



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 PM UTC

PDB ID : 6LEK / pdb_00006lek
BMRB ID : 36301
Title : Tertiary structure of Barnacle cement protein MrCP20
Authors : Mohanram, H.
Deposited on : 2019-11-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

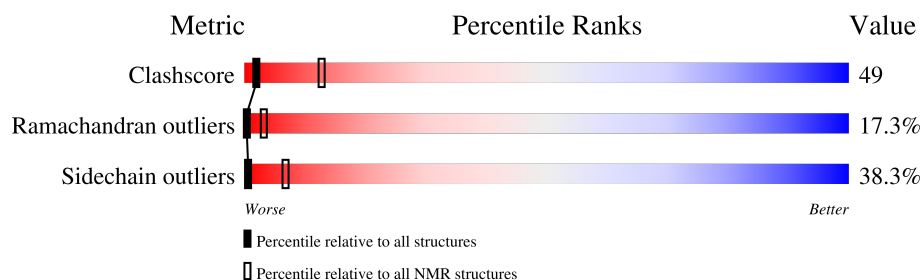
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 45%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	191	11% 29% 14% 43% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:17-A:54, A:63-A:88, A:99-A:113, A:123-A:133, A:149-A:153, A:162-A:169 (103)	4.97	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 7, 9, 10
2	3, 8
Single-model clusters	2

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2599 atoms, of which 1185 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cement protein-20k.

Mol	Chain	Residues	Atoms						Trace
1	A	185	Total	C	H	N	O	S	0
			2599	823	1185	257	301	33	

There are 7 discrepancies between the modelled and reference sequences:

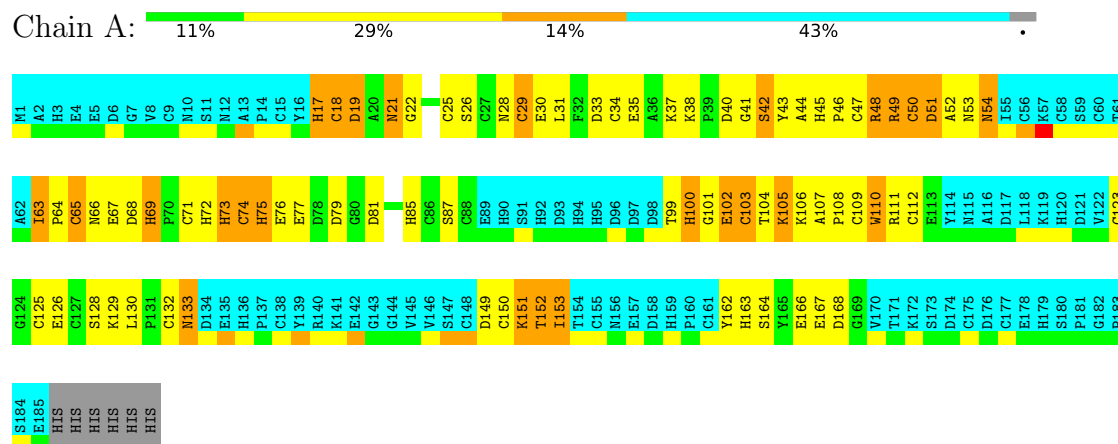
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9GRC4
A	186	HIS	-	expression tag	UNP Q9GRC4
A	187	HIS	-	expression tag	UNP Q9GRC4
A	188	HIS	-	expression tag	UNP Q9GRC4
A	189	HIS	-	expression tag	UNP Q9GRC4
A	190	HIS	-	expression tag	UNP Q9GRC4
A	191	HIS	-	expression tag	UNP Q9GRC4

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Cement protein-20k

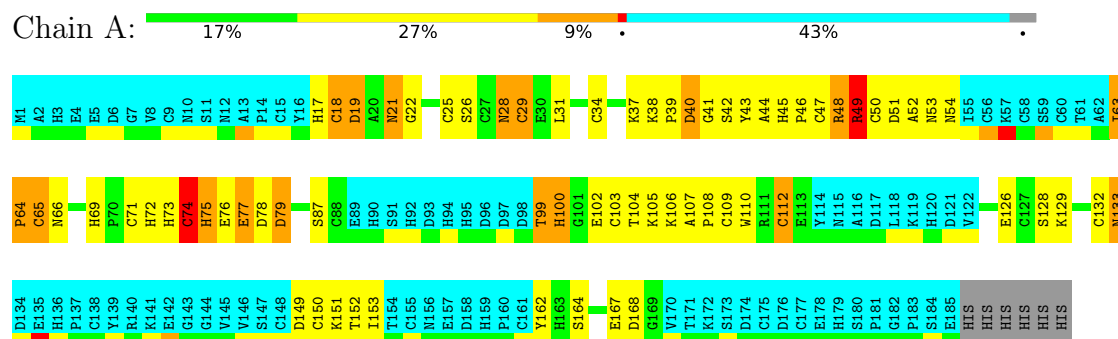


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

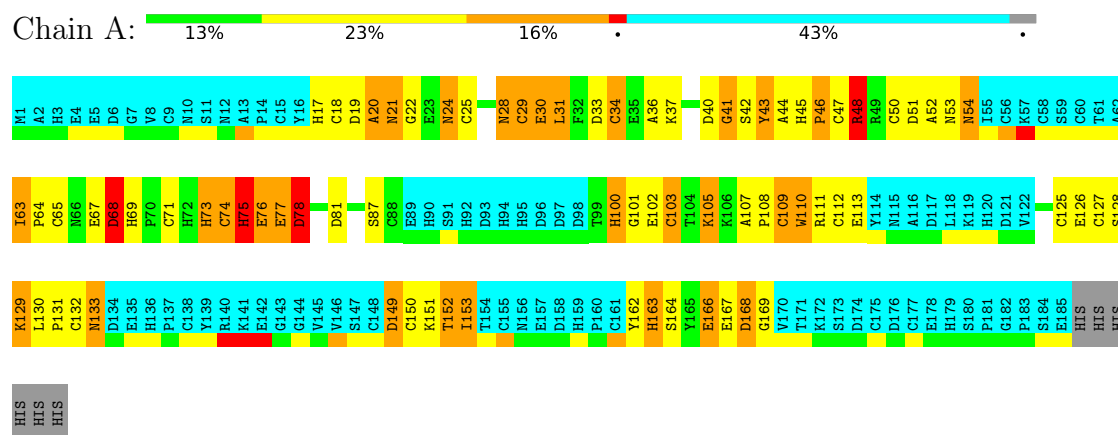
4.2.1 Score per residue for model 1

- Molecule 1: Cement protein-20k



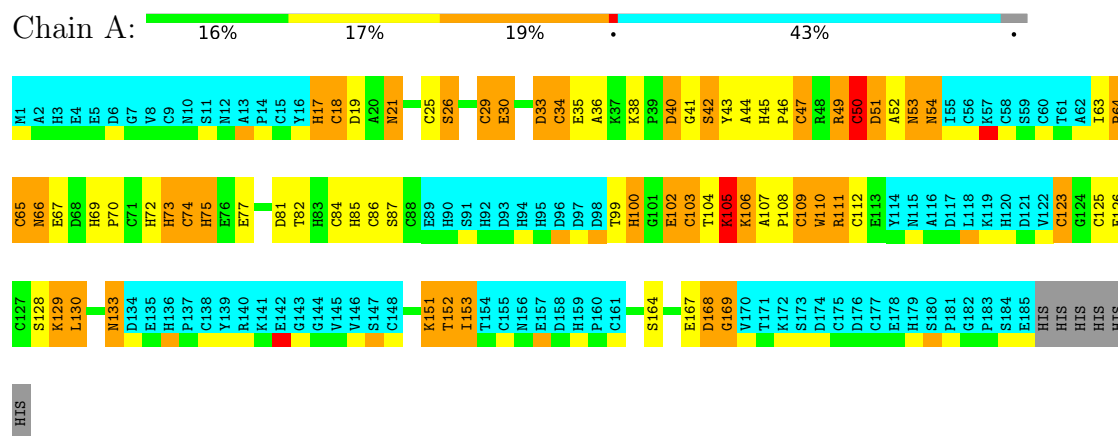
4.2.2 Score per residue for model 2

- Molecule 1: Cement protein-20k



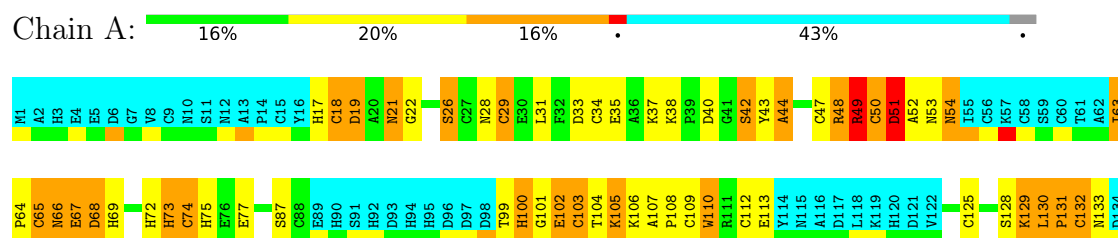
4.2.3 Score per residue for model 3

- Molecule 1: Cement protein-20k



4.2.4 Score per residue for model 4

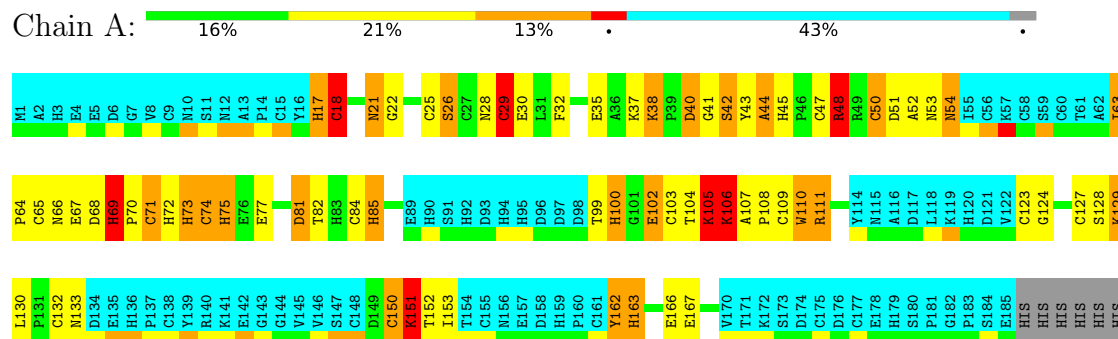
- Molecule 1: Cement protein-20k





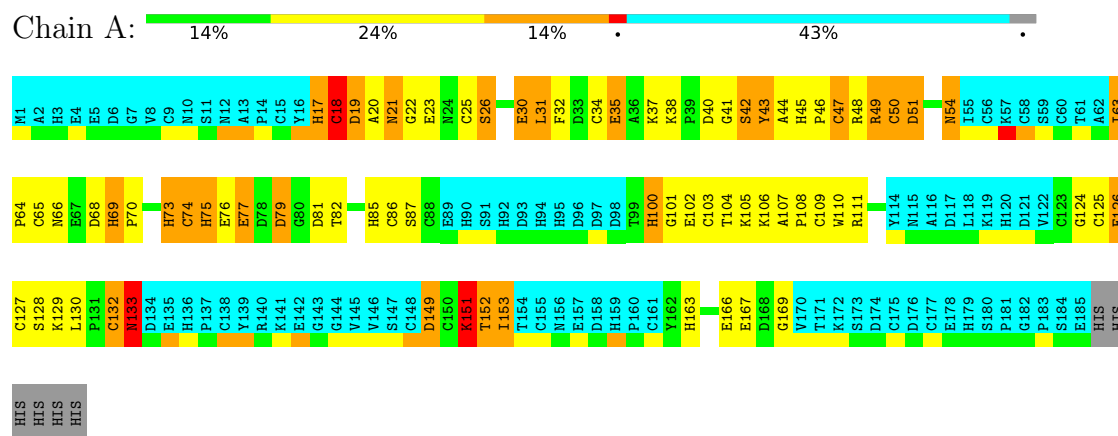
4.2.5 Score per residue for model 5

- Molecule 1: Cement protein-20k



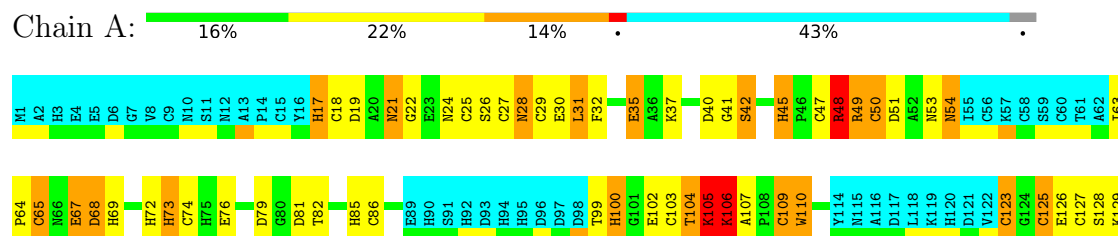
4.2.6 Score per residue for model 6 (medoid)

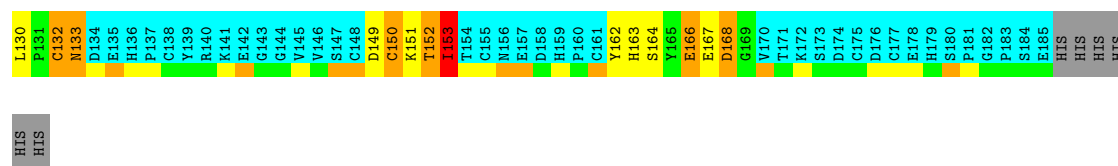
- Molecule 1: Cement protein-20k



4.2.7 Score per residue for model 7

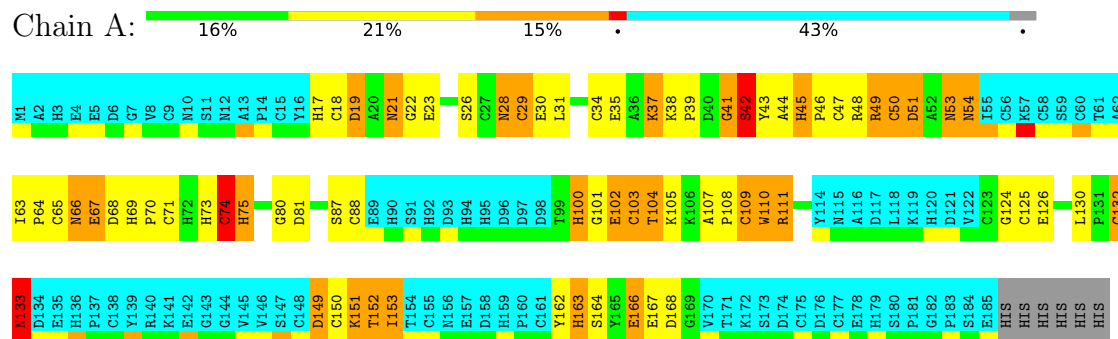
- Molecule 1: Cement protein-20k





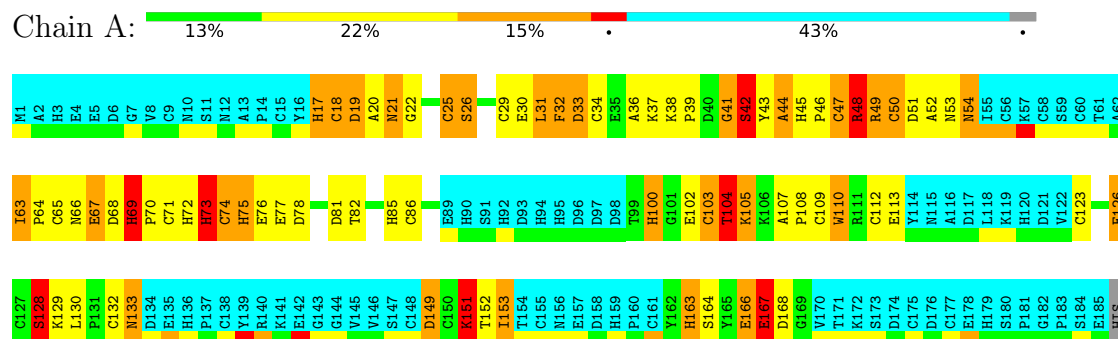
4.2.8 Score per residue for model 8

- Molecule 1: Cement protein-20k



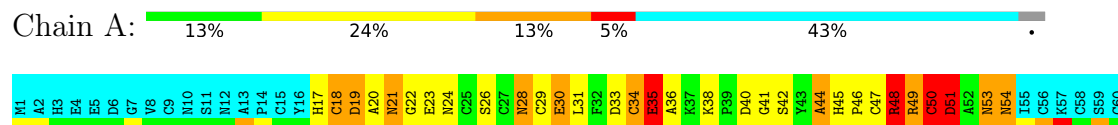
4.2.9 Score per residue for model 9

- Molecule 1: Cement protein-20k



4.2.10 Score per residue for model 10

- Molecule 1: Cement protein-20k





5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	954
Number of shifts mapped to atoms	954
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	790	662	666	72±10
All	All	7900	6620	6634	717

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:HIS:CB	1:A:70:PRO:HD2	1.05	1.79	6	3
1:A:103:CYS:SG	1:A:109:CYS:CB	1.04	2.44	8	2
1:A:69:HIS:HB3	1:A:70:PRO:CD	1.03	1.82	6	4
1:A:69:HIS:HB3	1:A:70:PRO:HD2	1.01	1.27	6	5
1:A:18:CYS:O	1:A:21:ASN:ND2	1.00	1.94	4	4
1:A:40:ASP:O	1:A:42:SER:N	0.99	1.96	2	1
1:A:69:HIS:CB	1:A:70:PRO:CD	0.98	2.41	6	3
1:A:103:CYS:CB	1:A:109:CYS:SG	0.97	2.51	8	3
1:A:52:ALA:HB2	1:A:65:CYS:HA	0.97	1.35	5	2
1:A:107:ALA:HB1	1:A:108:PRO:HD2	0.96	1.29	4	9
1:A:21:ASN:HD22	1:A:21:ASN:N	0.91	1.63	4	2
1:A:76:GLU:O	1:A:78:ASP:N	0.89	2.05	2	1
1:A:32:PHE:O	1:A:33:ASP:O	0.89	1.91	9	1
1:A:34:CYS:CB	1:A:47:CYS:SG	0.88	2.62	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:CYS:CB	1:A:109:CYS:HG	0.86	1.82	9	1
1:A:68:ASP:O	1:A:69:HIS:O	0.86	1.92	6	1
1:A:52:ALA:N	1:A:63:ILE:O	0.85	2.07	5	3
1:A:44:ALA:HB1	1:A:53:ASN:C	0.85	1.96	5	1
1:A:47:CYS:O	1:A:49:ARG:N	0.85	2.10	10	5
1:A:105:LYS:O	1:A:107:ALA:N	0.84	2.10	3	3
1:A:21:ASN:H	1:A:21:ASN:ND2	0.83	1.71	6	7
1:A:63:ILE:CG2	1:A:64:PRO:HD2	0.83	2.02	1	1
1:A:44:ALA:HB1	1:A:52:ALA:HB1	0.82	1.49	2	1
1:A:67:GLU:C	1:A:69:HIS:HD1	0.81	1.82	8	1
1:A:132:CYS:SG	1:A:150:CYS:CB	0.80	2.69	5	1
1:A:21:ASN:ND2	1:A:21:ASN:N	0.80	2.24	4	7
1:A:73:HIS:O	1:A:74:CYS:O	0.78	2.00	6	5
1:A:18:CYS:O	1:A:19:ASP:O	0.78	2.01	1	1
1:A:63:ILE:HG22	1:A:64:PRO:HD2	0.78	1.52	1	2
1:A:63:ILE:HG22	1:A:64:PRO:CD	0.77	2.08	1	1
1:A:132:CYS:CB	1:A:150:CYS:SG	0.77	2.71	5	1
1:A:99:THR:O	1:A:100:HIS:CB	0.77	2.31	4	2
1:A:63:ILE:CB	1:A:64:PRO:HD2	0.76	2.10	1	4
1:A:21:ASN:ND2	1:A:21:ASN:H	0.76	1.75	4	2
1:A:72:HIS:O	1:A:74:CYS:N	0.76	2.18	7	3
1:A:110:TRP:C	1:A:110:TRP:CD1	0.76	2.63	5	8
1:A:107:ALA:HB1	1:A:108:PRO:CD	0.75	2.10	4	8
1:A:103:CYS:SG	1:A:107:ALA:O	0.75	2.44	7	1
1:A:103:CYS:CB	1:A:109:CYS:HA	0.74	2.12	6	3
1:A:67:GLU:O	1:A:69:HIS:N	0.73	2.21	8	5
1:A:44:ALA:HB1	1:A:53:ASN:HB3	0.73	1.60	9	2
1:A:54:ASN:ND2	1:A:54:ASN:N	0.73	2.37	9	4
1:A:46:PRO:HA	1:A:52:ALA:HB3	0.73	1.59	1	1
1:A:34:CYS:HA	1:A:47:CYS:CB	0.73	2.14	4	2
1:A:18:CYS:O	1:A:22:GLY:N	0.73	2.21	4	5
1:A:45:HIS:CE1	1:A:46:PRO:O	0.73	2.42	3	1
1:A:22:GLY:O	1:A:26:SER:O	0.73	2.05	4	6
1:A:52:ALA:O	1:A:63:ILE:HG12	0.72	1.85	1	1
1:A:25:CYS:O	1:A:26:SER:C	0.72	2.32	5	3
1:A:67:GLU:O	1:A:68:ASP:C	0.71	2.32	10	4
1:A:47:CYS:O	1:A:48:ARG:O	0.71	2.09	7	2
1:A:43:TYR:O	1:A:44:ALA:CB	0.71	2.39	4	3
1:A:73:HIS:O	1:A:74:CYS:C	0.70	2.32	3	7
1:A:166:GLU:O	1:A:168:ASP:N	0.70	2.25	7	3
1:A:43:TYR:O	1:A:44:ALA:HB3	0.70	1.85	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:THR:HG22	1:A:153:ILE:HG22	0.70	1.63	7	1
1:A:66:ASN:H	1:A:66:ASN:ND2	0.70	1.84	3	1
1:A:17:HIS:CE1	1:A:22:GLY:HA3	0.69	2.22	4	3
1:A:66:ASN:ND2	1:A:66:ASN:N	0.69	2.39	3	1
1:A:69:HIS:HB2	1:A:70:PRO:HD2	0.69	1.65	6	3
1:A:110:TRP:CH2	1:A:152:THR:HG23	0.69	2.22	10	1
1:A:151:LYS:HE2	1:A:152:THR:HG23	0.69	1.64	9	2
1:A:17:HIS:ND1	1:A:18:CYS:N	0.68	2.41	6	4
1:A:105:LYS:O	1:A:106:LYS:C	0.68	2.36	7	3
1:A:132:CYS:O	1:A:133:ASN:C	0.68	2.35	9	2
1:A:45:HIS:N	1:A:46:PRO:CD	0.68	2.57	1	1
1:A:104:THR:O	1:A:105:LYS:O	0.68	2.10	5	2
1:A:18:CYS:O	1:A:19:ASP:C	0.68	2.35	8	4
1:A:21:ASN:N	1:A:21:ASN:ND2	0.67	2.42	10	1
1:A:20:ALA:HB2	1:A:67:GLU:CD	0.67	2.14	9	1
1:A:22:GLY:O	1:A:26:SER:N	0.67	2.27	4	2
1:A:49:ARG:O	1:A:50:CYS:C	0.67	2.38	3	5
1:A:100:HIS:O	1:A:110:TRP:CD1	0.67	2.48	4	4
1:A:20:ALA:HB2	1:A:51:ASP:OD2	0.67	1.90	2	1
1:A:17:HIS:CG	1:A:18:CYS:N	0.66	2.63	6	1
1:A:54:ASN:ND2	1:A:54:ASN:H	0.66	1.89	6	4
1:A:34:CYS:CB	1:A:47:CYS:HG	0.65	1.98	8	2
1:A:17:HIS:HB2	1:A:29:CYS:O	0.65	1.91	5	2
1:A:153:ILE:HG22	1:A:164:SER:O	0.65	1.92	2	1
1:A:74:CYS:O	1:A:75:HIS:C	0.64	2.39	3	7
1:A:152:THR:HG22	1:A:164:SER:O	0.64	1.91	3	2
1:A:152:THR:O	1:A:164:SER:O	0.64	2.15	8	2
1:A:51:ASP:HB2	1:A:65:CYS:HA	0.64	1.69	1	1
1:A:46:PRO:HG3	1:A:51:ASP:C	0.63	2.16	2	1
1:A:67:GLU:C	1:A:69:HIS:ND1	0.63	2.56	8	1
1:A:105:LYS:HE3	1:A:107:ALA:HB3	0.63	1.70	2	3
1:A:63:ILE:HB	1:A:64:PRO:HD2	0.62	1.71	1	4
1:A:36:ALA:HB1	1:A:44:ALA:HA	0.62	1.70	9	2
1:A:99:THR:O	1:A:151:LYS:HB2	0.62	1.95	10	1
1:A:63:ILE:CB	1:A:64:PRO:CD	0.62	2.76	1	1
1:A:48:ARG:O	1:A:50:CYS:N	0.62	2.32	9	1
1:A:51:ASP:HA	1:A:64:PRO:C	0.62	2.19	4	4
1:A:52:ALA:H	1:A:63:ILE:CG1	0.61	2.07	1	1
1:A:103:CYS:HB3	1:A:109:CYS:HA	0.61	1.71	6	4
1:A:34:CYS:HA	1:A:47:CYS:HB3	0.61	1.72	4	1
1:A:105:LYS:CE	1:A:107:ALA:HB3	0.61	2.25	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:THR:O	1:A:100:HIS:HB2	0.61	1.96	4	2
1:A:46:PRO:HD3	1:A:52:ALA:HA	0.61	1.72	2	1
1:A:54:ASN:N	1:A:54:ASN:HD22	0.60	1.93	9	4
1:A:133:ASN:HA	1:A:149:ASP:N	0.60	2.11	9	2
1:A:54:ASN:HD22	1:A:54:ASN:N	0.60	1.93	7	2
1:A:100:HIS:HB3	1:A:151:LYS:CD	0.60	2.27	5	1
1:A:44:ALA:HB1	1:A:53:ASN:HB2	0.60	1.73	8	2
1:A:38:LYS:HG2	1:A:42:SER:N	0.60	2.12	4	1
1:A:63:ILE:CG2	1:A:64:PRO:CD	0.60	2.77	1	1
1:A:34:CYS:HB2	1:A:47:CYS:SG	0.60	2.37	1	2
1:A:34:CYS:HA	1:A:47:CYS:HB2	0.59	1.74	3	1
1:A:64:PRO:O	1:A:66:ASN:N	0.59	2.35	4	2
1:A:47:CYS:O	1:A:48:ARG:C	0.59	2.43	2	3
1:A:73:HIS:C	1:A:74:CYS:SG	0.59	2.85	10	1
1:A:150:CYS:O	1:A:153:ILE:HG23	0.59	1.97	5	1
1:A:47:CYS:C	1:A:49:ARG:H	0.59	2.05	1	1
1:A:101:GLY:CA	1:A:111:ARG:HA	0.59	2.28	8	2
1:A:152:THR:HG22	1:A:166:GLU:O	0.59	1.98	8	1
1:A:130:LEU:HD22	1:A:169:GLY:CA	0.58	2.27	3	1
1:A:63:ILE:N	1:A:63:ILE:HD13	0.58	2.13	1	1
1:A:102:GLU:HG3	1:A:152:THR:C	0.58	2.23	3	1
1:A:105:LYS:C	1:A:107:ALA:N	0.58	2.60	5	4
1:A:101:GLY:N	1:A:110:TRP:NE1	0.58	2.51	10	1
1:A:30:GLU:O	1:A:30:GLU:HG2	0.58	1.99	3	1
1:A:44:ALA:HB1	1:A:53:ASN:CB	0.58	2.28	9	3
1:A:34:CYS:C	1:A:47:CYS:HB2	0.58	2.24	10	1
1:A:44:ALA:HB1	1:A:52:ALA:CB	0.57	2.25	2	1
1:A:132:CYS:O	1:A:133:ASN:O	0.57	2.22	8	2
1:A:153:ILE:HB	1:A:162:TYR:HA	0.57	1.75	8	1
1:A:100:HIS:CG	1:A:123:CYS:HB3	0.57	2.35	10	1
1:A:51:ASP:HA	1:A:64:PRO:HA	0.57	1.75	7	2
1:A:64:PRO:HB3	1:A:73:HIS:C	0.57	2.25	1	1
1:A:40:ASP:O	1:A:41:GLY:C	0.57	2.47	2	1
1:A:54:ASN:HB2	1:A:63:ILE:HD11	0.57	1.76	2	1
1:A:50:CYS:O	1:A:65:CYS:CB	0.57	2.53	9	2
1:A:74:CYS:O	1:A:75:HIS:O	0.57	2.23	10	3
1:A:125:CYS:O	1:A:125:CYS:SG	0.57	2.62	7	1
1:A:151:LYS:CE	1:A:152:THR:HG23	0.57	2.30	9	1
1:A:21:ASN:HB3	1:A:46:PRO:HB2	0.57	1.76	8	1
1:A:110:TRP:CZ2	1:A:152:THR:HG23	0.56	2.34	10	1
1:A:31:LEU:HD13	1:A:32:PHE:H	0.56	1.61	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:CYS:HA	1:A:30:GLU:HA	0.56	1.76	9	1
1:A:110:TRP:C	1:A:110:TRP:HD1	0.56	2.08	5	1
1:A:152:THR:HG22	1:A:162:TYR:CE2	0.56	2.35	10	1
1:A:30:GLU:O	1:A:30:GLU:CG	0.56	2.54	3	1
1:A:44:ALA:CB	1:A:52:ALA:HB1	0.56	2.28	2	1
1:A:163:HIS:O	1:A:164:SER:C	0.55	2.49	4	1
1:A:32:PHE:C	1:A:33:ASP:O	0.55	2.49	9	1
1:A:99:THR:O	1:A:152:THR:OG1	0.55	2.20	10	1
1:A:166:GLU:O	1:A:167:GLU:C	0.55	2.49	9	1
1:A:65:CYS:C	1:A:67:GLU:H	0.55	2.09	9	2
1:A:52:ALA:HB2	1:A:66:ASN:ND2	0.55	2.17	4	1
1:A:132:CYS:O	1:A:149:ASP:HA	0.55	2.02	2	1
1:A:53:ASN:O	1:A:53:ASN:CG	0.54	2.50	8	1
1:A:34:CYS:N	1:A:47:CYS:HB3	0.54	2.17	9	1
1:A:21:ASN:H	1:A:21:ASN:HD22	0.54	1.45	2	3
1:A:132:CYS:HB2	1:A:149:ASP:O	0.54	2.03	4	2
1:A:33:ASP:C	1:A:47:CYS:HB3	0.54	2.28	9	1
1:A:52:ALA:HB2	1:A:65:CYS:CA	0.54	2.24	5	1
1:A:44:ALA:CB	1:A:53:ASN:HB3	0.54	2.32	9	1
1:A:72:HIS:O	1:A:73:HIS:O	0.54	2.25	5	2
1:A:33:ASP:O	1:A:48:ARG:N	0.53	2.41	2	1
1:A:104:THR:HG22	1:A:162:TYR:CE2	0.53	2.37	8	1
1:A:99:THR:O	1:A:151:LYS:HB3	0.53	2.04	4	2
1:A:153:ILE:O	1:A:162:TYR:HA	0.53	2.02	5	2
1:A:102:GLU:C	1:A:103:CYS:SG	0.53	2.91	2	2
1:A:128:SER:O	1:A:130:LEU:N	0.53	2.42	3	1
1:A:151:LYS:HG3	1:A:169:GLY:HA3	0.53	1.80	6	1
1:A:102:GLU:HG2	1:A:110:TRP:CZ2	0.53	2.39	5	1
1:A:73:HIS:C	1:A:74:CYS:O	0.53	2.52	6	2
1:A:75:HIS:O	1:A:75:HIS:ND1	0.53	2.40	3	1
1:A:100:HIS:CG	1:A:151:LYS:HB3	0.53	2.39	8	1
1:A:34:CYS:O	1:A:45:HIS:O	0.53	2.27	10	1
1:A:47:CYS:C	1:A:49:ARG:N	0.53	2.65	1	1
1:A:153:ILE:CG2	1:A:164:SER:O	0.52	2.57	2	2
1:A:23:GLU:OE1	1:A:99:THR:HG23	0.52	2.04	10	1
1:A:107:ALA:CB	1:A:108:PRO:HD2	0.52	2.18	4	3
1:A:19:ASP:O	1:A:20:ALA:C	0.52	2.52	2	3
1:A:21:ASN:N	1:A:21:ASN:HD22	0.52	2.02	6	3
1:A:100:HIS:O	1:A:110:TRP:NE1	0.52	2.42	4	3
1:A:153:ILE:HG23	1:A:164:SER:O	0.52	2.04	8	1
1:A:46:PRO:HD3	1:A:53:ASN:CB	0.52	2.35	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:PRO:HD3	1:A:53:ASN:HB3	0.52	1.80	8	1
1:A:22:GLY:O	1:A:26:SER:CA	0.52	2.57	4	1
1:A:152:THR:HA	1:A:166:GLU:O	0.52	2.04	8	1
1:A:34:CYS:HA	1:A:47:CYS:SG	0.52	2.45	10	1
1:A:17:HIS:H	1:A:29:CYS:C	0.52	2.12	5	2
1:A:44:ALA:HA	1:A:53:ASN:O	0.52	2.04	1	1
1:A:50:CYS:O	1:A:64:PRO:HG2	0.52	2.05	1	1
1:A:45:HIS:N	1:A:46:PRO:HD3	0.51	2.20	1	1
1:A:66:ASN:N	1:A:66:ASN:HD22	0.51	2.03	3	1
1:A:100:HIS:HB2	1:A:151:LYS:HD3	0.51	1.81	9	1
1:A:49:ARG:O	1:A:51:ASP:N	0.51	2.43	8	5
1:A:17:HIS:CD2	1:A:31:LEU:N	0.51	2.78	6	1
1:A:64:PRO:O	1:A:65:CYS:C	0.51	2.53	3	5
1:A:167:GLU:O	1:A:168:ASP:C	0.51	2.53	3	1
1:A:65:CYS:C	1:A:67:GLU:N	0.51	2.66	9	3
1:A:128:SER:C	1:A:130:LEU:H	0.51	2.12	9	1
1:A:17:HIS:HB2	1:A:29:CYS:C	0.51	2.30	3	2
1:A:31:LEU:HD13	1:A:32:PHE:N	0.51	2.20	6	1
1:A:101:GLY:HA3	1:A:111:ARG:HA	0.51	1.82	8	2
1:A:153:ILE:HG13	1:A:162:TYR:CG	0.51	2.41	8	1
1:A:67:GLU:HB3	1:A:74:CYS:HA	0.51	1.82	9	1
1:A:34:CYS:SG	1:A:47:CYS:CB	0.51	2.98	6	2
1:A:102:GLU:CG	1:A:103:CYS:N	0.51	2.73	4	1
1:A:101:GLY:HA2	1:A:111:ARG:HA	0.51	1.82	2	2
1:A:150:CYS:O	1:A:151:LYS:C	0.51	2.53	10	1
1:A:76:GLU:O	1:A:77:GLU:C	0.51	2.52	2	1
1:A:102:GLU:HB3	1:A:152:THR:OG1	0.51	2.04	9	1
1:A:67:GLU:O	1:A:69:HIS:ND1	0.51	2.41	8	1
1:A:153:ILE:HD13	1:A:153:ILE:N	0.51	2.21	8	1
1:A:78:ASP:O	1:A:79:ASP:C	0.50	2.54	1	1
1:A:44:ALA:CB	1:A:53:ASN:HB2	0.50	2.35	3	1
1:A:43:TYR:O	1:A:44:ALA:HB2	0.50	2.05	8	2
1:A:103:CYS:HB2	1:A:109:CYS:C	0.50	2.30	7	1
1:A:39:PRO:C	1:A:41:GLY:H	0.50	2.14	8	2
1:A:74:CYS:O	1:A:76:GLU:N	0.50	2.44	9	1
1:A:108:PRO:HG2	1:A:167:GLU:CD	0.50	2.30	10	1
1:A:19:ASP:HB2	1:A:46:PRO:CA	0.50	2.36	2	1
1:A:130:LEU:HD13	1:A:169:GLY:HA2	0.50	1.84	3	1
1:A:20:ALA:HB2	1:A:67:GLU:OE2	0.50	2.07	9	1
1:A:38:LYS:CG	1:A:38:LYS:O	0.50	2.59	5	1
1:A:105:LYS:O	1:A:107:ALA:O	0.50	2.30	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:CYS:HB3	1:A:149:ASP:HA	0.50	1.83	8	1
1:A:112:CYS:HB3	1:A:124:GLY:N	0.50	2.21	10	1
1:A:52:ALA:H	1:A:63:ILE:HG12	0.50	1.67	1	1
1:A:102:GLU:HG3	1:A:149:ASP:C	0.49	2.33	8	1
1:A:110:TRP:CZ3	1:A:166:GLU:HB2	0.49	2.41	10	1
1:A:99:THR:O	1:A:100:HIS:HB3	0.49	2.07	4	1
1:A:50:CYS:O	1:A:64:PRO:CD	0.49	2.61	1	1
1:A:45:HIS:CD2	1:A:46:PRO:HD2	0.49	2.43	3	1
1:A:50:CYS:N	1:A:64:PRO:HG2	0.49	2.23	1	1
1:A:152:THR:O	1:A:153:ILE:C	0.49	2.56	10	4
1:A:21:ASN:CB	1:A:46:PRO:HB3	0.49	2.38	6	1
1:A:149:ASP:OD2	1:A:149:ASP:C	0.49	2.56	10	1
1:A:153:ILE:HB	1:A:162:TYR:CA	0.49	2.37	8	2
1:A:66:ASN:OD1	1:A:73:HIS:N	0.49	2.46	3	1
1:A:151:LYS:HG3	1:A:166:GLU:O	0.49	2.08	9	1
1:A:34:CYS:HG	1:A:47:CYS:CB	0.48	2.19	1	1
1:A:50:CYS:HA	1:A:66:ASN:HA	0.48	1.83	1	1
1:A:110:TRP:CH2	1:A:166:GLU:HB2	0.48	2.43	10	1
1:A:101:GLY:HA2	1:A:110:TRP:O	0.48	2.09	10	3
1:A:72:HIS:O	1:A:73:HIS:C	0.48	2.56	5	2
1:A:22:GLY:HA3	1:A:29:CYS:CB	0.48	2.37	10	1
1:A:22:GLY:O	1:A:26:SER:C	0.48	2.56	8	3
1:A:28:ASN:C	1:A:29:CYS:SG	0.48	2.96	8	2
1:A:17:HIS:O	1:A:31:LEU:O	0.48	2.31	8	2
1:A:17:HIS:ND1	1:A:22:GLY:HA3	0.48	2.23	4	1
1:A:17:HIS:CD2	1:A:30:GLU:H	0.48	2.27	6	1
1:A:36:ALA:HA	1:A:45:HIS:CB	0.48	2.38	2	1
1:A:163:HIS:CG	1:A:164:SER:N	0.48	2.81	7	1
1:A:102:GLU:HB2	1:A:151:LYS:HG2	0.48	1.83	8	1
1:A:63:ILE:N	1:A:63:ILE:CD1	0.48	2.76	1	1
1:A:65:CYS:HB2	1:A:69:HIS:O	0.48	2.08	1	1
1:A:49:ARG:N	1:A:73:HIS:HB2	0.48	2.24	4	1
1:A:38:LYS:HB3	1:A:39:PRO:HD2	0.48	1.85	8	1
1:A:52:ALA:HB2	1:A:66:ASN:CG	0.48	2.34	3	1
1:A:17:HIS:ND1	1:A:22:GLY:HA2	0.48	2.24	10	2
1:A:129:LYS:O	1:A:130:LEU:HD12	0.48	2.08	7	1
1:A:152:THR:CG2	1:A:166:GLU:O	0.48	2.61	8	1
1:A:153:ILE:O	1:A:162:TYR:N	0.47	2.46	5	1
1:A:102:GLU:HG2	1:A:151:LYS:CD	0.47	2.38	8	1
1:A:34:CYS:N	1:A:47:CYS:CB	0.47	2.77	9	1
1:A:42:SER:O	1:A:42:SER:OG	0.47	2.32	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ALA:C	1:A:63:ILE:CG1	0.47	2.87	1	1
1:A:109:CYS:O	1:A:110:TRP:HB2	0.47	2.09	7	1
1:A:52:ALA:HB2	1:A:66:ASN:OD1	0.47	2.08	3	1
1:A:54:ASN:N	1:A:54:ASN:ND2	0.47	2.62	5	2
1:A:103:CYS:O	1:A:152:THR:O	0.47	2.32	4	1
1:A:17:HIS:N	1:A:30:GLU:N	0.47	2.62	5	1
1:A:48:ARG:CB	1:A:73:HIS:CB	0.47	2.93	7	1
1:A:105:LYS:C	1:A:107:ALA:H	0.47	2.17	10	6
1:A:48:ARG:C	1:A:50:CYS:H	0.47	2.18	7	1
1:A:37:LYS:CB	1:A:42:SER:O	0.47	2.62	9	1
1:A:151:LYS:HB2	1:A:168:ASP:CB	0.47	2.40	3	1
1:A:133:ASN:HA	1:A:149:ASP:H	0.47	1.70	4	1
1:A:107:ALA:CB	1:A:108:PRO:CD	0.47	2.83	4	6
1:A:19:ASP:O	1:A:22:GLY:N	0.47	2.47	2	2
1:A:151:LYS:C	1:A:153:ILE:H	0.47	2.18	4	3
1:A:65:CYS:O	1:A:67:GLU:N	0.47	2.48	9	3
1:A:30:GLU:HG2	1:A:130:LEU:HD22	0.47	1.86	10	1
1:A:45:HIS:N	1:A:53:ASN:HB3	0.47	2.24	10	1
1:A:51:ASP:N	1:A:66:ASN:N	0.47	2.62	1	1
1:A:52:ALA:O	1:A:63:ILE:CG1	0.46	2.60	1	1
1:A:102:GLU:HG2	1:A:151:LYS:HG2	0.46	1.86	8	1
1:A:18:CYS:O	1:A:29:CYS:SG	0.46	2.73	10	1
1:A:51:ASP:HB2	1:A:64:PRO:O	0.46	2.09	1	1
1:A:102:GLU:O	1:A:110:TRP:CD2	0.46	2.68	1	1
1:A:17:HIS:H	1:A:30:GLU:N	0.46	2.08	5	2
1:A:65:CYS:HB3	1:A:68:ASP:CB	0.46	2.39	5	2
1:A:153:ILE:O	1:A:162:TYR:CA	0.46	2.64	5	1
1:A:69:HIS:HB3	1:A:70:PRO:HD3	0.46	1.79	6	1
1:A:26:SER:O	1:A:28:ASN:N	0.46	2.48	7	1
1:A:50:CYS:O	1:A:65:CYS:HB3	0.46	2.11	9	1
1:A:43:TYR:O	1:A:54:ASN:C	0.46	2.58	1	1
1:A:100:HIS:CD2	1:A:151:LYS:HG2	0.46	2.45	6	1
1:A:102:GLU:O	1:A:110:TRP:CE3	0.46	2.68	10	1
1:A:102:GLU:CB	1:A:151:LYS:HG2	0.46	2.41	8	1
1:A:19:ASP:CG	1:A:126:GLU:C	0.46	2.84	9	1
1:A:68:ASP:C	1:A:69:HIS:O	0.46	2.56	6	1
1:A:110:TRP:HH2	1:A:152:THR:HG23	0.46	1.69	10	1
1:A:100:HIS:CG	1:A:101:GLY:N	0.46	2.83	4	1
1:A:100:HIS:CD2	1:A:167:GLU:HA	0.46	2.46	6	1
1:A:20:ALA:O	1:A:24:ASN:HB2	0.46	2.11	2	1
1:A:110:TRP:CG	1:A:111:ARG:N	0.46	2.82	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:CYS:HB3	1:A:68:ASP:O	0.46	2.11	6	1
1:A:45:HIS:N	1:A:53:ASN:HB2	0.46	2.26	7	1
1:A:50:CYS:HA	1:A:65:CYS:O	0.46	2.10	1	1
1:A:100:HIS:CD2	1:A:168:ASP:O	0.46	2.69	2	1
1:A:153:ILE:O	1:A:163:HIS:HB2	0.46	2.10	4	1
1:A:32:PHE:O	1:A:32:PHE:CD1	0.46	2.68	5	1
1:A:102:GLU:CB	1:A:151:LYS:HD3	0.46	2.41	5	1
1:A:128:SER:C	1:A:130:LEU:N	0.46	2.74	9	1
1:A:104:THR:C	1:A:105:LYS:O	0.46	2.59	5	2
1:A:52:ALA:N	1:A:65:CYS:N	0.46	2.64	9	1
1:A:18:CYS:HB3	1:A:22:GLY:N	0.45	2.27	1	1
1:A:151:LYS:HG2	1:A:168:ASP:N	0.45	2.26	3	1
1:A:100:HIS:CE1	1:A:123:CYS:HA	0.45	2.47	9	1
1:A:46:PRO:CA	1:A:52:ALA:HB3	0.45	2.38	1	1
1:A:150:CYS:O	1:A:151:LYS:HB2	0.45	2.10	7	1
1:A:133:ASN:CB	1:A:149:ASP:HA	0.45	2.41	6	1
1:A:104:THR:O	1:A:105:LYS:C	0.45	2.59	7	1
1:A:48:ARG:O	1:A:74:CYS:HB2	0.45	2.11	1	1
1:A:50:CYS:O	1:A:64:PRO:CG	0.45	2.64	1	1
1:A:52:ALA:C	1:A:63:ILE:HG12	0.45	2.37	1	1
1:A:19:ASP:O	1:A:21:ASN:N	0.45	2.49	2	1
1:A:151:LYS:HD3	1:A:152:THR:N	0.45	2.26	3	1
1:A:150:CYS:O	1:A:151:LYS:O	0.45	2.35	10	1
1:A:17:HIS:O	1:A:31:LEU:N	0.45	2.49	7	1
1:A:35:GLU:C	1:A:45:HIS:CD2	0.45	2.94	7	1
1:A:26:SER:C	1:A:28:ASN:H	0.45	2.20	10	1
1:A:133:ASN:O	1:A:133:ASN:CG	0.45	2.60	1	1
1:A:102:GLU:HG3	1:A:103:CYS:N	0.45	2.25	4	1
1:A:104:THR:HG22	1:A:104:THR:O	0.45	2.12	6	1
1:A:18:CYS:CB	1:A:21:ASN:ND2	0.45	2.80	9	1
1:A:50:CYS:HA	1:A:65:CYS:C	0.45	2.36	1	1
1:A:33:ASP:O	1:A:47:CYS:HB2	0.45	2.12	3	2
1:A:17:HIS:CD2	1:A:29:CYS:O	0.45	2.70	4	1
1:A:17:HIS:CE1	1:A:18:CYS:O	0.44	2.71	1	1
1:A:44:ALA:HB1	1:A:53:ASN:O	0.44	2.11	5	1
1:A:18:CYS:HB2	1:A:21:ASN:ND2	0.44	2.27	10	1
1:A:75:HIS:C	1:A:75:HIS:CD2	0.44	2.95	10	1
1:A:152:THR:HG22	1:A:166:GLU:H	0.44	1.73	2	1
1:A:133:ASN:CA	1:A:149:ASP:HA	0.44	2.42	6	1
1:A:24:ASN:ND2	1:A:63:ILE:N	0.44	2.65	2	1
1:A:128:SER:O	1:A:129:LYS:C	0.44	2.60	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:HIS:CG	1:A:29:CYS:O	0.44	2.70	4	1
1:A:44:ALA:HB1	1:A:54:ASN:N	0.44	2.27	5	1
1:A:49:ARG:HA	1:A:69:HIS:CE1	0.44	2.48	7	1
1:A:51:ASP:HB2	1:A:64:PRO:HA	0.44	1.90	2	1
1:A:18:CYS:H	1:A:22:GLY:CA	0.44	2.25	4	1
1:A:67:GLU:CB	1:A:74:CYS:CB	0.44	2.96	5	1
1:A:17:HIS:HD1	1:A:18:CYS:N	0.44	2.09	8	1
1:A:63:ILE:HG22	1:A:64:PRO:HD3	0.44	1.89	1	1
1:A:50:CYS:O	1:A:65:CYS:HB2	0.44	2.12	9	2
1:A:133:ASN:HA	1:A:149:ASP:HA	0.44	1.88	6	1
1:A:37:LYS:HB2	1:A:44:ALA:N	0.44	2.28	8	1
1:A:130:LEU:HD22	1:A:168:ASP:O	0.44	2.12	3	1
1:A:45:HIS:C	1:A:53:ASN:HB2	0.44	2.38	9	1
1:A:17:HIS:HB2	1:A:29:CYS:HB2	0.43	1.90	8	2
1:A:37:LYS:HG3	1:A:44:ALA:HB3	0.43	1.90	8	1
1:A:162:TYR:CD1	1:A:162:TYR:O	0.43	2.70	4	1
1:A:100:HIS:CG	1:A:151:LYS:HG2	0.43	2.48	6	1
1:A:101:GLY:CA	1:A:110:TRP:O	0.43	2.65	8	1
1:A:69:HIS:C	1:A:71:CYS:H	0.43	2.21	5	3
1:A:100:HIS:HB3	1:A:124:GLY:H	0.43	1.73	10	1
1:A:64:PRO:HA	1:A:71:CYS:CB	0.43	2.44	1	1
1:A:36:ALA:HA	1:A:45:HIS:N	0.43	2.28	10	1
1:A:81:ASP:O	1:A:85:HIS:HB3	0.43	2.14	5	1
1:A:100:HIS:HB3	1:A:151:LYS:HB3	0.43	1.88	8	1
1:A:34:CYS:HB3	1:A:46:PRO:O	0.43	2.14	2	1
1:A:50:CYS:HB2	1:A:73:HIS:CG	0.43	2.48	2	1
1:A:129:LYS:C	1:A:130:LEU:HD12	0.43	2.39	7	1
1:A:100:HIS:CD2	1:A:168:ASP:HB3	0.43	2.48	10	1
1:A:34:CYS:O	1:A:35:GLU:C	0.43	2.61	10	1
1:A:21:ASN:OD1	1:A:47:CYS:HA	0.42	2.14	4	1
1:A:126:GLU:O	1:A:127:CYS:HB3	0.42	2.14	7	2
1:A:162:TYR:N	1:A:162:TYR:CD2	0.42	2.84	10	1
1:A:33:ASP:C	1:A:34:CYS:SG	0.42	3.02	3	1
1:A:39:PRO:C	1:A:41:GLY:N	0.42	2.76	8	1
1:A:67:GLU:O	1:A:67:GLU:CG	0.42	2.66	8	1
1:A:75:HIS:CE1	1:A:100:HIS:CE1	0.42	3.07	3	1
1:A:130:LEU:HD22	1:A:169:GLY:HA2	0.42	1.90	3	1
1:A:50:CYS:CB	1:A:65:CYS:HB3	0.42	2.45	10	1
1:A:112:CYS:HB3	1:A:123:CYS:C	0.42	2.39	10	1
1:A:21:ASN:HD22	1:A:22:GLY:N	0.42	2.11	2	1
1:A:51:ASP:HA	1:A:65:CYS:N	0.42	2.29	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:CYS:HB2	1:A:66:ASN:HA	0.42	1.89	1	1
1:A:102:GLU:OE2	1:A:153:ILE:HG12	0.42	2.14	2	1
1:A:20:ALA:O	1:A:24:ASN:OD1	0.42	2.38	2	1
1:A:17:HIS:HB2	1:A:30:GLU:HA	0.42	1.92	3	1
1:A:65:CYS:O	1:A:66:ASN:C	0.42	2.62	8	1
1:A:46:PRO:C	1:A:47:CYS:SG	0.42	3.02	9	1
1:A:46:PRO:HD3	1:A:53:ASN:CG	0.42	2.40	3	1
1:A:18:CYS:HA	1:A:31:LEU:O	0.42	2.14	7	2
1:A:17:HIS:HB2	1:A:29:CYS:CB	0.42	2.45	1	2
1:A:64:PRO:HG3	1:A:74:CYS:SG	0.42	2.55	1	1
1:A:20:ALA:O	1:A:24:ASN:CG	0.42	2.63	2	1
1:A:128:SER:OG	1:A:129:LYS:N	0.42	2.52	3	1
1:A:103:CYS:HB2	1:A:109:CYS:O	0.42	2.14	7	1
1:A:104:THR:O	1:A:107:ALA:HB3	0.42	2.15	7	1
1:A:18:CYS:HB3	1:A:21:ASN:ND2	0.42	2.30	9	1
1:A:100:HIS:HB3	1:A:151:LYS:CE	0.42	2.44	5	1
1:A:128:SER:HB3	1:A:130:LEU:HD23	0.42	1.92	6	1
1:A:50:CYS:HB2	1:A:66:ASN:HB3	0.42	1.91	1	1
1:A:73:HIS:O	1:A:75:HIS:N	0.42	2.53	1	1
1:A:20:ALA:HA	1:A:23:GLU:OE2	0.42	2.15	6	1
1:A:100:HIS:HA	1:A:124:GLY:HA3	0.42	1.92	8	1
1:A:151:LYS:HD2	1:A:168:ASP:O	0.42	2.14	8	1
1:A:99:THR:C	1:A:112:CYS:HB2	0.41	2.39	1	1
1:A:100:HIS:HB3	1:A:151:LYS:HD2	0.41	1.92	5	1
1:A:124:GLY:O	1:A:125:CYS:C	0.41	2.61	6	1
1:A:18:CYS:O	1:A:22:GLY:CA	0.41	2.68	1	1
1:A:51:ASP:HA	1:A:64:PRO:CA	0.41	2.45	4	1
1:A:101:GLY:O	1:A:151:LYS:HG3	0.41	2.15	2	1
1:A:126:GLU:N	1:A:126:GLU:CD	0.41	2.78	2	1
1:A:50:CYS:O	1:A:68:ASP:CB	0.41	2.69	5	1
1:A:17:HIS:ND1	1:A:21:ASN:HB2	0.41	2.31	9	1
1:A:64:PRO:HB3	1:A:73:HIS:CB	0.41	2.45	1	1
1:A:19:ASP:CB	1:A:46:PRO:CA	0.41	2.99	2	1
1:A:102:GLU:HG2	1:A:151:LYS:CG	0.41	2.45	8	1
1:A:132:CYS:SG	1:A:150:CYS:HA	0.41	2.56	10	1
1:A:19:ASP:HB2	1:A:46:PRO:C	0.41	2.41	2	1
1:A:149:ASP:OD2	1:A:149:ASP:O	0.41	2.38	7	1
1:A:100:HIS:HA	1:A:112:CYS:HB2	0.41	1.92	3	1
1:A:125:CYS:C	1:A:127:CYS:H	0.41	2.23	2	1
1:A:100:HIS:CE1	1:A:123:CYS:CB	0.41	3.04	7	1
1:A:103:CYS:HA	1:A:109:CYS:HA	0.41	1.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ARG:HB3	1:A:73:HIS:HA	0.41	1.93	7	1
1:A:18:CYS:O	1:A:19:ASP:HB2	0.41	2.16	3	1
1:A:123:CYS:C	1:A:125:CYS:N	0.41	2.79	3	1
1:A:21:ASN:OD1	1:A:51:ASP:O	0.41	2.39	6	1
1:A:18:CYS:C	1:A:21:ASN:HD22	0.41	2.20	8	1
1:A:100:HIS:CB	1:A:151:LYS:HB3	0.41	2.46	8	1
1:A:51:ASP:O	1:A:52:ALA:HB2	0.41	2.17	2	1
1:A:47:CYS:O	1:A:65:CYS:SG	0.41	2.77	5	1
1:A:101:GLY:O	1:A:149:ASP:O	0.41	2.39	6	1
1:A:100:HIS:CB	1:A:151:LYS:HB2	0.41	2.46	9	1
1:A:102:GLU:HG2	1:A:149:ASP:O	0.40	2.15	1	1
1:A:21:ASN:ND2	1:A:22:GLY:N	0.40	2.70	2	1
1:A:18:CYS:HA	1:A:22:GLY:CA	0.40	2.46	5	1
1:A:124:GLY:C	1:A:126:GLU:N	0.40	2.78	8	1
1:A:51:ASP:O	1:A:66:ASN:ND2	0.40	2.54	1	1
1:A:67:GLU:HB2	1:A:69:HIS:ND1	0.40	2.30	8	1
1:A:21:ASN:HB3	1:A:46:PRO:HD2	0.40	1.92	10	1
1:A:19:ASP:CB	1:A:46:PRO:HA	0.40	2.46	2	1
1:A:130:LEU:N	1:A:131:PRO:CD	0.40	2.83	4	1
1:A:151:LYS:HD3	1:A:168:ASP:C	0.40	2.42	4	1
1:A:50:CYS:CB	1:A:65:CYS:HB2	0.40	2.46	8	1
1:A:18:CYS:O	1:A:22:GLY:HA3	0.40	2.16	10	1
1:A:74:CYS:C	1:A:75:HIS:O	0.40	2.63	10	1
1:A:19:ASP:C	1:A:21:ASN:N	0.40	2.79	2	1
1:A:151:LYS:CG	1:A:169:GLY:HA2	0.40	2.46	2	1
1:A:73:HIS:O	1:A:74:CYS:SG	0.40	2.79	7	1
1:A:37:LYS:HB3	1:A:42:SER:O	0.40	2.16	9	1
1:A:102:GLU:CD	1:A:103:CYS:N	0.40	2.79	5	1
1:A:111:ARG:CB	1:A:124:GLY:C	0.40	2.95	5	1
1:A:32:PHE:C	1:A:48:ARG:HB2	0.40	2.41	9	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/191 (54%)	59±4 (57±4%)	26±4 (26±4%)	18±3 (17±3%)	0	3
All	All	1030/1910 (54%)	587 (57%)	265 (26%)	178 (17%)	0	3

All 60 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	41	GLY	9
1	A	48	ARG	9
1	A	75	HIS	8
1	A	19	ASP	7
1	A	40	ASP	7
1	A	74	CYS	7
1	A	73	HIS	7
1	A	49	ARG	6
1	A	151	LYS	6
1	A	153	ILE	6
1	A	77	GLU	5
1	A	65	CYS	5
1	A	68	ASP	5
1	A	50	CYS	5
1	A	82	THR	5
1	A	28	ASN	4
1	A	167	GLU	4
1	A	44	ALA	4
1	A	129	LYS	3
1	A	18	CYS	3
1	A	26	SER	3
1	A	51	ASP	3
1	A	105	LYS	3
1	A	106	LYS	3
1	A	35	GLU	3
1	A	66	ASN	3
1	A	69	HIS	3
1	A	133	ASN	3
1	A	64	PRO	2
1	A	131	PRO	2
1	A	17	HIS	2
1	A	100	HIS	2
1	A	32	PHE	2
1	A	42	SER	2
1	A	104	THR	2
1	A	39	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	20	ALA	1
1	A	46	PRO	1
1	A	54	ASN	1
1	A	78	ASP	1
1	A	123	CYS	1
1	A	168	ASP	1
1	A	169	GLY	1
1	A	29	CYS	1
1	A	162	TYR	1
1	A	79	ASP	1
1	A	132	CYS	1
1	A	27	CYS	1
1	A	76	GLU	1
1	A	110	TRP	1
1	A	152	THR	1
1	A	45	HIS	1
1	A	80	GLY	1
1	A	33	ASP	1
1	A	128	SER	1
1	A	163	HIS	1
1	A	166	GLU	1
1	A	101	GLY	1
1	A	108	PRO	1
1	A	164	SER	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	92/172 (53%)	57±4 (62±4%)	35±4 (38±4%)	0 7
All	All	920/1720 (53%)	568 (62%)	352 (38%)	0 7

All 79 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	21	ASN	10

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Mol	Chain	Res	Type	Models (Total)
1	A	63	ILE	10
1	A	29	CYS	8
1	A	81	ASP	8
1	A	54	ASN	8
1	A	37	LYS	7
1	A	100	HIS	7
1	A	105	LYS	7
1	A	163	HIS	7
1	A	42	SER	7
1	A	102	GLU	7
1	A	151	LYS	7
1	A	18	CYS	6
1	A	38	LYS	6
1	A	77	GLU	6
1	A	106	LYS	6
1	A	133	ASN	6
1	A	167	GLU	6
1	A	30	GLU	6
1	A	48	ARG	6
1	A	103	CYS	6
1	A	110	TRP	6
1	A	130	LEU	6
1	A	35	GLU	6
1	A	51	ASP	6
1	A	25	CYS	5
1	A	49	ARG	5
1	A	31	LEU	5
1	A	109	CYS	5
1	A	149	ASP	5
1	A	152	THR	5
1	A	153	ILE	5
1	A	166	GLU	5
1	A	50	CYS	5
1	A	67	GLU	5
1	A	85	HIS	5
1	A	28	ASN	4
1	A	74	CYS	4
1	A	79	ASP	4
1	A	104	THR	4
1	A	112	CYS	4
1	A	128	SER	4
1	A	129	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	150	CYS	4
1	A	168	ASP	4
1	A	66	ASN	4
1	A	86	CYS	4
1	A	111	ARG	4
1	A	132	CYS	4
1	A	45	HIS	4
1	A	40	ASP	3
1	A	76	GLU	3
1	A	99	THR	3
1	A	24	ASN	3
1	A	34	CYS	3
1	A	71	CYS	3
1	A	73	HIS	3
1	A	113	GLU	3
1	A	47	CYS	3
1	A	53	ASN	3
1	A	126	GLU	3
1	A	125	CYS	3
1	A	17	HIS	3
1	A	123	CYS	3
1	A	65	CYS	2
1	A	72	HIS	2
1	A	75	HIS	2
1	A	43	TYR	2
1	A	68	ASP	2
1	A	78	ASP	2
1	A	33	ASP	2
1	A	84	CYS	2
1	A	26	SER	2
1	A	165	TYR	2
1	A	69	HIS	2
1	A	127	CYS	2
1	A	88	CYS	2
1	A	23	GLU	1
1	A	164	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 44% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: m20_2.str

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	954
Number of shifts mapped to atoms	954
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	48

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	183	0.27 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	131	0.43 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}'$	109	0.70 ± 0.29	Should be applied
^{15}N	174	-1.28 ± 0.34	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 537 atoms were assigned a chemical shift out of a possible 1199. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	422/509 (83%)	162/206 (79%)	163/206 (79%)	97/97 (100%)
Sidechain	99/571 (17%)	16/358 (4%)	76/191 (40%)	7/22 (32%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	16/119 (13%)	8/63 (13%)	0/45 (0%)	8/11 (73%)
Overall	537/1199 (45%)	186/627 (30%)	239/442 (54%)	112/130 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 953 atoms were assigned a chemical shift out of a possible 2146. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	759/913 (83%)	293/369 (79%)	292/370 (79%)	174/174 (100%)
Sidechain	162/1024 (16%)	21/645 (3%)	131/346 (38%)	10/33 (30%)
Aromatic	32/209 (15%)	16/111 (14%)	0/78 (0%)	16/20 (80%)
Overall	953/2146 (44%)	330/1125 (29%)	423/794 (53%)	200/227 (88%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	2	ALA	N	0.00	106.13 – 140.55	-35.8
1	A	4	GLU	N	0.00	103.74 – 137.78	-35.5
1	A	23	GLU	N	0.00	103.74 – 137.78	-35.5
1	A	76	GLU	N	0.00	103.74 – 137.78	-35.5
1	A	113	GLU	N	0.00	103.74 – 137.78	-35.5
1	A	178	GLU	N	0.00	103.74 – 137.78	-35.5
1	A	22	GLY	CA	0.00	38.93 – 51.79	-35.3
1	A	141	LYS	N	0.00	102.74 – 139.42	-33.0
1	A	19	ASP	N	0.00	102.08 – 139.36	-32.4
1	A	121	ASP	N	0.00	102.08 – 139.36	-32.4
1	A	168	ASP	N	0.00	102.08 – 139.36	-32.4
1	A	12	ASN	N	0.00	99.66 – 138.23	-30.8
1	A	22	GLY	N	0.00	91.59 – 127.52	-30.5
1	A	41	GLY	N	0.00	91.59 – 127.52	-30.5
1	A	12	ASN	CA	0.00	44.28 – 62.79	-28.9
1	A	21	ASN	CA	0.00	44.28 – 62.79	-28.9
1	A	59	SER	CA	0.00	48.46 – 68.96	-28.6
1	A	184	SER	CA	0.00	48.46 – 68.96	-28.6
1	A	4	GLU	CA	0.00	47.03 – 67.62	-27.8
1	A	35	GLU	CA	0.00	47.03 – 67.62	-27.8
1	A	157	GLU	CA	0.00	47.03 – 67.62	-27.8
1	A	98	ASP	CA	0.00	44.71 – 64.67	-27.4

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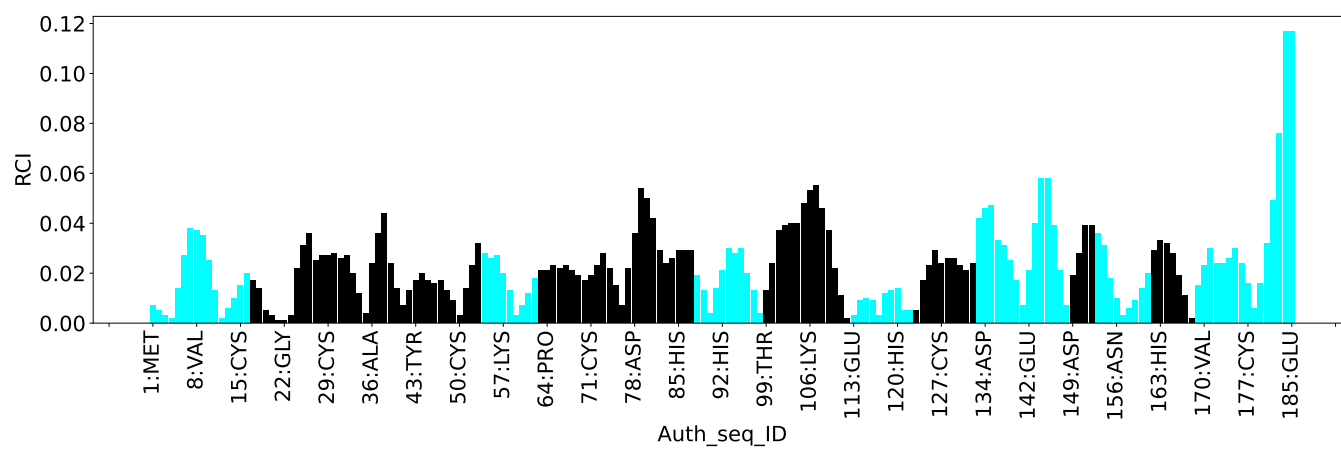
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	117	ASP	CA	0.00	44.71 – 64.67	-27.4
1	A	168	ASP	CA	0.00	44.71 – 64.67	-27.4
1	A	123	CYS	N	0.00	98.14 – 142.06	-27.4
1	A	148	CYS	N	0.00	98.14 – 142.06	-27.4
1	A	90	HIS	CA	0.00	45.04 – 67.94	-24.7
1	A	50	CYS	CA	0.00	40.80 – 75.33	-16.8
1	A	112	CYS	CA	0.00	40.80 – 75.33	-16.8
1	A	28	ASN	HD21	0.00	4.94 – 9.72	-15.3
1	A	19	ASP	H	0.00	5.52 – 11.08	-14.9
1	A	121	ASP	H	0.00	5.52 – 11.08	-14.9
1	A	168	ASP	H	0.00	5.52 – 11.08	-14.9
1	A	4	GLU	H	0.00	5.45 – 11.20	-14.5
1	A	23	GLU	H	0.00	5.45 – 11.20	-14.5
1	A	76	GLU	H	0.00	5.45 – 11.20	-14.5
1	A	113	GLU	H	0.00	5.45 – 11.20	-14.5
1	A	178	GLU	H	0.00	5.45 – 11.20	-14.5
1	A	2	ALA	H	0.00	5.31 – 11.08	-14.2
1	A	141	LYS	H	0.00	5.24 – 11.12	-13.9
1	A	12	ASN	H	0.00	5.28 – 11.36	-13.7
1	A	22	GLY	H	0.00	5.23 – 11.42	-13.5
1	A	41	GLY	H	0.00	5.23 – 11.42	-13.5
1	A	123	CYS	H	0.00	5.02 – 11.74	-12.5
1	A	148	CYS	H	0.00	5.02 – 11.74	-12.5
1	A	90	HIS	ND1	0.00	97.69 – 289.13	-10.1
1	A	120	HIS	ND1	0.00	97.69 – 289.13	-10.1
1	A	136	HIS	ND1	0.00	97.69 – 289.13	-10.1

7.1.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	849
Intra-residue ($ i-j =0$)	76
Sequential ($ i-j =1$)	379
Medium range ($ i-j >1$ and $ i-j <5$)	164
Long range ($ i-j \geq 5$)	170
Inter-chain	0
Hydrogen bond restraints	56
Disulfide bond restraints	4
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	4.4
Number of long range restraints per residue ¹	1.0

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	34.5	0.2
0.2-0.5 (Medium)	113.3	0.5
>0.5 (Large)	80.4	2.35

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

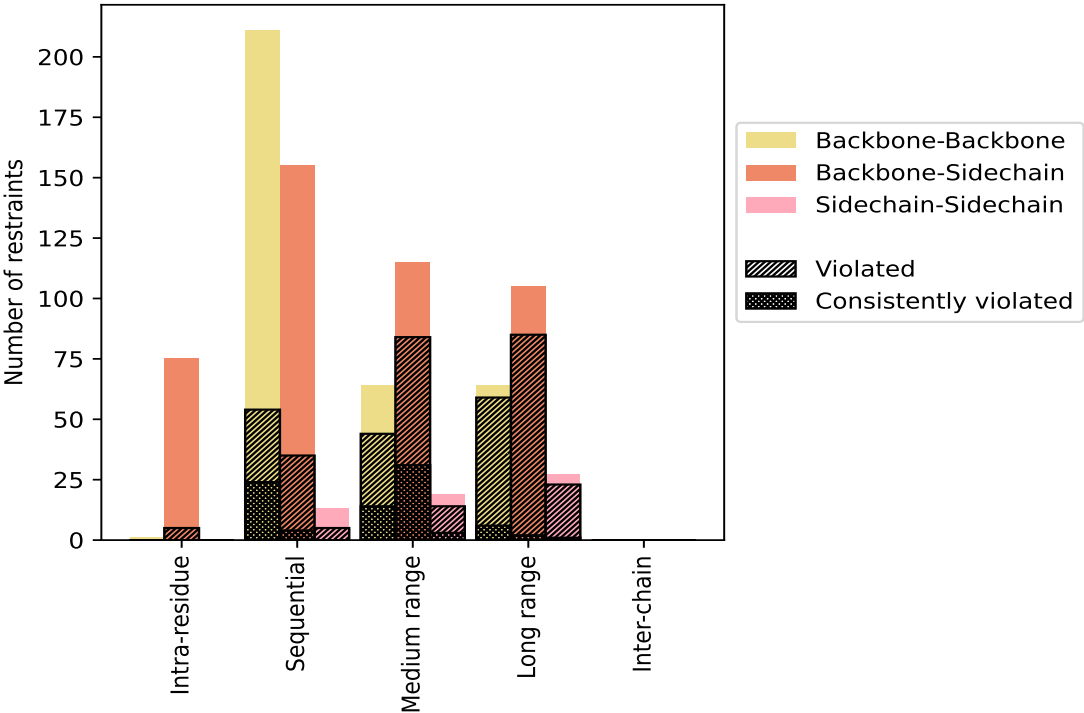
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	76	9.0	5	6.6	0.6	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	75	8.8	5	6.7	0.6	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	379	44.6	94	24.8	11.1	28	7.4	3.3
Backbone-Backbone	211	24.9	54	25.6	6.4	24	11.4	2.8
Backbone-Sidechain	155	18.3	35	22.6	4.1	4	2.6	0.5
Sidechain-Sidechain	13	1.5	5	38.5	0.6	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	164	19.3	118	72.0	13.9	43	26.2	5.1
Backbone-Backbone	64	7.5	44	68.8	5.2	14	21.9	1.6
Backbone-Sidechain	81	9.5	60	74.1	7.1	26	32.1	3.1
Sidechain-Sidechain	19	2.2	14	73.7	1.6	3	15.8	0.4
Long range (i-j ≥5)	170	20.0	141	82.9	16.6	7	4.1	0.8
Backbone-Backbone	64	7.5	59	92.2	6.9	6	9.4	0.7
Backbone-Sidechain	83	9.8	63	75.9	7.4	0	0.0	0.0
Sidechain-Sidechain	23	2.7	19	82.6	2.2	1	4.3	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	56	6.6	46	82.1	5.4	7	12.5	0.8
Disulfide bond	4	0.5	4	100.0	0.5	0	0.0	0.0
Total	849	100.0	408	48.1	48.1	85	10.0	10.0
Backbone-Backbone	340	40.0	157	46.2	18.5	44	12.9	5.2
Backbone-Sidechain	450	53.0	209	46.4	24.6	37	8.2	4.4
Sidechain-Sidechain	59	6.9	42	71.2	4.9	4	6.8	0.5

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

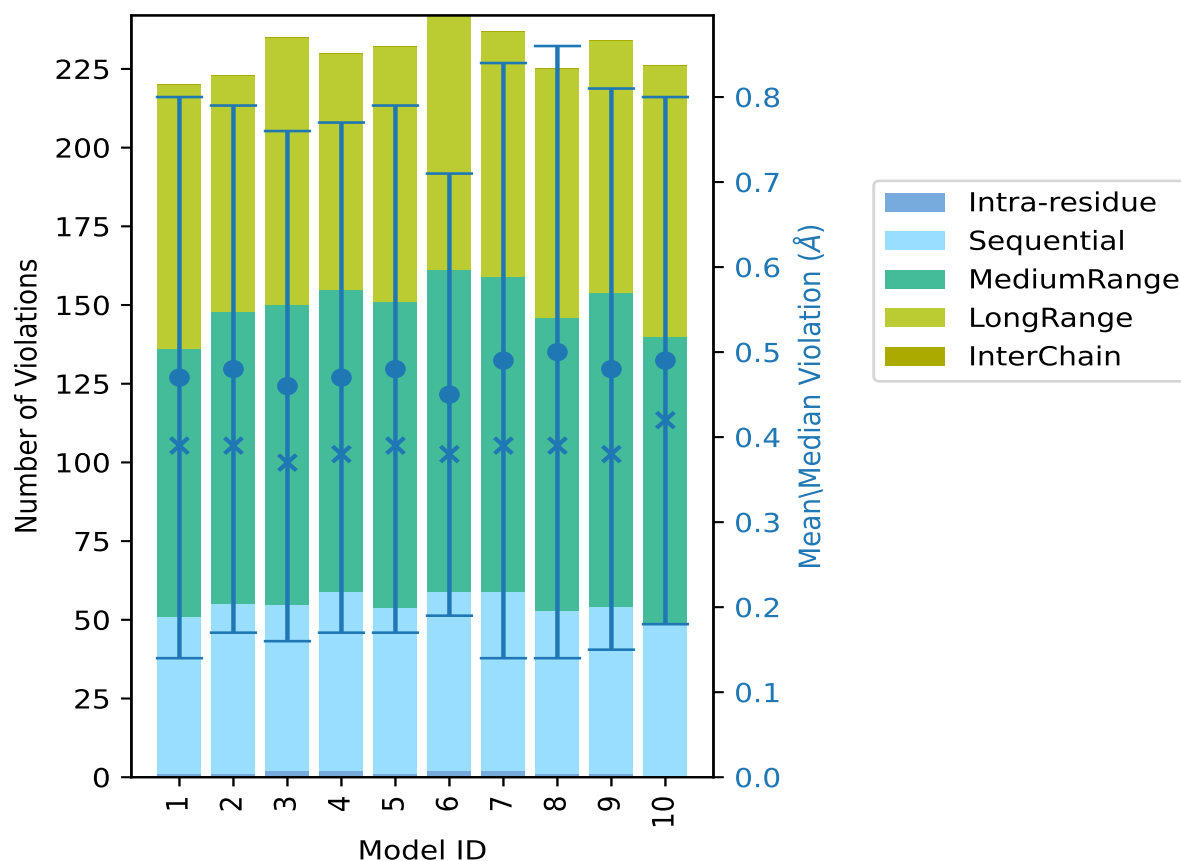
9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	50	85	84	0	220	0.47	2.35	0.33	0.39
2	1	54	93	75	0	223	0.48	1.83	0.31	0.39
3	2	53	95	85	0	235	0.46	1.61	0.3	0.37
4	2	57	96	75	0	230	0.47	1.55	0.3	0.38
5	1	53	97	81	0	232	0.48	1.91	0.31	0.39
6	2	57	102	81	0	242	0.45	1.73	0.26	0.38
7	2	57	100	78	0	237	0.49	2.05	0.35	0.39
8	1	52	93	79	0	225	0.5	2.1	0.36	0.39
9	1	53	100	80	0	234	0.48	1.58	0.33	0.38
10	0	49	91	86	0	226	0.49	1.82	0.31	0.42

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 431(IR:71, SQ:285, MR:46, LR:29, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
4	16	9	27	0	56	1	10.0
0	9	8	14	0	31	2	20.0
0	11	7	23	0	41	3	30.0

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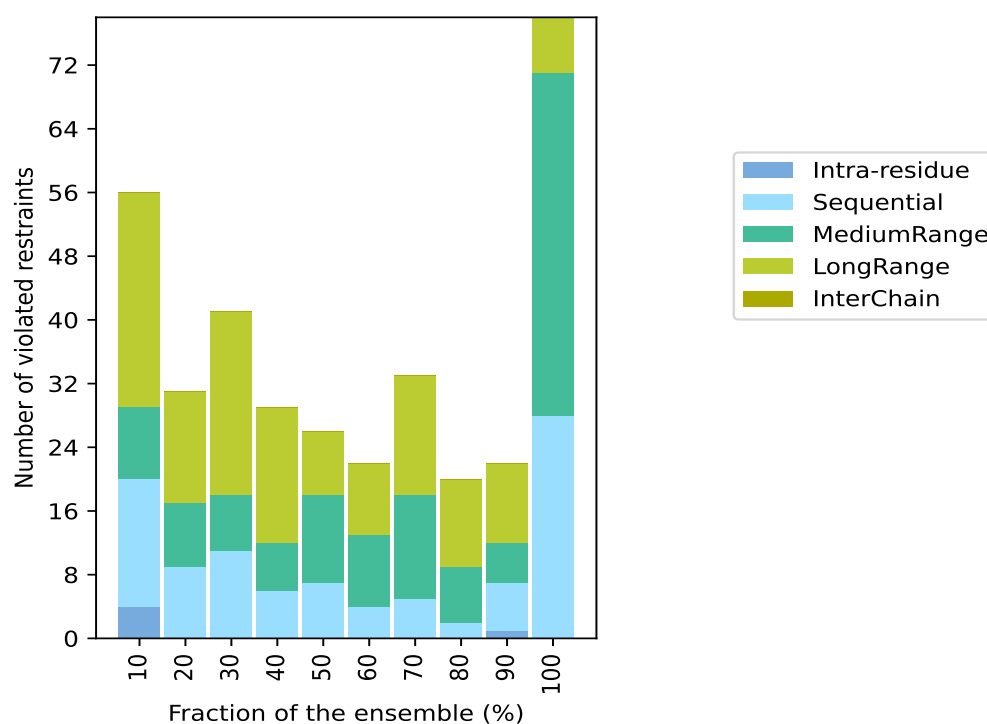
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	6	6	17	0	29	4	40.0
0	7	11	8	0	26	5	50.0
0	4	9	9	0	22	6	60.0
0	5	13	15	0	33	7	70.0
0	2	7	11	0	20	8	80.0
1	6	5	10	0	22	9	90.0
0	28	43	7	0	78	10	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

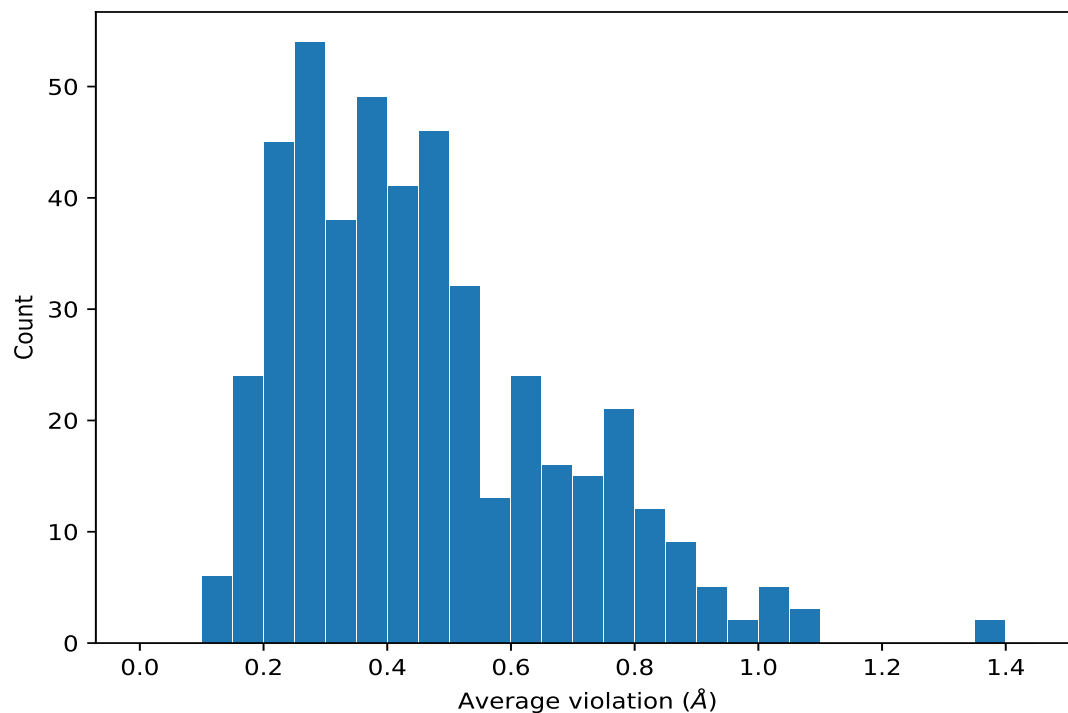


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	10	1.36	0.35	1.28
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	10	1.36	0.35	1.28
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	10	1.05	0.18	1.06
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	10	1.05	0.18	1.06
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	10	1.04	0.52	1.1
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	10	1.0	0.02	1.0
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	10	1.0	0.02	1.0
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	10	0.9	0.11	0.9
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	10	0.9	0.11	0.9
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	10	0.88	0.31	0.82
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	10	0.86	0.04	0.85
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	10	0.86	0.04	0.85
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	10	0.85	0.36	0.69
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	10	0.84	0.3	0.86
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	10	0.84	0.3	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	10	0.84	0.3	0.86
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	10	0.83	0.1	0.84
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	10	0.83	0.1	0.84
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	10	0.82	0.37	0.75
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	10	0.8	0.37	1.0
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	10	0.8	0.37	1.0
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	10	0.8	0.02	0.8
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	10	0.8	0.02	0.8
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	10	0.79	0.26	0.82
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	10	0.79	0.26	0.82
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	10	0.79	0.03	0.78
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	10	0.79	0.03	0.78
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	10	0.78	0.14	0.78
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	10	0.76	0.07	0.78
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	10	0.76	0.07	0.78
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	10	0.73	0.05	0.72
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	10	0.73	0.24	0.7
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	10	0.72	0.56	0.4
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	10	0.71	0.05	0.71
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	10	0.7	0.1	0.73
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	10	0.7	0.1	0.73
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	10	0.7	0.25	0.78
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	10	0.68	0.34	0.64
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	10	0.68	0.34	0.64
(1,275)	1:99:A:THR:H	1:152:A:THR:H	10	0.64	0.19	0.7
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	10	0.64	0.23	0.76
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	10	0.64	0.2	0.56
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	10	0.64	0.2	0.56
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	10	0.63	0.03	0.63
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	10	0.62	0.32	0.49
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	10	0.61	0.02	0.6
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	10	0.61	0.02	0.6
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	10	0.6	0.03	0.59
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	10	0.6	0.43	0.55
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	10	0.57	0.28	0.56
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	10	0.57	0.28	0.56
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	10	0.56	0.01	0.56
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	10	0.55	0.01	0.56
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	10	0.53	0.02	0.52
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	10	0.53	0.02	0.52
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	10	0.51	0.06	0.5
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	10	0.49	0.01	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	10	0.49	0.01	0.49
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	10	0.49	0.06	0.49
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	10	0.49	0.06	0.49
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	10	0.48	0.3	0.41
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	10	0.47	0.02	0.48
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	10	0.47	0.09	0.47
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	10	0.46	0.21	0.38
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	10	0.45	0.0	0.45
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	10	0.45	0.06	0.44
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	10	0.45	0.06	0.44
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	10	0.44	0.02	0.45
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	10	0.41	0.02	0.42
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	10	0.41	0.02	0.42
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	10	0.4	0.19	0.36
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	10	0.4	0.19	0.36
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	10	0.4	0.03	0.4
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	10	0.4	0.03	0.4
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	10	0.4	0.12	0.37
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	10	0.4	0.12	0.37
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	10	0.39	0.12	0.4
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	10	0.36	0.01	0.36
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	10	0.36	0.08	0.39
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	10	0.36	0.08	0.39
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	10	0.36	0.12	0.37
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	10	0.35	0.01	0.36
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	10	0.35	0.07	0.33
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	10	0.35	0.07	0.33
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	10	0.35	0.02	0.36
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	10	0.34	0.02	0.34
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	10	0.34	0.13	0.33
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	10	0.32	0.01	0.32
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	10	0.32	0.01	0.32
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	10	0.32	0.07	0.34
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	10	0.32	0.07	0.34
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	10	0.31	0.09	0.29
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	10	0.31	0.05	0.32
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	10	0.3	0.07	0.3
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	10	0.3	0.07	0.3
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	10	0.3	0.14	0.28
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	10	0.3	0.01	0.3
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	10	0.29	0.01	0.29
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	10	0.29	0.01	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	10	0.29	0.02	0.29
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	10	0.29	0.13	0.25
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	10	0.29	0.13	0.26
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	10	0.28	0.04	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	10	0.28	0.04	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	10	0.28	0.04	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	10	0.28	0.04	0.28
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	10	0.28	0.01	0.28
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	10	0.25	0.0	0.25
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	10	0.25	0.02	0.24
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	10	0.25	0.02	0.24
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	10	0.25	0.02	0.24
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	10	0.24	0.05	0.24
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	10	0.24	0.05	0.24
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	10	0.24	0.02	0.25
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	10	0.21	0.01	0.21
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	10	0.2	0.06	0.19
(3,31)	1:87:A:SER:O	1:91:A:SER:H	10	0.18	0.05	0.17
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	9	1.01	0.36	0.87
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	9	0.94	0.46	0.76
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	9	0.94	0.46	0.76
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	9	0.94	0.25	0.86
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	9	0.86	0.29	0.95
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	9	0.84	0.47	0.64
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	9	0.77	0.31	0.79
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	9	0.77	0.31	0.79
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	9	0.76	0.6	0.41
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	9	0.75	0.32	0.68
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	9	0.75	0.32	0.68
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	9	0.74	0.37	0.68
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	9	0.68	0.34	0.57
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	9	0.67	0.35	0.6
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	9	0.64	0.26	0.59
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	9	0.6	0.2	0.53
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	9	0.52	0.18	0.55
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	9	0.51	0.12	0.48
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	9	0.49	0.16	0.53
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	9	0.49	0.16	0.53
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	9	0.46	0.23	0.53
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	9	0.44	0.14	0.39
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	9	0.41	0.15	0.45
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	9	0.36	0.01	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	9	0.34	0.1	0.4
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	9	0.3	0.04	0.3
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	9	0.3	0.04	0.3
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	9	0.27	0.06	0.28
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	9	0.23	0.03	0.23
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	9	0.23	0.05	0.24
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	9	0.2	0.09	0.17
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	8	0.82	0.53	0.68
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	8	0.78	0.51	0.62
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	8	0.78	0.51	0.62
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	8	0.75	0.29	0.74
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	8	0.7	0.31	0.67
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	8	0.69	0.28	0.76
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	8	0.59	0.18	0.64
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	8	0.58	0.28	0.53
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	8	0.57	0.28	0.58
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	8	0.54	0.35	0.46
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	8	0.54	0.35	0.48
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	8	0.54	0.32	0.44
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	8	0.51	0.29	0.48
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	8	0.51	0.2	0.42
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	8	0.48	0.21	0.48
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	8	0.44	0.26	0.33
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	8	0.4	0.17	0.41
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	8	0.39	0.41	0.2
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	8	0.38	0.14	0.36
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	8	0.38	0.26	0.27
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	8	0.37	0.23	0.28
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	8	0.37	0.23	0.28
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	8	0.36	0.14	0.32
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	8	0.35	0.11	0.32
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	8	0.35	0.11	0.32
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	8	0.35	0.11	0.32
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	8	0.34	0.1	0.39
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	8	0.32	0.16	0.33
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	8	0.27	0.09	0.3
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	8	0.23	0.09	0.24
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	8	0.22	0.05	0.22
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	8	0.22	0.05	0.22
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	8	0.2	0.09	0.17
(1,523)	1:157:A:GLU:H	1:159:A:HIS:H	7	1.05	0.2	1.18
(1,478)	1:133:A:ASN:HA	1:149:A:ASP:HA	7	1.0	0.27	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,186)	1:50:A:CYS:H	1:73:A:HIS:H	7	0.87	0.58	0.59
(3,55)	1:56:A:CYS:O	1:59:A:SER:H	7	0.86	0.41	0.76
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD21	7	0.79	0.42	0.82
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD22	7	0.79	0.42	0.82
(1,104)	1:49:A:ARG:H	1:74:A:CYS:HA	7	0.77	0.36	0.88
(1,573)	1:23:A:GLU:HA	1:27:A:CYS:H	7	0.75	0.45	0.74
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB2	7	0.74	0.31	0.61
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB3	7	0.74	0.31	0.61
(1,51)	1:18:A:CYS:H	1:30:A:GLU:H	7	0.7	0.26	0.59
(1,494)	1:132:A:CYS:HB2	1:150:A:CYS:H	7	0.7	0.42	0.72
(1,494)	1:132:A:CYS:HB3	1:150:A:CYS:H	7	0.7	0.42	0.72
(1,515)	1:154:A:THR:HA	1:161:A:CYS:H	7	0.64	0.53	0.49
(1,554)	1:19:A:ASP:HB2	1:21:A:ASN:H	7	0.64	0.37	0.54
(1,547)	1:18:A:CYS:HB2	1:20:A:ALA:H	7	0.64	0.33	0.67
(1,547)	1:18:A:CYS:HB3	1:20:A:ALA:H	7	0.64	0.33	0.67
(3,56)	1:56:A:CYS:O	1:59:A:SER:N	7	0.63	0.42	0.52
(1,219)	1:21:A:ASN:H	1:47:A:CYS:H	7	0.59	0.32	0.52
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG21	7	0.54	0.33	0.39
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG22	7	0.54	0.33	0.39
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG23	7	0.54	0.33	0.39
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB2	7	0.54	0.19	0.47
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB3	7	0.54	0.19	0.47
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB2	7	0.54	0.19	0.47
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB3	7	0.54	0.19	0.47
(1,177)	1:24:A:ASN:HD21	1:54:A:ASN:H	7	0.53	0.2	0.59
(3,47)	1:37:A:LYS:O	1:44:A:ALA:H	7	0.49	0.15	0.49
(1,638)	1:67:A:GLU:HA	1:69:A:HIS:H	7	0.48	0.17	0.51
(1,320)	1:17:A:HIS:HE1	1:21:A:ASN:HD22	7	0.47	0.16	0.39
(1,457)	1:155:A:CYS:SG	1:161:A:CYS:CB	7	0.47	0.24	0.44
(1,498)	1:140:A:ARG:H	1:142:A:GLU:H	7	0.43	0.3	0.3
(1,418)	1:75:A:HIS:HB2	1:112:A:CYS:H	7	0.43	0.21	0.45
(1,418)	1:75:A:HIS:HB3	1:112:A:CYS:H	7	0.43	0.21	0.45
(1,412)	1:63:A:ILE:HG12	1:66:A:ASN:H	7	0.4	0.25	0.39
(1,412)	1:63:A:ILE:HG13	1:66:A:ASN:H	7	0.4	0.25	0.39
(1,559)	1:20:A:ALA:HA	1:24:A:ASN:H	7	0.35	0.08	0.33
(1,356)	1:154:A:THR:HG1	1:156:A:ASN:H	7	0.31	0.22	0.17
(1,324)	1:52:A:ALA:H	1:54:A:ASN:HD22	7	0.31	0.13	0.25
(1,216)	1:100:A:HIS:HD1	1:102:A:GLU:H	7	0.3	0.09	0.3
(1,315)	1:100:A:HIS:HD1	1:123:A:CYS:H	7	0.29	0.11	0.32
(1,73)	1:162:A:TYR:H	1:163:A:HIS:HD1	7	0.29	0.14	0.22
(1,758)	1:140:A:ARG:HA	1:141:A:LYS:H	7	0.29	0.07	0.27
(3,5)	1:105:A:LYS:O	1:107:A:ALA:H	7	0.27	0.07	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,690)	1:66:A:ASN:HA	1:67:A:GLU:H	7	0.26	0.04	0.27
(1,772)	1:157:A:GLU:HA	1:158:A:ASP:H	7	0.25	0.05	0.28
(3,14)	1:140:A:ARG:O	1:142:A:GLU:N	7	0.23	0.06	0.2
(3,40)	1:19:A:ASP:O	1:23:A:GLU:N	7	0.23	0.1	0.21
(1,398)	1:43:A:TYR:HB2	1:60:A:CYS:H	6	0.69	0.45	0.57
(1,398)	1:43:A:TYR:HB3	1:60:A:CYS:H	6	0.69	0.45	0.57
(1,361)	1:66:A:ASN:H	1:69:A:HIS:HD1	6	0.66	0.43	0.63
(1,416)	1:66:A:ASN:HD21	1:69:A:HIS:HD1	6	0.65	0.23	0.74
(1,416)	1:66:A:ASN:HD22	1:69:A:HIS:HD1	6	0.65	0.23	0.74
(3,15)	1:153:A:ILE:O	1:163:A:HIS:H	6	0.64	0.28	0.8
(1,93)	1:63:A:ILE:HB	1:66:A:ASN:H	6	0.53	0.2	0.47
(1,456)	1:132:A:CYS:CB	1:150:A:CYS:SG	6	0.5	0.11	0.52
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD21	6	0.5	0.18	0.45
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD22	6	0.5	0.18	0.45
(1,512)	1:154:A:THR:HA	1:162:A:TYR:HA	6	0.49	0.19	0.51
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD21	6	0.43	0.15	0.4
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD22	6	0.43	0.15	0.4
(1,71)	1:38:A:LYS:H	1:40:A:ASP:H	6	0.43	0.11	0.48
(1,455)	1:132:A:CYS:SG	1:150:A:CYS:CB	6	0.42	0.17	0.39
(1,158)	1:20:A:ALA:HB1	1:75:A:HIS:H	6	0.4	0.17	0.34
(1,158)	1:20:A:ALA:HB2	1:75:A:HIS:H	6	0.4	0.17	0.34
(1,158)	1:20:A:ALA:HB3	1:75:A:HIS:H	6	0.4	0.17	0.34
(1,295)	1:29:A:CYS:HG	1:31:A:LEU:H	6	0.37	0.16	0.36
(1,458)	1:155:A:CYS:CB	1:161:A:CYS:SG	6	0.37	0.11	0.36
(1,683)	1:58:A:CYS:HA	1:59:A:SER:H	6	0.36	0.02	0.36
(1,109)	1:75:A:HIS:HD1	1:112:A:CYS:H	6	0.36	0.23	0.25
(1,149)	1:20:A:ALA:HB1	1:127:A:CYS:H	6	0.35	0.16	0.4
(1,149)	1:20:A:ALA:HB2	1:127:A:CYS:H	6	0.35	0.16	0.4
(1,149)	1:20:A:ALA:HB3	1:127:A:CYS:H	6	0.35	0.16	0.4
(1,576)	1:26:A:SER:HB2	1:27:A:CYS:H	6	0.35	0.17	0.35
(1,484)	1:135:A:GLU:HB2	1:136:A:HIS:H	6	0.31	0.12	0.33
(1,484)	1:135:A:GLU:HB3	1:136:A:HIS:H	6	0.31	0.12	0.33
(3,2)	1:100:A:HIS:O	1:112:A:CYS:N	6	0.31	0.15	0.31
(1,651)	1:11:A:SER:HA	1:12:A:ASN:H	6	0.27	0.07	0.28
(1,22)	1:161:A:CYS:H	1:163:A:HIS:HD1	6	0.25	0.08	0.27
(1,562)	1:20:A:ALA:HA	1:22:A:GLY:H	6	0.22	0.05	0.22
(1,13)	1:75:A:HIS:HE1	1:77:A:GLU:H	6	0.22	0.07	0.24
(3,21)	1:82:A:THR:O	1:86:A:CYS:H	6	0.22	0.04	0.23
(3,54)	1:52:A:ALA:O	1:63:A:ILE:N	6	0.18	0.09	0.14
(3,28)	1:85:A:HIS:O	1:89:A:GLU:N	6	0.17	0.03	0.16
(1,522)	1:155:A:CYS:HB2	1:161:A:CYS:H	5	0.99	0.52	1.2
(1,522)	1:155:A:CYS:HB3	1:161:A:CYS:H	5	0.99	0.52	1.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,550)	1:18:A:CYS:HB2	1:21:A:ASN:H	5	0.85	0.67	0.48
(1,550)	1:18:A:CYS:HB3	1:21:A:ASN:H	5	0.85	0.67	0.48
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG2	5	0.68	0.28	0.83
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG3	5	0.68	0.28	0.83
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG2	5	0.57	0.08	0.56
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG3	5	0.57	0.08	0.56
(1,628)	1:91:A:SER:HA	1:95:A:HIS:H	5	0.52	0.28	0.38
(1,459)	1:100:A:HIS:H	1:112:A:CYS:H	5	0.51	0.29	0.44
(1,95)	1:81:A:ASP:H	1:85:A:HIS:HD1	5	0.49	0.03	0.5
(1,170)	1:153:A:ILE:HG21	1:155:A:CYS:H	5	0.49	0.23	0.39
(1,170)	1:153:A:ILE:HG22	1:155:A:CYS:H	5	0.49	0.23	0.39
(1,170)	1:153:A:ILE:HG23	1:155:A:CYS:H	5	0.49	0.23	0.39
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB2	5	0.49	0.18	0.56
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB3	5	0.49	0.18	0.56
(1,497)	1:138:A:CYS:H	1:144:A:GLY:H	5	0.43	0.31	0.28
(1,532)	1:43:A:TYR:HB2	1:55:A:ILE:HD11	5	0.43	0.08	0.49
(1,532)	1:43:A:TYR:HB3	1:55:A:ILE:HD11	5	0.43	0.08	0.49
(3,10)	1:136:A:HIS:O	1:146:A:VAL:N	5	0.42	0.34	0.23
(1,528)	1:38:A:LYS:HA	1:43:A:TYR:HA	5	0.41	0.21	0.54
(1,34)	1:166:A:GLU:HB2	1:168:A:ASP:H	5	0.38	0.2	0.31
(1,546)	1:18:A:CYS:HA	1:22:A:GLY:H	5	0.36	0.22	0.39
(3,48)	1:37:A:LYS:O	1:44:A:ALA:N	5	0.32	0.15	0.29
(1,444)	1:159:A:HIS:HB2	1:161:A:CYS:H	5	0.3	0.12	0.28
(1,444)	1:159:A:HIS:HB3	1:161:A:CYS:H	5	0.3	0.12	0.28
(1,419)	1:81:A:ASP:HB2	1:85:A:HIS:HD1	5	0.3	0.03	0.29
(1,419)	1:81:A:ASP:HB3	1:85:A:HIS:HD1	5	0.3	0.03	0.29
(1,106)	1:71:A:CYS:H	1:72:A:HIS:HD1	5	0.28	0.16	0.28
(1,20)	1:112:A:CYS:HG	1:125:A:CYS:H	5	0.28	0.15	0.22
(1,750)	1:131:A:PRO:HA	1:132:A:CYS:H	5	0.27	0.04	0.26
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB2	5	0.27	0.13	0.32
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB3	5	0.27	0.13	0.32
(1,351)	1:123:A:CYS:H	1:125:A:CYS:H	5	0.25	0.09	0.25
(1,188)	1:100:A:HIS:HE1	1:123:A:CYS:H	5	0.25	0.16	0.14
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG2	5	0.24	0.08	0.21
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG3	5	0.24	0.08	0.21
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG2	5	0.24	0.08	0.21
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG3	5	0.24	0.08	0.21
(1,691)	1:67:A:GLU:HA	1:68:A:ASP:H	5	0.22	0.1	0.21
(1,745)	1:125:A:CYS:HA	1:126:A:GLU:H	5	0.19	0.08	0.18
(1,620)	1:89:A:GLU:HA	1:93:A:ASP:H	5	0.19	0.08	0.15
(3,13)	1:140:A:ARG:O	1:142:A:GLU:H	5	0.15	0.05	0.12
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG2	4	0.79	0.6	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG3	4	0.79	0.6	0.5
(1,481)	1:134:A:ASP:H	1:148:A:CYS:H	4	0.72	0.25	0.82
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB2	4	0.68	0.16	0.74
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB3	4	0.68	0.16	0.74
(3,16)	1:153:A:ILE:O	1:163:A:HIS:N	4	0.64	0.08	0.66
(1,56)	1:17:A:HIS:HD1	1:21:A:ASN:H	4	0.62	0.17	0.58
(1,103)	1:49:A:ARG:H	1:74:A:CYS:HG	4	0.6	0.24	0.66
(1,105)	1:49:A:ARG:H	1:74:A:CYS:H	4	0.53	0.38	0.33
(1,121)	1:18:A:CYS:HG	1:20:A:ALA:H	4	0.52	0.18	0.58
(1,15)	1:66:A:ASN:HD22	1:67:A:GLU:H	4	0.5	0.17	0.53
(1,234)	1:112:A:CYS:H	1:125:A:CYS:H	4	0.47	0.21	0.42
(3,42)	1:20:A:ALA:O	1:24:A:ASN:N	4	0.44	0.16	0.44
(1,504)	1:145:A:VAL:HB	1:146:A:VAL:H	4	0.4	0.04	0.42
(1,299)	1:29:A:CYS:HA	1:31:A:LEU:H	4	0.4	0.06	0.39
(1,542)	1:53:A:ASN:HA	1:62:A:ALA:HA	4	0.38	0.17	0.41
(3,37)	1:18:A:CYS:O	1:22:A:GLY:H	4	0.38	0.17	0.39
(1,415)	1:66:A:ASN:HD21	1:68:A:ASP:H	4	0.37	0.14	0.34
(1,415)	1:66:A:ASN:HD22	1:68:A:ASP:H	4	0.37	0.14	0.34
(1,241)	1:101:A:GLY:H	1:123:A:CYS:HB3	4	0.37	0.27	0.25
(1,32)	1:152:A:THR:HG21	1:168:A:ASP:H	4	0.36	0.13	0.34
(1,32)	1:152:A:THR:HG22	1:168:A:ASP:H	4	0.36	0.13	0.34
(1,32)	1:152:A:THR:HG23	1:168:A:ASP:H	4	0.36	0.13	0.34
(1,527)	1:37:A:LYS:H	1:44:A:ALA:H	4	0.35	0.23	0.28
(3,50)	1:54:A:ASN:O	1:61:A:THR:N	4	0.34	0.16	0.37
(1,749)	1:129:A:LYS:HA	1:130:A:LEU:H	4	0.32	0.01	0.32
(1,362)	1:65:A:CYS:HG	1:69:A:HIS:HD1	4	0.31	0.06	0.33
(1,139)	1:75:A:HIS:HD1	1:124:A:GLY:H	4	0.3	0.02	0.29
(1,538)	1:54:A:ASN:H	1:61:A:THR:H	4	0.3	0.02	0.3
(2,1)	1:34:A:CYS:SG	1:47:A:CYS:SG	4	0.28	0.12	0.3
(1,168)	1:29:A:CYS:H	1:128:A:SER:HG	4	0.27	0.22	0.17
(1,500)	1:140:A:ARG:HG2	1:141:A:LYS:H	4	0.27	0.11	0.26
(1,500)	1:140:A:ARG:HG3	1:141:A:LYS:H	4	0.27	0.11	0.26
(3,11)	1:138:A:CYS:O	1:144:A:GLY:H	4	0.26	0.08	0.25
(1,163)	1:100:A:HIS:H	1:152:A:THR:H	4	0.25	0.09	0.27
(1,271)	1:99:A:THR:H	1:152:A:THR:HG1	4	0.25	0.08	0.26
(1,462)	1:103:A:CYS:HB2	1:104:A:THR:H	4	0.24	0.12	0.2
(1,462)	1:103:A:CYS:HB3	1:104:A:THR:H	4	0.24	0.12	0.2
(1,446)	1:166:A:GLU:HG2	1:168:A:ASP:H	4	0.24	0.09	0.22
(1,446)	1:166:A:GLU:HG3	1:168:A:ASP:H	4	0.24	0.09	0.22
(3,52)	1:50:A:CYS:O	1:65:A:CYS:N	4	0.23	0.08	0.23
(2,3)	1:132:A:CYS:SG	1:150:A:CYS:SG	4	0.22	0.17	0.12
(1,544)	1:55:A:ILE:HA	1:60:A:CYS:HA	4	0.2	0.14	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,719)	1:97:A:ASP:HA	1:98:A:ASP:H	4	0.16	0.03	0.15
(1,33)	1:152:A:THR:H	1:168:A:ASP:H	4	0.16	0.04	0.16
(3,26)	1:84:A:CYS:O	1:88:A:CYS:N	4	0.12	0.01	0.12
(1,386)	1:17:A:HIS:HD1	1:21:A:ASN:HB2	3	0.65	0.16	0.75
(1,386)	1:17:A:HIS:HD1	1:21:A:ASN:HB3	3	0.65	0.16	0.75
(1,310)	1:100:A:HIS:HD1	1:168:A:ASP:H	3	0.61	0.37	0.59
(1,29)	1:17:A:HIS:H	1:29:A:CYS:HA	3	0.57	0.52	0.23
(1,133)	1:28:A:ASN:H	1:29:A:CYS:HG	3	0.5	0.26	0.5
(1,496)	1:137:A:PRO:HA	1:145:A:VAL:HA	3	0.5	0.39	0.32
(1,30)	1:17:A:HIS:H	1:31:A:LEU:HB3	3	0.47	0.11	0.49
(1,381)	1:10:A:ASN:HD21	1:11:A:SER:HB2	3	0.47	0.11	0.46
(1,381)	1:10:A:ASN:HD21	1:11:A:SER:HB3	3	0.47	0.11	0.46
(1,381)	1:10:A:ASN:HD22	1:11:A:SER:HB2	3	0.47	0.11	0.46
(1,381)	1:10:A:ASN:HD22	1:11:A:SER:HB3	3	0.47	0.11	0.46
(1,535)	1:44:A:ALA:HB1	1:55:A:ILE:HG23	3	0.46	0.24	0.6
(1,535)	1:44:A:ALA:HB2	1:55:A:ILE:HG23	3	0.46	0.24	0.6
(1,535)	1:44:A:ALA:HB3	1:55:A:ILE:HG23	3	0.46	0.24	0.6
(1,634)	1:93:A:ASP:HA	1:95:A:HIS:H	3	0.46	0.29	0.44
(1,476)	1:103:A:CYS:HB2	1:109:A:CYS:HA	3	0.46	0.07	0.46
(1,476)	1:103:A:CYS:HB3	1:109:A:CYS:HA	3	0.46	0.07	0.46
(1,212)	1:17:A:HIS:HA	1:30:A:GLU:H	3	0.46	0.2	0.47
(1,417)	1:66:A:ASN:HD21	1:69:A:HIS:HE1	3	0.46	0.17	0.57
(1,417)	1:66:A:ASN:HD22	1:69:A:HIS:HE1	3	0.46	0.17	0.57
(1,173)	1:29:A:CYS:H	1:129:A:LYS:H	3	0.45	0.19	0.45
(1,26)	1:17:A:HIS:H	1:31:A:LEU:HB2	3	0.44	0.1	0.4
(1,293)	1:17:A:HIS:HB2	1:31:A:LEU:H	3	0.43	0.36	0.26
(1,224)	1:11:A:SER:H	1:16:A:TYR:H	3	0.42	0.37	0.18
(1,490)	1:139:A:TYR:HB2	1:140:A:ARG:H	3	0.41	0.02	0.42
(1,490)	1:139:A:TYR:HB3	1:140:A:ARG:H	3	0.41	0.02	0.42
(1,322)	1:17:A:HIS:HD1	1:21:A:ASN:HD22	3	0.41	0.18	0.51
(1,213)	1:30:A:GLU:H	1:128:A:SER:HG	3	0.37	0.22	0.29
(1,451)	1:34:A:CYS:SG	1:47:A:CYS:CB	3	0.36	0.11	0.3
(1,537)	1:56:A:CYS:H	1:59:A:SER:H	3	0.36	0.32	0.15
(1,516)	1:155:A:CYS:HB2	1:156:A:ASN:H	3	0.36	0.05	0.39
(1,516)	1:155:A:CYS:HB3	1:156:A:ASN:H	3	0.36	0.05	0.39
(1,292)	1:18:A:CYS:H	1:31:A:LEU:H	3	0.35	0.06	0.31
(1,517)	1:156:A:ASN:HB2	1:157:A:GLU:H	3	0.33	0.01	0.32
(1,517)	1:156:A:ASN:HB3	1:157:A:GLU:H	3	0.33	0.01	0.32
(1,112)	1:75:A:HIS:HD1	1:77:A:GLU:H	3	0.31	0.16	0.32
(1,767)	1:152:A:THR:HA	1:153:A:ILE:H	3	0.29	0.03	0.27
(1,721)	1:99:A:THR:HA	1:100:A:HIS:H	3	0.29	0.07	0.29
(1,519)	1:158:A:ASP:HB2	1:159:A:HIS:H	3	0.29	0.0	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,519)	1:158:A:ASP:HB3	1:159:A:HIS:H	3	0.29	0.0	0.29
(1,701)	1:78:A:ASP:HA	1:79:A:ASP:H	3	0.28	0.11	0.35
(1,131)	1:17:A:HIS:HB2	1:28:A:ASN:H	3	0.27	0.07	0.22
(3,43)	1:21:A:ASN:O	1:25:A:CYS:H	3	0.27	0.15	0.23
(1,340)	1:105:A:LYS:HB3	1:162:A:TYR:H	3	0.26	0.13	0.25
(3,38)	1:18:A:CYS:O	1:22:A:GLY:N	3	0.25	0.11	0.26
(1,437)	1:135:A:GLU:HB2	1:184:A:SER:H	3	0.23	0.1	0.19
(1,437)	1:135:A:GLU:HB3	1:184:A:SER:H	3	0.23	0.1	0.19
(1,135)	1:17:A:HIS:HB3	1:28:A:ASN:H	3	0.22	0.06	0.19
(1,454)	1:103:A:CYS:CB	1:109:A:CYS:SG	3	0.21	0.07	0.25
(1,503)	1:142:A:GLU:HB2	1:143:A:GLY:H	3	0.2	0.02	0.2
(1,503)	1:142:A:GLU:HB3	1:143:A:GLY:H	3	0.2	0.02	0.2
(1,245)	1:101:A:GLY:H	1:152:A:THR:H	3	0.18	0.07	0.16
(1,278)	1:59:A:SER:H	1:61:A:THR:HG21	3	0.18	0.06	0.19
(1,278)	1:59:A:SER:H	1:61:A:THR:HG22	3	0.18	0.06	0.19
(1,278)	1:59:A:SER:H	1:61:A:THR:HG23	3	0.18	0.06	0.19
(1,773)	1:158:A:ASP:HA	1:159:A:HIS:H	3	0.16	0.04	0.13
(1,147)	1:10:A:ASN:HD22	1:16:A:TYR:H	3	0.14	0.0	0.14
(1,363)	1:136:A:HIS:HD1	1:183:A:PRO:HB3	3	0.12	0.0	0.12
(1,408)	1:53:A:ASN:HD21	1:63:A:ILE:H	2	0.64	0.18	0.64
(1,408)	1:53:A:ASN:HD22	1:63:A:ILE:H	2	0.64	0.18	0.64
(1,460)	1:100:A:HIS:HB2	1:101:A:GLY:H	2	0.56	0.28	0.56
(1,460)	1:100:A:HIS:HB3	1:101:A:GLY:H	2	0.56	0.28	0.56
(1,118)	1:152:A:THR:HG21	1:166:A:GLU:H	2	0.54	0.09	0.54
(1,118)	1:152:A:THR:HG22	1:166:A:GLU:H	2	0.54	0.09	0.54
(1,118)	1:152:A:THR:HG23	1:166:A:GLU:H	2	0.54	0.09	0.54
(1,391)	1:24:A:ASN:HD21	1:54:A:ASN:HB2	2	0.48	0.34	0.48
(1,391)	1:24:A:ASN:HD21	1:54:A:ASN:HB3	2	0.48	0.34	0.48
(1,391)	1:24:A:ASN:HD22	1:54:A:ASN:HB2	2	0.48	0.34	0.48
(1,391)	1:24:A:ASN:HD22	1:54:A:ASN:HB3	2	0.48	0.34	0.48
(1,113)	1:75:A:HIS:HD1	1:126:A:GLU:H	2	0.41	0.22	0.41
(1,452)	1:47:A:CYS:SG	1:34:A:CYS:CB	2	0.4	0.07	0.4
(1,442)	1:153:A:ILE:HG12	1:155:A:CYS:H	2	0.37	0.19	0.37
(1,442)	1:153:A:ILE:HG13	1:155:A:CYS:H	2	0.37	0.19	0.37
(1,549)	1:18:A:CYS:HB2	1:19:A:ASP:H	2	0.36	0.01	0.36
(1,549)	1:18:A:CYS:HB3	1:19:A:ASP:H	2	0.36	0.01	0.36
(1,728)	1:106:A:LYS:HA	1:107:A:ALA:H	2	0.32	0.01	0.32
(1,48)	1:10:A:ASN:H	1:13:A:ALA:H	2	0.31	0.06	0.31
(1,717)	1:95:A:HIS:HA	1:96:A:ASP:H	2	0.29	0.01	0.29
(1,379)	1:10:A:ASN:HB2	1:17:A:HIS:H	2	0.28	0.15	0.28
(1,379)	1:10:A:ASN:HB3	1:17:A:HIS:H	2	0.28	0.15	0.28
(1,181)	1:75:A:HIS:HD2	1:123:A:CYS:H	2	0.28	0.06	0.28

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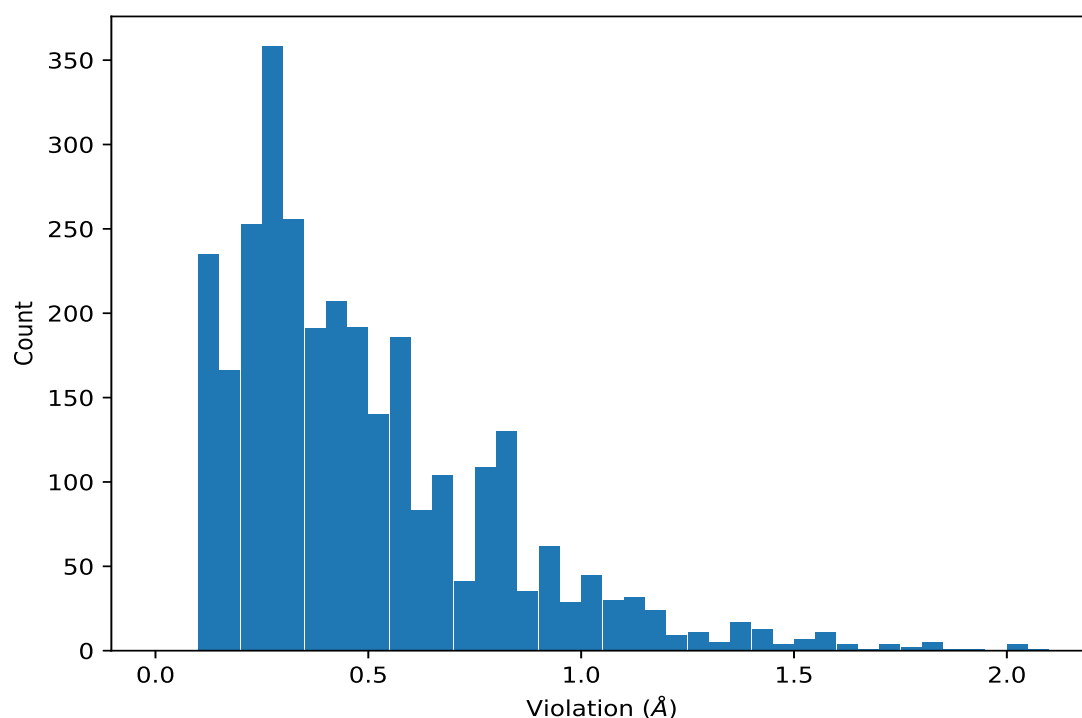
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,467)	1:106:A:LYS:HB2	1:107:A:ALA:H	2	0.26	0.13	0.26
(1,467)	1:106:A:LYS:HB3	1:107:A:ALA:H	2	0.26	0.13	0.26
(1,35)	1:100:A:HIS:HD2	1:168:A:ASP:H	2	0.25	0.12	0.25
(1,463)	1:104:A:THR:HG1	1:105:A:LYS:H	2	0.24	0.15	0.24
(1,639)	1:65:A:CYS:HA	1:67:A:GLU:H	2	0.24	0.1	0.24
(1,479)	1:133:A:ASN:HB2	1:134:A:ASP:H	2	0.22	0.12	0.22
(1,479)	1:133:A:ASN:HB3	1:134:A:ASP:H	2	0.22	0.12	0.22
(1,413)	1:63:A:ILE:HG12	1:66:A:ASN:HD21	2	0.22	0.02	0.22
(1,413)	1:63:A:ILE:HG12	1:66:A:ASN:HD22	2	0.22	0.02	0.22
(1,413)	1:63:A:ILE:HG13	1:66:A:ASN:HD21	2	0.22	0.02	0.22
(1,413)	1:63:A:ILE:HG13	1:66:A:ASN:HD22	2	0.22	0.02	0.22
(3,44)	1:21:A:ASN:O	1:25:A:CYS:N	2	0.2	0.03	0.2
(1,480)	1:133:A:ASN:HD21	1:134:A:ASP:H	2	0.2	0.02	0.2
(1,190)	1:75:A:HIS:HD1	1:123:A:CYS:H	2	0.19	0.04	0.19
(3,18)	1:157:A:GLU:O	1:159:A:HIS:N	2	0.19	0.01	0.19
(1,693)	1:70:A:PRO:HA	1:71:A:CYS:H	2	0.18	0.04	0.18
(1,24)	1:10:A:ASN:HD22	1:17:A:HIS:H	2	0.17	0.04	0.17
(1,569)	1:22:A:GLY:HA2	1:26:A:SER:H	2	0.17	0.07	0.17
(1,569)	1:22:A:GLY:HA3	1:26:A:SER:H	2	0.17	0.07	0.17
(1,569)	1:22:A:GLY:HA2	1:26:A:SER:H	2	0.17	0.07	0.17
(1,569)	1:22:A:GLY:HA3	1:26:A:SER:H	2	0.17	0.07	0.17
(2,2)	1:103:A:CYS:SG	1:109:A:CYS:SG	2	0.16	0.04	0.16
(1,114)	1:159:A:HIS:HD1	1:161:A:CYS:H	2	0.15	0.04	0.15
(1,585)	1:83:A:HIS:HA	1:87:A:SER:H	2	0.15	0.03	0.15
(1,57)	1:10:A:ASN:H	1:16:A:TYR:H	2	0.13	0.02	0.13
(1,338)	1:105:A:LYS:HG2	1:162:A:TYR:H	2	0.13	0.03	0.13
(1,137)	1:172:A:LYS:H	1:174:A:ASP:H	2	0.12	0.02	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	8	2.1
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	7	2.05
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	7	2.05
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	1	2.01
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	1	2.01
(1,515)	1:154:A:THR:HA	1:161:A:CYS:H	5	1.91
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	8	1.87
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG2	2	1.83
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG3	2	1.83
(3,55)	1:56:A:CYS:O	1:59:A:SER:H	7	1.82
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	10	1.82
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	8	1.8
(1,550)	1:18:A:CYS:HB2	1:21:A:ASN:H	5	1.75
(1,550)	1:18:A:CYS:HB3	1:21:A:ASN:H	5	1.75
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	5	1.74
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	5	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	6	1.73
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	6	1.73
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	7	1.7
(3,56)	1:56:A:CYS:O	1:59:A:SER:N	7	1.63
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	8	1.61
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	3	1.61
(1,186)	1:50:A:CYS:H	1:73:A:HIS:H	5	1.6
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	8	1.59
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	9	1.58
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	8	1.58
(1,522)	1:155:A:CYS:HB2	1:161:A:CYS:H	7	1.57
(1,522)	1:155:A:CYS:HB3	1:161:A:CYS:H	7	1.57
(1,550)	1:18:A:CYS:HB2	1:21:A:ASN:H	3	1.56
(1,550)	1:18:A:CYS:HB3	1:21:A:ASN:H	3	1.56
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	3	1.56
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	3	1.56
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	4	1.55
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	4	1.55
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD21	2	1.54
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD22	2	1.54
(1,478)	1:133:A:ASN:HA	1:149:A:ASP:HA	8	1.52
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	10	1.5
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	10	1.5
(1,186)	1:50:A:CYS:H	1:73:A:HIS:H	1	1.5
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	5	1.5
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	4	1.49
(1,162)	1:99:A:THR:H	1:110:A:TRP:HE1	10	1.49
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	7	1.48
(1,186)	1:50:A:CYS:H	1:73:A:HIS:H	9	1.46
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	7	1.45
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	9	1.45
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	3	1.45
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	9	1.43
(1,522)	1:155:A:CYS:HB2	1:161:A:CYS:H	9	1.43
(1,522)	1:155:A:CYS:HB3	1:161:A:CYS:H	9	1.43
(1,398)	1:43:A:TYR:HB2	1:60:A:CYS:H	2	1.43
(1,398)	1:43:A:TYR:HB3	1:60:A:CYS:H	2	1.43
(1,361)	1:66:A:ASN:H	1:69:A:HIS:HD1	8	1.43
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	4	1.42
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	9	1.42
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	9	1.42
(1,573)	1:23:A:GLU:HA	1:27:A:CYS:H	5	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	1	1.4
(1,494)	1:132:A:CYS:HB2	1:150:A:CYS:H	9	1.4
(1,494)	1:132:A:CYS:HB3	1:150:A:CYS:H	9	1.4
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	3	1.4
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	9	1.39
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	7	1.38
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	8	1.38
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	8	1.38
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	4	1.37
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	1	1.37
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	10	1.37
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	10	1.37
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	10	1.36
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	9	1.36
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	9	1.36
(1,554)	1:19:A:ASP:HB2	1:21:A:ASN:H	2	1.35
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	8	1.35
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	2	1.34
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	2	1.33
(1,523)	1:157:A:GLU:H	1:159:A:HIS:H	10	1.32
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	9	1.3
(1,29)	1:17:A:HIS:H	1:29:A:CYS:HA	2	1.3
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	3	1.26
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	3	1.25
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	3	1.25
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	5	1.25
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	5	1.25
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	7	1.25
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	7	1.25
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	9	1.25
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	7	1.25
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	5	1.25
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	5	1.25
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	3	1.24
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	2	1.24
(1,547)	1:18:A:CYS:HB2	1:20:A:ALA:H	3	1.23
(1,547)	1:18:A:CYS:HB3	1:20:A:ALA:H	3	1.23
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	10	1.23
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	6	1.21
(1,523)	1:157:A:GLU:H	1:159:A:HIS:H	3	1.21
(1,219)	1:21:A:ASN:H	1:47:A:CYS:H	5	1.21
(1,104)	1:49:A:ARG:H	1:74:A:CYS:HA	9	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	9	1.2
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	9	1.2
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	4	1.2
(1,522)	1:155:A:CYS:HB2	1:161:A:CYS:H	4	1.2
(1,522)	1:155:A:CYS:HB3	1:161:A:CYS:H	4	1.2
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	9	1.19
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	6	1.19
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	6	1.19
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	8	1.19
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	8	1.19
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	1	1.19
(1,523)	1:157:A:GLU:H	1:159:A:HIS:H	6	1.19
(1,105)	1:49:A:ARG:H	1:74:A:CYS:H	1	1.19
(1,523)	1:157:A:GLU:H	1:159:A:HIS:H	5	1.18
(1,478)	1:133:A:ASN:HA	1:149:A:ASP:HA	7	1.18
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	3	1.18
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG21	9	1.17
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG22	9	1.17
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG23	9	1.17
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	9	1.16
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	9	1.16
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	9	1.16
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	5	1.16
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	4	1.16
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	9	1.15
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	9	1.15
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	8	1.15
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	8	1.15
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	8	1.15
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	6	1.15
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	6	1.15
(1,573)	1:23:A:GLU:HA	1:27:A:CYS:H	3	1.14
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	10	1.14
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	10	1.14
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	2	1.14
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	2	1.14
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	7	1.13
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB2	5	1.13
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB3	5	1.13
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	1	1.12
(1,573)	1:23:A:GLU:HA	1:27:A:CYS:H	4	1.12
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	7	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	7	1.12
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	7	1.12
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	4	1.12
(1,498)	1:140:A:ARG:H	1:142:A:GLU:H	2	1.12
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	2	1.11
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	1	1.11
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	1	1.11
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	10	1.11
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	4	1.1
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD21	9	1.1
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD22	9	1.1
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	4	1.1
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	4	1.1
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	4	1.1
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	4	1.09
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	6	1.09
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	6	1.09
(1,398)	1:43:A:TYR:HB2	1:60:A:CYS:H	8	1.09
(1,398)	1:43:A:TYR:HB3	1:60:A:CYS:H	8	1.09
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	9	1.08
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	9	1.08
(1,483)	1:135:A:GLU:HA	1:147:A:SER:HA	10	1.08
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	9	1.08
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	4	1.07
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	3	1.07
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB2	8	1.07
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB3	8	1.07
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	9	1.07
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	9	1.07
(1,310)	1:100:A:HIS:HD1	1:168:A:ASP:H	7	1.07
(1,51)	1:18:A:CYS:H	1:30:A:GLU:H	3	1.07
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	8	1.06
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	8	1.06
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	6	1.06
(1,459)	1:100:A:HIS:H	1:112:A:CYS:H	10	1.06
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	8	1.06
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	7	1.06
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	7	1.05
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	7	1.05
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	4	1.05
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	4	1.05
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	1	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	1	1.05
(1,104)	1:49:A:ARG:H	1:74:A:CYS:HA	1	1.05
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	7	1.04
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	7	1.04
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	6	1.04
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	6	1.04
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	7	1.04
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	7	1.04
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	7	1.04
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB2	2	1.04
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB3	2	1.04
(1,496)	1:137:A:PRO:HA	1:145:A:VAL:HA	10	1.04
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG2	4	1.04
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG3	4	1.04
(1,541)	1:51:A:ASP:HA	1:64:A:PRO:HA	1	1.03
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	4	1.03
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	4	1.03
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	10	1.03
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	10	1.03
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	2	1.03
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	3	1.02
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	3	1.02
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	2	1.02
(1,478)	1:133:A:ASN:HA	1:149:A:ASP:HA	5	1.02
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	2	1.02
(3,10)	1:136:A:HIS:O	1:146:A:VAL:N	10	1.01
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	5	1.01
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	5	1.01
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	9	1.01
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	9	1.01
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	6	1.01
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	6	1.01
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	9	1.01
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	9	1.01
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	10	1.01
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	10	1.01
(1,554)	1:19:A:ASP:HB2	1:21:A:ASN:H	9	1.01
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	1	1.01
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	6	1.0
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	6	1.0
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	1	1.0
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	1	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	5	1.0
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	5	1.0
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	8	1.0
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	8	1.0
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	3	1.0
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	2	0.99
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	3	0.99
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	3	0.99
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	2	0.99
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	2	0.99
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	3	0.99
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	3	0.99
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	1	0.99
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	1	0.99
(1,104)	1:49:A:ARG:H	1:74:A:CYS:HA	3	0.99
(1,51)	1:18:A:CYS:H	1:30:A:GLU:H	5	0.99
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	10	0.98
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	8	0.97
(1,586)	1:83:A:HIS:HB2	1:86:A:CYS:H	4	0.97
(1,586)	1:83:A:HIS:HB3	1:86:A:CYS:H	4	0.97
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	10	0.97
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	2	0.97
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	2	0.97
(1,457)	1:155:A:CYS:SG	1:161:A:CYS:CB	4	0.97
(1,628)	1:91:A:SER:HA	1:95:A:HIS:H	7	0.96
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	2	0.96
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	2	0.96
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	7	0.96
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	7	0.96
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	10	0.96
(1,497)	1:138:A:CYS:H	1:144:A:GLY:H	10	0.96
(1,494)	1:132:A:CYS:HB2	1:150:A:CYS:H	4	0.96
(1,494)	1:132:A:CYS:HB3	1:150:A:CYS:H	4	0.96
(1,478)	1:133:A:ASN:HA	1:149:A:ASP:HA	4	0.96
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	10	0.95
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	6	0.95
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	7	0.94
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	4	0.94
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	4	0.94
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	7	0.94
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	7	0.94
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	1	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	1	0.94
(1,507)	1:147:A:SER:HB2	1:149:A:ASP:H	8	0.94
(1,507)	1:147:A:SER:HB3	1:149:A:ASP:H	8	0.94
(1,494)	1:132:A:CYS:HB2	1:150:A:CYS:H	7	0.94
(1,494)	1:132:A:CYS:HB3	1:150:A:CYS:H	7	0.94
(1,224)	1:11:A:SER:H	1:16:A:TYR:H	5	0.94
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	10	0.93
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	10	0.93
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	2	0.93
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	10	0.93
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	6	0.93
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	6	0.93
(1,481)	1:134:A:ASP:H	1:148:A:CYS:H	10	0.93
(1,416)	1:66:A:ASN:HD21	1:69:A:HIS:HD1	8	0.93
(1,416)	1:66:A:ASN:HD22	1:69:A:HIS:HD1	8	0.93
(1,293)	1:17:A:HIS:HB2	1:31:A:LEU:H	10	0.93
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	10	0.92
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	10	0.92
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	2	0.92
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	1	0.92
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	1	0.92
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	3	0.92
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	3	0.92
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	4	0.92
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	4	0.92
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	9	0.92
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	7	0.92
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	6	0.91
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	6	0.91
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	1	0.91
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	1	0.91
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	4	0.91
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	4	0.91
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	10	0.91
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	10	0.91
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	2	0.91
(3,15)	1:153:A:ILE:O	1:163:A:HIS:H	2	0.9
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	2	0.9
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	2	0.9
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	1	0.9
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	8	0.9
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	3	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	3	0.9
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD21	7	0.9
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD22	7	0.9
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	1	0.9
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	6	0.9
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	1	0.9
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	1	0.9
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	1	0.9
(1,523)	1:157:A:GLU:H	1:159:A:HIS:H	4	0.9
(1,361)	1:66:A:ASN:H	1:69:A:HIS:HD1	9	0.9
(1,56)	1:17:A:HIS:HD1	1:21:A:ASN:H	4	0.9
(1,51)	1:18:A:CYS:H	1:30:A:GLU:H	1	0.9
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	1	0.89
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	1	0.89
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	8	0.89
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	8	0.89
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	6	0.89
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	3	0.89
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	1	0.89
(1,275)	1:99:A:THR:H	1:152:A:THR:H	10	0.88
(1,104)	1:49:A:ARG:H	1:74:A:CYS:HA	5	0.88
(3,15)	1:153:A:ILE:O	1:163:A:HIS:H	8	0.87
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	2	0.87
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	2	0.87
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	2	0.87
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	2	0.87
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	10	0.87
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	10	0.87
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	4	0.87
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	9	0.87
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	9	0.87
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	5	0.87
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	5	0.87
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	5	0.87
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	5	0.87
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG21	5	0.87
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG22	5	0.87
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG23	5	0.87
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	6	0.86
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	1	0.86
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	1	0.86
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	1	0.86
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	7	0.86
(1,275)	1:99:A:THR:H	1:152:A:THR:H	5	0.86
(1,219)	1:21:A:ASN:H	1:47:A:CYS:H	10	0.86
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	10	0.86
(3,55)	1:56:A:CYS:O	1:59:A:SER:H	2	0.85
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	2	0.85
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	2	0.85
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	3	0.85
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	3	0.85
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	8	0.85
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	8	0.85
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	9	0.85
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	9	0.85
(1,600)	1:85:A:HIS:HB2	1:87:A:SER:H	8	0.85
(1,600)	1:85:A:HIS:HB3	1:87:A:SER:H	8	0.85
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	5	0.85
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	5	0.85
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	1	0.85
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	2	0.85
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD21	1	0.85
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD22	1	0.85
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB2	5	0.84
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB3	5	0.84
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB2	5	0.84
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB3	5	0.84
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	5	0.84
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	5	0.84
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	5	0.84
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	6	0.84
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	10	0.84
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	1	0.84
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	5	0.84
(1,478)	1:133:A:ASN:HA	1:149:A:ASP:HA	10	0.84
(1,460)	1:100:A:HIS:HB2	1:101:A:GLY:H	10	0.84
(1,460)	1:100:A:HIS:HB3	1:101:A:GLY:H	10	0.84
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG2	6	0.84
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG3	6	0.84
(1,321)	1:20:A:ALA:HA	1:21:A:ASN:HD22	2	0.84
(1,109)	1:75:A:HIS:HD1	1:112:A:CYS:H	10	0.84
(3,15)	1:153:A:ILE:O	1:163:A:HIS:H	5	0.83
(1,634)	1:93:A:ASP:HA	1:95:A:HIS:H	3	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	4	0.83
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	9	0.83
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	9	0.83
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	3	0.83
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	3	0.83
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	4	0.83
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	4	0.83
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	9	0.83
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	3	0.83
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	3	0.83
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	3	0.83
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	2	0.83
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG2	3	0.83
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG3	3	0.83
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	9	0.83
(1,241)	1:101:A:GLY:H	1:123:A:CYS:HB3	10	0.83
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	6	0.83
(1,103)	1:49:A:ARG:H	1:74:A:CYS:HG	7	0.83
(3,55)	1:56:A:CYS:O	1:59:A:SER:H	9	0.82
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	6	0.82
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	6	0.82
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	8	0.82
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	8	0.82
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	5	0.82
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	5	0.82
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD21	5	0.82
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD22	5	0.82
(1,537)	1:56:A:CYS:H	1:59:A:SER:H	8	0.82
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	6	0.82
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	6	0.82
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	9	0.82
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	9	0.82
(1,481)	1:134:A:ASP:H	1:148:A:CYS:H	5	0.82
(1,481)	1:134:A:ASP:H	1:148:A:CYS:H	8	0.82
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	6	0.82
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	6	0.82
(1,408)	1:53:A:ASN:HD21	1:63:A:ILE:H	8	0.82
(1,408)	1:53:A:ASN:HD22	1:63:A:ILE:H	8	0.82
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB2	4	0.82
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB3	4	0.82
(1,391)	1:24:A:ASN:HD21	1:54:A:ASN:HB2	2	0.82
(1,391)	1:24:A:ASN:HD21	1:54:A:ASN:HB3	2	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:24:A:ASN:HD22	1:54:A:ASN:HB2	2	0.82
(1,391)	1:24:A:ASN:HD22	1:54:A:ASN:HB3	2	0.82
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	6	0.82
(1,133)	1:28:A:ASN:H	1:29:A:CYS:HG	4	0.82
(1,104)	1:49:A:ARG:H	1:74:A:CYS:HA	2	0.82
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	10	0.81
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	4	0.81
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	4	0.81
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	5	0.81
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	5	0.81
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	8	0.81
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	8	0.81
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	3	0.81
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	3	0.81
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	3	0.81
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	4	0.81
(1,412)	1:63:A:ILE:HG12	1:66:A:ASN:H	1	0.81
(1,412)	1:63:A:ILE:HG13	1:66:A:ASN:H	1	0.81
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB2	7	0.81
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB3	7	0.81
(1,93)	1:63:A:ILE:HB	1:66:A:ASN:H	5	0.81
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB2	9	0.8
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB3	9	0.8
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB2	9	0.8
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB3	9	0.8
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	3	0.8
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	3	0.8
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	6	0.8
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	6	0.8
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	4	0.8
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	1	0.8
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	1	0.8
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	2	0.8
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	2	0.8
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	8	0.8
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	8	0.8
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	10	0.8
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	10	0.8
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	1	0.8
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	1	0.8
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	8	0.8
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	10	0.8
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	10	0.8
(1,523)	1:157:A:GLU:H	1:159:A:HIS:H	7	0.8
(1,478)	1:133:A:ASN:HA	1:149:A:ASP:HA	9	0.8
(1,418)	1:75:A:HIS:HB2	1:112:A:CYS:H	8	0.8
(1,418)	1:75:A:HIS:HB3	1:112:A:CYS:H	8	0.8
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	1	0.8
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	5	0.8
(1,103)	1:49:A:ARG:H	1:74:A:CYS:HG	10	0.8
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	2	0.79
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	2	0.79
(1,638)	1:67:A:GLU:HA	1:69:A:HIS:H	1	0.79
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	1	0.79
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	1	0.79
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	2	0.79
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	2	0.79
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	10	0.79
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	10	0.79
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	6	0.79
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	6	0.79
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	4	0.79
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	4	0.79
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	2	0.79
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	2	0.79
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	10	0.79
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	10	0.79
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	2	0.79
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	4	0.79
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	4	0.79
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	8	0.79
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	8	0.79
(1,234)	1:112:A:CYS:H	1:125:A:CYS:H	10	0.79
(1,177)	1:24:A:ASN:HD21	1:54:A:ASN:H	6	0.79
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	6	0.79
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	5	0.78
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	5	0.78
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	5	0.78
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	7	0.78
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	7	0.78
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	7	0.78
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	7	0.78
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	6	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	6	0.78
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	8	0.78
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	8	0.78
(1,547)	1:18:A:CYS:HB2	1:20:A:ALA:H	5	0.78
(1,547)	1:18:A:CYS:HB3	1:20:A:ALA:H	5	0.78
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	6	0.78
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	6	0.78
(1,523)	1:157:A:GLU:H	1:159:A:HIS:H	9	0.78
(1,416)	1:66:A:ASN:HD21	1:69:A:HIS:HD1	2	0.78
(1,416)	1:66:A:ASN:HD22	1:69:A:HIS:HD1	2	0.78
(1,416)	1:66:A:ASN:HD21	1:69:A:HIS:HD1	9	0.78
(1,416)	1:66:A:ASN:HD22	1:69:A:HIS:HD1	9	0.78
(1,356)	1:154:A:THR:HG1	1:156:A:ASN:H	5	0.78
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	4	0.78
(1,93)	1:63:A:ILE:HB	1:66:A:ASN:H	9	0.78
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	6	0.77
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	3	0.77
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	9	0.77
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	9	0.77
(1,630)	1:91:A:SER:HB2	1:93:A:ASP:H	7	0.77
(1,630)	1:91:A:SER:HB3	1:93:A:ASP:H	7	0.77
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	6	0.77
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	1	0.77
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	1	0.77
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	2	0.77
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	2	0.77
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	9	0.77
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	9	0.77
(1,547)	1:18:A:CYS:HB2	1:20:A:ALA:H	6	0.77
(1,547)	1:18:A:CYS:HB3	1:20:A:ALA:H	6	0.77
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	10	0.77
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	10	0.77
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	10	0.77
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	7	0.77
(1,455)	1:132:A:CYS:SG	1:150:A:CYS:CB	9	0.77
(1,386)	1:17:A:HIS:HD1	1:21:A:ASN:HB2	1	0.77
(1,386)	1:17:A:HIS:HD1	1:21:A:ASN:HB3	1	0.77
(1,170)	1:153:A:ILE:HG21	1:155:A:CYS:H	2	0.77
(1,170)	1:153:A:ILE:HG22	1:155:A:CYS:H	2	0.77
(1,170)	1:153:A:ILE:HG23	1:155:A:CYS:H	2	0.77
(3,55)	1:56:A:CYS:O	1:59:A:SER:H	4	0.76
(3,15)	1:153:A:ILE:O	1:163:A:HIS:H	7	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	8	0.76
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	10	0.76
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	10	0.76
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	8	0.76
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	8	0.76
(1,589)	1:83:A:HIS:HB2	1:85:A:HIS:H	4	0.76
(1,589)	1:83:A:HIS:HB3	1:85:A:HIS:H	4	0.76
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	6	0.76
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	7	0.76
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	7	0.76
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	7	0.76
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	7	0.76
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	3	0.76
(3,47)	1:37:A:LYS:O	1:44:A:ALA:H	3	0.75
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	7	0.75
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	10	0.75
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	8	0.75
(1,605)	1:86:A:CYS:HB2	1:88:A:CYS:H	4	0.75
(1,605)	1:86:A:CYS:HB3	1:88:A:CYS:H	4	0.75
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	1	0.75
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	2	0.75
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	10	0.75
(1,595)	1:84:A:CYS:HB2	1:87:A:SER:H	10	0.75
(1,595)	1:84:A:CYS:HB3	1:87:A:SER:H	10	0.75
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	3	0.75
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	5	0.75
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	7	0.75
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD21	7	0.75
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD22	7	0.75
(1,386)	1:17:A:HIS:HD1	1:21:A:ASN:HB2	4	0.75
(1,386)	1:17:A:HIS:HD1	1:21:A:ASN:HB3	4	0.75
(1,170)	1:153:A:ILE:HG21	1:155:A:CYS:H	5	0.75
(1,170)	1:153:A:ILE:HG22	1:155:A:CYS:H	5	0.75
(1,170)	1:153:A:ILE:HG23	1:155:A:CYS:H	5	0.75
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	5	0.74
(1,573)	1:23:A:GLU:HA	1:27:A:CYS:H	10	0.74
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	6	0.74
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	10	0.74
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	5	0.74
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	9	0.74
(1,398)	1:43:A:TYR:HB2	1:60:A:CYS:H	1	0.74
(1,398)	1:43:A:TYR:HB3	1:60:A:CYS:H	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	5	0.74
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	7	0.73
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	3	0.73
(3,16)	1:153:A:ILE:O	1:163:A:HIS:N	2	0.73
(1,628)	1:91:A:SER:HA	1:95:A:HIS:H	4	0.73
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	3	0.73
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	8	0.73
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	8	0.73
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	7	0.73
(1,275)	1:99:A:THR:H	1:152:A:THR:H	2	0.73
(1,158)	1:20:A:ALA:HB1	1:75:A:HIS:H	2	0.73
(1,158)	1:20:A:ALA:HB2	1:75:A:HIS:H	2	0.73
(1,158)	1:20:A:ALA:HB3	1:75:A:HIS:H	2	0.73
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	8	0.72
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	9	0.72
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	9	0.72
(1,546)	1:18:A:CYS:HA	1:22:A:GLY:H	2	0.72
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	7	0.72
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	6	0.72
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	8	0.72
(1,494)	1:132:A:CYS:HB2	1:150:A:CYS:H	6	0.72
(1,494)	1:132:A:CYS:HB3	1:150:A:CYS:H	6	0.72
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	9	0.72
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	5	0.72
(1,275)	1:99:A:THR:H	1:152:A:THR:H	6	0.72
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	10	0.72
(1,34)	1:166:A:GLU:HB2	1:168:A:ASP:H	3	0.72
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	4	0.72
(3,16)	1:153:A:ILE:O	1:163:A:HIS:N	8	0.71
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	2	0.71
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	1	0.71
(1,512)	1:154:A:THR:HA	1:162:A:TYR:HA	4	0.71
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	6	0.71
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	5	0.7
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	2	0.7
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	2	0.7
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	10	0.7
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	10	0.7
(1,527)	1:37:A:LYS:H	1:44:A:ALA:H	2	0.7
(1,416)	1:66:A:ASN:HD21	1:69:A:HIS:HD1	5	0.7
(1,416)	1:66:A:ASN:HD22	1:69:A:HIS:HD1	5	0.7
(1,361)	1:66:A:ASN:H	1:69:A:HIS:HD1	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	3	0.7
(1,275)	1:99:A:THR:H	1:152:A:THR:H	7	0.7
(1,275)	1:99:A:THR:H	1:152:A:THR:H	9	0.7
(1,177)	1:24:A:ASN:HD21	1:54:A:ASN:H	4	0.7
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	7	0.7
(1,15)	1:66:A:ASN:HD22	1:67:A:GLU:H	6	0.7
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	4	0.69
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	2	0.69
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	9	0.69
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	10	0.69
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	6	0.69
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	7	0.69
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	3	0.69
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	8	0.69
(1,512)	1:154:A:THR:HA	1:162:A:TYR:HA	8	0.69
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	6	0.69
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	6	0.69
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	7	0.69
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	7	0.69
(1,212)	1:17:A:HIS:HA	1:30:A:GLU:H	9	0.69
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	7	0.68
(1,615)	1:88:A:CYS:HA	1:91:A:SER:HA	7	0.68
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	4	0.68
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	6	0.68
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	6	0.68
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	10	0.68
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	10	0.68
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	6	0.68
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	3	0.68
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	3	0.68
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	8	0.68
(1,320)	1:17:A:HIS:HE1	1:21:A:ASN:HD22	8	0.68
(1,173)	1:29:A:CYS:H	1:129:A:LYS:H	5	0.68
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	1	0.67
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	4	0.67
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	3	0.67
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	3	0.67
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	4	0.67
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	4	0.67
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	3	0.67
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	6	0.67
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	6	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	9	0.67
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	9	0.67
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	4	0.67
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	4	0.67
(1,547)	1:18:A:CYS:HB2	1:20:A:ALA:H	8	0.67
(1,547)	1:18:A:CYS:HB3	1:20:A:ALA:H	8	0.67
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	5	0.67
(1,535)	1:44:A:ALA:HB1	1:55:A:ILE:HG23	6	0.67
(1,535)	1:44:A:ALA:HB2	1:55:A:ILE:HG23	6	0.67
(1,535)	1:44:A:ALA:HB3	1:55:A:ILE:HG23	6	0.67
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	1	0.67
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB2	6	0.67
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB3	6	0.67
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	4	0.67
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	5	0.67
(1,121)	1:18:A:CYS:HG	1:20:A:ALA:H	5	0.67
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	10	0.67
(3,55)	1:56:A:CYS:O	1:59:A:SER:H	8	0.66
(3,42)	1:20:A:ALA:O	1:24:A:ASN:N	2	0.66
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	3	0.66
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	7	0.66
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	5	0.66
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	9	0.66
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	8	0.66
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	8	0.66
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	6	0.66
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	6	0.66
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	6	0.66
(1,515)	1:154:A:THR:HA	1:161:A:CYS:H	8	0.66
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	3	0.66
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	4	0.66
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	4	0.66
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	1	0.66
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	4	0.66
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	4	0.66
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG2	6	0.66
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG3	6	0.66
(1,275)	1:99:A:THR:H	1:152:A:THR:H	4	0.66
(1,213)	1:30:A:GLU:H	1:128:A:SER:HG	9	0.66
(1,177)	1:24:A:ASN:HD21	1:54:A:ASN:H	2	0.66
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB2	6	0.66
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB3	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	3	0.65
(1,633)	1:92:A:HIS:HB2	1:94:A:HIS:H	7	0.65
(1,633)	1:92:A:HIS:HB3	1:94:A:HIS:H	7	0.65
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	5	0.65
(1,528)	1:38:A:LYS:HA	1:43:A:TYR:HA	4	0.65
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	9	0.65
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	6	0.65
(1,478)	1:133:A:ASN:HA	1:149:A:ASP:HA	3	0.65
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	8	0.65
(1,121)	1:18:A:CYS:HG	1:20:A:ALA:H	10	0.65
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	5	0.65
(3,55)	1:56:A:CYS:O	1:59:A:SER:H	3	0.64
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	3	0.64
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	6	0.64
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	7	0.64
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	5	0.64
(1,602)	1:85:A:HIS:HA	1:87:A:SER:H	9	0.64
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	7	0.64
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	7	0.64
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD21	3	0.64
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD22	3	0.64
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	5	0.64
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	5	0.64
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	8	0.64
(1,456)	1:132:A:CYS:CB	1:150:A:CYS:SG	8	0.64
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG2	5	0.64
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG3	5	0.64
(1,320)	1:17:A:HIS:HE1	1:21:A:ASN:HD22	6	0.64
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	6	0.64
(1,250)	1:101:A:GLY:H	1:123:A:CYS:HB2	10	0.64
(1,168)	1:29:A:CYS:H	1:128:A:SER:HG	5	0.64
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	4	0.64
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	4	0.64
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	3	0.64
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	1	0.63
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	2	0.63
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	1	0.63
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	3	0.63
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	3	0.63
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	5	0.63
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	5	0.63
(1,118)	1:152:A:THR:HG21	1:166:A:GLU:H	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:152:A:THR:HG22	1:166:A:GLU:H	4	0.63
(1,118)	1:152:A:THR:HG23	1:166:A:GLU:H	4	0.63
(1,113)	1:75:A:HIS:HD1	1:126:A:GLU:H	6	0.63
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	9	0.63
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	5	0.62
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	7	0.62
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	9	0.62
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	4	0.62
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	3	0.62
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	3	0.62
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	7	0.62
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	7	0.62
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	7	0.62
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	10	0.62
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	1	0.62
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	1	0.62
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	4	0.62
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	4	0.62
(1,320)	1:17:A:HIS:HE1	1:21:A:ASN:HD22	9	0.62
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	1	0.62
(1,219)	1:21:A:ASN:H	1:47:A:CYS:H	2	0.62
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	3	0.62
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	8	0.61
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	10	0.61
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	9	0.61
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	6	0.61
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	6	0.61
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	3	0.61
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	9	0.61
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	9	0.61
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	6	0.61
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	6	0.61
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	9	0.61
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	9	0.61
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	10	0.61
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	10	0.61
(1,566)	1:21:A:ASN:HB2	1:24:A:ASN:H	7	0.61
(1,566)	1:21:A:ASN:HB3	1:24:A:ASN:H	7	0.61
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	9	0.61
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	7	0.61
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	5	0.61
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	5	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	5	0.61
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	9	0.61
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB2	4	0.61
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB3	4	0.61
(1,497)	1:138:A:CYS:H	1:144:A:GLY:H	1	0.61
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	10	0.61
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	10	0.61
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	7	0.61
(1,418)	1:75:A:HIS:HB2	1:112:A:CYS:H	3	0.61
(1,418)	1:75:A:HIS:HB3	1:112:A:CYS:H	3	0.61
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	1	0.6
(3,16)	1:153:A:ILE:O	1:163:A:HIS:N	7	0.6
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	6	0.6
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	1	0.6
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	1	0.6
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	5	0.6
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	5	0.6
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	8	0.6
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	8	0.6
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	2	0.6
(1,535)	1:44:A:ALA:HB1	1:55:A:ILE:HG23	8	0.6
(1,535)	1:44:A:ALA:HB2	1:55:A:ILE:HG23	8	0.6
(1,535)	1:44:A:ALA:HB3	1:55:A:ILE:HG23	8	0.6
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	2	0.6
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	8	0.6
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	8	0.6
(1,381)	1:10:A:ASN:HD21	1:11:A:SER:HB2	5	0.6
(1,381)	1:10:A:ASN:HD21	1:11:A:SER:HB3	5	0.6
(1,381)	1:10:A:ASN:HD22	1:11:A:SER:HB2	5	0.6
(1,381)	1:10:A:ASN:HD22	1:11:A:SER:HB3	5	0.6
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	1	0.6
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	7	0.6
(1,56)	1:17:A:HIS:HD1	1:21:A:ASN:H	8	0.6
(1,50)	1:17:A:HIS:H	1:30:A:GLU:H	2	0.6
(1,30)	1:17:A:HIS:H	1:31:A:LEU:HB3	3	0.6
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	5	0.6
(3,47)	1:37:A:LYS:O	1:44:A:ALA:H	8	0.59
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	4	0.59
(3,37)	1:18:A:CYS:O	1:22:A:GLY:H	10	0.59
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	2	0.59
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	10	0.59
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	7	0.59
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	8	0.59
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	9	0.59
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	3	0.59
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	3	0.59
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	5	0.59
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	5	0.59
(1,594)	1:84:A:CYS:HB2	1:86:A:CYS:H	7	0.59
(1,594)	1:84:A:CYS:HB3	1:86:A:CYS:H	7	0.59
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	2	0.59
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	2	0.59
(1,576)	1:26:A:SER:HB2	1:27:A:CYS:H	3	0.59
(1,542)	1:53:A:ASN:HA	1:62:A:ALA:HA	8	0.59
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	1	0.59
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	1	0.59
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	2	0.59
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	2	0.59
(1,412)	1:63:A:ILE:HG12	1:66:A:ASN:H	5	0.59
(1,412)	1:63:A:ILE:HG13	1:66:A:ASN:H	5	0.59
(1,310)	1:100:A:HIS:HD1	1:168:A:ASP:H	8	0.59
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	9	0.59
(1,186)	1:50:A:CYS:H	1:73:A:HIS:H	7	0.59
(1,177)	1:24:A:ASN:HD21	1:54:A:ASN:H	8	0.59
(1,51)	1:18:A:CYS:H	1:30:A:GLU:H	8	0.59
(3,56)	1:56:A:CYS:O	1:59:A:SER:N	9	0.58
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	10	0.58
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	8	0.58
(3,29)	1:86:A:CYS:O	1:90:A:HIS:H	9	0.58
(3,10)	1:136:A:HIS:O	1:146:A:VAL:N	5	0.58
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	1	0.58
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	3	0.58
(1,494)	1:132:A:CYS:HB2	1:150:A:CYS:H	2	0.58
(1,494)	1:132:A:CYS:HB3	1:150:A:CYS:H	2	0.58
(1,456)	1:132:A:CYS:CB	1:150:A:CYS:SG	6	0.58
(1,456)	1:132:A:CYS:CB	1:150:A:CYS:SG	10	0.58
(1,417)	1:66:A:ASN:HD21	1:69:A:HIS:HE1	6	0.58
(1,417)	1:66:A:ASN:HD22	1:69:A:HIS:HE1	6	0.58
(1,415)	1:66:A:ASN:HD21	1:68:A:ASP:H	10	0.58
(1,415)	1:66:A:ASN:HD22	1:68:A:ASP:H	10	0.58
(1,412)	1:63:A:ILE:HG12	1:66:A:ASN:H	9	0.58
(1,412)	1:63:A:ILE:HG13	1:66:A:ASN:H	9	0.58
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD21	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD22	8	0.58
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	2	0.58
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	2	0.58
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	2	0.58
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	9	0.58
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB2	1	0.58
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB3	1	0.58
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	1	0.58
(1,26)	1:17:A:HIS:H	1:31:A:LEU:HB2	3	0.58
(3,56)	1:56:A:CYS:O	1:59:A:SER:N	2	0.57
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	6	0.57
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	7	0.57
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	5	0.57
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	2	0.57
(1,606)	1:86:A:CYS:HA	1:88:A:CYS:H	10	0.57
(1,590)	1:83:A:HIS:HB2	1:86:A:CYS:H	4	0.57
(1,590)	1:83:A:HIS:HB3	1:86:A:CYS:H	4	0.57
(1,583)	1:82:A:THR:HB	1:84:A:CYS:H	6	0.57
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	1	0.57
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	2	0.57
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	4	0.57
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	8	0.57
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	10	0.57
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	8	0.57
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	8	0.57
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	7	0.57
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	7	0.57
(1,528)	1:38:A:LYS:HA	1:43:A:TYR:HA	2	0.57
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB2	7	0.57
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB3	7	0.57
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	3	0.57
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	3	0.57
(1,417)	1:66:A:ASN:HD21	1:69:A:HIS:HE1	8	0.57
(1,417)	1:66:A:ASN:HD22	1:69:A:HIS:HE1	8	0.57
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	3	0.57
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	9	0.57
(1,149)	1:20:A:ALA:HB1	1:127:A:CYS:H	10	0.57
(1,149)	1:20:A:ALA:HB2	1:127:A:CYS:H	10	0.57
(1,149)	1:20:A:ALA:HB3	1:127:A:CYS:H	10	0.57
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	8	0.57
(1,106)	1:71:A:CYS:H	1:72:A:HIS:HD1	1	0.57
(1,56)	1:17:A:HIS:HD1	1:21:A:ASN:H	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	10	0.56
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	4	0.56
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	3	0.56
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	3	0.56
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	5	0.56
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	5	0.56
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	1	0.56
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	2	0.56
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	4	0.56
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	8	0.56
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	10	0.56
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	3	0.56
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	6	0.56
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	3	0.56
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	3	0.56
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	6	0.56
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	6	0.56
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	9	0.56
(1,442)	1:153:A:ILE:HG12	1:155:A:CYS:H	8	0.56
(1,442)	1:153:A:ILE:HG13	1:155:A:CYS:H	8	0.56
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	4	0.56
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	4	0.56
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	2	0.56
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	2	0.56
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG2	9	0.56
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG3	9	0.56
(1,361)	1:66:A:ASN:H	1:69:A:HIS:HD1	2	0.56
(1,322)	1:17:A:HIS:HD1	1:21:A:ASN:HD22	6	0.56
(1,295)	1:29:A:CYS:HG	1:31:A:LEU:H	4	0.56
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	6	0.56
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG21	3	0.56
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG22	3	0.56
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG23	3	0.56
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB2	10	0.56
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB3	10	0.56
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	8	0.55
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	2	0.55
(3,7)	1:134:A:ASP:O	1:148:A:CYS:H	5	0.55
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB2	6	0.55
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB3	6	0.55
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB2	6	0.55
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB3	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	6	0.55
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	1	0.55
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	6	0.55
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	6	0.55
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	3	0.55
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	4	0.55
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	4	0.55
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	3	0.55
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	5	0.55
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	9	0.55
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	5	0.55
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	7	0.55
(1,577)	1:82:A:THR:HA	1:83:A:HIS:H	9	0.55
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	9	0.55
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	9	0.55
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	10	0.55
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	10	0.55
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	8	0.55
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	2	0.55
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	6	0.55
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	6	0.55
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	7	0.55
(1,476)	1:103:A:CYS:HB2	1:109:A:CYS:HA	5	0.55
(1,476)	1:103:A:CYS:HB3	1:109:A:CYS:HA	5	0.55
(1,295)	1:29:A:CYS:HG	1:31:A:LEU:H	9	0.55
(1,71)	1:38:A:LYS:H	1:40:A:ASP:H	1	0.55
(1,51)	1:18:A:CYS:H	1:30:A:GLU:H	4	0.55
(1,20)	1:112:A:CYS:HG	1:125:A:CYS:H	1	0.55
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	3	0.54
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	6	0.54
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	1	0.54
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	6	0.54
(1,638)	1:67:A:GLU:HA	1:69:A:HIS:H	4	0.54
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	4	0.54
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	4	0.54
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	7	0.54
(1,554)	1:19:A:ASP:HB2	1:21:A:ASN:H	7	0.54
(1,554)	1:19:A:ASP:HB2	1:21:A:ASN:H	10	0.54
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	4	0.54
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	4	0.54
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	4	0.54
(1,528)	1:38:A:LYS:HA	1:43:A:TYR:HA	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	7	0.54
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	7	0.54
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	2	0.54
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	10	0.54
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	10	0.54
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	4	0.54
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	10	0.54
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	10	0.54
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG2	3	0.54
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG3	3	0.54
(1,275)	1:99:A:THR:H	1:152:A:THR:H	3	0.54
(1,95)	1:81:A:ASP:H	1:85:A:HIS:HD1	7	0.54
(1,32)	1:152:A:THR:HG21	1:168:A:ASP:H	10	0.54
(1,32)	1:152:A:THR:HG22	1:168:A:ASP:H	10	0.54
(1,32)	1:152:A:THR:HG23	1:168:A:ASP:H	10	0.54
(1,15)	1:66:A:ASN:HD22	1:67:A:GLU:H	5	0.54
(1,11)	1:135:A:GLU:H	1:136:A:HIS:HE1	10	0.54
(3,47)	1:37:A:LYS:O	1:44:A:ALA:H	9	0.53
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	10	0.53
(3,16)	1:153:A:ILE:O	1:163:A:HIS:N	5	0.53
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	3	0.53
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	6	0.53
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	6	0.53
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	7	0.53
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	7	0.53
(1,587)	1:83:A:HIS:HA	1:84:A:CYS:H	6	0.53
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	6	0.53
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	1	0.53
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	1	0.53
(1,522)	1:155:A:CYS:HB2	1:161:A:CYS:H	1	0.53
(1,522)	1:155:A:CYS:HB3	1:161:A:CYS:H	1	0.53
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	2	0.53
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	8	0.53
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	4	0.53
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	4	0.53
(1,458)	1:155:A:CYS:CB	1:161:A:CYS:SG	4	0.53
(1,457)	1:155:A:CYS:SG	1:161:A:CYS:CB	6	0.53
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	5	0.53
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	5	0.53
(1,234)	1:112:A:CYS:H	1:125:A:CYS:H	8	0.53
(1,188)	1:100:A:HIS:HE1	1:123:A:CYS:H	8	0.53
(1,103)	1:49:A:ARG:H	1:74:A:CYS:HG	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	6	0.53
(3,56)	1:56:A:CYS:O	1:59:A:SER:N	4	0.52
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	10	0.52
(3,48)	1:37:A:LYS:O	1:44:A:ALA:N	8	0.52
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	10	0.52
(2,4)	1:155:A:CYS:SG	1:161:A:CYS:SG	4	0.52
(2,3)	1:132:A:CYS:SG	1:150:A:CYS:SG	10	0.52
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	2	0.52
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	9	0.52
(1,547)	1:18:A:CYS:HB2	1:20:A:ALA:H	1	0.52
(1,547)	1:18:A:CYS:HB3	1:20:A:ALA:H	1	0.52
(1,543)	1:53:A:ASN:HA	1:61:A:THR:H	1	0.52
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	1	0.52
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	1	0.52
(1,512)	1:154:A:THR:HA	1:162:A:TYR:HA	10	0.52
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	2	0.52
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	2	0.52
(1,457)	1:155:A:CYS:SG	1:161:A:CYS:CB	3	0.52
(1,451)	1:34:A:CYS:SG	1:47:A:CYS:CB	10	0.52
(1,414)	1:65:A:CYS:HB2	1:69:A:HIS:HD1	3	0.52
(1,414)	1:65:A:CYS:HB3	1:69:A:HIS:HD1	3	0.52
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG2	8	0.52
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG3	8	0.52
(1,219)	1:21:A:ASN:H	1:47:A:CYS:H	9	0.52
(1,121)	1:18:A:CYS:HG	1:20:A:ALA:H	4	0.52
(1,95)	1:81:A:ASP:H	1:85:A:HIS:HD1	3	0.52
(1,93)	1:63:A:ILE:HB	1:66:A:ASN:H	8	0.52
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	9	0.52
(1,15)	1:66:A:ASN:HD22	1:67:A:GLU:H	9	0.52
(3,50)	1:54:A:ASN:O	1:61:A:THR:N	10	0.51
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	10	0.51
(1,638)	1:67:A:GLU:HA	1:69:A:HIS:H	7	0.51
(1,638)	1:67:A:GLU:HA	1:69:A:HIS:H	10	0.51
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	8	0.51
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	1	0.51
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	1	0.51
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	2	0.51
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	2	0.51
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	8	0.51
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	8	0.51
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	9	0.51
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	9	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	4	0.51
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	5	0.51
(1,515)	1:154:A:THR:HA	1:161:A:CYS:H	2	0.51
(1,498)	1:140:A:ARG:H	1:142:A:GLU:H	9	0.51
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	4	0.51
(1,324)	1:52:A:ALA:H	1:54:A:ASN:HD22	6	0.51
(1,322)	1:17:A:HIS:HD1	1:21:A:ASN:HD22	8	0.51
(1,158)	1:20:A:ALA:HB1	1:75:A:HIS:H	7	0.51
(1,158)	1:20:A:ALA:HB2	1:75:A:HIS:H	7	0.51
(1,158)	1:20:A:ALA:HB3	1:75:A:HIS:H	7	0.51
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	1	0.51
(3,55)	1:56:A:CYS:O	1:59:A:SER:H	6	0.5
(3,42)	1:20:A:ALA:O	1:24:A:ASN:N	3	0.5
(3,2)	1:100:A:HIS:O	1:112:A:CYS:N	4	0.5
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	5	0.5
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	3	0.5
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	4	0.5
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	7	0.5
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	9	0.5
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	6	0.5
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	8	0.5
(1,612)	1:87:A:SER:HB2	1:90:A:HIS:H	10	0.5
(1,612)	1:87:A:SER:HB3	1:90:A:HIS:H	10	0.5
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	7	0.5
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	10	0.5
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	6	0.5
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	6	0.5
(1,512)	1:154:A:THR:HA	1:162:A:TYR:HA	2	0.5
(1,477)	1:105:A:LYS:H	1:107:A:ALA:H	10	0.5
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB2	3	0.5
(1,405)	1:53:A:ASN:H	1:66:A:ASN:HB3	3	0.5
(1,286)	1:17:A:HIS:H	1:31:A:LEU:H	6	0.5
(1,219)	1:21:A:ASN:H	1:47:A:CYS:H	3	0.5
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	3	0.5
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	10	0.5
(1,133)	1:28:A:ASN:H	1:29:A:CYS:HG	9	0.5
(1,112)	1:75:A:HIS:HD1	1:77:A:GLU:H	5	0.5
(1,95)	1:81:A:ASP:H	1:85:A:HIS:HD1	9	0.5
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB2	2	0.5
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB3	2	0.5
(1,71)	1:38:A:LYS:H	1:40:A:ASP:H	7	0.5
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,47)	1:37:A:LYS:O	1:44:A:ALA:H	6	0.49
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	3	0.49
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	4	0.49
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	7	0.49
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	3	0.49
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	1	0.49
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	2	0.49
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	6	0.49
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	1	0.49
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	1	0.49
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	2	0.49
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	3	0.49
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	5	0.49
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	6	0.49
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	8	0.49
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	6	0.49
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	5	0.49
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	5	0.49
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	7	0.49
(1,532)	1:43:A:TYR:HB2	1:55:A:ILE:HD11	5	0.49
(1,532)	1:43:A:TYR:HB3	1:55:A:ILE:HD11	5	0.49
(1,532)	1:43:A:TYR:HB2	1:55:A:ILE:HD11	6	0.49
(1,532)	1:43:A:TYR:HB3	1:55:A:ILE:HD11	6	0.49
(1,532)	1:43:A:TYR:HB2	1:55:A:ILE:HD11	8	0.49
(1,532)	1:43:A:TYR:HB3	1:55:A:ILE:HD11	8	0.49
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	1	0.49
(1,515)	1:154:A:THR:HA	1:161:A:CYS:H	6	0.49
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	2	0.49
(1,418)	1:75:A:HIS:HB2	1:112:A:CYS:H	6	0.49
(1,418)	1:75:A:HIS:HB3	1:112:A:CYS:H	6	0.49
(1,73)	1:162:A:TYR:H	1:163:A:HIS:HD1	10	0.49
(1,71)	1:38:A:LYS:H	1:40:A:ASP:H	3	0.49
(1,30)	1:17:A:HIS:H	1:31:A:LEU:HB3	5	0.49
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	1	0.48
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	2	0.48
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	6	0.48
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	10	0.48
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	9	0.48
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	6	0.48
(3,1)	1:100:A:HIS:O	1:112:A:CYS:H	5	0.48
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	5	0.48
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:92:A:HIS:HA	1:93:A:ASP:H	10	0.48
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	2	0.48
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	5	0.48
(1,607)	1:86:A:CYS:HA	1:87:A:SER:H	9	0.48
(1,576)	1:26:A:SER:HB2	1:27:A:CYS:H	5	0.48
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	1	0.48
(1,550)	1:18:A:CYS:HB2	1:21:A:ASN:H	4	0.48
(1,550)	1:18:A:CYS:HB3	1:21:A:ASN:H	4	0.48
(1,498)	1:140:A:ARG:H	1:142:A:GLU:H	10	0.48
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	6	0.48
(1,458)	1:155:A:CYS:CB	1:161:A:CYS:SG	9	0.48
(1,444)	1:159:A:HIS:HB2	1:161:A:CYS:H	7	0.48
(1,444)	1:159:A:HIS:HB3	1:161:A:CYS:H	7	0.48
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	10	0.48
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	10	0.48
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG2	1	0.48
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG3	1	0.48
(1,299)	1:29:A:CYS:HA	1:31:A:LEU:H	8	0.48
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	2	0.48
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	7	0.48
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	6	0.48
(1,71)	1:38:A:LYS:H	1:40:A:ASP:H	6	0.48
(3,48)	1:37:A:LYS:O	1:44:A:ALA:N	9	0.47
(3,43)	1:21:A:ASN:O	1:25:A:CYS:H	2	0.47
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	5	0.47
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	1	0.47
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	10	0.47
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB2	1	0.47
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB3	1	0.47
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB2	1	0.47
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB3	1	0.47
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	9	0.47
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	1	0.47
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	2	0.47
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	4	0.47
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	4	0.47
(1,559)	1:20:A:ALA:HA	1:24:A:ASN:H	4	0.47
(1,554)	1:19:A:ASP:HB2	1:21:A:ASN:H	4	0.47
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB2	9	0.47
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB3	9	0.47
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	2	0.47
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:110:A:TRP:HB2	1:111:A:ARG:H	7	0.47
(1,471)	1:110:A:TRP:HB3	1:111:A:ARG:H	7	0.47
(1,456)	1:132:A:CYS:CB	1:150:A:CYS:SG	2	0.47
(1,452)	1:47:A:CYS:SG	1:34:A:CYS:CB	2	0.47
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	10	0.47
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	10	0.47
(1,408)	1:53:A:ASN:HD21	1:63:A:ILE:H	3	0.47
(1,408)	1:53:A:ASN:HD22	1:63:A:ILE:H	3	0.47
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD21	6	0.47
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD22	6	0.47
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	4	0.47
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	4	0.47
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	5	0.47
(1,212)	1:17:A:HIS:HA	1:30:A:GLU:H	7	0.47
(1,149)	1:20:A:ALA:HB1	1:127:A:CYS:H	7	0.47
(1,149)	1:20:A:ALA:HB2	1:127:A:CYS:H	7	0.47
(1,149)	1:20:A:ALA:HB3	1:127:A:CYS:H	7	0.47
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	4	0.46
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	9	0.46
(3,37)	1:18:A:CYS:O	1:22:A:GLY:H	3	0.46
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	7	0.46
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	2	0.46
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	9	0.46
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	1	0.46
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	1	0.46
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB2	2	0.46
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB3	2	0.46
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB2	2	0.46
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB3	2	0.46
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	7	0.46
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	9	0.46
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	2	0.46
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	2	0.46
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	5	0.46
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	5	0.46
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	9	0.46
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	9	0.46
(1,559)	1:20:A:ALA:HA	1:24:A:ASN:H	9	0.46
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	5	0.46
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	5	0.46
(1,554)	1:19:A:ASP:HB2	1:21:A:ASN:H	5	0.46
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	1	0.46
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	8	0.46
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	8	0.46
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	5	0.46
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	5	0.46
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	1	0.46
(1,476)	1:103:A:CYS:HB2	1:109:A:CYS:HA	7	0.46
(1,476)	1:103:A:CYS:HB3	1:109:A:CYS:HA	7	0.46
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	1	0.46
(1,459)	1:100:A:HIS:H	1:112:A:CYS:H	3	0.46
(1,456)	1:132:A:CYS:CB	1:150:A:CYS:SG	1	0.46
(1,381)	1:10:A:ASN:HD21	1:11:A:SER:HB2	1	0.46
(1,381)	1:10:A:ASN:HD21	1:11:A:SER:HB3	1	0.46
(1,381)	1:10:A:ASN:HD22	1:11:A:SER:HB2	1	0.46
(1,381)	1:10:A:ASN:HD22	1:11:A:SER:HB3	1	0.46
(1,356)	1:154:A:THR:HG1	1:156:A:ASN:H	10	0.46
(1,315)	1:100:A:HIS:HD1	1:123:A:CYS:H	9	0.46
(1,95)	1:81:A:ASP:H	1:85:A:HIS:HD1	5	0.46
(1,51)	1:18:A:CYS:H	1:30:A:GLU:H	7	0.46
(1,34)	1:166:A:GLU:HB2	1:168:A:ASP:H	9	0.46
(3,50)	1:54:A:ASN:O	1:61:A:THR:N	6	0.45
(3,47)	1:37:A:LYS:O	1:44:A:ALA:H	4	0.45
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	8	0.45
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	3	0.45
(3,2)	1:100:A:HIS:O	1:112:A:CYS:N	3	0.45
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	3	0.45
(1,638)	1:67:A:GLU:HA	1:69:A:HIS:H	2	0.45
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	5	0.45
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	6	0.45
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	8	0.45
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	5	0.45
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	5	0.45
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	6	0.45
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	5	0.45
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	5	0.45
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	1	0.45
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	2	0.45
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	3	0.45
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	5	0.45
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	6	0.45
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	7	0.45
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	10	0.45
(1,576)	1:26:A:SER:HB2	1:27:A:CYS:H	9	0.45
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	3	0.45
(1,546)	1:18:A:CYS:HA	1:22:A:GLY:H	10	0.45
(1,542)	1:53:A:ASN:HA	1:62:A:ALA:HA	5	0.45
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	10	0.45
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	1	0.45
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	4	0.45
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	1	0.45
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	1	0.45
(1,484)	1:135:A:GLU:HB2	1:136:A:HIS:H	4	0.45
(1,484)	1:135:A:GLU:HB3	1:136:A:HIS:H	4	0.45
(1,418)	1:75:A:HIS:HB2	1:112:A:CYS:H	1	0.45
(1,418)	1:75:A:HIS:HB3	1:112:A:CYS:H	1	0.45
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG2	4	0.45
(1,399)	1:45:A:HIS:H	1:46:A:PRO:HG3	4	0.45
(1,324)	1:52:A:ALA:H	1:54:A:ASN:HD22	5	0.45
(1,173)	1:29:A:CYS:H	1:129:A:LYS:H	3	0.45
(1,118)	1:152:A:THR:HG21	1:166:A:GLU:H	10	0.45
(1,118)	1:152:A:THR:HG22	1:166:A:GLU:H	10	0.45
(1,118)	1:152:A:THR:HG23	1:166:A:GLU:H	10	0.45
(1,109)	1:75:A:HIS:HD1	1:112:A:CYS:H	3	0.45
(1,95)	1:81:A:ASP:H	1:85:A:HIS:HD1	6	0.45
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	10	0.45
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	2	0.44
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	9	0.44
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	10	0.44
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	4	0.44
(1,634)	1:93:A:ASP:HA	1:95:A:HIS:H	4	0.44
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	1	0.44
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	1	0.44
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	7	0.44
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	7	0.44
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	8	0.44
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	8	0.44
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	7	0.44
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	7	0.44
(1,609)	1:87:A:SER:HA	1:88:A:CYS:H	4	0.44
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	3	0.44
(1,573)	1:23:A:GLU:HA	1:27:A:CYS:H	9	0.44
(1,544)	1:55:A:ILE:HA	1:60:A:CYS:HA	8	0.44
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	7	0.44
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	7	0.44
(1,490)	1:139:A:TYR:HB2	1:140:A:ARG:H	7	0.44
(1,490)	1:139:A:TYR:HB3	1:140:A:ARG:H	7	0.44
(1,462)	1:103:A:CYS:HB2	1:104:A:THR:H	5	0.44
(1,462)	1:103:A:CYS:HB3	1:104:A:THR:H	5	0.44
(1,459)	1:100:A:HIS:H	1:112:A:CYS:H	7	0.44
(1,457)	1:155:A:CYS:SG	1:161:A:CYS:CB	7	0.44
(1,429)	1:101:A:GLY:H	1:124:A:GLY:HA2	6	0.44
(1,429)	1:101:A:GLY:H	1:124:A:GLY:HA3	6	0.44
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD21	5	0.44
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD22	5	0.44
(1,403)	1:52:A:ALA:H	1:66:A:ASN:HD21	8	0.44
(1,403)	1:52:A:ALA:H	1:66:A:ASN:HD22	8	0.44
(1,292)	1:18:A:CYS:H	1:31:A:LEU:H	6	0.44
(1,73)	1:162:A:TYR:H	1:163:A:HIS:HD1	9	0.44
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	6	0.44
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	1	0.43
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	10	0.43
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	10	0.43
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	6	0.43
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	6	0.43
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	9	0.43
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	9	0.43
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	10	0.43
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	10	0.43
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	4	0.43
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	10	0.43
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	2	0.43
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	2	0.43
(1,504)	1:145:A:VAL:HB	1:146:A:VAL:H	3	0.43
(1,504)	1:145:A:VAL:HB	1:146:A:VAL:H	4	0.43
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	8	0.43
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	8	0.43
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	3	0.43
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	8	0.43
(1,455)	1:132:A:CYS:SG	1:150:A:CYS:CB	2	0.43
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB2	7	0.43
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB3	7	0.43
(1,416)	1:66:A:ASN:HD21	1:69:A:HIS:HD1	7	0.43
(1,416)	1:66:A:ASN:HD22	1:69:A:HIS:HD1	7	0.43
(1,386)	1:17:A:HIS:HD1	1:21:A:ASN:HB2	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:17:A:HIS:HD1	1:21:A:ASN:HB3	2	0.43
(1,379)	1:10:A:ASN:HB2	1:17:A:HIS:H	5	0.43
(1,379)	1:10:A:ASN:HB3	1:17:A:HIS:H	5	0.43
(1,340)	1:105:A:LYS:HB3	1:162:A:TYR:H	5	0.43
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	9	0.43
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	9	0.43
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	9	0.43
(1,299)	1:29:A:CYS:HA	1:31:A:LEU:H	1	0.43
(1,295)	1:29:A:CYS:HG	1:31:A:LEU:H	6	0.43
(1,243)	1:101:A:GLY:H	1:152:A:THR:HG1	5	0.43
(1,116)	1:166:A:GLU:H	1:168:A:ASP:H	10	0.43
(3,56)	1:56:A:CYS:O	1:59:A:SER:N	8	0.42
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	8	0.42
(3,40)	1:19:A:ASP:O	1:23:A:GLU:N	6	0.42
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	7	0.42
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	5	0.42
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	2	0.42
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	3	0.42
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	7	0.42
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	10	0.42
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	3	0.42
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	3	0.42
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	10	0.42
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	10	0.42
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	1	0.42
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	1	0.42
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	8	0.42
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	8	0.42
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	10	0.42
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	5	0.42
(1,547)	1:18:A:CYS:HB2	1:20:A:ALA:H	4	0.42
(1,547)	1:18:A:CYS:HB3	1:20:A:ALA:H	4	0.42
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	8	0.42
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	9	0.42
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	10	0.42
(1,504)	1:145:A:VAL:HB	1:146:A:VAL:H	6	0.42
(1,490)	1:139:A:TYR:HB2	1:140:A:ARG:H	1	0.42
(1,490)	1:139:A:TYR:HB3	1:140:A:ARG:H	1	0.42
(1,484)	1:135:A:GLU:HB2	1:136:A:HIS:H	7	0.42
(1,484)	1:135:A:GLU:HB3	1:136:A:HIS:H	7	0.42
(1,458)	1:155:A:CYS:CB	1:161:A:CYS:SG	7	0.42
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	9	0.42
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD21	4	0.42
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD22	4	0.42
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD21	10	0.42
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD22	10	0.42
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB2	10	0.42
(1,401)	1:49:A:ARG:H	1:74:A:CYS:HB3	10	0.42
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	1	0.42
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	1	0.42
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	1	0.42
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	9	0.42
(1,216)	1:100:A:HIS:HD1	1:102:A:GLU:H	1	0.42
(1,177)	1:24:A:ASN:HD21	1:54:A:ASN:H	7	0.42
(1,93)	1:63:A:ILE:HB	1:66:A:ASN:H	3	0.42
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	2	0.42
(1,56)	1:17:A:HIS:HD1	1:21:A:ASN:H	6	0.42
(1,36)	1:166:A:GLU:HB3	1:168:A:ASP:H	4	0.42
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	6	0.42
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	3	0.42
(3,47)	1:37:A:LYS:O	1:44:A:ALA:H	2	0.41
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	10	0.41
(3,30)	1:86:A:CYS:O	1:90:A:HIS:N	9	0.41
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	10	0.41
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	7	0.41
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	7	0.41
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	1	0.41
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	1	0.41
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	2	0.41
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	2	0.41
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	4	0.41
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	4	0.41
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	7	0.41
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	1	0.41
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	8	0.41
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	7	0.41
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	7	0.41
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	9	0.41
(1,500)	1:140:A:ARG:HG2	1:141:A:LYS:H	6	0.41
(1,500)	1:140:A:ARG:HG3	1:141:A:LYS:H	6	0.41
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	8	0.41
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	8	0.41
(1,459)	1:100:A:HIS:H	1:112:A:CYS:H	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:132:A:CYS:SG	1:150:A:CYS:CB	3	0.41
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	9	0.41
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	9	0.41
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	3	0.41
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	3	0.41
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	4	0.41
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	4	0.41
(1,415)	1:66:A:ASN:HD21	1:68:A:ASP:H	3	0.41
(1,415)	1:66:A:ASN:HD22	1:68:A:ASP:H	3	0.41
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	4	0.41
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	5	0.41
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	5	0.41
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	7	0.41
(3,56)	1:56:A:CYS:O	1:59:A:SER:N	3	0.4
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	8	0.4
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	4	0.4
(3,2)	1:100:A:HIS:O	1:112:A:CYS:N	1	0.4
(2,1)	1:34:A:CYS:SG	1:47:A:CYS:SG	1	0.4
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	1	0.4
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	3	0.4
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	3	0.4
(1,621)	1:89:A:GLU:HA	1:92:A:HIS:H	10	0.4
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	2	0.4
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	2	0.4
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	3	0.4
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	3	0.4
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	3	0.4
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	3	0.4
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	5	0.4
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	9	0.4
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	2	0.4
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	9	0.4
(1,532)	1:43:A:TYR:HB2	1:55:A:ILE:HD11	1	0.4
(1,532)	1:43:A:TYR:HB3	1:55:A:ILE:HD11	1	0.4
(1,531)	1:42:A:SER:HB2	1:56:A:CYS:H	6	0.4
(1,531)	1:42:A:SER:HB3	1:56:A:CYS:H	6	0.4
(1,516)	1:155:A:CYS:HB2	1:156:A:ASN:H	9	0.4
(1,516)	1:155:A:CYS:HB3	1:156:A:ASN:H	9	0.4
(1,484)	1:135:A:GLU:HB2	1:136:A:HIS:H	9	0.4
(1,484)	1:135:A:GLU:HB3	1:136:A:HIS:H	9	0.4
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	7	0.4
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:55:A:ILE:H	1:56:A:CYS:HB2	8	0.4
(1,409)	1:55:A:ILE:H	1:56:A:CYS:HB3	8	0.4
(1,398)	1:43:A:TYR:HB2	1:60:A:CYS:H	7	0.4
(1,398)	1:43:A:TYR:HB3	1:60:A:CYS:H	7	0.4
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	8	0.4
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	8	0.4
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	5	0.4
(1,186)	1:50:A:CYS:H	1:73:A:HIS:H	2	0.4
(1,149)	1:20:A:ALA:HB1	1:127:A:CYS:H	2	0.4
(1,149)	1:20:A:ALA:HB2	1:127:A:CYS:H	2	0.4
(1,149)	1:20:A:ALA:HB3	1:127:A:CYS:H	2	0.4
(1,149)	1:20:A:ALA:HB1	1:127:A:CYS:H	6	0.4
(1,149)	1:20:A:ALA:HB2	1:127:A:CYS:H	6	0.4
(1,149)	1:20:A:ALA:HB3	1:127:A:CYS:H	6	0.4
(1,136)	1:28:A:ASN:H	1:28:A:ASN:HD22	7	0.4
(1,93)	1:63:A:ILE:HB	1:66:A:ASN:H	1	0.4
(1,73)	1:162:A:TYR:H	1:163:A:HIS:HD1	6	0.4
(1,32)	1:152:A:THR:HG21	1:168:A:ASP:H	3	0.4
(1,32)	1:152:A:THR:HG22	1:168:A:ASP:H	3	0.4
(1,32)	1:152:A:THR:HG23	1:168:A:ASP:H	3	0.4
(1,26)	1:17:A:HIS:H	1:31:A:LEU:HB2	5	0.4
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	1	0.39
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	1	0.39
(1,635)	1:93:A:ASP:HA	1:94:A:HIS:H	4	0.39
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	4	0.39
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	4	0.39
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	9	0.39
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	9	0.39
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	4	0.39
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	4	0.39
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	8	0.39
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	8	0.39
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	6	0.39
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	6	0.39
(1,546)	1:18:A:CYS:HA	1:22:A:GLY:H	9	0.39
(1,539)	1:50:A:CYS:H	1:65:A:CYS:H	5	0.39
(1,527)	1:37:A:LYS:H	1:44:A:ALA:H	8	0.39
(1,516)	1:155:A:CYS:HB2	1:156:A:ASN:H	7	0.39
(1,516)	1:155:A:CYS:HB3	1:156:A:ASN:H	7	0.39
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	1	0.39
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	2	0.39
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG2	8	0.39
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG3	8	0.39
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG2	8	0.39
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG3	8	0.39
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	5	0.39
(1,467)	1:106:A:LYS:HB2	1:107:A:ALA:H	7	0.39
(1,467)	1:106:A:LYS:HB3	1:107:A:ALA:H	7	0.39
(1,463)	1:104:A:THR:HG1	1:105:A:LYS:H	4	0.39
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	2	0.39
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	2	0.39
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	8	0.39
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	8	0.39
(1,412)	1:63:A:ILE:HG12	1:66:A:ASN:H	8	0.39
(1,412)	1:63:A:ILE:HG13	1:66:A:ASN:H	8	0.39
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	2	0.39
(1,324)	1:52:A:ALA:H	1:54:A:ASN:HD22	7	0.39
(1,320)	1:17:A:HIS:HE1	1:21:A:ASN:HD22	1	0.39
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	4	0.39
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG21	1	0.39
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG22	1	0.39
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG23	1	0.39
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG21	6	0.39
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG22	6	0.39
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG23	6	0.39
(1,170)	1:153:A:ILE:HG21	1:155:A:CYS:H	10	0.39
(1,170)	1:153:A:ILE:HG22	1:155:A:CYS:H	10	0.39
(1,170)	1:153:A:ILE:HG23	1:155:A:CYS:H	10	0.39
(3,42)	1:20:A:ALA:O	1:24:A:ASN:N	5	0.38
(3,38)	1:18:A:CYS:O	1:22:A:GLY:N	3	0.38
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	3	0.38
(3,11)	1:138:A:CYS:O	1:144:A:GLY:H	5	0.38
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	6	0.38
(2,1)	1:34:A:CYS:SG	1:47:A:CYS:SG	10	0.38
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	10	0.38
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	8	0.38
(1,638)	1:67:A:GLU:HA	1:69:A:HIS:H	6	0.38
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	9	0.38
(1,628)	1:91:A:SER:HA	1:95:A:HIS:H	3	0.38
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	2	0.38
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	7	0.38
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	7	0.38
(1,512)	1:154:A:THR:HA	1:162:A:TYR:HA	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:139:A:TYR:HB2	1:140:A:ARG:H	8	0.38
(1,490)	1:139:A:TYR:HB3	1:140:A:ARG:H	8	0.38
(1,457)	1:155:A:CYS:SG	1:161:A:CYS:CB	10	0.38
(1,444)	1:159:A:HIS:HB2	1:161:A:CYS:H	9	0.38
(1,444)	1:159:A:HIS:HB3	1:161:A:CYS:H	9	0.38
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	1	0.38
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	1	0.38
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	10	0.38
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	10	0.38
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD21	2	0.38
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD22	2	0.38
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	3	0.38
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	3	0.38
(1,351)	1:123:A:CYS:H	1:125:A:CYS:H	6	0.38
(1,320)	1:17:A:HIS:HE1	1:21:A:ASN:HD22	4	0.38
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	1	0.38
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	7	0.38
(1,217)	1:102:A:GLU:H	1:110:A:TRP:HE1	7	0.38
(1,216)	1:100:A:HIS:HD1	1:102:A:GLU:H	2	0.38
(1,216)	1:100:A:HIS:HD1	1:102:A:GLU:H	8	0.38
(1,177)	1:24:A:ASN:HD21	1:54:A:ASN:H	10	0.38
(1,105)	1:49:A:ARG:H	1:74:A:CYS:H	10	0.38
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	1	0.38
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	1	0.37
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	5	0.37
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	6	0.37
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	10	0.37
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	7	0.37
(1,758)	1:140:A:ARG:HA	1:141:A:LYS:H	9	0.37
(1,721)	1:99:A:THR:HA	1:100:A:HIS:H	7	0.37
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	3	0.37
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	4	0.37
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	1	0.37
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	2	0.37
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	4	0.37
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	8	0.37
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	10	0.37
(1,701)	1:78:A:ASP:HA	1:79:A:ASP:H	9	0.37
(1,683)	1:58:A:CYS:HA	1:59:A:SER:H	2	0.37
(1,683)	1:58:A:CYS:HA	1:59:A:SER:H	4	0.37
(1,683)	1:58:A:CYS:HA	1:59:A:SER:H	9	0.37
(1,681)	1:56:A:CYS:HA	1:57:A:LYS:H	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	1	0.37
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	3	0.37
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	6	0.37
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	7	0.37
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	4	0.37
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	6	0.37
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	10	0.37
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	2	0.37
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB2	3	0.37
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB3	3	0.37
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB2	3	0.37
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB3	3	0.37
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	1	0.37
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	5	0.37
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	6	0.37
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	7	0.37
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	4	0.37
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	4	0.37
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	4	0.37
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	4	0.37
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	9	0.37
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	9	0.37
(1,611)	1:87:A:SER:HB2	1:89:A:GLU:H	5	0.37
(1,611)	1:87:A:SER:HB3	1:89:A:GLU:H	5	0.37
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	5	0.37
(1,549)	1:18:A:CYS:HB2	1:19:A:ASP:H	8	0.37
(1,549)	1:18:A:CYS:HB3	1:19:A:ASP:H	8	0.37
(1,542)	1:53:A:ASN:HA	1:62:A:ALA:HA	1	0.37
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	1	0.37
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	3	0.37
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	6	0.37
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	7	0.37
(1,476)	1:103:A:CYS:HB2	1:109:A:CYS:HA	3	0.37
(1,476)	1:103:A:CYS:HB3	1:109:A:CYS:HA	3	0.37
(1,455)	1:132:A:CYS:SG	1:150:A:CYS:CB	8	0.37
(1,446)	1:166:A:GLU:HG2	1:168:A:ASP:H	3	0.37
(1,446)	1:166:A:GLU:HG3	1:168:A:ASP:H	3	0.37
(1,437)	1:135:A:GLU:HB2	1:184:A:SER:H	6	0.37
(1,437)	1:135:A:GLU:HB3	1:184:A:SER:H	6	0.37
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG2	2	0.37
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG3	2	0.37
(1,362)	1:65:A:CYS:HG	1:69:A:HIS:HD1	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	8	0.37
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	10	0.37
(1,131)	1:17:A:HIS:HB2	1:28:A:ASN:H	7	0.37
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	2	0.37
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	1	0.37
(1,48)	1:10:A:ASN:H	1:13:A:ALA:H	5	0.37
(1,35)	1:100:A:HIS:HD2	1:168:A:ASP:H	4	0.37
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	4	0.36
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	2	0.36
(1,758)	1:140:A:ARG:HA	1:141:A:LYS:H	2	0.36
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	3	0.36
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	5	0.36
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	7	0.36
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	9	0.36
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	1	0.36
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	2	0.36
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	4	0.36
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	8	0.36
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	10	0.36
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	3	0.36
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	6	0.36
(1,691)	1:67:A:GLU:HA	1:68:A:ASP:H	1	0.36
(1,683)	1:58:A:CYS:HA	1:59:A:SER:H	3	0.36
(1,683)	1:58:A:CYS:HA	1:59:A:SER:H	8	0.36
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	8	0.36
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	9	0.36
(1,651)	1:11:A:SER:HA	1:12:A:ASN:H	5	0.36
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	4	0.36
(1,618)	1:88:A:CYS:HB2	1:90:A:HIS:H	7	0.36
(1,618)	1:88:A:CYS:HB3	1:90:A:HIS:H	7	0.36
(1,559)	1:20:A:ALA:HA	1:24:A:ASN:H	6	0.36
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	10	0.36
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	5	0.36
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	5	0.36
(1,501)	1:141:A:LYS:HB2	1:142:A:GLU:H	9	0.36
(1,501)	1:141:A:LYS:HB3	1:142:A:GLU:H	9	0.36
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	2	0.36
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	2	0.36
(1,315)	1:100:A:HIS:HD1	1:123:A:CYS:H	3	0.36
(1,163)	1:100:A:HIS:H	1:152:A:THR:H	5	0.36
(1,158)	1:20:A:ALA:HB1	1:75:A:HIS:H	5	0.36
(1,158)	1:20:A:ALA:HB2	1:75:A:HIS:H	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:20:A:ALA:HB3	1:75:A:HIS:H	5	0.36
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	7	0.36
(3,54)	1:52:A:ALA:O	1:63:A:ILE:N	1	0.35
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	6	0.35
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	9	0.35
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	9	0.35
(3,17)	1:157:A:GLU:O	1:159:A:HIS:H	6	0.35
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	3	0.35
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	7	0.35
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	8	0.35
(1,777)	1:163:A:HIS:HA	1:164:A:SER:H	9	0.35
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	5	0.35
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	7	0.35
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	6	0.35
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	3	0.35
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	5	0.35
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	9	0.35
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	5	0.35
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	7	0.35
(1,704)	1:82:A:THR:HA	1:83:A:HIS:H	9	0.35
(1,701)	1:78:A:ASP:HA	1:79:A:ASP:H	2	0.35
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	10	0.35
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	5	0.35
(1,628)	1:91:A:SER:HA	1:95:A:HIS:H	5	0.35
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	8	0.35
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	8	0.35
(1,620)	1:89:A:GLU:HA	1:93:A:ASP:H	10	0.35
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	6	0.35
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	6	0.35
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	7	0.35
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	3	0.35
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	10	0.35
(1,517)	1:156:A:ASN:HB2	1:157:A:GLU:H	1	0.35
(1,517)	1:156:A:ASN:HB3	1:157:A:GLU:H	1	0.35
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	1	0.35
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	1	0.35
(1,479)	1:133:A:ASN:HB2	1:134:A:ASP:H	3	0.35
(1,479)	1:133:A:ASN:HB3	1:134:A:ASP:H	3	0.35
(1,455)	1:132:A:CYS:SG	1:150:A:CYS:CB	10	0.35
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB2	5	0.35
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB3	5	0.35
(1,419)	1:81:A:ASP:HB2	1:85:A:HIS:HD1	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:81:A:ASP:HB3	1:85:A:HIS:HD1	7	0.35
(1,362)	1:65:A:CYS:HG	1:69:A:HIS:HD1	6	0.35
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	5	0.35
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	5	0.35
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	5	0.35
(1,299)	1:29:A:CYS:HA	1:31:A:LEU:H	2	0.35
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	7	0.35
(1,89)	1:24:A:ASN:H	1:24:A:ASN:HD22	6	0.35
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	2	0.35
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	6	0.35
(1,71)	1:38:A:LYS:H	1:40:A:ASP:H	10	0.35
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	5	0.35
(1,51)	1:18:A:CYS:H	1:30:A:GLU:H	9	0.35
(1,26)	1:17:A:HIS:H	1:31:A:LEU:HB2	2	0.35
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	9	0.35
(3,52)	1:50:A:CYS:O	1:65:A:CYS:N	8	0.34
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	2	0.34
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	9	0.34
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	3	0.34
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	2	0.34
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	7	0.34
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	7	0.34
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	4	0.34
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	7	0.34
(1,700)	1:77:A:GLU:HA	1:78:A:ASP:H	1	0.34
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	4	0.34
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	5	0.34
(1,651)	1:11:A:SER:HA	1:12:A:ASN:H	1	0.34
(1,639)	1:65:A:CYS:HA	1:67:A:GLU:H	1	0.34
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	4	0.34
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	5	0.34
(1,627)	1:90:A:HIS:HB2	1:93:A:ASP:H	9	0.34
(1,627)	1:90:A:HIS:HB3	1:93:A:ASP:H	9	0.34
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	5	0.34
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	6	0.34
(1,575)	1:23:A:GLU:HB2	1:26:A:SER:H	4	0.34
(1,575)	1:23:A:GLU:HB3	1:26:A:SER:H	4	0.34
(1,549)	1:18:A:CYS:HB2	1:19:A:ASP:H	6	0.34
(1,549)	1:18:A:CYS:HB3	1:19:A:ASP:H	6	0.34
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	4	0.34
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	5	0.34
(1,525)	1:34:A:CYS:HB2	1:47:A:CYS:H	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:34:A:CYS:HB3	1:47:A:CYS:H	5	0.34
(1,515)	1:154:A:THR:HA	1:161:A:CYS:H	3	0.34
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	3	0.34
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	4	0.34
(1,504)	1:145:A:VAL:HB	1:146:A:VAL:H	9	0.34
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	7	0.34
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	7	0.34
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD21	2	0.34
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD22	2	0.34
(1,381)	1:10:A:ASN:HD21	1:11:A:SER:HB2	3	0.34
(1,381)	1:10:A:ASN:HD21	1:11:A:SER:HB3	3	0.34
(1,381)	1:10:A:ASN:HD22	1:11:A:SER:HB2	3	0.34
(1,381)	1:10:A:ASN:HD22	1:11:A:SER:HB3	3	0.34
(1,315)	1:100:A:HIS:HD1	1:123:A:CYS:H	5	0.34
(1,139)	1:75:A:HIS:HD1	1:124:A:GLY:H	7	0.34
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	5	0.34
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	7	0.34
(1,75)	1:151:A:LYS:H	1:153:A:ILE:H	7	0.34
(1,22)	1:161:A:CYS:H	1:163:A:HIS:HD1	4	0.34
(3,14)	1:140:A:ARG:O	1:142:A:GLU:N	4	0.33
(3,5)	1:105:A:LYS:O	1:107:A:ALA:H	8	0.33
(1,767)	1:152:A:THR:HA	1:153:A:ILE:H	2	0.33
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	8	0.33
(1,750)	1:131:A:PRO:HA	1:132:A:CYS:H	3	0.33
(1,749)	1:129:A:LYS:HA	1:130:A:LEU:H	4	0.33
(1,749)	1:129:A:LYS:HA	1:130:A:LEU:H	7	0.33
(1,745)	1:125:A:CYS:HA	1:126:A:GLU:H	6	0.33
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	5	0.33
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	10	0.33
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	3	0.33
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	9	0.33
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	2	0.33
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	7	0.33
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	8	0.33
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	9	0.33
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	10	0.33
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	1	0.33
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	2	0.33
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	8	0.33
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	10	0.33
(1,705)	1:83:A:HIS:HA	1:84:A:CYS:H	6	0.33
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	2	0.33
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	3	0.33
(1,657)	1:20:A:ALA:HA	1:21:A:ASN:H	7	0.33
(1,651)	1:11:A:SER:HA	1:12:A:ASN:H	2	0.33
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	4	0.33
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	4	0.33
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	3	0.33
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	3	0.33
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	9	0.33
(1,559)	1:20:A:ALA:HA	1:24:A:ASN:H	7	0.33
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD21	10	0.33
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD22	10	0.33
(1,550)	1:18:A:CYS:HB2	1:21:A:ASN:H	10	0.33
(1,550)	1:18:A:CYS:HB3	1:21:A:ASN:H	10	0.33
(1,538)	1:54:A:ASN:H	1:61:A:THR:H	7	0.33
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	7	0.33
(1,534)	1:45:A:HIS:HA	1:53:A:ASN:H	5	0.33
(1,515)	1:154:A:THR:HA	1:161:A:CYS:H	10	0.33
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	2	0.33
(1,452)	1:47:A:CYS:SG	1:34:A:CYS:CB	10	0.33
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD21	1	0.33
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD22	1	0.33
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG2	7	0.33
(1,389)	1:22:A:GLY:H	1:46:A:PRO:HG3	7	0.33
(1,356)	1:154:A:THR:HG1	1:156:A:ASN:H	3	0.33
(1,299)	1:29:A:CYS:HA	1:31:A:LEU:H	4	0.33
(1,275)	1:99:A:THR:H	1:152:A:THR:H	8	0.33
(1,271)	1:99:A:THR:H	1:152:A:THR:HG1	9	0.33
(1,188)	1:100:A:HIS:HE1	1:123:A:CYS:H	10	0.33
(1,181)	1:75:A:HIS:HD2	1:123:A:CYS:H	10	0.33
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	3	0.33
(1,30)	1:17:A:HIS:H	1:31:A:LEU:HB3	2	0.33
(1,23)	1:55:A:ILE:H	1:57:A:LYS:H	4	0.33
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	4	0.32
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	7	0.32
(3,40)	1:19:A:ASP:O	1:23:A:GLU:N	7	0.32
(3,37)	1:18:A:CYS:O	1:22:A:GLY:H	5	0.32
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	5	0.32
(3,5)	1:105:A:LYS:O	1:107:A:ALA:H	9	0.32
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	9	0.32
(1,758)	1:140:A:ARG:HA	1:141:A:LYS:H	4	0.32
(1,749)	1:129:A:LYS:HA	1:130:A:LEU:H	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:106:A:LYS:HA	1:107:A:ALA:H	3	0.32
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	1	0.32
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	5	0.32
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	8	0.32
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	1	0.32
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	3	0.32
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	4	0.32
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	6	0.32
(1,706)	1:84:A:CYS:HA	1:85:A:HIS:H	4	0.32
(1,683)	1:58:A:CYS:HA	1:59:A:SER:H	6	0.32
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	3	0.32
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB2	8	0.32
(1,643)	1:67:A:GLU:HB2	1:76:A:GLU:HB3	8	0.32
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB2	8	0.32
(1,643)	1:67:A:GLU:HB3	1:76:A:GLU:HB3	8	0.32
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	2	0.32
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	2	0.32
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	1	0.32
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	6	0.32
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	7	0.32
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	3	0.32
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	1	0.32
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	1	0.32
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	7	0.32
(1,545)	1:55:A:ILE:HA	1:59:A:SER:H	2	0.32
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	3	0.32
(1,517)	1:156:A:ASN:HB2	1:157:A:GLU:H	2	0.32
(1,517)	1:156:A:ASN:HB3	1:157:A:GLU:H	2	0.32
(1,517)	1:156:A:ASN:HB2	1:157:A:GLU:H	8	0.32
(1,517)	1:156:A:ASN:HB3	1:157:A:GLU:H	8	0.32
(1,510)	1:153:A:ILE:HB	1:154:A:THR:H	6	0.32
(1,500)	1:140:A:ARG:HG2	1:141:A:LYS:H	10	0.32
(1,500)	1:140:A:ARG:HG3	1:141:A:LYS:H	10	0.32
(1,496)	1:137:A:PRO:HA	1:145:A:VAL:HA	3	0.32
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG2	9	0.32
(1,431)	1:110:A:TRP:HE1	1:151:A:LYS:HG3	9	0.32
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB2	3	0.32
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB3	3	0.32
(1,419)	1:81:A:ASP:HB2	1:85:A:HIS:HD1	6	0.32
(1,419)	1:81:A:ASP:HB3	1:85:A:HIS:HD1	6	0.32
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD21	9	0.32
(1,406)	1:53:A:ASN:H	1:66:A:ASN:HD22	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:100:A:HIS:HD1	1:123:A:CYS:H	2	0.32
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	7	0.32
(1,186)	1:50:A:CYS:H	1:73:A:HIS:H	3	0.32
(1,158)	1:20:A:ALA:HB1	1:75:A:HIS:H	10	0.32
(1,158)	1:20:A:ALA:HB2	1:75:A:HIS:H	10	0.32
(1,158)	1:20:A:ALA:HB3	1:75:A:HIS:H	10	0.32
(1,112)	1:75:A:HIS:HD1	1:77:A:GLU:H	10	0.32
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	4	0.32
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	8	0.32
(3,51)	1:50:A:CYS:O	1:65:A:CYS:H	5	0.31
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	7	0.31
(3,14)	1:140:A:ARG:O	1:142:A:GLU:N	5	0.31
(3,8)	1:134:A:ASP:O	1:148:A:CYS:N	5	0.31
(3,5)	1:105:A:LYS:O	1:107:A:ALA:H	4	0.31
(3,5)	1:105:A:LYS:O	1:107:A:ALA:H	6	0.31
(1,728)	1:106:A:LYS:HA	1:107:A:ALA:H	5	0.31
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	9	0.31
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	2	0.31
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	6	0.31
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	10	0.31
(1,710)	1:88:A:CYS:HA	1:89:A:GLU:H	5	0.31
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	4	0.31
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	1	0.31
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	8	0.31
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	10	0.31
(1,691)	1:67:A:GLU:HA	1:68:A:ASP:H	3	0.31
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	9	0.31
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	2	0.31
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	2	0.31
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	1	0.31
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	1	0.31
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	2	0.31
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	2	0.31
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	10	0.31
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	3	0.31
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	10	0.31
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	10	0.31
(1,538)	1:54:A:ASN:H	1:61:A:THR:H	2	0.31
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	5	0.31
(1,362)	1:65:A:CYS:HG	1:69:A:HIS:HD1	9	0.31
(1,351)	1:123:A:CYS:H	1:125:A:CYS:H	8	0.31
(1,292)	1:18:A:CYS:H	1:31:A:LEU:H	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,271)	1:99:A:THR:H	1:152:A:THR:HG1	7	0.31
(1,170)	1:153:A:ILE:HG21	1:155:A:CYS:H	8	0.31
(1,170)	1:153:A:ILE:HG22	1:155:A:CYS:H	8	0.31
(1,170)	1:153:A:ILE:HG23	1:155:A:CYS:H	8	0.31
(1,135)	1:17:A:HIS:HB3	1:28:A:ASN:H	1	0.31
(1,34)	1:166:A:GLU:HB2	1:168:A:ASP:H	8	0.31
(3,56)	1:56:A:CYS:O	1:59:A:SER:N	6	0.3
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	4	0.3
(3,11)	1:138:A:CYS:O	1:144:A:GLY:H	10	0.3
(1,772)	1:157:A:GLU:HA	1:158:A:ASP:H	6	0.3
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	1	0.3
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	3	0.3
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	2	0.3
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	6	0.3
(1,749)	1:129:A:LYS:HA	1:130:A:LEU:H	5	0.3
(1,717)	1:95:A:HIS:HA	1:96:A:ASP:H	4	0.3
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	3	0.3
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	4	0.3
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	7	0.3
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	9	0.3
(1,713)	1:91:A:SER:HA	1:92:A:HIS:H	10	0.3
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	3	0.3
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	1	0.3
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	2	0.3
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	3	0.3
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	5	0.3
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	6	0.3
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	7	0.3
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	10	0.3
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	2	0.3
(1,690)	1:66:A:ASN:HA	1:67:A:GLU:H	1	0.3
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	5	0.3
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	9	0.3
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	7	0.3
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	7	0.3
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	7	0.3
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	7	0.3
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	8	0.3
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	8	0.3
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	5	0.3
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	9	0.3
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	2	0.3
(1,524)	1:33:A:ASP:H	1:48:A:ARG:H	3	0.3
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	3	0.3
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	10	0.3
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	10	0.3
(1,498)	1:140:A:ARG:H	1:142:A:GLU:H	5	0.3
(1,456)	1:132:A:CYS:CB	1:150:A:CYS:SG	3	0.3
(1,451)	1:34:A:CYS:SG	1:47:A:CYS:CB	4	0.3
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD21	8	0.3
(1,411)	1:63:A:ILE:HB	1:66:A:ASN:HD22	8	0.3
(1,398)	1:43:A:TYR:HB2	1:60:A:CYS:H	6	0.3
(1,398)	1:43:A:TYR:HB3	1:60:A:CYS:H	6	0.3
(1,295)	1:29:A:CYS:HG	1:31:A:LEU:H	7	0.3
(1,292)	1:18:A:CYS:H	1:31:A:LEU:H	5	0.3
(1,275)	1:99:A:THR:H	1:152:A:THR:H	1	0.3
(1,234)	1:112:A:CYS:H	1:125:A:CYS:H	6	0.3
(1,216)	1:100:A:HIS:HD1	1:102:A:GLU:H	6	0.3
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	6	0.3
(1,139)	1:75:A:HIS:HD1	1:124:A:GLY:H	4	0.3
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	7	0.3
(1,31)	1:152:A:THR:HG1	1:168:A:ASP:H	8	0.3
(1,13)	1:75:A:HIS:HE1	1:77:A:GLU:H	4	0.3
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	5	0.29
(3,50)	1:54:A:ASN:O	1:61:A:THR:N	1	0.29
(3,48)	1:37:A:LYS:O	1:44:A:ALA:N	4	0.29
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	8	0.29
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	10	0.29
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	3	0.29
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	1	0.29
(1,772)	1:157:A:GLU:HA	1:158:A:ASP:H	3	0.29
(1,772)	1:157:A:GLU:HA	1:158:A:ASP:H	5	0.29
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	3	0.29
(1,750)	1:131:A:PRO:HA	1:132:A:CYS:H	6	0.29
(1,721)	1:99:A:THR:HA	1:100:A:HIS:H	4	0.29
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	5	0.29
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	1	0.29
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	2	0.29
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	6	0.29
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	5	0.29
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	7	0.29
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	7	0.29
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	9	0.29
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	1	0.29
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	2	0.29
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	3	0.29
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	5	0.29
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	6	0.29
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	8	0.29
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	4	0.29
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	6	0.29
(1,690)	1:66:A:ASN:HA	1:67:A:GLU:H	7	0.29
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	6	0.29
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	6	0.29
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	6	0.29
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	6	0.29
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	8	0.29
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	8	0.29
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	8	0.29
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	8	0.29
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	1	0.29
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	1	0.29
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	10	0.29
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	10	0.29
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	9	0.29
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	9	0.29
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	5	0.29
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	6	0.29
(1,559)	1:20:A:ALA:HA	1:24:A:ASN:H	2	0.29
(1,556)	1:19:A:ASP:HB2	1:22:A:GLY:H	3	0.29
(1,556)	1:19:A:ASP:HB3	1:22:A:GLY:H	3	0.29
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	7	0.29
(1,519)	1:158:A:ASP:HB2	1:159:A:HIS:H	4	0.29
(1,519)	1:158:A:ASP:HB3	1:159:A:HIS:H	4	0.29
(1,519)	1:158:A:ASP:HB2	1:159:A:HIS:H	9	0.29
(1,519)	1:158:A:ASP:HB3	1:159:A:HIS:H	9	0.29
(1,516)	1:155:A:CYS:HB2	1:156:A:ASN:H	4	0.29
(1,516)	1:155:A:CYS:HB3	1:156:A:ASN:H	4	0.29
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	5	0.29
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	2	0.29
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	2	0.29
(1,495)	1:136:A:HIS:H	1:146:A:VAL:H	9	0.29
(1,481)	1:134:A:ASP:H	1:148:A:CYS:H	3	0.29
(1,458)	1:155:A:CYS:CB	1:161:A:CYS:SG	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:81:A:ASP:HB2	1:85:A:HIS:HD1	5	0.29
(1,419)	1:81:A:ASP:HB3	1:85:A:HIS:HD1	5	0.29
(1,418)	1:75:A:HIS:HB2	1:112:A:CYS:H	9	0.29
(1,418)	1:75:A:HIS:HB3	1:112:A:CYS:H	9	0.29
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	3	0.29
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	3	0.29
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	3	0.29
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	8	0.29
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	8	0.29
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	8	0.29
(1,320)	1:17:A:HIS:HE1	1:21:A:ASN:HD22	7	0.29
(1,315)	1:100:A:HIS:HD1	1:123:A:CYS:H	6	0.29
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG21	4	0.29
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG22	4	0.29
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG23	4	0.29
(1,216)	1:100:A:HIS:HD1	1:102:A:GLU:H	3	0.29
(1,213)	1:30:A:GLU:H	1:128:A:SER:HG	4	0.29
(1,163)	1:100:A:HIS:H	1:152:A:THR:H	9	0.29
(1,106)	1:71:A:CYS:H	1:72:A:HIS:HD1	6	0.29
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	10	0.29
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	4	0.29
(1,32)	1:152:A:THR:HG21	1:168:A:ASP:H	4	0.29
(1,32)	1:152:A:THR:HG22	1:168:A:ASP:H	4	0.29
(1,32)	1:152:A:THR:HG23	1:168:A:ASP:H	4	0.29
(1,22)	1:161:A:CYS:H	1:163:A:HIS:HD1	8	0.29
(1,22)	1:161:A:CYS:H	1:163:A:HIS:HD1	9	0.29
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	4	0.28
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	6	0.28
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	2	0.28
(3,5)	1:105:A:LYS:O	1:107:A:ALA:H	1	0.28
(3,3)	1:102:A:GLU:O	1:110:A:TRP:H	8	0.28
(1,772)	1:157:A:GLU:HA	1:158:A:ASP:H	10	0.28
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	10	0.28
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	9	0.28
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	5	0.28
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	8	0.28
(1,714)	1:92:A:HIS:HA	1:93:A:ASP:H	10	0.28
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	1	0.28
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	4	0.28
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	6	0.28
(1,711)	1:89:A:GLU:HA	1:90:A:HIS:H	4	0.28
(1,708)	1:86:A:CYS:HA	1:87:A:SER:H	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	7	0.28
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	9	0.28
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	2	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	1	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	1	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	1	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	1	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	2	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	2	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	2	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	2	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	3	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	3	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	3	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	3	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	5	0.28
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	5	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	5	0.28
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	5	0.28
(1,573)	1:23:A:GLU:HA	1:27:A:CYS:H	2	0.28
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	2	0.28
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	5	0.28
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	5	0.28
(1,562)	1:20:A:ALA:HA	1:22:A:GLY:H	3	0.28
(1,538)	1:54:A:ASN:H	1:61:A:THR:H	3	0.28
(1,532)	1:43:A:TYR:HB2	1:55:A:ILE:HD11	3	0.28
(1,532)	1:43:A:TYR:HB3	1:55:A:ILE:HD11	3	0.28
(1,519)	1:158:A:ASP:HB2	1:159:A:HIS:H	7	0.28
(1,519)	1:158:A:ASP:HB3	1:159:A:HIS:H	7	0.28
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB2	1	0.28
(1,514)	1:154:A:THR:HB	1:155:A:CYS:HB3	1	0.28
(1,509)	1:153:A:ILE:H	1:163:A:HIS:H	3	0.28
(1,497)	1:138:A:CYS:H	1:144:A:GLY:H	8	0.28
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	1	0.28
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	1	0.28
(1,460)	1:100:A:HIS:HB2	1:101:A:GLY:H	7	0.28
(1,460)	1:100:A:HIS:HB3	1:101:A:GLY:H	7	0.28
(1,444)	1:159:A:HIS:HB2	1:161:A:CYS:H	4	0.28
(1,444)	1:159:A:HIS:HB3	1:161:A:CYS:H	4	0.28
(1,415)	1:66:A:ASN:HD21	1:68:A:ASP:H	7	0.28
(1,415)	1:66:A:ASN:HD22	1:68:A:ASP:H	7	0.28
(1,320)	1:17:A:HIS:HE1	1:21:A:ASN:HD22	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:29:A:CYS:HG	1:31:A:LEU:H	2	0.28
(1,245)	1:101:A:GLY:H	1:152:A:THR:H	5	0.28
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	5	0.28
(1,139)	1:75:A:HIS:HD1	1:124:A:GLY:H	5	0.28
(1,139)	1:75:A:HIS:HD1	1:124:A:GLY:H	9	0.28
(1,109)	1:75:A:HIS:HD1	1:112:A:CYS:H	1	0.28
(1,106)	1:71:A:CYS:H	1:72:A:HIS:HD1	9	0.28
(1,105)	1:49:A:ARG:H	1:74:A:CYS:H	4	0.28
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	7	0.28
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	9	0.28
(1,20)	1:112:A:CYS:HG	1:125:A:CYS:H	9	0.28
(1,13)	1:75:A:HIS:HE1	1:77:A:GLU:H	7	0.28
(1,13)	1:75:A:HIS:HE1	1:77:A:GLU:H	9	0.28
(3,31)	1:87:A:SER:O	1:91:A:SER:H	4	0.27
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	9	0.27
(3,14)	1:140:A:ARG:O	1:142:A:GLU:N	3	0.27
(1,767)	1:152:A:THR:HA	1:153:A:ILE:H	7	0.27
(1,767)	1:152:A:THR:HA	1:153:A:ILE:H	8	0.27
(1,758)	1:140:A:ARG:HA	1:141:A:LYS:H	3	0.27
(1,758)	1:140:A:ARG:HA	1:141:A:LYS:H	6	0.27
(1,717)	1:95:A:HIS:HA	1:96:A:ASP:H	3	0.27
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	1	0.27
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	2	0.27
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	2	0.27
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	8	0.27
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	9	0.27
(1,712)	1:90:A:HIS:HA	1:91:A:SER:H	10	0.27
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	3	0.27
(1,690)	1:66:A:ASN:HA	1:67:A:GLU:H	8	0.27
(1,690)	1:66:A:ASN:HA	1:67:A:GLU:H	10	0.27
(1,626)	1:90:A:HIS:HB2	1:92:A:HIS:H	10	0.27
(1,626)	1:90:A:HIS:HB3	1:92:A:HIS:H	10	0.27
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	9	0.27
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	4	0.27
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	4	0.27
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	7	0.27
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	7	0.27
(1,562)	1:20:A:ALA:HA	1:22:A:GLY:H	8	0.27
(1,562)	1:20:A:ALA:HA	1:22:A:GLY:H	9	0.27
(1,559)	1:20:A:ALA:HA	1:24:A:ASN:H	5	0.27
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	3	0.27
(1,538)	1:54:A:ASN:H	1:61:A:THR:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	6	0.27
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	4	0.27
(1,458)	1:155:A:CYS:CB	1:161:A:CYS:SG	3	0.27
(1,454)	1:103:A:CYS:CB	1:109:A:CYS:SG	1	0.27
(1,451)	1:34:A:CYS:SG	1:47:A:CYS:CB	2	0.27
(1,419)	1:81:A:ASP:HB2	1:85:A:HIS:HD1	9	0.27
(1,419)	1:81:A:ASP:HB3	1:85:A:HIS:HD1	9	0.27
(1,416)	1:66:A:ASN:HD21	1:69:A:HIS:HD1	10	0.27
(1,416)	1:66:A:ASN:HD22	1:69:A:HIS:HD1	10	0.27
(1,289)	1:149:A:ASP:H	1:170:A:VAL:H	8	0.27
(1,105)	1:49:A:ARG:H	1:74:A:CYS:H	8	0.27
(1,93)	1:63:A:ILE:HB	1:66:A:ASN:H	6	0.27
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	9	0.27
(1,34)	1:166:A:GLU:HB2	1:168:A:ASP:H	2	0.27
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	3	0.26
(3,38)	1:18:A:CYS:O	1:22:A:GLY:N	5	0.26
(3,15)	1:153:A:ILE:O	1:163:A:HIS:H	9	0.26
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	8	0.26
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	4	0.26
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	6	0.26
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	4	0.26
(1,750)	1:131:A:PRO:HA	1:132:A:CYS:H	2	0.26
(1,750)	1:131:A:PRO:HA	1:132:A:CYS:H	4	0.26
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	6	0.26
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	8	0.26
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	9	0.26
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	9	0.26
(1,707)	1:85:A:HIS:HA	1:86:A:CYS:H	5	0.26
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	9	0.26
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	9	0.26
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	10	0.26
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	10	0.26
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	10	0.26
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	10	0.26
(1,613)	1:87:A:SER:HB2	1:91:A:SER:HA	9	0.26
(1,613)	1:87:A:SER:HB3	1:91:A:SER:HA	9	0.26
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	6	0.26
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	6	0.26
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	1	0.26
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	2	0.26
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	7	0.26
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	7	0.26
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	2	0.26
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	2	0.26
(1,515)	1:154:A:THR:HA	1:161:A:CYS:H	1	0.26
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA2	7	0.26
(1,493)	1:139:A:TYR:HA	1:143:A:GLY:HA3	7	0.26
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG2	1	0.26
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG3	1	0.26
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG2	1	0.26
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG3	1	0.26
(1,484)	1:135:A:GLU:HB2	1:136:A:HIS:H	5	0.26
(1,484)	1:135:A:GLU:HB3	1:136:A:HIS:H	5	0.26
(1,446)	1:166:A:GLU:HG2	1:168:A:ASP:H	9	0.26
(1,446)	1:166:A:GLU:HG3	1:168:A:ASP:H	9	0.26
(1,419)	1:81:A:ASP:HB2	1:85:A:HIS:HD1	3	0.26
(1,419)	1:81:A:ASP:HB3	1:85:A:HIS:HD1	3	0.26
(1,293)	1:17:A:HIS:HB2	1:31:A:LEU:H	6	0.26
(1,241)	1:101:A:GLY:H	1:123:A:CYS:HB3	1	0.26
(1,234)	1:112:A:CYS:H	1:125:A:CYS:H	3	0.26
(1,232)	1:17:A:HIS:HB3	1:29:A:CYS:H	6	0.26
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	3	0.26
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	8	0.26
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	2	0.25
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	1	0.25
(3,45)	1:33:A:ASP:O	1:48:A:ARG:H	5	0.25
(3,40)	1:19:A:ASP:O	1:23:A:GLU:N	8	0.25
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	1	0.25
(3,21)	1:82:A:THR:O	1:86:A:CYS:H	10	0.25
(1,766)	1:151:A:LYS:HA	1:152:A:THR:H	8	0.25
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	9	0.25
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	1	0.25
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	5	0.25
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	6	0.25
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	8	0.25
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	1	0.25
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	2	0.25
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	3	0.25
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	5	0.25
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	6	0.25
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	7	0.25
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	8	0.25
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:66:A:ASN:HA	1:67:A:GLU:H	2	0.25
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	9	0.25
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	7	0.25
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	7	0.25
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	7	0.25
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	2	0.25
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	3	0.25
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	3	0.25
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	7	0.25
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	5	0.25
(1,576)	1:26:A:SER:HB2	1:27:A:CYS:H	8	0.25
(1,565)	1:21:A:ASN:HB2	1:25:A:CYS:H	3	0.25
(1,565)	1:21:A:ASN:HB3	1:25:A:CYS:H	3	0.25
(1,559)	1:20:A:ALA:HA	1:24:A:ASN:H	3	0.25
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	9	0.25
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	6	0.25
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	6	0.25
(1,498)	1:140:A:ARG:H	1:142:A:GLU:H	6	0.25
(1,457)	1:155:A:CYS:SG	1:161:A:CYS:CB	1	0.25
(1,454)	1:103:A:CYS:CB	1:109:A:CYS:SG	6	0.25
(1,351)	1:123:A:CYS:H	1:125:A:CYS:H	5	0.25
(1,340)	1:105:A:LYS:HB3	1:162:A:TYR:H	4	0.25
(1,324)	1:52:A:ALA:H	1:54:A:ASN:HD22	1	0.25
(1,205)	1:110:A:TRP:HE1	1:152:A:THR:H	4	0.25
(1,163)	1:100:A:HIS:H	1:152:A:THR:H	7	0.25
(1,48)	1:10:A:ASN:H	1:13:A:ALA:H	3	0.25
(1,22)	1:161:A:CYS:H	1:163:A:HIS:HD1	2	0.25
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	9	0.25
(3,54)	1:52:A:ALA:O	1:63:A:ILE:N	5	0.24
(3,52)	1:50:A:CYS:O	1:65:A:CYS:N	6	0.24
(3,31)	1:87:A:SER:O	1:91:A:SER:H	5	0.24
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	2	0.24
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	6	0.24
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	8	0.24
(3,21)	1:82:A:THR:O	1:86:A:CYS:H	4	0.24
(1,758)	1:140:A:ARG:HA	1:141:A:LYS:H	5	0.24
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	1	0.24
(1,716)	1:94:A:HIS:HA	1:95:A:HIS:H	2	0.24
(1,709)	1:87:A:SER:HA	1:88:A:CYS:H	4	0.24
(1,690)	1:66:A:ASN:HA	1:67:A:GLU:H	6	0.24
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	8	0.24
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	6	0.24
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	5	0.24
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	5	0.24
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	8	0.24
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	8	0.24
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	1	0.24
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	2	0.24
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	8	0.24
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	10	0.24
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	7	0.24
(1,569)	1:22:A:GLY:HA2	1:26:A:SER:H	9	0.24
(1,569)	1:22:A:GLY:HA3	1:26:A:SER:H	9	0.24
(1,569)	1:22:A:GLY:HA2	1:26:A:SER:H	9	0.24
(1,569)	1:22:A:GLY:HA3	1:26:A:SER:H	9	0.24
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	8	0.24
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	3	0.24
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	3	0.24
(1,462)	1:103:A:CYS:HB2	1:104:A:THR:H	3	0.24
(1,462)	1:103:A:CYS:HB3	1:104:A:THR:H	3	0.24
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	5	0.24
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	5	0.24
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	10	0.24
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	10	0.24
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	10	0.24
(1,278)	1:59:A:SER:H	1:61:A:THR:HG21	6	0.24
(1,278)	1:59:A:SER:H	1:61:A:THR:HG22	6	0.24
(1,278)	1:59:A:SER:H	1:61:A:THR:HG23	6	0.24
(1,257)	1:112:A:CYS:H	1:126:A:GLU:H	5	0.24
(1,241)	1:101:A:GLY:H	1:123:A:CYS:HB3	3	0.24
(1,219)	1:21:A:ASN:H	1:47:A:CYS:H	8	0.24
(1,158)	1:20:A:ALA:HB1	1:75:A:HIS:H	9	0.24
(1,158)	1:20:A:ALA:HB2	1:75:A:HIS:H	9	0.24
(1,158)	1:20:A:ALA:HB3	1:75:A:HIS:H	9	0.24
(1,103)	1:49:A:ARG:H	1:74:A:CYS:HG	8	0.24
(1,15)	1:66:A:ASN:HD22	1:67:A:GLU:H	8	0.24
(3,44)	1:21:A:ASN:O	1:25:A:CYS:N	2	0.23
(3,43)	1:21:A:ASN:O	1:25:A:CYS:H	4	0.23
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	10	0.23
(3,21)	1:82:A:THR:O	1:86:A:CYS:H	1	0.23
(3,21)	1:82:A:THR:O	1:86:A:CYS:H	8	0.23
(3,15)	1:153:A:ILE:O	1:163:A:HIS:H	4	0.23
(3,12)	1:138:A:CYS:O	1:144:A:GLY:N	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	1:136:A:HIS:O	1:146:A:VAL:N	2	0.23
(3,5)	1:105:A:LYS:O	1:107:A:ALA:H	2	0.23
(2,1)	1:34:A:CYS:SG	1:47:A:CYS:SG	6	0.23
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	2	0.23
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	6	0.23
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	10	0.23
(1,693)	1:70:A:PRO:HA	1:71:A:CYS:H	3	0.23
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	6	0.23
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	8	0.23
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	8	0.23
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	8	0.23
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	1	0.23
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	1	0.23
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	8	0.23
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	10	0.23
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	6	0.23
(1,522)	1:155:A:CYS:HB2	1:161:A:CYS:H	5	0.23
(1,522)	1:155:A:CYS:HB3	1:161:A:CYS:H	5	0.23
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	4	0.23
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	4	0.23
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	6	0.23
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	6	0.23
(1,413)	1:63:A:ILE:HG12	1:66:A:ASN:HD21	2	0.23
(1,413)	1:63:A:ILE:HG12	1:66:A:ASN:HD22	2	0.23
(1,413)	1:63:A:ILE:HG13	1:66:A:ASN:HD21	2	0.23
(1,413)	1:63:A:ILE:HG13	1:66:A:ASN:HD22	2	0.23
(1,324)	1:52:A:ALA:H	1:54:A:ASN:HD22	9	0.23
(1,190)	1:75:A:HIS:HD1	1:123:A:CYS:H	8	0.23
(1,183)	1:75:A:HIS:HE1	1:123:A:CYS:H	3	0.23
(1,170)	1:153:A:ILE:HG21	1:155:A:CYS:H	6	0.23
(1,170)	1:153:A:ILE:HG22	1:155:A:CYS:H	6	0.23
(1,170)	1:153:A:ILE:HG23	1:155:A:CYS:H	6	0.23
(1,158)	1:20:A:ALA:HB1	1:75:A:HIS:H	1	0.23
(1,158)	1:20:A:ALA:HB2	1:75:A:HIS:H	1	0.23
(1,158)	1:20:A:ALA:HB3	1:75:A:HIS:H	1	0.23
(1,121)	1:18:A:CYS:HG	1:20:A:ALA:H	6	0.23
(1,104)	1:49:A:ARG:H	1:74:A:CYS:HA	8	0.23
(1,29)	1:17:A:HIS:H	1:29:A:CYS:HA	8	0.23
(1,18)	1:100:A:HIS:HD1	1:123:A:CYS:HB2	9	0.23
(3,52)	1:50:A:CYS:O	1:65:A:CYS:N	9	0.22
(3,47)	1:37:A:LYS:O	1:44:A:ALA:H	10	0.22
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:82:A:THR:O	1:86:A:CYS:H	2	0.22
(3,13)	1:140:A:ARG:O	1:142:A:GLU:H	5	0.22
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	7	0.22
(3,2)	1:100:A:HIS:O	1:112:A:CYS:N	10	0.22
(1,773)	1:158:A:ASP:HA	1:159:A:HIS:H	10	0.22
(1,753)	1:134:A:ASP:HA	1:135:A:GLU:H	1	0.22
(1,750)	1:131:A:PRO:HA	1:132:A:CYS:H	1	0.22
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	8	0.22
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	3	0.22
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	7	0.22
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	10	0.22
(1,673)	1:46:A:PRO:HA	1:47:A:CYS:H	2	0.22
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	8	0.22
(1,651)	1:11:A:SER:HA	1:12:A:ASN:H	3	0.22
(1,651)	1:11:A:SER:HA	1:12:A:ASN:H	8	0.22
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	10	0.22
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	10	0.22
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	8	0.22
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	3	0.22
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	2	0.22
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	2	0.22
(1,608)	1:86:A:CYS:HB2	1:89:A:GLU:H	10	0.22
(1,608)	1:86:A:CYS:HB3	1:89:A:GLU:H	10	0.22
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	1	0.22
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	3	0.22
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	2	0.22
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	5	0.22
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	9	0.22
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	8	0.22
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD21	4	0.22
(1,555)	1:19:A:ASP:HB3	1:21:A:ASN:HD22	4	0.22
(1,503)	1:142:A:GLU:HB2	1:143:A:GLY:H	10	0.22
(1,503)	1:142:A:GLU:HB3	1:143:A:GLY:H	10	0.22
(1,480)	1:133:A:ASN:HD21	1:134:A:ASP:H	6	0.22
(1,458)	1:155:A:CYS:CB	1:161:A:CYS:SG	1	0.22
(1,435)	1:135:A:GLU:H	1:184:A:SER:HB2	5	0.22
(1,435)	1:135:A:GLU:H	1:184:A:SER:HB3	5	0.22
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	3	0.22
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	3	0.22
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	9	0.22
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	9	0.22
(1,417)	1:66:A:ASN:HD21	1:69:A:HIS:HE1	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:66:A:ASN:HD22	1:69:A:HIS:HE1	2	0.22
(1,415)	1:66:A:ASN:HD21	1:68:A:ASP:H	6	0.22
(1,415)	1:66:A:ASN:HD22	1:68:A:ASP:H	6	0.22
(1,362)	1:65:A:CYS:HG	1:69:A:HIS:HD1	3	0.22
(1,331)	1:20:A:ALA:HB1	1:125:A:CYS:H	4	0.22
(1,331)	1:20:A:ALA:HB2	1:125:A:CYS:H	4	0.22
(1,331)	1:20:A:ALA:HB3	1:125:A:CYS:H	4	0.22
(1,271)	1:99:A:THR:H	1:152:A:THR:HG1	4	0.22
(1,181)	1:75:A:HIS:HD2	1:123:A:CYS:H	1	0.22
(1,131)	1:17:A:HIS:HB2	1:28:A:ASN:H	3	0.22
(1,131)	1:17:A:HIS:HB2	1:28:A:ASN:H	5	0.22
(1,109)	1:75:A:HIS:HD1	1:112:A:CYS:H	5	0.22
(1,104)	1:49:A:ARG:H	1:74:A:CYS:HA	7	0.22
(1,73)	1:162:A:TYR:H	1:163:A:HIS:HD1	8	0.22
(1,71)	1:38:A:LYS:H	1:40:A:ASP:H	5	0.22
(1,33)	1:152:A:THR:H	1:168:A:ASP:H	3	0.22
(1,22)	1:161:A:CYS:H	1:163:A:HIS:HD1	10	0.22
(1,20)	1:112:A:CYS:HG	1:125:A:CYS:H	5	0.22
(3,42)	1:20:A:ALA:O	1:24:A:ASN:N	9	0.21
(3,40)	1:19:A:ASP:O	1:23:A:GLU:N	4	0.21
(3,31)	1:87:A:SER:O	1:91:A:SER:H	9	0.21
(3,28)	1:85:A:HIS:O	1:89:A:GLU:N	10	0.21
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	2	0.21
(3,13)	1:140:A:ARG:O	1:142:A:GLU:H	4	0.21
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	3	0.21
(2,2)	1:103:A:CYS:SG	1:109:A:CYS:SG	7	0.21
(1,745)	1:125:A:CYS:HA	1:126:A:GLU:H	5	0.21
(1,721)	1:99:A:THR:HA	1:100:A:HIS:H	10	0.21
(1,719)	1:97:A:ASP:HA	1:98:A:ASP:H	3	0.21
(1,691)	1:67:A:GLU:HA	1:68:A:ASP:H	6	0.21
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	1	0.21
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	1	0.21
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	3	0.21
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB2	9	0.21
(1,623)	1:89:A:GLU:HB2	1:91:A:SER:HB3	9	0.21
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB2	9	0.21
(1,623)	1:89:A:GLU:HB3	1:91:A:SER:HB3	9	0.21
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	2	0.21
(1,601)	1:85:A:HIS:HD1	1:88:A:CYS:H	4	0.21
(1,582)	1:82:A:THR:HG1	1:85:A:HIS:H	4	0.21
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	1	0.21
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	4	0.21
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	6	0.21
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	6	0.21
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	9	0.21
(1,502)	1:141:A:LYS:HG2	1:142:A:GLU:H	9	0.21
(1,502)	1:141:A:LYS:HG3	1:142:A:GLU:H	9	0.21
(1,500)	1:140:A:ARG:HG2	1:141:A:LYS:H	4	0.21
(1,500)	1:140:A:ARG:HG3	1:141:A:LYS:H	4	0.21
(1,498)	1:140:A:ARG:H	1:142:A:GLU:H	3	0.21
(1,494)	1:132:A:CYS:HB2	1:150:A:CYS:H	3	0.21
(1,494)	1:132:A:CYS:HB3	1:150:A:CYS:H	3	0.21
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG2	2	0.21
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG3	2	0.21
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG2	2	0.21
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG3	2	0.21
(1,444)	1:159:A:HIS:HB2	1:161:A:CYS:H	8	0.21
(1,444)	1:159:A:HIS:HB3	1:161:A:CYS:H	8	0.21
(1,438)	1:135:A:GLU:HB2	1:185:A:GLU:H	10	0.21
(1,438)	1:135:A:GLU:HB3	1:185:A:GLU:H	10	0.21
(1,301)	1:135:A:GLU:H	1:185:A:GLU:H	5	0.21
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	9	0.21
(1,219)	1:21:A:ASN:H	1:47:A:CYS:H	7	0.21
(1,216)	1:100:A:HIS:HD1	1:102:A:GLU:H	5	0.21
(1,212)	1:17:A:HIS:HA	1:30:A:GLU:H	4	0.21
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	4	0.21
(1,186)	1:50:A:CYS:H	1:73:A:HIS:H	6	0.21
(1,173)	1:29:A:CYS:H	1:129:A:LYS:H	7	0.21
(1,168)	1:29:A:CYS:H	1:128:A:SER:HG	10	0.21
(1,67)	1:75:A:HIS:HE1	1:76:A:GLU:H	4	0.21
(1,24)	1:10:A:ASN:HD22	1:17:A:HIS:H	6	0.21
(1,14)	1:67:A:GLU:H	1:69:A:HIS:HE1	6	0.21
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	5	0.2
(3,48)	1:37:A:LYS:O	1:44:A:ALA:N	2	0.2
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	9	0.2
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	3	0.2
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	1	0.2
(3,25)	1:84:A:CYS:O	1:88:A:CYS:H	8	0.2
(3,18)	1:157:A:GLU:O	1:159:A:HIS:N	9	0.2
(3,14)	1:140:A:ARG:O	1:142:A:GLU:N	1	0.2
(3,11)	1:138:A:CYS:O	1:144:A:GLY:H	7	0.2
(1,772)	1:157:A:GLU:HA	1:158:A:ASP:H	7	0.2
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	1	0.2
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	5	0.2
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	6	0.2
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	6	0.2
(1,642)	1:150:A:CYS:HA	1:153:A:ILE:H	9	0.2
(1,638)	1:67:A:GLU:HA	1:69:A:HIS:H	8	0.2
(1,628)	1:91:A:SER:HA	1:95:A:HIS:H	9	0.2
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	8	0.2
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	9	0.2
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	8	0.2
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	1	0.2
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	1	0.2
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	4	0.2
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	3	0.2
(1,511)	1:153:A:ILE:HB	1:154:A:THR:HG1	4	0.2
(1,503)	1:142:A:GLU:HB2	1:143:A:GLY:H	6	0.2
(1,503)	1:142:A:GLU:HB3	1:143:A:GLY:H	6	0.2
(1,475)	1:102:A:GLU:H	1:110:A:TRP:H	9	0.2
(1,453)	1:103:A:CYS:SG	1:109:A:CYS:CB	10	0.2
(1,418)	1:75:A:HIS:HB2	1:112:A:CYS:H	7	0.2
(1,418)	1:75:A:HIS:HB3	1:112:A:CYS:H	7	0.2
(1,413)	1:63:A:ILE:HG12	1:66:A:ASN:HD21	7	0.2
(1,413)	1:63:A:ILE:HG12	1:66:A:ASN:HD22	7	0.2
(1,413)	1:63:A:ILE:HG13	1:66:A:ASN:HD21	7	0.2
(1,413)	1:63:A:ILE:HG13	1:66:A:ASN:HD22	7	0.2
(1,339)	1:105:A:LYS:H	1:162:A:TYR:H	7	0.2
(1,247)	1:100:A:HIS:HE1	1:101:A:GLY:H	10	0.2
(1,109)	1:75:A:HIS:HD1	1:112:A:CYS:H	2	0.2
(1,20)	1:112:A:CYS:HG	1:125:A:CYS:H	3	0.2
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	8	0.19
(3,49)	1:54:A:ASN:O	1:61:A:THR:H	8	0.19
(3,31)	1:87:A:SER:O	1:91:A:SER:H	6	0.19
(3,28)	1:85:A:HIS:O	1:89:A:GLU:N	9	0.19
(3,14)	1:140:A:ARG:O	1:142:A:GLU:N	7	0.19
(3,2)	1:100:A:HIS:O	1:112:A:CYS:N	2	0.19
(1,772)	1:157:A:GLU:HA	1:158:A:ASP:H	4	0.19
(1,772)	1:157:A:GLU:HA	1:158:A:ASP:H	9	0.19
(1,715)	1:93:A:ASP:HA	1:94:A:HIS:H	4	0.19
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	6	0.19
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	10	0.19
(1,576)	1:26:A:SER:HB2	1:27:A:CYS:H	7	0.19
(1,484)	1:135:A:GLU:HB2	1:136:A:HIS:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:135:A:GLU:HB3	1:136:A:HIS:H	2	0.19
(1,459)	1:100:A:HIS:H	1:112:A:CYS:H	4	0.19
(1,457)	1:155:A:CYS:SG	1:161:A:CYS:CB	9	0.19
(1,455)	1:132:A:CYS:SG	1:150:A:CYS:CB	6	0.19
(1,446)	1:166:A:GLU:HG2	1:168:A:ASP:H	8	0.19
(1,446)	1:166:A:GLU:HG3	1:168:A:ASP:H	8	0.19
(1,437)	1:135:A:GLU:HB2	1:184:A:SER:H	10	0.19
(1,437)	1:135:A:GLU:HB3	1:184:A:SER:H	10	0.19
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	5	0.19
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	5	0.19
(1,423)	1:88:A:CYS:HB2	1:90:A:HIS:HD1	6	0.19
(1,423)	1:88:A:CYS:HB3	1:90:A:HIS:HD1	6	0.19
(1,412)	1:63:A:ILE:HG12	1:66:A:ASN:H	6	0.19
(1,412)	1:63:A:ILE:HG13	1:66:A:ASN:H	6	0.19
(1,398)	1:43:A:TYR:HB2	1:60:A:CYS:H	5	0.19
(1,398)	1:43:A:TYR:HB3	1:60:A:CYS:H	5	0.19
(1,361)	1:66:A:ASN:H	1:69:A:HIS:HD1	7	0.19
(1,351)	1:123:A:CYS:H	1:125:A:CYS:H	9	0.19
(1,324)	1:52:A:ALA:H	1:54:A:ASN:HD22	10	0.19
(1,278)	1:59:A:SER:H	1:61:A:THR:HG21	1	0.19
(1,278)	1:59:A:SER:H	1:61:A:THR:HG22	1	0.19
(1,278)	1:59:A:SER:H	1:61:A:THR:HG23	1	0.19
(1,242)	1:101:A:GLY:H	1:168:A:ASP:H	1	0.19
(1,177)	1:24:A:ASN:HD21	1:54:A:ASN:H	3	0.19
(1,135)	1:17:A:HIS:HB3	1:28:A:ASN:H	6	0.19
(1,133)	1:28:A:ASN:H	1:29:A:CYS:HG	3	0.19
(1,128)	1:172:A:LYS:HB3	1:174:A:ASP:H	4	0.19
(1,114)	1:159:A:HIS:HD1	1:161:A:CYS:H	7	0.19
(1,113)	1:75:A:HIS:HD1	1:126:A:GLU:H	8	0.19
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	2	0.19
(1,73)	1:162:A:TYR:H	1:163:A:HIS:HD1	2	0.19
(1,32)	1:152:A:THR:HG21	1:168:A:ASP:H	9	0.19
(1,32)	1:152:A:THR:HG22	1:168:A:ASP:H	9	0.19
(1,32)	1:152:A:THR:HG23	1:168:A:ASP:H	9	0.19
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	1	0.19
(1,13)	1:75:A:HIS:HE1	1:77:A:GLU:H	3	0.19
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	1	0.18
(3,41)	1:20:A:ALA:O	1:24:A:ASN:H	6	0.18
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	5	0.18
(3,31)	1:87:A:SER:O	1:91:A:SER:H	3	0.18
(3,18)	1:157:A:GLU:O	1:159:A:HIS:N	7	0.18
(3,14)	1:140:A:ARG:O	1:142:A:GLU:N	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	1:138:A:CYS:O	1:144:A:GLY:H	9	0.18
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	4	0.18
(3,4)	1:102:A:GLU:O	1:110:A:TRP:N	1	0.18
(1,745)	1:125:A:CYS:HA	1:126:A:GLU:H	1	0.18
(1,718)	1:96:A:ASP:HA	1:97:A:ASP:H	7	0.18
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	10	0.18
(1,651)	1:11:A:SER:HA	1:12:A:ASN:H	7	0.18
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	10	0.18
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	10	0.18
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	6	0.18
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	6	0.18
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	8	0.18
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	8	0.18
(1,620)	1:89:A:GLU:HA	1:93:A:ASP:H	9	0.18
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	3	0.18
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	6	0.18
(1,578)	1:82:A:THR:HA	1:84:A:CYS:H	7	0.18
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	10	0.18
(1,567)	1:21:A:ASN:HD21	1:24:A:ASN:H	4	0.18
(1,567)	1:21:A:ASN:HD22	1:24:A:ASN:H	4	0.18
(1,562)	1:20:A:ALA:HA	1:22:A:GLY:H	5	0.18
(1,562)	1:20:A:ALA:HA	1:22:A:GLY:H	7	0.18
(1,553)	1:19:A:ASP:HA	1:21:A:ASN:H	3	0.18
(1,442)	1:153:A:ILE:HG12	1:155:A:CYS:H	5	0.18
(1,442)	1:153:A:ILE:HG13	1:155:A:CYS:H	5	0.18
(1,421)	1:83:A:HIS:HB2	1:85:A:HIS:HD1	7	0.18
(1,421)	1:83:A:HIS:HB3	1:85:A:HIS:HD1	7	0.18
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB2	2	0.18
(1,387)	1:18:A:CYS:H	1:30:A:GLU:HB3	2	0.18
(1,230)	1:74:A:CYS:HA	1:125:A:CYS:H	8	0.18
(1,224)	1:11:A:SER:H	1:16:A:TYR:H	9	0.18
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	1	0.18
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	7	0.17
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	9	0.17
(3,44)	1:21:A:ASN:O	1:25:A:CYS:N	4	0.17
(3,40)	1:19:A:ASP:O	1:23:A:GLU:N	2	0.17
(1,775)	1:161:A:CYS:HA	1:162:A:TYR:H	5	0.17
(1,758)	1:140:A:ARG:HA	1:141:A:LYS:H	10	0.17
(1,751)	1:132:A:CYS:HA	1:133:A:ASN:H	6	0.17
(1,690)	1:66:A:ASN:HA	1:67:A:GLU:H	4	0.17
(1,658)	1:23:A:GLU:HA	1:24:A:ASN:H	4	0.17
(1,631)	1:92:A:HIS:HA	1:94:A:HIS:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	10	0.17
(1,585)	1:83:A:HIS:HA	1:87:A:SER:H	10	0.17
(1,580)	1:82:A:THR:HA	1:86:A:CYS:H	5	0.17
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	1	0.17
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	2	0.17
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	8	0.17
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	10	0.17
(1,571)	1:23:A:GLU:HA	1:24:A:ASN:H	4	0.17
(1,568)	1:21:A:ASN:HA	1:24:A:ASN:H	1	0.17
(1,528)	1:38:A:LYS:HA	1:43:A:TYR:HA	1	0.17
(1,503)	1:142:A:GLU:HB2	1:143:A:GLY:H	3	0.17
(1,503)	1:142:A:GLU:HB3	1:143:A:GLY:H	3	0.17
(1,498)	1:140:A:ARG:H	1:142:A:GLU:H	4	0.17
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG2	4	0.17
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG3	4	0.17
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG2	4	0.17
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG3	4	0.17
(1,480)	1:133:A:ASN:HD21	1:134:A:ASP:H	5	0.17
(1,462)	1:103:A:CYS:HB2	1:104:A:THR:H	10	0.17
(1,462)	1:103:A:CYS:HB3	1:104:A:THR:H	10	0.17
(1,361)	1:66:A:ASN:H	1:69:A:HIS:HD1	6	0.17
(1,356)	1:154:A:THR:HG1	1:156:A:ASN:H	2	0.17
(1,310)	1:100:A:HIS:HD1	1:168:A:ASP:H	10	0.17
(1,207)	1:110:A:TRP:HE1	1:152:A:THR:HG21	7	0.17
(1,207)	1:110:A:TRP:HE1	1:152:A:THR:HG22	7	0.17
(1,207)	1:110:A:TRP:HE1	1:152:A:THR:HG23	7	0.17
(1,33)	1:152:A:THR:H	1:168:A:ASP:H	6	0.17
(1,29)	1:17:A:HIS:H	1:29:A:CYS:HA	1	0.17
(3,46)	1:33:A:ASP:O	1:48:A:ARG:N	5	0.16
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	1	0.16
(3,39)	1:19:A:ASP:O	1:23:A:GLU:H	3	0.16
(3,31)	1:87:A:SER:O	1:91:A:SER:H	7	0.16
(3,28)	1:85:A:HIS:O	1:89:A:GLU:N	1	0.16
(3,28)	1:85:A:HIS:O	1:89:A:GLU:N	8	0.16
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	5	0.16
(1,719)	1:97:A:ASP:HA	1:98:A:ASP:H	5	0.16
(1,667)	1:39:A:PRO:HA	1:40:A:ASP:H	2	0.16
(1,640)	1:110:A:TRP:HA	1:139:A:TYR:H	9	0.16
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	4	0.16
(1,562)	1:20:A:ALA:HA	1:22:A:GLY:H	1	0.16
(1,546)	1:18:A:CYS:HA	1:22:A:GLY:H	7	0.16
(1,533)	1:44:A:ALA:HB1	1:54:A:ASN:HD22	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:44:A:ALA:HB2	1:54:A:ASN:HD22	2	0.16
(1,533)	1:44:A:ALA:HB3	1:54:A:ASN:HD22	2	0.16
(1,530)	1:39:A:PRO:HA	1:40:A:ASP:H	2	0.16
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	6	0.16
(1,527)	1:37:A:LYS:H	1:44:A:ALA:H	6	0.16
(1,497)	1:138:A:CYS:H	1:144:A:GLY:H	2	0.16
(1,497)	1:138:A:CYS:H	1:144:A:GLY:H	7	0.16
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG2	7	0.16
(1,492)	1:139:A:TYR:HE1	1:140:A:ARG:HG3	7	0.16
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG2	7	0.16
(1,492)	1:139:A:TYR:HE2	1:140:A:ARG:HG3	7	0.16
(1,444)	1:159:A:HIS:HB2	1:161:A:CYS:H	2	0.16
(1,444)	1:159:A:HIS:HB3	1:161:A:CYS:H	2	0.16
(1,418)	1:75:A:HIS:HB2	1:112:A:CYS:H	10	0.16
(1,418)	1:75:A:HIS:HB3	1:112:A:CYS:H	10	0.16
(1,356)	1:154:A:THR:HG1	1:156:A:ASN:H	4	0.16
(1,356)	1:154:A:THR:HG1	1:156:A:ASN:H	6	0.16
(1,338)	1:105:A:LYS:HG2	1:162:A:TYR:H	3	0.16
(1,315)	1:100:A:HIS:HD1	1:123:A:CYS:H	10	0.16
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	10	0.16
(1,245)	1:101:A:GLY:H	1:152:A:THR:H	4	0.16
(1,220)	1:101:A:GLY:H	1:124:A:GLY:H	10	0.16
(1,135)	1:17:A:HIS:HB3	1:28:A:ASN:H	8	0.16
(1,109)	1:75:A:HIS:HD1	1:112:A:CYS:H	9	0.16
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	6	0.16
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	2	0.16
(1,13)	1:75:A:HIS:HE1	1:77:A:GLU:H	10	0.16
(3,54)	1:52:A:ALA:O	1:63:A:ILE:N	2	0.15
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	10	0.15
(3,31)	1:87:A:SER:O	1:91:A:SER:H	8	0.15
(3,28)	1:85:A:HIS:O	1:89:A:GLU:N	2	0.15
(3,14)	1:140:A:ARG:O	1:142:A:GLU:N	8	0.15
(1,639)	1:65:A:CYS:HA	1:67:A:GLU:H	8	0.15
(1,620)	1:89:A:GLU:HA	1:93:A:ASP:H	1	0.15
(1,620)	1:89:A:GLU:HA	1:93:A:ASP:H	2	0.15
(1,537)	1:56:A:CYS:H	1:59:A:SER:H	10	0.15
(1,529)	1:38:A:LYS:HA	1:42:A:SER:H	10	0.15
(1,512)	1:154:A:THR:HA	1:162:A:TYR:HA	9	0.15
(1,496)	1:137:A:PRO:HA	1:145:A:VAL:HA	6	0.15
(1,322)	1:17:A:HIS:HD1	1:21:A:ASN:HD22	7	0.15
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	2	0.15
(1,241)	1:101:A:GLY:H	1:123:A:CYS:HB3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:11:A:SER:H	1:16:A:TYR:H	6	0.15
(1,216)	1:100:A:HIS:HD1	1:102:A:GLU:H	9	0.15
(1,213)	1:30:A:GLU:H	1:128:A:SER:HG	6	0.15
(1,190)	1:75:A:HIS:HD1	1:123:A:CYS:H	9	0.15
(1,154)	1:75:A:HIS:H	1:75:A:HIS:HE1	1	0.15
(1,120)	1:17:A:HIS:HD1	1:20:A:ALA:H	5	0.15
(1,106)	1:71:A:CYS:H	1:72:A:HIS:HD1	5	0.15
(1,73)	1:162:A:TYR:H	1:163:A:HIS:HD1	1	0.15
(1,57)	1:10:A:ASN:H	1:16:A:TYR:H	4	0.15
(1,34)	1:166:A:GLU:HB2	1:168:A:ASP:H	7	0.15
(1,33)	1:152:A:THR:H	1:168:A:ASP:H	1	0.15
(1,10)	1:45:A:HIS:H	1:45:A:HIS:HD2	3	0.15
(3,31)	1:87:A:SER:O	1:91:A:SER:H	2	0.14
(3,27)	1:85:A:HIS:O	1:89:A:GLU:H	7	0.14
(3,26)	1:84:A:CYS:O	1:88:A:CYS:N	9	0.14
(3,21)	1:82:A:THR:O	1:86:A:CYS:H	6	0.14
(3,10)	1:136:A:HIS:O	1:146:A:VAL:N	4	0.14
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	9	0.14
(1,786)	1:175:A:CYS:HA	1:176:A:ASP:H	6	0.14
(1,719)	1:97:A:ASP:HA	1:98:A:ASP:H	7	0.14
(1,719)	1:97:A:ASP:HA	1:98:A:ASP:H	9	0.14
(1,693)	1:70:A:PRO:HA	1:71:A:CYS:H	4	0.14
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	1	0.14
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	9	0.14
(1,576)	1:26:A:SER:HB2	1:27:A:CYS:H	1	0.14
(1,551)	1:19:A:ASP:HA	1:23:A:GLU:H	9	0.14
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	5	0.14
(1,528)	1:38:A:LYS:HA	1:43:A:TYR:HA	9	0.14
(1,527)	1:37:A:LYS:H	1:44:A:ALA:H	3	0.14
(1,491)	1:139:A:TYR:HE1	1:140:A:ARG:H	8	0.14
(1,491)	1:139:A:TYR:HE2	1:140:A:ARG:H	8	0.14
(1,484)	1:135:A:GLU:HB2	1:136:A:HIS:H	6	0.14
(1,484)	1:135:A:GLU:HB3	1:136:A:HIS:H	6	0.14
(1,446)	1:166:A:GLU:HG2	1:168:A:ASP:H	2	0.14
(1,446)	1:166:A:GLU:HG3	1:168:A:ASP:H	2	0.14
(1,437)	1:135:A:GLU:HB2	1:184:A:SER:H	1	0.14
(1,437)	1:135:A:GLU:HB3	1:184:A:SER:H	1	0.14
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB2	8	0.14
(1,430)	1:110:A:TRP:HE1	1:111:A:ARG:HB3	8	0.14
(1,412)	1:63:A:ILE:HG12	1:66:A:ASN:H	2	0.14
(1,412)	1:63:A:ILE:HG13	1:66:A:ASN:H	2	0.14
(1,391)	1:24:A:ASN:HD21	1:54:A:ASN:HB2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:24:A:ASN:HD21	1:54:A:ASN:HB3	3	0.14
(1,391)	1:24:A:ASN:HD22	1:54:A:ASN:HB2	3	0.14
(1,391)	1:24:A:ASN:HD22	1:54:A:ASN:HB3	3	0.14
(1,271)	1:99:A:THR:H	1:152:A:THR:HG1	10	0.14
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG21	2	0.14
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG22	2	0.14
(1,244)	1:101:A:GLY:H	1:152:A:THR:HG23	2	0.14
(1,196)	1:52:A:ALA:H	1:54:A:ASN:HD21	1	0.14
(1,188)	1:100:A:HIS:HE1	1:123:A:CYS:H	3	0.14
(1,149)	1:20:A:ALA:HB1	1:127:A:CYS:H	3	0.14
(1,149)	1:20:A:ALA:HB2	1:127:A:CYS:H	3	0.14
(1,149)	1:20:A:ALA:HB3	1:127:A:CYS:H	3	0.14
(1,147)	1:10:A:ASN:HD22	1:16:A:TYR:H	2	0.14
(1,147)	1:10:A:ASN:HD22	1:16:A:TYR:H	5	0.14
(1,137)	1:172:A:LYS:H	1:174:A:ASP:H	5	0.14
(1,130)	1:172:A:LYS:HB2	1:174:A:ASP:H	6	0.14
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	9	0.14
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB2	8	0.14
(1,86)	1:149:A:ASP:H	1:150:A:CYS:HB3	8	0.14
(3,40)	1:19:A:ASP:O	1:23:A:GLU:N	1	0.13
(3,37)	1:18:A:CYS:O	1:22:A:GLY:H	7	0.13
(3,28)	1:85:A:HIS:O	1:89:A:GLU:N	6	0.13
(3,10)	1:136:A:HIS:O	1:146:A:VAL:N	3	0.13
(2,3)	1:132:A:CYS:SG	1:150:A:CYS:SG	1	0.13
(1,773)	1:158:A:ASP:HA	1:159:A:HIS:H	3	0.13
(1,726)	1:104:A:THR:HA	1:105:A:LYS:H	4	0.13
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	10	0.13
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB2	3	0.13
(1,644)	1:72:A:HIS:HA	1:79:A:ASP:HB3	3	0.13
(1,624)	1:90:A:HIS:HA	1:94:A:HIS:H	4	0.13
(1,579)	1:82:A:THR:HA	1:85:A:HIS:H	10	0.13
(1,573)	1:23:A:GLU:HA	1:27:A:CYS:H	6	0.13
(1,554)	1:19:A:ASP:HB2	1:21:A:ASN:H	6	0.13
(1,552)	1:19:A:ASP:HA	1:22:A:GLY:H	9	0.13
(1,550)	1:18:A:CYS:HB2	1:21:A:ASN:H	6	0.13
(1,550)	1:18:A:CYS:HB3	1:21:A:ASN:H	6	0.13
(1,544)	1:55:A:ILE:HA	1:60:A:CYS:HA	1	0.13
(1,544)	1:55:A:ILE:HA	1:60:A:CYS:HA	5	0.13
(1,500)	1:140:A:ARG:HG2	1:141:A:LYS:H	2	0.13
(1,500)	1:140:A:ARG:HG3	1:141:A:LYS:H	2	0.13
(1,467)	1:106:A:LYS:HB2	1:107:A:ALA:H	10	0.13
(1,467)	1:106:A:LYS:HB3	1:107:A:ALA:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:100:A:HIS:HB2	1:168:A:ASP:H	10	0.13
(1,427)	1:100:A:HIS:HB3	1:168:A:ASP:H	10	0.13
(1,379)	1:10:A:ASN:HB2	1:17:A:HIS:H	2	0.13
(1,379)	1:10:A:ASN:HB3	1:17:A:HIS:H	2	0.13
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	6	0.13
(1,188)	1:100:A:HIS:HE1	1:123:A:CYS:H	7	0.13
(1,168)	1:29:A:CYS:H	1:128:A:SER:HG	3	0.13
(1,149)	1:20:A:ALA:HB1	1:127:A:CYS:H	5	0.13
(1,149)	1:20:A:ALA:HB2	1:127:A:CYS:H	5	0.13
(1,149)	1:20:A:ALA:HB3	1:127:A:CYS:H	5	0.13
(1,147)	1:10:A:ASN:HD22	1:16:A:TYR:H	3	0.13
(1,127)	1:174:A:ASP:H	1:179:A:HIS:HD2	6	0.13
(1,73)	1:162:A:TYR:H	1:163:A:HIS:HD1	7	0.13
(1,35)	1:100:A:HIS:HD2	1:168:A:ASP:H	5	0.13
(1,24)	1:10:A:ASN:HD22	1:17:A:HIS:H	1	0.13
(1,20)	1:112:A:CYS:HG	1:125:A:CYS:H	4	0.13
(3,54)	1:52:A:ALA:O	1:63:A:ILE:N	7	0.12
(3,54)	1:52:A:ALA:O	1:63:A:ILE:N	8	0.12
(3,54)	1:52:A:ALA:O	1:63:A:ILE:N	10	0.12
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	3	0.12
(3,52)	1:50:A:CYS:O	1:65:A:CYS:N	1	0.12
(3,48)	1:37:A:LYS:O	1:44:A:ALA:N	10	0.12
(3,40)	1:19:A:ASP:O	1:23:A:GLU:N	10	0.12
(3,38)	1:18:A:CYS:O	1:22:A:GLY:N	10	0.12
(3,31)	1:87:A:SER:O	1:91:A:SER:H	1	0.12
(3,26)	1:84:A:CYS:O	1:88:A:CYS:N	3	0.12
(3,13)	1:140:A:ARG:O	1:142:A:GLU:H	3	0.12
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	6	0.12
(3,9)	1:136:A:HIS:O	1:146:A:VAL:H	7	0.12
(3,5)	1:105:A:LYS:O	1:107:A:ALA:H	7	0.12
(2,3)	1:132:A:CYS:SG	1:150:A:CYS:SG	8	0.12
(2,2)	1:103:A:CYS:SG	1:109:A:CYS:SG	6	0.12
(1,773)	1:158:A:ASP:HA	1:159:A:HIS:H	6	0.12
(1,745)	1:125:A:CYS:HA	1:126:A:GLU:H	3	0.12
(1,701)	1:78:A:ASP:HA	1:79:A:ASP:H	7	0.12
(1,691)	1:67:A:GLU:HA	1:68:A:ASP:H	9	0.12
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	4	0.12
(1,656)	1:19:A:ASP:HA	1:20:A:ALA:H	8	0.12
(1,652)	1:14:A:PRO:HA	1:15:A:CYS:H	4	0.12
(1,641)	1:109:A:CYS:H	1:138:A:CYS:H	7	0.12
(1,634)	1:93:A:ASP:HA	1:95:A:HIS:H	5	0.12
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:83:A:HIS:HA	1:87:A:SER:H	7	0.12
(1,572)	1:23:A:GLU:HA	1:26:A:SER:H	4	0.12
(1,570)	1:23:A:GLU:HA	1:25:A:CYS:H	4	0.12
(1,544)	1:55:A:ILE:HA	1:60:A:CYS:HA	10	0.12
(1,537)	1:56:A:CYS:H	1:59:A:SER:H	5	0.12
(1,535)	1:44:A:ALA:HB1	1:55:A:ILE:HG23	1	0.12
(1,535)	1:44:A:ALA:HB2	1:55:A:ILE:HG23	1	0.12
(1,535)	1:44:A:ALA:HB3	1:55:A:ILE:HG23	1	0.12
(1,526)	1:36:A:ALA:HA	1:45:A:HIS:HA	8	0.12
(1,454)	1:103:A:CYS:CB	1:109:A:CYS:SG	4	0.12
(1,428)	1:100:A:HIS:HD1	1:124:A:GLY:HA2	4	0.12
(1,428)	1:100:A:HIS:HD1	1:124:A:GLY:HA3	4	0.12
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB2	9	0.12
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB3	9	0.12
(1,382)	1:11:A:SER:H	1:12:A:ASN:HB2	7	0.12
(1,382)	1:11:A:SER:H	1:12:A:ASN:HB3	7	0.12
(1,363)	1:136:A:HIS:HD1	1:183:A:PRO:HB3	1	0.12
(1,363)	1:136:A:HIS:HD1	1:183:A:PRO:HB3	5	0.12
(1,363)	1:136:A:HIS:HD1	1:183:A:PRO:HB3	6	0.12
(1,351)	1:123:A:CYS:H	1:125:A:CYS:H	7	0.12
(1,324)	1:52:A:ALA:H	1:54:A:ASN:HD22	4	0.12
(1,315)	1:100:A:HIS:HD1	1:123:A:CYS:H	8	0.12
(1,309)	1:100:A:HIS:HD1	1:123:A:CYS:HB3	3	0.12
(1,152)	1:179:A:HIS:HD1	1:180:A:SER:H	5	0.12
(1,112)	1:75:A:HIS:HD1	1:77:A:GLU:H	2	0.12
(1,84)	1:147:A:SER:HG	1:149:A:ASP:H	8	0.12
(3,50)	1:54:A:ASN:O	1:61:A:THR:N	9	0.11
(3,43)	1:21:A:ASN:O	1:25:A:CYS:H	6	0.11
(3,31)	1:87:A:SER:O	1:91:A:SER:H	10	0.11
(3,26)	1:84:A:CYS:O	1:88:A:CYS:N	5	0.11
(3,22)	1:82:A:THR:O	1:86:A:CYS:N	10	0.11
(3,13)	1:140:A:ARG:O	1:142:A:GLU:H	1	0.11
(2,3)	1:132:A:CYS:SG	1:150:A:CYS:SG	9	0.11
(2,1)	1:34:A:CYS:SG	1:47:A:CYS:SG	4	0.11
(1,745)	1:125:A:CYS:HA	1:126:A:GLU:H	8	0.11
(1,691)	1:67:A:GLU:HA	1:68:A:ASP:H	5	0.11
(1,645)	1:71:A:CYS:HB2	1:75:A:HIS:HA	9	0.11
(1,645)	1:71:A:CYS:HB3	1:75:A:HIS:HA	9	0.11
(1,620)	1:89:A:GLU:HA	1:93:A:ASP:H	6	0.11
(1,603)	1:86:A:CYS:HA	1:90:A:HIS:H	5	0.11
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	2	0.11
(1,542)	1:53:A:ASN:HA	1:62:A:ALA:HA	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:46:A:PRO:HA	1:52:A:ALA:HA	9	0.11
(1,473)	1:110:A:TRP:HE1	1:111:A:ARG:H	3	0.11
(1,462)	1:103:A:CYS:HB2	1:104:A:THR:H	2	0.11
(1,462)	1:103:A:CYS:HB3	1:104:A:THR:H	2	0.11
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB2	4	0.11
(1,425)	1:96:A:ASP:H	1:98:A:ASP:HB3	4	0.11
(1,412)	1:63:A:ILE:HG12	1:66:A:ASN:H	3	0.11
(1,412)	1:63:A:ILE:HG13	1:66:A:ASN:H	3	0.11
(1,356)	1:154:A:THR:HG1	1:156:A:ASN:H	8	0.11
(1,340)	1:105:A:LYS:HB3	1:162:A:TYR:H	7	0.11
(1,245)	1:101:A:GLY:H	1:152:A:THR:H	1	0.11
(1,188)	1:100:A:HIS:HE1	1:123:A:CYS:H	4	0.11
(1,168)	1:29:A:CYS:H	1:128:A:SER:HG	1	0.11
(1,163)	1:100:A:HIS:H	1:152:A:THR:H	6	0.11
(1,137)	1:172:A:LYS:H	1:174:A:ASP:H	2	0.11
(1,114)	1:159:A:HIS:HD1	1:161:A:CYS:H	9	0.11
(1,88)	1:65:A:CYS:H	1:69:A:HIS:HD1	6	0.11
(1,87)	1:63:A:ILE:HB	1:65:A:CYS:H	3	0.11
(1,57)	1:10:A:ASN:H	1:16:A:TYR:H	2	0.11
(1,19)	1:10:A:ASN:H	1:17:A:HIS:H	4	0.11
(1,13)	1:75:A:HIS:HE1	1:77:A:GLU:H	8	0.11
(3,53)	1:52:A:ALA:O	1:63:A:ILE:H	4	0.1
(3,26)	1:84:A:CYS:O	1:88:A:CYS:N	7	0.1
(3,13)	1:140:A:ARG:O	1:142:A:GLU:H	7	0.1
(3,2)	1:100:A:HIS:O	1:112:A:CYS:N	8	0.1
(1,592)	1:84:A:CYS:HA	1:88:A:CYS:H	1	0.1
(1,569)	1:22:A:GLY:HA2	1:26:A:SER:H	3	0.1
(1,569)	1:22:A:GLY:HA3	1:26:A:SER:H	3	0.1
(1,569)	1:22:A:GLY:HA2	1:26:A:SER:H	3	0.1
(1,569)	1:22:A:GLY:HA3	1:26:A:SER:H	3	0.1
(1,547)	1:18:A:CYS:HB2	1:20:A:ALA:H	7	0.1
(1,547)	1:18:A:CYS:HB3	1:20:A:ALA:H	7	0.1
(1,546)	1:18:A:CYS:HA	1:22:A:GLY:H	4	0.1
(1,540)	1:52:A:ALA:H	1:63:A:ILE:H	3	0.1
(1,494)	1:132:A:CYS:HB2	1:150:A:CYS:H	1	0.1
(1,494)	1:132:A:CYS:HB3	1:150:A:CYS:H	1	0.1
(1,479)	1:133:A:ASN:HB2	1:134:A:ASP:H	9	0.1
(1,479)	1:133:A:ASN:HB3	1:134:A:ASP:H	9	0.1
(1,463)	1:104:A:THR:HG1	1:105:A:LYS:H	6	0.1
(1,383)	1:11:A:SER:H	1:16:A:TYR:HB2	1	0.1
(1,383)	1:11:A:SER:H	1:16:A:TYR:HB3	1	0.1
(1,338)	1:105:A:LYS:HG2	1:162:A:TYR:H	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:100:A:HIS:HD1	1:112:A:CYS:H	5	0.1
(1,311)	1:100:A:HIS:HD1	1:152:A:THR:HG1	8	0.1
(1,295)	1:29:A:CYS:HG	1:31:A:LEU:H	8	0.1
(1,293)	1:17:A:HIS:HB2	1:31:A:LEU:H	9	0.1
(1,278)	1:59:A:SER:H	1:61:A:THR:HG21	8	0.1
(1,278)	1:59:A:SER:H	1:61:A:THR:HG22	8	0.1
(1,278)	1:59:A:SER:H	1:61:A:THR:HG23	8	0.1
(1,106)	1:71:A:CYS:H	1:72:A:HIS:HD1	4	0.1
(1,33)	1:152:A:THR:H	1:168:A:ASP:H	10	0.1
(1,22)	1:161:A:CYS:H	1:163:A:HIS:HD1	7	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found