEL.PDB	O, B_PHE_927	N, B_ILE_931	H, B_ILE_931	2.95	1.96	8.93
MODEL.PDB	O, B_LYS_933	N, B_SER_937	H, B_SER_937	2.86	1.90	14.74
MODEL.PDB	O, B_ILE_934	N, B_LEU_938	H, B_LEU_938	2.84	1.84	5.40
MODEL.PDB	O, B_GLN_935	N, B_SER_939	H, B_SER_939	2.86	1.91	16.55
MODEL.PDB	O, B_ASP_936	N, B_SER_940	H, B_SER_940	2.84	1.85	9.53
MODEL.PDB	O, B_LEU_945	N, B_LEU_948	H, B_LEU_948	2.89	1.91	12.12
MODEL.PDB	OD1, B_ASN_953	NE2, B_GLN_949	HE21, B_GLN_949	2.81	1.84	12.61
MODEL.PDB	O, B_GLY_946	N, B_ASP_950	H, B_ASP_950	2.84	1.86	10.71
MODEL.PDB	O, B_GLN_949	N, B_ASN_953	H, B_ASN_953	2.81	1.82	8.84
MODEL.PDB	O, B_ASP_950	N, B_GLN_954	H, B_GLN_954	2.73	1.74	10.35
MODEL.PDB	O, B_ASN_953	N, B_GLN_957	H, B_GLN_957	2.83	1.85	10.89
MODEL.PDB	O, B_ALA_956	N, B_ASN_960	H, B_ASN_960	2.82	1.84	11.78
MODEL.PDB	O, B_GLN_957	N, B_THR_961	H, B_THR_961	2.92	1.94	12.31
MODEL.PDB	O, B_LEU_959	N, B_VAL_963	H, B_VAL_963	2.95	1.98	13.04
MODEL.PDB	O, C_GLN_755	N, B_PHE_970	H, B_PHE_970	2.79	1.86	17.89
MODEL.PDB	O, B_ASN_969	N, B_ALA_972	H, B_ALA_972	2.95	1.98	13.71
MODEL.PDB	OE1, B_GLN_992	N, B_ILE_973	H, B_ILE_973	2.82	1.85	13.37
MODEL.PDB	O, B_ASN_978	N, B_SER_982	H, B_SER_982	2.96	2.05	20.99
MODEL.PDB	OD2, B_ASP_979	NE, B_ARG_983	HE, B_ARG_983	2.71	1.71	5.22
MODEL.PDB	OD1, B_ASP_979	NH2, B_ARG_983	HH21, B_ARG_983	2.61	1.64	12.14
MODEL.PDB	O, B_ASP_985	N, B_ALA_989	H, B_ALA_989	2.88	1.93	16.37
MODEL.PDB	O, B_LYS_986	N, B_GLU_990	H, B_GLU_990	2.92	1.99	18.69
MODEL.PDB	OE2, B_GLU_988	NE2, B_GLN_992	HE21, B_GLN_992	2.70	1.70	2.13
MODEL.PDB	O, B_ALA_989	N, B_ILE_993	H, B_ILE_993	2.78	1.81	11.44
MODEL.PDB	O, B_GLU_990	N, B_ASP_994	H, B_ASP_994	2.78	1.80	11.51
MODEL.PDB	OD1, C_ASP_994	NH1, B_ARG_995	HH12, B_ARG_995	2.64	1.64	8.73
MODEL.PDB	O, B_PHE_970	NH2, B_ARG_995	HH21, B_ARG_995	2.82	1.88	17.56
MODEL.PDB	O, B_ILE_993	N, B_ILE_997	H, B_ILE_997	2.82	1.83	8.71
MODEL.PDB	O, B_ASP_994	N, B_THR_998	H, B_THR_998	2.95	1.95	7.15
MODEL.PDB	O, C_SER_60	N, C_SER_31	H, C_SER_31	2.75	1.76	9.01
MODEL.PDB	O, C_GLY_219	OG1, C_THR_33	HG1, C_THR_33	2.62	1.76	21.23
MODEL.PDB	O, C_PRO_217	NH2, C_ARG_34	HH21, C_ARG_34	2.77	1.86	19.83
MODEL.PDB	O, C_GLY_283	OH, C_TYR_38	HH, C_TYR_38	2.94	2.07	20.40
MODEL.PDB	O, B_PHE_565	N, C_PHE_43	H, C_PHE_43	2.83	1.82	3.14
MODEL.PDB	O, C_PHE_275	N, C_THR_51	H, C_THR_51	2.97	1.98	7.47
MODEL.PDB	OD2, C_ASP_53	OG1, C_THR_51	HG1, C_THR_51	2.80	2.01	28.71
MODEL.PDB	O, C_SER_31	N, C_PHE_59	H, C_PHE_59	2.76	1.85	20.94
MODEL.PDB	O, C_THR_29	N, C_VAL_62	H, C_VAL_62	2.91	1.93	10.93
MODEL.PDB	O, C_VAL_267	N, C_THR_63	H, C_THR_63	2.90	1.93	13.24
MODEL.PDB	O, C_TYR_265	N, C_PHE_65	H, C_PHE_65	2.83	1.83	5.20
MODEL.PDB	O, C_THR_73	OG, C_SER_71	HG, C_SER_71	2.63	1.79	23.54
MODEL.PDB	O, C_THR_76	OG1, C_THR_73	HG1, C_THR_73	2.80	1.86	7.69
MODEL.PDB	OD2, C_ASP_138	N, C_LYS_77	H, C_LYS_77	2.83	1.96	24.89
MODEL.PDB	O, C_LYS_77	NH2, C_ARG_78	HH21, C_ARG_78	2.65	1.70	15.27
MODEL.PDB	O, C_ARG_78	N, C_ASP_80	H, C_ASP_80	2.99	2.11	23.88
MODEL.PDB	O, C_PHE_238	N, C_LEU_84	H, C_LEU_84	2.77	1.77	5.40
MODEL.PDB	O, C_ASN_87	N, C_GLY_89	H, C_GLY_89	2.80	1.93	24.56
MODEL.PDB	O, C_GLY_268	N, C_TYR_91	H, C_TYR_91	2.80	1.85	16.61
MODEL.PDB	O, C_PHE_192	N, C_PHE_92	H, C_PHE_92	2.90	1.90	5.12
MODEL.PDB	OD1, C_ASP_253	NZ, C_LYS_97	HZ2, C_LYS_97	2.69	1.77	19.23
MODEL.PDB	O, C_ASN_121	NH1, C_ARG_102	HH11, C_ARG_102	2.76	1.80	14.78
MODEL.PDB	O, C_ILE_119	N, C_TRP_104	H, C_TRP_104	2.85	1.88	13.53
MODEL.PDB	O, C_GLN_239	N, C_ILE_105	H, C_ILE_105	2.93	1.93	8.32
MODEL.PDB	O, C_LEU_117	N, C_PHE_106	H, C_PHE_106	2.81	1.82	8.05
MODEL.PDB	O, C_ARG_237	N, C_GLY_107	H, C_GLY_107	2.90	1.91	10.24
MODEL.PDB	OE2, B_GLU_471	NZ, C_LYS_113	HZ1, C_LYS_113	2.68	1.73	15.31
MODEL.PDB	O, C_PHE_106	N, C_LEU_117	H, C_LEU_117	2.74	1.80	17.34

MODEL.PDB	O, C_LYS_129	N, C_LEU_118	H, C_LEU_118	2.76	1.75	3.99
MODEL.PDB	O, C_TRP_104	N, C_ILE_119	H, C_ILE_119	2.92	1.99	18.69
MODEL.PDB	O, C_VAL_127	N, C_VAL_120	H, C_VAL_120	2.85	1.86	9.48
MODEL.PDB	OD1, C_ASN_125	ND2, C_ASN_122	HD21, C_ASN_122	2.84	1.89	16.55
MODEL.PDB	O, C_ASN_122	N, C_THR_124	H, C_THR_124	2.82	1.94	23.27
MODEL.PDB	O, C_SER_172	N, C_VAL_126	H, C_VAL_126	2.89	1.93	14.70
MODEL.PDB	O, C_LEU_118	N, C_LYS_129	H, C_LYS_129	2.84	1.84	6.56
MODEL.PDB	OE2, C_GLU_169	NZ, C_LYS_129	HZ3, C_LYS_129	2.46	1.53	17.71
MODEL.PDB	O, C_CYS_131	N, C_PHE_133	H, C_PHE_133	2.94	2.10	27.94
MODEL.PDB	OD1, C_ASP_111	N, C_PHE_135	H, C_PHE_135	2.88	1.95	19.37
MODEL.PDB	O, C_HIS_146	N, C_ASN_149	H, C_ASN_149	2.95	1.99	14.41
MODEL.PDB	OE1, C_GLU_154	NZ, C_LYS_150	HZ3, C_LYS_150	2.61	1.79	28.77
MODEL.PDB	O, C_VAL_159	N, C_SER_161	H, C_SER_161	2.87	2.06	29.95
MODEL.PDB	O, C_GLU_180	N, C_GLY_184	H, C_GLY_184	2.88	1.91	13.23
MODEL.PDB	OD1, C_ASN_185	N, C_PHE_186	H, C_PHE_186	2.64	1.76	24.15
MODEL.PDB	O, C_PHE_92	N, C_PHE_192	H, C_PHE_192	2.74	1.77	13.27
MODEL.PDB	O, C_VAL_90	N, C_PHE_194	H, C_PHE_194	2.96	1.96	5.15
MODEL.PDB	OH, C_TYR_204	NZ, C_LYS_195	HZ2, C_LYS_195	2.89	1.88	6.24
MODEL.PDB	O, C_ILE_233	ND2, C_ASN_196	HD22, C_ASN_196	2.84	1.98	26.20
MODEL.PDB	O, C_TYR_200	N, C_ILE_197	H, C_ILE_197	2.93	1.92	4.38
MODEL.PDB	O, C_ILE_197	N, C_TYR_200	H, C_TYR_200	2.84	1.91	17.89
MODEL.PDB	O, C_LEU_229	N, C_PHE_201	H, C_PHE_201	2.81	1.82	10.62
MODEL.PDB	OD2, C_ASP_228	NZ, C_LYS_202	HZ2, C_LYS_202	2.76	1.94	28.81
MODEL.PDB	O, C_VAL_193	N, C_TYR_204	H, C_TYR_204	2.93	1.98	16.05
MODEL.PDB	O, C_GLU_224	N, C_SER_205	H, C_SER_205	2.89	1.94	14.89
MODEL.PDB	OE2, C_GLU_191	OG1, C_THR_208	HG1, C_THR_208	2.86	1.90	5.11
MODEL.PDB	O, C_ILE_203	N, C_LEU_226	H, C_LEU_226	2.82	1.81	2.77
MODEL.PDB	O, C_GLY_107	N, C_ARG_237	H, C_ARG_237	3.00	2.09	21.59
MODEL.PDB	O, C_LEU_84	N, C_PHE_238	H, C_PHE_238	2.77	1.89	23.69
MODEL.PDB	O, C_ILE_105	N, C_GLN_239	H, C_GLN_239	2.81	1.86	14.63
MODEL.PDB	O, C_ASN_81	NE2, C_GLN_239	HE21, C_GLN_239	2.97	2.09	24.23
MODEL.PDB	O, C_GLY_103	N, C_LEU_241	H, C_LEU_241	2.84	1.88	14.32
MODEL.PDB	OE1, C_GLU_156	NH1, C_ARG_246	HH12, C_ARG_246	2.76	1.76	7.38
MODEL.PDB	OE2, C_GLU_156	NH2, C_ARG_246	HH22, C_ARG_246	2.61	1.71	21.34
MODEL.PDB	O, C_SER_255	OG, C_SER_247	HG, C_SER_247	2.85	1.91	7.40
MODEL.PDB	OD1, C_ASN_99	N, C_LEU_249	H, C_LEU_249	2.95	1.96	10.13
MODEL.PDB	O, C_GLY_184	N, C_ASP_253	H, C_ASP_253	2.93	2.00	18.63
MODEL.PDB	O, C_SER_255	N, C_GLY_257	H, C_GLY_257	2.96	2.09	25.74
MODEL.PDB	O, C_GLU_96	N, C_ALA_264	H, C_ALA_264	2.77	1.83	17.25
MODEL.PDB	O, C_PHE_65	N, C_TYR_265	H, C_TYR_265	2.92	1.94	12.01
MODEL.PDB	O, C_ALA_93	N, C_TYR_266	H, C_TYR_266	2.76	1.76	6.11
MODEL.PDB	O, C_PHE_55	N, C_GLN_271	H, C_GLN_271	2.96	2.00	14.44
MODEL.PDB	OD2, C_ASP_290	NH2, C_ARG_273	HH22, C_ARG_273	2.55	1.66	21.76
MODEL.PDB	O, C_THR_51	N, C_PHE_275	H, C_PHE_275	2.93	1.93	8.43
MODEL.PDB	O, C_HIS_49	N, C_LEU_277	H, C_LEU_277	2.76	1.75	5.61
MODEL.PDB	O, C_ASP_287	N, C_LYS_278	H, C_LYS_278	2.95	1.94	6.11
MODEL.PDB	O, C_THR_284	N, C_ASN_280	H, C_ASN_280	2.78	1.78	5.39
MODEL.PDB	O, C_ASN_280	N, C_GLY_283	H, C_GLY_283	2.90	1.96	17.14
MODEL.PDB	O, C_LYS_278	N, C_THR_286	H, C_THR_286	2.94	1.94	7.11
MODEL.PDB	O, C_LEU_276	N, C_VAL_289	H, C_VAL_289	2.86	1.89	13.26
MODEL.PDB	OD1, C_ASP_294	N, C_LEU_296	H, C_LEU_296	2.75	1.80	15.93
MODEL.PDB	O, C_ASP_294	N, C_GLU_298	H, C_GLU_298	2.90	1.98	19.20
MODEL.PDB	O, C_PRO_295	N, C_THR_299	H, C_THR_299	2.94	2.03	21.12
MODEL.PDB	O, C_SER_297	N, C_CYS_301	H, C_CYS_301	2.99	2.02	14.63
MODEL.PDB	O, C_GLU_298	N, C_THR_302	H, C_THR_302	2.78	1.81	13.04
MODEL.PDB	O, C_THR_299	N, C_LEU_303	H, C_LEU_303	2.80	1.82	9.35
MODEL.PDB	O, C_CYS_301	NZ, C_LYS_304	HZ1, C_LYS_304	2.67	1.68	9.78
MODEL.PDB	O, C_THR_307	OG, C_SER_305	HG, C_SER_305	2.82	1.93	17.29

MODEL.PDB	O, C_ARG_685	NZ, C_LYS_310	HZ3, C_LYS_310	2.70	1.83	24.75
MODEL.PDB	O, C_GLU_309	OH, C_TYR_313	HH, C_TYR_313	2.72	1.91	26.67
MODEL.PDB	OE2, C_GLU_298	OG1, C_THR_315	HG1, C_THR_315	2.64	1.70	8.17
MODEL.PDB	O, C_GLY_593	N, C_PHE_318	H, C_PHE_318	2.93	1.95	11.12
MODEL.PDB	O, C_CYS_538	N, C_THR_323	H, C_THR_323	2.86	1.86	7.66
MODEL.PDB	O, C_ASN_542	N, C_ARG_328	H, C_ARG_328	2.84	1.83	5.03
MODEL.PDB	OE1, C_GLN_580	NE, C_ARG_328	HE, C_ARG_328	2.78	1.86	19.60
MODEL.PDB	OD2, C_ASP_578	NH1, C_ARG_328	HH12, C_ARG_328	2.60	1.78	28.67
MODEL.PDB	OE1, C_GLN_580	NH2, C_ARG_328	HH21, C_ARG_328	2.90	2.05	27.29
MODEL.PDB	O, C_CYS_336	N, C_PHE_338	H, C_PHE_338	2.85	2.02	28.34
MODEL.PDB	O, C_PHE_338	N, C_VAL_341	H, C_VAL_341	2.94	2.11	29.17
MODEL.PDB	O, C_GLY_339	N, C_ASN_343	H, C_ASN_343	2.81	1.85	14.75
MODEL.PDB	OD2, C_ASP_467	OH, C_TYR_351	HH, C_TYR_351	2.53	1.60	11.08
MODEL.PDB	O, C_SER_399	N, C_ASN_354	H, C_ASN_354	2.98	2.02	15.21
MODEL.PDB	OD1, C_ASP_398	NE, C_ARG_355	HE, C_ARG_355	2.62	1.64	10.97
MODEL.PDB	OD2, C_ASP_398	NH2, C_ARG_355	HH21, C_ARG_355	2.58	1.57	3.27
MODEL.PDB	O, C_VAL_395	N, C_ILE_358	H, C_ILE_358	2.79	1.80	7.71
MODEL.PDB	OD1, C_ASN_394	OG, C_SER_359	HG, C_SER_359	2.97	2.15	25.84
MODEL.PDB	O, C_ASN_334	N, C_VAL_362	H, C_VAL_362	2.71	1.78	18.56
MODEL.PDB	O, C_CYS_525	N, C_ALA_363	H, C_ALA_363	2.77	1.77	6.71
MODEL.PDB	OD1, C_ASP_364	N, C_SER_366	H, C_SER_366	2.74	1.81	19.19
MODEL.PDB	OD1, C_ASP_364	OG, C_SER_366	HG, C_SER_366	2.68	1.81	20.57
MODEL.PDB	O, C_TYR_365	N, C_TYR_369	H, C_TYR_369	2.89	1.95	18.35
MODEL.PDB	O, C_ALA_435	N, C_THR_376	H, C_THR_376	2.96	1.97	8.80
MODEL.PDB	OH, C_TYR_380	NZ, C_LYS_378	HZ3, C_LYS_378	2.93	1.99	17.96
MODEL.PDB	O, A_ARG_983	N, C_SER_383	H, C_SER_383	2.91	1.90	2.08
MODEL.PDB	O, C_VAL_524	N, C_PHE_392	H, C_PHE_392	2.76	1.77	8.68
MODEL.PDB	O, C_GLU_516	N, C_THR_393	H, C_THR_393	2.81	1.85	15.38
MODEL.PDB	O, C_ILE_358	N, C_VAL_395	H, C_VAL_395	2.96	1.96	7.50
MODEL.PDB	O, C_SER_514	N, C_TYR_396	H, C_TYR_396	2.96	1.98	10.39
MODEL.PDB	O, C_LYS_356	N, C_ALA_397	H, C_ALA_397	2.95	1.94	4.02
MODEL.PDB	O, C_VAL_512	N, C_ASP_398	H, C_ASP_398	2.96	1.95	4.31
MODEL.PDB	O, C_ASN_354	N, C_SER_399	H, C_SER_399	2.83	1.90	19.13
MODEL.PDB	O, C_VAL_510	N, C_PHE_400	H, C_PHE_400	2.99	2.01	10.93
MODEL.PDB	O, C_ALA_348	N, C_VAL_401	H, C_VAL_401	2.98	2.14	27.38
MODEL.PDB	O, C_ASP_405	NE, C_ARG_408	HE, C_ARG_408	2.82	1.92	21.75
MODEL.PDB	O, C_ASP_405	NH1, C_ARG_408	HH11, C_ARG_408	2.91	2.03	24.55
MODEL.PDB	O, C_GLU_406	N, C_GLN_409	H, C_GLN_409	2.99	2.08	21.28
MODEL.PDB	OD2, C_ASP_420	N, C_GLY_416	H, C_GLY_416	2.76	1.76	4.26
MODEL.PDB	O, C_GLY_416	N, C_ASP_420	H, C_ASP_420	2.85	1.85	5.05
MODEL.PDB	O, C_ILE_418	N, C_ASN_422	H, C_ASN_422	2.84	1.91	18.43
MODEL.PDB	O, C_LYS_417	ND2, C_ASN_422	HD21, C_ASN_422	2.95	2.09	25.91
MODEL.PDB	O, C_ARG_454	ND2, C_ASN_422	HD22, C_ASN_422	2.96	2.05	20.86
MODEL.PDB	O, C_ILE_418	N, C_TYR_423	H, C_TYR_423	2.90	1.93	12.86
MODEL.PDB	O, C_LEU_461	NZ, C_LYS_424	HZ1, C_LYS_424	2.82	2.00	28.66
MODEL.PDB	OD1, C_ASN_460	NZ, C_LYS_424	HZ2, C_LYS_424	2.69	1.71	11.25
MODEL.PDB	OD1, C_ASP_428	N, C_PHE_429	H, C_PHE_429	2.74	1.87	24.99
MODEL.PDB	O, C_LYS_378	N, C_VAL_433	H, C_VAL_433	2.75	1.75	6.16
MODEL.PDB	O, C_VAL_511	N, C_ILE_434	H, C_ILE_434	2.97	2.08	22.89
MODEL.PDB	OD2, C_ASP_442	OG, C_SER_438	HG, C_SER_438	2.57	1.73	23.01
MODEL.PDB	O, C_SER_438	N, C_LEU_441	H, C_LEU_441	2.95	1.96	8.73
MODEL.PDB	O, C_SER_438	N, C_ASP_442	H, C_ASP_442	2.90	1.92	12.85
MODEL.PDB	O, C_ASN_439	OG, C_SER_443	HG, C_SER_443	2.61	1.82	28.48
MODEL.PDB	O, C_LYS_444	N, C_GLY_447	H, C_GLY_447	2.98	2.07	22.07
MODEL.PDB	OD1, C_ASN_448	N, C_ASN_450	H, C_ASN_450	2.93	1.96	12.28
MODEL.PDB	O, C_GLN_493	N, C_TYR_453	H, C_TYR_453	2.89	1.92	13.12
MODEL.PDB	OD1, C_ASN_422	N, C_ARG_454	H, C_ARG_454	2.74	1.74	7.03
MODEL.PDB	O, C_PRO_491	N, C_LEU_455	H, C_LEU_455	2.83	1.82	2.24

MODEL.PDB	O, C_PHE_490	NH1, C_ARG_457	HH11, C_ARG_457	2.86	1.92	18.01
MODEL.PDB	O, C_PHE_456	NH2, C_ARG_457	HH21, C_ARG_457	2.95	2.01	17.42
MODEL.PDB	OH, C_TYR_421	N, C_SER_459	H, C_SER_459	2.92	1.96	13.91
MODEL.PDB	OD1, C_ASP_420	ND2, C_ASN_460	HD22, C_ASN_460	2.79	1.85	17.42
MODEL.PDB	OE2, C_GLU_465	N, C_LYS_462	H, C_LYS_462	2.96	1.95	1.74
MODEL.PDB	O, C_ALA_352	NH1, C_ARG_466	HH12, C_ARG_466	2.71	1.78	17.54
MODEL.PDB	OD1, C_ASP_467	N, C_SER_469	H, C_SER_469	2.85	1.87	11.33
MODEL.PDB	OD1, C_ASP_467	OG, C_SER_469	HG, C_SER_469	2.78	1.89	17.62
MODEL.PDB	OE1, C_GLN_474	OH, C_TYR_489	HH, C_TYR_489	2.76	1.82	9.42
MODEL.PDB	O, C_TYR_453	N, C_GLN_493	H, C_GLN_493	2.75	1.78	12.98
MODEL.PDB	O, C_SER_494	NE2, C_GLN_493	HE21, C_GLN_493	2.89	1.89	5.58
MODEL.PDB	O, C_TYR_451	N, C_TYR_495	H, C_TYR_495	2.84	1.85	10.31
MODEL.PDB	O, C_ASN_448	N, C_PHE_497	H, C_PHE_497	2.83	1.94	22.51
MODEL.PDB	O, C_ILE_402	N, C_TYR_508	H, C_TYR_508	2.92	1.93	10.25
MODEL.PDB	O, C_TRP_436	N, C_ARG_509	H, C_ARG_509	2.93	2.11	29.53
MODEL.PDB	OD1, C_ASP_442	NH1, C_ARG_509	HH11, C_ARG_509	2.58	1.62	14.24
MODEL.PDB	O, C_PHE_400	N, C_VAL_510	H, C_VAL_510	2.83	1.83	4.85
MODEL.PDB	O, C_ASP_398	N, C_VAL_512	H, C_VAL_512	2.98	2.00	12.14
MODEL.PDB	O, C_CYS_432	N, C_LEU_513	H, C_LEU_513	2.91	1.92	10.29
MODEL.PDB	O, C_TYR_396	N, C_SER_514	H, C_SER_514	2.85	1.85	7.11
MODEL.PDB	O, C_PHE_392	N, C_THR_523	H, C_THR_523	2.78	1.77	1.47
MODEL.PDB	O, C_PHE_392	N, C_VAL_524	H, C_VAL_524	2.84	1.84	7.50
MODEL.PDB	O, C_VAL_327	N, C_THR_531	H, C_THR_531	2.96	2.00	14.18
MODEL.PDB	OE1, C_GLU_554	NZ, C_LYS_535	HZ3, C_LYS_535	2.65	1.79	24.99
MODEL.PDB	OE2, C_GLU_554	NZ, C_LYS_535	HZ3, C_LYS_535	2.72	1.89	27.95
MODEL.PDB	O, C_LEU_552	N, C_ASN_536	H, C_ASN_536	2.83	1.84	8.37
MODEL.PDB	OE2, C_GLU_324	NZ, C_LYS_537	HZ3, C_LYS_537	2.54	1.67	24.70
MODEL.PDB	O, C_GLY_550	N, C_VAL_539	H, C_VAL_539	2.99	2.00	10.70
MODEL.PDB	O, C_GLY_548	N, C_PHE_541	H, C_PHE_541	2.93	1.94	8.02
MODEL.PDB	O, C_ILE_326	N, C_ASN_542	H, C_ASN_542	2.98	2.01	12.93
MODEL.PDB	O, C_LEU_546	N, C_PHE_543	H, C_PHE_543	2.98	2.00	12.02
MODEL.PDB	O, C_ALA_522	ND2, C_ASN_544	HD22, C_ASN_544	2.88	1.87	4.17
MODEL.PDB	OD1, C_ASN_542	N, C_GLY_545	H, C_GLY_545	2.95	2.04	21.14
MODEL.PDB	O, C_PHE_543	N, C_LEU_546	H, C_LEU_546	2.91	1.92	9.15
MODEL.PDB	OD2, A_ASP_745	OG1, C_THR_549	HG1, C_THR_549	2.94	2.12	25.69
MODEL.PDB	O, C_THR_588	N, C_VAL_551	H, C_VAL_551	2.81	1.80	4.39
MODEL.PDB	O, C_ILE_584	N, C_SER_555	H, C_SER_555	2.94	1.99	16.70
MODEL.PDB	OD1, C_ASP_586	OG, C_SER_555	HG, C_SER_555	2.61	1.67	9.67
MODEL.PDB	OD2, C_ASP_574	NZ, C_LYS_557	HZ3, C_LYS_557	2.58	1.76	27.92
MODEL.PDB	O, C_ALA_575	N, C_GLY_566	H, C_GLY_566	2.84	1.87	13.47
MODEL.PDB	O, A_PHE_43	N, C_ARG_567	H, C_ARG_567	2.91	1.94	12.53
MODEL.PDB	O, C_ILE_569	OG1, C_THR_572	HG1, C_THR_572	2.80	1.89	13.83
MODEL.PDB	O, C_LEU_585	N, C_VAL_576	H, C_VAL_576	2.93	1.96	11.99
MODEL.PDB	O, C_GLN_564	N, C_ARG_577	H, C_ARG_577	2.95	1.94	1.92
MODEL.PDB	O, C_GLN_563	NE, C_ARG_577	HE, C_ARG_577	2.88	2.06	29.54
MODEL.PDB	O, C_GLN_563	NH2, C_ARG_577	HH21, C_ARG_577	2.73	1.86	25.33
MODEL.PDB	OD1, C_ASP_578	N, C_THR_581	H, C_THR_581	2.66	1.70	14.58
MODEL.PDB	O, C_VAL_576	N, C_LEU_585	H, C_LEU_585	2.94	1.97	13.37
MODEL.PDB	O, C_THR_553	N, C_ASP_586	H, C_ASP_586	2.90	2.06	28.07
MODEL.PDB	O, C_ASP_574	N, C_ILE_587	H, C_ILE_587	2.65	1.66	9.43
MODEL.PDB	O, C_SER_316	N, C_VAL_595	H, C_VAL_595	2.92	1.92	3.30
MODEL.PDB	O, C_LEU_611	N, C_SER_596	H, C_SER_596	2.89	1.90	10.46
MODEL.PDB	O, C_TYR_313	N, C_VAL_597	H, C_VAL_597	2.90	1.91	11.17
MODEL.PDB	O, C_ALA_609	N, C_ILE_598	H, C_ILE_598	2.76	1.80	13.17
MODEL.PDB	O, C_ILE_651	N, C_VAL_610	H, C_VAL_610	2.81	1.80	1.72
MODEL.PDB	O, C_SER_596	N, C_LEU_611	H, C_LEU_611	2.72	1.72	4.81
MODEL.PDB	O, C_GLY_594	N, C_GLN_613	H, C_GLN_613	2.89	1.91	11.46
MODEL.PDB	O, C_ALA_647	N, C_ASP_614	H, C_ASP_614	2.81	1.82	6.96

MODEL.PDB	O, C_ASP_627	NE2, C_GLN_628	HE21, C_GLN_628	2.82	1.92	21.92
MODEL.PDB	O, C_GLN_628	N, C_THR_630	H, C_THR_630	2.76	1.84	18.98
MODEL.PDB	O, C_GLU_619	NH2, C_ARG_634	HH21, C_ARG_634	2.74	1.90	27.43
MODEL.PDB	OD2, C_ASP_294	OG, C_SER_637	HG, C_SER_637	2.56	1.75	25.96
MODEL.PDB	O, C_LEU_650	N, C_PHE_643	H, C_PHE_643	2.81	1.92	22.91
MODEL.PDB	O, C_GLY_648	OG1, C_THR_645	HG1, C_THR_645	2.71	1.80	15.84
MODEL.PDB	OD2, A_ASP_848	NH2, C_ARG_646	HH22, C_ARG_646	2.63	1.79	27.55
MODEL.PDB	O, C_PHE_643	N, C_LEU_650	H, C_LEU_650	2.73	1.75	9.99
MODEL.PDB	O, C_VAL_610	N, C_ILE_651	H, C_ILE_651	2.78	1.80	10.59
MODEL.PDB	O, C_ASN_641	N, C_GLY_652	H, C_GLY_652	2.79	1.78	1.50
MODEL.PDB	O, C_ILE_692	N, C_GLU_654	H, C_GLU_654	2.81	1.89	19.55
MODEL.PDB	O, C_THR_696	OG, C_SER_659	HG, C_SER_659	2.86	2.07	28.50
MODEL.PDB	O, C_THR_676	OH, C_TYR_660	HH, C_TYR_660	2.66	1.82	23.84
MODEL.PDB	OE1, C_GLU_661	N, C_CYS_662	H, C_CYS_662	2.69	1.71	11.63
MODEL.PDB	O, C_ILE_670	N, C_ILE_666	H, C_ILE_666	2.88	1.97	20.86
MODEL.PDB	O, A_PRO_863	N, C_ALA_668	H, C_ALA_668	2.82	1.86	14.51
MODEL.PDB	O, A_LEU_864	N, C_GLY_669	H, C_GLY_669	2.73	1.84	22.00
MODEL.PDB	O, C_TYR_695	N, C_CYS_671	H, C_CYS_671	2.88	1.91	13.00
MODEL.PDB	O, C_ILE_664	N, C_ALA_672	H, C_ALA_672	2.79	1.82	13.83
MODEL.PDB	OD2, C_ASP_663	OG, C_SER_673	HG, C_SER_673	2.61	1.66	4.96
MODEL.PDB	OG, C_SER_689	OG1, C_THR_676	HG1, C_THR_676	2.79	1.86	11.33
MODEL.PDB	OE1, C_GLN_677	ND2, C_ASN_679	HD21, C_ASN_679	2.90	1.93	13.29
MODEL.PDB	O, C_ASN_679	NH1, C_ARG_683	HH11, C_ARG_683	2.73	1.73	8.46
MODEL.PDB	O, C_ALA_684	NH2, C_ARG_685	HH21, C_ARG_685	2.74	1.79	14.98
MODEL.PDB	O, C_ALA_688	N, C_SER_691	H, C_SER_691	2.96	1.98	12.29
MODEL.PDB	O, C_CYS_671	N, C_TYR_695	H, C_TYR_695	2.78	1.80	9.89
MODEL.PDB	O, C_GLU_661	OH, C_TYR_695	HH, C_TYR_695	2.57	1.63	8.69
MODEL.PDB	O, C_GLY_669	N, C_MET_697	H, C_MET_697	2.91	1.93	11.90
MODEL.PDB	O, C_VAL_705	N, C_TYR_707	H, C_TYR_707	2.85	1.99	25.15
MODEL.PDB	OD2, A_ASP_796	ND2, C_ASN_709	HD21, C_ASN_709	2.70	1.85	25.89
MODEL.PDB	OD1, C_ASN_717	N, C_PHE_718	H, C_PHE_718	2.83	1.93	22.04
MODEL.PDB	OE1, C_GLN_926	N, C_ILE_720	H, C_ILE_720	2.82	1.82	5.94
MODEL.PDB	OD2, C_ASP_775	NZ, C_LYS_733	HZ3, C_LYS_733	2.58	1.60	11.03
MODEL.PDB	O, C_THR_732	N, C_THR_734	H, C_THR_734	2.83	1.99	27.90
MODEL.PDB	O, C_THR_859	N, C_SER_735	H, C_SER_735	3.00	2.04	15.40
MODEL.PDB	O, C_GLY_857	N, C_ASP_737	H, C_ASP_737	2.74	1.76	10.16
MODEL.PDB	O, C_ASP_737	N, C_TYR_741	H, C_TYR_741	2.84	1.88	14.81
MODEL.PDB	O, C_CYS_738	N, C_ILE_742	H, C_ILE_742	3.00	2.01	9.31
MODEL.PDB	O, C_THR_739	N, C_CYS_743	H, C_CYS_743	2.88	1.97	20.77
MODEL.PDB	OE2, C_GLU_748	OG1, C_THR_747	HG1, C_THR_747	2.89	2.01	18.92
MODEL.PDB	O, C_THR_747	N, C_ASN_751	H, C_ASN_751	2.94	1.97	14.54
MODEL.PDB	O, C_CYS_749	N, C_LEU_753	H, C_LEU_753	2.92	1.96	15.41
MODEL.PDB	O, C_SER_758	N, C_GLN_762	H, C_GLN_762	2.95	1.99	14.82
MODEL.PDB	O, C_PHE_759	N, C_LEU_763	H, C_LEU_763	2.94	1.94	6.26
MODEL.PDB	O, C_THR_761	N, C_ARG_765	H, C_ARG_765	2.87	1.91	13.67
MODEL.PDB	O, C_ASN_764	N, C_THR_768	H, C_THR_768	2.93	1.94	11.17
MODEL.PDB	O, C_ASN_764	OG1, C_THR_768	HG1, C_THR_768	2.97	2.07	16.22
MODEL.PDB	O, C_ARG_765	N, C_GLY_769	H, C_GLY_769	2.89	1.90	8.91
MODEL.PDB	O, C_LEU_767	N, C_ALA_771	H, C_ALA_771	2.92	1.96	15.95
MODEL.PDB	O, C_GLU_773	N, C_ASN_777	H, C_ASN_777	2.85	1.90	15.65
MODEL.PDB	O, C_LYS_776	N, C_GLU_780	H, C_GLU_780	2.74	1.75	8.57
MODEL.PDB	O, C_GLN_779	N, C_ALA_783	H, C_ALA_783	2.87	1.93	18.26
MODEL.PDB	O, B_ALA_701	N, C_ILE_788	H, C_ILE_788	2.78	1.81	13.05
MODEL.PDB	O, B_ASN_703	N, C_LYS_790	H, C_LYS_790	2.96	1.97	9.28
MODEL.PDB	OG, B_SER_704	NZ, C_LYS_790	HZ1, C_LYS_790	2.84	1.83	1.48
MODEL.PDB	O, C_THR_791	NZ, C_LYS_790	HZ3, C_LYS_790	3.00	2.14	26.67
MODEL.PDB	O, C_ASP_796	N, C_GLY_798	H, C_GLY_798	2.69	1.76	18.92
MODEL.PDB	OD1, C_ASN_928	N, C_ASN_801	H, C_ASN_801	2.79	1.83	13.49

MODEL.PDB	OD1, C_ASN_801	N, C_SER_803	H, C_SER_803	2.98	2.00	12.86
MODEL.PDB	O, C_LYS_811	N, C_LYS_814	H, C_LYS_814	2.88	1.98	22.49
MODEL.PDB	OG, C_SER_816	N, C_GLU_819	H, C_GLU_819	2.87	1.89	10.14
MODEL.PDB	O, C_SER_816	N, C_ASP_820	H, C_ASP_820	2.98	1.97	2.32
MODEL.PDB	O, C_ILE_818	N, C_LEU_822	H, C_LEU_822	2.83	1.88	16.04
MODEL.PDB	O, C_THR_941	NZ, C_LYS_825	HZ1, C_LYS_825	2.75	1.90	26.39
MODEL.PDB	O, C_SER_939	NZ, C_LYS_825	HZ2, C_LYS_825	2.75	1.89	25.56
MODEL.PDB	OE1, C_GLN_949	N, C_THR_827	H, C_THR_827	2.83	1.89	17.39
MODEL.PDB	OD2, C_ASP_839	N, C_LEU_841	H, C_LEU_841	2.74	1.77	12.63
MODEL.PDB	O, C_GLY_842	N, C_ILE_844	H, C_ILE_844	2.97	2.11	25.44
MODEL.PDB	O, C_ARG_847	N, C_LEU_849	H, C_LEU_849	2.76	1.85	21.40
MODEL.PDB	O, C_ALA_829	NE2, C_GLN_853	HE21, C_GLN_853	2.91	2.02	23.17
MODEL.PDB	OD1, B_ASP_614	NZ, C_LYS_854	HZ2, C_LYS_854	2.69	1.71	10.87
MODEL.PDB	O, C_SER_735	N, C_THR_859	H, C_THR_859	2.93	2.02	20.98
MODEL.PDB	O, C_LYS_733	N, C_LEU_861	H, C_LEU_861	2.79	1.82	12.47
MODEL.PDB	OD1, C_ASP_775	N, C_LEU_864	H, C_LEU_864	2.76	1.77	10.42
MODEL.PDB	O, C_ASP_867	N, C_ALA_871	H, C_ALA_871	2.87	1.88	10.37
MODEL.PDB	O, C_MET_869	N, C_TYR_873	H, C_TYR_873	2.99	2.02	12.67
MODEL.PDB	O, C_ILE_870	N, C_THR_874	H, C_THR_874	2.98	2.00	12.06
MODEL.PDB	OE1, C_GLU_819	OG1, C_THR_874	HG1, C_THR_874	2.71	1.77	10.99
MODEL.PDB	O, C_ALA_871	N, C_SER_875	H, C_SER_875	3.00	2.01	8.94
MODEL.PDB	O, C_THR_874	N, C_LEU_878	H, C_LEU_878	2.92	1.97	16.46
MODEL.PDB	O, C_SER_875	N, C_ALA_879	H, C_ALA_879	2.82	1.83	9.71
MODEL.PDB	O, C_LEU_877	N, C_THR_881	H, C_THR_881	2.92	1.93	10.72
MODEL.PDB	O, C_ALA_879	N, C_THR_883	H, C_THR_883	2.97	2.03	17.08
MODEL.PDB	O, C_GLY_880	N, C_SER_884	H, C_SER_884	2.81	1.86	15.30
MODEL.PDB	O, C_THR_887	N, C_GLY_891	H, C_GLY_891	2.92	1.93	8.63
MODEL.PDB	O, C_THR_881	NE2, C_GLN_901	HE22, C_GLN_901	2.78	1.85	18.56
MODEL.PDB	O, C_PHE_898	N, C_MET_902	H, C_MET_902	2.93	1.96	13.47
MODEL.PDB	O, C_ALA_899	N, C_ALA_903	H, C_ALA_903	2.87	1.90	12.92
MODEL.PDB	O, C_GLY_885	NH2, C_ARG_905	HH21, C_ARG_905	2.82	1.97	26.49
MODEL.PDB	O, C_MET_902	N, C_PHE_906	H, C_PHE_906	2.85	1.86	8.76
MODEL.PDB	O, C_TYR_904	N, C_GLY_908	H, C_GLY_908	2.76	1.80	15.11
MODEL.PDB	O, C_ASN_907	N, C_GLY_910	H, C_GLY_910	2.99	2.15	27.40
MODEL.PDB	O, C_PHE_906	N, C_VAL_911	H, C_VAL_911	2.94	1.95	9.20
MODEL.PDB	O, C_ASN_914	N, C_GLU_918	H, C_GLU_918	2.97	1.96	1.50
MODEL.PDB	O, C_VAL_915	ND2, C_ASN_919	HD21, C_ASN_919	2.89	1.92	12.77
MODEL.PDB	O, C_GLY_798	NE2, C_GLN_920	HE21, C_GLN_920	2.95	2.00	16.18
MODEL.PDB	O, C_GLN_920	N, C_ALA_924	H, C_ALA_924	2.98	1.99	9.05
MODEL.PDB	O, C_LEU_922	N, C_GLN_926	H, C_GLN_926	2.91	1.93	10.60
MODEL.PDB	O, C_ILE_923	N, C_PHE_927	H, C_PHE_927	2.93	1.96	12.72
MODEL.PDB	O, C_ALA_924	N, C_ASN_928	H, C_ASN_928	2.92	1.93	9.88
MODEL.PDB	O, C_ASN_925	OG, C_SER_929	HG, C_SER_929	2.74	1.83	13.62
MODEL.PDB	O, C_GLN_926	N, C_ALA_930	H, C_ALA_930	2.91	1.97	16.97
MODEL.PDB	O, C_PHE_927	N, C_ILE_931	H, C_ILE_931	3.00	2.00	7.96
MODEL.PDB	O, C_LYS_933	N, C_SER_937	H, C_SER_937	2.87	1.89	11.80
MODEL.PDB	O, C_ILE_934	N, C_LEU_938	H, C_LEU_938	2.91	1.91	7.48
MODEL.PDB	O, C_GLN_935	N, C_SER_939	H, C_SER_939	2.83	1.89	17.96
MODEL.PDB	OD1, C_ASN_953	NE2, C_GLN_949	HE21, C_GLN_949	2.95	1.94	2.22
MODEL.PDB	O, C_GLY_946	N, C_ASP_950	H, C_ASP_950	2.84	1.85	9.19
MODEL.PDB	O, C_GLN_949	N, C_ASN_953	H, C_ASN_953	2.77	1.79	9.50
MODEL.PDB	O, C_ASP_950	N, C_GLN_954	H, C_GLN_954	2.84	1.86	10.76
MODEL.PDB	O, C_VAL_952	N, C_ALA_956	H, C_ALA_956	2.97	1.98	9.55
MODEL.PDB	O, C_ASN_953	N, C_GLN_957	H, C_GLN_957	2.82	1.85	12.26
MODEL.PDB	O, C_GLN_954	N, C_ALA_958	H, C_ALA_958	2.91	1.95	15.56
MODEL.PDB	O, C_ASN_955	N, C_LEU_959	H, C_LEU_959	2.99	1.99	6.77
MODEL.PDB	O, C_ALA_956	N, C_ASN_960	H, C_ASN_960	2.93	1.95	10.97
MODEL.PDB	O, C_GLN_957	N, C_THR_961	H, C_THR_961	2.89	1.95	17.35

MODEL.PDB	O, C_GLN_957	OG1, C_THR_961	HG1, C_THR_961	2.62	1.72	16.71
MODEL.PDB	O, C_ALA_958	N, C_LEU_962	H, C_LEU_962	2.96	1.99	14.16
MODEL.PDB	O, C_LEU_959	N, C_VAL_963	H, C_VAL_963	2.89	1.90	7.75
MODEL.PDB	O, C_ASN_960	N, C_LYS_964	H, C_LYS_964	2.92	1.96	15.00
MODEL.PDB	OG, C_SER_967	NZ, C_LYS_964	HZ2, C_LYS_964	2.75	1.91	27.16
MODEL.PDB	OG, A_SER_758	NE2, C_GLN_965	HE21, C_GLN_965	2.97	2.12	27.09
MODEL.PDB	O, A_GLN_755	N, C_PHE_970	H, C_PHE_970	2.83	1.85	12.65
MODEL.PDB	O, C_ASN_969	N, C_ALA_972	H, C_ALA_972	2.99	2.02	13.68
MODEL.PDB	OE1, C_GLN_992	N, C_ILE_973	H, C_ILE_973	2.85	1.91	16.70
MODEL.PDB	O, C_LEU_966	OG, C_SER_975	HG, C_SER_975	2.60	1.67	11.20
MODEL.PDB	O, B_THR_547	ND2, C_ASN_978	HD21, C_ASN_978	2.84	1.92	19.82
MODEL.PDB	O, C_ASN_978	N, C_SER_982	H, C_SER_982	2.79	1.87	19.11
MODEL.PDB	O, C_ASP_979	N, C_ARG_983	H, C_ARG_983	2.93	1.97	15.14
MODEL.PDB	OE1, C_GLU_748	NZ, C_LYS_986	HZ2, C_LYS_986	2.53	1.54	9.58
MODEL.PDB	OD2, C_ASP_985	N, C_VAL_987	H, C_VAL_987	2.92	1.98	17.86
MODEL.PDB	O, C_ASP_985	N, C_ALA_989	H, C_ALA_989	2.82	1.89	18.83
MODEL.PDB	O, C_ALA_989	N, C_ILE_993	H, C_ILE_993	2.87	1.88	9.75
MODEL.PDB	O, C_GLU_990	N, C_ASP_994	H, C_ASP_994	2.75	1.77	11.32
MODEL.PDB	OD1, A_ASP_994	NH1, C_ARG_995	HH12, C_ARG_995	2.65	1.64	2.91
MODEL.PDB	O, C_PHE_970	NH2, C_ARG_995	HH21, C_ARG_995	2.82	1.85	12.87
MODEL.PDB	OD2, A_ASP_994	NH2, C_ARG_995	HH22, C_ARG_995	2.64	1.67	12.83
MODEL.PDB	O, C_ILE_993	N, C_ILE_997	H, C_ILE_997	2.81	1.84	12.90
MODEL.PDB	O, C_ASP_994	N, C_THR_998	H, C_THR_998	2.94	1.94	4.03

Table 3: The side chain and main chain hydrogen bonding networks. In this table, the residue naming scheme is **Chain ID_residue name_residue number**, $\angle ADH$ represents the angle formed by acceptor (A), donor (D) and hydrogen (H) ($\angle ADH$).

PDB	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH$(°)
MODEL.PDB	OE2, A_GLU_191	NH1, A_ARG_34	HH11, A_ARG_34	2.67	1.78	22.19
MODEL.PDB	OD1, A_ASP_40	NH1, A_ARG_44	HH12, A_ARG_44	2.70	1.70	6.73
MODEL.PDB	OD2, A_ASP_40	NH2, A_ARG_44	HH22, A_ARG_44	2.63	1.66	12.76
MODEL.PDB	OD2, A_ASP_138	NH1, A_ARG_78	HH11, A_ARG_78	2.69	1.82	24.44
MODEL.PDB	OE1, A_GLU_191	OH, A_TYR_91	HH, A_TYR_91	2.70	1.78	13.73
MODEL.PDB	OH, A_TYR_37	NZ, A_LYS_195	HZ2, A_LYS_195	2.76	1.80	13.93
MODEL.PDB	OE2, C_GLU_516	OH, A_TYR_200	HH, A_TYR_200	2.56	1.75	25.87
MODEL.PDB	OE2, A_GLU_224	NZ, A_LYS_206	HZ3, A_LYS_206	2.70	1.79	20.97
MODEL.PDB	OD1, A_ASP_215	NE, A_ARG_214	HE, A_ARG_214	2.96	2.08	24.64
MODEL.PDB	OD1, A_ASP_215	NH1, A_ARG_214	HH11, A_ARG_214	2.72	1.80	19.02
MODEL.PDB	OE2, A_GLU_191	OG, A_SER_221	HG, A_SER_221	2.68	1.80	18.27
MODEL.PDB	OD1, A_ASP_290	NH2, A_ARG_273	HH21, A_ARG_273	2.62	1.69	18.86
MODEL.PDB	OD1, A_ASN_280	OG1, A_THR_286	HG1, A_THR_286	2.71	1.94	29.85
MODEL.PDB	OG, A_SER_50	NZ, A_LYS_304	HZ3, A_LYS_304	2.91	1.95	14.53
MODEL.PDB	OD1, A_ASP_663	NZ, A_LYS_310	HZ2, A_LYS_310	2.63	1.74	22.20
MODEL.PDB	OE2, A_GLU_298	OG, A_SER_316	HG, A_SER_316	2.68	1.73	6.59
MODEL.PDB	OD2, B_ASP_737	NH1, A_ARG_319	HH12, A_ARG_319	2.74	1.78	15.71
MODEL.PDB	OD1, A_ASP_398	NE, A_ARG_355	HE, A_ARG_355	2.67	1.68	10.27
MODEL.PDB	OD2, A_ASP_398	NH2, A_ARG_355	HH21, A_ARG_355	2.63	1.83	29.83
MODEL.PDB	OD1, A_ASN_394	OG, A_SER_359	HG, A_SER_359	2.65	1.78	19.43
MODEL.PDB	OG, A_SER_383	NZ, A_LYS_386	HZ1, A_LYS_386	2.87	2.00	24.63
MODEL.PDB	OE1, A_GLU_516	ND2, A_ASN_394	HD21, A_ASN_394	2.79	1.83	15.55
MODEL.PDB	OE1, A_GLN_506	ND2, A_ASN_437	HD22, A_ASN_437	2.76	1.75	1.26
MODEL.PDB	OE1, A_GLN_498	ND2, A_ASN_448	HD21, A_ASN_448	2.95	2.09	25.72
MODEL.PDB	OE1, A_GLU_471	NZ, A_LYS_458	HZ1, A_LYS_458	2.43	1.55	23.29
MODEL.PDB	OE2, A_GLU_465	ND2, A_ASN_460	HD21, A_ASN_460	2.81	1.80	4.71
MODEL.PDB	OD1, A_ASP_467	NE, A_ARG_466	HE, A_ARG_466	2.70	1.70	7.41
MODEL.PDB	OD2, A_ASP_467	NH1, A_ARG_466	HH11, A_ARG_466	2.66	1.80	25.17
MODEL.PDB	OD2, A_ASP_442	NE, A_ARG_509	HE, A_ARG_509	2.69	1.74	14.88
MODEL.PDB	OD1, A_ASP_442	NH1, A_ARG_509	HH11, A_ARG_509	2.80	1.80	3.45
MODEL.PDB	OD2, A_ASP_574	NZ, A_LYS_557	HZ1, A_LYS_557	2.65	1.80	26.29
MODEL.PDB	OD1, A_ASP_568	NZ, A_LYS_557	HZ2, A_LYS_557	2.72	1.90	29.52
MODEL.PDB	OE1, A_GLN_564	NH2, A_ARG_577	HH22, A_ARG_577	2.71	1.88	28.37
MODEL.PDB	OH, A_TYR_636	NE2, A_GLN_607	HE22, A_GLN_607	2.96	2.00	15.28
MODEL.PDB	OD2, A_ASP_627	NE2, A_GLN_628	HE21, A_GLN_628	2.77	1.86	20.74
MODEL.PDB	OG1, A_THR_632	OG1, A_THR_630	HG1, A_THR_630	2.93	2.01	13.87
MODEL.PDB	OD1, A_ASN_658	OH, A_TYR_660	HH, A_TYR_660	2.82	1.96	21.62
MODEL.PDB	OD2, A_ASP_663	OG, A_SER_673	HG, A_SER_673	2.68	1.81	20.07
MODEL.PDB	OD1, A_ASN_710	OG, A_SER_708	HG, A_SER_708	2.64	1.84	27.39
MODEL.PDB	OD2, A_ASP_775	NZ, A_LYS_733	HZ3, A_LYS_733	2.60	1.62	11.48
MODEL.PDB	OG1, C_THR_961	NH2, A_ARG_765	HH22, A_ARG_765	2.95	1.98	13.10
MODEL.PDB	OD2, A_ASP_808	OG, A_SER_810	HG, A_SER_810	2.73	1.94	28.41
MODEL.PDB	OD1, A_ASP_820	NH1, A_ARG_815	HH11, A_ARG_815	2.65	1.73	19.61
MODEL.PDB	OG1, A_THR_734	NZ, A_LYS_854	HZ3, A_LYS_854	2.90	2.01	23.94
MODEL.PDB	OD2, C_ASP_614	OG1, A_THR_859	HG1, A_THR_859	2.83	1.95	19.70
MODEL.PDB	OE2, A_GLU_819	OG1, A_THR_874	HG1, A_THR_874	2.63	1.71	12.98
MODEL.PDB	OD1, A_ASP_936	NE2, A_GLN_935	HE21, A_GLN_935	2.78	1.84	17.00
MODEL.PDB	OD1, A_ASN_953	NE2, A_GLN_949	HE21, A_GLN_949	2.96	1.95	3.82
MODEL.PDB	OE1, A_GLN_965	OG, A_SER_968	HG, A_SER_968	2.75	1.97	29.51
MODEL.PDB	OD2, B_ASP_994	NH1, A_ARG_995	HH12, A_ARG_995	2.69	1.68	3.63
MODEL.PDB	OD1, B_ASP_994	NH2, A_ARG_995	HH22, A_ARG_995	2.66	1.65	4.49
MODEL.PDB	OE2, B_GLU_191	NH1, B_ARG_34	HH11, B_ARG_34	2.59	1.61	10.99
MODEL.PDB	OG1, B_THR_114	OG1, B_THR_109	HG1, B_THR_109	2.95	2.04	16.45
MODEL.PDB	OG1, B_THR_167	NE2, B_GLN_115	HE22, B_GLN_115	2.93	1.99	17.65
MODEL.PDB	OD1, B_ASN_211	ND2, B_ASN_185	HD22, B_ASN_185	2.96	1.98	11.82
MODEL.PDB	OD1, B_ASP_53	NZ, B_LYS_195	HZ1, B_LYS_195	2.67	1.77	21.61
MODEL.PDB	OH, B_TYR_37	NZ, B_LYS_195	HZ2, B_LYS_195	2.81	1.83	10.84

MODEL.PDB	OE2, B_GLU_224	NZ, B_LYS_206	HZ1, B_LYS_206	2.61	1.63	10.77
MODEL.PDB	OE1, B_GLU_154	OG, B_SER_247	HG, B_SER_247	2.58	1.63	5.81
MODEL.PDB	OD2, B_ASP_290	NE, B_ARG_273	HE, B_ARG_273	2.67	1.80	24.19
MODEL.PDB	OD1, B_ASP_290	NH2, B_ARG_273	HH21, B_ARG_273	2.63	1.66	12.98
MODEL.PDB	OD2, B_ASP_287	NZ, B_LYS_278	HZ1, B_LYS_278	2.60	1.60	3.72
MODEL.PDB	OG, B_SER_50	NZ, B_LYS_304	HZ1, B_LYS_304	2.84	1.83	5.53
MODEL.PDB	OD2, B_ASP_663	NZ, B_LYS_310	HZ3, B_LYS_310	2.62	1.67	16.87
MODEL.PDB	OE1, B_GLN_580	NE, B_ARG_328	HE, B_ARG_328	2.68	1.70	11.58
MODEL.PDB	OD2, B_ASP_398	NH2, B_ARG_355	HH21, B_ARG_355	2.60	1.63	13.35
MODEL.PDB	OG1, B_THR_523	OG, B_SER_359	HG, B_SER_359	2.73	1.79	9.26
MODEL.PDB	OD1, B_ASP_364	OG, B_SER_366	HG, B_SER_366	2.74	1.87	20.38
MODEL.PDB	OG, B_SER_373	OG, B_SER_371	HG, B_SER_371	2.84	1.90	10.21
MODEL.PDB	OG1, B_THR_376	NZ, B_LYS_378	HZ3, B_LYS_378	2.86	1.89	13.06
MODEL.PDB	OE2, B_GLU_516	OG1, B_THR_393	HG1, B_THR_393	2.60	1.68	12.70
MODEL.PDB	OD2, B_ASP_398	OH, B_TYR_423	HH, B_TYR_423	2.64	1.73	15.03
MODEL.PDB	OD1, B_ASN_460	NZ, B_LYS_424	HZ2, B_LYS_424	2.64	1.68	12.99
MODEL.PDB	OE1, B_GLN_506	ND2, B_ASN_437	HD22, B_ASN_437	2.76	1.76	7.71
MODEL.PDB	OD2, B_ASP_442	OG, B_SER_438	HG, B_SER_438	2.68	1.74	9.15
MODEL.PDB	OD1, B_ASN_440	NZ, B_LYS_444	HZ1, B_LYS_444	2.69	1.88	29.21
MODEL.PDB	OD2, B_ASP_442	OH, B_TYR_451	HH, B_TYR_451	2.68	1.72	0.75
MODEL.PDB	OD1, B_ASP_420	ND2, B_ASN_460	HD21, B_ASN_460	2.68	1.79	21.99
MODEL.PDB	OD1, B_ASN_487	OH, B_TYR_489	HH, B_TYR_489	2.67	1.80	20.09
MODEL.PDB	OD1, B_ASP_442	NH1, B_ARG_509	HH11, B_ARG_509	2.67	1.81	24.93
MODEL.PDB	OD2, B_ASP_389	NZ, B_LYS_528	HZ3, B_LYS_528	2.66	1.77	22.25
MODEL.PDB	OE2, B_GLU_554	NZ, B_LYS_535	HZ3, B_LYS_535	2.58	1.58	6.75
MODEL.PDB	OD2, B_ASP_586	NZ, B_LYS_557	HZ3, B_LYS_557	2.63	1.78	26.14
MODEL.PDB	OE1, B_GLU_619	OG, B_SER_591	HG, B_SER_591	2.62	1.73	18.48
MODEL.PDB	OG1, B_THR_632	NE, B_ARG_634	HE, B_ARG_634	2.87	1.95	20.06
MODEL.PDB	OD2, B_ASP_614	NH1, B_ARG_646	HH12, B_ARG_646	2.84	1.93	20.79
MODEL.PDB	OD1, B_ASN_710	OG, B_SER_708	HG, B_SER_708	2.65	1.81	23.38
MODEL.PDB	OD2, C_ASP_796	ND2, B_ASN_709	HD21, B_ASN_709	2.69	1.82	25.22
MODEL.PDB	OG1, B_THR_734	OG1, B_THR_732	HG1, B_THR_732	2.80	2.02	29.06
MODEL.PDB	OD2, B_ASP_775	NZ, B_LYS_733	HZ1, B_LYS_733	2.58	1.59	8.03
MODEL.PDB	OE1, A_GLU_702	NZ, B_LYS_790	HZ2, B_LYS_790	2.57	1.72	25.91
MODEL.PDB	OD1, B_ASN_801	NE2, B_GLN_804	HE21, B_GLN_804	2.93	1.97	14.52
MODEL.PDB	OD1, B_ASP_820	NE, B_ARG_815	HE, B_ARG_815	2.83	1.98	26.93
MODEL.PDB	OD1, B_ASP_820	NH1, B_ARG_815	HH11, B_ARG_815	2.70	1.79	20.55
MODEL.PDB	OD1, B_ASP_867	NH2, B_ARG_815	HH21, B_ARG_815	2.92	2.02	21.93
MODEL.PDB	OD2, A_ASP_614	OG1, B_THR_859	HG1, B_THR_859	2.98	2.16	26.02
MODEL.PDB	OE2, B_GLU_819	OG1, B_THR_874	HG1, B_THR_874	2.73	1.83	16.33
MODEL.PDB	OD1, B_ASN_953	NE2, B_GLN_949	HE21, B_GLN_949	2.81	1.84	12.61
MODEL.PDB	OD2, B_ASP_979	NE, B_ARG_983	HE, B_ARG_983	2.71	1.71	5.22
MODEL.PDB	OD1, B_ASP_979	NH2, B_ARG_983	HH21, B_ARG_983	2.61	1.64	12.14
MODEL.PDB	OE2, B_GLU_988	NE2, B_GLN_992	HE21, B_GLN_992	2.70	1.70	2.13
MODEL.PDB	OD1, C_ASP_994	NH1, B_ARG_995	HH12, B_ARG_995	2.64	1.64	8.73
MODEL.PDB	OD2, C_ASP_53	OG1, C_THR_51	HG1, C_THR_51	2.80	2.01	28.71
MODEL.PDB	OD1, C_ASP_253	NZ, C_LYS_97	HZ2, C_LYS_97	2.69	1.77	19.23
MODEL.PDB	OE2, B_GLU_471	NZ, C_LYS_113	HZ1, C_LYS_113	2.68	1.73	15.31
MODEL.PDB	OD1, C_ASN_125	ND2, C_ASN_122	HD21, C_ASN_122	2.84	1.89	16.55
MODEL.PDB	OE2, C_GLU_169	NZ, C_LYS_129	HZ3, C_LYS_129	2.46	1.53	17.71
MODEL.PDB	OE1, C_GLU_154	NZ, C_LYS_150	HZ3, C_LYS_150	2.61	1.79	28.77
MODEL.PDB	OH, C_TYR_204	NZ, C_LYS_195	HZ2, C_LYS_195	2.89	1.88	6.24
MODEL.PDB	OD2, C_ASP_228	NZ, C_LYS_202	HZ2, C_LYS_202	2.76	1.94	28.81
MODEL.PDB	OE2, C_GLU_191	OG1, C_THR_208	HG1, C_THR_208	2.86	1.90	5.11
MODEL.PDB	OE1, C_GLU_156	NH1, C_ARG_246	HH12, C_ARG_246	2.76	1.76	7.38
MODEL.PDB	OE2, C_GLU_156	NH2, C_ARG_246	HH22, C_ARG_246	2.61	1.71	21.34
MODEL.PDB	OD2, C_ASP_290	NH2, C_ARG_273	HH22, C_ARG_273	2.55	1.66	21.76
MODEL.PDB	OE2, C_GLU_298	OG1, C_THR_315	HG1, C_THR_315	2.64	1.70	8.17

MODEL.PDB	OE1, C_GLN_580	NE, C_ARG_328	HE, C_ARG_328	2.78	1.86	19.60
MODEL.PDB	OD2, C_ASP_578	NH1, C_ARG_328	HH12, C_ARG_328	2.60	1.78	28.67
MODEL.PDB	OE1, C_GLN_580	NH2, C_ARG_328	HH21, C_ARG_328	2.90	2.05	27.29
MODEL.PDB	OD2, C_ASP_467	OH, C_TYR_351	HH, C_TYR_351	2.53	1.60	11.08
MODEL.PDB	OD1, C_ASP_398	NE, C_ARG_355	HE, C_ARG_355	2.62	1.64	10.97
MODEL.PDB	OD2, C_ASP_398	NH2, C_ARG_355	HH21, C_ARG_355	2.58	1.57	3.27
MODEL.PDB	OD1, C_ASN_394	OG, C_SER_359	HG, C_SER_359	2.97	2.15	25.84
MODEL.PDB	OD1, C_ASP_364	OG, C_SER_366	HG, C_SER_366	2.68	1.81	20.57
MODEL.PDB	OH, C_TYR_380	NZ, C_LYS_378	HZ3, C_LYS_378	2.93	1.99	17.96
MODEL.PDB	OD1, C_ASN_460	NZ, C_LYS_424	HZ2, C_LYS_424	2.69	1.71	11.25
MODEL.PDB	OD2, C_ASP_442	OG, C_SER_438	HG, C_SER_438	2.57	1.73	23.01
MODEL.PDB	OD1, C_ASP_420	ND2, C_ASN_460	HD22, C_ASN_460	2.79	1.85	17.42
MODEL.PDB	OD1, C_ASP_467	OG, C_SER_469	HG, C_SER_469	2.78	1.89	17.62
MODEL.PDB	OE1, C_GLN_474	OH, C_TYR_489	HH, C_TYR_489	2.76	1.82	9.42
MODEL.PDB	OD1, C_ASP_442	NH1, C_ARG_509	HH11, C_ARG_509	2.58	1.62	14.24
MODEL.PDB	OE1, C_GLU_554	NZ, C_LYS_535	HZ3, C_LYS_535	2.65	1.79	24.99
MODEL.PDB	OE2, C_GLU_554	NZ, C_LYS_535	HZ3, C_LYS_535	2.72	1.89	27.95
MODEL.PDB	OE2, C_GLU_324	NZ, C_LYS_537	HZ3, C_LYS_537	2.54	1.67	24.70
MODEL.PDB	OD2, A_ASP_745	OG1, C_THR_549	HG1, C_THR_549	2.94	2.12	25.69
MODEL.PDB	OD1, C_ASP_586	OG, C_SER_555	HG, C_SER_555	2.61	1.67	9.67
MODEL.PDB	OD2, C_ASP_574	NZ, C_LYS_557	HZ3, C_LYS_557	2.58	1.76	27.92
MODEL.PDB	OD2, C_ASP_294	OG, C_SER_637	HG, C_SER_637	2.56	1.75	25.96
MODEL.PDB	OD2, A_ASP_848	NH2, C_ARG_646	HH22, C_ARG_646	2.63	1.79	27.55
MODEL.PDB	OD2, C_ASP_663	OG, C_SER_673	HG, C_SER_673	2.61	1.66	4.96
MODEL.PDB	OG, C_SER_689	OG1, C_THR_676	HG1, C_THR_676	2.79	1.86	11.33
MODEL.PDB	OE1, C_GLN_677	ND2, C_ASN_679	HD21, C_ASN_679	2.90	1.93	13.29
MODEL.PDB	OD2, A_ASP_796	ND2, C_ASN_709	HD21, C_ASN_709	2.70	1.85	25.89
MODEL.PDB	OD2, C_ASP_775	NZ, C_LYS_733	HZ3, C_LYS_733	2.58	1.60	11.03
MODEL.PDB	OE2, C_GLU_748	OG1, C_THR_747	HG1, C_THR_747	2.89	2.01	18.92
MODEL.PDB	OG, B_SER_704	NZ, C_LYS_790	HZ1, C_LYS_790	2.84	1.83	1.48
MODEL.PDB	OD1, B_ASP_614	NZ, C_LYS_854	HZ2, C_LYS_854	2.69	1.71	10.87
MODEL.PDB	OE1, C_GLU_819	OG1, C_THR_874	HG1, C_THR_874	2.71	1.77	10.99
MODEL.PDB	OD1, C_ASN_953	NE2, C_GLN_949	HE21, C_GLN_949	2.95	1.94	2.22
MODEL.PDB	OG, C_SER_967	NZ, C_LYS_964	HZ2, C_LYS_964	2.75	1.91	27.16
MODEL.PDB	OG, A_SER_758	NE2, C_GLN_965	HE21, C_GLN_965	2.97	2.12	27.09
MODEL.PDB	OE1, C_GLU_748	NZ, C_LYS_986	HZ2, C_LYS_986	2.53	1.54	9.58
MODEL.PDB	OD1, A_ASP_994	NH1, C_ARG_995	HH12, C_ARG_995	2.65	1.64	2.91
MODEL.PDB	OD2, A_ASP_994	NH2, C_ARG_995	HH22, C_ARG_995	2.64	1.67	12.83

Table 4: Side chain hydrogen bonding network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**, $\angle ADH$ represents the angle formed by acceptor (A), donor (D) and hydrogen (H) ($\angle ADH$).

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
MODEL	A_ARG_319	NH1	B_ASP_737	OD2	2.735
MODEL	A_ARG_319	NH1	B_ASP_745	OD1	3.587
MODEL	A_ARG_319	NH2	B_ASP_737	OD2	3.982
MODEL	A_LYS_790	NZ	C_GLU_702	OE1	2.623
MODEL	A_LYS_790	NZ	C_GLU_702	OE2	2.744
MODEL	A_ARG_995	NH1	B_ASP_994	OD1	3.497
MODEL	A_ARG_995	NH1	B_ASP_994	OD2	2.691
MODEL	A_ARG_995	NH2	B_ASP_994	OD1	2.657
MODEL	A_ARG_995	NH2	B_ASP_994	OD2	3.473
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE1	3.621
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE2	2.620
MODEL	B_ARG_319	NH1	C_ASP_745	OD1	2.606
MODEL	B_ARG_319	NH1	C_ASP_745	OD2	3.565
MODEL	B_ARG_319	NH2	C_ASP_745	OD1	3.325
MODEL	B_ARG_319	NH2	C_ASP_745	OD2	2.636
MODEL	B_LYS_790	NZ	A_GLU_702	OE1	2.570
MODEL	B_LYS_790	NZ	A_GLU_702	OE2	3.570
MODEL	B_LYS_854	NZ	A_ASP_614	OD1	3.487
MODEL	B_LYS_986	NZ	C_ASP_427	OD2	3.985
MODEL	B_ARG_995	NH1	C_ASP_994	OD1	2.636
MODEL	B_ARG_995	NH1	C_ASP_994	OD2	3.371
MODEL	B_ARG_995	NH2	C_ASP_994	OD1	3.182
MODEL	B_ARG_995	NH2	C_ASP_994	OD2	2.637
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE1	2.711
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE2	3.989
MODEL	C_LYS_113	NZ	B_GLU_471	OE2	2.679
MODEL	C_ARG_319	NH1	A_ASP_745	OD1	3.819
MODEL	C_LYS_458	NZ	A_ASP_389	OD2	3.696
MODEL	C_ARG_646	NH1	A_ASP_848	OD2	3.643
MODEL	C_ARG_646	NH2	A_ASP_848	OD1	3.695
MODEL	C_ARG_646	NH2	A_ASP_848	OD2	2.627
MODEL	C_ARG_847	NH1	B_GLU_619	OE1	3.034
MODEL	C_LYS_854	NZ	B_ASP_614	OD1	2.686
MODEL	C_ARG_995	NH1	A_ASP_994	OD1	2.647
MODEL	C_ARG_995	NH1	A_ASP_994	OD2	3.498
MODEL	C_ARG_995	NH2	A_ASP_994	OD1	3.382
MODEL	C_ARG_995	NH2	A_ASP_994	OD2	2.636
MODEL	C_ARG_1019	NH1	B_GLU_1017	OE2	2.726
MODEL	C_ARG_1019	NH2	B_GLU_1017	OE2	3.415
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE1	3.509
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE2	2.596

Table 5: Interfacial salt bridging network analysis within the PDB entries. In this table, the residue naming scheme is **Chain ID_residue name_residue number**.

Count	Residue A	Residue B
12	ARG995	ASP994
6	ARG319	ASP745
6	ARG1039	GLU1031
4	LYS790	GLU702
3	ARG646	ASP848
2	ARG319	ASP737
2	LYS854	ASP614
2	ARG1019	GLU1017
1	LYS986	ASP427
1	ARG847	GLU619
1	LYS113	GLU471
1	LYS458	ASP389

Table 6: Counting of interfacial salt bridges within the PDB entries in Table 5.

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
MODEL	A_ARG_34	NH1	A_GLU_191	OE2	2.674
MODEL	A_ARG_44	NH1	A_ASP_40	OD1	2.695
MODEL	A_ARG_44	NH1	A_ASP_40	OD2	3.232
MODEL	A_ARG_44	NH2	A_ASP_40	OD1	3.625
MODEL	A_ARG_44	NH2	A_ASP_40	OD2	2.635
MODEL	A_ARG_78	NH1	A_ASP_138	OD2	2.688
MODEL	A_ARG_102	NH1	A_GLU_96	OE1	3.329
MODEL	A_LYS_195	NZ	A_ASP_53	OD1	2.683
MODEL	A_LYS_195	NZ	A_ASP_53	OD2	2.722
MODEL	A_LYS_206	NZ	A_GLU_224	OE1	2.749
MODEL	A_LYS_206	NZ	A_GLU_224	OE2	2.697
MODEL	A_ARG_214	NH1	A_ASP_215	OD1	2.721
MODEL	A_ARG_214	NH1	A_ASP_215	OD2	3.669
MODEL	A_ARG_273	NH2	A_ASP_290	OD1	2.616
MODEL	A_ARG_273	NH2	A_ASP_290	OD2	3.058
MODEL	A_LYS_278	NZ	A_ASP_287	OD2	3.755
MODEL	A_LYS_310	NZ	A_ASP_663	OD1	2.628
MODEL	A_LYS_310	NZ	A_ASP_663	OD2	2.667
MODEL	A_ARG_319	NH1	B_ASP_737	OD2	2.735
MODEL	A_ARG_319	NH1	B_ASP_745	OD1	3.587
MODEL	A_ARG_319	NH2	B_ASP_737	OD2	3.982
MODEL	A_ARG_328	NH1	A_ASP_578	OD2	3.263
MODEL	A_ARG_328	NH2	A_ASP_578	OD2	3.964
MODEL	A_ARG_355	NH2	A_ASP_398	OD1	3.101
MODEL	A_ARG_355	NH2	A_ASP_398	OD2	2.632
MODEL	A_LYS_356	NZ	A_GLU_340	OE1	2.636
MODEL	A_ARG_403	NH1	A_GLU_406	OE2	3.089
MODEL	A_LYS_458	NZ	A_GLU_471	OE1	2.430
MODEL	A_ARG_466	NH1	A_ASP_467	OD1	3.188
MODEL	A_ARG_466	NH1	A_ASP_467	OD2	2.659
MODEL	A_ARG_509	NH1	A_ASP_442	OD1	2.803
MODEL	A_ARG_509	NH1	A_ASP_442	OD2	3.407
MODEL	A_LYS_537	NZ	A_GLU_324	OE1	2.730
MODEL	A_LYS_537	NZ	A_GLU_324	OE2	2.652
MODEL	A_LYS_557	NZ	A_ASP_568	OD1	2.715
MODEL	A_LYS_557	NZ	A_ASP_568	OD2	2.782
MODEL	A_LYS_557	NZ	A_ASP_574	OD1	2.869
MODEL	A_LYS_557	NZ	A_ASP_574	OD2	2.649
MODEL	A_ARG_567	NH1	A_ASP_571	OD1	2.606
MODEL	A_ARG_567	NH2	A_ASP_571	OD1	2.720
MODEL	A_LYS_733	NZ	A_ASP_775	OD1	3.202
MODEL	A_LYS_733	NZ	A_ASP_775	OD2	2.601
MODEL	A_LYS_790	NZ	C_GLU_702	OE1	2.623
MODEL	A_LYS_790	NZ	C_GLU_702	OE2	2.744
MODEL	A_LYS_811	NZ	A_ASP_820	OD2	2.461
MODEL	A_ARG_815	NH1	A_ASP_820	OD1	2.649
MODEL	A_LYS_986	NZ	A_GLU_748	OE2	2.597
MODEL	A_ARG_995	NH1	B_ASP_994	OD1	3.497
MODEL	A_ARG_995	NH1	B_ASP_994	OD2	2.691
MODEL	A_ARG_995	NH2	B_ASP_994	OD1	2.657
MODEL	A_ARG_995	NH2	B_ASP_994	OD2	3.473
MODEL	A_ARG_1019	NH1	A_GLU_773	OE1	2.777
MODEL	A_ARG_1019	NH2	A_GLU_780	OE1	3.073
MODEL	A_ARG_1019	NH2	A_GLU_780	OE2	3.823
MODEL	A_LYS_1028	NZ	A_GLU_725	OE1	2.878
MODEL	A_LYS_1028	NZ	A_GLU_725	OE2	2.589
MODEL	A_ARG_1039	NH1	A_GLU_1031	OE1	2.697

MODEL	A_ARG_1039	NH1	A_GLU_1031	OE2	3.642
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE1	3.621
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE2	2.620
MODEL	A_HIS_1064	NE2	A_GLU_725	OE1	2.720
MODEL	A_HIS_1083	ND1	A_ASP_1084	OD1	3.726
MODEL	A_HIS_1083	NE2	A_ASP_1084	OD1	2.954
MODEL	A_HIS_1083	NE2	A_ASP_1084	OD2	3.064
MODEL	A_LYS_1086	NZ	A_ASP_1084	OD2	2.860
MODEL	B_ARG_34	NH1	B_GLU_191	OE2	2.594
MODEL	B_ARG_78	NH2	B_ASP_80	OD1	3.853
MODEL	B_ARG_78	NH2	B_ASP_80	OD2	3.115
MODEL	B_LYS_195	NZ	B_ASP_53	OD1	2.671
MODEL	B_LYS_195	NZ	B_ASP_53	OD2	2.656
MODEL	B_LYS_206	NZ	B_GLU_224	OE1	3.459
MODEL	B_LYS_206	NZ	B_GLU_224	OE2	2.611
MODEL	B_ARG_273	NH2	B_ASP_290	OD1	2.633
MODEL	B_ARG_273	NH2	B_ASP_290	OD2	3.259
MODEL	B_LYS_278	NZ	B_ASP_287	OD2	2.604
MODEL	B_LYS_310	NZ	B_ASP_663	OD1	2.691
MODEL	B_LYS_310	NZ	B_ASP_663	OD2	2.615
MODEL	B_ARG_319	NH1	C_ASP_745	OD1	2.606
MODEL	B_ARG_319	NH1	C_ASP_745	OD2	3.565
MODEL	B_ARG_319	NH2	C_ASP_745	OD1	3.325
MODEL	B_ARG_319	NH2	C_ASP_745	OD2	2.636
MODEL	B_ARG_328	NH1	B_ASP_578	OD2	3.286
MODEL	B_ARG_328	NH2	B_ASP_578	OD1	3.906
MODEL	B_ARG_328	NH2	B_ASP_578	OD2	2.659
MODEL	B_ARG_355	NH2	B_ASP_398	OD2	2.596
MODEL	B_ARG_403	NH1	B_GLU_406	OE2	2.630
MODEL	B_ARG_403	NH2	B_GLU_406	OE2	3.754
MODEL	B_ARG_408	NH1	B_ASP_405	OD1	2.895
MODEL	B_ARG_408	NH1	B_ASP_405	OD2	2.755
MODEL	B_ARG_408	NH2	B_ASP_405	OD2	3.887
MODEL	B_ARG_454	NH1	B_ASP_467	OD2	2.590
MODEL	B_LYS_462	NZ	B_GLU_465	OE2	3.504
MODEL	B_ARG_509	NH1	B_ASP_442	OD1	2.673
MODEL	B_ARG_509	NH1	B_ASP_442	OD2	3.881
MODEL	B_LYS_528	NZ	B_ASP_389	OD2	2.658
MODEL	B_LYS_535	NZ	B_GLU_554	OE2	2.577
MODEL	B_LYS_537	NZ	B_GLU_324	OE1	2.634
MODEL	B_LYS_537	NZ	B_GLU_324	OE2	2.706
MODEL	B_LYS_557	NZ	B_ASP_586	OD1	2.689
MODEL	B_LYS_557	NZ	B_ASP_586	OD2	2.627
MODEL	B_ARG_567	NH1	B_ASP_571	OD1	2.826
MODEL	B_ARG_567	NH1	B_ASP_571	OD2	2.786
MODEL	B_ARG_567	NH2	B_ASP_571	OD1	3.551
MODEL	B_HIS_625	ND1	B_ASP_627	OD2	3.516
MODEL	B_HIS_625	NE2	B_ASP_627	OD2	3.967
MODEL	B_ARG_646	NH1	B_ASP_614	OD2	2.839
MODEL	B_LYS_733	NZ	B_ASP_775	OD1	3.016
MODEL	B_LYS_733	NZ	B_ASP_775	OD2	2.582
MODEL	B_LYS_776	NZ	B_GLU_780	OE1	2.710
MODEL	B_LYS_776	NZ	B_GLU_780	OE2	2.672
MODEL	B_LYS_790	NZ	A_GLU_702	OE1	2.570
MODEL	B_LYS_790	NZ	A_GLU_702	OE2	3.570
MODEL	B_ARG_815	NH1	B_ASP_820	OD1	2.696
MODEL	B_ARG_815	NH2	B_ASP_867	OD1	2.920
MODEL	B_ARG_815	NH2	B_GLU_868	OE2	3.311

MODEL	B_LYS_854	NZ	A_ASP_614	OD1	3.487
MODEL	B_ARG_983	NH2	B_ASP_979	OD1	2.614
MODEL	B_ARG_983	NH2	B_ASP_979	OD2	3.538
MODEL	B_LYS_986	NZ	C_ASP_427	OD2	3.985
MODEL	B_ARG_995	NH1	C_ASP_994	OD1	2.636
MODEL	B_ARG_995	NH1	C_ASP_994	OD2	3.371
MODEL	B_ARG_995	NH2	C_ASP_994	OD1	3.182
MODEL	B_ARG_995	NH2	C_ASP_994	OD2	2.637
MODEL	B_ARG_1019	NH1	B_GLU_773	OE1	3.284
MODEL	B_ARG_1019	NH1	B_GLU_773	OE2	2.600
MODEL	B_LYS_1028	NZ	B_GLU_725	OE1	2.732
MODEL	B_LYS_1028	NZ	B_GLU_725	OE2	2.670
MODEL	B_ARG_1039	NH1	B_GLU_1031	OE1	2.669
MODEL	B_ARG_1039	NH1	B_GLU_1031	OE2	3.057
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE1	2.711
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE2	3.989
MODEL	B_LYS_1045	NZ	B_ASP_1041	OD1	2.637
MODEL	B_HIS_1064	NE2	B_GLU_725	OE2	2.768
MODEL	B_LYS_1086	NZ	B_ASP_1084	OD2	2.620
MODEL	C_LYS_97	NZ	C_GLU_96	OE2	2.761
MODEL	C_LYS_97	NZ	C_ASP_253	OD1	2.693
MODEL	C_LYS_97	NZ	C_ASP_253	OD2	2.866
MODEL	C_LYS_113	NZ	B_GLU_471	OE2	2.679
MODEL	C_LYS_129	NZ	C_GLU_169	OE1	2.582
MODEL	C_LYS_129	NZ	C_GLU_169	OE2	2.463
MODEL	C_LYS_150	NZ	C_GLU_154	OE1	2.608
MODEL	C_LYS_150	NZ	C_GLU_154	OE2	2.752
MODEL	C_ARG_158	NH2	C_GLU_154	OE2	3.189
MODEL	C_LYS_187	NZ	C_GLU_180	OE2	2.873
MODEL	C_LYS_202	NZ	C_ASP_228	OD2	2.762
MODEL	C_ARG_246	NH1	C_GLU_156	OE1	2.756
MODEL	C_ARG_246	NH1	C_GLU_156	OE2	3.170
MODEL	C_ARG_246	NH2	C_GLU_156	OE1	3.528
MODEL	C_ARG_246	NH2	C_GLU_156	OE2	2.612
MODEL	C_ARG_273	NH1	C_ASP_290	OD1	2.966
MODEL	C_ARG_273	NH1	C_ASP_290	OD2	3.840
MODEL	C_ARG_273	NH2	C_ASP_290	OD1	2.966
MODEL	C_ARG_273	NH2	C_ASP_290	OD2	2.552
MODEL	C_LYS_310	NZ	C_ASP_663	OD1	3.129
MODEL	C_ARG_319	NH1	A_ASP_745	OD1	3.819
MODEL	C_ARG_328	NH1	C_ASP_578	OD2	2.598
MODEL	C_ARG_328	NH2	C_ASP_578	OD1	3.708
MODEL	C_ARG_328	NH2	C_ASP_578	OD2	2.801
MODEL	C_ARG_355	NH2	C_ASP_398	OD1	3.407
MODEL	C_ARG_355	NH2	C_ASP_398	OD2	2.579
MODEL	C_LYS_356	NZ	C_GLU_340	OE1	2.568
MODEL	C_ARG_403	NH1	C_GLU_406	OE1	3.581
MODEL	C_ARG_403	NH1	C_GLU_406	OE2	2.672
MODEL	C_ARG_403	NH2	C_GLU_406	OE2	2.658
MODEL	C_LYS_458	NZ	A_ASP_389	OD2	3.696
MODEL	C_LYS_462	NZ	C_GLU_465	OE1	2.614
MODEL	C_LYS_462	NZ	C_GLU_465	OE2	2.647
MODEL	C_ARG_509	NH1	C_ASP_442	OD1	2.578
MODEL	C_LYS_528	NZ	C_ASP_389	OD1	3.189
MODEL	C_LYS_528	NZ	C_ASP_389	OD2	3.148
MODEL	C_LYS_535	NZ	C_GLU_554	OE1	2.654
MODEL	C_LYS_535	NZ	C_GLU_554	OE2	2.723
MODEL	C_LYS_537	NZ	C_GLU_324	OE2	2.535

MODEL	C_LYS_557	NZ	C_ASP_568	OD1	2.816
MODEL	C_LYS_557	NZ	C_ASP_568	OD2	2.819
MODEL	C_LYS_557	NZ	C_ASP_574	OD1	3.661
MODEL	C_LYS_557	NZ	C_ASP_574	OD2	2.584
MODEL	C_ARG_567	NH1	C_ASP_571	OD1	3.523
MODEL	C_ARG_567	NH1	C_ASP_571	OD2	2.610
MODEL	C_ARG_567	NH2	C_ASP_571	OD1	2.539
MODEL	C_ARG_567	NH2	C_ASP_571	OD2	3.300
MODEL	C_ARG_646	NH1	A_ASP_848	OD2	3.643
MODEL	C_ARG_646	NH2	A_ASP_848	OD1	3.695
MODEL	C_ARG_646	NH2	A_ASP_848	OD2	2.627
MODEL	C_LYS_733	NZ	C_ASP_775	OD1	3.066
MODEL	C_LYS_733	NZ	C_ASP_775	OD2	2.575
MODEL	C_LYS_811	NZ	C_ASP_820	OD2	3.817
MODEL	C_ARG_815	NH1	C_ASP_820	OD1	2.929
MODEL	C_ARG_815	NH1	C_ASP_820	OD2	2.916
MODEL	C_ARG_815	NH2	C_ASP_820	OD1	3.727
MODEL	C_ARG_847	NH1	B_GLU_619	OE1	3.034
MODEL	C_LYS_854	NZ	B_ASP_614	OD1	2.686
MODEL	C_LYS_986	NZ	C_GLU_748	OE1	2.531
MODEL	C_ARG_995	NH1	A_ASP_994	OD1	2.647
MODEL	C_ARG_995	NH1	A_ASP_994	OD2	3.498
MODEL	C_ARG_995	NH2	A_ASP_994	OD1	3.382
MODEL	C_ARG_995	NH2	A_ASP_994	OD2	2.636
MODEL	C_ARG_1019	NH1	B_GLU_1017	OE2	2.726
MODEL	C_ARG_1019	NH1	C_GLU_773	OE2	2.647
MODEL	C_ARG_1019	NH2	B_GLU_1017	OE2	3.415
MODEL	C_LYS_1028	NZ	C_GLU_725	OE1	2.678
MODEL	C_LYS_1028	NZ	C_GLU_725	OE2	2.787
MODEL	C_ARG_1039	NH1	C_GLU_1031	OE1	3.735
MODEL	C_ARG_1039	NH1	C_GLU_1031	OE2	2.669
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE1	3.509
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE2	2.596
MODEL	C_HIS_1064	NE2	C_GLU_725	OE1	2.774
MODEL	C_LYS_1086	NZ	C_ASP_1084	OD2	2.855

Table 7: MODE-specific salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
MODEL	A_ARG_319	NH1	B_ASP_737	OD2	2.735
MODEL	A_ARG_319	NH1	B_ASP_745	OD1	3.587
MODEL	A_ARG_319	NH2	B_ASP_737	OD2	3.982
MODEL	A_LYS_790	NZ	C_GLU_702	OE1	2.623
MODEL	A_LYS_790	NZ	C_GLU_702	OE2	2.744
MODEL	A_ARG_995	NH1	B_ASP_994	OD1	3.497
MODEL	A_ARG_995	NH1	B_ASP_994	OD2	2.691
MODEL	A_ARG_995	NH2	B_ASP_994	OD1	2.657
MODEL	A_ARG_995	NH2	B_ASP_994	OD2	3.473
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE1	3.621
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE2	2.620
MODEL	B_ARG_319	NH1	C_ASP_745	OD1	2.606
MODEL	B_ARG_319	NH1	C_ASP_745	OD2	3.565
MODEL	B_ARG_319	NH2	C_ASP_745	OD1	3.325
MODEL	B_ARG_319	NH2	C_ASP_745	OD2	2.636
MODEL	B_LYS_790	NZ	A_GLU_702	OE1	2.570
MODEL	B_LYS_790	NZ	A_GLU_702	OE2	3.570
MODEL	B_LYS_854	NZ	A_ASP_614	OD1	3.487
MODEL	B_LYS_986	NZ	C_ASP_427	OD2	3.985
MODEL	B_ARG_995	NH1	C_ASP_994	OD1	2.636
MODEL	B_ARG_995	NH1	C_ASP_994	OD2	3.371
MODEL	B_ARG_995	NH2	C_ASP_994	OD1	3.182
MODEL	B_ARG_995	NH2	C_ASP_994	OD2	2.637
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE1	2.711
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE2	3.989
MODEL	C_LYS_113	NZ	B_GLU_471	OE2	2.679
MODEL	C_ARG_319	NH1	A_ASP_745	OD1	3.819
MODEL	C_LYS_458	NZ	A_ASP_389	OD2	3.696
MODEL	C_ARG_646	NH1	A_ASP_848	OD2	3.643
MODEL	C_ARG_646	NH2	A_ASP_848	OD1	3.695
MODEL	C_ARG_646	NH2	A_ASP_848	OD2	2.627
MODEL	C_ARG_847	NH1	B_GLU_619	OE1	3.034
MODEL	C_LYS_854	NZ	B_ASP_614	OD1	2.686
MODEL	C_ARG_995	NH1	A_ASP_994	OD1	2.647
MODEL	C_ARG_995	NH1	A_ASP_994	OD2	3.498
MODEL	C_ARG_995	NH2	A_ASP_994	OD1	3.382
MODEL	C_ARG_995	NH2	A_ASP_994	OD2	2.636
MODEL	C_ARG_1019	NH1	B_GLU_1017	OE2	2.726
MODEL	C_ARG_1019	NH2	B_GLU_1017	OE2	3.415
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE1	3.509
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE2	2.596

Table 8: MODE-specific interfacial salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**