Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 07:34 AM EDT

PDB ID	:	2NSW
BMRB ID	:	7327
Title	:	NMR Solution Structure of the Pheromone En-2
Authors	:	Placzek, W.J.; Etezady-Esfarjani, T.; Herrmann, T.; Peti, W.; Wuthrich, K.
Deposited on	:	2006-11-06

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 (i) 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 (1)) were used in the production of this report:

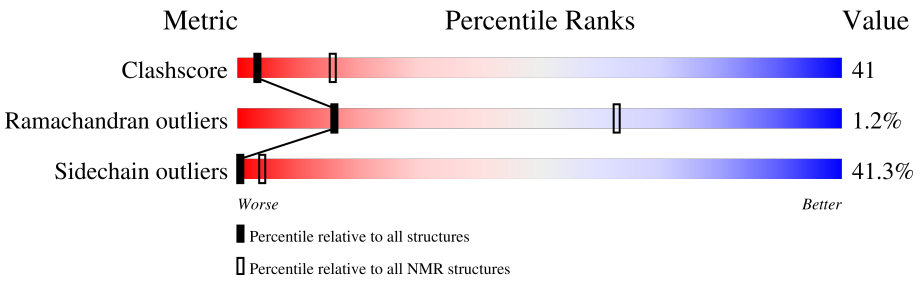
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 60%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	60	23% 42% 15% 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:2-A:26, A:30-A:52 (48)	0.27	3

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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 13, 15, 18, 20
2	5, 6, 8, 10, 19
3	7, 9, 16, 17
4	11, 12, 14

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 795 atoms, of which 362 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mating pheromone En-2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	60	795	258	362	69	97	9	0

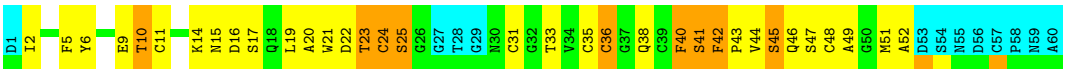
4 Residue-property plots (i)

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: Mating pheromone En-2

Chain A: 23% 42% 15% 20%



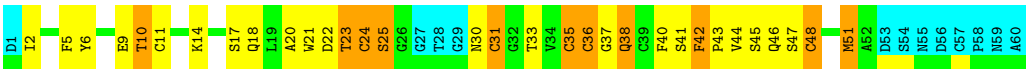
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Mating pheromone En-2

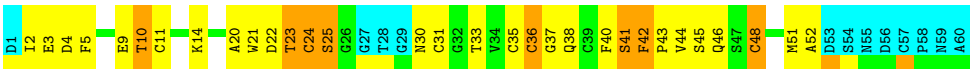
Chain A: 27% 35% 18% 20%



4.2.2 Score per residue for model 2

• Molecule 1: Mating pheromone En-2

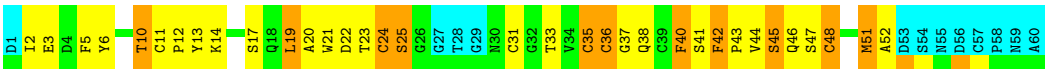
Chain A: 28% 38% 13% 20%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Mating pheromone En-2

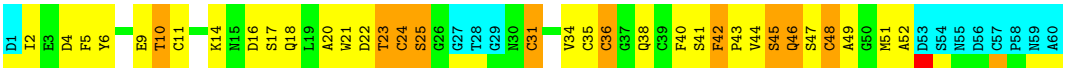
Chain A: 23% 38% 18% 20%



4.2.4 Score per residue for model 4

- Molecule 1: Mating pheromone En-2

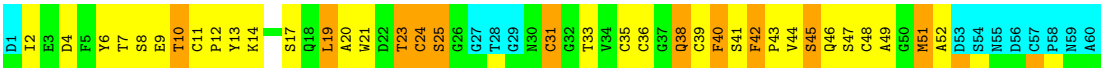
Chain A: 23% 40% 17% 20%



4.2.5 Score per residue for model 5

- Molecule 1: Mating pheromone En-2

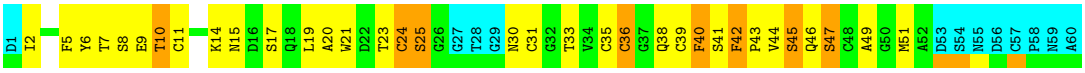
Chain A: 20% 42% 18% 20%



4.2.6 Score per residue for model 6

- Molecule 1: Mating pheromone En-2

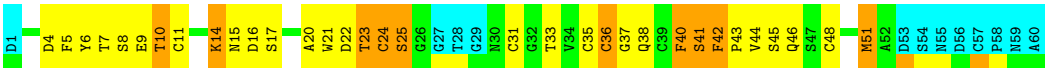
Chain A: 23% 43% 13% 20%



4.2.7 Score per residue for model 7

- Molecule 1: Mating pheromone En-2

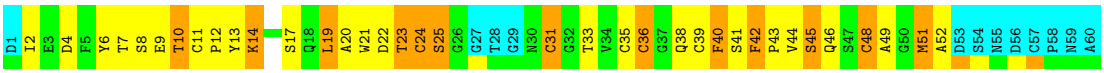
Chain A: 25% 38% 17% 20%



4.2.8 Score per residue for model 8

- Molecule 1: Mating pheromone En-2

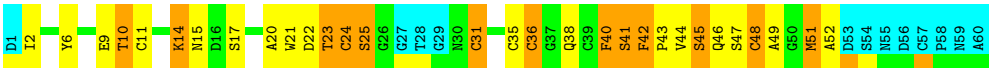
Chain A: 20% 38% 22% 20%



4.2.9 Score per residue for model 9

- Molecule 1: Mating pheromone En-2

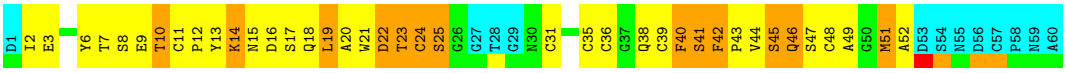
Chain A: 30% 28% 22% 20%



4.2.10 Score per residue for model 10

- Molecule 1: Mating pheromone En-2

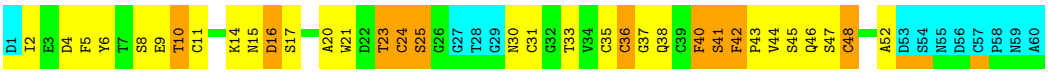
Chain A: 15% 43% 22% 20%



4.2.11 Score per residue for model 11

- Molecule 1: Mating pheromone En-2

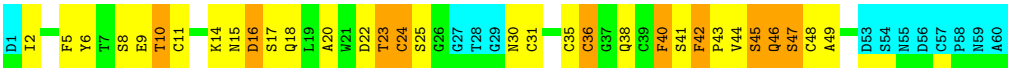
Chain A: 23% 40% 17% 20%



4.2.12 Score per residue for model 12

- Molecule 1: Mating pheromone En-2

Chain A: 27% 37% 17% 20%



4.2.13 Score per residue for model 13

- Molecule 1: Mating pheromone En-2

Chain A: 28% 33% 17% • 20%

D1 I2 Y6 T10 C11 K14 N15 D16 S17 A20 W21 D22 T23 C24 S25 G26 G27 T28 G29 N30 C31 C35 C36 G37 Q38 C39 F40 S41 F42 P43 V44 S45 Q46 S47 C48 A49 G50 M51 A52 D53 S54 N55 D56 C57 P58 N59 A60

4.2.14 Score per residue for model 14

- Molecule 1: Mating pheromone En-2

Chain A: 20% 45% 15% 20%

D1 I2 E3 D4 F5 Y6 E9 T10 C11 K14 N15 D16 S17 Q18 L19 A20 W21 D22 T23 C24 S25 G26 G27 T28 G29 N30 C31 G32 T33 V34 C35 C36 G37 Q38 C39 F40 S41 F42 P43 V44 S45 Q46 S47 C48 A52 D53 S54 N55 D56 C57 P58 N59 A60

4.2.15 Score per residue for model 15

- Molecule 1: Mating pheromone En-2

Chain A: 27% 40% 13% 20%

D1 I2 F5 Y6 E9 T10 Y13 K14 N15 D16 S17 Q18 L19 A20 W21 D22 T23 C24 S25 G26 G27 T28 G29 N30 C31 G32 T33 V34 C35 C36 G37 Q38 C39 F40 S41 F42 P43 V44 S45 Q46 S47 C48 A52 D53 S54 N55 D56 C57 P58 N59 A60

4.2.16 Score per residue for model 16

- Molecule 1: Mating pheromone En-2

Chain A: 22% 40% 18% 20%

D1 I2 E3 D4 F5 Y6 T7 S8 E9 T10 C11 K14 N15 D16 S17 Q18 L19 A20 W21 D22 T23 C24 S25 G26 G27 T28 G29 N30 C31 V34 C35 C36 G37 Q38 C39 F40 S41 F42 P43 V44 S45 Q46 S47 C48 A49 G50 M51 A52 D53 S54 N55 D56 C57 P58 N59 A60

4.2.17 Score per residue for model 17

- Molecule 1: Mating pheromone En-2

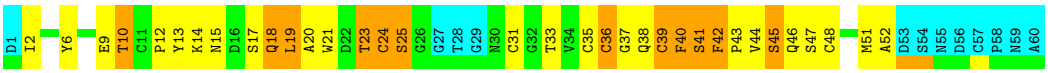
Chain A: 28% 38% 13% 20%

D1 I2 E3 D4 F5 Y6 T7 S8 E9 T10 K14 N15 D16 S17 W21 D22 T23 C24 S25 G26 G27 T28 G29 N30 C31 V34 C35 C36 G37 Q38 C39 F40 S41 F42 P43 V44 S45 Q46 S47 C48 A49 D53 S54 N55 D56 C57 P58 N59 A60

4.2.18 Score per residue for model 18

- Molecule 1: Mating pheromone En-2

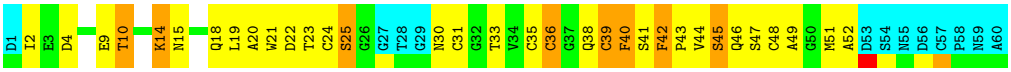
Chain A: 23% 37% 20% 20%



4.2.19 Score per residue for model 19

- Molecule 1: Mating pheromone En-2

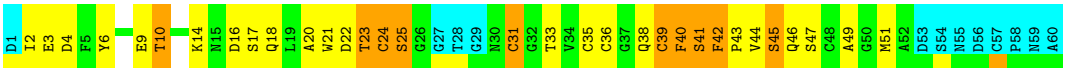
Chain A: 25% 42% 13% 20%



4.2.20 Score per residue for model 20

- Molecule 1: Mating pheromone En-2

Chain A: 27% 37% 17% 20%



5 Refinement protocol and experimental data overview (i)

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
DYANA	refinement	

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	389
Number of shifts mapped to atoms	389
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	354	304	305	27±3
All	All	7080	6080	6100	543

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:THR:HG23	1:A:38:GLN:O	0.88	1.69	18	20
1:A:19:LEU:HD13	1:A:20:ALA:N	0.82	1.89	18	6
1:A:36:CYS:SG	1:A:49:ALA:HB2	0.74	2.23	17	12
1:A:15:ASN:HB3	1:A:19:LEU:HD22	0.71	1.61	6	2
1:A:15:ASN:CB	1:A:19:LEU:HD22	0.67	2.19	6	2
1:A:5:PHE:CG	1:A:44:VAL:HG21	0.66	2.25	1	12
1:A:42:PHE:CD2	1:A:43:PRO:HA	0.64	2.27	11	20
1:A:19:LEU:HD13	1:A:19:LEU:C	0.64	2.13	18	6
1:A:23:THR:HG22	1:A:24:CYS:N	0.62	2.10	10	7
1:A:42:PHE:CG	1:A:43:PRO:HA	0.60	2.31	3	20
1:A:21:TRP:CE3	1:A:25:SER:OG	0.60	2.54	19	7
1:A:21:TRP:CZ2	1:A:51:MET:CB	0.59	2.86	10	11
1:A:6:TYR:CG	1:A:17:SER:CB	0.56	2.89	13	1
1:A:48:CYS:O	1:A:52:ALA:HB2	0.56	2.01	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:CB	1:A:39:CYS:SG	0.56	2.94	19	3
1:A:15:ASN:O	1:A:16:ASP:CB	0.56	2.54	14	4
1:A:6:TYR:CG	1:A:17:SER:OG	0.55	2.58	13	1
1:A:36:CYS:SG	1:A:37:GLY:N	0.55	2.79	7	8
1:A:34:VAL:CG1	1:A:38:GLN:NE2	0.55	2.70	16	1
1:A:19:LEU:CD1	1:A:20:ALA:N	0.55	2.69	18	1
1:A:21:TRP:CD2	1:A:25:SER:OG	0.54	2.59	3	9
1:A:24:CYS:SG	1:A:25:SER:N	0.53	2.80	14	12
1:A:5:PHE:CB	1:A:44:VAL:HG21	0.53	2.33	1	2
1:A:42:PHE:CE1	1:A:46:GLN:HB2	0.52	2.40	8	20
1:A:13:TYR:CD1	1:A:19:LEU:HD11	0.52	2.40	3	4
1:A:15:ASN:HB2	1:A:19:LEU:HD22	0.52	1.82	14	1
1:A:18:GLN:O	1:A:22:ASP:CB	0.52	2.58	14	3
1:A:39:CYS:HB3	1:A:40:PHE:CE1	0.51	2.40	19	3
1:A:24:CYS:O	1:A:31:CYS:CB	0.51	2.59	3	11
1:A:21:TRP:CZ2	1:A:51:MET:HB3	0.51	2.41	9	7
1:A:11:CYS:SG	1:A:20:ALA:CB	0.50	2.99	8	15
1:A:21:TRP:HB2	1:A:40:PHE:CZ	0.50	2.42	15	17
1:A:41:SER:O	1:A:44:VAL:HB	0.49	2.07	15	20
1:A:42:PHE:CZ	1:A:46:GLN:HB2	0.49	2.43	8	11
1:A:10:THR:CG2	1:A:38:GLN:O	0.49	2.57	10	13
1:A:23:THR:CG2	1:A:24:CYS:N	0.48	2.77	10	3
1:A:13:TYR:HB3	1:A:19:LEU:HD12	0.47	1.84	15	4
1:A:6:TYR:CG	1:A:17:SER:HB3	0.47	2.45	9	13
1:A:41:SER:O	1:A:44:VAL:CB	0.47	2.63	15	19
1:A:23:THR:CG2	1:A:30:ASN:OD1	0.47	2.63	12	2
1:A:40:PHE:CD1	1:A:40:PHE:N	0.47	2.83	6	1
1:A:6:TYR:CG	1:A:17:SER:HB2	0.47	2.45	17	4
1:A:7:THR:N	1:A:39:CYS:O	0.47	2.48	8	3
1:A:21:TRP:CE2	1:A:25:SER:HB2	0.46	2.46	18	15
1:A:21:TRP:CD1	1:A:25:SER:OG	0.46	2.68	17	1
1:A:42:PHE:N	1:A:45:SER:HB3	0.46	2.26	6	15
1:A:36:CYS:SG	1:A:45:SER:O	0.46	2.73	20	12
1:A:42:PHE:HA	1:A:44:VAL:N	0.46	2.25	15	18
1:A:12:PRO:HG2	1:A:13:TYR:CE2	0.45	2.46	8	5
1:A:7:THR:OG1	1:A:10:THR:CG2	0.45	2.64	7	2
1:A:21:TRP:O	1:A:25:SER:N	0.45	2.49	6	1
1:A:21:TRP:CZ2	1:A:51:MET:SD	0.45	3.09	1	1
1:A:44:VAL:O	1:A:47:SER:N	0.45	2.49	16	14
1:A:42:PHE:HA	1:A:43:PRO:C	0.45	2.32	1	20
1:A:36:CYS:N	1:A:48:CYS:SG	0.45	2.89	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:TRP:CD2	1:A:25:SER:CB	0.45	2.99	19	1
1:A:31:CYS:HB2	1:A:52:ALA:HB1	0.45	1.89	14	1
1:A:21:TRP:CG	1:A:25:SER:OG	0.44	2.70	17	1
1:A:36:CYS:O	1:A:40:PHE:O	0.44	2.36	10	16
1:A:19:LEU:C	1:A:19:LEU:CD1	0.44	2.86	18	1
1:A:14:LYS:O	1:A:15:ASN:CB	0.44	2.66	9	2
1:A:5:PHE:CG	1:A:44:VAL:CG2	0.44	2.99	1	2
1:A:18:GLN:O	1:A:22:ASP:N	0.44	2.50	19	6
1:A:36:CYS:SG	1:A:49:ALA:CB	0.44	3.03	17	2
1:A:25:SER:O	1:A:51:MET:SD	0.43	2.77	1	1
1:A:33:THR:O	1:A:36:CYS:SG	0.43	2.77	19	12
1:A:21:TRP:O	1:A:25:SER:OG	0.43	2.36	17	1
1:A:14:LYS:N	1:A:14:LYS:CD	0.43	2.82	17	2
1:A:22:ASP:O	1:A:22:ASP:OD1	0.43	2.37	17	1
1:A:6:TYR:CD2	1:A:17:SER:HB3	0.43	2.48	12	2
1:A:20:ALA:HB1	1:A:39:CYS:SG	0.43	2.53	20	3
1:A:7:THR:OG1	1:A:7:THR:O	0.42	2.36	7	1
1:A:19:LEU:HD13	1:A:20:ALA:CA	0.42	2.45	18	1
1:A:18:GLN:NE2	1:A:18:GLN:O	0.42	2.53	18	1
1:A:33:THR:HA	1:A:36:CYS:SG	0.41	2.55	20	1
1:A:35:CYS:C	1:A:48:CYS:SG	0.41	2.99	3	2
1:A:21:TRP:CE2	1:A:25:SER:OG	0.41	2.56	17	1
1:A:44:VAL:C	1:A:46:GLN:N	0.41	2.74	20	5
1:A:30:ASN:OD1	1:A:30:ASN:C	0.41	2.59	13	1
1:A:31:CYS:SG	1:A:52:ALA:O	0.41	2.79	13	8
1:A:13:TYR:CG	1:A:19:LEU:CD1	0.41	3.03	10	1
1:A:14:LYS:HD3	1:A:14:LYS:N	0.41	2.31	19	2
1:A:14:LYS:N	1:A:14:LYS:HD3	0.41	2.31	10	1
1:A:34:VAL:HG12	1:A:38:GLN:NE2	0.40	2.32	4	1
1:A:7:THR:O	1:A:7:THR:OG1	0.40	2.37	5	2
1:A:41:SER:O	1:A:44:VAL:HG23	0.40	2.17	15	1
1:A:34:VAL:O	1:A:38:GLN:HB2	0.40	2.17	17	1
1:A:14:LYS:O	1:A:19:LEU:HD23	0.40	2.17	16	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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	48/60 (80%)	40±2 (83±4%)	7±1 (15±3%)	1±1 (1±1%)	16 63
All	All	960/1200 (80%)	801 (83%)	147 (15%)	12 (1%)	16 63

All 2 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	36	CYS	9
1	A	16	ASP	3

6.3.2 Protein sidechains (i)

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	41/50 (82%)	24±2 (59±4%)	17±2 (41±4%)	0 4
All	All	820/1000 (82%)	481 (59%)	339 (41%)	0 4

All 30 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	14	LYS	20
1	A	23	THR	20
1	A	24	CYS	20
1	A	35	CYS	20
1	A	42	PHE	20
1	A	45	SER	20
1	A	10	THR	19
1	A	25	SER	19
1	A	2	ILE	18
1	A	9	GLU	17
1	A	48	CYS	16
1	A	40	PHE	15
1	A	31	CYS	10
1	A	51	MET	10
1	A	4	ASP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	41	SER	10
1	A	8	SER	9
1	A	36	CYS	8
1	A	22	ASP	8
1	A	16	ASP	8
1	A	30	ASN	6
1	A	3	GLU	6
1	A	19	LEU	6
1	A	46	GLN	5
1	A	47	SER	5
1	A	15	ASN	5
1	A	38	GLN	4
1	A	39	CYS	3
1	A	17	SER	1
1	A	18	GLN	1

6.3.3 RNA (i)

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 monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 60% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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	389
Number of shifts mapped to atoms	389
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	48	-0.36 ± 0.22	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	4	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 60%, i.e. 330 atoms were assigned a chemical shift out of a possible 550. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	137/240 (57%)	98/98 (100%)	39/96 (41%)	0/46 (0%)
Sidechain	165/250 (66%)	149/162 (92%)	16/82 (20%)	0/6 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	28/60 (47%)	28/29 (97%)	0/30 (0%)	0/1 (0%)
Overall	330/550 (60%)	275/289 (95%)	55/208 (26%)	0/53 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 59%, i.e. 389 atoms were assigned a chemical shift out of a possible 661. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	169/300 (56%)	121/123 (98%)	48/120 (40%)	0/57 (0%)
Sidechain	192/301 (64%)	174/193 (90%)	18/100 (18%)	0/8 (0%)
Aromatic	28/60 (47%)	28/29 (97%)	0/30 (0%)	0/1 (0%)
Overall	389/661 (59%)	323/345 (94%)	66/250 (26%)	0/66 (0%)

7.1.4 Statistically unusual chemical shifts (i)

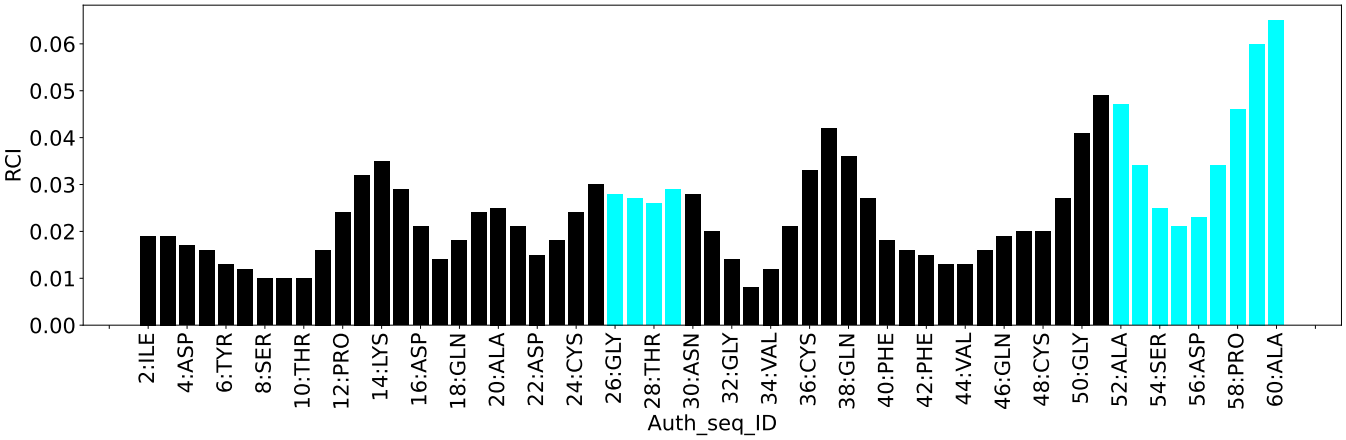
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	25	SER	HB3	2.42	2.49 – 5.20	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

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:


RCI
0.00
0.01
0.02
0.03
0.04
0.05
0.06
2:ILE
4:ASP
6:TYR
8:SER
10:THR
12:PRO
14:LYS
16:ASP
18:GLN
20:ALA
22:ASP
24:CYS
26:GLY
28:THR
30:ASN
32:GLY
34:VAL
36:CYS
38:GLN
40:PHE
42:PHE
44:VAL
46:GLN
48:CYS
50:GLY
52:ALA
54:SER
56:ASP
58:PRO
60:ALA
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	699
Intra-residue (|i-j|=0)	164
Sequential (|i-j|=1)	210
Medium range (|i-j|>1 and |i-j|<5)	116
Long range (|i-j|≥5)	197
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	12
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.7
Number of long range restraints per residue[1]	3.5

[1]Long 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 (i)

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 (i)

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)	9.8	0.2
0.2-0.5 (Medium)	13.3	0.5
>0.5 (Large)	20.3	2.28

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 (i)

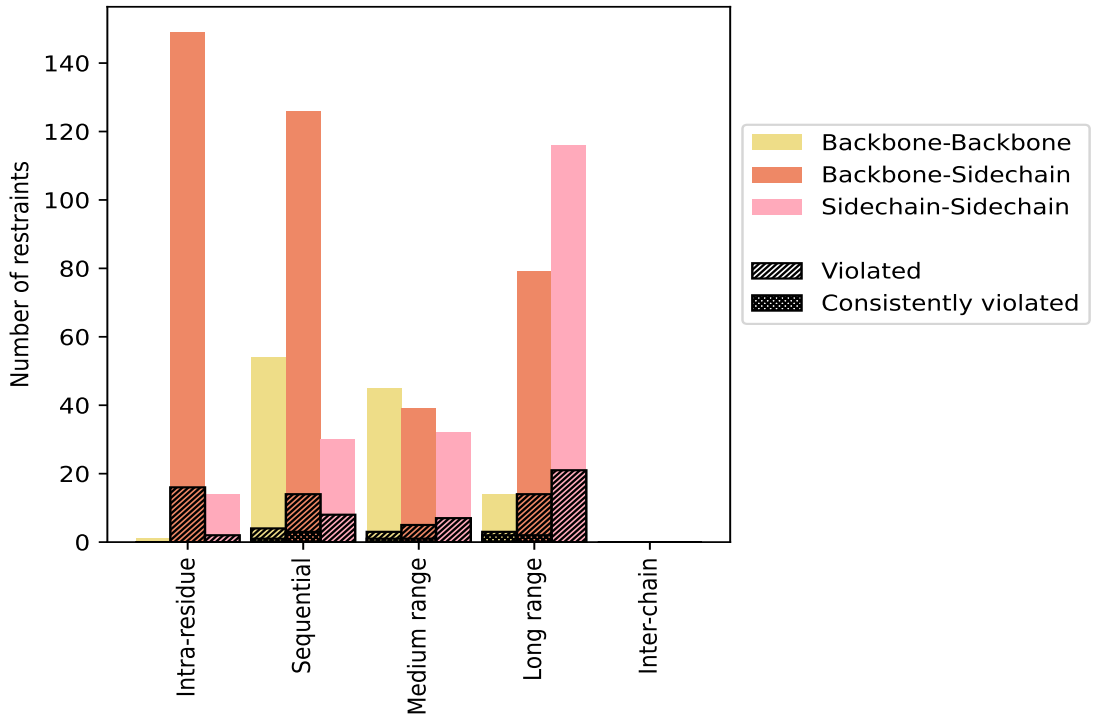
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	164	23.5	18	11.0	2.6	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	149	21.3	16	10.7	2.3	0	0.0	0.0
Sidechain-Sidechain	14	2.0	2	14.3	0.3	0	0.0	0.0
Sequential (|i-j|=1)	210	30.0	26	12.4	3.7	4	1.9	0.6
Backbone-Backbone	54	7.7	4	7.4	0.6	1	1.9	0.1
Backbone-Sidechain	126	18.0	14	11.1	2.0	3	2.4	0.4
Sidechain-Sidechain	30	4.3	8	26.7	1.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	116	16.6	15	12.9	2.1	2	1.7	0.3
Backbone-Backbone	45	6.4	3	6.7	0.4	1	2.2	0.1
Backbone-Sidechain	39	5.6	5	12.8	0.7	1	2.6	0.1
Sidechain-Sidechain	32	4.6	7	21.9	1.0	0	0.0	0.0
Long range (|i-j|≥5)	197	28.2	35	17.8	5.0	4	2.0	0.6
Backbone-Backbone	14	2.0	3	21.4	0.4	2	14.3	0.3
Backbone-Sidechain	79	11.3	14	17.7	2.0	2	2.5	0.3
Sidechain-Sidechain	104	14.9	18	17.3	2.6	0	0.0	0.0
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	12	1.7	3	25.0	0.4	0	0.0	0.0
Total	699	100.0	97	13.9	13.9	10	1.4	1.4
Backbone-Backbone	114	16.3	10	8.8	1.4	4	3.5	0.6
Backbone-Sidechain	393	56.2	49	12.5	7.0	6	1.5	0.9
Sidechain-Sidechain	192	27.5	38	19.8	5.4	0	0.0	0.0

[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	6	9	8	21	0	44	0.65	2.16	0.5	0.47
2	6	12	7	21	0	46	0.66	2.19	0.49	0.52
3	4	12	6	15	0	37	0.53	1.72	0.39	0.45
4	6	14	7	18	0	45	0.66	2.21	0.48	0.5
5	7	11	4	15	0	37	0.53	1.77	0.38	0.46
6	6	12	9	20	0	47	0.61	2.16	0.47	0.49
7	7	10	5	16	0	38	0.55	2.06	0.45	0.4
8	7	12	5	17	0	41	0.55	1.76	0.41	0.45
9	6	9	9	18	0	42	0.63	1.76	0.49	0.46
10	7	11	3	14	0	35	0.62	1.79	0.42	0.56
11	8	14	8	20	0	50	0.66	2.23	0.49	0.5

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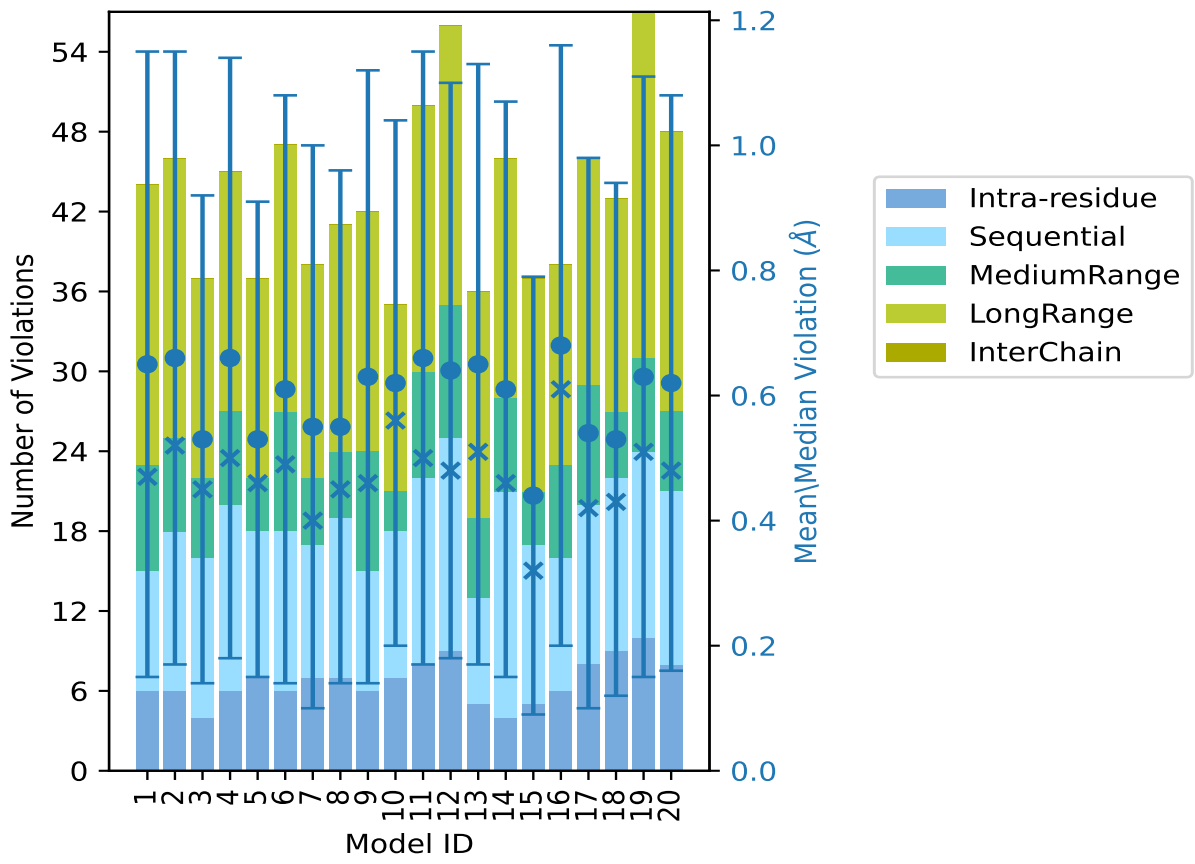
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	9	16	10	21	0	56	0.64	2.03	0.46	0.48
13	5	8	6	17	0	36	0.65	2.16	0.48	0.51
14	4	17	7	18	0	46	0.61	2.05	0.46	0.46
15	5	12	4	16	0	37	0.44	1.74	0.35	0.32
16	6	10	7	15	0	38	0.68	1.75	0.48	0.61
17	8	12	9	17	0	46	0.54	2.0	0.44	0.42
18	9	13	5	16	0	43	0.53	1.66	0.41	0.43
19	10	14	7	26	0	57	0.63	2.22	0.48	0.51
20	8	13	6	21	0	48	0.62	2.28	0.46	0.48

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

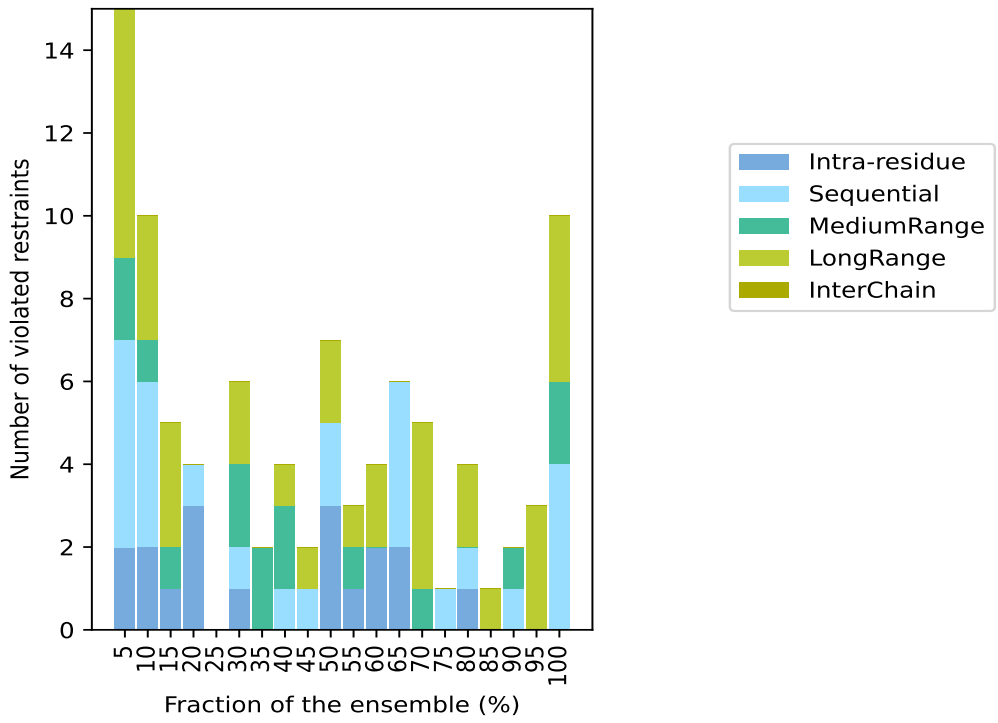
9.3 Distance violation statistics for the ensemble (i)

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, 593(IR:146, SQ:184, MR:101, LR:162, 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]	%
2	5	2	6	0	15	1	5.0
2	4	1	3	0	10	2	10.0
1	0	1	3	0	5	3	15.0
3	1	0	0	0	4	4	20.0
0	0	0	0	0	0	5	25.0
1	1	2	2	0	6	6	30.0
0	0	2	0	0	2	7	35.0
0	1	2	1	0	4	8	40.0
0	1	0	1	0	2	9	45.0
3	2	0	2	0	7	10	50.0
1	0	1	1	0	3	11	55.0
2	0	0	2	0	4	12	60.0
2	4	0	0	0	6	13	65.0
0	0	1	4	0	5	14	70.0
0	1	0	0	0	1	15	75.0
1	1	0	2	0	4	16	80.0
0	0	0	1	0	1	17	85.0
0	1	1	0	0	2	18	90.0
0	0	0	3	0	3	19	95.0
0	4	2	4	0	10	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

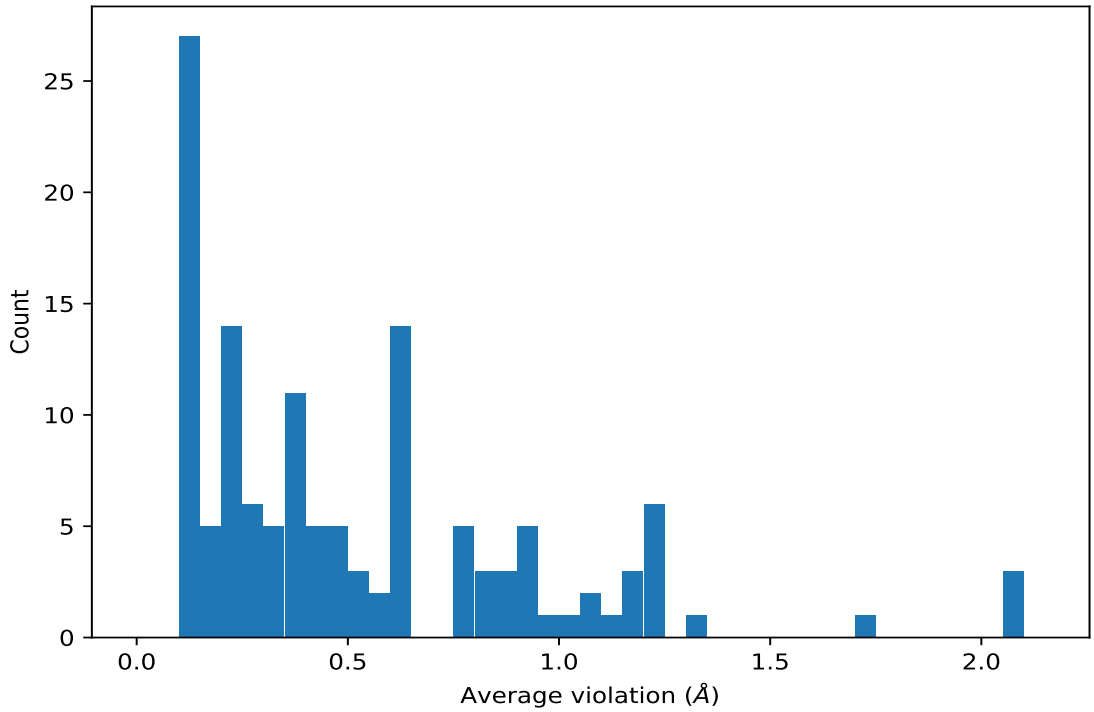
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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)
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	20	1.74	0.05	1.74
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	20	1.3	0.24	1.31
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	20	1.07	0.06	1.08
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	20	0.9	0.29	0.93
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	20	0.79	0.08	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	20	0.79	0.08	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	20	0.79	0.08	0.8
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	20	0.63	0.11	0.66
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	20	0.62	0.13	0.61
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	20	0.62	0.13	0.61
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	20	0.46	0.0	0.46
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	20	0.34	0.01	0.34
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	20	0.21	0.02	0.2
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	19	0.79	0.16	0.73
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	19	0.47	0.15	0.5
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	19	0.47	0.15	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	19	0.16	0.03	0.16
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	19	0.16	0.03	0.16
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	18	0.82	0.24	0.86
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	18	0.82	0.24	0.86
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	18	0.82	0.24	0.86
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	18	0.13	0.02	0.12
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	17	1.02	0.49	1.21
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	16	1.14	0.02	1.14
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	16	0.62	0.1	0.6
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	16	0.62	0.1	0.6
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	16	0.62	0.1	0.6
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	16	0.42	0.13	0.43
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	16	0.42	0.13	0.43
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	16	0.38	0.03	0.38
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	15	0.59	0.3	0.58
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	15	0.59	0.3	0.58
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	14	2.08	0.18	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	14	2.08	0.18	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	14	2.08	0.18	2.16
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	14	1.21	0.35	1.23
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	14	1.21	0.35	1.23
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	14	1.21	0.35	1.23
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	14	1.2	0.33	1.29
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	14	1.2	0.33	1.29
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	14	1.2	0.33	1.29
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	14	0.88	0.44	0.94
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	14	0.88	0.44	0.94
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	14	0.88	0.44	0.94
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	14	0.62	0.27	0.72
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	14	0.62	0.27	0.72
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	14	0.62	0.27	0.72
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	13	1.19	0.02	1.19
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	13	1.19	0.02	1.19
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	13	1.19	0.02	1.19
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	13	0.6	0.09	0.62
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	13	0.45	0.0	0.45
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	13	0.27	0.02	0.28
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	13	0.21	0.04	0.22
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	13	0.14	0.02	0.14
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	13	0.14	0.02	0.14
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	13	0.14	0.02	0.14
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	12	0.97	0.02	0.96

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	12	0.52	0.0	0.52
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	12	0.5	0.22	0.43
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	12	0.5	0.22	0.43
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	12	0.26	0.05	0.28
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	11	0.38	0.16	0.33
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	11	0.38	0.16	0.33
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	11	0.38	0.16	0.33
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	11	0.38	0.16	0.33
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	11	0.38	0.16	0.33
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	11	0.38	0.16	0.33
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	11	0.2	0.07	0.19
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	11	0.14	0.02	0.13
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	11	0.13	0.01	0.13
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	10	1.06	0.02	1.06
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	10	0.94	0.28	1.06
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	10	0.9	0.07	0.88
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	10	0.9	0.07	0.88
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	10	0.9	0.07	0.88
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	10	0.78	0.02	0.78
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	10	0.44	0.03	0.45
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	10	0.44	0.03	0.45
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	10	0.33	0.01	0.34
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	10	0.29	0.19	0.2
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	9	0.46	0.19	0.54
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	9	0.32	0.1	0.36
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	9	0.32	0.1	0.36
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	8	0.63	0.01	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	8	0.63	0.01	0.63
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	8	0.39	0.26	0.3
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	8	0.39	0.26	0.3
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	8	0.39	0.26	0.3
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	8	0.26	0.07	0.28
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	8	0.21	0.08	0.2
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	8	0.21	0.08	0.2
(1,251)	1:A:26:GLY:HA2	1:A:28:THR:H	7	0.64	0.35	0.66
(1,607)	1:A:16:ASP:HB2	1:A:19:LEU:HB3	7	0.43	0.12	0.44
(1,536)	1:A:21:TRP:HZ3	1:A:25:SER:HB2	6	0.26	0.13	0.22
(1,385)	1:A:3:GLU:H	1:A:3:GLU:HG2	6	0.25	0.1	0.32
(1,366)	1:A:24:CYS:HB3	1:A:35:CYS:HB2	6	0.21	0.1	0.19
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB2	6	0.19	0.01	0.18
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB3	6	0.19	0.01	0.18
(1,641)	1:A:19:LEU:HB3	1:A:20:ALA:HA	6	0.15	0.02	0.14

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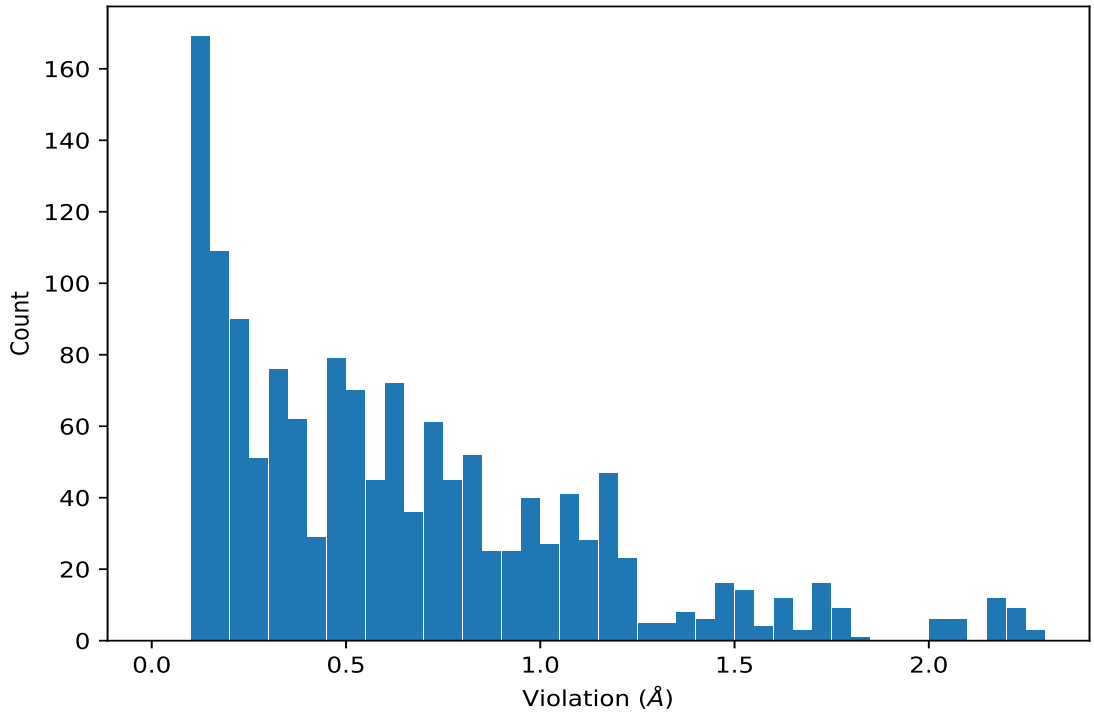
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,50)	1:A:25:SER:HA	1:A:52:ALA:H	6	0.13	0.02	0.12
(1,45)	1:A:15:ASN:HB2	1:A:16:ASP:H	4	0.36	0.01	0.36
(1,614)	1:A:46:GLN:HA	1:A:46:GLN:HG2	4	0.3	0.01	0.3
(1,294)	1:A:17:SER:HA	1:A:17:SER:HB3	4	0.24	0.01	0.24
(1,559)	1:A:54:SER:HA	1:A:54:SER:HB2	4	0.11	0.0	0.11
(1,98)	1:A:51:MET:HG3	1:A:53:ASP:H	3	0.63	0.68	0.2
(1,688)	1:A:11:CYS:SG	1:A:39:CYS:CB	3	0.23	0.01	0.22
(1,565)	1:A:36:CYS:HB3	1:A:45:SER:HA	3	0.14	0.03	0.13
(1,46)	1:A:37:GLY:H	1:A:45:SER:HB2	3	0.13	0.01	0.13
(1,46)	1:A:37:GLY:H	1:A:45:SER:HB3	3	0.13	0.01	0.13
(1,198)	1:A:41:SER:H	1:A:41:SER:HB2	3	0.12	0.0	0.12
(1,609)	1:A:11:CYS:HA	1:A:38:GLN:HB2	3	0.12	0.0	0.12
(1,609)	1:A:11:CYS:HA	1:A:38:GLN:HB3	3	0.12	0.0	0.12
(1,601)	1:A:23:THR:HG21	1:A:30:ASN:HB2	2	0.24	0.01	0.24
(1,601)	1:A:23:THR:HG22	1:A:30:ASN:HB2	2	0.24	0.01	0.24
(1,601)	1:A:23:THR:HG23	1:A:30:ASN:HB2	2	0.24	0.01	0.24
(1,554)	1:A:19:LEU:HD11	1:A:20:ALA:HA	2	0.21	0.01	0.21
(1,554)	1:A:19:LEU:HD12	1:A:20:ALA:HA	2	0.21	0.01	0.21
(1,554)	1:A:19:LEU:HD13	1:A:20:ALA:HA	2	0.21	0.01	0.21
(1,279)	1:A:12:PRO:HD3	1:A:13:TYR:HD1	2	0.12	0.01	0.12
(1,279)	1:A:12:PRO:HD3	1:A:13:TYR:HD2	2	0.12	0.01	0.12
(1,353)	1:A:6:TYR:HE1	1:A:39:CYS:HB3	2	0.12	0.01	0.12
(1,353)	1:A:6:TYR:HE2	1:A:39:CYS:HB3	2	0.12	0.01	0.12
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG11	2	0.12	0.01	0.12
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG12	2	0.12	0.01	0.12
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG13	2	0.12	0.01	0.12
(1,43)	1:A:16:ASP:H	1:A:17:SER:HA	2	0.12	0.0	0.12
(1,181)	1:A:9:GLU:HB3	1:A:10:THR:HB	2	0.12	0.0	0.12
(1,263)	1:A:44:VAL:HA	1:A:48:CYS:H	2	0.12	0.0	0.12
(1,612)	1:A:30:ASN:HA	1:A:30:ASN:HB3	2	0.12	0.0	0.12
(1,435)	1:A:14:LYS:H	1:A:14:LYS:HB2	2	0.11	0.0	0.11
(1,435)	1:A:14:LYS:H	1:A:14:LYS:HB3	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard 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)
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	20	2.28
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	20	2.28
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	20	2.28
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	11	2.23
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	11	2.23
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	11	2.23
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	19	2.22
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	19	2.22
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	19	2.22
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	4	2.21
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	4	2.21
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	4	2.21
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	2	2.19
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	2	2.19
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	2	2.19
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	1	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	1	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	1	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	6	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	6	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	6	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	13	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	13	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	13	2.16
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	7	2.06
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	7	2.06
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	7	2.06
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	14	2.05
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	14	2.05
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	14	2.05
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	12	2.03
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	12	2.03
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	12	2.03
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	17	2.0
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	17	2.0
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	17	2.0
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	19	1.82
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	6	1.79
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	10	1.79
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	5	1.77
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	13	1.77
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	20	1.77
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	8	1.76
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	9	1.76
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	12	1.76
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	16	1.75
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	4	1.74
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	15	1.74
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	9	1.74
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	9	1.74
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	9	1.74
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	11	1.73
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	11	1.73
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	11	1.73
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	1	1.72
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	3	1.72
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	17	1.72
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	2	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	9	1.71
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	9	1.71
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	9	1.71
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	19	1.7
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	11	1.66
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	14	1.66
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	18	1.66
(1,558)	1:A:47:SER:HA	1:A:50:GLY:HA2	7	1.64
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	6	1.64
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD11	16	1.64
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD12	16	1.64
(1,169)	1:A:13:TYR:HA	1:A:19:LEU:HD13	16	1.64
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	4	1.62
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	4	1.62
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	4	1.62
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	16	1.61
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	20	1.6
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	20	1.6
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	20	1.6
(1,98)	1:A:51:MET:HG3	1:A:53:ASP:H	1	1.59
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	12	1.59
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	11	1.57
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	16	1.55
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	9	1.54
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	1	1.53
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	1	1.53
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	1	1.53
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	14	1.52
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	1	1.52
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	1	1.52
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	1	1.52
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	8	1.52
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	11	1.5
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	4	1.5
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	4	1.5
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	4	1.5
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	17	1.5
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	19	1.49
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	13	1.48
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	13	1.48
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	13	1.48
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	19	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	19	1.48
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	19	1.48
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	2	1.47
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	2	1.47
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	2	1.47
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	2	1.47
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	12	1.46
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	7	1.46
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	7	1.46
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	7	1.46
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	10	1.46
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	16	1.43
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	16	1.43
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	16	1.43
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	2	1.4
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	2	1.4
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	2	1.4
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	4	1.38
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	4	1.38
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	1	1.37
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	1	1.37
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	1	1.37
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	12	1.35
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	12	1.35
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	12	1.35
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	11	1.33
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	11	1.33
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	11	1.33
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	9	1.33
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	19	1.31
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	5	1.28
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	18	1.28
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	14	1.25
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	14	1.25
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	14	1.25
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	6	1.24
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	6	1.24
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	6	1.24
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	13	1.24
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	13	1.24
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	13	1.24
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	12	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	13	1.23
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	13	1.23
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	13	1.23
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	18	1.21
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	4	1.21
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	4	1.21
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	4	1.21
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	9	1.21
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	9	1.21
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	9	1.21
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	3	1.2
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	3	1.2
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	3	1.2
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	8	1.2
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	8	1.2
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	8	1.2
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	10	1.19
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	10	1.19
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	10	1.19
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	11	1.19
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	11	1.19
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	11	1.19
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	14	1.19
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	14	1.19
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	14	1.19
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	18	1.19
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	18	1.19
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	18	1.19
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	19	1.19
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	19	1.19
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	19	1.19
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	19	1.19
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	14	1.19
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	12	1.18
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	12	1.18
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	12	1.18
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	16	1.18
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	16	1.18
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	16	1.18
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	6	1.18
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	6	1.18
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	6	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	12	1.18
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	2	1.17
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	2	1.17
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	2	1.17
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	19	1.17
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	12	1.16
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	12	1.16
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	12	1.16
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	14	1.16
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	14	1.16
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	11	1.16
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	16	1.16
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	19	1.16
(1,512)	1:A:2:ILE:HG21	1:A:3:GLU:HB2	20	1.15
(1,512)	1:A:2:ILE:HG22	1:A:3:GLU:HB2	20	1.15
(1,512)	1:A:2:ILE:HG23	1:A:3:GLU:HB2	20	1.15
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	10	1.15
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	2	1.15
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	1	1.15
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	20	1.15
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	20	1.15
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	9	1.14
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	9	1.14
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	9	1.14
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	3	1.14
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	4	1.14
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	5	1.14
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	6	1.14
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	9	1.14
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	14	1.14
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	18	1.14
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	2	1.13
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	15	1.13
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	17	1.13
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	2	1.12
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	2	1.12
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	2	1.12
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	12	1.12
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	3	1.11
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	13	1.11
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	11	1.11
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	12	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	18	1.11
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	7	1.1
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	15	1.1
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	8	1.1
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	5	1.1
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	10	1.1
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	13	1.1
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	16	1.09
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	16	1.09
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	16	1.09
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	8	1.09
(1,242)	1:A:17:SER:HB3	1:A:18:GLN:HA	10	1.09
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	9	1.09
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	2	1.09
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	11	1.08
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	11	1.08
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	11	1.08
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	4	1.08
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	14	1.08
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	18	1.08
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	19	1.08
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	16	1.07
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	16	1.07
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	6	1.07
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	2	1.07
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	11	1.07
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	12	1.07
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	18	1.07
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	20	1.07
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	6	1.07
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	7	1.07
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	17	1.06
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	17	1.06
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	17	1.06
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	20	1.06
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	20	1.06
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	20	1.06
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	9	1.06
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	9	1.06
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	9	1.06
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	8	1.06
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	10	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	19	1.06
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	14	1.05
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	14	1.05
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	14	1.05
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	11	1.05
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	8	1.05
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	6	1.04
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	2	1.04
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	16	1.04
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	1	1.03
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	1	1.03
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	1	1.03
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	1	1.03
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	7	1.03
(1,186)	1:A:14:LYS:HA	1:A:14:LYS:HD2	17	1.03
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	3	1.03
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	10	1.02
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	9	1.02
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	9	1.02
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	3	1.02
(1,251)	1:A:26:GLY:HA2	1:A:28:THR:H	12	1.02
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	10	1.02
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	5	1.01
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	12	1.01
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	12	1.01
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	12	1.01
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	12	1.01
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	12	1.01
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	12	1.01
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	1	1.01
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	20	1.0
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	20	1.0
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	8	1.0
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	12	0.99
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	11	0.99
(1,251)	1:A:26:GLY:HA2	1:A:28:THR:H	19	0.99
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	19	0.98
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	20	0.98
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	20	0.98
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	20	0.98
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	2	0.98
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	2	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	2	0.98
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	9	0.97
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	12	0.97
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	4	0.97
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	4	0.97
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	4	0.97
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	13	0.97
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	13	0.97
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	13	0.97
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	17	0.97
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	17	0.97
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	17	0.97
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	18	0.97
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	4	0.96
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	8	0.96
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	13	0.96
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	16	0.96
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	13	0.96
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	13	0.96
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	13	0.96
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	20	0.96
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	20	0.96
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	20	0.96
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	11	0.96
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	6	0.95
(1,583)	1:A:36:CYS:HB2	1:A:45:SER:HA	17	0.95
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	6	0.95
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	6	0.95
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	6	0.95
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	20	0.95
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	20	0.95
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	9	0.94
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	18	0.94
(1,251)	1:A:26:GLY:HA2	1:A:28:THR:H	6	0.94
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	1	0.93
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	1	0.93
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	1	0.93
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	11	0.93
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	11	0.93
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	11	0.93
(1,369)	1:A:21:TRP:HH2	1:A:51:MET:HG2	1	0.93
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	17	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	17	0.93
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	17	0.93
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	5	0.92
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	3	0.92
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	2	0.91
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	2	0.91
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	2	0.91
(1,262)	1:A:21:TRP:HA	1:A:24:CYS:HB2	14	0.91
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	6	0.9
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	6	0.9
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	6	0.9
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	15	0.9
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	15	0.9
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	15	0.9
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	17	0.89
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	17	0.89
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	17	0.89
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	14	0.88
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	14	0.88
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	14	0.88
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	3	0.88
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	3	0.88
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	3	0.88
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	5	0.87
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	5	0.87
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	5	0.87
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	4	0.87
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	4	0.87
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	4	0.87
(1,162)	1:A:32:GLY:HA3	1:A:49:ALA:HA	15	0.87
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	3	0.86
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	3	0.86
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	3	0.86
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	10	0.86
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	10	0.86
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	10	0.86
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	1	0.85
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	1	0.85
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	1	0.85
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	14	0.84
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	14	0.84
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	14	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	19	0.83
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	19	0.83
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	19	0.83
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	19	0.83
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	13	0.83
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	7	0.83
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	7	0.83
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	7	0.83
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	6	0.82
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	6	0.82
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	6	0.82
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	19	0.82
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	19	0.82
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	19	0.82
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	19	0.82
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	19	0.82
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	19	0.82
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	20	0.82
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	13	0.82
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	13	0.82
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	13	0.82
(1,482)	1:A:7:THR:HG21	1:A:41:SER:HB3	20	0.81
(1,482)	1:A:7:THR:HG22	1:A:41:SER:HB3	20	0.81
(1,482)	1:A:7:THR:HG23	1:A:41:SER:HB3	20	0.81
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	2	0.81
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	2	0.81
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	14	0.81
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	14	0.81
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	14	0.81
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	1	0.81
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	4	0.81
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	4	0.81
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	4	0.81
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	17	0.8
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	16	0.8
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	16	0.8
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	16	0.8
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	14	0.8
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	16	0.8
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	16	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	5	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	5	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	16	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	16	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	16	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	20	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	20	0.8
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	20	0.8
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	1	0.79
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	1	0.79
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	7	0.79
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	7	0.79
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	3	0.79
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	13	0.79
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	19	0.79
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	2	0.79
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	2	0.79
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	2	0.79
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	10	0.78
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	1	0.78
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	18	0.78
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	18	0.78
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	18	0.78
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	7	0.78
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	7	0.78
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	7	0.78
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	8	0.78
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	8	0.78
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	8	0.78
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	1	0.77
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	2	0.77
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	6	0.77
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	4	0.76
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	7	0.76
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	7	0.76
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	5	0.76
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	17	0.76
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	10	0.75
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	10	0.75
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	10	0.75
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	1	0.75
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	1	0.75
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	12	0.75
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	12	0.75
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	12	0.75
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	1	0.75
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	1	0.75
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	4	0.75
(1,199)	1:A:41:SER:HB2	1:A:42:PHE:H	12	0.75
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	11	0.75
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	11	0.75
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	11	0.75
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	12	0.74
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	19	0.74
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	19	0.74
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	19	0.74
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	11	0.74
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	11	0.74
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	11	0.74
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	14	0.74
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	14	0.74
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	18	0.74
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	18	0.74
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	18	0.74
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	2	0.73
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	10	0.73
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	3	0.73
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	3	0.73
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	11	0.73
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	11	0.73
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	18	0.73
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	18	0.73
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	9	0.73
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	9	0.73
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	9	0.73
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	16	0.72
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	5	0.72
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	5	0.72
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	5	0.72
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	8	0.72
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	8	0.72
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	8	0.72
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	16	0.72
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	16	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	16	0.72
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	2	0.72
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	2	0.72
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	15	0.71
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	15	0.71
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	15	0.71
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	13	0.71
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	15	0.71
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	16	0.71
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	16	0.71
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	17	0.71
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	6	0.7
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	12	0.7
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	17	0.7
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	17	0.7
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	17	0.7
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	13	0.7
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	13	0.7
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	13	0.7
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	7	0.7
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	7	0.7
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	7	0.7
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	7	0.7
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	7	0.7
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	7	0.7
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	9	0.7
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	6	0.7
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	6	0.7
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	6	0.7
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	12	0.69
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	12	0.69
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	12	0.69
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	4	0.69
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	14	0.68
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	8	0.68
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	4	0.68
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	11	0.68
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	3	0.68
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	3	0.68
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	3	0.68
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	19	0.68
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	19	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	19	0.68
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	7	0.68
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	20	0.68
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	18	0.67
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	2	0.67
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	2	0.67
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	20	0.67
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	8	0.66
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	8	0.66
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	6	0.66
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	9	0.66
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	14	0.66
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	8	0.66
(1,251)	1:A:26:GLY:HA2	1:A:28:THR:H	11	0.66
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	15	0.66
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	15	0.66
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	16	0.65
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	12	0.65
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	12	0.65
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	12	0.65
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	14	0.65
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	17	0.65
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	17	0.65
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	2	0.64
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	2	0.64
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	5	0.64
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	5	0.64
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	11	0.64
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	11	0.64
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	6	0.64
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	6	0.64
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	5	0.64
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	19	0.63
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	8	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	8	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	8	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	17	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	17	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	19	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	19	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	20	0.63
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	20	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	19	0.63
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	19	0.63
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	19	0.63
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	5	0.62
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	15	0.62
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	10	0.62
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	2	0.62
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	2	0.62
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	2	0.62
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	14	0.62
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	14	0.62
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	14	0.62
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE1	4	0.62
(1,377)	1:A:4:ASP:HB2	1:A:5:PHE:HE2	4	0.62
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	8	0.62
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	8	0.62
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	12	0.62
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	15	0.62
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	8	0.62
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	8	0.62
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	18	0.61
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	3	0.61
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	13	0.61
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	7	0.61
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	7	0.61
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	7	0.61
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	7	0.61
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	7	0.61
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	7	0.61
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	6	0.61
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	6	0.61
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	6	0.61
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	18	0.61
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	18	0.61
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	10	0.6
(1,607)	1:A:16:ASP:HB2	1:A:19:LEU:HB3	11	0.6
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	7	0.6
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	10	0.6
(1,496)	1:A:19:LEU:HD21	1:A:22:ASP:HB3	4	0.6
(1,496)	1:A:19:LEU:HD22	1:A:22:ASP:HB3	4	0.6
(1,496)	1:A:19:LEU:HD23	1:A:22:ASP:HB3	4	0.6
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	17	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	17	0.6
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	17	0.6
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	17	0.6
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	17	0.6
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	17	0.6
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	10	0.6
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	10	0.6
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	19	0.6
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	19	0.6
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	4	0.6
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	4	0.6
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	11	0.59
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	19	0.59
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	19	0.59
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	13	0.59
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	13	0.59
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	5	0.59
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	5	0.59
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	11	0.58
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	11	0.58
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	11	0.58
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	14	0.58
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	14	0.58
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	14	0.58
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	20	0.58
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	20	0.58
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	6	0.58
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	6	0.58
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG21	12	0.58
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG22	12	0.58
(1,197)	1:A:27:GLY:HA2	1:A:28:THR:HG23	12	0.58
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	16	0.57
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	16	0.57
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	16	0.57
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	3	0.57
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	3	0.57
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	5	0.57
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	5	0.57
(1,282)	1:A:25:SER:HB2	1:A:52:ALA:H	3	0.57
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	5	0.56
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	5	0.56
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD11	17	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD12	17	0.56
(1,480)	1:A:13:TYR:HB2	1:A:19:LEU:HD13	17	0.56
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	20	0.56
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	20	0.56
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	20	0.56
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	4	0.56
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	4	0.56
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	7	0.56
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	9	0.56
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	9	0.56
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	10	0.56
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	10	0.56
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	19	0.55
(1,251)	1:A:26:GLY:HA2	1:A:28:THR:H	18	0.55
(1,607)	1:A:16:ASP:HB2	1:A:19:LEU:HB3	9	0.54
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	9	0.54
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	9	0.54
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	9	0.54
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	15	0.54
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	17	0.54
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	17	0.54
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	2	0.53
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	12	0.53
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	12	0.53
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	4	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	5	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	6	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	8	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	9	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	10	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	12	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	13	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	16	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	17	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	19	0.52
(1,320)	1:A:36:CYS:H	1:A:36:CYS:HB3	20	0.52
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	20	0.51
(1,536)	1:A:21:TRP:HZ3	1:A:25:SER:HB2	17	0.51
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	1	0.51
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	1	0.51
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	1	0.51
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	19	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	19	0.51
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	19	0.51
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	2	0.51
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	2	0.51
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	3	0.5
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	6	0.5
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	6	0.5
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	12	0.5
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	12	0.5
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	20	0.5
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	4	0.5
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	4	0.5
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	4	0.5
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	16	0.5
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	16	0.5
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	16	0.5
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	11	0.5
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	11	0.5
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	11	0.5
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	11	0.5
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	11	0.5
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	11	0.5
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	11	0.5
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	11	0.5
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	11	0.5
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	11	0.5
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	14	0.5
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	14	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	4	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	4	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	4	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	5	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	5	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	5	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	15	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	15	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	15	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	18	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	18	0.5
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	18	0.5
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	13	0.5
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:A:2:ILE:HG21	1:A:17:SER:HB3	6	0.49
(1,511)	1:A:2:ILE:HG22	1:A:17:SER:HB3	6	0.49
(1,511)	1:A:2:ILE:HG23	1:A:17:SER:HB3	6	0.49
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	7	0.49
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	7	0.49
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	4	0.49
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	2	0.48
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	2	0.48
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	15	0.48
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	4	0.48
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	4	0.48
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD11	3	0.48
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD12	3	0.48
(1,354)	1:A:16:ASP:HB2	1:A:19:LEU:HD13	3	0.48
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	1	0.47
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	1	0.47
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	1	0.47
(1,266)	1:A:27:GLY:HA3	1:A:53:ASP:HA	1	0.47
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	16	0.46
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	16	0.46
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	18	0.46
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	18	0.46
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	20	0.46
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	20	0.46
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	12	0.46
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	12	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	1	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	2	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	3	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	4	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	5	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	6	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	7	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	8	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	9	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	10	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	11	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	12	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	13	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	14	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	15	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	17	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	18	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	19	0.46
(1,243)	1:A:11:CYS:H	1:A:12:PRO:HD2	20	0.46
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	20	0.46
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	20	0.46
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	2	0.45
(1,607)	1:A:16:ASP:HB2	1:A:19:LEU:HB3	14	0.45
(1,593)	1:A:59:ASN:HB2	1:A:60:ALA:HB1	8	0.45
(1,593)	1:A:59:ASN:HB2	1:A:60:ALA:HB2	8	0.45
(1,593)	1:A:59:ASN:HB2	1:A:60:ALA:HB3	8	0.45
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	5	0.45
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	8	0.45
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	8	0.45
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	10	0.45
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	10	0.45
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	11	0.45
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	11	0.45
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	12	0.45
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	12	0.45
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	19	0.45
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	19	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	2	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	3	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	4	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	8	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	9	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	10	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	11	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	12	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	14	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	16	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	18	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	19	0.45
(1,402)	1:A:3:GLU:H	1:A:3:GLU:HB2	20	0.45
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	12	0.45
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	12	0.45
(1,607)	1:A:16:ASP:HB2	1:A:19:LEU:HB3	1	0.44
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	2	0.44
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	2	0.44
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	17	0.44
(1,607)	1:A:16:ASP:HB2	1:A:19:LEU:HB3	12	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	13	0.43
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	13	0.43
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	18	0.43
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	18	0.43
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	20	0.43
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	20	0.43
(1,574)	1:A:25:SER:HB2	1:A:48:CYS:HA	8	0.43
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	15	0.43
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	15	0.43
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	6	0.43
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	6	0.43
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	6	0.42
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	10	0.42
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	10	0.42
(1,366)	1:A:24:CYS:HB3	1:A:35:CYS:HB2	20	0.41
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	16	0.41
(1,94)	1:A:46:GLN:HG3	1:A:47:SER:H	7	0.4
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	11	0.4
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	11	0.4
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	12	0.4
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	12	0.4
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	9	0.4
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	14	0.4
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	19	0.4
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	2	0.39
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	2	0.39
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	6	0.39
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	19	0.39
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	19	0.39
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	19	0.39
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	19	0.39
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	19	0.39
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	19	0.39
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	5	0.39
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	1	0.39
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	2	0.39
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	4	0.39
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	18	0.39
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	7	0.39
(1,14)	1:A:14:LYS:HD2	1:A:15:ASN:H	17	0.39
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	2	0.38
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	15	0.38
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	15	0.38
(1,45)	1:A:15:ASN:HB2	1:A:16:ASP:H	12	0.38
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	17	0.38
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	17	0.38
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	3	0.38
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	3	0.38
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	3	0.38
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	6	0.38
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	11	0.38
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	12	0.38
(1,621)	1:A:3:GLU:HA	1:A:3:GLU:HG3	4	0.37
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	8	0.37
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	8	0.37
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	11	0.37
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	11	0.37
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	4	0.37
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	4	0.37
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	4	0.37
(1,45)	1:A:15:ASN:HB2	1:A:16:ASP:H	13	0.37
(1,436)	1:A:14:LYS:HB2	1:A:14:LYS:HD2	7	0.37
(1,436)	1:A:14:LYS:HB3	1:A:14:LYS:HD2	7	0.37
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	9	0.37
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	9	0.37
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	15	0.37
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	19	0.37
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	19	0.37
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB2	19	0.37
(1,233)	1:A:37:GLY:HA3	1:A:45:SER:HB3	19	0.37
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	12	0.36
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	12	0.36
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	5	0.36
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	4	0.36
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	4	0.36
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	4	0.36
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	4	0.36
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	4	0.36
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	4	0.36
(1,45)	1:A:15:ASN:HB2	1:A:16:ASP:H	11	0.36
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	5	0.36
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	9	0.35
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:A:15:ASN:HB2	1:A:16:ASP:H	14	0.35
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	7	0.35
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	4	0.34
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	5	0.34
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	6	0.34
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	12	0.34
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	17	0.34
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	19	0.34
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	9	0.34
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	9	0.34
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	9	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	1	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	2	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	5	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	6	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	8	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	9	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	11	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	13	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	15	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	16	0.34
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	17	0.34
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	9	0.33
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	11	0.33
(1,607)	1:A:16:ASP:HB2	1:A:19:LEU:HB3	2	0.33
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	1	0.33
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	3	0.33
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	13	0.33
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	1	0.33
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	1	0.33
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	1	0.33
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	1	0.33
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	1	0.33
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	1	0.33
(1,385)	1:A:3:GLU:H	1:A:3:GLU:HG2	7	0.33
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	13	0.33
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	13	0.33
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	14	0.33
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	14	0.33
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	3	0.33
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	4	0.33
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	12	0.33
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	14	0.33
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	18	0.33
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	19	0.33
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	12	0.32
(1,614)	1:A:46:GLN:HA	1:A:46:GLN:HG2	17	0.32
(1,385)	1:A:3:GLU:H	1:A:3:GLU:HG2	1	0.32
(1,385)	1:A:3:GLU:H	1:A:3:GLU:HG2	15	0.32
(1,104)	1:A:44:VAL:H	1:A:45:SER:HA	20	0.32
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	15	0.31
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	6	0.31
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	19	0.31
(1,614)	1:A:46:GLN:HA	1:A:46:GLN:HG2	1	0.31
(1,550)	1:A:41:SER:HA	1:A:41:SER:HB2	20	0.31
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	6	0.31
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	6	0.31
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	6	0.31
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	6	0.31
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	6	0.31
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	6	0.31
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	20	0.31
(1,385)	1:A:3:GLU:H	1:A:3:GLU:HG2	5	0.31
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	13	0.31
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	13	0.31
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	8	0.31
(1,285)	1:A:17:SER:H	1:A:17:SER:HB2	10	0.31
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	14	0.3
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	8	0.3
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	11	0.3
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	12	0.3
(1,614)	1:A:46:GLN:HA	1:A:46:GLN:HG2	20	0.3
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	7	0.3
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	7	0.3
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	18	0.3
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	17	0.3
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	17	0.3
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	9	0.29
(1,614)	1:A:46:GLN:HA	1:A:46:GLN:HG2	13	0.29
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	1	0.29
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	11	0.29
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	15	0.29
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	20	0.29
(1,536)	1:A:21:TRP:HZ3	1:A:25:SER:HB2	3	0.29
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	14	0.29
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	14	0.29
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	14	0.29
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	14	0.29
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	14	0.29
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	14	0.29
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	20	0.29
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	20	0.29
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	20	0.29
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	20	0.29
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	20	0.29
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	20	0.29
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	20	0.29
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	20	0.29
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	14	0.28
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	18	0.28
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	4	0.28
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	6	0.28
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG2	18	0.28
(1,384)	1:A:12:PRO:HD2	1:A:38:GLN:HG3	18	0.28
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	15	0.27
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	15	0.27
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	19	0.27
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	19	0.27
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	3	0.26
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	9	0.26
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	10	0.26
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	12	0.26
(1,439)	1:A:12:PRO:HG3	1:A:13:TYR:HE1	14	0.26
(1,439)	1:A:12:PRO:HG3	1:A:13:TYR:HE2	14	0.26
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	20	0.26
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	1	0.25
(1,601)	1:A:23:THR:HG21	1:A:30:ASN:HB2	7	0.25
(1,601)	1:A:23:THR:HG22	1:A:30:ASN:HB2	7	0.25
(1,601)	1:A:23:THR:HG23	1:A:30:ASN:HB2	7	0.25
(1,536)	1:A:21:TRP:HZ3	1:A:25:SER:HB2	1	0.25
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	7	0.25
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	7	0.25
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	7	0.25
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	4	0.25
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	4	0.25
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	19	0.25
(1,688)	1:A:11:CYS:SG	1:A:39:CYS:CB	18	0.24
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	17	0.24
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	10	0.24
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	10	0.24
(1,294)	1:A:17:SER:HA	1:A:17:SER:HB3	7	0.24
(1,294)	1:A:17:SER:HA	1:A:17:SER:HB3	17	0.24
(1,294)	1:A:17:SER:HA	1:A:17:SER:HB3	20	0.24
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	1	0.24
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	1	0.24
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	1	0.23
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	5	0.23
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	15	0.23
(1,601)	1:A:23:THR:HG21	1:A:30:ASN:HB2	13	0.23
(1,601)	1:A:23:THR:HG22	1:A:30:ASN:HB2	13	0.23
(1,601)	1:A:23:THR:HG23	1:A:30:ASN:HB2	13	0.23
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	15	0.23
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	17	0.23
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	17	0.23
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	17	0.23
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	7	0.23
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	7	0.23
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	7	0.23
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	2	0.23
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	8	0.23
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	15	0.23
(1,688)	1:A:11:CYS:SG	1:A:39:CYS:CB	19	0.22
(1,688)	1:A:11:CYS:SG	1:A:39:CYS:CB	20	0.22
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	14	0.22
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	7	0.22
(1,594)	1:A:56:ASP:HA	1:A:56:ASP:HB2	14	0.22
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	3	0.22
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	3	0.22
(1,554)	1:A:19:LEU:HD11	1:A:20:ALA:HA	6	0.22
(1,554)	1:A:19:LEU:HD12	1:A:20:ALA:HA	6	0.22
(1,554)	1:A:19:LEU:HD13	1:A:20:ALA:HA	6	0.22
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	1	0.22
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	13	0.22
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	13	0.22
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	13	0.22
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	13	0.22
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	13	0.22
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	13	0.22
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	13	0.22
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	13	0.22
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	11	0.22
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	14	0.22
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	18	0.22
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	19	0.22
(1,366)	1:A:24:CYS:HB3	1:A:35:CYS:HB2	18	0.22
(1,366)	1:A:24:CYS:HB3	1:A:35:CYS:HB2	19	0.22
(1,294)	1:A:17:SER:HA	1:A:17:SER:HB3	13	0.22
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	11	0.22
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	14	0.22
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	11	0.21
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	18	0.21
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	14	0.21
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	14	0.21
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	11	0.21
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	11	0.21
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	12	0.21
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	12	0.21
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB2	17	0.21
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB3	17	0.21
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	11	0.21
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	11	0.21
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	4	0.21
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	5	0.21
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	18	0.21
(1,98)	1:A:51:MET:HG3	1:A:53:ASP:H	17	0.2
(1,607)	1:A:16:ASP:HB2	1:A:19:LEU:HB3	6	0.2
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB2	4	0.2
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB3	4	0.2
(1,554)	1:A:19:LEU:HD11	1:A:20:ALA:HA	4	0.2
(1,554)	1:A:19:LEU:HD12	1:A:20:ALA:HA	4	0.2
(1,554)	1:A:19:LEU:HD13	1:A:20:ALA:HA	4	0.2
(1,536)	1:A:21:TRP:HZ3	1:A:25:SER:HB2	4	0.2
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	16	0.2
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	16	0.2
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	16	0.2
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	20	0.2
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE1	15	0.2
(1,281)	1:A:12:PRO:HD3	1:A:13:TYR:HE2	15	0.2
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	1	0.2
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	2	0.2
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	3	0.2
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	10	0.2
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	12	0.2
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	13	0.2
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	2	0.19
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	5	0.19
(1,641)	1:A:19:LEU:HB3	1:A:20:ALA:HA	18	0.19
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	4	0.19
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	10	0.19
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	9	0.19
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	9	0.19
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	5	0.19
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	5	0.19
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	6	0.19
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	6	0.19
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	8	0.19
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	8	0.19
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	7	0.19
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	17	0.19
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	6	0.18
(1,66)	1:A:27:GLY:H	1:A:53:ASP:HB2	19	0.18
(1,66)	1:A:27:GLY:H	1:A:53:ASP:HB3	19	0.18
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	8	0.18
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	8	0.18
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	19	0.18
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	19	0.18
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB2	9	0.18
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB3	9	0.18
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB2	12	0.18
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB3	12	0.18
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB2	13	0.18
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB3	13	0.18
(1,565)	1:A:36:CYS:HB3	1:A:45:SER:HA	15	0.18
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	3	0.18
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	10	0.18
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	4	0.18
(1,536)	1:A:21:TRP:HZ3	1:A:25:SER:HB2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD11	9	0.18
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD12	9	0.18
(1,479)	1:A:14:LYS:HE2	1:A:19:LEU:HD13	9	0.18
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	17	0.18
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	17	0.18
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	17	0.18
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	9	0.18
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	9	0.18
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	9	0.18
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	10	0.18
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	10	0.18
(1,283)	1:A:25:SER:HB2	1:A:51:MET:H	19	0.18
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	9	0.18
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	17	0.18
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	17	0.18
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	17	0.18
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	20	0.17
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	19	0.17
(1,581)	1:A:3:GLU:HB2	1:A:17:SER:HB2	5	0.17
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB2	16	0.17
(1,566)	1:A:34:VAL:HA	1:A:38:GLN:HB3	16	0.17
(1,50)	1:A:25:SER:HA	1:A:52:ALA:H	10	0.17
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	20	0.17
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	20	0.17
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	20	0.17
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	19	0.17
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	19	0.17
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	6	0.17
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	16	0.17
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	12	0.17
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	12	0.17
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	12	0.17
(1,579)	1:A:6:TYR:HD1	1:A:17:SER:HB2	5	0.16
(1,579)	1:A:6:TYR:HD2	1:A:17:SER:HB2	5	0.16
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	3	0.16
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	3	0.16
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	3	0.16
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	7	0.16
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	7	0.16
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	15	0.16
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	15	0.16
(1,366)	1:A:24:CYS:HB3	1:A:35:CYS:HB2	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	6	0.16
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	6	0.16
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	6	0.16
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	11	0.16
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	11	0.16
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	11	0.16
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	18	0.16
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	18	0.16
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	18	0.16
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	18	0.15
(1,641)	1:A:19:LEU:HB3	1:A:20:ALA:HA	8	0.15
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	2	0.15
(1,636)	1:A:32:GLY:HA3	1:A:52:ALA:HB1	17	0.15
(1,636)	1:A:32:GLY:HA3	1:A:52:ALA:HB2	17	0.15
(1,636)	1:A:32:GLY:HA3	1:A:52:ALA:HB3	17	0.15
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	17	0.15
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	15	0.15
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD11	2	0.15
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD12	2	0.15
(1,477)	1:A:13:TYR:HD1	1:A:19:LEU:HD13	2	0.15
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD11	2	0.15
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD12	2	0.15
(1,477)	1:A:13:TYR:HD2	1:A:19:LEU:HD13	2	0.15
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	12	0.15
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	12	0.15
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	14	0.15
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	14	0.15
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	18	0.15
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	18	0.15
(1,251)	1:A:26:GLY:HA2	1:A:28:THR:H	8	0.15
(1,248)	1:A:5:PHE:HB3	1:A:6:TYR:H	6	0.15
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	14	0.15
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	14	0.15
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	14	0.15
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	5	0.14
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	6	0.14
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	8	0.14
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	19	0.14
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	15	0.14
(1,641)	1:A:19:LEU:HB3	1:A:20:ALA:HA	10	0.14
(1,639)	1:A:16:ASP:HB2	1:A:19:LEU:HB2	19	0.14
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	15	0.14
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	19	0.14
(1,46)	1:A:37:GLY:H	1:A:45:SER:HB2	2	0.14
(1,46)	1:A:37:GLY:H	1:A:45:SER:HB3	2	0.14
(1,414)	1:A:3:GLU:HB3	1:A:4:ASP:H	8	0.14
(1,389)	1:A:21:TRP:HH2	1:A:25:SER:HB3	17	0.14
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	11	0.14
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	11	0.14
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	17	0.14
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	17	0.14
(1,366)	1:A:24:CYS:HB3	1:A:35:CYS:HB2	3	0.14
(1,251)	1:A:26:GLY:HA2	1:A:28:THR:H	3	0.14
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	16	0.14
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	16	0.14
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	16	0.14
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	10	0.13
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	15	0.13
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	3	0.13
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	7	0.13
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	8	0.13
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	16	0.13
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG11	7	0.13
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG12	7	0.13
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG13	7	0.13
(1,641)	1:A:19:LEU:HB3	1:A:20:ALA:HA	3	0.13
(1,641)	1:A:19:LEU:HB3	1:A:20:ALA:HA	5	0.13
(1,641)	1:A:19:LEU:HB3	1:A:20:ALA:HA	15	0.13
(1,575)	1:A:6:TYR:HE1	1:A:17:SER:HB2	3	0.13
(1,575)	1:A:6:TYR:HE2	1:A:17:SER:HB2	3	0.13
(1,565)	1:A:36:CYS:HB3	1:A:45:SER:HA	11	0.13
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	2	0.13
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	19	0.13
(1,50)	1:A:25:SER:HA	1:A:52:ALA:H	9	0.13
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	9	0.13
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	9	0.13
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	9	0.13
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD11	19	0.13
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD12	19	0.13
(1,481)	1:A:16:ASP:HB3	1:A:19:LEU:HD13	19	0.13
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD11	16	0.13
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD12	16	0.13
(1,478)	1:A:13:TYR:HB3	1:A:19:LEU:HD13	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:A:37:GLY:H	1:A:45:SER:HB2	11	0.13
(1,46)	1:A:37:GLY:H	1:A:45:SER:HB3	11	0.13
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	1	0.13
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	1	0.13
(1,353)	1:A:6:TYR:HE1	1:A:39:CYS:HB3	20	0.13
(1,353)	1:A:6:TYR:HE2	1:A:39:CYS:HB3	20	0.13
(1,318)	1:A:14:LYS:HE3	1:A:15:ASN:HB2	18	0.13
(1,279)	1:A:12:PRO:HD3	1:A:13:TYR:HD1	7	0.13
(1,279)	1:A:12:PRO:HD3	1:A:13:TYR:HD2	7	0.13
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	4	0.13
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	4	0.13
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	4	0.13
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	11	0.12
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	16	0.12
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	18	0.12
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	9	0.12
(1,618)	1:A:3:GLU:HB2	1:A:3:GLU:HG2	16	0.12
(1,612)	1:A:30:ASN:HA	1:A:30:ASN:HB3	5	0.12
(1,609)	1:A:11:CYS:HA	1:A:38:GLN:HB2	6	0.12
(1,609)	1:A:11:CYS:HA	1:A:38:GLN:HB3	6	0.12
(1,609)	1:A:11:CYS:HA	1:A:38:GLN:HB2	19	0.12
(1,609)	1:A:11:CYS:HA	1:A:38:GLN:HB3	19	0.12
(1,565)	1:A:36:CYS:HB3	1:A:45:SER:HA	2	0.12
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	6	0.12
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	8	0.12
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	9	0.12
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	11	0.12
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	14	0.12
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	15	0.12
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	18	0.12
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	12	0.12
(1,50)	1:A:25:SER:HA	1:A:52:ALA:H	5	0.12
(1,50)	1:A:25:SER:HA	1:A:52:ALA:H	17	0.12
(1,46)	1:A:37:GLY:H	1:A:45:SER:HB2	1	0.12
(1,46)	1:A:37:GLY:H	1:A:45:SER:HB3	1	0.12
(1,43)	1:A:16:ASP:H	1:A:17:SER:HA	14	0.12
(1,385)	1:A:3:GLU:H	1:A:3:GLU:HG2	13	0.12
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	13	0.12
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	13	0.12
(1,366)	1:A:24:CYS:HB3	1:A:35:CYS:HB2	14	0.12
(1,350)	1:A:52:ALA:H	1:A:53:ASP:HB2	17	0.12
(1,350)	1:A:52:ALA:H	1:A:53:ASP:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,263)	1:A:44:VAL:HA	1:A:48:CYS:H	8	0.12
(1,198)	1:A:41:SER:H	1:A:41:SER:HB2	2	0.12
(1,198)	1:A:41:SER:H	1:A:41:SER:HB2	7	0.12
(1,198)	1:A:41:SER:H	1:A:41:SER:HB2	18	0.12
(1,181)	1:A:9:GLU:HB3	1:A:10:THR:HB	15	0.12
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	1	0.12
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	1	0.12
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	1	0.12
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	3	0.12
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	3	0.12
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	3	0.12
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	7	0.12
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	7	0.12
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	7	0.12
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	15	0.12
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	15	0.12
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	15	0.12
(1,175)	1:A:52:ALA:HB1	1:A:53:ASP:HA	20	0.12
(1,175)	1:A:52:ALA:HB2	1:A:53:ASP:HA	20	0.12
(1,175)	1:A:52:ALA:HB3	1:A:53:ASP:HA	20	0.12
(1,142)	1:A:25:SER:H	1:A:26:GLY:H	12	0.12
(1,98)	1:A:51:MET:HG3	1:A:53:ASP:H	8	0.11
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	2	0.11
(1,80)	1:A:35:CYS:H	1:A:35:CYS:HB2	3	0.11
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	6	0.11
(1,74)	1:A:16:ASP:HB2	1:A:18:GLN:H	12	0.11
(1,693)	1:A:35:CYS:CB	1:A:48:CYS:SG	15	0.11
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	9	0.11
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	12	0.11
(1,692)	1:A:35:CYS:SG	1:A:48:CYS:CB	20	0.11
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG11	17	0.11
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG12	17	0.11
(1,669)	1:A:21:TRP:HE3	1:A:44:VAL:HG13	17	0.11
(1,612)	1:A:30:ASN:HA	1:A:30:ASN:HB3	7	0.11
(1,609)	1:A:11:CYS:HA	1:A:38:GLN:HB2	8	0.11
(1,609)	1:A:11:CYS:HA	1:A:38:GLN:HB3	8	0.11
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB2	4	0.11
(1,605)	1:A:27:GLY:HA3	1:A:53:ASP:HB3	4	0.11
(1,559)	1:A:54:SER:HA	1:A:54:SER:HB2	6	0.11
(1,559)	1:A:54:SER:HA	1:A:54:SER:HB2	11	0.11
(1,559)	1:A:54:SER:HA	1:A:54:SER:HB2	12	0.11
(1,559)	1:A:54:SER:HA	1:A:54:SER:HB2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	1	0.11
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	4	0.11
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	5	0.11
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	7	0.11
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	12	0.11
(1,547)	1:A:53:ASP:HA	1:A:54:SER:HA	20	0.11
(1,541)	1:A:6:TYR:HA	1:A:17:SER:HB2	2	0.11
(1,536)	1:A:21:TRP:HZ3	1:A:25:SER:HB2	10	0.11
(1,50)	1:A:25:SER:HA	1:A:52:ALA:H	1	0.11
(1,50)	1:A:25:SER:HA	1:A:52:ALA:H	8	0.11
(1,488)	1:A:7:THR:HG21	1:A:11:CYS:H	16	0.11
(1,488)	1:A:7:THR:HG22	1:A:11:CYS:H	16	0.11
(1,488)	1:A:7:THR:HG23	1:A:11:CYS:H	16	0.11
(1,483)	1:A:7:THR:HG21	1:A:41:SER:H	14	0.11
(1,483)	1:A:7:THR:HG22	1:A:41:SER:H	14	0.11
(1,483)	1:A:7:THR:HG23	1:A:41:SER:H	14	0.11
(1,473)	1:A:13:TYR:HB2	1:A:19:LEU:HG	18	0.11
(1,435)	1:A:14:LYS:H	1:A:14:LYS:HB2	9	0.11
(1,435)	1:A:14:LYS:H	1:A:14:LYS:HB3	9	0.11
(1,435)	1:A:14:LYS:H	1:A:14:LYS:HB2	16	0.11
(1,435)	1:A:14:LYS:H	1:A:14:LYS:HB3	16	0.11
(1,43)	1:A:16:ASP:H	1:A:17:SER:HA	13	0.11
(1,385)	1:A:3:GLU:H	1:A:3:GLU:HG2	17	0.11
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB2	17	0.11
(1,373)	1:A:12:PRO:HD2	1:A:38:GLN:HB3	17	0.11
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB2	2	0.11
(1,370)	1:A:40:PHE:HB3	1:A:45:SER:HB3	2	0.11
(1,360)	1:A:22:ASP:HB2	1:A:23:THR:H	20	0.11
(1,353)	1:A:6:TYR:HE1	1:A:39:CYS:HB3	18	0.11
(1,353)	1:A:6:TYR:HE2	1:A:39:CYS:HB3	18	0.11
(1,279)	1:A:12:PRO:HD3	1:A:13:TYR:HD1	14	0.11
(1,279)	1:A:12:PRO:HD3	1:A:13:TYR:HD2	14	0.11
(1,278)	1:A:23:THR:HA	1:A:23:THR:HB	19	0.11
(1,263)	1:A:44:VAL:HA	1:A:48:CYS:H	6	0.11
(1,181)	1:A:9:GLU:HB3	1:A:10:THR:HB	14	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found