



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:18 AM UTC

PDB ID : 2Y1S / pdb_00002y1s
Title : Microvirin lectin
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Deposited on : 2010-12-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

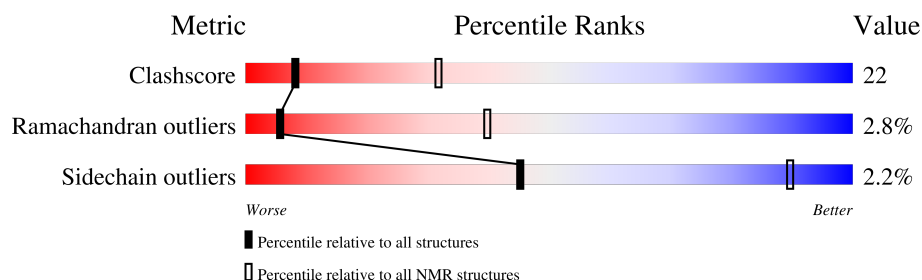
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	

2 Ensemble composition and analysis

This entry contains 40 models. Model 31 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:4-A:106 (103)	0.21	31

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 7 clusters and 9 single-model clusters were found.

Cluster number	Models
1	6, 12, 15, 21, 25, 27, 31, 32, 33, 39
2	10, 14, 18, 24, 35, 37
3	5, 8, 13, 17
4	4, 22, 28, 34
5	11, 38, 40
6	16, 20
7	26, 29
Single-model clusters	1; 2; 3; 7; 9; 19; 23; 30; 36

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1612 atoms, of which 762 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mannan-binding lectin.

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1612	516	762	141	185	8	

There is a discrepancy between the modelled and reference sequences:

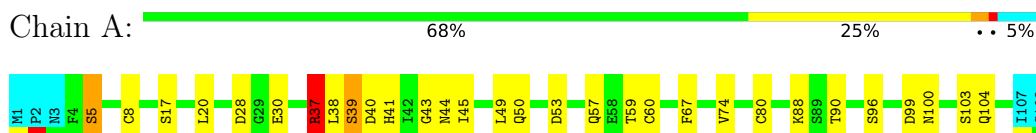
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ARG	HIS	conflict	UNP Q2MDE2

4 Residue-property plots

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: Mannan-binding lectin

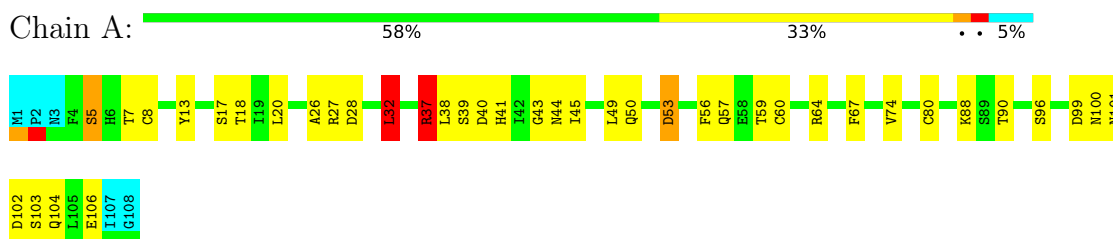


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

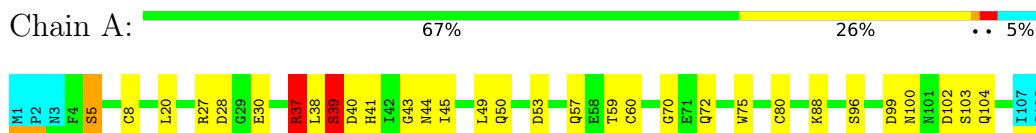
4.2.1 Score per residue for model 1

- Molecule 1: Mannan-binding lectin



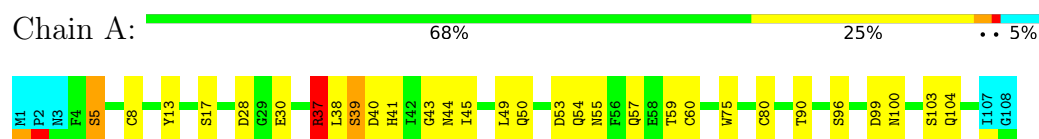
4.2.2 Score per residue for model 2

- Molecule 1: Mannan-binding lectin



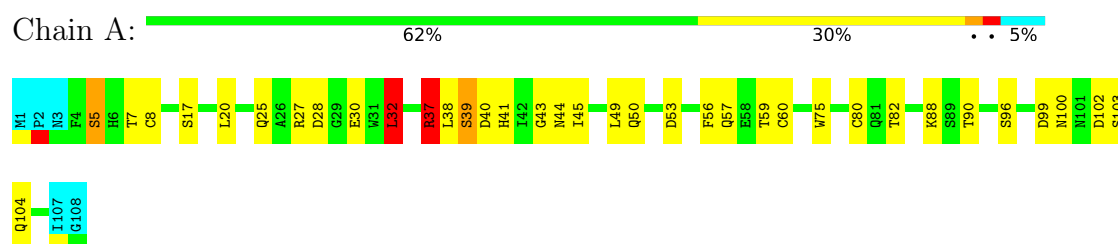
4.2.3 Score per residue for model 3

- Molecule 1: Mannan-binding lectin



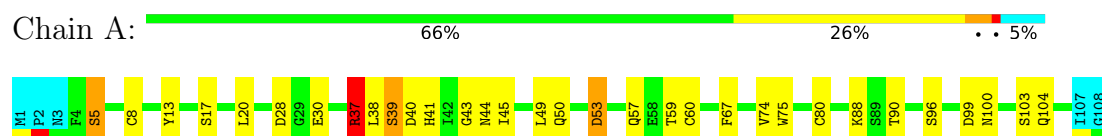
4.2.4 Score per residue for model 4

- Molecule 1: Mannan-binding lectin



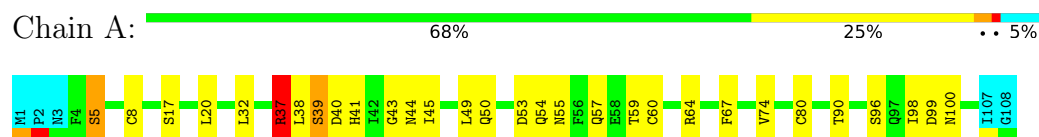
4.2.5 Score per residue for model 5

- Molecule 1: Mannan-binding lectin



4.2.6 Score per residue for model 6

- Molecule 1: Mannan-binding lectin



4.2.7 Score per residue for model 7

- Molecule 1: Mannan-binding lectin





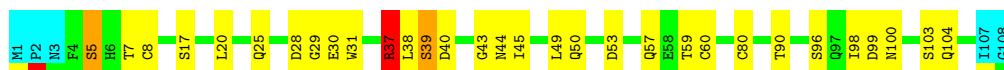
4.2.8 Score per residue for model 8

- Molecule 1: Mannan-binding lectin



4.2.9 Score per residue for model 9

- Molecule 1: Mannan-binding lectin



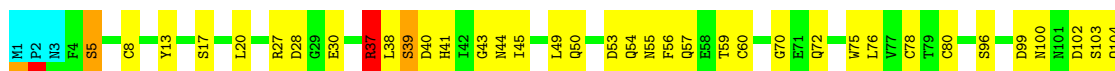
4.2.10 Score per residue for model 10

- Molecule 1: Mannan-binding lectin



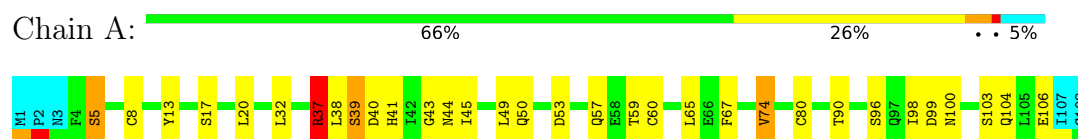
4.2.11 Score per residue for model 11

- Molecule 1: Mannan-binding lectin



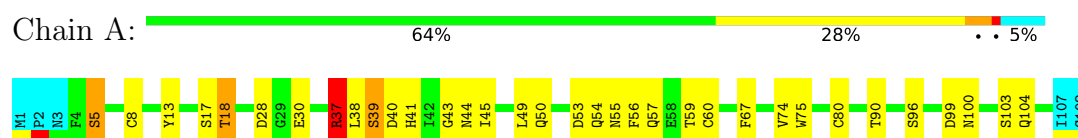
4.2.12 Score per residue for model 12

- Molecule 1: Mannan-binding lectin



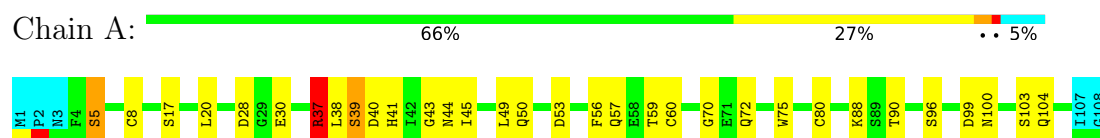
4.2.13 Score per residue for model 13

- Molecule 1: Mannan-binding lectin



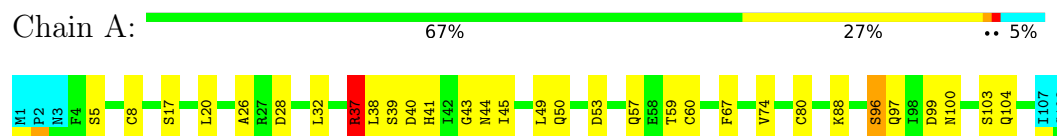
4.2.14 Score per residue for model 14

- Molecule 1: Mannan-binding lectin



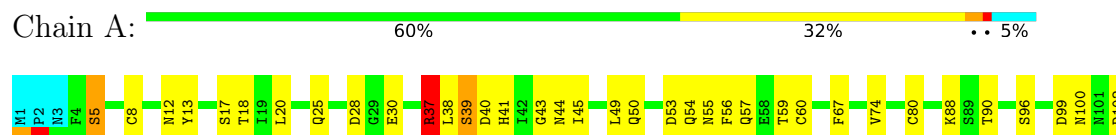
4.2.15 Score per residue for model 15

- Molecule 1: Mannan-binding lectin



4.2.16 Score per residue for model 16

- Molecule 1: Mannan-binding lectin

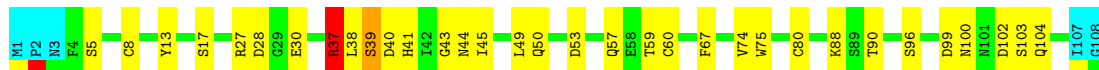




4.2.17 Score per residue for model 17

- Molecule 1: Mannan-binding lectin

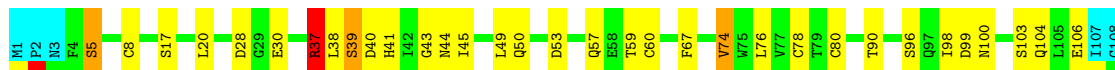
Chain A: 65% 29% 5%



4.2.18 Score per residue for model 18

- Molecule 1: Mannan-binding lectin

Chain A: 65% 27% 5%



4.2.19 Score per residue for model 19

- Molecule 1: Mannan-binding lectin

Chain A: 60% 32% 5%



4.2.20 Score per residue for model 20

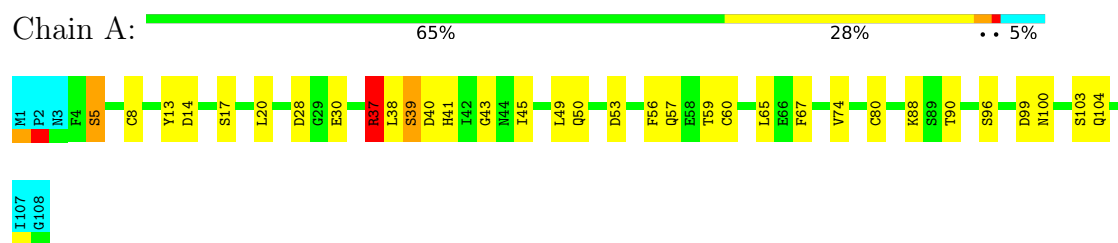
- Molecule 1: Mannan-binding lectin

Chain A: 67% 24% 5%



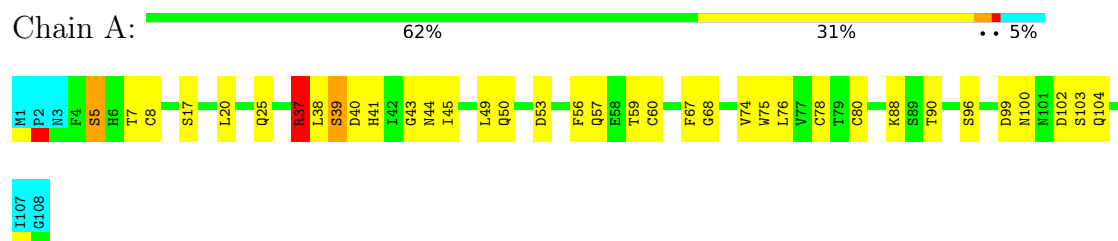
4.2.21 Score per residue for model 21

- Molecule 1: Mannan-binding lectin



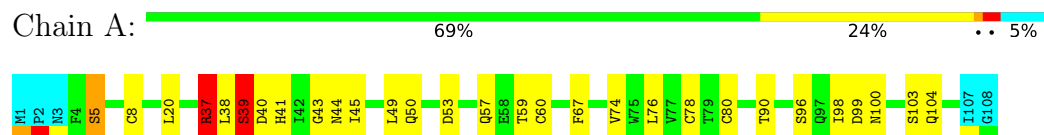
4.2.22 Score per residue for model 22

- Molecule 1: Mannan-binding lectin



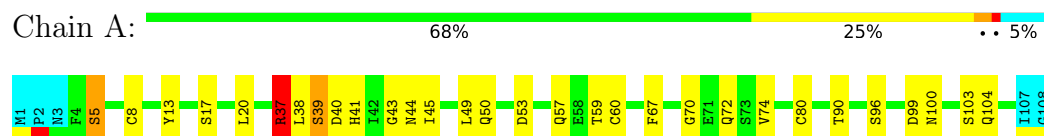
4.2.23 Score per residue for model 23

- Molecule 1: Mannan-binding lectin



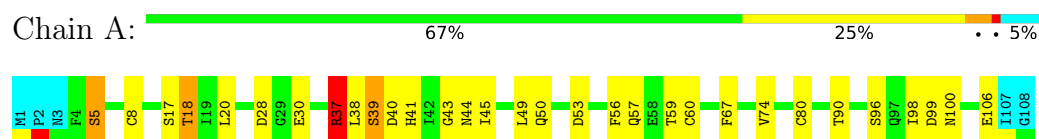
4.2.24 Score per residue for model 24

- Molecule 1: Mannan-binding lectin



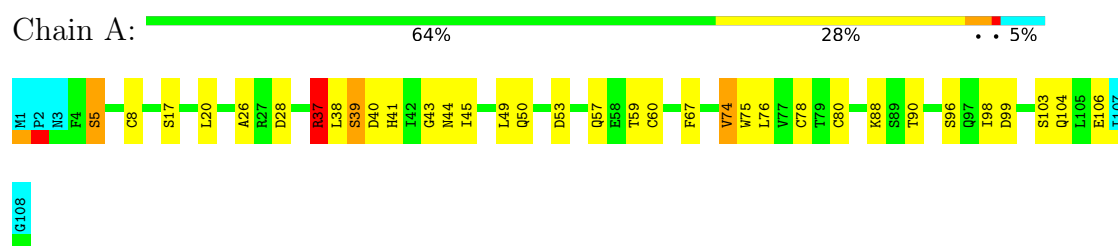
4.2.25 Score per residue for model 25

- Molecule 1: Mannan-binding lectin



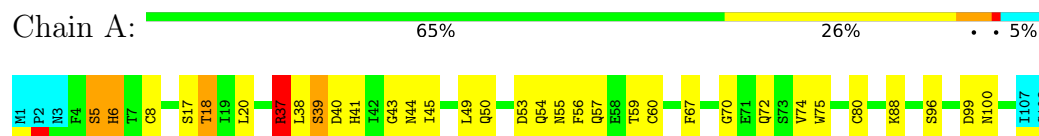
4.2.26 Score per residue for model 26

- Molecule 1: Mannan-binding lectin



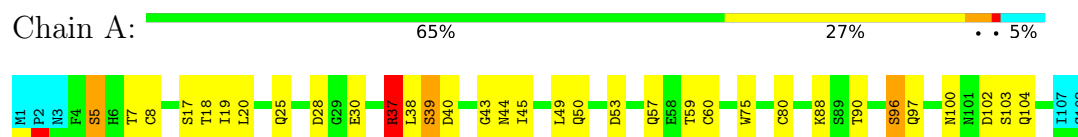
4.2.27 Score per residue for model 27

- Molecule 1: Mannan-binding lectin



4.2.28 Score per residue for model 28

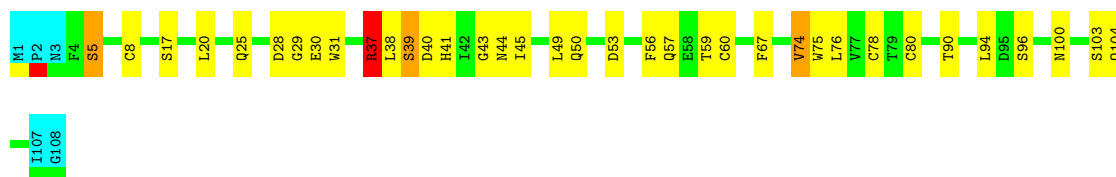
- Molecule 1: Mannan-binding lectin



4.2.29 Score per residue for model 29

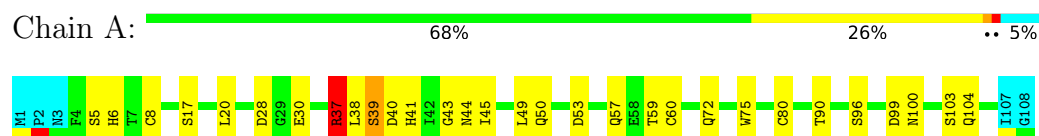
- Molecule 1: Mannan-binding lectin





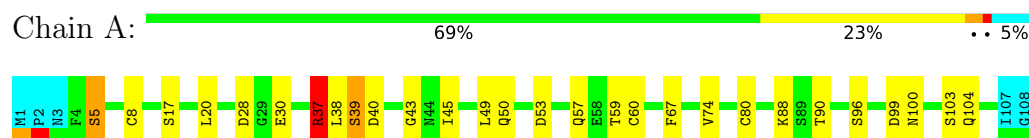
4.2.30 Score per residue for model 30

- Molecule 1: Mannan-binding lectin



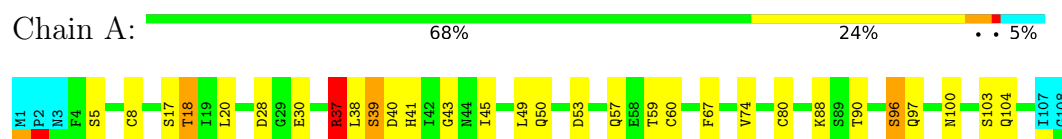
4.2.31 Score per residue for model 31 (medoid)

- Molecule 1: Mannan-binding lectin



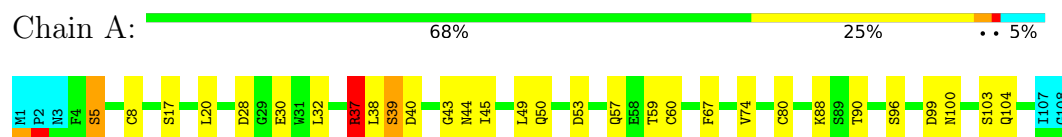
4.2.32 Score per residue for model 32

- Molecule 1: Mannan-binding lectin



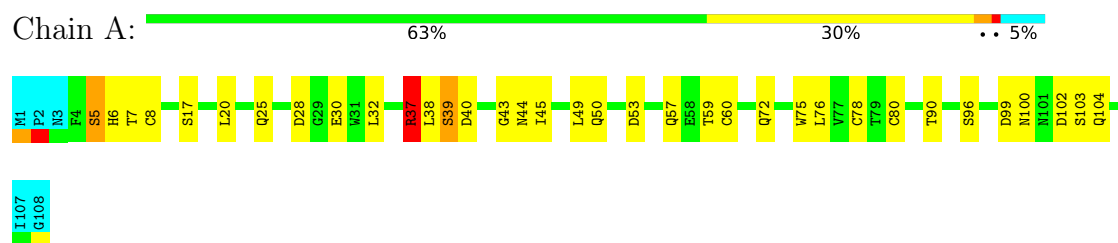
4.2.33 Score per residue for model 33

- Molecule 1: Mannan-binding lectin



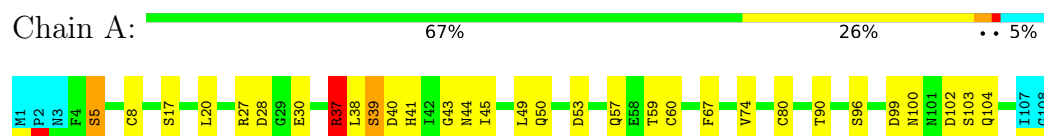
4.2.34 Score per residue for model 34

- Molecule 1: Mannan-binding lectin



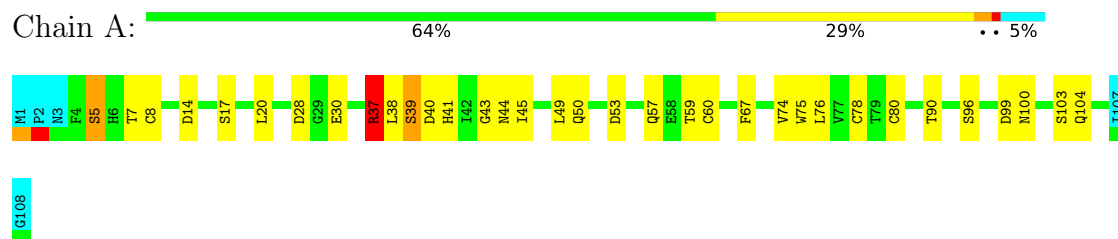
4.2.35 Score per residue for model 35

- Molecule 1: Mannan-binding lectin



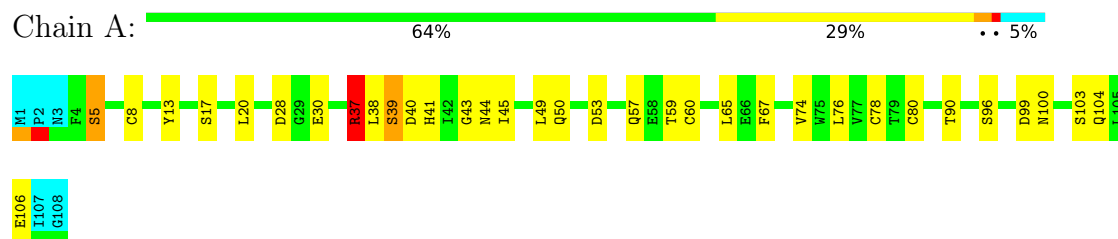
4.2.36 Score per residue for model 36

- Molecule 1: Mannan-binding lectin



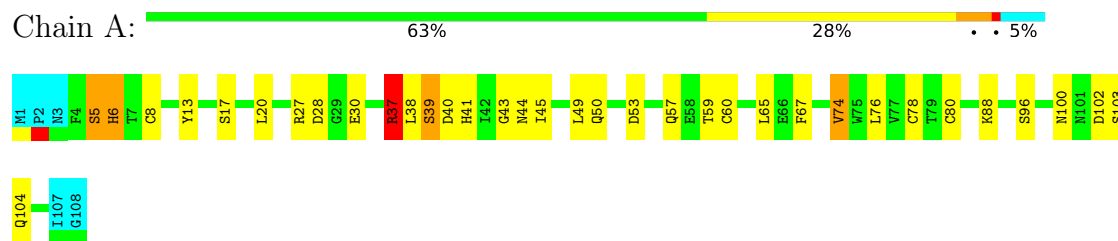
4.2.37 Score per residue for model 37

- Molecule 1: Mannan-binding lectin



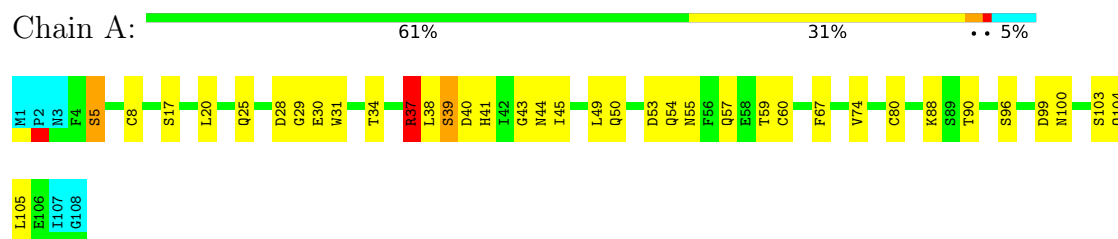
4.2.38 Score per residue for model 38

- Molecule 1: Mannan-binding lectin



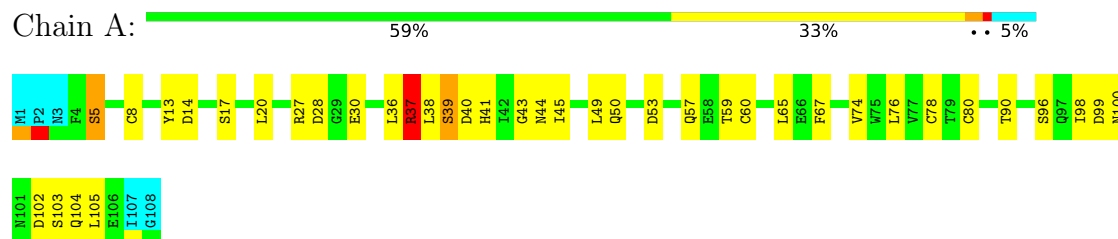
4.2.39 Score per residue for model 39

- Molecule 1: Mannan-binding lectin



4.2.40 Score per residue for model 40

- Molecule 1: Mannan-binding lectin



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE*, *SIMULATED ANNEALING*.

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
Xplor-NIH	refinement	
X-PLOR	structure solution	

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	1206
Number of shifts mapped to atoms	1205
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.67±0.00	2±1/829 (0.2± 0.1%)	1.32±0.01	0±0/1126 (0.0± 0.0%)
All	All	1.67	62/33160 (0.2%)	1.32	0/45040 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.0
All	All	0	40

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	43	GLY	N-CA	5.98	1.50	1.45	3	40
1	A	32	LEU	N-CA	5.84	1.50	1.45	33	9
1	A	68	GLY	N-CA	5.15	1.50	1.45	22	1
1	A	37	ARG	CD-NE	5.05	1.53	1.46	22	10
1	A	64	ARG	NE-CZ	-5.02	1.27	1.33	6	2

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	37	ARG	Sidechain	40

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	814	724	724	34±3
All	All	32560	28960	28960	1348

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ARG:HH21	1:A:37:ARG:CG	0.75	1.94	37	40
1:A:45:ILE:HG23	1:A:45:ILE:O	0.74	1.82	18	37
1:A:82:THR:HG22	1:A:88:LYS:NZ	0.72	2.00	4	1
1:A:37:ARG:NH2	1:A:39:SER:OG	0.68	2.27	2	40
1:A:8:CYS:SG	1:A:100:ASN:ND2	0.67	2.67	2	39
1:A:49:LEU:HD21	1:A:80:CYS:SG	0.67	2.30	36	40
1:A:20:LEU:HD11	1:A:38:LEU:HD11	0.65	1.66	23	36
1:A:45:ILE:HG21	1:A:50:GLN:OE1	0.64	1.93	35	3
1:A:37:ARG:CG	1:A:37:ARG:NH2	0.62	2.61	1	40
1:A:50:GLN:NE2	1:A:53:ASP:OD2	0.62	2.33	26	35
1:A:57:GLN:H	1:A:57:GLN:CD	0.62	2.03	32	40
1:A:17:SER:O	1:A:37:ARG:NE	0.61	2.33	7	38
1:A:6:HIS:ND1	1:A:6:HIS:N	0.60	2.46	7	4
1:A:67:PHE:CE2	1:A:74:VAL:HG12	0.60	2.32	24	30
1:A:6:HIS:CE1	1:A:72:GLN:NE2	0.59	2.70	34	2
1:A:25:GLN:OE1	1:A:31:TRP:CE2	0.59	2.55	39	3
1:A:27:ARG:NH2	1:A:102:ASP:OD2	0.59	2.36	11	9
1:A:53:ASP:OD1	1:A:53:ASP:N	0.59	2.35	8	11
1:A:103:SER:O	1:A:104:GLN:NE2	0.59	2.35	32	24
1:A:44:ASN:ND2	1:A:59:THR:OG1	0.59	2.36	4	37
1:A:25:GLN:NE2	1:A:29:GLY:C	0.59	2.61	39	3
1:A:37:ARG:NH2	1:A:37:ARG:HG2	0.59	2.11	2	40
1:A:38:LEU:O	1:A:40:ASP:N	0.59	2.36	23	40
1:A:25:GLN:NE2	1:A:29:GLY:O	0.59	2.36	29	3
1:A:25:GLN:OE1	1:A:31:TRP:CD2	0.58	2.56	39	2
1:A:56:PHE:CE1	1:A:57:GLN:OE1	0.58	2.56	16	11
1:A:37:ARG:HH21	1:A:37:ARG:HG2	0.57	1.57	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLN:HE21	1:A:29:GLY:C	0.57	2.07	29	3
1:A:82:THR:HG22	1:A:88:LYS:HZ3	0.57	1.59	4	1
1:A:5:SER:O	1:A:8:CYS:O	0.57	2.23	25	40
1:A:96:SER:OG	1:A:97:GLN:N	0.57	2.36	15	4
1:A:49:LEU:HD12	1:A:90:THR:OG1	0.56	2.01	12	29
1:A:7:THR:OG1	1:A:100:ASN:ND2	0.55	2.40	22	9
1:A:45:ILE:O	1:A:45:ILE:CG2	0.55	2.54	2	37
1:A:28:ASP:OD1	1:A:30:GLU:N	0.55	2.39	13	28
1:A:18:THR:HG21	1:A:57:GLN:OE1	0.55	2.02	16	1
1:A:50:GLN:CG	1:A:53:ASP:OD2	0.54	2.55	20	6
1:A:37:ARG:CZ	1:A:39:SER:OG	0.54	2.55	2	2
1:A:20:LEU:CD1	1:A:38:LEU:HD11	0.54	2.33	23	3
1:A:38:LEU:O	1:A:39:SER:C	0.53	2.51	32	40
1:A:57:GLN:CD	1:A:57:GLN:N	0.53	2.66	32	38
1:A:38:LEU:C	1:A:40:ASP:N	0.52	2.65	23	40
1:A:28:ASP:OD2	1:A:30:GLU:OE1	0.51	2.29	9	2
1:A:50:GLN:CD	1:A:53:ASP:OD2	0.51	2.54	18	20
1:A:99:ASP:O	1:A:99:ASP:OD1	0.50	2.29	40	8
1:A:59:THR:C	1:A:60:CYS:SG	0.50	2.94	14	38
1:A:100:ASN:O	1:A:100:ASN:CG	0.50	2.54	36	32
1:A:37:ARG:NH2	1:A:39:SER:CB	0.50	2.75	25	35
1:A:27:ARG:CZ	1:A:102:ASP:OD2	0.50	2.60	2	1
1:A:13:TYR:CD2	1:A:13:TYR:O	0.50	2.65	8	10
1:A:49:LEU:CD1	1:A:90:THR:OG1	0.50	2.60	3	34
1:A:103:SER:O	1:A:104:GLN:OE1	0.50	2.29	39	13
1:A:99:ASP:OD1	1:A:99:ASP:C	0.50	2.55	16	34
1:A:25:GLN:O	1:A:102:ASP:O	0.50	2.30	22	7
1:A:36:LEU:HD13	1:A:105:LEU:CD2	0.50	2.36	40	1
1:A:14:ASP:OD1	1:A:14:ASP:N	0.49	2.44	21	3
1:A:44:ASN:CG	1:A:59:THR:OG1	0.49	2.55	3	27
1:A:99:ASP:OD1	1:A:106:GLU:O	0.49	2.30	37	5
1:A:41:HIS:C	1:A:53:ASP:O	0.49	2.55	2	4
1:A:99:ASP:OD1	1:A:99:ASP:O	0.48	2.32	12	16
1:A:67:PHE:CD2	1:A:74:VAL:HG12	0.48	2.44	29	19
1:A:37:ARG:HH21	1:A:37:ARG:HG3	0.48	1.67	29	4
1:A:76:LEU:HD11	1:A:78:CYS:SG	0.47	2.49	22	12
1:A:28:ASP:OD1	1:A:28:ASP:C	0.47	2.57	13	21
1:A:38:LEU:C	1:A:40:ASP:H	0.44	2.21	23	1
1:A:38:LEU:O	1:A:41:HIS:N	0.44	2.49	16	26
1:A:94:LEU:HD12	1:A:94:LEU:N	0.44	2.27	29	1
1:A:18:THR:O	1:A:18:THR:OG1	0.43	2.33	27	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:THR:HG21	1:A:105:LEU:HD22	0.43	1.90	39	1
1:A:101:ASN:ND2	1:A:106:GLU:OE2	0.43	2.47	1	1
1:A:44:ASN:ND2	1:A:60:CYS:SG	0.43	2.90	23	16
1:A:13:TYR:HB2	1:A:65:LEU:HD11	0.43	1.89	37	5
1:A:54:GLN:O	1:A:55:ASN:CB	0.43	2.66	39	8
1:A:94:LEU:HD12	1:A:94:LEU:H	0.42	1.74	29	1
1:A:32:LEU:HD12	1:A:32:LEU:N	0.42	2.30	1	2
1:A:42:ILE:N	1:A:53:ASP:O	0.42	2.53	7	1
1:A:70:GLY:C	1:A:72:GLN:H	0.42	2.23	19	7
1:A:28:ASP:C	1:A:28:ASP:OD1	0.41	2.63	29	1
1:A:26:ALA:HB3	1:A:28:ASP:OD1	0.41	2.14	1	3
1:A:50:GLN:HE21	1:A:53:ASP:CG	0.41	2.24	33	1
1:A:75:TRP:CD1	1:A:75:TRP:N	0.41	2.85	3	17
1:A:56:PHE:CG	1:A:57:GLN:N	0.41	2.89	11	6
1:A:12:ASN:OD1	1:A:13:TYR:N	0.41	2.54	16	1
1:A:75:TRP:N	1:A:75:TRP:CD1	0.41	2.85	29	1
1:A:70:GLY:C	1:A:72:GLN:N	0.40	2.79	14	1
1:A:17:SER:OG	1:A:19:ILE:CD1	0.40	2.70	28	1
1:A:9:SER:O	1:A:10:SER:CB	0.40	2.69	19	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/108 (95%)	90±9 (87±9%)	8±1 (8±1%)	3±0 (3±0%)	6	41
All	All	4032/4320 (93%)	3595 (89%)	324 (8%)	113 (3%)	6	40

All 3 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	96	SER	40
1	A	39	SER	38
1	A	5	SER	35

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	94/98 (96%)	91±4 (97±4%)	2±1 (2±1%)	45	90
All	All	3739/3920 (95%)	3658 (98%)	81 (2%)	45	90

All 8 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	37	ARG	40
1	A	88	LYS	19
1	A	74	VAL	6
1	A	18	THR	5
1	A	53	ASP	4
1	A	6	HIS	3
1	A	32	LEU	2
1	A	39	SER	2

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *data.doc.csh*

7.1.1 Bookkeeping

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

Total number of shifts	1206
Number of shifts mapped to atoms	1205
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	HIS	HE2	7.054	.	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	108	-0.21 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	100	-0.03 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	106	0.33 ± 0.18	None needed (< 0.5 ppm)
^{15}N	102	-0.03 ± 0.40	None needed (< 0.5 ppm)

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 88%, i.e. 1154 atoms were assigned a chemical shift out of a possible 1314. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	511/518 (99%)	208/211 (99%)	205/206 (100%)	98/101 (97%)
Sidechain	586/697 (84%)	385/444 (87%)	186/228 (82%)	15/25 (60%)
Aromatic	57/99 (58%)	40/50 (80%)	14/44 (32%)	3/5 (60%)
Overall	1154/1314 (88%)	633/705 (90%)	405/478 (85%)	116/131 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1205 atoms were assigned a chemical shift out of a possible 1377. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	533/542 (98%)	217/221 (98%)	214/216 (99%)	102/105 (97%)
Sidechain	615/736 (84%)	404/470 (86%)	195/240 (81%)	16/26 (62%)
Aromatic	57/99 (58%)	40/50 (80%)	14/44 (32%)	3/5 (60%)
Overall	1205/1377 (88%)	661/741 (89%)	423/500 (85%)	121/136 (89%)

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.

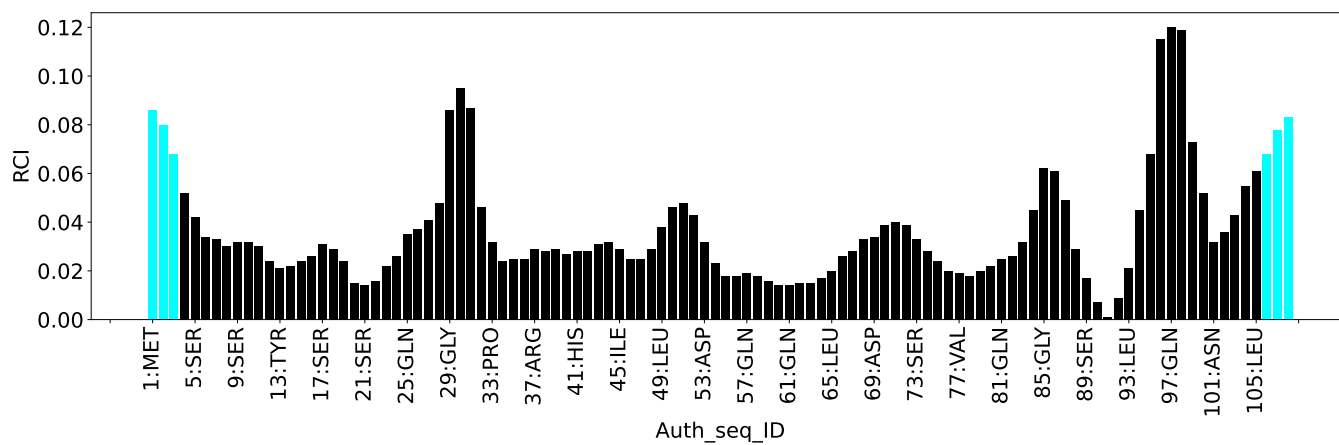
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	91	GLN	C	77.39	166.94 – 185.80	-52.5
1	A	25	GLN	HB2	0.03	0.80 – 3.29	-8.1
1	A	81	GLN	HB2	0.29	0.80 – 3.29	-7.1
1	A	25	GLN	HG2	0.62	1.01 – 3.62	-6.5
1	A	81	GLN	HG2	0.79	1.01 – 3.62	-5.8

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:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1344
Intra-residue ($ i-j =0$)	362
Sequential ($ i-j =1$)	432
Medium range ($ i-j >1$ and $ i-j <5$)	118
Long range ($ i-j \geq 5$)	395
Inter-chain	0
Hydrogen bond restraints	34
Disulfide bond restraints	3
Total dihedral-angle restraints	141
Number of unmapped restraints	0
Number of restraints per residue	13.8
Number of long range restraints per residue ¹	4.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	11.9	0.2
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.3	9.16
10.0-20.0 (Medium)	0.1	13.65
>20.0 (Large)	0.5	139.94

9 Distance violation analysis ⓘ

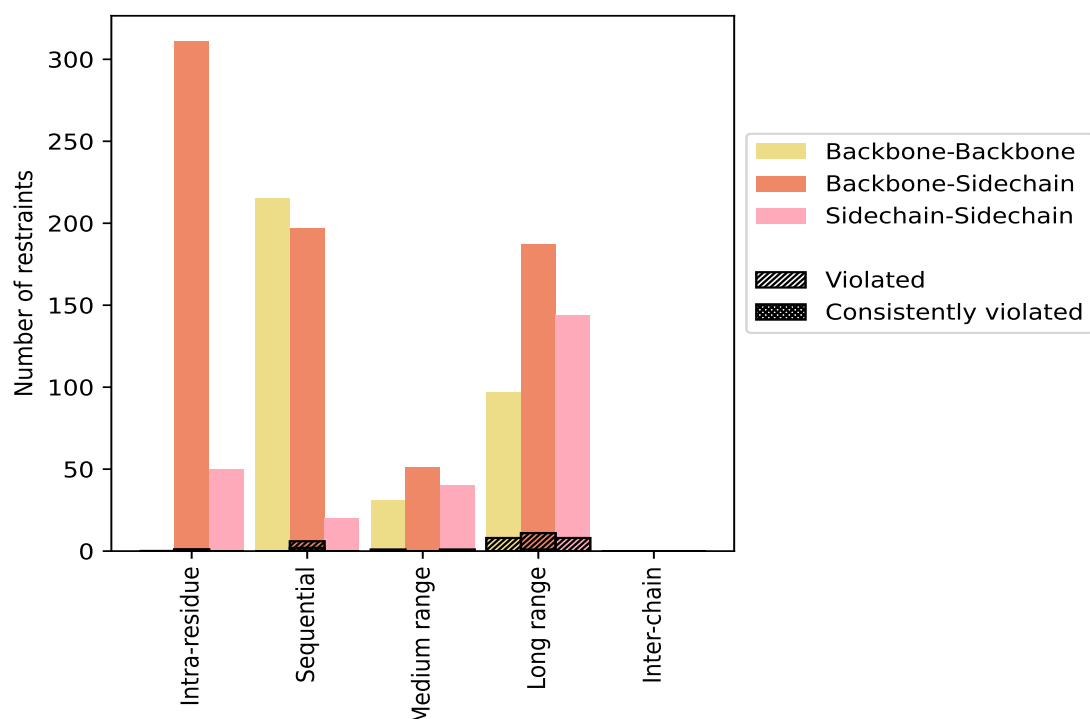
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	362	26.9	1	0.3	0.1	1	0.3	0.1
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	311	23.1	1	0.3	0.1	1	0.3	0.1
Sidechain-Sidechain	50	3.7	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	432	32.1	6	1.4	0.4	2	0.5	0.1
Backbone-Backbone	215	16.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	197	14.7	6	3.0	0.4	2	1.0	0.1
Sidechain-Sidechain	20	1.5	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	118	8.8	2	1.7	0.1	0	0.0	0.0
Backbone-Backbone	31	2.3	1	3.2	0.1	0	0.0	0.0
Backbone-Sidechain	47	3.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	40	3.0	1	2.5	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	395	29.4	22	5.6	1.6	1	0.3	0.1
Backbone-Backbone	97	7.2	8	8.2	0.6	0	0.0	0.0
Backbone-Sidechain	157	11.7	6	3.8	0.4	1	0.6	0.1
Sidechain-Sidechain	141	10.5	8	5.7	0.6	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	34	2.5	5	14.7	0.4	0	0.0	0.0
Disulfide bond	3	0.2	0	0.0	0.0	0	0.0	0.0
Total	1344	100.0	36	2.7	2.7	4	0.3	0.3
Backbone-Backbone	344	25.6	9	2.6	0.7	0	0.0	0.0
Backbone-Sidechain	746	55.5	18	2.4	1.3	4	0.5	0.3
Sidechain-Sidechain	254	18.9	9	3.5	0.7	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	1	2	0	9	0	12	0.13	0.16	0.02	0.13
2	1	4	1	8	0	14	0.13	0.17	0.02	0.13
3	1	3	0	13	0	17	0.13	0.18	0.02	0.12
4	1	4	0	9	0	14	0.13	0.17	0.02	0.12
5	1	2	0	9	0	12	0.13	0.17	0.02	0.12
6	1	4	1	8	0	14	0.12	0.15	0.02	0.12
7	1	4	0	9	0	14	0.13	0.15	0.01	0.12
8	1	4	0	10	0	15	0.12	0.16	0.02	0.12
9	1	4	0	7	0	12	0.12	0.14	0.01	0.12
10	1	3	0	12	0	16	0.13	0.16	0.02	0.12

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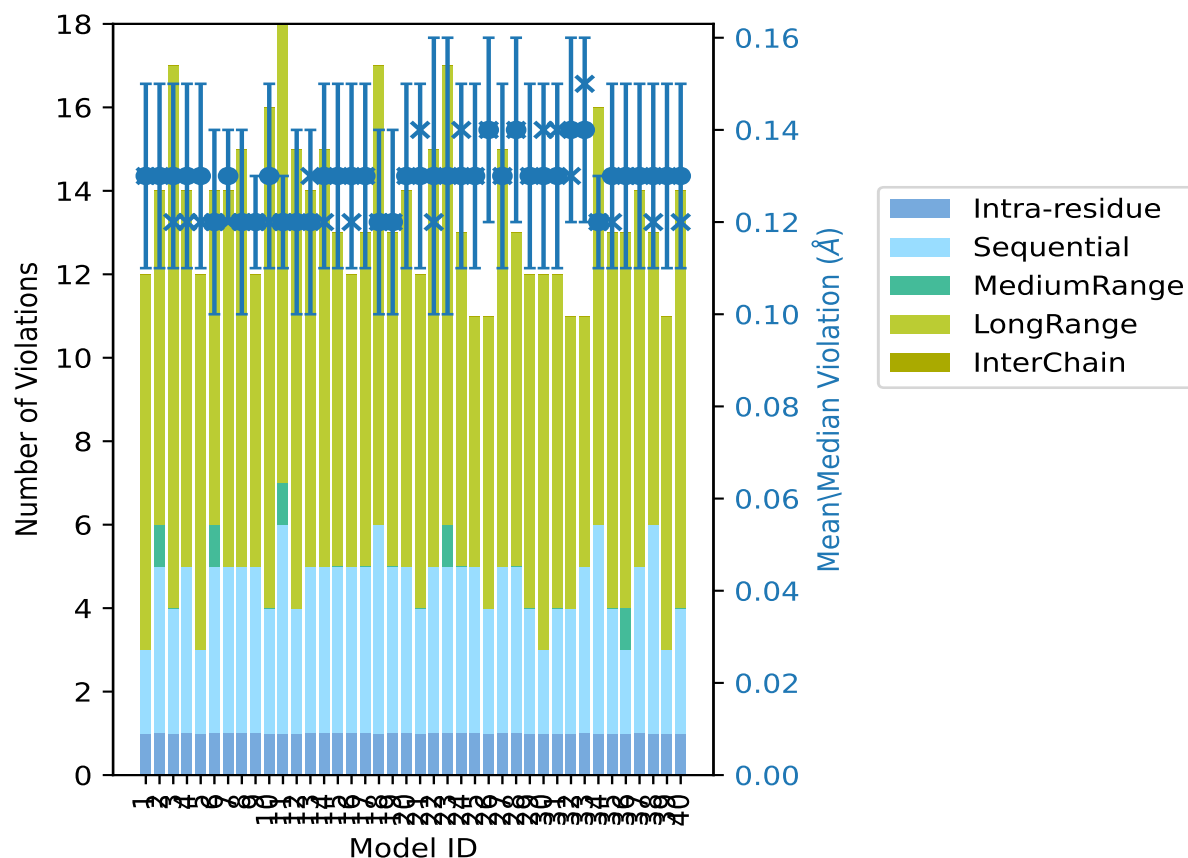
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	5	1	11	0	18	0.12	0.15	0.01	0.12
12	1	3	0	11	0	15	0.12	0.16	0.02	0.12
13	1	4	0	9	0	14	0.12	0.19	0.02	0.13
14	1	4	0	10	0	15	0.13	0.17	0.02	0.12
15	1	4	0	8	0	13	0.13	0.16	0.02	0.13
16	1	4	0	7	0	12	0.13	0.16	0.02	0.12
17	1	4	0	8	0	13	0.13	0.18	0.02	0.13
18	1	5	0	11	0	17	0.12	0.16	0.02	0.12
19	1	4	0	8	0	13	0.12	0.17	0.02	0.12
20	1	4	0	9	0	14	0.13	0.16	0.02	0.13
21	1	3	0	8	0	12	0.13	0.16	0.02	0.14
22	1	4	0	10	0	15	0.13	0.19	0.03	0.12
23	1	4	1	11	0	17	0.13	0.19	0.03	0.13
24	1	4	0	8	0	13	0.13	0.17	0.02	0.14
25	1	4	0	6	0	11	0.13	0.16	0.02	0.13
26	1	3	0	7	0	11	0.14	0.19	0.02	0.14
27	1	4	0	10	0	15	0.13	0.17	0.02	0.13
28	1	4	0	8	0	13	0.14	0.2	0.02	0.14
29	1	3	0	8	0	12	0.13	0.16	0.02	0.13
30	1	2	0	9	0	12	0.13	0.16	0.02	0.14
31	1	3	0	8	0	12	0.13	0.17	0.02	0.14
32	1	3	0	7	0	11	0.14	0.18	0.02	0.13
33	1	4	0	6	0	11	0.14	0.17	0.02	0.15
34	1	5	0	10	0	16	0.12	0.13	0.01	0.12
35	1	3	0	9	0	13	0.13	0.16	0.02	0.12
36	1	2	1	9	0	13	0.13	0.18	0.02	0.13
37	1	4	0	9	0	14	0.13	0.17	0.02	0.13
38	1	5	0	7	0	13	0.13	0.16	0.02	0.12
39	1	2	0	8	0	11	0.13	0.16	0.02	0.13
40	1	3	0	10	0	14	0.13	0.16	0.02	0.12

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1276(IR:361, SQ:426, MR:116, LR:373, 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	%
0	0	0	2	0	2	1	2.5
0	0	1	3	0	4	2	5.0
0	1	1	1	0	3	3	7.5
0	0	0	1	0	1	4	10.0
0	0	0	2	0	2	5	12.5
0	0	0	0	0	0	6	15.0

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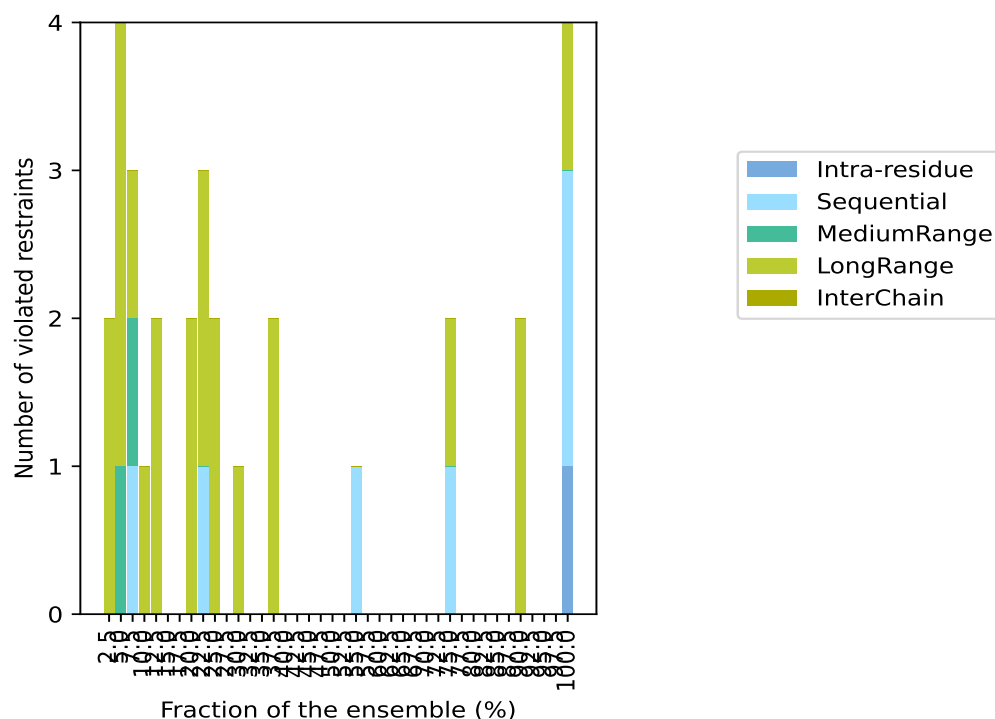
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	7	17.5
0	0	0	2	0	2	8	20.0
0	1	0	2	0	3	9	22.5
0	0	0	2	0	2	10	25.0
0	0	0	0	0	0	11	27.5
0	0	0	1	0	1	12	30.0
0	0	0	0	0	0	13	32.5
0	0	0	0	0	0	14	35.0
0	0	0	2	0	2	15	37.5
0	0	0	0	0	0	16	40.0
0	0	0	0	0	0	17	42.5
0	0	0	0	0	0	18	45.0
0	0	0	0	0	0	19	47.5
0	0	0	0	0	0	20	50.0
0	0	0	0	0	0	21	52.5
0	1	0	0	0	1	22	55.0
0	0	0	0	0	0	23	57.5
0	0	0	0	0	0	24	60.0
0	0	0	0	0	0	25	62.5
0	0	0	0	0	0	26	65.0
0	0	0	0	0	0	27	67.5
0	0	0	0	0	0	28	70.0
0	0	0	0	0	0	29	72.5
0	1	0	1	0	2	30	75.0
0	0	0	0	0	0	31	77.5
0	0	0	0	0	0	32	80.0
0	0	0	0	0	0	33	82.5
0	0	0	0	0	0	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	2	0	2	36	90.0
0	0	0	0	0	0	37	92.5
0	0	0	0	0	0	38	95.0
0	0	0	0	0	0	39	97.5
1	2	0	1	0	4	40	100.0

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

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

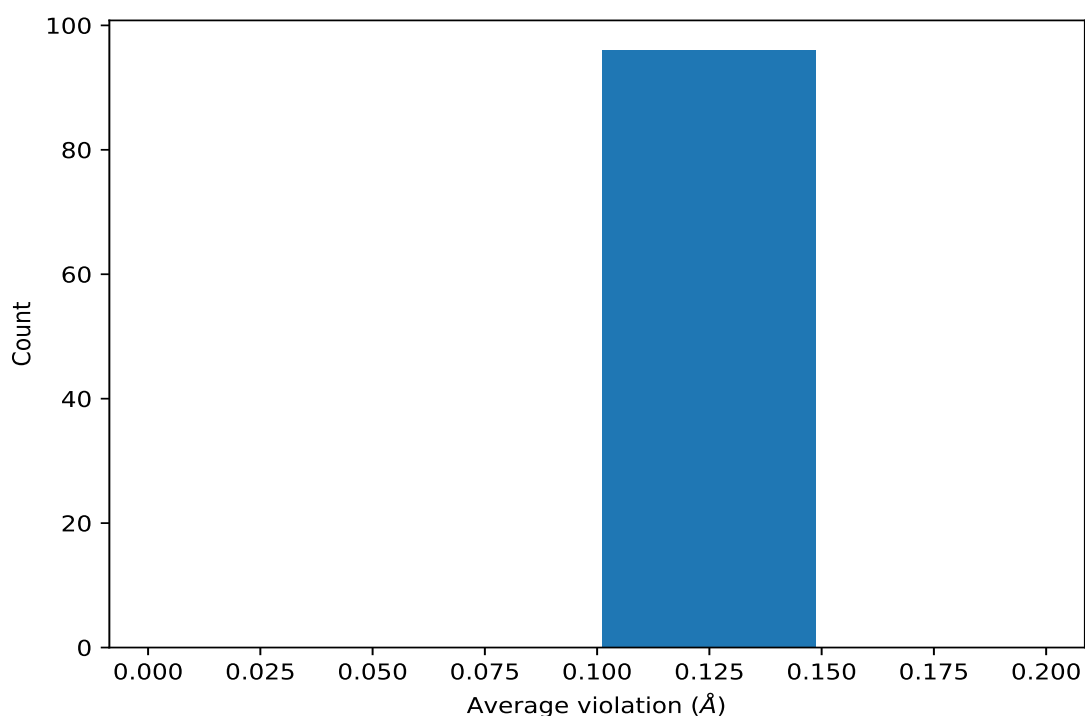
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	40	0.15	0.02	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	40	0.15	0.02	0.16
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	40	0.14	0.01	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	40	0.13	0.01	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	40	0.13	0.01	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	40	0.13	0.01	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	40	0.13	0.01	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	36	0.13	0.02	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	36	0.13	0.02	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	36	0.13	0.02	0.13
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	36	0.12	0.02	0.12
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	36	0.12	0.02	0.12
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	30	0.13	0.02	0.13
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	30	0.13	0.02	0.13
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	30	0.13	0.02	0.13
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	30	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	30	0.13	0.02	0.12
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	30	0.13	0.02	0.12
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	30	0.13	0.02	0.12
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	30	0.13	0.02	0.12
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	30	0.13	0.02	0.12
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	29	0.13	0.02	0.14
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	25	0.13	0.03	0.12
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	24	0.14	0.02	0.14
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	22	0.11	0.01	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	22	0.11	0.01	0.11
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	15	0.11	0.01	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	15	0.11	0.01	0.12
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	15	0.11	0.01	0.11
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	12	0.11	0.01	0.11
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	10	0.12	0.01	0.12
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	10	0.12	0.02	0.11
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	9	0.12	0.01	0.12
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	9	0.12	0.01	0.12
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	9	0.12	0.01	0.12
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	9	0.12	0.01	0.12
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	9	0.12	0.01	0.12
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	9	0.12	0.01	0.12
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	9	0.11	0.01	0.11
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	9	0.11	0.01	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	9	0.11	0.0	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	9	0.11	0.0	0.11
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	8	0.12	0.0	0.12
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	8	0.11	0.01	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	8	0.11	0.01	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	8	0.11	0.01	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	8	0.11	0.01	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	8	0.11	0.01	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	8	0.11	0.01	0.11
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	8	0.11	0.01	0.11
(2,11)	1:24:A:CYS:H	1:32:A:LEU:O	5	0.12	0.02	0.12
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE1	5	0.12	0.01	0.12
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE2	5	0.12	0.01	0.12
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD1	5	0.11	0.02	0.1
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD2	5	0.11	0.02	0.1
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD1	5	0.11	0.02	0.1
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD2	5	0.11	0.02	0.1
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD1	5	0.11	0.02	0.1

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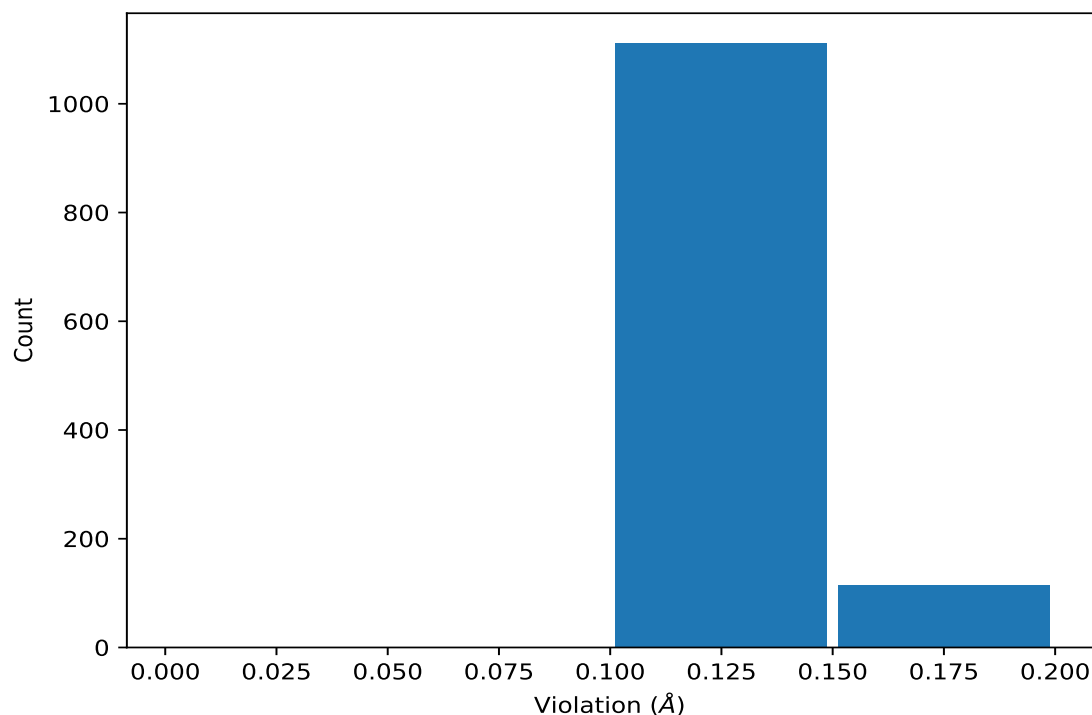
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD2	5	0.11	0.02	0.1
(1,114)	1:21:A:SER:HA	1:36:A:LEU:H	4	0.11	0.01	0.11
(1,764)	1:19:A:ILE:HG21	1:21:A:SER:HB2	3	0.13	0.02	0.14
(1,764)	1:19:A:ILE:HG21	1:21:A:SER:HB3	3	0.13	0.02	0.14
(1,764)	1:19:A:ILE:HG22	1:21:A:SER:HB2	3	0.13	0.02	0.14
(1,764)	1:19:A:ILE:HG22	1:21:A:SER:HB3	3	0.13	0.02	0.14
(1,764)	1:19:A:ILE:HG23	1:21:A:SER:HB2	3	0.13	0.02	0.14
(1,764)	1:19:A:ILE:HG23	1:21:A:SER:HB3	3	0.13	0.02	0.14
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD11	3	0.1	0.0	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD12	3	0.1	0.0	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD13	3	0.1	0.0	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD21	3	0.1	0.0	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD22	3	0.1	0.0	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD23	3	0.1	0.0	0.1
(1,225)	1:41:A:HIS:HB2	1:42:A:ILE:H	3	0.1	0.0	0.1
(1,225)	1:41:A:HIS:HB3	1:42:A:ILE:H	3	0.1	0.0	0.1
(1,750)	1:18:A:THR:HB	1:38:A:LEU:HB2	2	0.12	0.0	0.12
(1,750)	1:18:A:THR:HB	1:38:A:LEU:HB3	2	0.12	0.0	0.12
(1,772)	1:19:A:ILE:HA	1:38:A:LEU:H	2	0.12	0.0	0.12
(1,332)	1:55:A:ASN:HA	1:57:A:GLN:H	2	0.11	0.01	0.11
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD11	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD12	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD13	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD11	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD12	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD13	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD11	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD12	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD13	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD11	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD12	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD13	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD11	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD12	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD13	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD11	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD12	2	0.11	0.0	0.11
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD13	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	28	0.2
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	22	0.19
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	26	0.19
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	13	0.19
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	13	0.19
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	23	0.19
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	23	0.19
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	32	0.18
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	36	0.18
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	23	0.18
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	23	0.18
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	23	0.18
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	23	0.18
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	23	0.18
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	23	0.18
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	32	0.18
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	32	0.18
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	32	0.18
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	3	0.18
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	3	0.18
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	33	0.17
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	37	0.17
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	22	0.17
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	22	0.17
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	22	0.17
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	22	0.17
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	22	0.17
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	22	0.17
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	4	0.17
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	4	0.17
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	4	0.17
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	27	0.17
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	27	0.17
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	27	0.17
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	31	0.17
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	31	0.17
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	31	0.17
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	19	0.17
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	19	0.17
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	2	0.17
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	2	0.17
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	2	0.17
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	2	0.17
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	2	0.17
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	5	0.17
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	5	0.17
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	14	0.17
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	14	0.17
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	24	0.17
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	24	0.17
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	25	0.16
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	30	0.16
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	38	0.16
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	5	0.16
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	17	0.16
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	23	0.16
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	40	0.16
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	10	0.16
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	10	0.16
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	10	0.16
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	10	0.16
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	10	0.16
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	10	0.16
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	16	0.16
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	16	0.16
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	16	0.16
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	22	0.16
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	22	0.16
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	22	0.16
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	33	0.16
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	33	0.16
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	33	0.16
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	17	0.16
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	17	0.16
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	39	0.16
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	39	0.16
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	12	0.16
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	12	0.16
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	14	0.16
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	14	0.16
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	14	0.16
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	29	0.16
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	29	0.16
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	29	0.16
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	26	0.16
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	26	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	1	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	1	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	8	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	8	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	10	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	16	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	16	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	18	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	18	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	20	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	20	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	21	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	21	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	22	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	22	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	30	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	30	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	33	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	33	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	35	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	35	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	37	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	37	0.16
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	38	0.16
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	38	0.16
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	24	0.15
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	33	0.15
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	37	0.15
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	39	0.15
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	40	0.15
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	1	0.15
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	8	0.15
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	10	0.15
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	12	0.15
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	22	0.15
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	30	0.15
(2,11)	1:24:A:CYS:H	1:32:A:LEU:O	37	0.15
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	4	0.15
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	20	0.15
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	24	0.15
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	5	0.15
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	5	0.15
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	5	0.15
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	5	0.15
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	5	0.15
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	5	0.15
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	33	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	33	0.15
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	33	0.15
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	33	0.15
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	33	0.15
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	33	0.15
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	36	0.15
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	36	0.15
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	36	0.15
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	36	0.15
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	36	0.15
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	36	0.15
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	40	0.15
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	40	0.15
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	40	0.15
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	40	0.15
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	40	0.15
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	40	0.15
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	6	0.15
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	6	0.15
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	6	0.15
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	7	0.15
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	7	0.15
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	7	0.15
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	11	0.15
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	11	0.15
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	11	0.15
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	15	0.15
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	15	0.15
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	15	0.15
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	20	0.15
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	20	0.15
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	20	0.15
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	28	0.15
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	28	0.15
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	28	0.15
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	10	0.15
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	10	0.15
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	13	0.15
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	13	0.15
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	30	0.15
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	30	0.15
(1,764)	1:19:A:ILE:HG21	1:21:A:SER:HB2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,764)	1:19:A:ILE:HG21	1:21:A:SER:HB3	2	0.15
(1,764)	1:19:A:ILE:HG22	1:21:A:SER:HB2	2	0.15
(1,764)	1:19:A:ILE:HG22	1:21:A:SER:HB3	2	0.15
(1,764)	1:19:A:ILE:HG23	1:21:A:SER:HB2	2	0.15
(1,764)	1:19:A:ILE:HG23	1:21:A:SER:HB3	2	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	1	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	8	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	10	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	12	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	15	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	22	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	23	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	25	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	26	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	27	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	33	0.15
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	35	0.15
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	10	0.15
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	10	0.15
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	31	0.15
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	31	0.15
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	39	0.15
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	39	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	2	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	2	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	2	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	18	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	18	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	18	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	25	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	25	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	25	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	35	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	35	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	35	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	36	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	36	0.15
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	36	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	18	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	18	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	25	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	25	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	27	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	27	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	30	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	30	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	35	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	35	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	38	0.15
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	38	0.15
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	6	0.15
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	6	0.15
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	7	0.15
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	7	0.15
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	11	0.15
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	11	0.15
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	17	0.15
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	17	0.15
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	28	0.15
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	28	0.15
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	32	0.15
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	32	0.15
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	40	0.15
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	40	0.15
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	18	0.14
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	21	0.14
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	23	0.14
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	31	0.14
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	4	0.14
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	28	0.14
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	1	0.14
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	1	0.14
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	1	0.14
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	1	0.14
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	1	0.14
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	1	0.14
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	30	0.14
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	30	0.14
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	30	0.14
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	30	0.14
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	30	0.14
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	30	0.14
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	37	0.14
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	37	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	37	0.14
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	37	0.14
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	37	0.14
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	37	0.14
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	26	0.14
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	26	0.14
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	26	0.14
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	32	0.14
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	32	0.14
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	32	0.14
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	12	0.14
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	12	0.14
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	36	0.14
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	36	0.14
(1,764)	1:19:A:ILE:HG21	1:21:A:SER:HB2	23	0.14
(1,764)	1:19:A:ILE:HG21	1:21:A:SER:HB3	23	0.14
(1,764)	1:19:A:ILE:HG22	1:21:A:SER:HB2	23	0.14
(1,764)	1:19:A:ILE:HG22	1:21:A:SER:HB3	23	0.14
(1,764)	1:19:A:ILE:HG23	1:21:A:SER:HB2	23	0.14
(1,764)	1:19:A:ILE:HG23	1:21:A:SER:HB3	23	0.14
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	26	0.14
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	26	0.14
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	26	0.14
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	26	0.14
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	26	0.14
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	26	0.14
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	29	0.14
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	29	0.14
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	29	0.14
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	29	0.14
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	29	0.14
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	29	0.14
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD1	10	0.14
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD2	10	0.14
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD1	10	0.14
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD2	10	0.14
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD1	10	0.14
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD2	10	0.14
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	2	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	3	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	4	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	6	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	7	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	9	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	14	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	16	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	17	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	20	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	21	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	24	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	28	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	30	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	31	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	36	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	39	0.14
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	40	0.14
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	19	0.14
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	19	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	5	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	5	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	7	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	7	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	9	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	9	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	13	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	13	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	18	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	18	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	21	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	21	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	23	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	23	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	24	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	24	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	27	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	27	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	29	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	29	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	33	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	33	0.14
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	40	0.14
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	40	0.14
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	3	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	3	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	3	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	11	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	11	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	11	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	15	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	15	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	15	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	21	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	21	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	21	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	24	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	24	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	24	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	28	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	28	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	28	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	31	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	31	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	31	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	37	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	37	0.14
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	37	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	1	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	1	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	6	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	6	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	13	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	13	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	14	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	14	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	16	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	16	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	17	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	17	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	21	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	21	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	24	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	24	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	28	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	28	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	29	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	29	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	32	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	32	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	39	0.14
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	39	0.14
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	19	0.14
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	28	0.14
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	4	0.14
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	4	0.14
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	9	0.14
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	9	0.14
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	15	0.14
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	15	0.14
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	25	0.14
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	25	0.14
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	26	0.14
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	26	0.14
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	27	0.14
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	27	0.14
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	31	0.14
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	31	0.14
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	36	0.14
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	36	0.14
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	3	0.13
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	13	0.13
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	27	0.13
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	29	0.13
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	34	0.13
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	9	0.13
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	20	0.13
(2,11)	1:24:A:CYS:H	1:32:A:LEU:O	5	0.13
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	7	0.13
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	8	0.13
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	11	0.13
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	38	0.13
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	8	0.13
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	8	0.13
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	8	0.13
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	8	0.13
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	8	0.13
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	9	0.13
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	9	0.13
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	9	0.13
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	9	0.13
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	9	0.13
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	9	0.13
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	12	0.13
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	12	0.13
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	12	0.13
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	12	0.13
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	12	0.13
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	12	0.13
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	27	0.13
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	27	0.13
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	27	0.13
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	27	0.13
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	27	0.13
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	27	0.13
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	28	0.13
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	28	0.13
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	28	0.13
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	28	0.13
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	28	0.13
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	28	0.13
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	3	0.13
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	3	0.13
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	3	0.13
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	8	0.13
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	8	0.13
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	8	0.13
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	38	0.13
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	38	0.13
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	38	0.13
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	40	0.13
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	40	0.13
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	40	0.13
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	2	0.13
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	2	0.13
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	15	0.13
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	15	0.13
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	21	0.13
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	24	0.13
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	24	0.13
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	25	0.13
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	25	0.13
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	26	0.13
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	26	0.13
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	33	0.13
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	33	0.13
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	35	0.13
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	35	0.13
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD1	27	0.13
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD2	27	0.13
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD1	27	0.13
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD2	27	0.13
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD1	27	0.13
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD2	27	0.13
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE1	1	0.13
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE2	1	0.13
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	11	0.13
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	2	0.13
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	11	0.13
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	13	0.13
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	18	0.13
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	29	0.13
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	32	0.13
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	34	0.13
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	37	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	3	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	3	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	6	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	6	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	14	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	14	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	15	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	15	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	16	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	16	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	17	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	17	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	20	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	20	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	25	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	25	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	26	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	26	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	32	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	32	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	35	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	35	0.13
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	37	0.13
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	37	0.13
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	1	0.13
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	13	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	7	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	7	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	7	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	10	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	10	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	10	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	13	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	13	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	13	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	16	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	16	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	16	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	23	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	23	0.13
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	23	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	8	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	8	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	12	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	12	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	19	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	19	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	23	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	23	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	31	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	31	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	34	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	34	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	36	0.13
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	36	0.13
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	31	0.13
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	12	0.13
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	12	0.13
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	29	0.13
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	29	0.13
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	34	0.13
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	34	0.13
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	39	0.13
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	39	0.13
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	20	0.13
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	20	0.13
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	23	0.13
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	23	0.13
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	6	0.12
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	12	0.12
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	14	0.12
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	18	0.12
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	23	0.12
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	37	0.12
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	40	0.12
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	3	0.12
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	7	0.12
(2,11)	1:24:A:CYS:H	1:32:A:LEU:O	14	0.12
(2,11)	1:24:A:CYS:H	1:32:A:LEU:O	18	0.12
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	1	0.12
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	3	0.12
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	23	0.12
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	32	0.12
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	34	0.12
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	40	0.12
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	2	0.12
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	2	0.12
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	2	0.12
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	2	0.12
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	2	0.12
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	2	0.12
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	7	0.12
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	7	0.12
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	7	0.12
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	7	0.12
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	7	0.12
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	7	0.12
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	35	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	35	0.12
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	35	0.12
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	35	0.12
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	35	0.12
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	35	0.12
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	9	0.12
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	9	0.12
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	9	0.12
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	14	0.12
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	14	0.12
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	14	0.12
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	25	0.12
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	25	0.12
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	25	0.12
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	29	0.12
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	29	0.12
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	29	0.12
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	3	0.12
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	3	0.12
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	7	0.12
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	7	0.12
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	8	0.12
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	8	0.12
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	14	0.12
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	14	0.12
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	18	0.12
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	18	0.12
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	32	0.12
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	32	0.12
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	37	0.12
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	37	0.12
(1,772)	1:19:A:ILE:HA	1:38:A:LEU:H	17	0.12
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	12	0.12
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	12	0.12
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	12	0.12
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	12	0.12
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	12	0.12
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	12	0.12
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	36	0.12
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	36	0.12
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	36	0.12
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	36	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	36	0.12
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	36	0.12
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	39	0.12
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	39	0.12
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	39	0.12
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	39	0.12
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	39	0.12
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	39	0.12
(1,750)	1:18:A:THR:HB	1:38:A:LEU:HB2	28	0.12
(1,750)	1:18:A:THR:HB	1:38:A:LEU:HB3	28	0.12
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE1	19	0.12
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE2	19	0.12
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE1	34	0.12
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE2	34	0.12
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	3	0.12
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	4	0.12
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	39	0.12
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	10	0.12
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	10	0.12
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	10	0.12
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	10	0.12
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	10	0.12
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	10	0.12
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	12	0.12
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	12	0.12
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	12	0.12
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	12	0.12
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	12	0.12
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	12	0.12
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	19	0.12
(1,551)	1:90:A:THR:HB	1:90:A:THR:H	38	0.12
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	34	0.12
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	34	0.12
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	18	0.12
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	39	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	1	0.12
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	1	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	4	0.12
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	4	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	8	0.12
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	8	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	11	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	19	0.12
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	19	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	28	0.12
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	28	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	30	0.12
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	30	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	34	0.12
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	34	0.12
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	38	0.12
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	38	0.12
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	3	0.12
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	5	0.12
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	17	0.12
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	24	0.12
(1,404)	1:64:A:ARG:H	1:78:A:CYS:HA	22	0.12
(1,332)	1:55:A:ASN:HA	1:57:A:GLN:H	11	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	4	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	4	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	4	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	5	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	5	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	5	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	6	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	6	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	6	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	17	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	17	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	17	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	19	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	19	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	19	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	27	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	27	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	27	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	34	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	34	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	34	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	38	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	38	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	38	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	39	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	39	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	39	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	40	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	40	0.12
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	40	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	3	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	3	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	5	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	5	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	7	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	7	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	9	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	9	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	10	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	10	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	11	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	11	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	15	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	15	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	20	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	20	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	22	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	22	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	33	0.12
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	33	0.12
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	15	0.12
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	24	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	1	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	1	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	4	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	4	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	7	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	7	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	19	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	19	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	20	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	20	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	21	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	21	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	26	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	26	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	36	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	36	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	40	0.12
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	40	0.12
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	3	0.12
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	22	0.12
(1,114)	1:21:A:SER:HA	1:36:A:LEU:H	3	0.12
(1,111)	1:21:A:SER:HB2	1:22:A:ALA:H	19	0.12
(1,111)	1:21:A:SER:HB3	1:22:A:ALA:H	19	0.12
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	14	0.12
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	14	0.12
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	15	0.12
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	15	0.12
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	17	0.12
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	17	0.12
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	24	0.12
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	24	0.12
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	11	0.11
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	22	0.11
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	32	0.11
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	35	0.11
(2,22)	1:66:A:GLU:O	1:75:A:TRP:H	38	0.11
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	6	0.11
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	13	0.11
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	14	0.11
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	16	0.11
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	26	0.11
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	27	0.11
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	16	0.11
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	19	0.11
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	35	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	4	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	4	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	14	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	14	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	24	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	24	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	28	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	28	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	33	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	33	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	34	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	34	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	40	0.11
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	40	0.11
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	11	0.11
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	11	0.11
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	11	0.11
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	11	0.11
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	11	0.11
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	11	0.11
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	14	0.11
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	14	0.11
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	14	0.11
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	14	0.11
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	14	0.11
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	14	0.11
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	21	0.11
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	21	0.11
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	21	0.11
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	21	0.11
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	21	0.11
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	21	0.11
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	25	0.11
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	25	0.11
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	25	0.11
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	25	0.11
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	25	0.11
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	25	0.11
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	29	0.11
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	29	0.11
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	29	0.11
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	29	0.11
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	29	0.11
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	29	0.11
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	31	0.11
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	31	0.11
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	31	0.11
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	31	0.11
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	31	0.11
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	31	0.11
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	34	0.11
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	34	0.11
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	34	0.11
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	34	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	34	0.11
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	34	0.11
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	38	0.11
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	38	0.11
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	38	0.11
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	38	0.11
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	38	0.11
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	38	0.11
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD11	11	0.11
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD12	11	0.11
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD13	11	0.11
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD11	11	0.11
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD12	11	0.11
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD13	11	0.11
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD11	11	0.11
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD12	11	0.11
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD13	11	0.11
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD11	11	0.11
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD12	11	0.11
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD13	11	0.11
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD11	11	0.11
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD12	11	0.11
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD13	11	0.11
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD11	11	0.11
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD12	11	0.11
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD13	11	0.11
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	12	0.11
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	12	0.11
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	12	0.11
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	34	0.11
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	34	0.11
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	34	0.11
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	1	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	1	0.11
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	5	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	5	0.11
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	6	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	6	0.11
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	9	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	9	0.11
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	16	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	27	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	27	0.11
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	29	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	29	0.11
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	31	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	31	0.11
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	34	0.11
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	34	0.11
(1,772)	1:19:A:ILE:HA	1:38:A:LEU:H	18	0.11
(1,764)	1:19:A:ILE:HG21	1:21:A:SER:HB2	36	0.11
(1,764)	1:19:A:ILE:HG21	1:21:A:SER:HB3	36	0.11
(1,764)	1:19:A:ILE:HG22	1:21:A:SER:HB2	36	0.11
(1,764)	1:19:A:ILE:HG22	1:21:A:SER:HB3	36	0.11
(1,764)	1:19:A:ILE:HG23	1:21:A:SER:HB2	36	0.11
(1,764)	1:19:A:ILE:HG23	1:21:A:SER:HB3	36	0.11
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	10	0.11
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	10	0.11
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	10	0.11
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	10	0.11
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	10	0.11
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	10	0.11
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	15	0.11
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	15	0.11
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	15	0.11
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	15	0.11
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	15	0.11
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	15	0.11
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	30	0.11
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	30	0.11
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	30	0.11
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	30	0.11
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	30	0.11
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	30	0.11
(1,750)	1:18:A:THR:HB	1:38:A:LEU:HB2	30	0.11
(1,750)	1:18:A:THR:HB	1:38:A:LEU:HB3	30	0.11
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE1	3	0.11
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE2	3	0.11
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD11	14	0.11
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD12	14	0.11
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD13	14	0.11
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD21	14	0.11
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD22	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD23	14	0.11
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	5	0.11
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	17	0.11
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	30	0.11
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	32	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	6	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	6	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	6	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	6	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	6	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	6	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	18	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	18	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	18	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	18	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	18	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	18	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	27	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	27	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	27	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	27	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	27	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	27	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	37	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	37	0.11
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	37	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	37	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	37	0.11
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	37	0.11
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	2	0.11
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	2	0.11
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	4	0.11
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	4	0.11
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	9	0.11
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	9	0.11
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	11	0.11
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	11	0.11
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	38	0.11
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	38	0.11
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	10	0.11
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	25	0.11
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	27	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	2	0.11
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	2	0.11
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	10	0.11
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	11	0.11
(1,413)	1:65:A:LEU:HA	1:77:A:VAL:H	12	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	8	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	8	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	8	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	9	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	9	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	9	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	20	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	20	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	20	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	22	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	22	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	22	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD11	30	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD12	30	0.11
(1,311)	1:51:A:PHE:H	1:92:A:ILE:HD13	30	0.11
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	4	0.11
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	4	0.11
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	40	0.11
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	40	0.11
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	21	0.11
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	23	0.11
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	29	0.11
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	35	0.11
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	3	0.11
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	3	0.11
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	5	0.11
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	5	0.11
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	35	0.11
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	35	0.11
(1,225)	1:41:A:HIS:HB2	1:42:A:ILE:H	23	0.11
(1,225)	1:41:A:HIS:HB3	1:42:A:ILE:H	23	0.11
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	1	0.11
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	2	0.11
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	11	0.11
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	20	0.11
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	23	0.11
(1,114)	1:21:A:SER:HA	1:36:A:LEU:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:21:A:SER:HA	1:36:A:LEU:H	16	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	6	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	6	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	7	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	7	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	10	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	10	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	11	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	11	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	16	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	16	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	19	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	19	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	25	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	25	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	27	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	27	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	33	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	33	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	34	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	34	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	37	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	37	0.11
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	38	0.11
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	38	0.11
(2,29)	1:99:A:ASP:H	1:106:A:GLU:O	26	0.1
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	18	0.1
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	34	0.1
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	38	0.1
(2,14)	1:43:A:GLY:O	1:50:A:GLN:H	39	0.1
(2,11)	1:24:A:CYS:H	1:32:A:LEU:O	21	0.1
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	2	0.1
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	13	0.1
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	15	0.1
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	27	0.1
(2,5)	1:14:A:ASP:O	1:19:A:ILE:H	29	0.1
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	8	0.1
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	8	0.1
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB2	9	0.1
(1,1066)	1:59:A:THR:HB	1:81:A:GLN:HB3	9	0.1
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	3	0.1
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	3	0.1
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	3	0.1
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	3	0.1
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	3	0.1
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	4	0.1
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	4	0.1
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	4	0.1
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	4	0.1
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	4	0.1
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	4	0.1
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	6	0.1
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	6	0.1
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	6	0.1
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	6	0.1
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	6	0.1
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	6	0.1
(1,1017)	1:49:A:LEU:HD11	1:91:A:GLN:HA	18	0.1
(1,1017)	1:49:A:LEU:HD12	1:91:A:GLN:HA	18	0.1
(1,1017)	1:49:A:LEU:HD13	1:91:A:GLN:HA	18	0.1
(1,1017)	1:49:A:LEU:HD21	1:91:A:GLN:HA	18	0.1
(1,1017)	1:49:A:LEU:HD22	1:91:A:GLN:HA	18	0.1
(1,1017)	1:49:A:LEU:HD23	1:91:A:GLN:HA	18	0.1
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD11	10	0.1
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD12	10	0.1
(1,917)	1:38:A:LEU:HD11	1:98:A:ILE:HD13	10	0.1
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD11	10	0.1
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD12	10	0.1
(1,917)	1:38:A:LEU:HD12	1:98:A:ILE:HD13	10	0.1
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD11	10	0.1
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD12	10	0.1
(1,917)	1:38:A:LEU:HD13	1:98:A:ILE:HD13	10	0.1
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD11	10	0.1
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD12	10	0.1
(1,917)	1:38:A:LEU:HD21	1:98:A:ILE:HD13	10	0.1
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD11	10	0.1
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD12	10	0.1
(1,917)	1:38:A:LEU:HD22	1:98:A:ILE:HD13	10	0.1
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD11	10	0.1
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD12	10	0.1
(1,917)	1:38:A:LEU:HD23	1:98:A:ILE:HD13	10	0.1
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	13	0.1
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	13	0.1
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	17	0.1
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	17	0.1
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	17	0.1
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	18	0.1
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	18	0.1
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	18	0.1
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	21	0.1
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	21	0.1
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	21	0.1
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	24	0.1
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	24	0.1
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	24	0.1
(1,873)	1:34:A:THR:HG21	1:35:A:GLU:HA	35	0.1
(1,873)	1:34:A:THR:HG22	1:35:A:GLU:HA	35	0.1
(1,873)	1:34:A:THR:HG23	1:35:A:GLU:HA	35	0.1
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	4	0.1
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	4	0.1
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	20	0.1
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	20	0.1
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	23	0.1
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	23	0.1
(1,792)	1:21:A:SER:HB2	1:35:A:GLU:HA	40	0.1
(1,792)	1:21:A:SER:HB3	1:35:A:GLU:HA	40	0.1
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB2	22	0.1
(1,752)	1:18:A:THR:HG21	1:39:A:SER:HB3	22	0.1
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB2	22	0.1
(1,752)	1:18:A:THR:HG22	1:39:A:SER:HB3	22	0.1
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB2	22	0.1
(1,752)	1:18:A:THR:HG23	1:39:A:SER:HB3	22	0.1
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD1	12	0.1
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD2	12	0.1
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD1	12	0.1
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD2	12	0.1
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD1	12	0.1
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD2	12	0.1
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD1	13	0.1
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD2	13	0.1
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD1	13	0.1
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD2	13	0.1
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD1	13	0.1
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD2	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD1	14	0.1
(1,691)	1:11:A:ILE:HD11	1:67:A:PHE:HD2	14	0.1
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD1	14	0.1
(1,691)	1:11:A:ILE:HD12	1:67:A:PHE:HD2	14	0.1
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD1	14	0.1
(1,691)	1:11:A:ILE:HD13	1:67:A:PHE:HD2	14	0.1
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE1	9	0.1
(1,689)	1:11:A:ILE:HB	1:67:A:PHE:HE2	9	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD11	7	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD12	7	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD13	7	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD21	7	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD22	7	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD23	7	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD11	20	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD12	20	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD13	20	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD21	20	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD22	20	0.1
(1,681)	1:11:A:ILE:HB	1:20:A:LEU:HD23	20	0.1
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	8	0.1
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	10	0.1
(1,640)	1:4:A:PHE:HA	1:99:A:ASP:HA	36	0.1
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	13	0.1
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	13	0.1
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	13	0.1
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	13	0.1
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	13	0.1
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	13	0.1
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD11	23	0.1
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD12	23	0.1
(1,632)	1:4:A:PHE:HD1	1:11:A:ILE:HD13	23	0.1
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD11	23	0.1
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD12	23	0.1
(1,632)	1:4:A:PHE:HD2	1:11:A:ILE:HD13	23	0.1
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	18	0.1
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	18	0.1
(1,549)	1:89:A:SER:HB2	1:90:A:THR:H	37	0.1
(1,549)	1:89:A:SER:HB3	1:90:A:THR:H	37	0.1
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	12	0.1
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	31	0.1
(1,463)	1:76:A:LEU:H	1:92:A:ILE:H	36	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	22	0.1
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	22	0.1
(1,417)	1:66:A:GLU:HG2	1:67:A:PHE:H	36	0.1
(1,417)	1:66:A:GLU:HG3	1:67:A:PHE:H	36	0.1
(1,332)	1:55:A:ASN:HA	1:57:A:GLN:H	6	0.1
(1,294)	1:49:A:LEU:HD11	1:56:A:PHE:H	35	0.1
(1,294)	1:49:A:LEU:HD12	1:56:A:PHE:H	35	0.1
(1,294)	1:49:A:LEU:HD13	1:56:A:PHE:H	35	0.1
(1,294)	1:49:A:LEU:HD21	1:56:A:PHE:H	35	0.1
(1,294)	1:49:A:LEU:HD22	1:56:A:PHE:H	35	0.1
(1,294)	1:49:A:LEU:HD23	1:56:A:PHE:H	35	0.1
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG2	37	0.1
(1,270)	1:46:A:ASP:H	1:83:A:MET:HG3	37	0.1
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	11	0.1
(1,255)	1:44:A:ASN:H	1:56:A:PHE:H	19	0.1
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	12	0.1
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	12	0.1
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	22	0.1
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	22	0.1
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG2	31	0.1
(1,242)	1:43:A:GLY:H	1:50:A:GLN:HG3	31	0.1
(1,225)	1:41:A:HIS:HB2	1:42:A:ILE:H	2	0.1
(1,225)	1:41:A:HIS:HB3	1:42:A:ILE:H	2	0.1
(1,225)	1:41:A:HIS:HB2	1:42:A:ILE:H	22	0.1
(1,225)	1:41:A:HIS:HB3	1:42:A:ILE:H	22	0.1
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	6	0.1
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	8	0.1
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	15	0.1
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	16	0.1
(1,142)	1:25:A:GLN:HA	1:32:A:LEU:H	34	0.1
(1,114)	1:21:A:SER:HA	1:36:A:LEU:H	11	0.1
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	8	0.1
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	8	0.1
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	13	0.1
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	13	0.1
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	18	0.1
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	18	0.1
(1,1)	1:2:A:PRO:HB2	1:3:A:ASN:H	28	0.1
(1,1)	1:2:A:PRO:HB3	1:3:A:ASN:H	28	0.1

10 Dihedral-angle violation analysis ⓘ

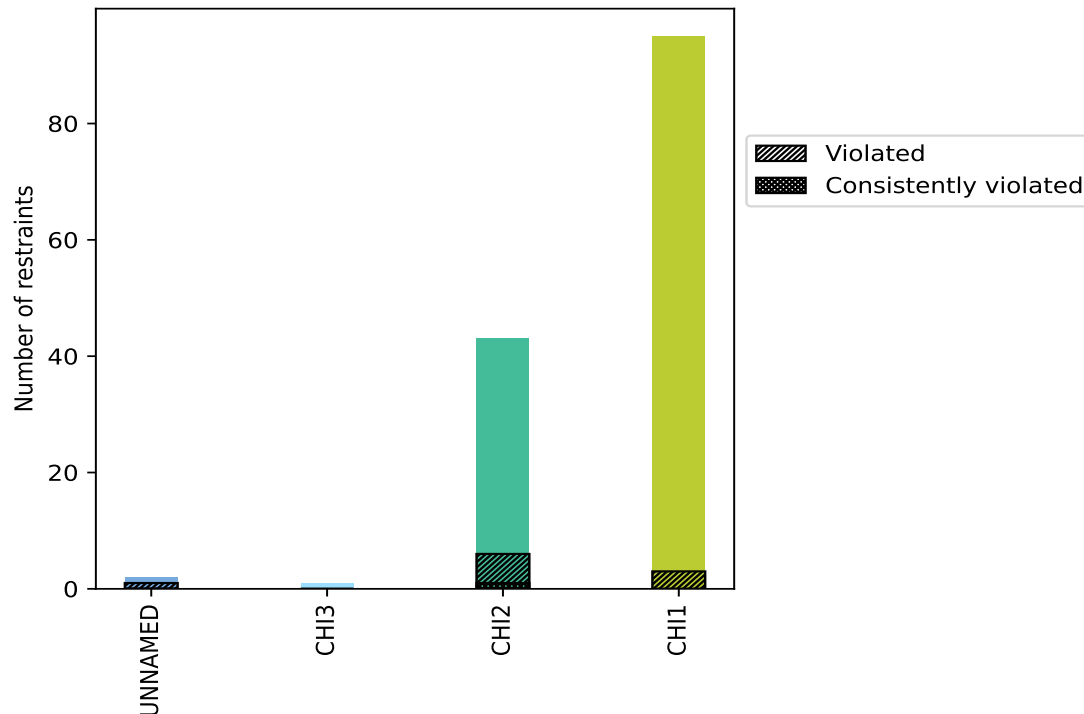
10.1 Summary of dihedral-angle violations ⓘ

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
UNNAMED	2	1.4	1	50.0	0.7	0	0.0	0.0
CHI3	1	0.7	0	0.0	0.0	0	0.0	0.0
CHI2	43	30.5	6	14.0	4.3	1	2.3	0.7
CHI1	95	67.4	3	3.2	2.1	0	0.0	0.0
Total	141	100.0	10	7.1	7.1	1	0.7	0.7

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations ⓘ



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

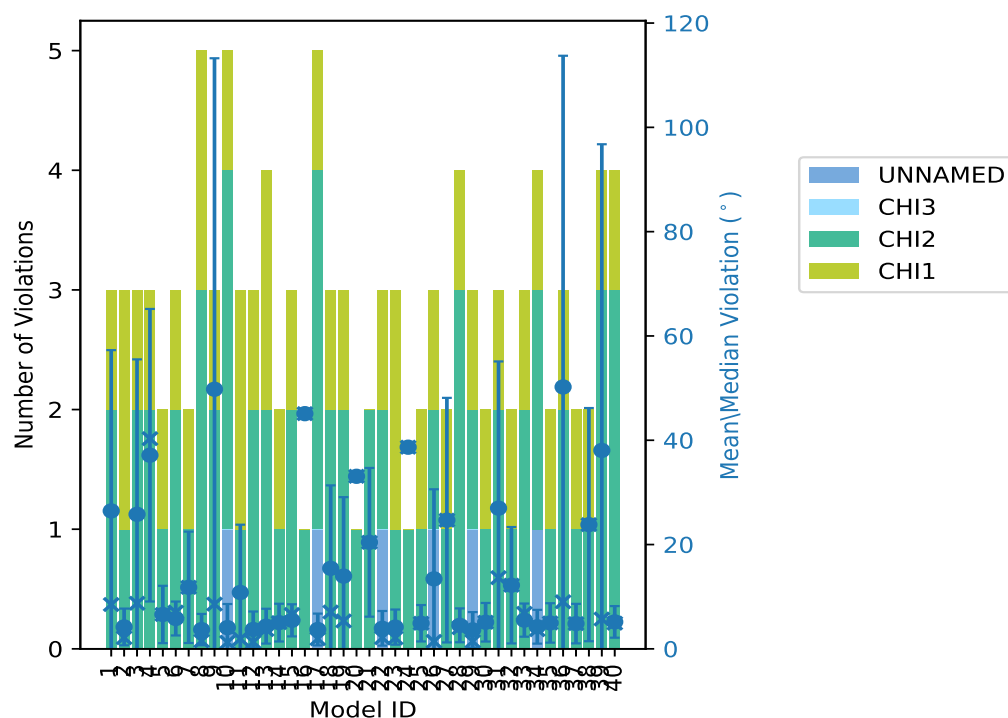
Model ID	Number of violations					Mean (°)	Max (°)	SD (°)	Median (°)
	UNNAMED	CHI3	CHI2	CHI1	Total				
1	0	0	2	1	3	26.45	69.84	30.83	8.5
2	0	0	1	2	3	4.2	9.16	3.52	2.14
3	0	0	2	1	3	25.8	67.58	29.71	8.74
4	0	0	2	1	3	37.13	69.78	28.05	40.31
5	0	0	1	1	2	6.59	12.09	5.5	6.59
6	0	0	2	1	3	5.82	9.04	3.25	7.05
7	0	0	1	1	2	11.8	22.47	10.68	11.8
8	0	0	3	2	5	3.69	7.95	3.01	1.52
9	0	0	2	1	3	49.78	139.44	63.47	8.58
10	1	0	3	1	5	4.07	12.83	4.53	1.26
11	0	0	1	2	3	10.81	29.19	13.0	1.92
12	0	0	2	1	3	3.71	8.59	3.45	1.31
13	0	0	2	2	4	4.35	8.96	3.34	3.7
14	0	0	1	1	2	5.03	8.65	3.62	5.03
15	0	0	2	1	3	5.47	8.56	3.08	6.59
16	0	0	1	0	1	45.1	45.1	0.0	45.1
17	1	0	3	1	5	3.71	9.12	3.05	1.94
18	0	0	2	1	3	15.44	37.72	15.91	7.06
19	0	0	2	1	3	13.95	35.23	15.14	5.35
20	0	0	1	0	1	33.09	33.09	0.0	33.09
21	0	0	2	0	2	20.43	34.69	14.26	20.43
22	1	0	1	1	3	3.94	8.6	3.32	2.14
23	0	0	1	2	3	4.17	8.92	3.37	2.1
24	0	0	1	0	1	38.67	38.67	0.0	38.67
25	0	0	1	1	2	4.91	8.4	3.49	4.91
26	1	0	1	1	3	13.42	37.72	17.18	1.43
27	0	0	1	1	2	24.68	48.13	23.45	24.68
28	0	0	3	1	4	4.51	8.72	3.25	4.06
29	1	0	1	1	3	3.64	8.46	3.41	1.44
30	0	0	1	1	2	5.1	8.8	3.7	5.1
31	0	0	2	1	3	26.98	66.11	28.13	13.65
32	0	0	1	1	2	12.2	23.36	11.16	12.2
33	0	0	2	1	3	5.51	8.58	3.18	6.82
34	1	0	2	1	4	4.24	8.6	3.24	3.68
35	0	0	1	1	2	4.97	8.75	3.78	4.97
36	0	0	2	1	3	50.22	139.94	63.51	9.03
37	0	0	1	1	2	4.84	8.63	3.79	4.84
38	0	0	1	1	2	23.82	46.17	22.36	23.82

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Model ID	Number of violations					Mean (°)	Max (°)	SD (°)	Median (°)
	UNNAMED	CHI3	CHI2	CHI1	Total				
39	0	0	3	1	4	38.05	139.63	58.71	5.72
40	0	0	3	1	4	5.17	9.03	3.03	4.93

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints					Fraction of the ensemble	
UNNAMED	CHI3	CHI2	CHI1	Total	Count ¹	%
0	0	1	0	1	1	2.5
0	0	1	0	1	2	5.0
0	0	2	1	3	3	7.5
0	0	0	1	1	4	10.0

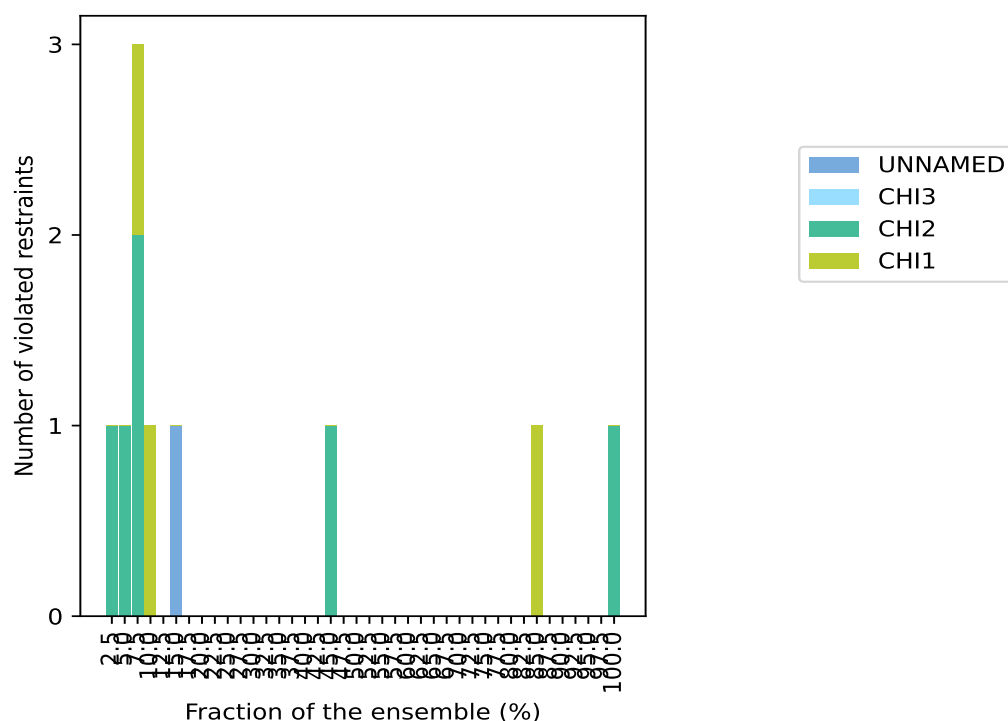
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Number of violated restraints					Fraction of the ensemble	
UNNAMED	CHI3	CHI2	CHI1	Total	Count ¹	%
0	0	0	0	0	5	12.5
1	0	0	0	1	6	15.0
0	0	0	0	0	7	17.5
0	0	0	0	0	8	20.0
0	0	0	0	0	9	22.5
0	0	0	0	0	10	25.0
0	0	0	0	0	11	27.5
0	0	0	0	0	12	30.0
0	0	0	0	0	13	32.5
0	0	0	0	0	14	35.0
0	0	0	0	0	15	37.5
0	0	0	0	0	16	40.0
0	0	0	0	0	17	42.5
0	0	1	0	1	18	45.0
0	0	0	0	0	19	47.5
0	0	0	0	0	20	50.0
0	0	0	0	0	21	52.5
0	0	0	0	0	22	55.0
0	0	0	0	0	23	57.5
0	0	0	0	0	24	60.0
0	0	0	0	0	25	62.5
0	0	0	0	0	26	65.0
0	0	0	0	0	27	67.5
0	0	0	0	0	28	70.0
0	0	0	0	0	29	72.5
0	0	0	0	0	30	75.0
0	0	0	0	0	31	77.5
0	0	0	0	0	32	80.0
0	0	0	0	0	33	82.5
0	0	0	1	1	34	85.0
0	0	0	0	0	35	87.5
0	0	0	0	0	36	90.0
0	0	0	0	0	37	92.5
0	0	0	0	0	38	95.0
0	0	0	0	0	39	97.5
0	0	1	0	1	40	100.0

¹ Number of models with violations

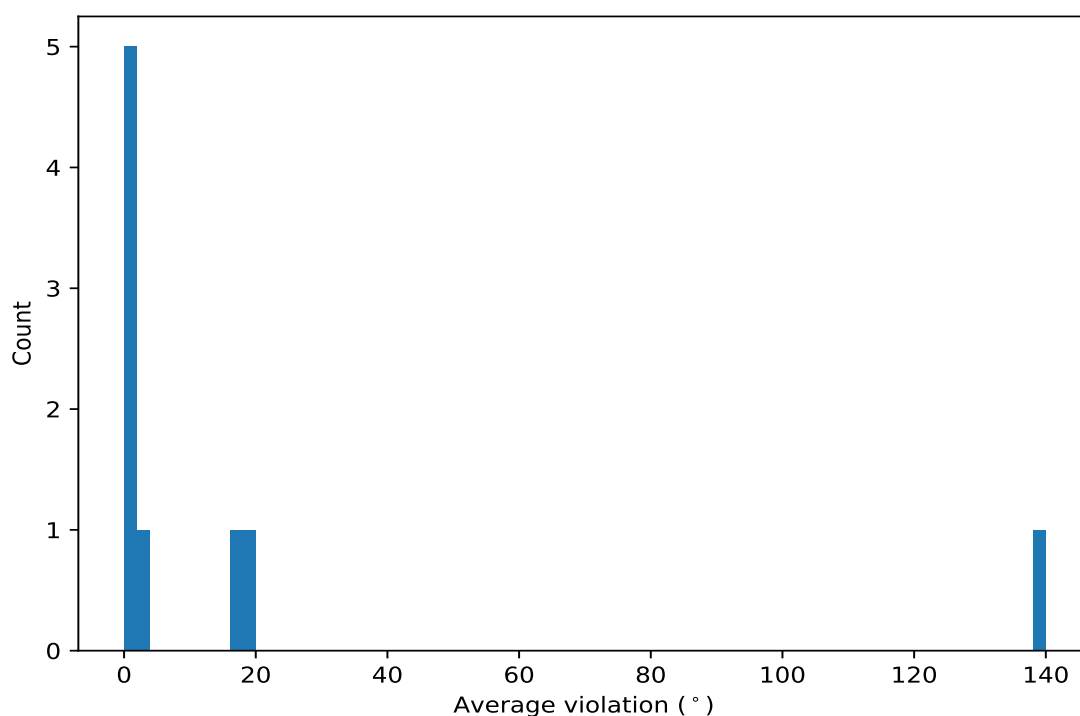
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

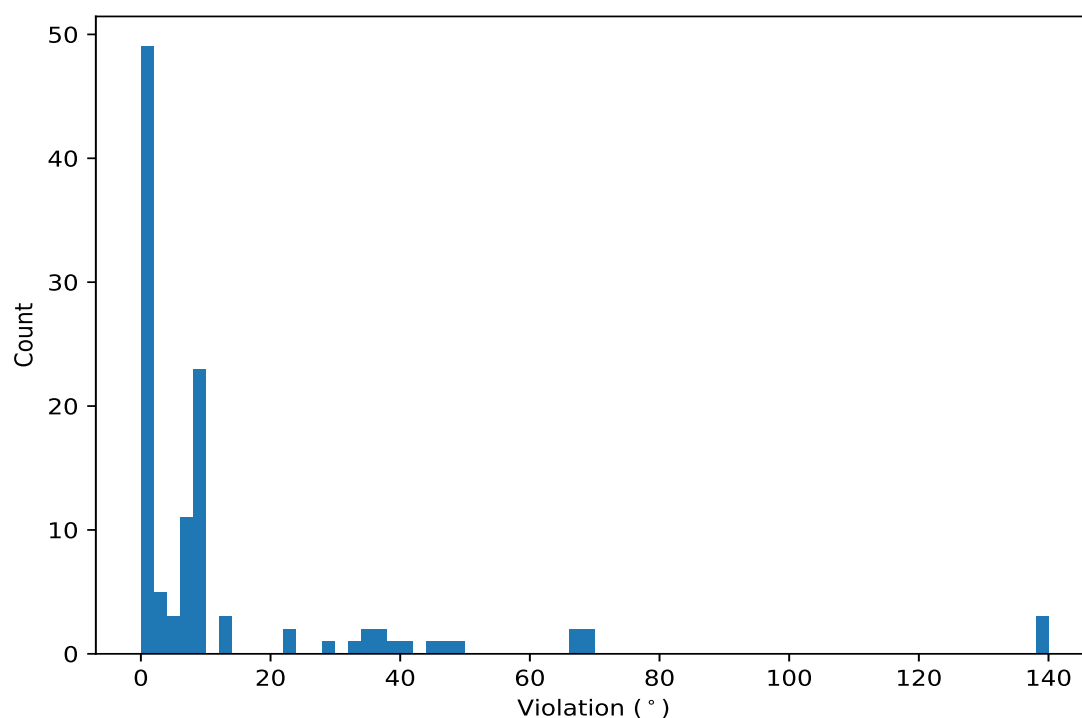
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	40	17.99	13.48	9.03
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	34	1.34	0.25	1.28
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	18	19.76	26.01	6.69
(1,118)	1:91:A:GLN:CB	1:91:A:GLN:CG	1:91:A:GLN:CD	1:91:A:GLN:NE2	6	1.18	0.17	1.1
(1,22)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:CB	1:20:A:LEU:CG	4	1.38	0.38	1.28
(1,4)	1:4:A:PHE:CA	1:4:A:PHE:CB	1:4:A:PHE:CG	1:4:A:PHE:CD1	3	139.67	0.21	139.63
(1,46)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:CB	1:39:A:SER:OG	3	1.85	0.38	2.1
(1,49)	1:41:A:HIS:CA	1:41:A:HIS:CB	1:41:A:HIS:CG	1:41:A:HIS:ND1	3	1.13	0.07	1.14
(1,41)	1:36:A:LEU:CA	1:36:A:LEU:CB	1:36:A:LEU:CG	1:36:A:LEU:CD1	2	2.73	0.04	2.73

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:4:A:PHE:CA	1:4:A:PHE:CB	1:4:A:PHE:CG	1:4:A:PHE:CD1	36	139.94
(1,4)	1:4:A:PHE:CA	1:4:A:PHE:CB	1:4:A:PHE:CG	1:4:A:PHE:CD1	39	139.63
(1,4)	1:4:A:PHE:CA	1:4:A:PHE:CB	1:4:A:PHE:CG	1:4:A:PHE:CD1	9	139.44
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	1	69.84
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	4	69.78
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	3	67.58
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	31	66.11
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	27	48.13
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	38	46.17
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	16	45.1
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	4	40.31
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	24	38.67
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	18	37.72
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	26	37.72
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	19	35.23
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	21	34.69
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	20	33.09
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	11	29.19
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	32	23.36
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	7	22.47
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	31	13.65

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	10	12.83
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	5	12.09
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	2	9.16
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	17	9.12
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	6	9.04
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	36	9.03
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	40	9.03
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	13	8.96
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	23	8.92
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	30	8.8
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	35	8.75
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	3	8.74
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	28	8.72
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	39	8.67
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	14	8.65
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	37	8.63
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	22	8.6
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	34	8.6
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	12	8.59
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	9	8.58
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	33	8.58
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	15	8.56
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	1	8.5
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	29	8.46
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	25	8.4
(1,7)	1:6:A:HIS:CA	1:6:A:HIS:CB	1:6:A:HIS:CG	1:6:A:HIS:ND1	8	7.95
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	40	7.18
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	18	7.06
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	6	7.05
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	33	6.82
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	8	6.74
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	28	6.64
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	15	6.59
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	21	6.18
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	34	6.14
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	13	6.1
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	19	5.35
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	17	5.05
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	10	4.12
(1,41)	1:36:A:LEU:CA	1:36:A:LEU:CB	1:36:A:LEU:CG	1:36:A:LEU:CD1	39	2.77
(1,41)	1:36:A:LEU:CA	1:36:A:LEU:CB	1:36:A:LEU:CG	1:36:A:LEU:CD1	40	2.69
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	22	2.14
(1,46)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:CB	1:39:A:SER:OG	2	2.14
(1,46)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:CB	1:39:A:SER:OG	23	2.1
(1,22)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:CB	1:20:A:LEU:CG	17	1.94
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	11	1.92
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	40	1.76
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	36	1.68
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	18	1.54
(1,22)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:CB	1:20:A:LEU:CG	8	1.52
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	23	1.49

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	28	1.48
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	38	1.46
(1,118)	1:91:A:GLN:CB	1:91:A:GLN:CG	1:91:A:GLN:CD	1:91:A:GLN:NE2	29	1.44
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	26	1.43
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	25	1.42
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	14	1.41
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	30	1.4
(1,118)	1:91:A:GLN:CB	1:91:A:GLN:CG	1:91:A:GLN:CD	1:91:A:GLN:NE2	17	1.39
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	6	1.37
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	9	1.32
(1,46)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:CB	1:39:A:SER:OG	11	1.31
(1,36)	1:32:A:LEU:CA	1:32:A:LEU:CB	1:32:A:LEU:CG	1:32:A:LEU:CD1	12	1.31
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	2	1.3
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	4	1.3
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	13	1.3
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	15	1.27
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	19	1.27
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	10	1.26
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	27	1.24
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	12	1.23
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	34	1.22
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	8	1.21
(1,49)	1:41:A:HIS:CA	1:41:A:HIS:CB	1:41:A:HIS:CG	1:41:A:HIS:ND1	28	1.21
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	35	1.2
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	31	1.18
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	39	1.14
(1,49)	1:41:A:HIS:CA	1:41:A:HIS:CB	1:41:A:HIS:CG	1:41:A:HIS:ND1	10	1.14
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	7	1.12
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	33	1.12
(1,118)	1:91:A:GLN:CB	1:91:A:GLN:CG	1:91:A:GLN:CD	1:91:A:GLN:NE2	26	1.11
(1,118)	1:91:A:GLN:CB	1:91:A:GLN:CG	1:91:A:GLN:CD	1:91:A:GLN:NE2	22	1.09
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	5	1.09
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	3	1.08
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	32	1.05
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	37	1.05
(1,49)	1:41:A:HIS:CA	1:41:A:HIS:CB	1:41:A:HIS:CG	1:41:A:HIS:ND1	17	1.05
(1,130)	1:100:A:ASN:CA	1:100:A:ASN:CB	1:100:A:ASN:CG	1:100:A:ASN:OD1	8	1.04
(1,22)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:CB	1:20:A:LEU:CG	13	1.04
(1,118)	1:91:A:GLN:CB	1:91:A:GLN:CG	1:91:A:GLN:CD	1:91:A:GLN:NE2	34	1.02
(1,79)	1:63:A:CYS:N	1:63:A:CYS:CA	1:63:A:CYS:CB	1:63:A:CYS:SG	29	1.02
(1,22)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:CB	1:20:A:LEU:CG	1	1.02
(1,118)	1:91:A:GLN:CB	1:91:A:GLN:CG	1:91:A:GLN:CD	1:91:A:GLN:NE2	10	1.01