Full wwPDB NMR Structure Validation Report (i)

Mar 5, 2026 – 09:38 PM UTC

PDB ID	:	2L4N / pdb_00002l4n
BMRB ID	:	17245
Title	:	Solution Structure of the Chemokine CCL21
Authors	:	Veldkamp, C.T.; Peterson, F.C.; Love, M.; Sandberg, J.L.
Deposited on	:	2010-10-10

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

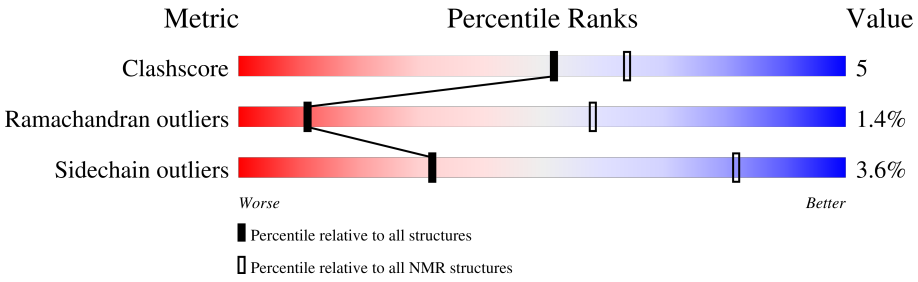
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 84%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	113	51% · 6% 38%

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:8-A:70 (63)	1.03	19

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

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

The models can be grouped into 4 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1127 atoms, of which 572 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-C motif chemokine 21.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	70	1127	348	572	102	100	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	LYS	-	expression tag	UNP O00585
A	113	LEU	-	expression tag	UNP O00585

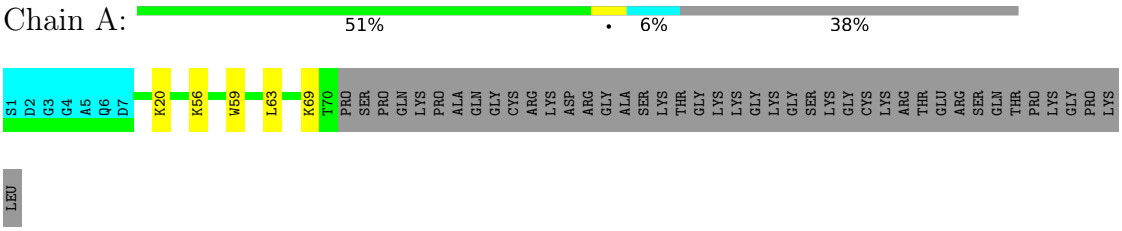
4 Residue-property plots

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: C-C motif chemokine 21

Chain A:



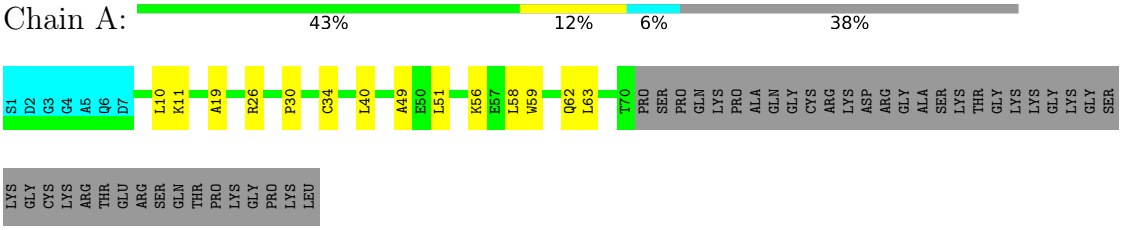
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: C-C motif chemokine 21

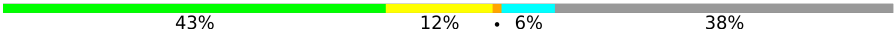
Chain A:

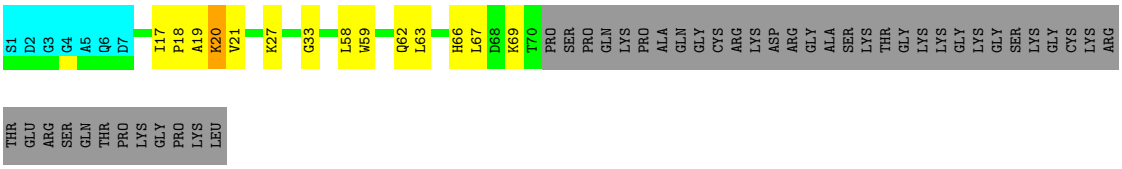


4.2.2 Score per residue for model 2

• Molecule 1: C-C motif chemokine 21

Chain A:

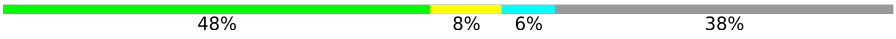


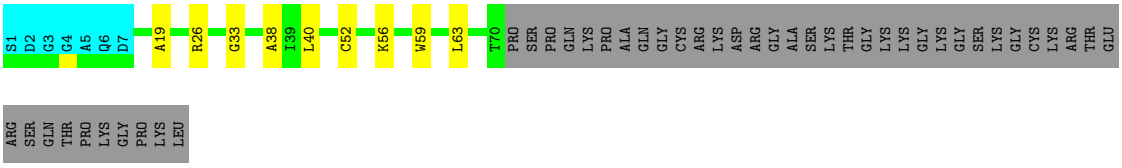


4.2.3 Score per residue for model 3

• Molecule 1: C-C motif chemokine 21

Chain A:

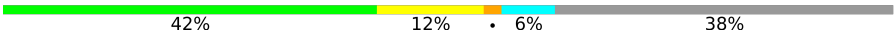


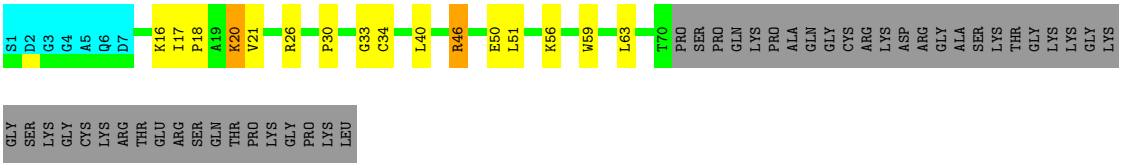


4.2.4 Score per residue for model 4

• Molecule 1: C-C motif chemokine 21

Chain A:

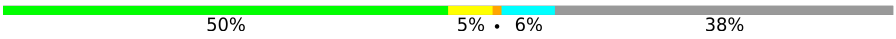


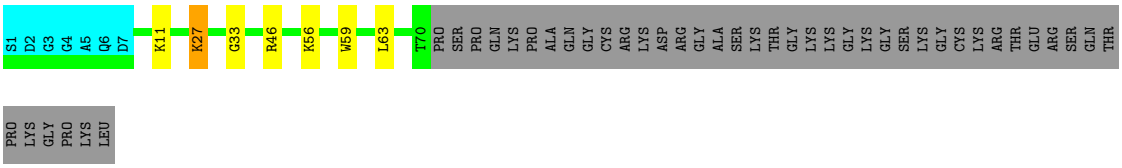


4.2.5 Score per residue for model 5

• Molecule 1: C-C motif chemokine 21

Chain A:

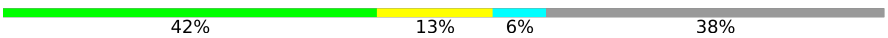


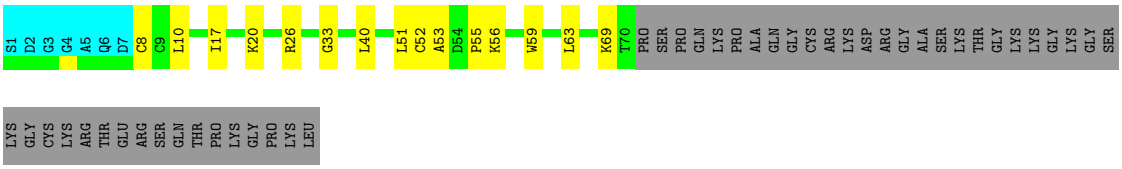


4.2.6 Score per residue for model 6

• Molecule 1: C-C motif chemokine 21

Chain A:



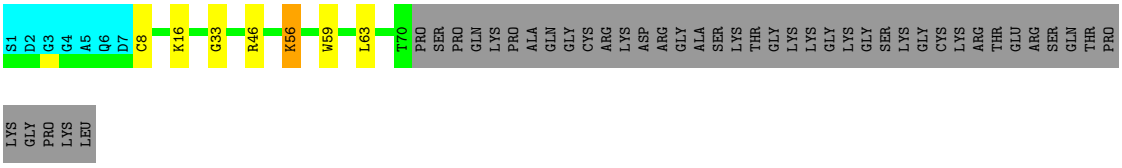


4.2.7 Score per residue for model 7

• Molecule 1: C-C motif chemokine 21

Chain A:



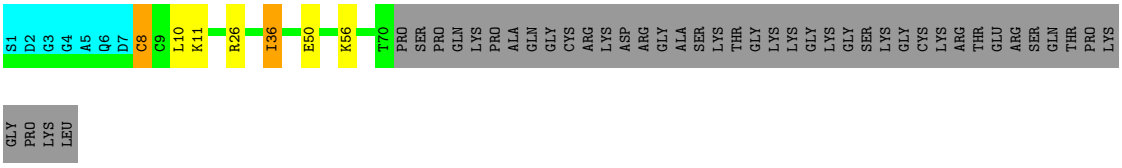


4.2.8 Score per residue for model 8

• Molecule 1: C-C motif chemokine 21

Chain A:

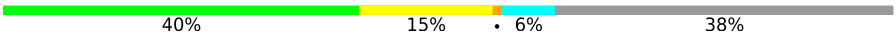


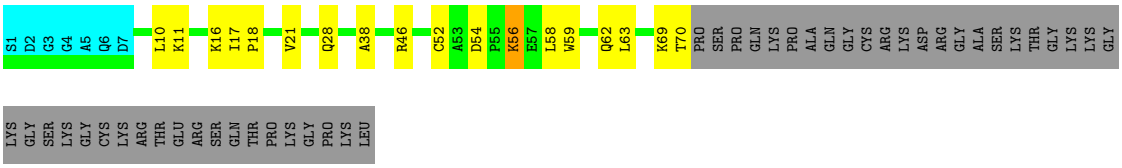


4.2.9 Score per residue for model 9

• Molecule 1: C-C motif chemokine 21

Chain A:



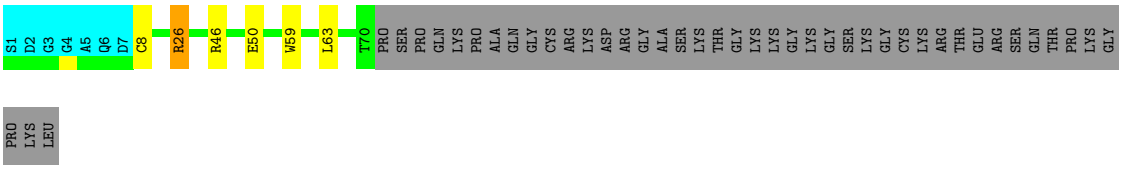


4.2.10 Score per residue for model 10

• Molecule 1: C-C motif chemokine 21

Chain A:

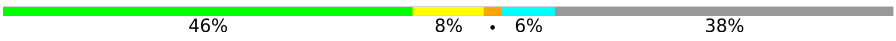


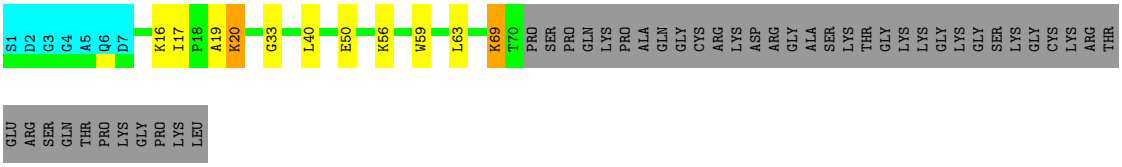


4.2.11 Score per residue for model 11

• Molecule 1: C-C motif chemokine 21

Chain A:

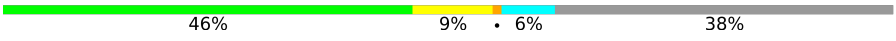


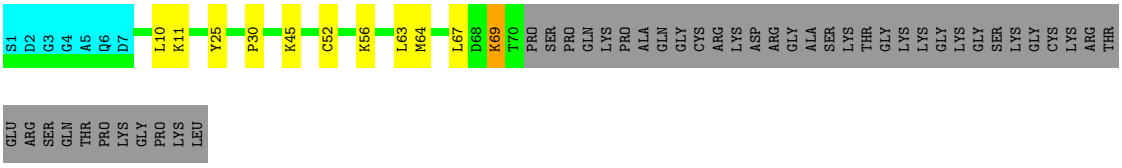


4.2.12 Score per residue for model 12

• Molecule 1: C-C motif chemokine 21

Chain A:

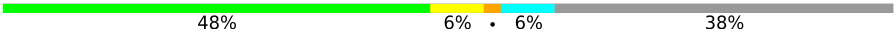


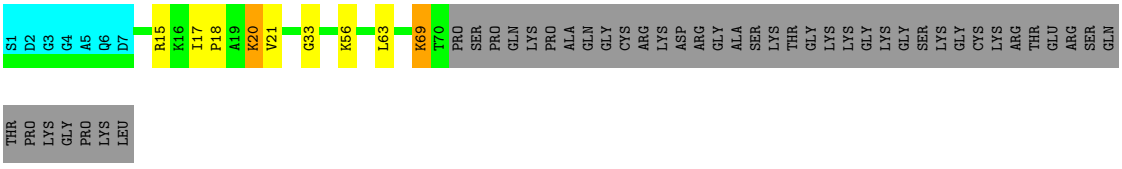


4.2.13 Score per residue for model 13

• Molecule 1: C-C motif chemokine 21

Chain A:



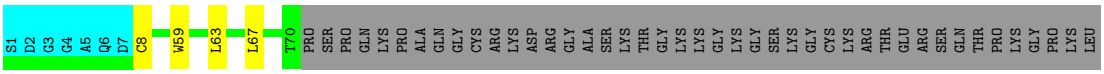


4.2.14 Score per residue for model 14

• Molecule 1: C-C motif chemokine 21

Chain A:

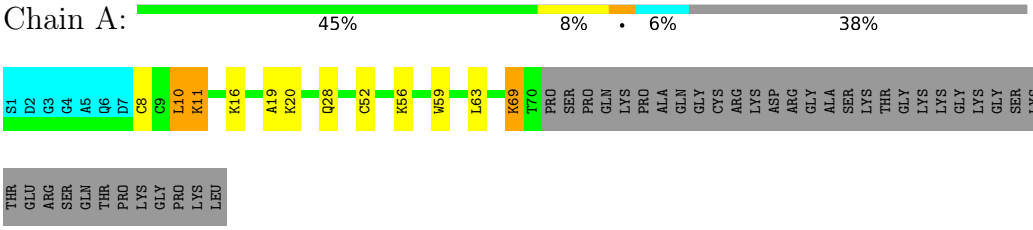




4.2.15 Score per residue for model 15

• Molecule 1: C-C motif chemokine 21

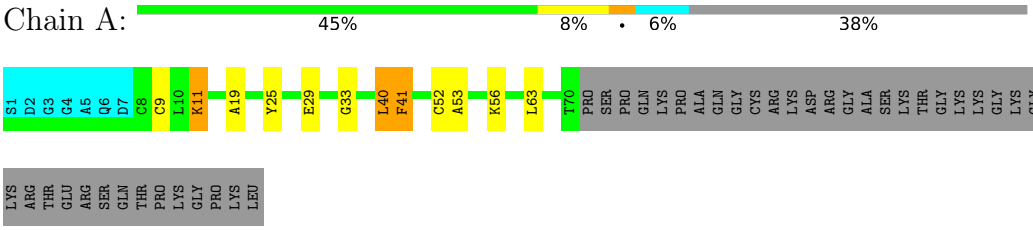
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: C-C motif chemokine 21

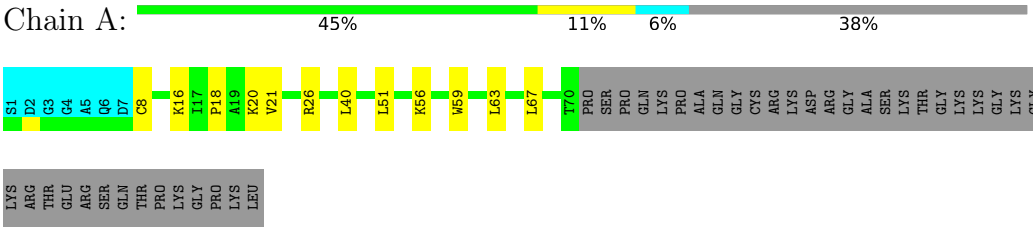
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: C-C motif chemokine 21

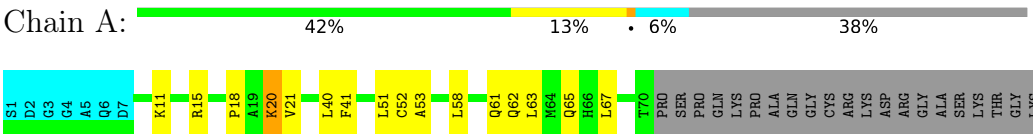
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: C-C motif chemokine 21

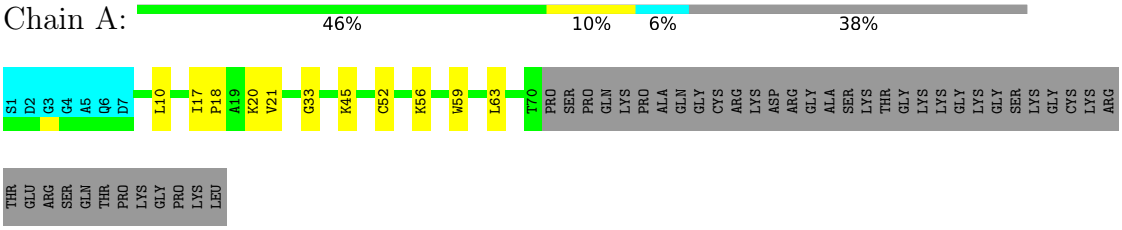
Chain A:





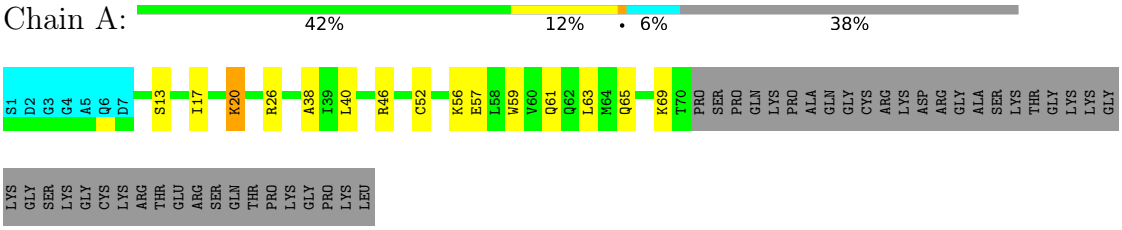
4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: C-C motif chemokine 21



4.2.20 Score per residue for model 20

• Molecule 1: C-C motif chemokine 21



5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1224
Number of shifts mapped to atoms	811
Number of unparsed shifts	0
Number of shifts with mapping errors	413
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality

6.1 Standard geometry

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	1.15±0.04	1±1/521 (0.1± 0.1%)	0.91±0.03	0±0/700 (0.0± 0.0%)
All	All	1.15	12/10420 (0.1%)	0.91	2/14000 (0.0%)

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	45	LYS	N-CA	-6.39	1.38	1.46	19	1
1	A	17	ILE	CA-CB	6.35	1.59	1.54	9	4
1	A	8	CYS	C-N	-6.17	1.25	1.33	17	3
1	A	11	LYS	N-CA	-6.08	1.38	1.46	5	2
1	A	51	LEU	C-N	-5.47	1.26	1.33	6	1
1	A	45	LYS	C-N	-5.07	1.27	1.33	12	1

All unique angle 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	41	PHE	CA-CB-CG	5.55	119.35	113.80	16	1
1	A	46	ARG	N-CA-CB	5.32	116.31	110.35	4	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	511	538	537	6±2
All	All	10220	10760	10740	114

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:PHE:CE1	1:A:63:LEU:HD13	0.56	2.35	18	1
1:A:59:TRP:O	1:A:63:LEU:HG	0.56	2.00	20	15
1:A:41:PHE:CZ	1:A:63:LEU:HD13	0.56	2.36	18	1
1:A:69:LYS:N	1:A:69:LYS:HE2	0.55	2.17	13	1
1:A:11:LYS:O	1:A:52:CYS:HB3	0.54	2.02	16	3
1:A:46:ARG:HD3	1:A:46:ARG:O	0.53	2.03	10	3
1:A:69:LYS:HD2	1:A:70:THR:N	0.52	2.19	9	1
1:A:11:LYS:HD3	1:A:11:LYS:O	0.51	2.05	15	1
1:A:63:LEU:O	1:A:67:LEU:HG	0.51	2.06	2	5
1:A:69:LYS:N	1:A:69:LYS:HE3	0.51	2.21	11	3
1:A:26:ARG:HB3	1:A:40:LEU:HB2	0.49	1.84	6	5
1:A:38:ALA:HB1	1:A:52:CYS:SG	0.49	2.48	3	2
1:A:10:LEU:CD1	1:A:11:LYS:HG2	0.49	2.38	8	1
1:A:40:LEU:HA	1:A:51:LEU:O	0.48	2.09	18	3
1:A:56:LYS:HE3	1:A:56:LYS:HA	0.48	1.86	7	1
1:A:10:LEU:HD23	1:A:52:CYS:SG	0.48	2.49	12	1
1:A:10:LEU:HD12	1:A:11:LYS:N	0.48	2.23	9	2
1:A:18:PRO:O	1:A:21:VAL:HG22	0.47	2.09	13	6
1:A:10:LEU:N	1:A:52:CYS:SG	0.47	2.86	6	3
1:A:10:LEU:H	1:A:10:LEU:HD23	0.47	1.68	15	1
1:A:65:GLN:O	1:A:69:LYS:HG3	0.47	2.09	20	1
1:A:26:ARG:HD3	1:A:26:ARG:C	0.46	2.34	10	2
1:A:66:HIS:O	1:A:69:LYS:HG2	0.46	2.10	2	1
1:A:20:LYS:HD2	1:A:20:LYS:H	0.46	1.70	13	6
1:A:25:TYR:HA	1:A:40:LEU:O	0.46	2.11	16	1
1:A:58:LEU:O	1:A:62:GLN:HG3	0.46	2.10	9	4
1:A:16:LYS:N	1:A:16:LYS:HD2	0.45	2.26	7	1
1:A:19:ALA:HB2	1:A:63:LEU:HD22	0.45	1.89	11	3
1:A:50:GLU:CD	1:A:50:GLU:H	0.45	2.20	10	1
1:A:25:TYR:CE1	1:A:64:MET:HA	0.45	2.47	12	1
1:A:36:ILE:HD13	1:A:36:ILE:H	0.44	1.73	8	1
1:A:16:LYS:HD2	1:A:59:TRP:CZ2	0.44	2.47	11	1
1:A:56:LYS:HA	1:A:56:LYS:CE	0.43	2.43	7	1
1:A:8:CYS:HA	1:A:28:GLN:OE1	0.43	2.13	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:PRO:HG2	1:A:21:VAL:CG2	0.43	2.42	9	1
1:A:61:GLN:O	1:A:65:GLN:HG3	0.43	2.13	18	1
1:A:10:LEU:HD11	1:A:50:GLU:O	0.43	2.14	8	1
1:A:19:ALA:N	1:A:63:LEU:HD22	0.43	2.27	16	3
1:A:54:ASP:OD1	1:A:56:LYS:HB2	0.43	2.14	9	1
1:A:41:PHE:CE2	1:A:53:ALA:HB2	0.43	2.49	18	2
1:A:56:LYS:N	1:A:56:LYS:HD2	0.43	2.29	1	3
1:A:15:ARG:HA	1:A:15:ARG:NE	0.43	2.28	18	1
1:A:10:LEU:HD12	1:A:11:LYS:HG2	0.42	1.90	8	1
1:A:53:ALA:O	1:A:55:PRO:HD3	0.42	2.15	6	1
1:A:30:PRO:HA	1:A:34:CYS:O	0.42	2.15	1	1
1:A:57:GLU:O	1:A:61:GLN:HG3	0.42	2.14	20	1
1:A:17:ILE:O	1:A:63:LEU:HD11	0.41	2.15	2	4
1:A:27:LYS:H	1:A:27:LYS:HE2	0.41	1.75	5	1
1:A:30:PRO:HA	1:A:34:CYS:HB2	0.41	1.93	4	1
1:A:46:ARG:HD3	1:A:46:ARG:H	0.41	1.76	4	1
1:A:16:LYS:HG2	1:A:59:TRP:CD1	0.41	2.50	17	1
1:A:40:LEU:HB3	1:A:50:GLU:HB3	0.40	1.93	11	1
1:A:26:ARG:HG3	1:A:50:GLU:OE2	0.40	2.15	4	1
1:A:49:ALA:O	1:A:51:LEU:HD12	0.40	2.17	1	1
1:A:28:GLN:HE21	1:A:38:ALA:HB3	0.40	1.76	9	1
1:A:16:LYS:HD2	1:A:59:TRP:NE1	0.40	2.32	15	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	62/113 (55%)	58±1 (94±2%)	3±1 (5±2%)	1±1 (1±1%)	11	58
All	All	1240/2260 (55%)	1161 (94%)	62 (5%)	17 (1%)	11	58

All 5 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	33	GLY	10
1	A	8	CYS	4
1	A	30	PRO	1
1	A	9	CYS	1
1	A	13	SER	1

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	58/96 (60%)	56±1 (96±2%)	2±1 (4±2%)	32 82
All	All	1160/1920 (60%)	1118 (96%)	42 (4%)	32 82

All 13 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	56	LYS	13
1	A	20	LYS	10
1	A	69	LYS	5
1	A	27	LYS	2
1	A	16	LYS	2
1	A	46	ARG	2
1	A	11	LYS	2
1	A	36	ILE	1
1	A	26	ARG	1
1	A	15	ARG	1
1	A	10	LEU	1
1	A	29	GLU	1
1	A	40	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1224
Number of shifts mapped to atoms	811
Number of unparsed shifts	0
Number of shifts with mapping errors	413
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- No matching atom found in the structure. All 413 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	PRO	HA	4.5	0.02	1
1	A	71	PRO	HB2	2.353	0.02	2
1	A	71	PRO	HB3	1.966	0.02	2
1	A	71	PRO	HD2	3.901	0.02	2
1	A	71	PRO	HD3	3.76	0.02	2
1	A	71	PRO	HG2	2.069	0.02	2
1	A	71	PRO	HG3	2.069	0.02	2
1	A	71	PRO	C	176.76	0.1	1
1	A	71	PRO	CA	63.204	0.1	1
1	A	71	PRO	CB	32.336	0.1	1
1	A	71	PRO	CD	50.945	0.1	1
1	A	71	PRO	CG	27.592	0.1	1
1	A	72	SER	H	8.521	0.02	1
1	A	72	SER	CA	56.652	0.1	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	SER	CB	63.898	0.1	1
1	A	72	SER	N	117.875	0.1	1
1	A	73	PRO	HA	4.496	0.02	1
1	A	73	PRO	HB2	2.362	0.02	2
1	A	73	PRO	HB3	1.972	0.02	2
1	A	73	PRO	HD2	3.987	0.02	2
1	A	73	PRO	HD3	3.849	0.02	2
1	A	73	PRO	HG2	2.079	0.02	2
1	A	73	PRO	HG3	2.079	0.02	2
1	A	73	PRO	C	176.862	0.1	1
1	A	73	PRO	CA	63.457	0.1	1
1	A	73	PRO	CB	32.336	0.1	1
1	A	73	PRO	CD	51.036	0.1	1
1	A	73	PRO	CG	27.592	0.1	1
1	A	74	GLN	H	8.438	0.02	1
1	A	74	GLN	HA	4.373	0.02	1
1	A	74	GLN	HB2	2.113	0.02	2
1	A	74	GLN	HB3	2.003	0.02	2
1	A	74	GLN	HG2	2.445	0.02	2
1	A	74	GLN	HG3	2.445	0.02	2
1	A	74	GLN	C	175.841	0.1	1
1	A	74	GLN	CA	55.766	0.1	1
1	A	74	GLN	CB	29.964	0.1	1
1	A	74	GLN	CG	33.978	0.1	1
1	A	74	GLN	N	120.647	0.1	1
1	A	75	LYS	H	8.415	0.02	1
1	A	75	LYS	CA	54.451	0.1	1
1	A	75	LYS	CB	32.883	0.1	1
1	A	75	LYS	N	124.261	0.1	1
1	A	76	PRO	HA	4.476	0.02	1
1	A	76	PRO	HB2	2.324	0.02	2
1	A	76	PRO	HB3	1.952	0.02	2
1	A	76	PRO	HD2	3.879	0.02	2
1	A	76	PRO	HD3	3.675	0.02	2
1	A	76	PRO	HG2	2.069	0.02	2
1	A	76	PRO	HG3	2.069	0.02	2
1	A	76	PRO	C	176.658	0.1	1
1	A	76	PRO	CA	63.204	0.1	1
1	A	76	PRO	CB	32.336	0.1	1
1	A	76	PRO	CD	50.58	0.1	1
1	A	76	PRO	CG	27.684	0.1	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	ALA	H	8.48	0.02	1
1	A	77	ALA	HA	4.383	0.02	1
1	A	77	ALA	HB1	1.427	0.02	1
1	A	77	ALA	HB2	1.427	0.02	1
1	A	77	ALA	HB3	1.427	0.02	1
1	A	77	ALA	C	177.811	0.1	1
1	A	77	ALA	CA	52.566	0.1	1
1	A	77	ALA	CB	19.474	0.1	1
1	A	77	ALA	N	124.618	0.1	1
1	A	78	GLN	H	8.439	0.02	1
1	A	78	GLN	HA	4.386	0.02	1
1	A	78	GLN	HB2	2.157	0.02	2
1	A	78	GLN	HB3	2.032	0.02	2
1	A	78	GLN	HG2	2.436	0.02	2
1	A	78	GLN	HG3	2.436	0.02	2
1	A	78	GLN	C	176.483	0.1	1
1	A	78	GLN	CA	56.078	0.1	1
1	A	78	GLN	CB	30.055	0.1	1
1	A	78	GLN	CG	33.978	0.1	1
1	A	78	GLN	N	119.782	0.1	1
1	A	79	GLY	H	8.446	0.02	1
1	A	79	GLY	HA2	4.024	0.02	2
1	A	79	GLY	HA3	4.024	0.02	2
1	A	79	GLY	C	175.841	0.1	1
1	A	79	GLY	CA	45.414	0.1	1
1	A	79	GLY	N	109.652	0.1	1
1	A	80	CYS	H	8.307	0.02	1
1	A	80	CYS	HA	4.671	0.02	1
1	A	80	CYS	HB2	2.745	0.02	2
1	A	80	CYS	HB3	2.745	0.02	2
1	A	80	CYS	C	176.308	0.1	1
1	A	80	CYS	CA	55.759	0.1	1
1	A	80	CYS	CB	41.914	0.1	1
1	A	80	CYS	N	118.444	0.1	1
1	A	81	ARG	H	8.373	0.02	1
1	A	81	ARG	HA	4.404	0.02	1
1	A	81	ARG	HB2	1.922	0.02	2
1	A	81	ARG	HB3	1.828	0.02	2
1	A	81	ARG	HD2	3.263	0.02	2
1	A	81	ARG	HD3	3.263	0.02	2
1	A	81	ARG	HG2	1.703	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	ARG	HG3	1.703	0.02	2
1	A	81	ARG	C	176.249	0.1	1
1	A	81	ARG	CA	56.49	0.1	1
1	A	81	ARG	CB	31.15	0.1	1
1	A	81	ARG	CD	43.83	0.1	1
1	A	81	ARG	CG	27.227	0.1	1
1	A	81	ARG	N	121.723	0.1	1
1	A	82	LYS	H	8.455	0.02	1
1	A	82	LYS	HA	4.364	0.02	1
1	A	82	LYS	HB2	1.908	0.02	2
1	A	82	LYS	HB3	1.807	0.02	2
1	A	82	LYS	HD2	1.737	0.02	2
1	A	82	LYS	HD3	1.737	0.02	2
1	A	82	LYS	HE2	3.046	0.02	2
1	A	82	LYS	HE3	3.046	0.02	2
1	A	82	LYS	HG2	1.485	0.02	2
1	A	82	LYS	HG3	1.485	0.02	2
1	A	82	LYS	C	176.191	0.1	1
1	A	82	LYS	CA	56.734	0.1	1
1	A	82	LYS	CB	33.066	0.1	1
1	A	82	LYS	CD	29.573	0.1	1
1	A	82	LYS	CE	42.515	0.1	1
1	A	82	LYS	CG	25.043	0.1	1
1	A	82	LYS	N	122.697	0.1	1
1	A	83	ASP	H	8.362	0.02	1
1	A	83	ASP	CA	54.299	0.1	1
1	A	83	ASP	CB	41.64	0.1	1
1	A	83	ASP	N	121.227	0.1	1
1	A	84	ARG	HA	4.373	0.02	1
1	A	84	ARG	HB2	1.982	0.02	2
1	A	84	ARG	HB3	1.88	0.02	2
1	A	84	ARG	HD2	3.259	0.02	2
1	A	84	ARG	HD3	3.259	0.02	2
1	A	84	ARG	HG2	1.701	0.02	2
1	A	84	ARG	HG3	1.701	0.02	2
1	A	84	ARG	C	176.979	0.1	1
1	A	84	ARG	CA	56.734	0.1	1
1	A	84	ARG	CB	30.694	0.1	1
1	A	84	ARG	CD	43.83	0.1	1
1	A	84	ARG	CG	27.136	0.1	1
1	A	85	GLY	H	8.494	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	GLY	HA2	3.993	0.02	2
1	A	85	GLY	HA3	3.993	0.02	2
1	A	85	GLY	C	174.075	0.1	1
1	A	85	GLY	CA	45.468	0.1	1
1	A	85	GLY	N	109.402	0.1	1
1	A	86	ALA	H	8.145	0.02	1
1	A	86	ALA	HA	4.372	0.02	1
1	A	86	ALA	HB1	1.449	0.02	1
1	A	86	ALA	HB2	1.449	0.02	1
1	A	86	ALA	HB3	1.449	0.02	1
1	A	86	ALA	C	178.001	0.1	1
1	A	86	ALA	CA	52.834	0.1	1
1	A	86	ALA	CB	19.565	0.1	1
1	A	86	ALA	N	123.603	0.1	1
1	A	87	SER	H	8.316	0.02	1
1	A	87	SER	HA	4.517	0.02	1
1	A	87	SER	HB2	3.922	0.02	2
1	A	87	SER	HB3	3.922	0.02	2
1	A	87	SER	C	174.849	0.1	1
1	A	87	SER	CA	58.629	0.1	1
1	A	87	SER	CB	64.126	0.1	1
1	A	87	SER	N	114.782	0.1	1
1	A	88	LYS	H	8.482	0.02	1
1	A	88	LYS	HA	4.424	0.02	1
1	A	88	LYS	HB2	1.952	0.02	2
1	A	88	LYS	HB3	1.838	0.02	2
1	A	88	LYS	HD2	1.741	0.02	2
1	A	88	LYS	HD3	1.741	0.02	2
1	A	88	LYS	HE2	3.035	0.02	2
1	A	88	LYS	HE3	3.035	0.02	2
1	A	88	LYS	HG2	1.53	0.02	2
1	A	88	LYS	HG3	1.53	0.02	2
1	A	88	LYS	C	177.037	0.1	1
1	A	88	LYS	CA	57.059	0.1	1
1	A	88	LYS	CB	33.066	0.1	1
1	A	88	LYS	CD	29.326	0.1	1
1	A	88	LYS	CG	25.129	0.1	1
1	A	88	LYS	N	123.133	0.1	1
1	A	89	THR	H	8.061	0.02	1
1	A	89	THR	HA	4.383	0.02	1
1	A	89	THR	HB	4.289	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	89	THR	HG21	1.244	0.02	1
1	A	89	THR	HG22	1.244	0.02	1
1	A	89	THR	HG23	1.244	0.02	1
1	A	89	THR	C	175.199	0.1	1
1	A	89	THR	CA	61.96	0.1	1
1	A	89	THR	CB	70.283	0.1	1
1	A	89	THR	CG2	21.754	0.1	1
1	A	89	THR	N	112.586	0.1	1
1	A	90	GLY	H	8.315	0.02	1
1	A	90	GLY	HA2	4.226	0.02	2
1	A	90	GLY	HA3	4.226	0.02	2
1	A	90	GLY	C	174.192	0.1	1
1	A	90	GLY	CA	45.414	0.1	1
1	A	90	GLY	N	110.812	0.1	1
1	A	91	LYS	H	8.219	0.02	1
1	A	91	LYS	HA	4.384	0.02	1
1	A	91	LYS	HB2	1.85	0.02	2
1	A	91	LYS	HB3	1.482	0.02	2
1	A	91	LYS	HD2	1.72	0.02	2
1	A	91	LYS	HD3	1.72	0.02	2
1	A	91	LYS	HE2	3.044	0.02	2
1	A	91	LYS	HE3	3.044	0.02	2
1	A	91	LYS	HG2	1.482	0.02	2
1	A	91	LYS	HG3	1.482	0.02	2
1	A	91	LYS	C	176.848	0.1	1
1	A	91	LYS	CA	56.544	0.1	1
1	A	91	LYS	CB	33.339	0.1	1
1	A	91	LYS	CD	29.573	0.1	1
1	A	91	LYS	CE	42.191	0.1	1
1	A	91	LYS	CG	25.043	0.1	1
1	A	91	LYS	N	120.822	0.1	1
1	A	92	LYS	H	8.426	0.02	1
1	A	92	LYS	HA	4.383	0.02	1
1	A	92	LYS	HB2	1.88	0.02	2
1	A	92	LYS	HB3	1.88	0.02	2
1	A	92	LYS	HD2	1.728	0.02	2
1	A	92	LYS	HD3	1.728	0.02	2
1	A	92	LYS	HE2	3.045	0.02	2
1	A	92	LYS	HE3	3.045	0.02	2
1	A	92	LYS	HG2	1.499	0.02	2
1	A	92	LYS	HG3	1.499	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	92	LYS	C	177.081	0.1	1
1	A	92	LYS	CA	56.707	0.1	1
1	A	92	LYS	CB	33.157	0.1	1
1	A	92	LYS	CD	29.417	0.1	1
1	A	92	LYS	CG	25.038	0.1	1
1	A	92	LYS	N	122.06	0.1	1
1	A	93	GLY	H	8.385	0.02	1
1	A	93	GLY	HA2	4.034	0.02	2
1	A	93	GLY	HA3	4.034	0.02	2
1	A	93	GLY	C	174.177	0.1	1
1	A	93	GLY	CA	45.36	0.1	1
1	A	93	GLY	N	109.899	0.1	1
1	A	94	LYS	H	8.329	0.02	1
1	A	94	LYS	HA	4.404	0.02	1
1	A	94	LYS	HB2	1.874	0.02	2
1	A	94	LYS	HB3	1.874	0.02	2
1	A	94	LYS	HD2	1.736	0.02	2
1	A	94	LYS	HD3	1.736	0.02	2
1	A	94	LYS	HE2	3.055	0.02	2
1	A	94	LYS	HE3	3.055	0.02	2
1	A	94	LYS	HG2	1.499	0.02	2
1	A	94	LYS	HG3	1.499	0.02	2
1	A	94	LYS	C	176.571	0.1	1
1	A	94	LYS	CA	56.666	0.1	1
1	A	94	LYS	CB	33.522	0.1	1
1	A	94	LYS	CD	29.417	0.1	1
1	A	94	LYS	CE	43.83	0.1	1
1	A	94	LYS	CG	25.129	0.1	1
1	A	94	LYS	N	120.98	0.1	1
1	A	95	GLY	H	8.536	0.02	1
1	A	95	GLY	HA2	4.055	0.02	2
1	A	95	GLY	HA3	4.055	0.02	2
1	A	95	GLY	C	174.206	0.1	1
1	A	95	GLY	CA	45.387	0.1	1
1	A	95	GLY	N	109.962	0.1	1
1	A	96	SER	H	8.254	0.02	1
1	A	96	SER	HA	4.517	0.02	1
1	A	96	SER	HB2	3.942	0.02	2
1	A	96	SER	HB3	3.942	0.02	2
1	A	96	SER	C	174.396	0.1	1
1	A	96	SER	CA	58.508	0.1	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	SER	CB	64.308	0.1	1
1	A	96	SER	N	115.623	0.1	1
1	A	97	LYS	H	8.491	0.02	1
1	A	97	LYS	HA	4.404	0.02	1
1	A	97	LYS	HB2	1.868	0.02	2
1	A	97	LYS	HB3	1.868	0.02	2
1	A	97	LYS	HD2	1.721	0.02	2
1	A	97	LYS	HD3	1.721	0.02	2
1	A	97	LYS	HE2	3.034	0.02	2
1	A	97	LYS	HE3	3.034	0.02	2
1	A	97	LYS	HG2	1.469	0.02	2
1	A	97	LYS	HG3	1.469	0.02	2
1	A	97	LYS	C	177.081	0.1	1
1	A	97	LYS	CA	56.815	0.1	1
1	A	97	LYS	CB	33.248	0.1	1
1	A	97	LYS	CD	29.417	0.1	1
1	A	97	LYS	CG	25.129	0.1	1
1	A	97	LYS	N	123.441	0.1	1
1	A	98	GLY	H	8.435	0.02	1
1	A	98	GLY	HA2	4.034	0.02	2
1	A	98	GLY	HA3	4.034	0.02	2
1	A	98	GLY	C	173.958	0.1	1
1	A	98	GLY	CA	45.414	0.1	1
1	A	98	GLY	N	109.184	0.1	1
1	A	99	CYS	H	8.413	0.02	1
1	A	99	CYS	HA	4.414	0.02	1
1	A	99	CYS	HB2	3.275	0.02	2
1	A	99	CYS	HB3	3.07	0.02	2
1	A	99	CYS	C	174.469	0.1	1
1	A	99	CYS	CA	55.732	0.1	1
1	A	99	CYS	CB	41.777	0.1	1
1	A	99	CYS	N	118.609	0.1	1
1	A	100	LYS	H	8.496	0.02	1
1	A	100	LYS	HA	4.381	0.02	1
1	A	100	LYS	HB2	1.88	0.02	2
1	A	100	LYS	HB3	1.88	0.02	2
1	A	100	LYS	HD2	1.737	0.02	2
1	A	100	LYS	HD3	1.737	0.02	2
1	A	100	LYS	HE2	3.066	0.02	2
1	A	100	LYS	HE3	3.066	0.02	2
1	A	100	LYS	HG2	1.489	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	LYS	HG3	1.489	0.02	2
1	A	100	LYS	C	176.264	0.1	1
1	A	100	LYS	CA	56.463	0.1	1
1	A	100	LYS	CB	33.43	0.1	1
1	A	100	LYS	CD	29.599	0.1	1
1	A	100	LYS	CE	41.64	0.1	1
1	A	100	LYS	CG	25.038	0.1	1
1	A	100	LYS	N	123.629	0.1	1
1	A	101	ARG	H	8.509	0.02	1
1	A	101	ARG	HA	4.407	0.02	1
1	A	101	ARG	HB2	1.925	0.02	2
1	A	101	ARG	HB3	1.825	0.02	2
1	A	101	ARG	HD2	3.259	0.02	2
1	A	101	ARG	HD3	3.259	0.02	2
1	A	101	ARG	HG2	1.703	0.02	2
1	A	101	ARG	HG3	1.703	0.02	2
1	A	101	ARG	C	176.439	0.1	1
1	A	101	ARG	CA	56.416	0.1	1
1	A	101	ARG	CB	31.15	0.1	1
1	A	101	ARG	CD	43.83	0.1	1
1	A	101	ARG	CG	27.319	0.1	1
1	A	101	ARG	N	123.442	0.1	1
1	A	102	THR	H	8.286	0.02	1
1	A	102	THR	HA	4.383	0.02	1
1	A	102	THR	HB	4.3	0.02	1
1	A	102	THR	HG21	1.239	0.02	1
1	A	102	THR	HG22	1.239	0.02	1
1	A	102	THR	HG23	1.239	0.02	1
1	A	102	THR	C	174.498	0.1	1
1	A	102	THR	CA	62.069	0.1	1
1	A	102	THR	CB	70.238	0.1	1
1	A	102	THR	CG2	21.754	0.1	1
1	A	102	THR	N	116.093	0.1	1
1	A	103	GLU	H	8.523	0.02	1
1	A	103	GLU	HA	4.388	0.02	1
1	A	103	GLU	HB2	2.095	0.02	2
1	A	103	GLU	HB3	1.98	0.02	2
1	A	103	GLU	HG2	2.323	0.02	2
1	A	103	GLU	HG3	2.323	0.02	2
1	A	103	GLU	C	176.352	0.1	1
1	A	103	GLU	CA	56.598	0.1	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	GLU	CB	30.603	0.1	1
1	A	103	GLU	CG	36.441	0.1	1
1	A	103	GLU	N	124.044	0.1	1
1	A	104	ARG	H	8.487	0.02	1
1	A	104	ARG	HA	4.396	0.02	1
1	A	104	ARG	HB2	1.927	0.02	2
1	A	104	ARG	HB3	1.825	0.02	2
1	A	104	ARG	HD2	3.249	0.02	2
1	A	104	ARG	HD3	3.249	0.02	2
1	A	104	ARG	HG2	1.668	0.02	2
1	A	104	ARG	HG3	1.668	0.02	2
1	A	104	ARG	C	176.352	0.1	1
1	A	104	ARG	CA	56.382	0.1	1
1	A	104	ARG	CB	31.515	0.1	1
1	A	104	ARG	CD	43.647	0.1	1
1	A	104	ARG	CG	27.136	0.1	1
1	A	104	ARG	N	122.268	0.1	1
1	A	105	SER	H	8.415	0.02	1
1	A	105	SER	HA	4.476	0.02	1
1	A	105	SER	HB2	3.911	0.02	2
1	A	105	SER	HB3	3.911	0.02	2
1	A	105	SER	C	174.484	0.1	1
1	A	105	SER	CA	58.562	0.1	1
1	A	105	SER	CB	64.126	0.1	1
1	A	105	SER	N	117.275	0.1	1
1	A	106	GLN	H	8.506	0.02	1
1	A	106	GLN	HA	4.486	0.02	1
1	A	106	GLN	HB2	2.188	0.02	2
1	A	106	GLN	HB3	2.023	0.02	2
1	A	106	GLN	HG2	2.415	0.02	2
1	A	106	GLN	HG3	2.415	0.02	2
1	A	106	GLN	C	175.841	0.1	1
1	A	106	GLN	CA	55.813	0.1	1
1	A	106	GLN	CB	29.964	0.1	1
1	A	106	GLN	CG	33.978	0.1	1
1	A	106	GLN	N	122.267	0.1	1
1	A	107	THR	H	8.297	0.02	1
1	A	107	THR	CA	60.092	0.1	1
1	A	107	THR	CB	70.101	0.1	1
1	A	107	THR	N	118.211	0.1	1
1	A	108	PRO	HA	4.486	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	PRO	HB2	2.34	0.02	2
1	A	108	PRO	HB3	1.957	0.02	2
1	A	108	PRO	HD2	3.906	0.02	2
1	A	108	PRO	HD3	3.76	0.02	2
1	A	108	PRO	HG2	2.059	0.02	2
1	A	108	PRO	HG3	2.059	0.02	2
1	A	108	PRO	C	176.862	0.1	1
1	A	108	PRO	CA	63.504	0.1	1
1	A	108	PRO	CB	32.485	0.1	1
1	A	108	PRO	CD	51.31	0.1	1
1	A	108	PRO	CG	27.775	0.1	1
1	A	109	LYS	H	8.453	0.02	1
1	A	109	LYS	HA	4.383	0.02	1
1	A	109	LYS	HB2	1.88	0.02	2
1	A	109	LYS	HB3	1.88	0.02	2
1	A	109	LYS	HD2	1.735	0.02	2
1	A	109	LYS	HD3	1.735	0.02	2
1	A	109	LYS	HE2	3.106	0.02	2
1	A	109	LYS	HE3	3.106	0.02	2
1	A	109	LYS	HG2	1.495	0.02	2
1	A	109	LYS	HG3	1.495	0.02	2
1	A	109	LYS	C	176.731	0.1	1
1	A	109	LYS	CA	56.463	0.1	1
1	A	109	LYS	CB	33.522	0.1	1
1	A	109	LYS	CD	29.234	0.1	1
1	A	109	LYS	CG	25.038	0.1	1
1	A	109	LYS	N	121.556	0.1	1
1	A	110	GLY	H	8.213	0.02	1
1	A	110	GLY	CA	44.222	0.1	1
1	A	110	GLY	N	110.094	0.1	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	109	-0.07 ± 0.34	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	99	-0.11 ± 0.24	None needed (< 0.5 ppm)
$^{13}C'$	98	-0.05 ± 0.17	None needed (< 0.5 ppm)
^{15}N	98	0.08 ± 0.68	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 765 atoms were assigned a chemical shift out of a possible 916. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	295/306 (96%)	117/122 (96%)	120/126 (95%)	58/58 (100%)
Sidechain	438/562 (78%)	297/364 (82%)	141/170 (83%)	0/28 (0%)
Aromatic	32/48 (67%)	18/23 (78%)	13/22 (59%)	1/3 (33%)
Overall	765/916 (84%)	432/509 (85%)	274/318 (86%)	59/89 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 811 atoms were assigned a chemical shift out of a possible 978. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	325/343 (95%)	130/138 (94%)	132/140 (94%)	63/65 (97%)
Sidechain	454/587 (77%)	308/379 (81%)	146/179 (82%)	0/29 (0%)
Aromatic	32/48 (67%)	18/23 (78%)	13/22 (59%)	1/3 (33%)
Overall	811/978 (83%)	456/540 (84%)	291/341 (85%)	64/97 (66%)

7.1.4 Statistically unusual chemical shifts

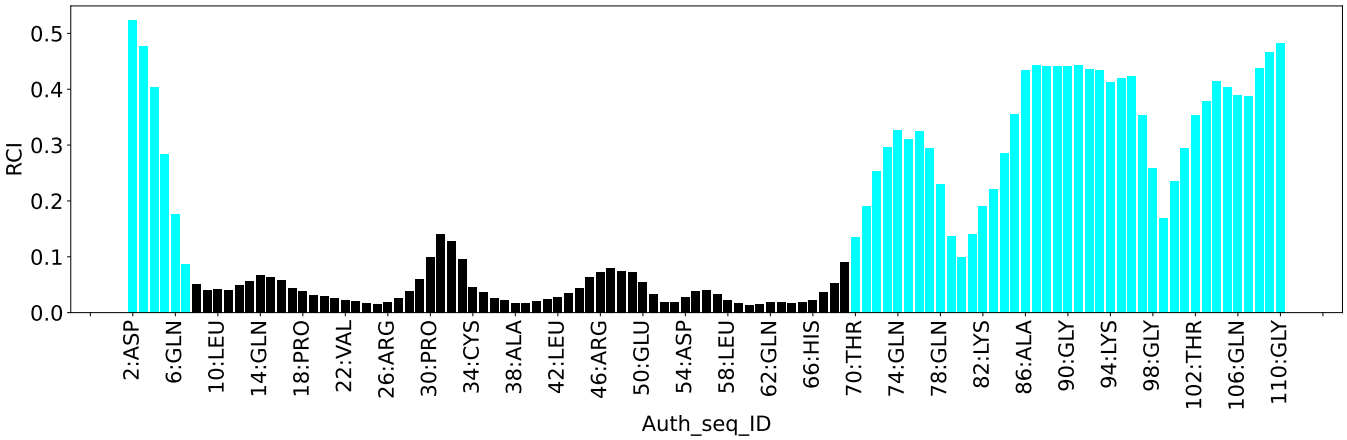
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	39	ILE	CG2	9.51	10.93 – 24.12	-6.1
1	A	60	VAL	HG21	-0.59	-0.58 – 2.19	-5.0
1	A	60	VAL	HG22	-0.59	-0.58 – 2.19	-5.0
1	A	60	VAL	HG23	-0.59	-0.58 – 2.19	-5.0

7.1.5 Random Coil Index (RCI) plots

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	592
Intra-residue (|i-j|=0)	265
Sequential (|i-j|=1)	150
Medium range (|i-j|>1 and |i-j|<5)	54
Long range (|i-j|≥5)	121
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	2
Total dihedral-angle restraints	89
Number of unmapped restraints	0
Number of restraints per residue	6.0
Number of long range restraints per residue[1]	1.1

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

8.2 Residual restraint violations

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)	10.8	0.2
0.2-0.5 (Medium)	3.5	0.4
>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)	7.3	3.15
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

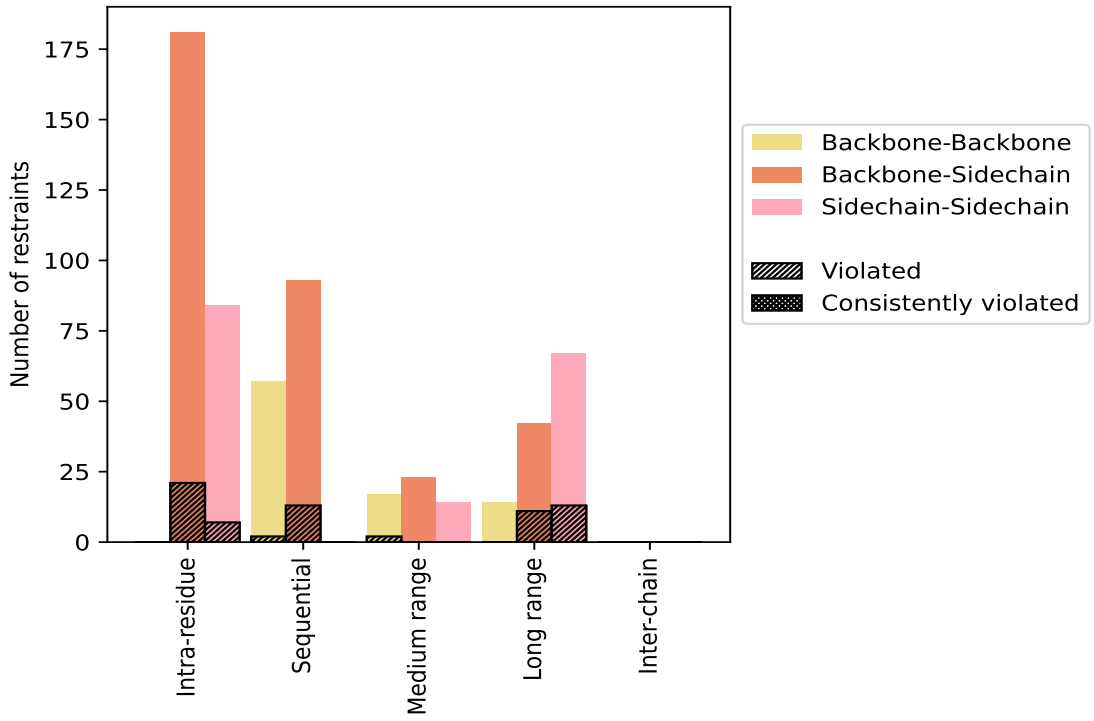
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	265	44.8	28	10.6	4.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	181	30.6	21	11.6	3.5	0	0.0	0.0
Sidechain-Sidechain	84	14.2	7	8.3	1.2	0	0.0	0.0
Sequential (|i-j|=1)	150	25.3	15	10.0	2.5	0	0.0	0.0
Backbone-Backbone	57	9.6	2	3.5	0.3	0	0.0	0.0
Backbone-Sidechain	93	15.7	13	14.0	2.2	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	54	9.1	2	3.7	0.3	0	0.0	0.0
Backbone-Backbone	17	2.9	2	11.8	0.3	0	0.0	0.0
Backbone-Sidechain	23	3.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	14	2.4	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	121	20.4	24	19.8	4.1	0	0.0	0.0
Backbone-Backbone	14	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	42	7.1	11	26.2	1.9	0	0.0	0.0
Sidechain-Sidechain	65	11.0	13	20.0	2.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	2	0.3	0	0.0	0.0	0	0.0	0.0
Total	592	100.0	69	11.7	11.7	0	0.0	0.0
Backbone-Backbone	88	14.9	4	4.5	0.7	0	0.0	0.0
Backbone-Sidechain	339	57.3	45	13.3	7.6	0	0.0	0.0
Sidechain-Sidechain	165	27.9	20	12.1	3.4	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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	8	2	1	4	0	15	0.17	0.26	0.06	0.14
2	7	3	2	4	0	16	0.17	0.3	0.05	0.14
3	7	4	0	4	0	15	0.15	0.3	0.05	0.12
4	8	1	1	3	0	13	0.17	0.3	0.06	0.18
5	5	3	1	6	0	15	0.16	0.29	0.05	0.15
6	7	6	1	6	0	20	0.16	0.31	0.06	0.14
7	8	7	2	2	0	19	0.15	0.27	0.05	0.14
8	6	3	1	3	0	13	0.16	0.27	0.05	0.15
9	8	4	2	3	0	17	0.16	0.29	0.05	0.13
10	6	4	1	3	0	14	0.17	0.29	0.06	0.16

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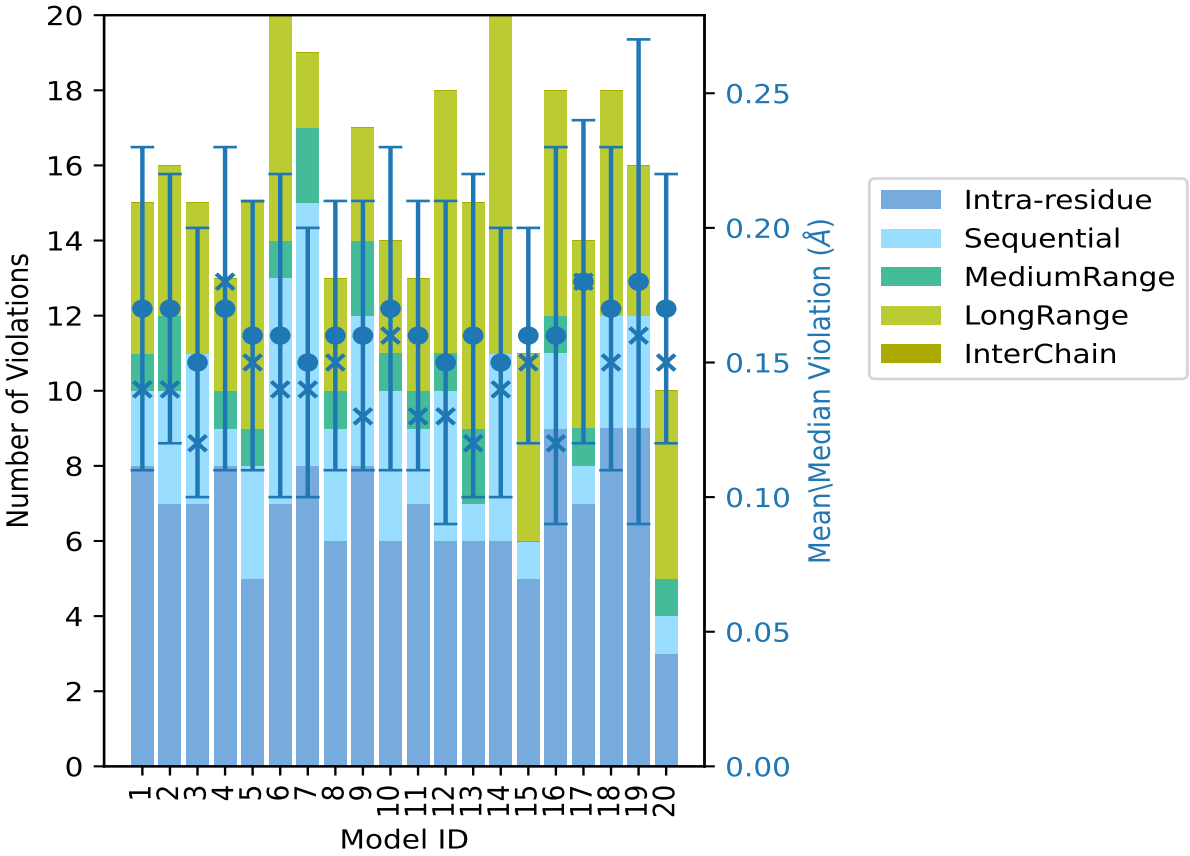
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	7	2	1	3	0	13	0.16	0.27	0.05	0.13
12	6	4	1	7	0	18	0.15	0.31	0.06	0.13
13	6	1	2	6	0	15	0.16	0.29	0.06	0.12
14	6	5	0	9	0	20	0.15	0.24	0.05	0.14
15	5	1	0	5	0	11	0.16	0.26	0.04	0.15
16	9	2	1	6	0	18	0.16	0.32	0.07	0.12
17	7	1	1	5	0	14	0.18	0.3	0.06	0.18
18	9	3	0	6	0	18	0.17	0.3	0.06	0.15
19	9	3	0	4	0	16	0.18	0.4	0.09	0.16
20	3	1	1	5	0	10	0.17	0.28	0.05	0.15

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

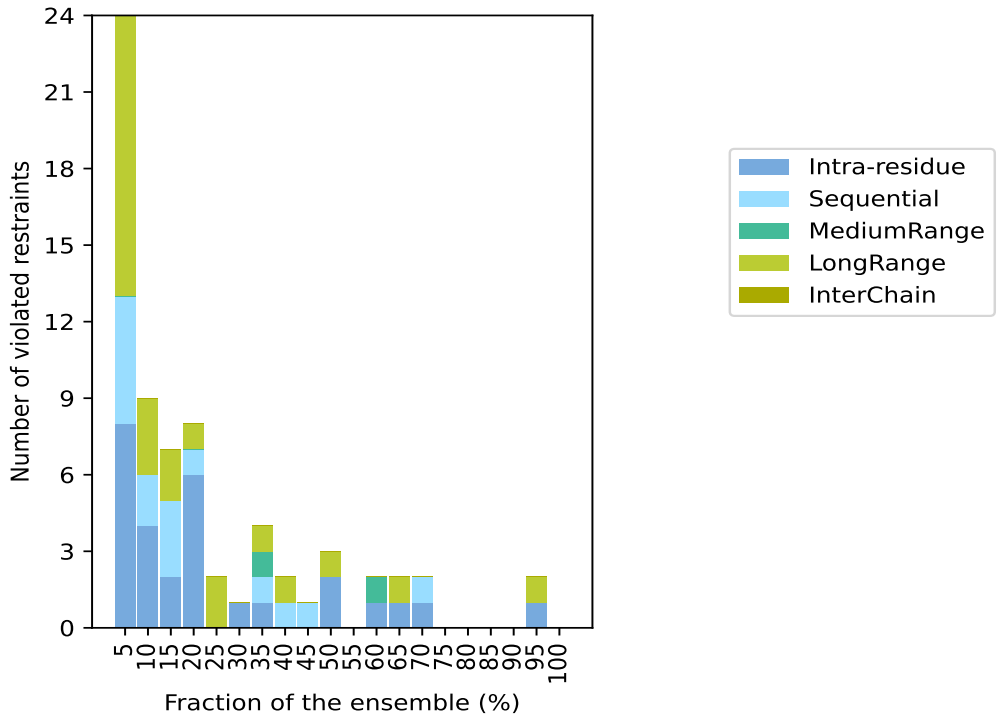
9.3 Distance violation statistics for the ensemble (i)

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, 521(IR:237, SQ:135, MR:52, LR:97, 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]	%
8	5	0	11	0	24	1	5.0
4	2	0	3	0	9	2	10.0
2	3	0	2	0	7	3	15.0
6	1	0	1	0	8	4	20.0
0	0	0	2	0	2	5	25.0
1	0	0	0	0	1	6	30.0
1	1	1	1	0	4	7	35.0
0	1	0	1	0	2	8	40.0
0	1	0	0	0	1	9	45.0
2	0	0	1	0	3	10	50.0
0	0	0	0	0	0	11	55.0
1	0	1	0	0	2	12	60.0
1	0	0	1	0	2	13	65.0
1	1	0	0	0	2	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
1	0	0	1	0	2	19	95.0
0	0	0	0	0	0	20	100.0

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

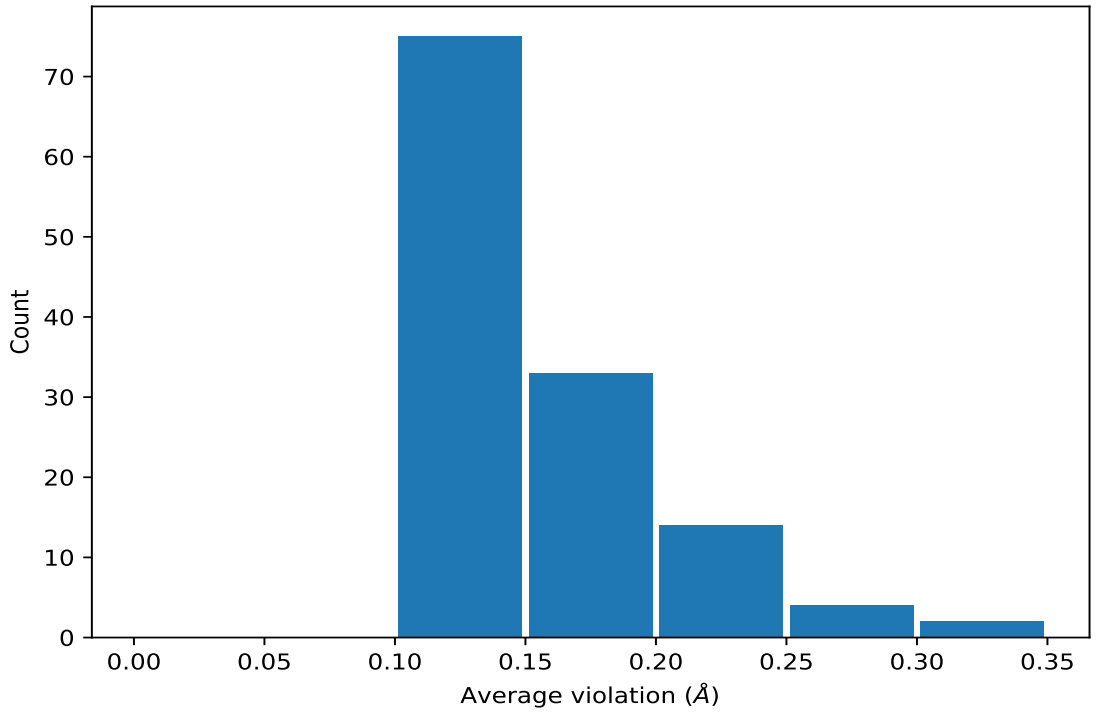
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation 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)
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	19	0.19	0.06	0.18
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	19	0.19	0.06	0.18
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	19	0.16	0.06	0.14
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	19	0.16	0.06	0.14
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	14	0.24	0.06	0.24
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	14	0.24	0.06	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	14	0.13	0.02	0.12
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	13	0.19	0.02	0.19
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	13	0.19	0.02	0.19
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	13	0.13	0.02	0.12
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	12	0.25	0.06	0.26
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	12	0.25	0.06	0.26
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	12	0.14	0.03	0.12
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	10	0.23	0.04	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	10	0.23	0.04	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	10	0.23	0.04	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	10	0.23	0.04	0.22
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	10	0.23	0.04	0.22
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	10	0.23	0.04	0.22
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	10	0.12	0.01	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	10	0.12	0.01	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	10	0.12	0.01	0.12
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	9	0.21	0.06	0.24
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	8	0.15	0.03	0.14
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	8	0.12	0.01	0.12
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	8	0.12	0.01	0.12
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	8	0.12	0.01	0.12
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	7	0.2	0.05	0.23
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE3	7	0.2	0.05	0.23
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	7	0.2	0.05	0.23
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	7	0.2	0.05	0.23
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB1	7	0.12	0.01	0.12
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB2	7	0.12	0.01	0.12
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB3	7	0.12	0.01	0.12
(1,121)	1:20:A:LYS:HG2	1:21:A:VAL:H	7	0.12	0.02	0.12
(1,121)	1:20:A:LYS:HG3	1:21:A:VAL:H	7	0.12	0.02	0.12
(1,568)	1:67:A:LEU:HA	1:69:A:LYS:H	7	0.12	0.01	0.11
(1,377)	1:45:A:LYS:HA	1:45:A:LYS:HB2	6	0.21	0.01	0.21
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB1	5	0.14	0.02	0.14
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB2	5	0.14	0.02	0.14
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB3	5	0.14	0.02	0.14
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB1	5	0.14	0.02	0.14
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB2	5	0.14	0.02	0.14
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB3	5	0.14	0.02	0.14
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD11	5	0.12	0.02	0.11
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD12	5	0.12	0.02	0.11
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD13	5	0.12	0.02	0.11
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE2	4	0.16	0.07	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE3	4	0.16	0.07	0.14
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD2	4	0.15	0.03	0.15
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD3	4	0.15	0.03	0.15
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD2	4	0.15	0.03	0.15
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD3	4	0.15	0.03	0.15
(1,133)	1:22:A:VAL:HB	1:23:A:ARG:H	4	0.15	0.0	0.15
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG2	4	0.14	0.06	0.11
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG3	4	0.14	0.06	0.11
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD2	4	0.14	0.01	0.14
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD3	4	0.14	0.01	0.14
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD2	4	0.13	0.02	0.14
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD3	4	0.13	0.02	0.14
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD2	4	0.13	0.02	0.14
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD3	4	0.13	0.02	0.14
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD2	4	0.13	0.02	0.12
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD3	4	0.13	0.02	0.12
(1,251)	1:30:A:PRO:HG3	1:38:A:ALA:H	4	0.11	0.01	0.12
(1,118)	1:20:A:LYS:HD2	1:21:A:VAL:H	3	0.25	0.03	0.23
(1,118)	1:20:A:LYS:HD3	1:21:A:VAL:H	3	0.25	0.03	0.23
(1,587)	1:69:A:LYS:HB2	1:70:A:THR:H	3	0.16	0.05	0.13
(1,587)	1:69:A:LYS:HB3	1:70:A:THR:H	3	0.16	0.05	0.13
(1,183)	1:25:A:TYR:HD1	1:63:A:LEU:HB2	3	0.13	0.01	0.14
(1,183)	1:25:A:TYR:HD1	1:63:A:LEU:HB3	3	0.13	0.01	0.14
(1,183)	1:25:A:TYR:HD2	1:63:A:LEU:HB2	3	0.13	0.01	0.14
(1,183)	1:25:A:TYR:HD2	1:63:A:LEU:HB3	3	0.13	0.01	0.14
(1,580)	1:69:A:LYS:H	1:69:A:LYS:HD2	3	0.13	0.01	0.13
(1,580)	1:69:A:LYS:H	1:69:A:LYS:HD3	3	0.13	0.01	0.13
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD11	3	0.12	0.0	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD12	3	0.12	0.0	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD13	3	0.12	0.0	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD21	3	0.12	0.0	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD22	3	0.12	0.0	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD23	3	0.12	0.0	0.12
(1,513)	1:61:A:GLN:H	1:61:A:GLN:HG2	3	0.12	0.01	0.12
(1,513)	1:61:A:GLN:H	1:61:A:GLN:HG3	3	0.12	0.01	0.12
(1,280)	1:37:A:PRO:HG2	1:38:A:ALA:H	3	0.11	0.01	0.11
(1,280)	1:37:A:PRO:HG3	1:38:A:ALA:H	3	0.11	0.01	0.11
(1,367)	1:44:A:ARG:HA	1:44:A:ARG:HD2	2	0.3	0.02	0.3
(1,367)	1:44:A:ARG:HA	1:44:A:ARG:HD3	2	0.3	0.02	0.3
(1,424)	1:51:A:LEU:HG	1:52:A:CYS:H	2	0.18	0.04	0.18
(1,36)	1:10:A:LEU:HD11	1:50:A:GLU:H	2	0.16	0.01	0.16
(1,36)	1:10:A:LEU:HD12	1:50:A:GLU:H	2	0.16	0.01	0.16

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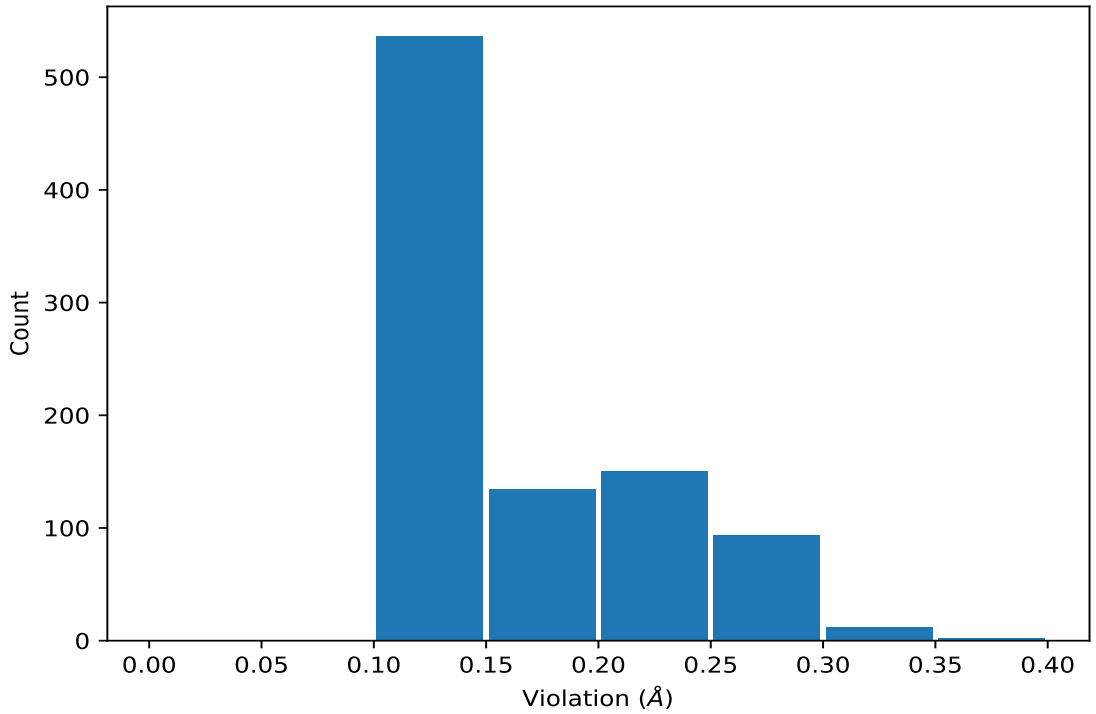
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,36)	1:10:A:LEU:HD13	1:50:A:GLU:H	2	0.16	0.01	0.16
(1,36)	1:10:A:LEU:HD21	1:50:A:GLU:H	2	0.16	0.01	0.16
(1,36)	1:10:A:LEU:HD22	1:50:A:GLU:H	2	0.16	0.01	0.16
(1,36)	1:10:A:LEU:HD23	1:50:A:GLU:H	2	0.16	0.01	0.16
(1,204)	1:26:A:ARG:HA	1:26:A:ARG:HD2	2	0.14	0.03	0.14
(1,204)	1:26:A:ARG:HA	1:26:A:ARG:HD3	2	0.14	0.03	0.14
(1,323)	1:40:A:LEU:HD21	1:52:A:CYS:H	2	0.12	0.0	0.12
(1,323)	1:40:A:LEU:HD22	1:52:A:CYS:H	2	0.12	0.0	0.12
(1,323)	1:40:A:LEU:HD23	1:52:A:CYS:H	2	0.12	0.0	0.12
(1,37)	1:10:A:LEU:HD11	1:50:A:GLU:HB2	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD11	1:50:A:GLU:HB3	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD12	1:50:A:GLU:HB2	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD12	1:50:A:GLU:HB3	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD13	1:50:A:GLU:HB2	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD13	1:50:A:GLU:HB3	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD21	1:50:A:GLU:HB2	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD21	1:50:A:GLU:HB3	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD22	1:50:A:GLU:HB2	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD22	1:50:A:GLU:HB3	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD23	1:50:A:GLU:HB2	2	0.11	0.0	0.11
(1,37)	1:10:A:LEU:HD23	1:50:A:GLU:HB3	2	0.11	0.0	0.11
(1,449)	1:56:A:LYS:HA	1:56:A:LYS:HD2	2	0.11	0.01	0.11
(1,449)	1:56:A:LYS:HA	1:56:A:LYS:HD3	2	0.11	0.01	0.11
(1,297)	1:39:A:ILE:HD11	1:40:A:LEU:H	2	0.11	0.0	0.11
(1,297)	1:39:A:ILE:HD12	1:40:A:LEU:H	2	0.11	0.0	0.11
(1,297)	1:39:A:ILE:HD13	1:40:A:LEU:H	2	0.11	0.0	0.11
(1,214)	1:27:A:LYS:H	1:27:A:LYS:HD2	2	0.1	0.0	0.1
(1,214)	1:27:A:LYS:H	1:27:A:LYS:HD3	2	0.1	0.0	0.1

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations ⓘ

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	19	0.4
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	19	0.4
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	19	0.34
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	19	0.34
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	19	0.34
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	19	0.34
(1,367)	1:44:A:ARG:HA	1:44:A:ARG:HD2	19	0.32
(1,367)	1:44:A:ARG:HA	1:44:A:ARG:HD3	19	0.32
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	16	0.32
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	16	0.32
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	12	0.31
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	12	0.31
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	6	0.31
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	6	0.31
(1,227)	1:27:A:LYS:HB2	1:27:A:LYS:HE2	17	0.3
(1,227)	1:27:A:LYS:HB2	1:27:A:LYS:HE3	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:27:A:LYS:HB3	1:27:A:LYS:HE2	17	0.3
(1,227)	1:27:A:LYS:HB3	1:27:A:LYS:HE3	17	0.3
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	2	0.3
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	2	0.3
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	3	0.3
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	3	0.3
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	4	0.3
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	4	0.3
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	4	0.3
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	4	0.3
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	4	0.3
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	4	0.3
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	4	0.3
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	4	0.3
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	4	0.3
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	4	0.3
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	4	0.3
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	4	0.3
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	18	0.3
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	18	0.3
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	18	0.3
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	18	0.3
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	18	0.3
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	18	0.3
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	18	0.3
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	18	0.3
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	18	0.3
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	18	0.3
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	18	0.3
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	18	0.3
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	6	0.3
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	5	0.29
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	5	0.29
(1,367)	1:44:A:ARG:HA	1:44:A:ARG:HD2	6	0.29
(1,367)	1:44:A:ARG:HA	1:44:A:ARG:HD3	6	0.29
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	12	0.29
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	12	0.29
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	9	0.29
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	9	0.29
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	13	0.29
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	13	0.29
(1,118)	1:20:A:LYS:HD2	1:21:A:VAL:H	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:20:A:LYS:HD3	1:21:A:VAL:H	10	0.29
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	16	0.29
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	16	0.29
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	16	0.29
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	16	0.29
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	16	0.29
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	16	0.29
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	16	0.29
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	16	0.29
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	16	0.29
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	16	0.29
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	16	0.29
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	16	0.29
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	18	0.28
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	18	0.28
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	20	0.28
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	20	0.28
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	10	0.28
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE2	16	0.27
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE3	16	0.27
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	8	0.27
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	8	0.27
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	13	0.27
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	13	0.27
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	9	0.27
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	9	0.27
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	11	0.27
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	11	0.27
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	7	0.27
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	15	0.26
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	15	0.26
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	1	0.26
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	1	0.26
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	17	0.26
(1,542)	1:64:A:MET:H	1:64:A:MET:HG2	2	0.25
(1,542)	1:64:A:MET:H	1:64:A:MET:HG3	2	0.25
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	1	0.25
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE3	1	0.25
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	1	0.25
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	1	0.25
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG2	7	0.25
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG3	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	1	0.25
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	1	0.25
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	10	0.25
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	10	0.25
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	4	0.25
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	4	0.25
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	5	0.25
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	5	0.25
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	2	0.24
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE3	2	0.24
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	2	0.24
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	2	0.24
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	15	0.24
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE3	15	0.24
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	15	0.24
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	15	0.24
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	14	0.24
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	14	0.24
(1,348)	1:41:A:PHE:HE1	1:63:A:LEU:HG	18	0.24
(1,78)	1:16:A:LYS:HA	1:16:A:LYS:HD2	17	0.24
(1,78)	1:16:A:LYS:HA	1:16:A:LYS:HD3	17	0.24
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	13	0.24
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	13	0.24
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	13	0.24
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	13	0.24
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	18	0.24
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	18	0.24
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	18	0.24
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	18	0.24
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	14	0.24
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	14	0.24
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	14	0.24
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	14	0.24
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	14	0.24
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	14	0.24
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	14	0.24
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	14	0.24
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	14	0.24
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	14	0.24
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	14	0.24
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	14	0.24
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:69:A:LYS:HB2	1:70:A:THR:H	14	0.23
(1,587)	1:69:A:LYS:HB3	1:70:A:THR:H	14	0.23
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	16	0.23
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE3	16	0.23
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	16	0.23
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	16	0.23
(1,377)	1:45:A:LYS:HA	1:45:A:LYS:HB2	20	0.23
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	1	0.23
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	1	0.23
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	11	0.23
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	11	0.23
(1,118)	1:20:A:LYS:HD2	1:21:A:VAL:H	7	0.23
(1,118)	1:20:A:LYS:HD3	1:21:A:VAL:H	7	0.23
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	17	0.23
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	17	0.23
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	17	0.23
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	17	0.23
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	19	0.23
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	19	0.23
(1,424)	1:51:A:LEU:HG	1:52:A:CYS:H	6	0.22
(1,377)	1:45:A:LYS:HA	1:45:A:LYS:HB2	3	0.22
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	4	0.22
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	4	0.22
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	18	0.22
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	18	0.22
(1,118)	1:20:A:LYS:HD2	1:21:A:VAL:H	5	0.22
(1,118)	1:20:A:LYS:HD3	1:21:A:VAL:H	5	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	4	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	4	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	4	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	4	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	7	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	7	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	7	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	7	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	8	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	8	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	8	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	8	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	20	0.22
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	20	0.22
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	20	0.22
(1,377)	1:45:A:LYS:HA	1:45:A:LYS:HB2	13	0.21
(1,377)	1:45:A:LYS:HA	1:45:A:LYS:HB2	18	0.21
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	11	0.21
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	11	0.21
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	17	0.21
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	17	0.21
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	11	0.21
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	11	0.21
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	11	0.21
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	11	0.21
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	3	0.21
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	3	0.21
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	3	0.21
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	3	0.21
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	3	0.21
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	3	0.21
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	3	0.21
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	3	0.21
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	3	0.21
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	3	0.21
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	3	0.21
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	3	0.21
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	9	0.21
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	9	0.21
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	9	0.21
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	9	0.21
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	9	0.21
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	9	0.21
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	9	0.21
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	9	0.21
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	9	0.21
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	9	0.21
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	9	0.21
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	9	0.21
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	12	0.2
(1,377)	1:45:A:LYS:HA	1:45:A:LYS:HB2	4	0.2
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	2	0.2
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	2	0.2
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	8	0.2
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	8	0.2
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	1	0.2
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	1	0.2
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	5	0.2
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	5	0.2
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE2	1	0.2
(1,45)	1:11:A:LYS:HB2	1:11:A:LYS:HE3	1	0.2
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE2	1	0.2
(1,45)	1:11:A:LYS:HB3	1:11:A:LYS:HE3	1	0.2
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	1	0.2
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	1	0.2
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	1	0.2
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	1	0.2
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	1	0.2
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	1	0.2
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	1	0.2
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	1	0.2
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	1	0.2
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	1	0.2
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	1	0.2
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	1	0.2
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	20	0.2
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	20	0.2
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	20	0.2
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	20	0.2
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	20	0.2
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	20	0.2
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	20	0.2
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	20	0.2
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	20	0.2
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	20	0.2
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	20	0.2
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	20	0.2
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	10	0.19
(1,377)	1:45:A:LYS:HA	1:45:A:LYS:HB2	6	0.19
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	7	0.19
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	7	0.19
(1,209)	1:26:A:ARG:HB2	1:40:A:LEU:HD11	5	0.19
(1,209)	1:26:A:ARG:HB2	1:40:A:LEU:HD12	5	0.19
(1,209)	1:26:A:ARG:HB2	1:40:A:LEU:HD13	5	0.19
(1,209)	1:26:A:ARG:HB2	1:40:A:LEU:HD21	5	0.19
(1,209)	1:26:A:ARG:HB2	1:40:A:LEU:HD22	5	0.19
(1,209)	1:26:A:ARG:HB2	1:40:A:LEU:HD23	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:26:A:ARG:HB3	1:40:A:LEU:HD11	5	0.19
(1,209)	1:26:A:ARG:HB3	1:40:A:LEU:HD12	5	0.19
(1,209)	1:26:A:ARG:HB3	1:40:A:LEU:HD13	5	0.19
(1,209)	1:26:A:ARG:HB3	1:40:A:LEU:HD21	5	0.19
(1,209)	1:26:A:ARG:HB3	1:40:A:LEU:HD22	5	0.19
(1,209)	1:26:A:ARG:HB3	1:40:A:LEU:HD23	5	0.19
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	3	0.19
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	3	0.19
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	7	0.19
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	7	0.19
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	19	0.19
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	19	0.19
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	12	0.19
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	12	0.19
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	2	0.19
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	2	0.19
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	2	0.19
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	2	0.19
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	2	0.19
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	2	0.19
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	2	0.19
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	2	0.19
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	2	0.19
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	2	0.19
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	2	0.19
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	2	0.19
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	19	0.18
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	9	0.18
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	9	0.18
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	16	0.18
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	16	0.18
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	17	0.18
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	17	0.18
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	6	0.18
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	6	0.18
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	19	0.18
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	19	0.18
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	4	0.18
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	4	0.18
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	2	0.18
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	2	0.18
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	4	0.18
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	8	0.18
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	8	0.18
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD2	18	0.18
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD3	18	0.18
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD2	18	0.18
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD3	18	0.18
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	10	0.18
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	10	0.18
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	10	0.18
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	10	0.18
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	10	0.18
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	10	0.18
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	10	0.18
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	10	0.18
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	10	0.18
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	10	0.18
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	10	0.18
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	10	0.18
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	17	0.18
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	17	0.18
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	17	0.18
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	17	0.18
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	17	0.18
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	17	0.18
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	17	0.18
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	17	0.18
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	17	0.18
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	17	0.18
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	17	0.18
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	17	0.18
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	14	0.17
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	9	0.17
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	10	0.17
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE2	7	0.17
(1,218)	1:27:A:LYS:HA	1:27:A:LYS:HE3	7	0.17
(1,204)	1:26:A:ARG:HA	1:26:A:ARG:HD2	5	0.17
(1,204)	1:26:A:ARG:HA	1:26:A:ARG:HD3	5	0.17
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	3	0.17
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	3	0.17
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	14	0.17
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	17	0.17
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD2	10	0.17
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD3	10	0.17
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD2	10	0.17
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD3	10	0.17
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	15	0.17
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	15	0.17
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	15	0.17
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	15	0.17
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	15	0.17
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	15	0.17
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	15	0.17
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	15	0.17
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	15	0.17
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	15	0.17
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	15	0.17
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	15	0.17
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB1	15	0.17
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB2	15	0.17
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB3	15	0.17
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB1	15	0.17
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB2	15	0.17
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB3	15	0.17
(1,404)	1:48:A:GLN:HB2	1:49:A:ALA:H	3	0.16
(1,404)	1:48:A:GLN:HB3	1:49:A:ALA:H	3	0.16
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	7	0.16
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	7	0.16
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	8	0.16
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	8	0.16
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	5	0.16
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	19	0.16
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD2	12	0.16
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD3	12	0.16
(1,36)	1:10:A:LEU:HD11	1:50:A:GLU:H	20	0.16
(1,36)	1:10:A:LEU:HD12	1:50:A:GLU:H	20	0.16
(1,36)	1:10:A:LEU:HD13	1:50:A:GLU:H	20	0.16
(1,36)	1:10:A:LEU:HD21	1:50:A:GLU:H	20	0.16
(1,36)	1:10:A:LEU:HD22	1:50:A:GLU:H	20	0.16
(1,36)	1:10:A:LEU:HD23	1:50:A:GLU:H	20	0.16
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	2	0.16
(1,584)	1:69:A:LYS:HB2	1:69:A:LYS:HD2	6	0.15
(1,584)	1:69:A:LYS:HB2	1:69:A:LYS:HD3	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,584)	1:69:A:LYS:HB3	1:69:A:LYS:HD2	6	0.15
(1,584)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	6	0.15
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE2	9	0.15
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE3	9	0.15
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	10	0.15
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE3	10	0.15
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	10	0.15
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	10	0.15
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	2	0.15
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	16	0.15
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD2	17	0.15
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD3	17	0.15
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	7	0.15
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD2	11	0.15
(1,376)	1:45:A:LYS:H	1:45:A:LYS:HD3	11	0.15
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	18	0.15
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	18	0.15
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	18	0.15
(1,299)	1:39:A:ILE:HD11	1:60:A:VAL:HG11	9	0.15
(1,299)	1:39:A:ILE:HD11	1:60:A:VAL:HG12	9	0.15
(1,299)	1:39:A:ILE:HD11	1:60:A:VAL:HG13	9	0.15
(1,299)	1:39:A:ILE:HD11	1:60:A:VAL:HG21	9	0.15
(1,299)	1:39:A:ILE:HD11	1:60:A:VAL:HG22	9	0.15
(1,299)	1:39:A:ILE:HD11	1:60:A:VAL:HG23	9	0.15
(1,299)	1:39:A:ILE:HD12	1:60:A:VAL:HG11	9	0.15
(1,299)	1:39:A:ILE:HD12	1:60:A:VAL:HG12	9	0.15
(1,299)	1:39:A:ILE:HD12	1:60:A:VAL:HG13	9	0.15
(1,299)	1:39:A:ILE:HD12	1:60:A:VAL:HG21	9	0.15
(1,299)	1:39:A:ILE:HD12	1:60:A:VAL:HG22	9	0.15
(1,299)	1:39:A:ILE:HD12	1:60:A:VAL:HG23	9	0.15
(1,299)	1:39:A:ILE:HD13	1:60:A:VAL:HG11	9	0.15
(1,299)	1:39:A:ILE:HD13	1:60:A:VAL:HG12	9	0.15
(1,299)	1:39:A:ILE:HD13	1:60:A:VAL:HG13	9	0.15
(1,299)	1:39:A:ILE:HD13	1:60:A:VAL:HG21	9	0.15
(1,299)	1:39:A:ILE:HD13	1:60:A:VAL:HG22	9	0.15
(1,299)	1:39:A:ILE:HD13	1:60:A:VAL:HG23	9	0.15
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD11	6	0.15
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD12	6	0.15
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD13	6	0.15
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	12	0.15
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	12	0.15
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	14	0.15
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG2	15	0.15
(1,149)	1:23:A:ARG:H	1:23:A:ARG:HG3	15	0.15
(1,133)	1:22:A:VAL:HB	1:23:A:ARG:H	5	0.15
(1,133)	1:22:A:VAL:HB	1:23:A:ARG:H	11	0.15
(1,121)	1:20:A:LYS:HG2	1:21:A:VAL:H	14	0.15
(1,121)	1:20:A:LYS:HG3	1:21:A:VAL:H	14	0.15
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD2	15	0.15
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD3	15	0.15
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD2	15	0.15
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD3	15	0.15
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	6	0.15
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	6	0.15
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	6	0.15
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	6	0.15
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	6	0.15
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	6	0.15
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	6	0.15
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	6	0.15
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	6	0.15
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	6	0.15
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	6	0.15
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	6	0.15
(1,36)	1:10:A:LEU:HD11	1:50:A:GLU:H	15	0.15
(1,36)	1:10:A:LEU:HD12	1:50:A:GLU:H	15	0.15
(1,36)	1:10:A:LEU:HD13	1:50:A:GLU:H	15	0.15
(1,36)	1:10:A:LEU:HD21	1:50:A:GLU:H	15	0.15
(1,36)	1:10:A:LEU:HD22	1:50:A:GLU:H	15	0.15
(1,36)	1:10:A:LEU:HD23	1:50:A:GLU:H	15	0.15
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB1	14	0.15
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB2	14	0.15
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB3	14	0.15
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB1	14	0.15
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB2	14	0.15
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB3	14	0.15
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	8	0.15
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	19	0.15
(1,7)	1:6:A:GLN:H	1:6:A:GLN:HG2	18	0.15
(1,7)	1:6:A:GLN:H	1:6:A:GLN:HG3	18	0.15
(1,580)	1:69:A:LYS:H	1:69:A:LYS:HD2	14	0.14
(1,580)	1:69:A:LYS:H	1:69:A:LYS:HD3	14	0.14
(1,568)	1:67:A:LEU:HA	1:69:A:LYS:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	14	0.14
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE3	14	0.14
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	14	0.14
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	14	0.14
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	12	0.14
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	20	0.14
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD2	6	0.14
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD3	6	0.14
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD2	13	0.14
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD3	13	0.14
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB1	15	0.14
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB2	15	0.14
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB3	15	0.14
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB1	17	0.14
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB2	17	0.14
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB3	17	0.14
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	19	0.14
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	19	0.14
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	19	0.14
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	7	0.14
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD11	1	0.14
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD12	1	0.14
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD13	1	0.14
(1,183)	1:25:A:TYR:HD1	1:63:A:LEU:HB2	13	0.14
(1,183)	1:25:A:TYR:HD1	1:63:A:LEU:HB3	13	0.14
(1,183)	1:25:A:TYR:HD2	1:63:A:LEU:HB2	13	0.14
(1,183)	1:25:A:TYR:HD2	1:63:A:LEU:HB3	13	0.14
(1,183)	1:25:A:TYR:HD1	1:63:A:LEU:HB2	20	0.14
(1,183)	1:25:A:TYR:HD1	1:63:A:LEU:HB3	20	0.14
(1,183)	1:25:A:TYR:HD2	1:63:A:LEU:HB2	20	0.14
(1,183)	1:25:A:TYR:HD2	1:63:A:LEU:HB3	20	0.14
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	10	0.14
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	10	0.14
(1,133)	1:22:A:VAL:HB	1:23:A:ARG:H	6	0.14
(1,133)	1:22:A:VAL:HB	1:23:A:ARG:H	18	0.14
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD2	10	0.14
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD3	10	0.14
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD2	10	0.14
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD3	10	0.14
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	5	0.14
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	5	0.14
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	5	0.14
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	5	0.14
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	5	0.14
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	5	0.14
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	5	0.14
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	5	0.14
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	5	0.14
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	5	0.14
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	5	0.14
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	12	0.14
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	12	0.14
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	12	0.14
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	12	0.14
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	12	0.14
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	12	0.14
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	12	0.14
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	12	0.14
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	12	0.14
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	12	0.14
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	12	0.14
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	12	0.14
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB1	13	0.14
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB2	13	0.14
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB3	13	0.14
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB1	13	0.14
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB2	13	0.14
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB3	13	0.14
(1,587)	1:69:A:LYS:HB2	1:70:A:THR:H	9	0.13
(1,587)	1:69:A:LYS:HB3	1:70:A:THR:H	9	0.13
(1,587)	1:69:A:LYS:HB2	1:70:A:THR:H	18	0.13
(1,587)	1:69:A:LYS:HB3	1:70:A:THR:H	18	0.13
(1,585)	1:69:A:LYS:HB2	1:69:A:LYS:HE2	16	0.13
(1,585)	1:69:A:LYS:HB2	1:69:A:LYS:HE3	16	0.13
(1,585)	1:69:A:LYS:HB3	1:69:A:LYS:HE2	16	0.13
(1,585)	1:69:A:LYS:HB3	1:69:A:LYS:HE3	16	0.13
(1,580)	1:69:A:LYS:H	1:69:A:LYS:HD2	18	0.13
(1,580)	1:69:A:LYS:H	1:69:A:LYS:HD3	18	0.13
(1,568)	1:67:A:LEU:HA	1:69:A:LYS:H	2	0.13
(1,513)	1:61:A:GLN:H	1:61:A:GLN:HG2	3	0.13
(1,513)	1:61:A:GLN:H	1:61:A:GLN:HG3	3	0.13
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	9	0.13
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:51:A:LEU:HG	1:52:A:CYS:H	9	0.13
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	12	0.13
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	12	0.13
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	12	0.13
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	14	0.13
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	14	0.13
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	14	0.13
(1,345)	1:41:A:PHE:HD1	1:67:A:LEU:HD11	14	0.13
(1,345)	1:41:A:PHE:HD1	1:67:A:LEU:HD12	14	0.13
(1,345)	1:41:A:PHE:HD1	1:67:A:LEU:HD13	14	0.13
(1,345)	1:41:A:PHE:HD1	1:67:A:LEU:HD21	14	0.13
(1,345)	1:41:A:PHE:HD1	1:67:A:LEU:HD22	14	0.13
(1,345)	1:41:A:PHE:HD1	1:67:A:LEU:HD23	14	0.13
(1,322)	1:40:A:LEU:HD11	1:52:A:CYS:HA	2	0.13
(1,322)	1:40:A:LEU:HD12	1:52:A:CYS:HA	2	0.13
(1,322)	1:40:A:LEU:HD13	1:52:A:CYS:HA	2	0.13
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	10	0.13
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	10	0.13
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	10	0.13
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	12	0.13
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	12	0.13
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	12	0.13
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	12	0.13
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	20	0.13
(1,234)	1:28:A:GLN:H	1:40:A:LEU:HD11	16	0.13
(1,234)	1:28:A:GLN:H	1:40:A:LEU:HD12	16	0.13
(1,234)	1:28:A:GLN:H	1:40:A:LEU:HD13	16	0.13
(1,234)	1:28:A:GLN:H	1:40:A:LEU:HD21	16	0.13
(1,234)	1:28:A:GLN:H	1:40:A:LEU:HD22	16	0.13
(1,234)	1:28:A:GLN:H	1:40:A:LEU:HD23	16	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	5	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	5	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	6	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	6	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	11	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	11	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	15	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	15	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	16	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	16	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	18	0.13
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:20:A:LYS:HG2	1:21:A:VAL:H	9	0.13
(1,121)	1:20:A:LYS:HG3	1:21:A:VAL:H	9	0.13
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	2	0.13
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	9	0.13
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD2	4	0.13
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD3	4	0.13
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD2	4	0.13
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD3	4	0.13
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD2	14	0.13
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD3	14	0.13
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD2	14	0.13
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD3	14	0.13
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	11	0.13
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	11	0.13
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	11	0.13
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	11	0.13
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	11	0.13
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	11	0.13
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	11	0.13
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	11	0.13
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	11	0.13
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	11	0.13
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	11	0.13
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	11	0.13
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE2	2	0.12
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE3	2	0.12
(1,580)	1:69:A:LYS:H	1:69:A:LYS:HD2	9	0.12
(1,580)	1:69:A:LYS:H	1:69:A:LYS:HD3	9	0.12
(1,568)	1:67:A:LEU:HA	1:69:A:LYS:H	13	0.12
(1,513)	1:61:A:GLN:H	1:61:A:GLN:HG2	9	0.12
(1,513)	1:61:A:GLN:H	1:61:A:GLN:HG3	9	0.12
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	18	0.12
(1,453)	1:56:A:LYS:HB2	1:56:A:LYS:HE3	18	0.12
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	18	0.12
(1,453)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	18	0.12
(1,449)	1:56:A:LYS:HA	1:56:A:LYS:HD2	17	0.12
(1,449)	1:56:A:LYS:HA	1:56:A:LYS:HD3	17	0.12
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	1	0.12
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	11	0.12
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	15	0.12
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	19	0.12
(1,418)	1:51:A:LEU:H	1:51:A:LEU:HG	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD2	3	0.12
(1,389)	1:46:A:ARG:HA	1:46:A:ARG:HD3	3	0.12
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	2	0.12
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	5	0.12
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	6	0.12
(1,383)	1:45:A:LYS:HB2	1:46:A:ARG:H	8	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	1	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	1	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	1	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	4	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	4	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	4	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	5	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	5	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	5	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	7	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	7	0.12
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	7	0.12
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB1	6	0.12
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB2	6	0.12
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB3	6	0.12
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB1	18	0.12
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB2	18	0.12
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB3	18	0.12
(1,323)	1:40:A:LEU:HD21	1:52:A:CYS:H	14	0.12
(1,323)	1:40:A:LEU:HD22	1:52:A:CYS:H	14	0.12
(1,323)	1:40:A:LEU:HD23	1:52:A:CYS:H	14	0.12
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	2	0.12
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	2	0.12
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	2	0.12
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	17	0.12
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	17	0.12
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	17	0.12
(1,280)	1:37:A:PRO:HG2	1:38:A:ALA:H	6	0.12
(1,280)	1:37:A:PRO:HG3	1:38:A:ALA:H	6	0.12
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	6	0.12
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	11	0.12
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	16	0.12
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	17	0.12
(1,251)	1:30:A:PRO:HG3	1:38:A:ALA:H	10	0.12
(1,251)	1:30:A:PRO:HG3	1:38:A:ALA:H	11	0.12
(1,240)	1:28:A:GLN:HB2	1:37:A:PRO:HA	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:28:A:GLN:HB3	1:37:A:PRO:HA	16	0.12
(1,210)	1:26:A:ARG:HD2	1:40:A:LEU:HD11	5	0.12
(1,210)	1:26:A:ARG:HD2	1:40:A:LEU:HD12	5	0.12
(1,210)	1:26:A:ARG:HD2	1:40:A:LEU:HD13	5	0.12
(1,210)	1:26:A:ARG:HD2	1:40:A:LEU:HD21	5	0.12
(1,210)	1:26:A:ARG:HD2	1:40:A:LEU:HD22	5	0.12
(1,210)	1:26:A:ARG:HD2	1:40:A:LEU:HD23	5	0.12
(1,210)	1:26:A:ARG:HD3	1:40:A:LEU:HD11	5	0.12
(1,210)	1:26:A:ARG:HD3	1:40:A:LEU:HD12	5	0.12
(1,210)	1:26:A:ARG:HD3	1:40:A:LEU:HD13	5	0.12
(1,210)	1:26:A:ARG:HD3	1:40:A:LEU:HD21	5	0.12
(1,210)	1:26:A:ARG:HD3	1:40:A:LEU:HD22	5	0.12
(1,210)	1:26:A:ARG:HD3	1:40:A:LEU:HD23	5	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD11	8	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD12	8	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD13	8	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD21	8	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD22	8	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD23	8	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD11	14	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD12	14	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD13	14	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD21	14	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD22	14	0.12
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD23	14	0.12
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	2	0.12
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	2	0.12
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	19	0.12
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	19	0.12
(1,121)	1:20:A:LYS:HG2	1:21:A:VAL:H	1	0.12
(1,121)	1:20:A:LYS:HG3	1:21:A:VAL:H	1	0.12
(1,121)	1:20:A:LYS:HG2	1:21:A:VAL:H	3	0.12
(1,121)	1:20:A:LYS:HG3	1:21:A:VAL:H	3	0.12
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	3	0.12
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	4	0.12
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	12	0.12
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	13	0.12
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	15	0.12
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD2	9	0.12
(1,81)	1:16:A:LYS:HB2	1:16:A:LYS:HD3	9	0.12
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD2	9	0.12
(1,81)	1:16:A:LYS:HB3	1:16:A:LYS:HD3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD2	7	0.12
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD3	7	0.12
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD2	16	0.12
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD3	16	0.12
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	8	0.12
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	8	0.12
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	8	0.12
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	8	0.12
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	8	0.12
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	8	0.12
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	8	0.12
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	8	0.12
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	8	0.12
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	8	0.12
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	8	0.12
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	8	0.12
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	13	0.12
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	13	0.12
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	13	0.12
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	13	0.12
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	13	0.12
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	13	0.12
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	13	0.12
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	13	0.12
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	13	0.12
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	13	0.12
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	13	0.12
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	13	0.12
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB1	6	0.12
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB2	6	0.12
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB3	6	0.12
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB1	6	0.12
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB2	6	0.12
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB3	6	0.12
(1,16)	1:8:A:CYS:HA	1:9:A:CYS:H	13	0.12
(1,568)	1:67:A:LEU:HA	1:69:A:LYS:H	4	0.11
(1,568)	1:67:A:LEU:HA	1:69:A:LYS:H	7	0.11
(1,568)	1:67:A:LEU:HA	1:69:A:LYS:H	9	0.11
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG2	4	0.11
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG3	4	0.11
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG2	8	0.11
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG2	12	0.11
(1,447)	1:56:A:LYS:H	1:56:A:LYS:HG3	12	0.11
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	18	0.11
(1,416)	1:50:A:GLU:HG2	1:51:A:LEU:H	12	0.11
(1,416)	1:50:A:GLU:HG3	1:51:A:LEU:H	12	0.11
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	3	0.11
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	3	0.11
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	3	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB1	13	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB2	13	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB3	13	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB1	19	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB2	19	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB3	19	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB1	20	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB2	20	0.11
(1,340)	1:41:A:PHE:HB2	1:53:A:ALA:HB3	20	0.11
(1,323)	1:40:A:LEU:HD21	1:52:A:CYS:H	17	0.11
(1,323)	1:40:A:LEU:HD22	1:52:A:CYS:H	17	0.11
(1,323)	1:40:A:LEU:HD23	1:52:A:CYS:H	17	0.11
(1,321)	1:40:A:LEU:HD11	1:52:A:CYS:H	5	0.11
(1,321)	1:40:A:LEU:HD12	1:52:A:CYS:H	5	0.11
(1,321)	1:40:A:LEU:HD13	1:52:A:CYS:H	5	0.11
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	11	0.11
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	11	0.11
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	11	0.11
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	16	0.11
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	16	0.11
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	16	0.11
(1,297)	1:39:A:ILE:HD11	1:40:A:LEU:H	7	0.11
(1,297)	1:39:A:ILE:HD12	1:40:A:LEU:H	7	0.11
(1,297)	1:39:A:ILE:HD13	1:40:A:LEU:H	7	0.11
(1,280)	1:37:A:PRO:HG2	1:38:A:ALA:H	14	0.11
(1,280)	1:37:A:PRO:HG3	1:38:A:ALA:H	14	0.11
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	2	0.11
(1,255)	1:31:A:SER:H	1:34:A:CYS:H	13	0.11
(1,251)	1:30:A:PRO:HG3	1:38:A:ALA:H	16	0.11
(1,230)	1:27:A:LYS:HG2	1:28:A:GLN:H	3	0.11
(1,230)	1:27:A:LYS:HG3	1:28:A:GLN:H	3	0.11
(1,204)	1:26:A:ARG:HA	1:26:A:ARG:HD2	11	0.11
(1,204)	1:26:A:ARG:HA	1:26:A:ARG:HD3	11	0.11
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD11	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD12	20	0.11
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD13	20	0.11
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD21	20	0.11
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD22	20	0.11
(1,200)	1:26:A:ARG:H	1:40:A:LEU:HD23	20	0.11
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD11	14	0.11
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD12	14	0.11
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD13	14	0.11
(1,183)	1:25:A:TYR:HD1	1:63:A:LEU:HB2	12	0.11
(1,183)	1:25:A:TYR:HD1	1:63:A:LEU:HB3	12	0.11
(1,183)	1:25:A:TYR:HD2	1:63:A:LEU:HB2	12	0.11
(1,183)	1:25:A:TYR:HD2	1:63:A:LEU:HB3	12	0.11
(1,179)	1:25:A:TYR:HB3	1:41:A:PHE:HE1	18	0.11
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD2	1	0.11
(1,152)	1:23:A:ARG:HA	1:23:A:ARG:HD3	1	0.11
(1,121)	1:20:A:LYS:HG2	1:21:A:VAL:H	8	0.11
(1,121)	1:20:A:LYS:HG3	1:21:A:VAL:H	8	0.11
(1,121)	1:20:A:LYS:HG2	1:21:A:VAL:H	12	0.11
(1,121)	1:20:A:LYS:HG3	1:21:A:VAL:H	12	0.11
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	6	0.11
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	16	0.11
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD2	19	0.11
(1,69)	1:15:A:ARG:HA	1:15:A:ARG:HD3	19	0.11
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB2	7	0.11
(1,38)	1:10:A:LEU:HD11	1:51:A:LEU:HB3	7	0.11
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB2	7	0.11
(1,38)	1:10:A:LEU:HD12	1:51:A:LEU:HB3	7	0.11
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB2	7	0.11
(1,38)	1:10:A:LEU:HD13	1:51:A:LEU:HB3	7	0.11
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB2	7	0.11
(1,38)	1:10:A:LEU:HD21	1:51:A:LEU:HB3	7	0.11
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB2	7	0.11
(1,38)	1:10:A:LEU:HD22	1:51:A:LEU:HB3	7	0.11
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB2	7	0.11
(1,38)	1:10:A:LEU:HD23	1:51:A:LEU:HB3	7	0.11
(1,37)	1:10:A:LEU:HD11	1:50:A:GLU:HB2	1	0.11
(1,37)	1:10:A:LEU:HD11	1:50:A:GLU:HB3	1	0.11
(1,37)	1:10:A:LEU:HD12	1:50:A:GLU:HB2	1	0.11
(1,37)	1:10:A:LEU:HD12	1:50:A:GLU:HB3	1	0.11
(1,37)	1:10:A:LEU:HD13	1:50:A:GLU:HB2	1	0.11
(1,37)	1:10:A:LEU:HD13	1:50:A:GLU:HB3	1	0.11
(1,37)	1:10:A:LEU:HD21	1:50:A:GLU:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:10:A:LEU:HD21	1:50:A:GLU:HB3	1	0.11
(1,37)	1:10:A:LEU:HD22	1:50:A:GLU:HB2	1	0.11
(1,37)	1:10:A:LEU:HD22	1:50:A:GLU:HB3	1	0.11
(1,37)	1:10:A:LEU:HD23	1:50:A:GLU:HB2	1	0.11
(1,37)	1:10:A:LEU:HD23	1:50:A:GLU:HB3	1	0.11
(1,37)	1:10:A:LEU:HD11	1:50:A:GLU:HB2	18	0.11
(1,37)	1:10:A:LEU:HD11	1:50:A:GLU:HB3	18	0.11
(1,37)	1:10:A:LEU:HD12	1:50:A:GLU:HB2	18	0.11
(1,37)	1:10:A:LEU:HD12	1:50:A:GLU:HB3	18	0.11
(1,37)	1:10:A:LEU:HD13	1:50:A:GLU:HB2	18	0.11
(1,37)	1:10:A:LEU:HD13	1:50:A:GLU:HB3	18	0.11
(1,37)	1:10:A:LEU:HD21	1:50:A:GLU:HB2	18	0.11
(1,37)	1:10:A:LEU:HD21	1:50:A:GLU:HB3	18	0.11
(1,37)	1:10:A:LEU:HD22	1:50:A:GLU:HB2	18	0.11
(1,37)	1:10:A:LEU:HD22	1:50:A:GLU:HB3	18	0.11
(1,37)	1:10:A:LEU:HD23	1:50:A:GLU:HB2	18	0.11
(1,37)	1:10:A:LEU:HD23	1:50:A:GLU:HB3	18	0.11
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB1	19	0.11
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB2	19	0.11
(1,18)	1:8:A:CYS:HB2	1:38:A:ALA:HB3	19	0.11
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB1	19	0.11
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB2	19	0.11
(1,18)	1:8:A:CYS:HB3	1:38:A:ALA:HB3	19	0.11
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE2	19	0.1
(1,583)	1:69:A:LYS:HA	1:69:A:LYS:HE3	19	0.1
(1,568)	1:67:A:LEU:HA	1:69:A:LYS:H	5	0.1
(1,513)	1:61:A:GLN:H	1:61:A:GLN:HG2	1	0.1
(1,513)	1:61:A:GLN:H	1:61:A:GLN:HG3	1	0.1
(1,472)	1:57:A:GLU:HG2	1:58:A:LEU:H	7	0.1
(1,472)	1:57:A:GLU:HG3	1:58:A:LEU:H	7	0.1
(1,450)	1:56:A:LYS:HA	1:56:A:LYS:HE2	16	0.1
(1,450)	1:56:A:LYS:HA	1:56:A:LYS:HE3	16	0.1
(1,449)	1:56:A:LYS:HA	1:56:A:LYS:HD2	13	0.1
(1,449)	1:56:A:LYS:HA	1:56:A:LYS:HD3	13	0.1
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	3	0.1
(1,442)	1:55:A:PRO:HB2	1:56:A:LYS:H	6	0.1
(1,391)	1:46:A:ARG:HA	1:47:A:SER:H	7	0.1
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	6	0.1
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	6	0.1
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	6	0.1
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB1	13	0.1
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB2	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:41:A:PHE:HE1	1:53:A:ALA:HB3	13	0.1
(1,300)	1:39:A:ILE:HD11	1:64:A:MET:H	3	0.1
(1,300)	1:39:A:ILE:HD12	1:64:A:MET:H	3	0.1
(1,300)	1:39:A:ILE:HD13	1:64:A:MET:H	3	0.1
(1,297)	1:39:A:ILE:HD11	1:40:A:LEU:H	4	0.1
(1,297)	1:39:A:ILE:HD12	1:40:A:LEU:H	4	0.1
(1,297)	1:39:A:ILE:HD13	1:40:A:LEU:H	4	0.1
(1,280)	1:37:A:PRO:HG2	1:38:A:ALA:H	7	0.1
(1,280)	1:37:A:PRO:HG3	1:38:A:ALA:H	7	0.1
(1,251)	1:30:A:PRO:HG3	1:38:A:ALA:H	14	0.1
(1,214)	1:27:A:LYS:H	1:27:A:LYS:HD2	10	0.1
(1,214)	1:27:A:LYS:H	1:27:A:LYS:HD3	10	0.1
(1,214)	1:27:A:LYS:H	1:27:A:LYS:HD2	16	0.1
(1,214)	1:27:A:LYS:H	1:27:A:LYS:HD3	16	0.1
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD11	8	0.1
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD12	8	0.1
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD13	8	0.1
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD11	12	0.1
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD12	12	0.1
(1,196)	1:26:A:ARG:H	1:39:A:ILE:HD13	12	0.1
(1,121)	1:20:A:LYS:HG2	1:21:A:VAL:H	16	0.1
(1,121)	1:20:A:LYS:HG3	1:21:A:VAL:H	16	0.1
(1,97)	1:19:A:ALA:H	1:63:A:LEU:HG	14	0.1
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD2	9	0.1
(1,44)	1:11:A:LYS:HB2	1:11:A:LYS:HD3	9	0.1
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD2	9	0.1
(1,44)	1:11:A:LYS:HB3	1:11:A:LYS:HD3	9	0.1
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD2	7	0.1
(1,39)	1:11:A:LYS:H	1:11:A:LYS:HD3	7	0.1
(1,13)	1:8:A:CYS:CB	1:34:A:CYS:CB	12	0.1

10 Dihedral-angle violation analysis

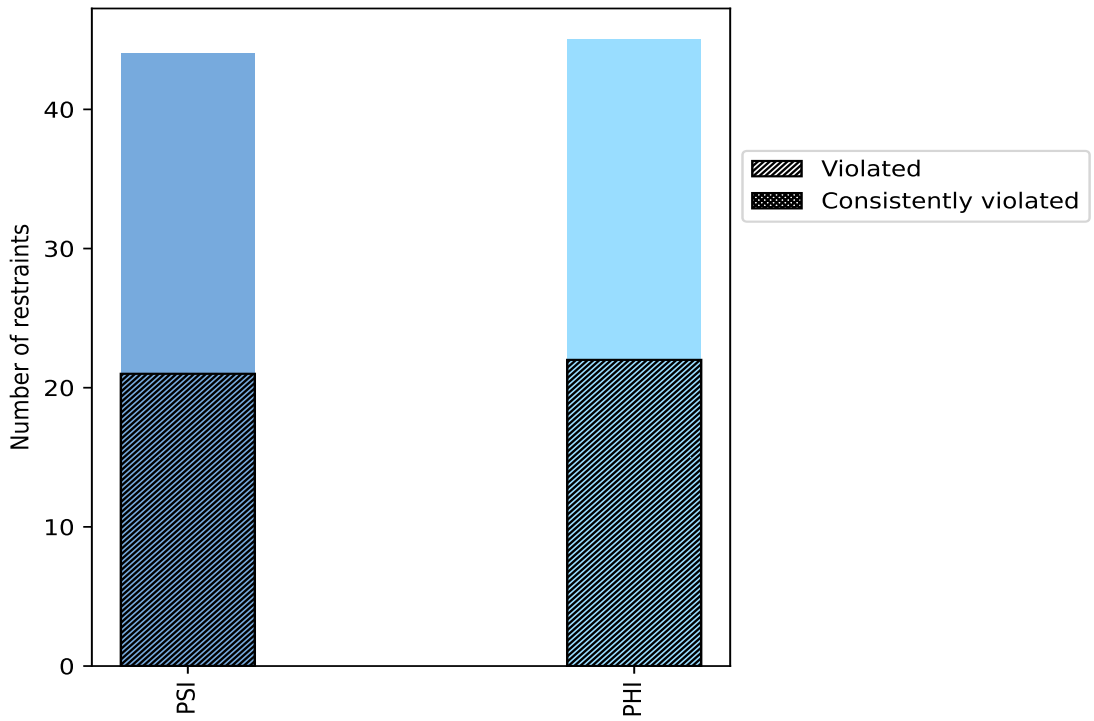
10.1 Summary of dihedral-angle violations

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]
PSI	44	49.4	21	47.7	23.6	0	0.0	0.0
PHI	45	50.6	22	48.9	24.7	0	0.0	0.0
Total	89	100.0	43	48.3	48.3	0	0.0	0.0

[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



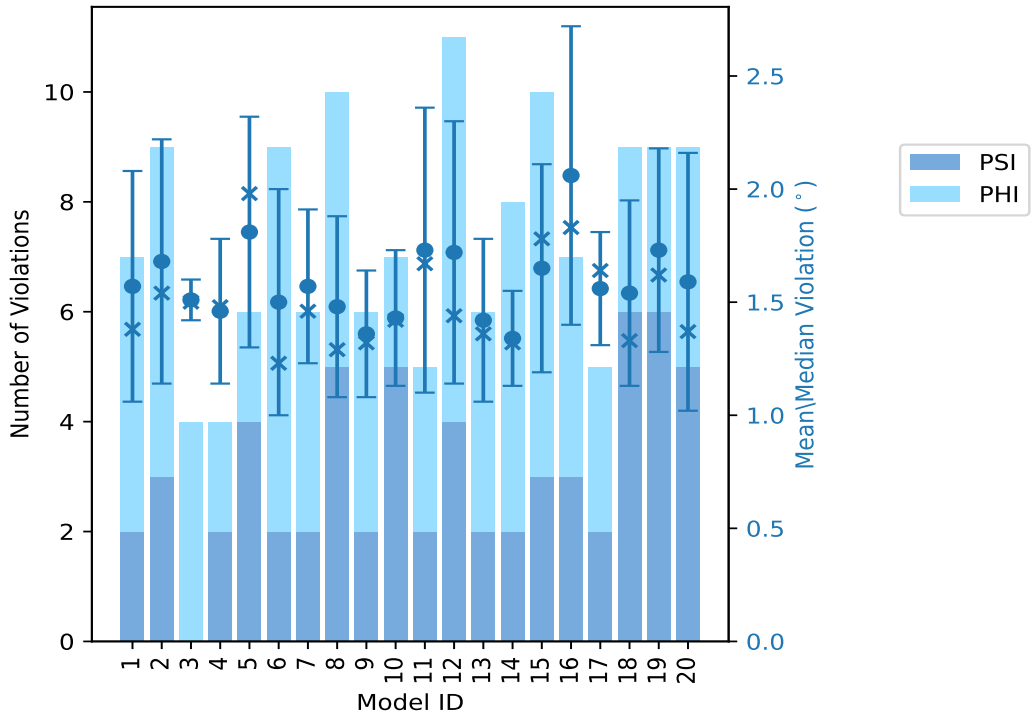
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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 (°)
	PSI	PHI	Total				
1	2	5	7	1.57	2.78	0.51	1.38
2	3	6	9	1.68	2.42	0.54	1.54
3	0	4	4	1.51	1.64	0.09	1.5
4	2	2	4	1.46	1.85	0.32	1.48
5	4	2	6	1.81	2.48	0.51	1.98
6	2	7	9	1.5	2.57	0.5	1.23
7	2	4	6	1.57	2.17	0.34	1.46
8	5	5	10	1.48	2.47	0.4	1.29
9	2	4	6	1.36	1.72	0.28	1.32
10	5	2	7	1.43	1.94	0.3	1.42
11	2	3	5	1.73	2.61	0.63	1.67
12	4	7	11	1.72	3.15	0.58	1.44
13	2	4	6	1.42	1.9	0.36	1.36
14	2	6	8	1.34	1.66	0.21	1.32
15	3	7	10	1.65	2.18	0.46	1.78
16	3	4	7	2.06	3.09	0.66	1.83
17	2	3	5	1.56	1.82	0.25	1.64
18	6	3	9	1.54	2.29	0.41	1.33
19	6	3	9	1.73	2.53	0.45	1.62
20	5	4	9	1.59	2.65	0.57	1.37

10.2.1 Bar graph : Dihedral violation statistics for each model



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

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	
PSI	PHI	Total	Count[1]	%
5	6	11	1	5.0
5	5	10	2	10.0
5	2	7	3	15.0
1	2	3	4	20.0
2	3	5	5	25.0
3	0	3	6	30.0
0	1	1	7	35.0
0	0	0	8	40.0
0	1	1	9	45.0
0	1	1	10	50.0
0	0	0	11	55.0

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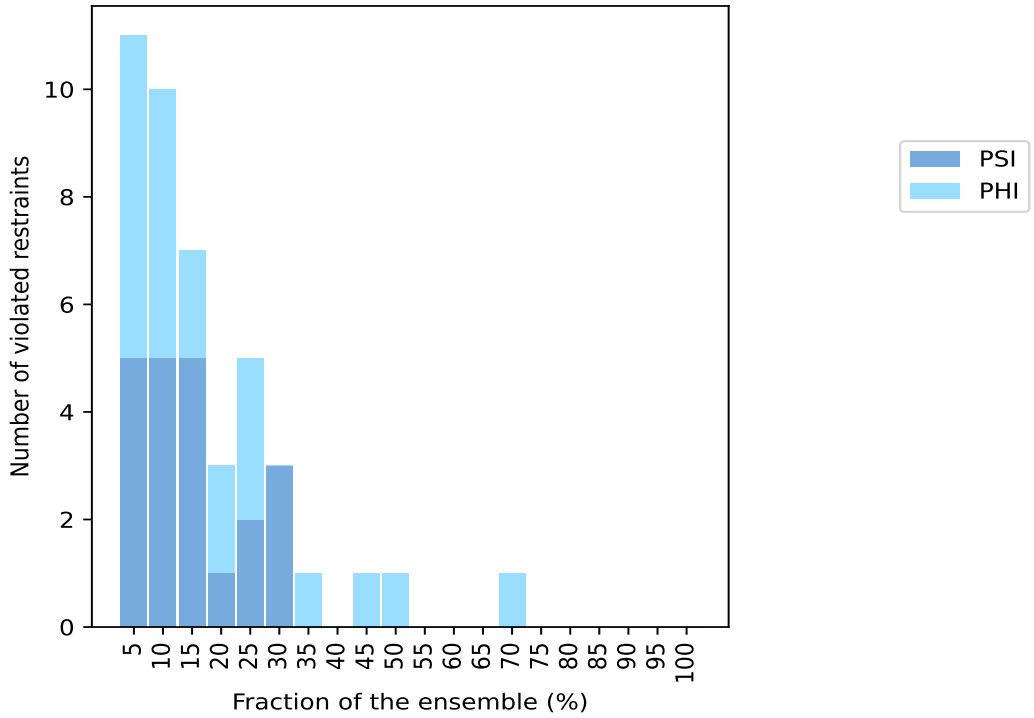
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	1	1	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

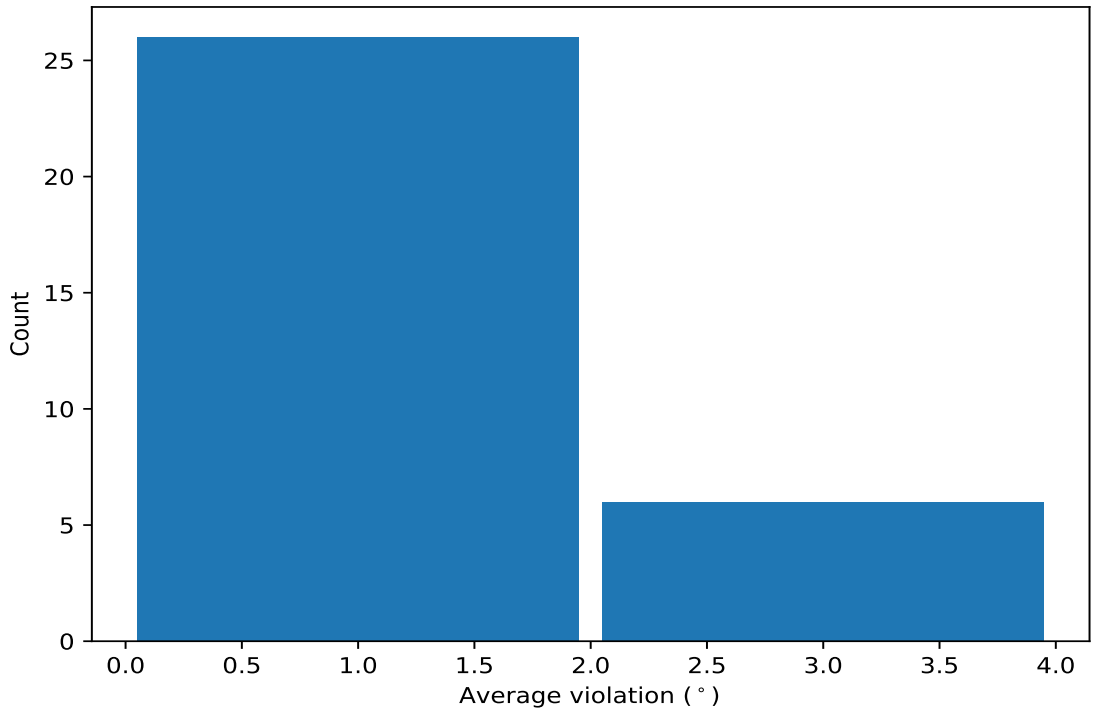


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	14	1.5	0.26	1.51
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	10	1.64	0.38	1.66
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	9	1.65	0.46	1.54
(1,27)	1:26:A:ARG:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	7	1.45	0.37	1.34
(1,5)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:TYR:N	6	2.22	0.44	2.1
(1,84)	1:67:A:LEU:N	1:67:A:LEU:CA	1:67:A:LEU:C	1:68:A:ASP:N	6	1.48	0.3	1.38
(1,60)	1:52:A:CYS:N	1:52:A:CYS:CA	1:52:A:CYS:C	1:53:A:ALA:N	6	1.25	0.21	1.2
(1,2)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:CYS:N	5	1.79	0.44	1.53
(1,58)	1:50:A:GLU:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	5	1.57	0.5	1.28
(1,7)	1:12:A:TYR:N	1:12:A:TYR:CA	1:12:A:TYR:C	1:13:A:SER:N	5	1.48	0.36	1.24
(1,78)	1:63:A:LEU:C	1:64:A:MET:N	1:64:A:MET:CA	1:64:A:MET:C	5	1.4	0.44	1.21
(1,52)	1:43:A:PRO:C	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	5	1.37	0.34	1.23
(1,36)	1:33:A:GLY:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	4	1.59	0.36	1.52
(1,24)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:ARG:N	4	1.49	0.6	1.23
(1,4)	1:10:A:LEU:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	4	1.48	0.47	1.27
(1,32)	1:30:A:PRO:C	1:31:A:SER:N	1:31:A:SER:CA	1:31:A:SER:C	3	2.05	0.31	2.11
(1,9)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:GLN:N	3	1.79	0.58	1.46
(1,86)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:LYS:N	3	1.57	0.23	1.51
(1,18)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:ALA:N	3	1.51	0.19	1.49
(1,57)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:LEU:N	3	1.41	0.47	1.14

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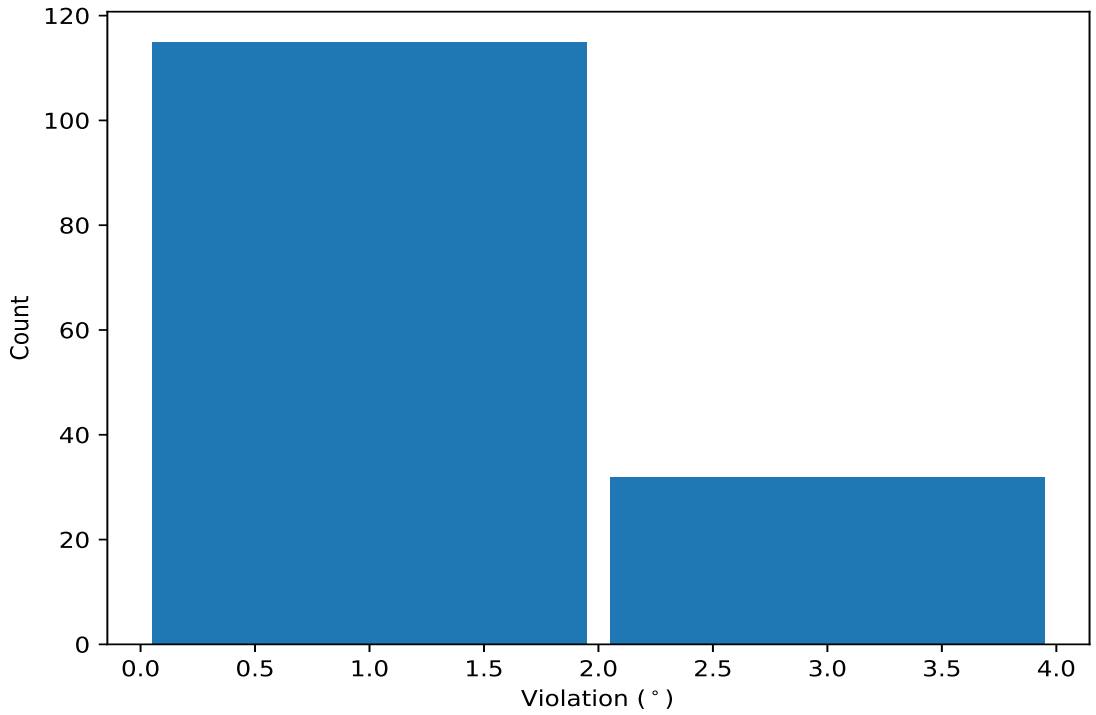
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,53)	1:44:A:ARG:C	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	3	1.39	0.33	1.24
(1,48)	1:40:A:LEU:N	1:40:A:LEU:CA	1:40:A:LEU:C	1:41:A:PHE:N	3	1.27	0.08	1.32
(1,34)	1:31:A:SER:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	2	2.22	0.35	2.22
(1,28)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:GLN:N	2	2.08	0.44	2.08
(1,55)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	2	2.08	0.01	2.08
(1,29)	1:27:A:LYS:C	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	2	2.01	0.98	2.01
(1,33)	1:31:A:SER:N	1:31:A:SER:CA	1:31:A:SER:C	1:32:A:LEU:N	2	1.94	0.83	1.94
(1,89)	1:69:A:LYS:C	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	2	1.6	0.59	1.6
(1,1)	1:6:A:GLN:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	2	1.56	0.3	1.56
(1,88)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:THR:N	2	1.44	0.26	1.44
(1,25)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:ARG:N	2	1.36	0.28	1.36
(1,40)	1:35:A:SER:C	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	2	1.22	0.17	1.22

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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 (°)
(1,5)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:TYR:N	12	3.15
(1,59)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:CYS:N	16	3.09
(1,29)	1:27:A:LYS:C	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	16	2.99
(1,33)	1:31:A:SER:N	1:31:A:SER:CA	1:31:A:SER:C	1:32:A:LEU:N	1	2.78
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	20	2.65
(1,9)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:GLN:N	11	2.61
(1,34)	1:31:A:SER:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	6	2.57
(1,28)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:GLN:N	19	2.53
(1,24)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:ARG:N	5	2.48
(1,2)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:CYS:N	8	2.47
(1,58)	1:50:A:GLU:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	2	2.42
(1,32)	1:30:A:PRO:C	1:31:A:SER:N	1:31:A:SER:CA	1:31:A:SER:C	12	2.39
(1,77)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:MET:N	18	2.29
(1,78)	1:63:A:LEU:C	1:64:A:MET:N	1:64:A:MET:CA	1:64:A:MET:C	2	2.26
(1,4)	1:10:A:LEU:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	11	2.26
(1,5)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:TYR:N	2	2.24
(1,89)	1:69:A:LYS:C	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	15	2.18
(1,36)	1:33:A:GLY:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	7	2.17
(1,27)	1:26:A:ARG:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	15	2.16
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	20	2.15
(1,5)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:TYR:N	19	2.15
(1,2)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:CYS:N	19	2.15
(1,7)	1:12:A:TYR:N	1:12:A:TYR:CA	1:12:A:TYR:C	1:13:A:SER:N	5	2.14
(1,32)	1:30:A:PRO:C	1:31:A:SER:N	1:31:A:SER:CA	1:31:A:SER:C	15	2.11
(1,84)	1:67:A:LEU:N	1:67:A:LEU:CA	1:67:A:LEU:C	1:68:A:ASP:N	6	2.1
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	2	2.1
(1,55)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	5	2.09
(1,57)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:LEU:N	12	2.07
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	18	2.07
(1,55)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	15	2.06
(1,5)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:TYR:N	20	2.06
(1,52)	1:43:A:PRO:C	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	16	2.03
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	10	1.94
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	8	1.93
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	18	1.92
(1,5)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:TYR:N	13	1.9
(1,86)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:LYS:N	5	1.88
(1,34)	1:31:A:SER:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	15	1.87
(1,58)	1:50:A:GLU:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	13	1.86
(1,1)	1:6:A:GLN:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	12	1.86
(1,53)	1:44:A:ARG:C	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	4	1.85
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	19	1.84
(1,37)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:SER:N	20	1.84
(1,5)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:TYR:N	16	1.83
(1,27)	1:26:A:ARG:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	17	1.82
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	7	1.8
(1,18)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:ALA:N	17	1.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	16	1.73
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	9	1.72
(1,88)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:THR:N	15	1.7
(1,85)	1:67:A:LEU:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	6	1.68
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	9	1.68
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	11	1.67
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	14	1.66
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	8	1.65
(1,32)	1:30:A:PRO:C	1:31:A:SER:N	1:31:A:SER:CA	1:31:A:SER:C	3	1.64
(1,28)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:GLN:N	17	1.64
(1,25)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:ARG:N	4	1.64
(1,60)	1:52:A:CYS:N	1:52:A:CYS:CA	1:52:A:CYS:C	1:53:A:ALA:N	19	1.62
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	10	1.62
(1,7)	1:12:A:TYR:N	1:12:A:TYR:CA	1:12:A:TYR:C	1:13:A:SER:N	10	1.61
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	19	1.55
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	2	1.54
(1,36)	1:33:A:GLY:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	12	1.54
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	1	1.54
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	14	1.54
(1,2)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:CYS:N	14	1.53
(1,86)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:LYS:N	1	1.51
(1,38)	1:34:A:CYS:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	3	1.51
(1,84)	1:67:A:LEU:N	1:67:A:LEU:CA	1:67:A:LEU:C	1:68:A:ASP:N	16	1.5
(1,36)	1:33:A:GLY:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	3	1.5
(1,18)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:ALA:N	13	1.49
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	17	1.48
(1,27)	1:26:A:ARG:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	7	1.47
(1,21)	1:20:A:LYS:C	1:21:A:VAL:N	1:21:A:VAL:CA	1:21:A:VAL:C	9	1.47
(1,9)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:GLN:N	7	1.46
(1,24)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:ARG:N	18	1.45
(1,84)	1:67:A:LEU:N	1:67:A:LEU:CA	1:67:A:LEU:C	1:68:A:ASP:N	12	1.44
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	6	1.44
(1,60)	1:52:A:CYS:N	1:52:A:CYS:CA	1:52:A:CYS:C	1:53:A:ALA:N	7	1.42
(1,2)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:CYS:N	10	1.42
(1,40)	1:35:A:SER:C	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	12	1.39
(1,2)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:CYS:N	12	1.39
(1,19)	1:19:A:ALA:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1	1.38
(1,4)	1:10:A:LEU:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	3	1.38
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	20	1.37
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	14	1.35
(1,27)	1:26:A:ARG:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	12	1.34
(1,84)	1:67:A:LEU:N	1:67:A:LEU:CA	1:67:A:LEU:C	1:68:A:ASP:N	19	1.33
(1,52)	1:43:A:PRO:C	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	8	1.33
(1,48)	1:40:A:LEU:N	1:40:A:LEU:CA	1:40:A:LEU:C	1:41:A:PHE:N	18	1.33
(1,86)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:LYS:N	8	1.32
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1	1.32
(1,48)	1:40:A:LEU:N	1:40:A:LEU:CA	1:40:A:LEU:C	1:41:A:PHE:N	4	1.32
(1,9)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:GLN:N	2	1.31
(1,78)	1:63:A:LEU:C	1:64:A:MET:N	1:64:A:MET:CA	1:64:A:MET:C	1	1.3
(1,18)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:ALA:N	19	1.29
(1,58)	1:50:A:GLU:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	14	1.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,84)	1:67:A:LEU:N	1:67:A:LEU:CA	1:67:A:LEU:C	1:68:A:ASP:N	10	1.27
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	16	1.26
(1,1)	1:6:A:GLN:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	8	1.26
(1,60)	1:52:A:CYS:N	1:52:A:CYS:CA	1:52:A:CYS:C	1:53:A:ALA:N	14	1.24
(1,53)	1:44:A:ARG:C	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	13	1.24
(1,7)	1:12:A:TYR:N	1:12:A:TYR:CA	1:12:A:TYR:C	1:13:A:SER:N	8	1.24
(1,83)	1:66:A:HIS:C	1:67:A:LEU:N	1:67:A:LEU:CA	1:67:A:LEU:C	2	1.23
(1,58)	1:50:A:GLU:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	5	1.23
(1,52)	1:43:A:PRO:C	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	6	1.23
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	18	1.23
(1,7)	1:12:A:TYR:N	1:12:A:TYR:CA	1:12:A:TYR:C	1:13:A:SER:N	18	1.23
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	12	1.23
(1,84)	1:67:A:LEU:N	1:67:A:LEU:CA	1:67:A:LEU:C	1:68:A:ASP:N	8	1.21
(1,78)	1:63:A:LEU:C	1:64:A:MET:N	1:64:A:MET:CA	1:64:A:MET:C	15	1.21
(1,27)	1:26:A:ARG:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	8	1.2
(1,88)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:THR:N	8	1.19
(1,7)	1:12:A:TYR:N	1:12:A:TYR:CA	1:12:A:TYR:C	1:13:A:SER:N	20	1.18
(1,60)	1:52:A:CYS:N	1:52:A:CYS:CA	1:52:A:CYS:C	1:53:A:ALA:N	18	1.16
(1,48)	1:40:A:LEU:N	1:40:A:LEU:CA	1:40:A:LEU:C	1:41:A:PHE:N	9	1.16
(1,36)	1:33:A:GLY:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	6	1.16
(1,4)	1:10:A:LEU:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1	1.16
(1,57)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:LEU:N	18	1.14
(1,27)	1:26:A:ARG:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	6	1.14
(1,52)	1:43:A:PRO:C	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	14	1.13
(1,52)	1:43:A:PRO:C	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	17	1.13
(1,78)	1:63:A:LEU:C	1:64:A:MET:N	1:64:A:MET:CA	1:64:A:MET:C	12	1.12
(1,15)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:ILE:N	10	1.12
(1,78)	1:63:A:LEU:C	1:64:A:MET:N	1:64:A:MET:CA	1:64:A:MET:C	19	1.11
(1,33)	1:31:A:SER:N	1:31:A:SER:CA	1:31:A:SER:C	1:32:A:LEU:N	15	1.11
(1,4)	1:10:A:LEU:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	9	1.1
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	15	1.09
(1,58)	1:50:A:GLU:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	7	1.08
(1,16)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	6	1.08
(1,53)	1:44:A:ARG:C	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	11	1.07
(1,25)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:ARG:N	6	1.07
(1,81)	1:65:A:GLN:C	1:66:A:HIS:N	1:66:A:HIS:CA	1:66:A:HIS:C	2	1.05
(1,40)	1:35:A:SER:C	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	15	1.05
(1,27)	1:26:A:ARG:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	20	1.04
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	20	1.04
(1,3)	1:9:A:CYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	5	1.04
(1,60)	1:52:A:CYS:N	1:52:A:CYS:CA	1:52:A:CYS:C	1:53:A:ALA:N	9	1.03
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	13	1.03
(1,29)	1:27:A:LYS:C	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	13	1.03
(1,60)	1:52:A:CYS:N	1:52:A:CYS:CA	1:52:A:CYS:C	1:53:A:ALA:N	10	1.02
(1,24)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:ARG:N	11	1.02
(1,89)	1:69:A:LYS:C	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	14	1.01
(1,57)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:LEU:N	20	1.01
(1,49)	1:40:A:LEU:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	4	1.01
(1,24)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:ARG:N	2	1.0