Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 06:20 AM EDT

PDB ID	:	2JWS
BMRB ID	:	15535
Title	:	Solution NMR structures of two designed proteins with 88% sequence identity but different fold and function
Authors	:	He, Y.; Chen, Y.; Alexander, P.; Bryan, P.; Orban, J.
Deposited on	:	2007-10-24

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:

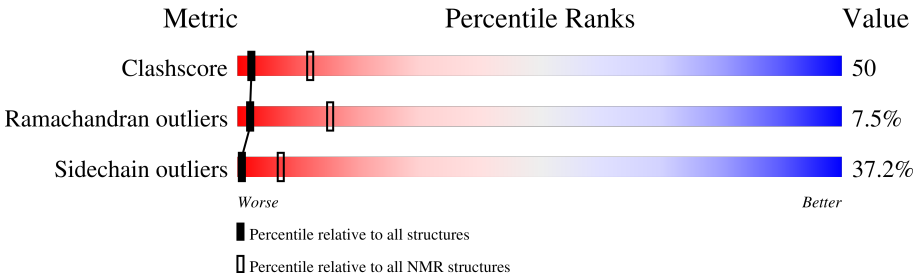
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 83%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	56	25% 38% 14% . 21%

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:9-A:52 (44)	0.18	3

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 921 atoms, of which 476 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ga88.

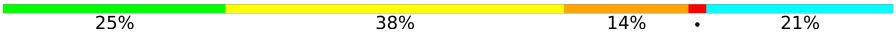
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	56	921	290	476	68	87	0

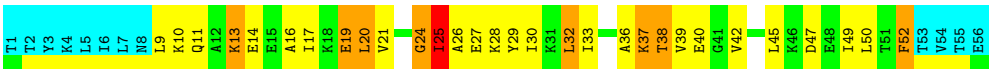
4 Residue-property plots

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: Ga88

Chain A: 

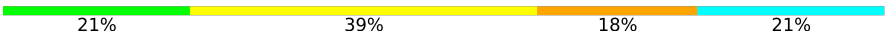


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

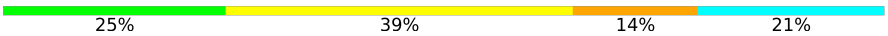
4.2.1 Score per residue for model 1

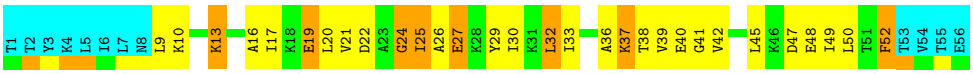
• Molecule 1: Ga88

Chain A: 

4.2.2 Score per residue for model 2

• Molecule 1: Ga88

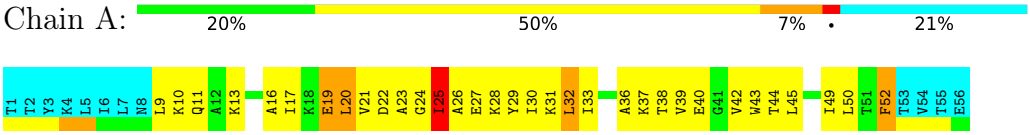
Chain A: 



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Ga88

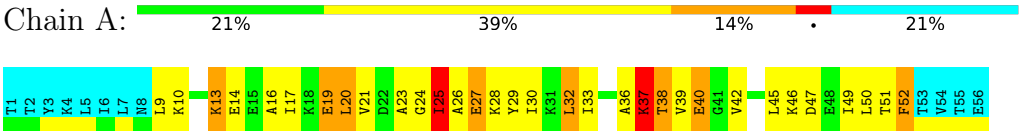
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Ga88

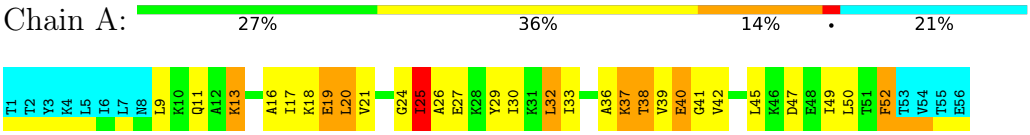
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Ga88

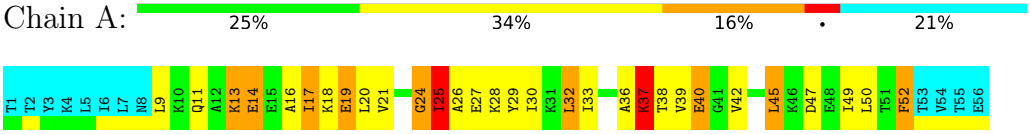
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Ga88

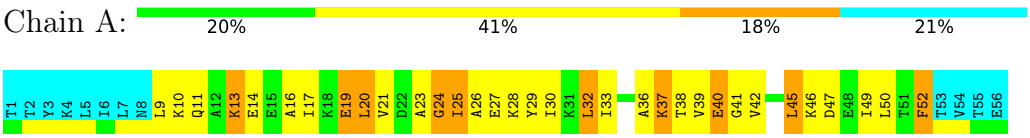
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Ga88

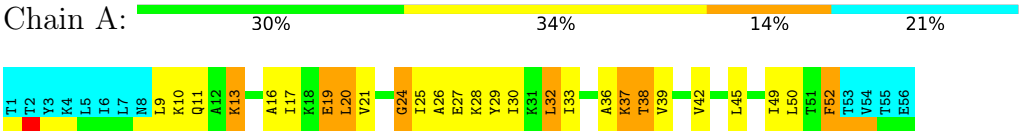
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Ga88

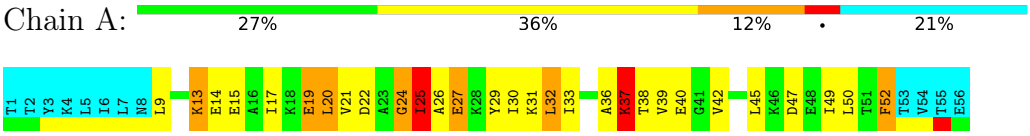
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Ga88

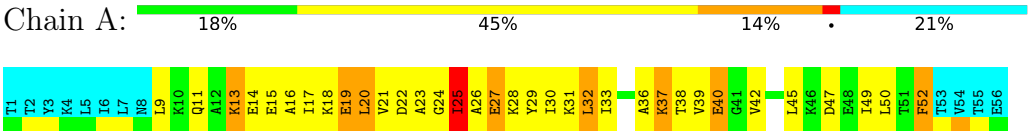
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Ga88

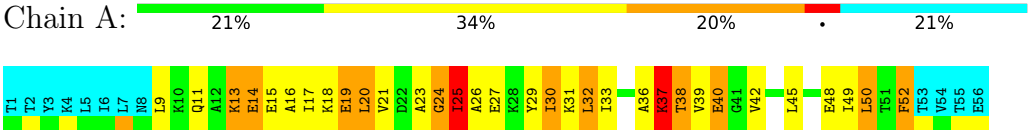
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Ga88

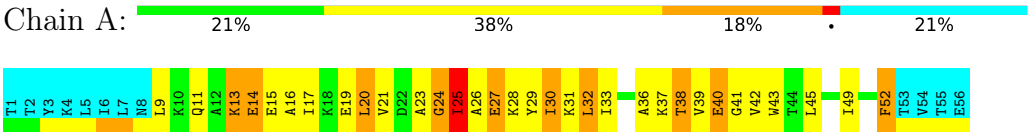
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Ga88

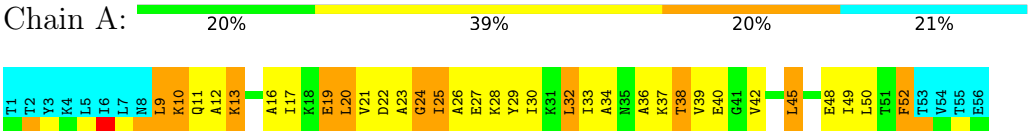
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Ga88

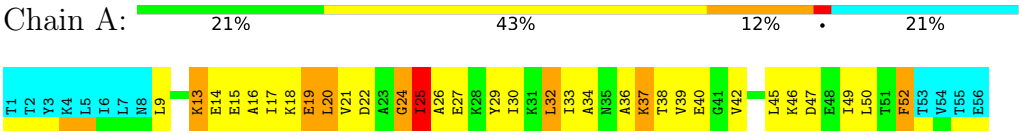
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Ga88

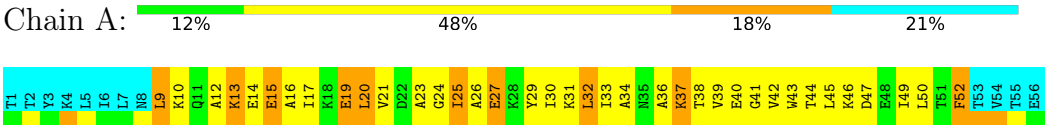
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Ga88

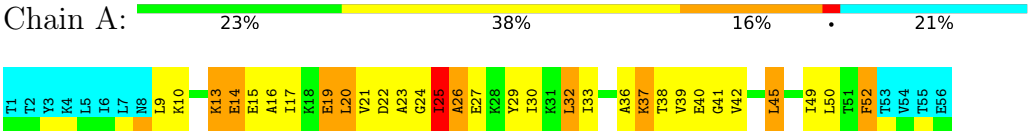
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Ga88

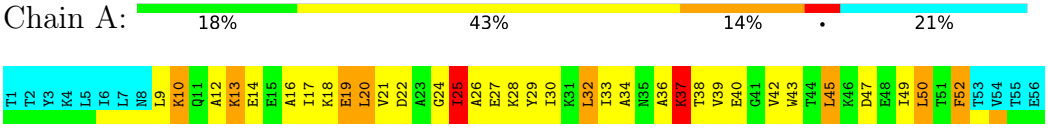
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Ga88

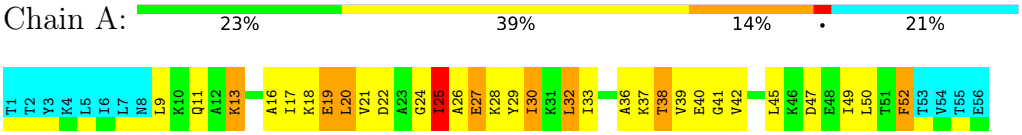
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Ga88

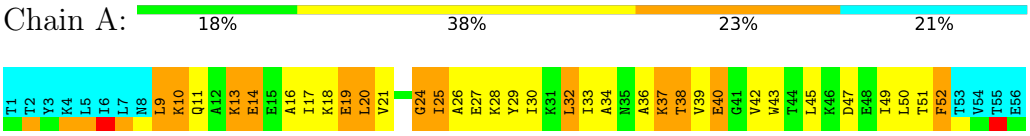
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Ga88

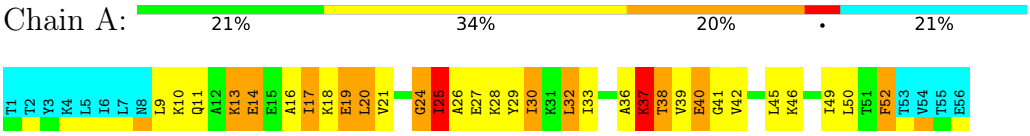
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Ga88

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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	648
Number of shifts mapped to atoms	647
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	347	370	371	36±4
All	All	6940	7400	7420	725

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 50.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:HD23	1:A:42:VAL:HG21	1.00	1.33	15	3
1:A:9:LEU:HD13	1:A:42:VAL:HG21	0.86	1.47	17	2
1:A:9:LEU:CD1	1:A:42:VAL:HG21	0.85	2.01	18	2
1:A:29:TYR:CG	1:A:49:ILE:HD13	0.83	2.08	4	13
1:A:9:LEU:CD2	1:A:42:VAL:HG21	0.81	2.06	15	2
1:A:29:TYR:CD1	1:A:49:ILE:HD13	0.80	2.12	4	10
1:A:52:PHE:CG	1:A:52:PHE:O	0.79	2.35	9	19
1:A:9:LEU:HD13	1:A:10:LYS:N	0.79	1.93	19	3
1:A:24:GLY:O	1:A:25:ILE:HG23	0.79	1.78	7	7
1:A:20:LEU:HD22	1:A:30:ILE:HG13	0.78	1.55	13	4
1:A:38:THR:O	1:A:42:VAL:HG23	0.78	1.78	15	20
1:A:9:LEU:HD22	1:A:9:LEU:O	0.77	1.79	19	3
1:A:17:ILE:O	1:A:21:VAL:HG23	0.76	1.80	5	20
1:A:32:LEU:HB2	1:A:45:LEU:HD23	0.74	1.58	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLU:O	1:A:17:ILE:HG22	0.73	1.83	4	7
1:A:20:LEU:HD22	1:A:30:ILE:CG1	0.72	2.15	13	4
1:A:25:ILE:HD12	1:A:52:PHE:CE1	0.70	2.20	19	1
1:A:23:ALA:HB3	1:A:25:ILE:HD11	0.69	1.62	15	6
1:A:23:ALA:CB	1:A:25:ILE:HD11	0.69	2.16	13	6
1:A:9:LEU:HD21	1:A:36:ALA:CB	0.69	2.17	13	11
1:A:45:LEU:O	1:A:49:ILE:HG22	0.69	1.88	13	20
1:A:19:GLU:HB3	1:A:50:LEU:HD13	0.67	1.67	2	5
1:A:25:ILE:N	1:A:25:ILE:HD13	0.66	2.05	12	2
1:A:20:LEU:HD22	1:A:30:ILE:HB	0.65	1.69	20	11
1:A:9:LEU:HD13	1:A:36:ALA:HB1	0.64	1.69	3	6
1:A:9:LEU:HD13	1:A:36:ALA:CB	0.64	2.22	6	6
1:A:16:ALA:HB1	1:A:33:ILE:CD1	0.62	2.24	15	19
1:A:9:LEU:HG	1:A:42:VAL:HG21	0.62	1.72	8	6
1:A:13:LYS:O	1:A:17:ILE:HD13	0.62	1.94	9	2
1:A:9:LEU:HD22	1:A:9:LEU:C	0.61	2.16	19	3
1:A:9:LEU:HD21	1:A:36:ALA:HB2	0.61	1.72	16	9
1:A:9:LEU:HD12	1:A:9:LEU:O	0.61	1.96	17	2
1:A:16:ALA:CB	1:A:33:ILE:HD12	0.60	2.26	15	16
1:A:32:LEU:CB	1:A:45:LEU:HD23	0.60	2.27	7	4
1:A:13:LYS:HB3	1:A:42:VAL:HG11	0.59	1.74	18	18
1:A:19:GLU:CG	1:A:50:LEU:HD13	0.59	2.28	14	16
1:A:27:GLU:O	1:A:30:ILE:HG22	0.59	1.97	8	14
1:A:9:LEU:HD21	1:A:36:ALA:HB1	0.59	1.74	18	6
1:A:16:ALA:HB1	1:A:33:ILE:HD12	0.59	1.72	15	6
1:A:25:ILE:HD12	1:A:25:ILE:N	0.58	2.13	3	5
1:A:9:LEU:HD12	1:A:39:VAL:CA	0.58	2.28	20	5
1:A:20:LEU:HD21	1:A:25:ILE:O	0.58	1.98	8	1
1:A:49:ILE:O	1:A:52:PHE:CD1	0.58	2.56	15	10
1:A:25:ILE:HG21	1:A:52:PHE:CE1	0.57	2.34	15	7
1:A:20:LEU:HG	1:A:25:ILE:HD12	0.57	1.75	13	4
1:A:36:ALA:O	1:A:37:LYS:CB	0.56	2.52	8	19
1:A:29:TYR:HA	1:A:32:LEU:HG	0.56	1.78	12	20
1:A:52:PHE:CD1	1:A:52:PHE:C	0.56	2.78	7	10
1:A:33:ILE:HG22	1:A:42:VAL:HA	0.55	1.78	20	6
1:A:24:GLY:C	1:A:25:ILE:HD13	0.55	2.22	20	2
1:A:41:GLY:O	1:A:45:LEU:HG	0.54	2.02	2	2
1:A:52:PHE:O	1:A:52:PHE:CD1	0.54	2.60	16	11
1:A:17:ILE:HD13	1:A:30:ILE:HG12	0.54	1.78	7	1
1:A:17:ILE:HD12	1:A:30:ILE:CD1	0.54	2.32	11	2
1:A:32:LEU:HB2	1:A:45:LEU:HD13	0.54	1.78	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:HD13	1:A:9:LEU:C	0.53	2.23	13	3
1:A:20:LEU:HD11	1:A:49:ILE:HG12	0.53	1.81	4	7
1:A:19:GLU:HG3	1:A:50:LEU:HD13	0.53	1.80	14	13
1:A:49:ILE:HD12	1:A:52:PHE:CD1	0.52	2.39	8	6
1:A:9:LEU:HD11	1:A:36:ALA:HB1	0.52	1.82	9	8
1:A:9:LEU:HD12	1:A:39:VAL:N	0.52	2.20	16	5
1:A:19:GLU:CB	1:A:50:LEU:HD13	0.52	2.34	2	10
1:A:29:TYR:CG	1:A:49:ILE:CD1	0.52	2.93	9	6
1:A:29:TYR:CD2	1:A:49:ILE:HD11	0.51	2.40	13	3
1:A:27:GLU:O	1:A:30:ILE:N	0.51	2.44	20	18
1:A:17:ILE:HD12	1:A:30:ILE:HG12	0.51	1.83	4	2
1:A:9:LEU:C	1:A:9:LEU:HD23	0.50	2.27	10	4
1:A:9:LEU:HD12	1:A:39:VAL:HA	0.50	1.82	16	3
1:A:29:TYR:O	1:A:32:LEU:HG	0.49	2.06	11	18
1:A:38:THR:HG22	1:A:41:GLY:H	0.49	1.67	15	1
1:A:23:ALA:HB1	1:A:25:ILE:HD11	0.49	1.82	13	1
1:A:39:VAL:HG13	1:A:40:GLU:N	0.49	2.22	16	19
1:A:41:GLY:O	1:A:45:LEU:N	0.49	2.41	7	3
1:A:25:ILE:N	1:A:25:ILE:CD1	0.49	2.76	12	4
1:A:49:ILE:O	1:A:52:PHE:HD1	0.49	1.91	12	5
1:A:9:LEU:HD23	1:A:42:VAL:CG2	0.48	2.23	19	1
1:A:25:ILE:HG21	1:A:52:PHE:CZ	0.48	2.43	1	7
1:A:29:TYR:CD2	1:A:32:LEU:HD11	0.47	2.44	1	6
1:A:17:ILE:HD11	1:A:34:ALA:HB2	0.47	1.86	19	1
1:A:29:TYR:CB	1:A:49:ILE:HG12	0.47	2.40	20	19
1:A:9:LEU:HD12	1:A:9:LEU:C	0.47	2.29	17	1
1:A:17:ILE:CD1	1:A:30:ILE:HG21	0.47	2.40	14	1
1:A:29:TYR:CD2	1:A:49:ILE:CD1	0.46	2.98	10	3
1:A:52:PHE:CD1	1:A:52:PHE:O	0.46	2.67	15	3
1:A:49:ILE:O	1:A:52:PHE:HD2	0.46	1.93	4	1
1:A:25:ILE:CG2	1:A:52:PHE:CZ	0.46	2.99	1	5
1:A:32:LEU:HD23	1:A:32:LEU:N	0.46	2.25	3	12
1:A:52:PHE:O	1:A:52:PHE:CD2	0.45	2.68	12	4
1:A:33:ILE:HG22	1:A:42:VAL:O	0.45	2.11	12	1
1:A:38:THR:C	1:A:42:VAL:HG23	0.45	2.30	19	2
1:A:29:TYR:CD2	1:A:32:LEU:CD1	0.45	2.99	4	9
1:A:20:LEU:HD22	1:A:30:ILE:CB	0.45	2.41	18	3
1:A:20:LEU:O	1:A:24:GLY:N	0.45	2.50	8	4
1:A:26:ALA:HB3	1:A:29:TYR:CD2	0.45	2.47	16	1
1:A:20:LEU:HG	1:A:25:ILE:CD1	0.45	2.42	7	1
1:A:40:GLU:O	1:A:43:TRP:CD1	0.44	2.70	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLU:CG	1:A:15:GLU:N	0.44	2.79	9	3
1:A:29:TYR:CD2	1:A:49:ILE:HD13	0.44	2.46	9	2
1:A:20:LEU:CD1	1:A:25:ILE:HD11	0.44	2.42	7	1
1:A:43:TRP:C	1:A:43:TRP:CD1	0.44	2.91	15	2
1:A:43:TRP:CD1	1:A:44:THR:N	0.43	2.86	3	2
1:A:32:LEU:HD12	1:A:45:LEU:HD12	0.43	1.91	10	1
1:A:9:LEU:HD11	1:A:36:ALA:CB	0.43	2.44	18	1
1:A:29:TYR:CD1	1:A:49:ILE:CD1	0.43	3.02	9	2
1:A:17:ILE:O	1:A:21:VAL:CG2	0.43	2.67	6	4
1:A:29:TYR:HA	1:A:32:LEU:CG	0.42	2.44	2	6
1:A:43:TRP:CD1	1:A:43:TRP:C	0.42	2.91	3	1
1:A:24:GLY:C	1:A:25:ILE:CG1	0.42	2.87	6	1
1:A:20:LEU:HD11	1:A:49:ILE:CG1	0.42	2.45	3	2
1:A:13:LYS:HB3	1:A:42:VAL:CG1	0.42	2.43	18	6
1:A:25:ILE:HB	1:A:52:PHE:CE1	0.42	2.50	8	1
1:A:30:ILE:O	1:A:34:ALA:CB	0.42	2.67	13	4
1:A:26:ALA:HB3	1:A:29:TYR:CE2	0.42	2.49	16	1
1:A:13:LYS:O	1:A:17:ILE:HG12	0.42	2.15	17	1
1:A:20:LEU:CD1	1:A:49:ILE:HG12	0.42	2.44	8	3
1:A:23:ALA:O	1:A:24:GLY:O	0.42	2.38	11	2
1:A:17:ILE:CD1	1:A:30:ILE:CG2	0.42	2.98	14	1
1:A:9:LEU:C	1:A:9:LEU:CD2	0.42	2.86	19	1
1:A:9:LEU:HB3	1:A:39:VAL:HG23	0.42	1.92	2	2
1:A:16:ALA:HB1	1:A:33:ILE:HD13	0.42	1.91	13	3
1:A:20:LEU:HG	1:A:25:ILE:HD11	0.41	1.90	7	1
1:A:29:TYR:CD2	1:A:32:LEU:HD12	0.41	2.50	3	1
1:A:52:PHE:O	1:A:52:PHE:CG	0.41	2.74	4	1
1:A:24:GLY:O	1:A:25:ILE:CG2	0.41	2.61	7	1
1:A:9:LEU:HB2	1:A:39:VAL:HG23	0.41	1.93	9	1
1:A:36:ALA:O	1:A:37:LYS:HB2	0.41	2.15	1	1
1:A:14:GLU:O	1:A:17:ILE:CG2	0.41	2.68	6	1
1:A:16:ALA:HB2	1:A:46:LYS:HD3	0.41	1.92	14	2
1:A:49:ILE:HD11	1:A:52:PHE:CZ	0.41	2.50	15	1
1:A:38:THR:O	1:A:41:GLY:N	0.41	2.54	16	1
1:A:49:ILE:CD1	1:A:52:PHE:CE1	0.41	3.03	16	1
1:A:41:GLY:O	1:A:45:LEU:HD23	0.41	2.14	12	1
1:A:49:ILE:HD11	1:A:52:PHE:CE1	0.40	2.51	7	1
1:A:40:GLU:HG2	1:A:43:TRP:CZ2	0.40	2.51	3	1
1:A:19:GLU:HG3	1:A:50:LEU:HD22	0.40	1.93	2	1
1:A:13:LYS:HG2	1:A:14:GLU:N	0.40	2.31	19	1
1:A:40:GLU:HA	1:A:43:TRP:CZ2	0.40	2.52	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:CD1	1:A:49:ILE:CG1	0.40	3.00	11	1
1:A:32:LEU:N	1:A:32:LEU:HD23	0.40	2.31	18	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	44/56 (79%)	36±1 (82±2%)	5±1 (11±2%)	3±1 (8±2%)	2	15
All	All	880/1120 (79%)	718 (82%)	96 (11%)	66 (8%)	2	15

All 4 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	24	GLY	20
1	A	26	ALA	20
1	A	25	ILE	15
1	A	37	LYS	11

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	36/48 (75%)	23±2 (63±6%)	13±2 (37±6%)	1	7
All	All	720/960 (75%)	452 (63%)	268 (37%)	1	7

All 26 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	13	LYS	20
1	A	19	GLU	20
1	A	20	LEU	20
1	A	32	LEU	20
1	A	52	PHE	20
1	A	25	ILE	17
1	A	11	GLN	13
1	A	28	LYS	13
1	A	47	ASP	13
1	A	37	LYS	12
1	A	18	LYS	10
1	A	22	ASP	10
1	A	38	THR	10
1	A	40	GLU	10
1	A	10	LYS	10
1	A	27	GLU	8
1	A	14	GLU	8
1	A	31	LYS	7
1	A	45	LEU	5
1	A	15	GLU	5
1	A	30	ILE	4
1	A	48	GLU	3
1	A	46	LYS	3
1	A	9	LEU	3
1	A	17	ILE	2
1	A	50	LEU	2

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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 83% for the well-defined parts and 82% 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	648
Number of shifts mapped to atoms	647
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

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

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	LEU	HG	1.424	0.001	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	56	-0.38 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	54	0.25 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	54	-0.12 ± 0.14	None needed (< 0.5 ppm)
^{15}N	55	0.34 ± 0.26	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 83%, i.e. 518 atoms were assigned a chemical shift out of a possible 622. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	222/222 (100%)	90/90 (100%)	88/88 (100%)	44/44 (100%)
Sidechain	270/369 (73%)	180/241 (75%)	90/119 (76%)	0/9 (0%)
Aromatic	26/31 (84%)	13/15 (87%)	12/15 (80%)	1/1 (100%)
Overall	518/622 (83%)	283/346 (82%)	190/222 (86%)	45/54 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 648 atoms were assigned a chemical shift out of a possible 794. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	276/282 (98%)	111/114 (97%)	110/112 (98%)	55/56 (98%)
Sidechain	340/472 (72%)	226/309 (73%)	114/152 (75%)	0/11 (0%)
Aromatic	32/40 (80%)	17/19 (89%)	14/20 (70%)	1/1 (100%)
Overall	648/794 (82%)	354/442 (80%)	238/284 (84%)	56/68 (82%)

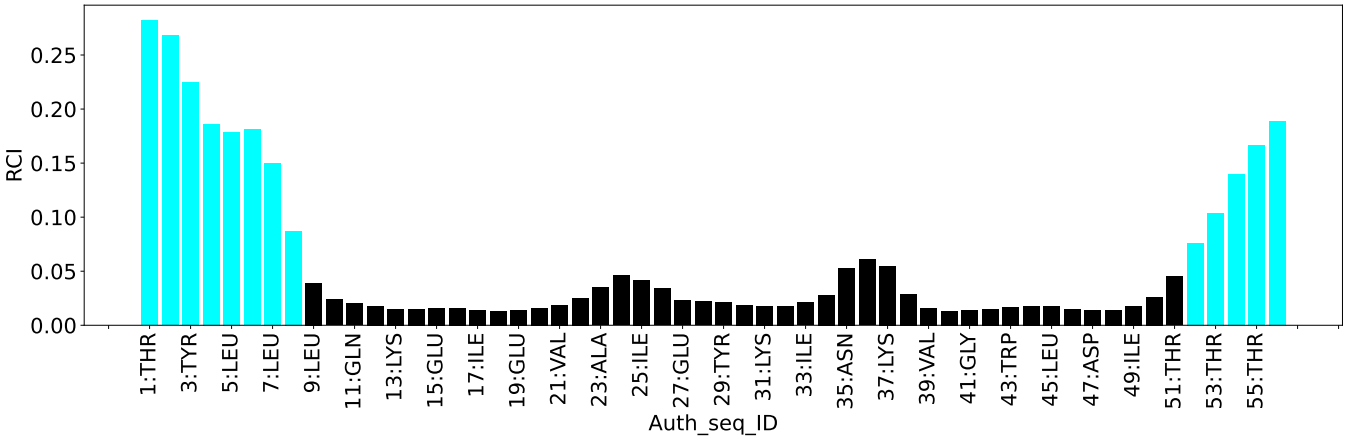
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

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:


RCI
0.25
0.20
0.15
0.10
0.05
0.00
1:THR
3:TYR
5:LEU
7:LEU
9:LEU
11:GLN
13:LYS
15:GLU
17:ILE
19:GLU
21:VAL
23:ALA
25:ILE
27:GLU
29:TYR
31:LYS
33:ILE
35:ASN
37:LYS
39:VAL
41:GLY
43:TRP
45:LEU
47:ASP
49:ILE
51:THR
53:THR
55:THR
Auth_seq_ID

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	1017
Intra-residue (|i-j|=0)	538
Sequential (|i-j|=1)	194
Medium range (|i-j|>1 and |i-j|<5)	171
Long range (|i-j|≥5)	64
Inter-chain	0
Hydrogen bond restraints	50
Disulfide bond restraints	0
Total dihedral-angle restraints	70
Number of unmapped restraints	5
Number of restraints per residue	19.4
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)	22.1	0.2
0.2-0.5 (Medium)	0.8	0.31
>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)	0.2	1.2
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

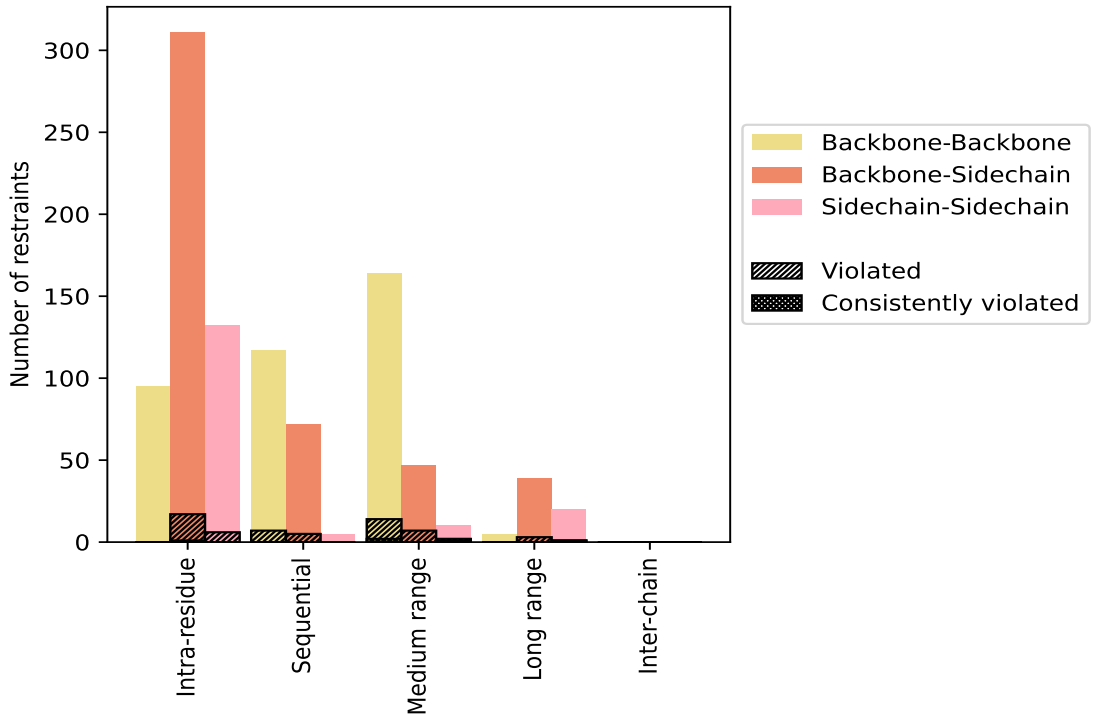
9.1 Summary of distance violations (i)

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)	538	52.9	23	4.3	2.3	1	0.2	0.1
Backbone-Backbone	95	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	311	30.6	17	5.5	1.7	1	0.3	0.1
Sidechain-Sidechain	132	13.0	6	4.5	0.6	0	0.0	0.0
Sequential (|i-j|=1)	194	19.1	12	6.2	1.2	0	0.0	0.0
Backbone-Backbone	117	11.5	7	6.0	0.7	0	0.0	0.0
Backbone-Sidechain	72	7.1	5	6.9	0.5	0	0.0	0.0
Sidechain-Sidechain	5	0.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	171	16.8	17	9.9	1.7	2	1.2	0.2
Backbone-Backbone	114	11.2	8	7.0	0.8	1	0.9	0.1
Backbone-Sidechain	47	4.6	7	14.9	0.7	0	0.0	0.0
Sidechain-Sidechain	10	1.0	2	20.0	0.2	1	10.0	0.1
Long range (|i-j|≥5)	64	6.3	4	6.2	0.4	1	1.6	0.1
Backbone-Backbone	5	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	39	3.8	3	7.7	0.3	0	0.0	0.0
Sidechain-Sidechain	20	2.0	1	5.0	0.1	1	5.0	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	50	4.9	6	12.0	0.6	1	2.0	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1017	100.0	62	6.1	6.1	5	0.5	0.5
Backbone-Backbone	381	37.5	21	5.5	2.1	2	0.5	0.2
Backbone-Sidechain	469	46.1	32	6.8	3.1	1	0.2	0.1
Sidechain-Sidechain	167	16.4	9	5.4	0.9	2	1.2	0.2

[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	7	3	8	2	0	20	0.13	0.2	0.02	0.13
2	6	4	7	2	0	19	0.13	0.17	0.02	0.13
3	7	5	7	1	0	20	0.14	0.21	0.03	0.14
4	9	5	9	1	0	24	0.14	0.2	0.03	0.13
5	7	2	6	2	0	17	0.14	0.19	0.02	0.13
6	10	4	7	2	0	23	0.14	0.21	0.03	0.13
7	7	2	9	3	0	21	0.14	0.21	0.03	0.13
8	7	6	10	2	0	25	0.14	0.19	0.03	0.13
9	7	5	9	3	0	24	0.14	0.23	0.03	0.14
10	9	3	7	2	0	21	0.15	0.31	0.05	0.15
11	9	3	6	3	0	21	0.14	0.2	0.03	0.14

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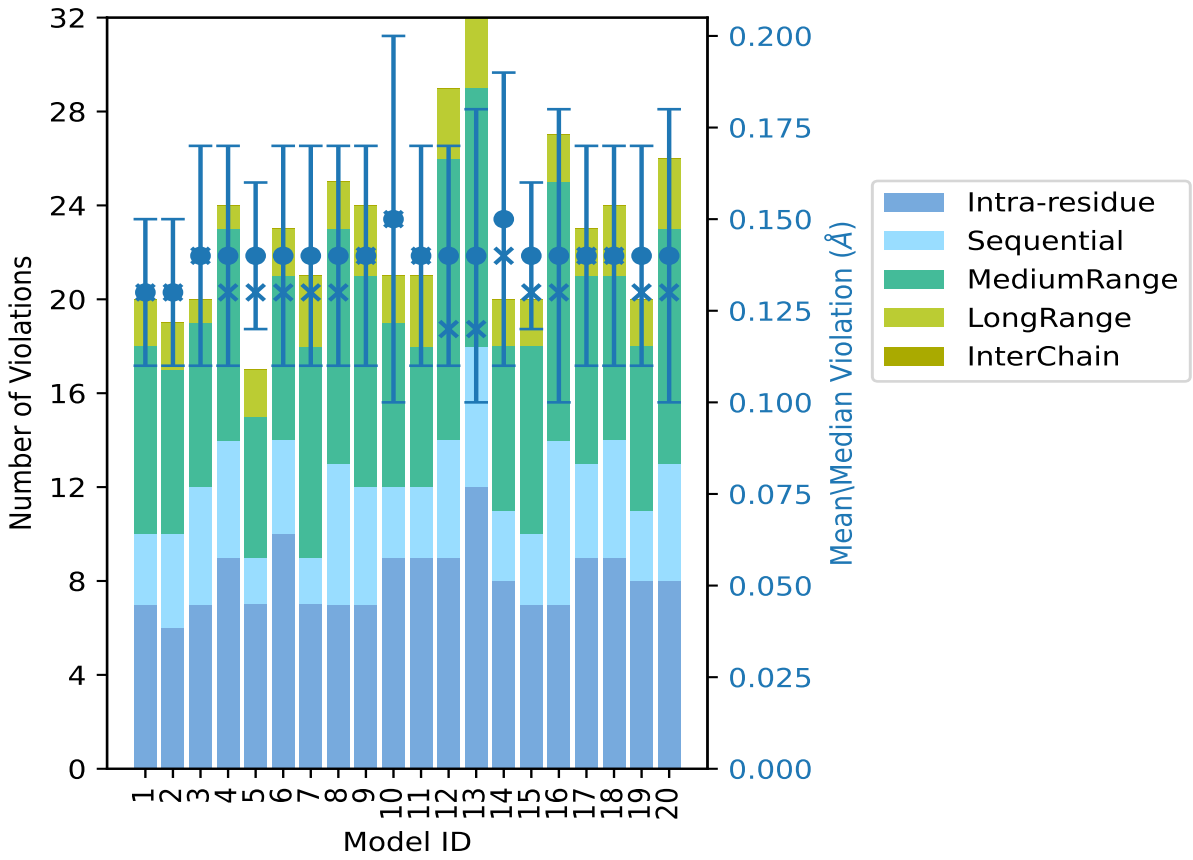
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	9	5	12	3	0	29	0.14	0.2	0.03	0.12
13	12	6	11	3	0	32	0.14	0.31	0.04	0.12
14	8	3	7	2	0	20	0.15	0.24	0.04	0.14
15	7	3	8	2	0	20	0.14	0.18	0.02	0.13
16	7	7	11	2	0	27	0.14	0.29	0.04	0.13
17	9	4	8	2	0	23	0.14	0.2	0.03	0.14
18	9	5	7	3	0	24	0.14	0.25	0.03	0.14
19	8	3	7	2	0	20	0.14	0.22	0.03	0.13
20	8	5	10	3	0	26	0.14	0.3	0.04	0.13

[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

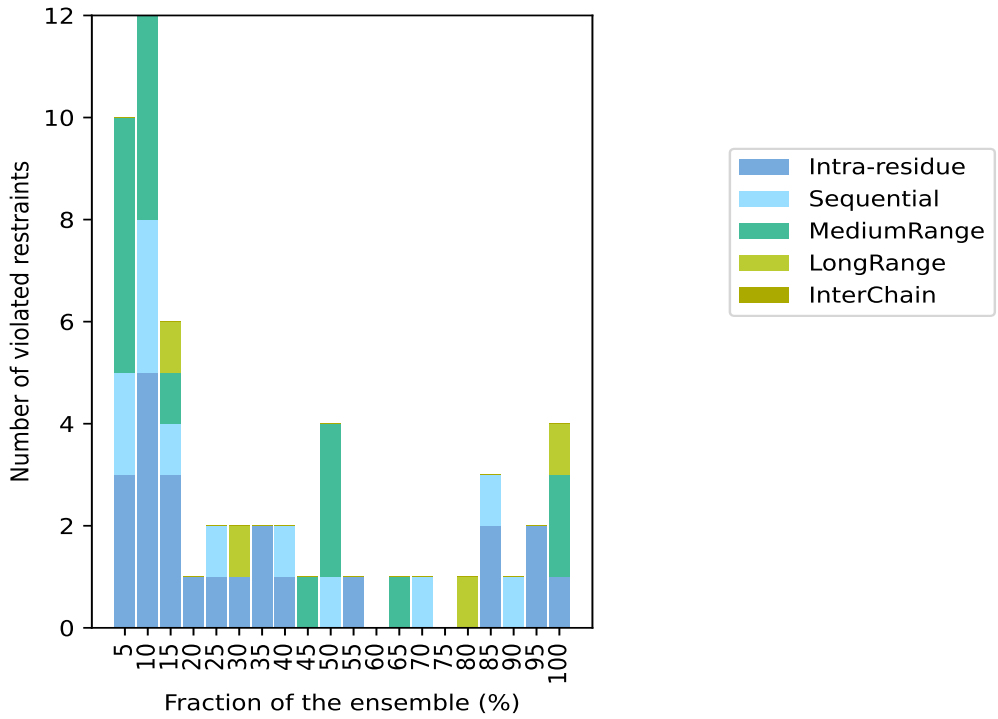
9.3 Distance violation statistics for the ensemble (i)

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, 911(IR:515, SQ:182, MR:154, LR:60, 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]	%
3	2	5	0	0	10	1	5.0
5	3	4	0	0	12	2	10.0
3	1	1	1	0	6	3	15.0
1	0	0	0	0	1	4	20.0
1	1	0	0	0	2	5	25.0
1	0	0	1	0	2	6	30.0
2	0	0	0	0	2	7	35.0
1	1	0	0	0	2	8	40.0
0	0	1	0	0	1	9	45.0
0	1	3	0	0	4	10	50.0
1	0	0	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	1	0	0	1	13	65.0
0	1	0	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	1	0	1	16	80.0
2	1	0	0	0	3	17	85.0
0	1	0	0	0	1	18	90.0
2	0	0	0	0	2	19	95.0
1	0	2	1	0	4	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

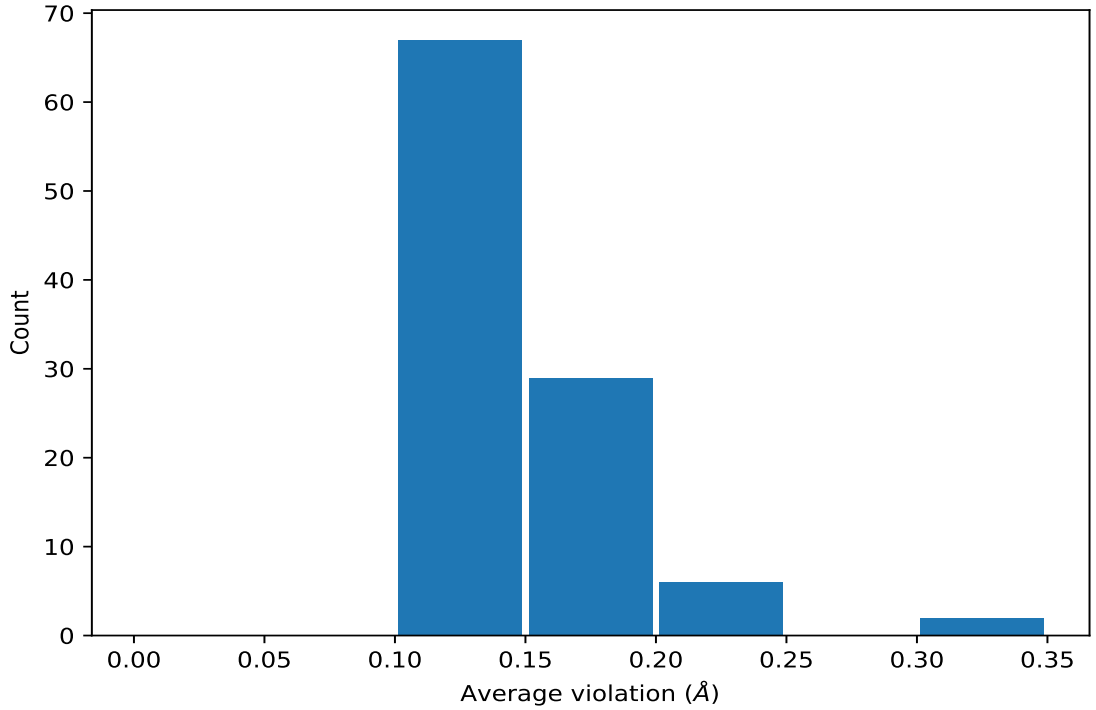
9.3.1 Bar graph : Distance violation statistics for the ensemble



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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	20	0.19	0.01	0.18
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	20	0.19	0.01	0.18
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	20	0.19	0.01	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	20	0.18	0.01	0.18
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	20	0.15	0.04	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	20	0.15	0.04	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	20	0.15	0.04	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	20	0.15	0.04	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	20	0.15	0.04	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	20	0.15	0.04	0.14
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	20	0.14	0.02	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	20	0.14	0.01	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	20	0.14	0.01	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	20	0.14	0.01	0.14
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	19	0.15	0.02	0.15
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	19	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	19	0.15	0.02	0.15
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	19	0.15	0.02	0.15
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	19	0.13	0.01	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	18	0.14	0.02	0.14
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	18	0.14	0.02	0.14
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	18	0.14	0.02	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	17	0.13	0.01	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	17	0.13	0.01	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	17	0.13	0.01	0.12
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	17	0.13	0.02	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	17	0.12	0.02	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	17	0.12	0.02	0.11
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	16	0.13	0.01	0.13
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	16	0.12	0.01	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	16	0.12	0.01	0.12
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	15	0.13	0.02	0.12
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	14	0.12	0.01	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	13	0.11	0.01	0.11
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	11	0.15	0.03	0.16
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	10	0.15	0.03	0.16
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	10	0.13	0.02	0.13
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	10	0.12	0.01	0.12
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	10	0.12	0.01	0.12
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	10	0.12	0.01	0.12
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	9	0.11	0.0	0.11
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	8	0.17	0.04	0.18
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	8	0.17	0.04	0.18
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	8	0.17	0.04	0.18
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	8	0.12	0.01	0.12
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	8	0.12	0.01	0.12
(1,528)	1:A:53:THR:HG21	1:A:53:THR:HA	7	0.2	0.0	0.2
(1,528)	1:A:53:THR:HG22	1:A:53:THR:HA	7	0.2	0.0	0.2
(1,528)	1:A:53:THR:HG23	1:A:53:THR:HA	7	0.2	0.0	0.2
(1,936)	1:A:53:THR:H	1:A:53:THR:HG21	7	0.14	0.01	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG22	7	0.14	0.01	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG23	7	0.14	0.01	0.14
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG12	6	0.15	0.01	0.15
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG13	6	0.15	0.01	0.15
(1,187)	1:A:19:GLU:HG2	1:A:47:ASP:H	6	0.12	0.01	0.12
(1,187)	1:A:19:GLU:HG3	1:A:47:ASP:H	6	0.12	0.01	0.12
(1,930)	1:A:53:THR:H	1:A:52:PHE:HA	5	0.2	0.04	0.22
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG2	5	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG3	5	0.11	0.0	0.11
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG2	4	0.15	0.02	0.15
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG3	4	0.15	0.02	0.15
(1,549)	1:A:29:TYR:HD1	1:A:29:TYR:HA	3	0.3	0.01	0.31
(1,549)	1:A:29:TYR:HD2	1:A:29:TYR:HA	3	0.3	0.01	0.31
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG11	3	0.19	0.0	0.19
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG12	3	0.19	0.0	0.19
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG13	3	0.19	0.0	0.19
(1,75)	1:A:9:LEU:HD11	1:A:9:LEU:HB2	3	0.13	0.01	0.14
(1,75)	1:A:9:LEU:HD12	1:A:9:LEU:HB2	3	0.13	0.01	0.14
(1,75)	1:A:9:LEU:HD13	1:A:9:LEU:HB2	3	0.13	0.01	0.14
(1,510)	1:A:51:THR:HA	1:A:54:VAL:HB	3	0.12	0.01	0.12
(1,594)	1:A:8:ASN:H	1:A:9:LEU:HB3	3	0.12	0.01	0.12
(2,32)	1:A:39:VAL:O	1:A:43:TRP:N	3	0.12	0.01	0.12
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG11	3	0.11	0.0	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG12	3	0.11	0.0	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG13	3	0.11	0.0	0.11
(1,746)	1:A:28:LYS:H	1:A:28:LYS:HG2	2	0.24	0.0	0.24
(1,746)	1:A:28:LYS:H	1:A:28:LYS:HG3	2	0.24	0.0	0.24
(1,32)	1:A:5:LEU:HD11	1:A:3:TYR:H	2	0.16	0.01	0.16
(1,32)	1:A:5:LEU:HD12	1:A:3:TYR:H	2	0.16	0.01	0.16
(1,32)	1:A:5:LEU:HD13	1:A:3:TYR:H	2	0.16	0.01	0.16
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD11	2	0.14	0.0	0.14
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD12	2	0.14	0.0	0.14
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD13	2	0.14	0.0	0.14
(1,74)	1:A:9:LEU:HD11	1:A:9:LEU:HB3	2	0.14	0.0	0.14
(1,74)	1:A:9:LEU:HD12	1:A:9:LEU:HB3	2	0.14	0.0	0.14
(1,74)	1:A:9:LEU:HD13	1:A:9:LEU:HB3	2	0.14	0.0	0.14
(1,940)	1:A:54:VAL:H	1:A:53:THR:H	2	0.14	0.02	0.14
(1,598)	1:A:9:LEU:H	1:A:8:ASN:HB2	2	0.13	0.01	0.13
(1,598)	1:A:9:LEU:H	1:A:8:ASN:HB3	2	0.13	0.01	0.13
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD11	2	0.12	0.01	0.12
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD12	2	0.12	0.01	0.12
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD13	2	0.12	0.01	0.12
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD11	2	0.12	0.01	0.12
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD12	2	0.12	0.01	0.12
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD13	2	0.12	0.01	0.12
(1,525)	1:A:53:THR:HB	1:A:52:PHE:HA	2	0.12	0.0	0.12
(1,190)	1:A:20:LEU:HA	1:A:20:LEU:HG	2	0.12	0.0	0.12
(1,868)	1:A:45:LEU:H	1:A:47:ASP:H	2	0.12	0.0	0.12
(1,238)	1:A:25:ILE:HA	1:A:27:GLU:H	2	0.11	0.0	0.11
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG11	2	0.11	0.0	0.11

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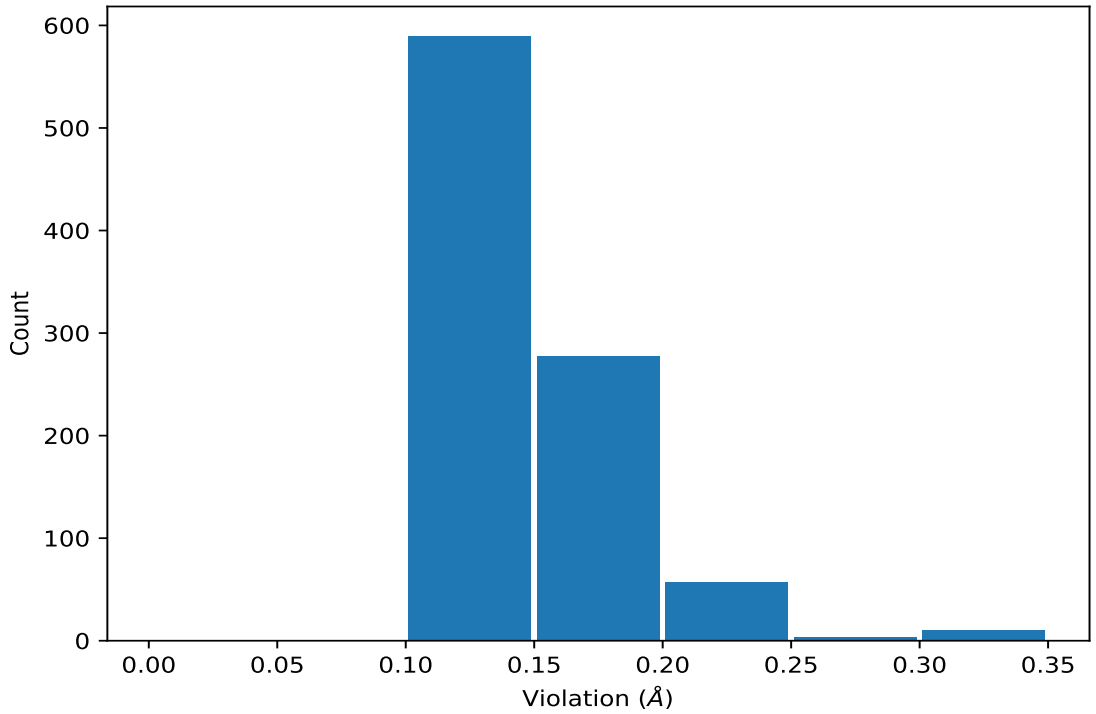
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG12	2	0.11	0.0	0.11
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG13	2	0.11	0.0	0.11
(2,38)	1:A:42:VAL:O	1:A:46:LYS:N	2	0.11	0.0	0.11
(2,50)	1:A:48:GLU:O	1:A:52:PHE:N	2	0.11	0.0	0.11

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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)
(1,549)	1:A:29:TYR:HD1	1:A:29:TYR:HA	10	0.31
(1,549)	1:A:29:TYR:HD2	1:A:29:TYR:HA	10	0.31
(1,549)	1:A:29:TYR:HD1	1:A:29:TYR:HA	13	0.31
(1,549)	1:A:29:TYR:HD2	1:A:29:TYR:HA	13	0.31
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	20	0.3
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	20	0.3
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	20	0.3
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	20	0.3
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	20	0.3
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	20	0.3
(1,549)	1:A:29:TYR:HD1	1:A:29:TYR:HA	16	0.29
(1,549)	1:A:29:TYR:HD2	1:A:29:TYR:HA	16	0.29
(1,930)	1:A:53:THR:H	1:A:52:PHE:HA	18	0.25
(1,746)	1:A:28:LYS:H	1:A:28:LYS:HG2	10	0.24
(1,746)	1:A:28:LYS:H	1:A:28:LYS:HG3	10	0.24
(1,20)	1:A:4:LYS:HA	1:A:4:LYS:HG2	14	0.24
(1,20)	1:A:4:LYS:HA	1:A:4:LYS:HG3	14	0.24
(1,930)	1:A:53:THR:H	1:A:52:PHE:HA	9	0.23
(1,746)	1:A:28:LYS:H	1:A:28:LYS:HG2	13	0.23
(1,746)	1:A:28:LYS:H	1:A:28:LYS:HG3	13	0.23
(1,930)	1:A:53:THR:H	1:A:52:PHE:HA	19	0.22
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	16	0.22
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	14	0.21
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	14	0.21
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	14	0.21
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	3	0.21
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	3	0.21
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	3	0.21
(1,528)	1:A:53:THR:HG21	1:A:53:THR:HA	6	0.21
(1,528)	1:A:53:THR:HG22	1:A:53:THR:HA	6	0.21
(1,528)	1:A:53:THR:HG23	1:A:53:THR:HA	6	0.21
(1,528)	1:A:53:THR:HG21	1:A:53:THR:HA	7	0.21
(1,528)	1:A:53:THR:HG22	1:A:53:THR:HA	7	0.21
(1,528)	1:A:53:THR:HG23	1:A:53:THR:HA	7	0.21
(1,930)	1:A:53:THR:H	1:A:52:PHE:HA	14	0.2
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	12	0.2
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	17	0.2
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	11	0.2
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	11	0.2
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	11	0.2
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	6	0.2
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	6	0.2
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	7	0.2
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	7	0.2
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	7	0.2
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	12	0.2
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	12	0.2
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	12	0.2
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	17	0.2
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	17	0.2
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	17	0.2
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG11	6	0.2
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG12	6	0.2
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG13	6	0.2
(1,528)	1:A:53:THR:HG21	1:A:53:THR:HA	1	0.2
(1,528)	1:A:53:THR:HG22	1:A:53:THR:HA	1	0.2
(1,528)	1:A:53:THR:HG23	1:A:53:THR:HA	1	0.2
(1,528)	1:A:53:THR:HG21	1:A:53:THR:HA	3	0.2
(1,528)	1:A:53:THR:HG22	1:A:53:THR:HA	3	0.2
(1,528)	1:A:53:THR:HG23	1:A:53:THR:HA	3	0.2
(1,528)	1:A:53:THR:HG21	1:A:53:THR:HA	4	0.2
(1,528)	1:A:53:THR:HG22	1:A:53:THR:HA	4	0.2
(1,528)	1:A:53:THR:HG23	1:A:53:THR:HA	4	0.2
(1,528)	1:A:53:THR:HG21	1:A:53:THR:HA	11	0.2
(1,528)	1:A:53:THR:HG22	1:A:53:THR:HA	11	0.2
(1,528)	1:A:53:THR:HG23	1:A:53:THR:HA	11	0.2
(1,528)	1:A:53:THR:HG21	1:A:53:THR:HA	12	0.2
(1,528)	1:A:53:THR:HG22	1:A:53:THR:HA	12	0.2
(1,528)	1:A:53:THR:HG23	1:A:53:THR:HA	12	0.2
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	18	0.19
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	19	0.19
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	20	0.19
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	8	0.19
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	13	0.19
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	17	0.19
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	8	0.19
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	8	0.19
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	8	0.19
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	10	0.19
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	10	0.19
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	10	0.19
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	4	0.19
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	4	0.19
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	9	0.19
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	9	0.19
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	9	0.19
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	13	0.19
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	13	0.19
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	13	0.19
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	16	0.19
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	16	0.19
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	16	0.19
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	19	0.19
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	19	0.19
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	19	0.19
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG11	5	0.19
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG12	5	0.19
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG13	5	0.19
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG11	13	0.19
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG12	13	0.19
(1,532)	1:A:54:VAL:HA	1:A:54:VAL:HG13	13	0.19
(1,40)	1:A:6:ILE:HB	1:A:6:ILE:HD11	20	0.19
(1,40)	1:A:6:ILE:HB	1:A:6:ILE:HD12	20	0.19
(1,40)	1:A:6:ILE:HB	1:A:6:ILE:HD13	20	0.19
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	3	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	4	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	6	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	7	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	8	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	11	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	12	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	14	0.18
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	15	0.18
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	9	0.18
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	9	0.18
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	9	0.18
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	9	0.18
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	18	0.18
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	18	0.18
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	18	0.18
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	18	0.18
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	19	0.18
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	19	0.18
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	19	0.18
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	1	0.18
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	1	0.18
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	1	0.18
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	11	0.18
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	11	0.18
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	11	0.18
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	14	0.18
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	14	0.18
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	14	0.18
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	15	0.18
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	15	0.18
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	15	0.18
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	20	0.18
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	20	0.18
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	20	0.18
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	9	0.18
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	16	0.17
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	1	0.17
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	5	0.17
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	9	0.17
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	10	0.17
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	17	0.17
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	2	0.17
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	16	0.17
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	18	0.17
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	15	0.17
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	9	0.17
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	9	0.17
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	9	0.17
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG12	6	0.17
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG13	6	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	4	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	4	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	4	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	4	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	5	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	5	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	5	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	5	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	8	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	8	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	8	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	11	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	11	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	11	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	11	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	12	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	12	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	12	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	12	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	14	0.17
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	14	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	14	0.17
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	14	0.17
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	2	0.17
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	2	0.17
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	2	0.17
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	5	0.17
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	5	0.17
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	5	0.17
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	8	0.17
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	8	0.17
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	8	0.17
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	10	0.17
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	10	0.17
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	10	0.17
(1,546)	1:A:49:ILE:HG21	1:A:32:LEU:HG	18	0.17
(1,546)	1:A:49:ILE:HG22	1:A:32:LEU:HG	18	0.17
(1,546)	1:A:49:ILE:HG23	1:A:32:LEU:HG	18	0.17
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	10	0.17
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	15	0.17
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	20	0.17
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	13	0.17
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	2	0.16
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	13	0.16
(2,26)	1:A:28:LYS:O	1:A:32:LEU:N	16	0.16
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	6	0.16
(1,936)	1:A:53:THR:H	1:A:53:THR:HG21	7	0.16
(1,936)	1:A:53:THR:H	1:A:53:THR:HG22	7	0.16
(1,936)	1:A:53:THR:H	1:A:53:THR:HG23	7	0.16
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	17	0.16
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	19	0.16
(1,816)	1:A:40:GLU:H	1:A:36:ALA:HA	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	2	0.16
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	2	0.16
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	8	0.16
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	8	0.16
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG12	17	0.16
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG13	17	0.16
(1,596)	1:A:8:ASN:H	1:A:9:LEU:H	12	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	11	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	11	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	11	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	14	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	14	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	14	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	15	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	15	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	15	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	17	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	17	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	17	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	20	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	20	0.16
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	20	0.16
(1,32)	1:A:5:LEU:HD11	1:A:3:TYR:H	4	0.16
(1,32)	1:A:5:LEU:HD12	1:A:3:TYR:H	4	0.16
(1,32)	1:A:5:LEU:HD13	1:A:3:TYR:H	4	0.16
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	8	0.16
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	8	0.16
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	8	0.16
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	8	0.16
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	8	0.16
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	8	0.16
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG2	10	0.16
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG3	10	0.16
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	10	0.15
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	16	0.15
(1,940)	1:A:54:VAL:H	1:A:53:THR:H	16	0.15
(1,936)	1:A:53:THR:H	1:A:53:THR:HG21	6	0.15
(1,936)	1:A:53:THR:H	1:A:53:THR:HG22	6	0.15
(1,936)	1:A:53:THR:H	1:A:53:THR:HG23	6	0.15
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	4	0.15
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	1	0.15
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	7	0.15
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	3	0.15
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	3	0.15
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	3	0.15
(1,807)	1:A:38:THR:H	1:A:38:THR:HG21	16	0.15
(1,807)	1:A:38:THR:H	1:A:38:THR:HG22	16	0.15
(1,807)	1:A:38:THR:H	1:A:38:THR:HG23	16	0.15
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	20	0.15
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	20	0.15
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG12	9	0.15
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG13	9	0.15
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG12	14	0.15
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG13	14	0.15
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	6	0.15
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	6	0.15
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	6	0.15
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	6	0.15
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	17	0.15
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	17	0.15
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	17	0.15
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	17	0.15
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	13	0.15
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	2	0.15
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	2	0.15
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	2	0.15
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	13	0.15
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	13	0.15
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	18	0.15
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	18	0.15
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	6	0.15
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	6	0.15
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	6	0.15
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	10	0.15
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	10	0.15
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	10	0.15
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	2	0.15
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	2	0.15
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	2	0.15
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	3	0.15
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	3	0.15
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	3	0.15
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	4	0.15
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	4	0.15
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	5	0.15
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	5	0.15
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	5	0.15
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	9	0.15
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	9	0.15
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	9	0.15
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	12	0.15
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	12	0.15
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	12	0.15
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	16	0.15
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	16	0.15
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	16	0.15
(1,32)	1:A:5:LEU:HD11	1:A:3:TYR:H	9	0.15
(1,32)	1:A:5:LEU:HD12	1:A:3:TYR:H	9	0.15
(1,32)	1:A:5:LEU:HD13	1:A:3:TYR:H	9	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	2	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	2	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	2	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	2	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	2	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	2	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	4	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	4	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	4	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	4	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	4	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	4	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	10	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	10	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	10	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	10	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	10	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	10	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	13	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	13	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	13	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	13	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	13	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	13	0.15
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	18	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	18	0.15
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	18	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	18	0.15
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	18	0.15
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	10	0.15
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG2	17	0.15
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG3	17	0.15
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG2	18	0.15
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG3	18	0.15
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	13	0.14
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	3	0.14
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	8	0.14
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	12	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG21	3	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG22	3	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG23	3	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG21	11	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG22	11	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG23	11	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG21	12	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG22	12	0.14
(1,936)	1:A:53:THR:H	1:A:53:THR:HG23	12	0.14
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	15	0.14
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	2	0.14
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	4	0.14
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	14	0.14
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	16	0.14
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	9	0.14
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	9	0.14
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	20	0.14
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	20	0.14
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	20	0.14
(1,75)	1:A:9:LEU:HD11	1:A:9:LEU:HB2	13	0.14
(1,75)	1:A:9:LEU:HD12	1:A:9:LEU:HB2	13	0.14
(1,75)	1:A:9:LEU:HD13	1:A:9:LEU:HB2	13	0.14
(1,75)	1:A:9:LEU:HD11	1:A:9:LEU:HB2	19	0.14
(1,75)	1:A:9:LEU:HD12	1:A:9:LEU:HB2	19	0.14
(1,75)	1:A:9:LEU:HD13	1:A:9:LEU:HB2	19	0.14
(1,74)	1:A:9:LEU:HD11	1:A:9:LEU:HB3	17	0.14
(1,74)	1:A:9:LEU:HD12	1:A:9:LEU:HB3	17	0.14
(1,74)	1:A:9:LEU:HD13	1:A:9:LEU:HB3	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:A:9:LEU:HD11	1:A:9:LEU:HB3	18	0.14
(1,74)	1:A:9:LEU:HD12	1:A:9:LEU:HB3	18	0.14
(1,74)	1:A:9:LEU:HD13	1:A:9:LEU:HB3	18	0.14
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD11	17	0.14
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD12	17	0.14
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD13	17	0.14
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD11	18	0.14
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD12	18	0.14
(1,68)	1:A:9:LEU:HB3	1:A:9:LEU:HD13	18	0.14
(1,598)	1:A:9:LEU:H	1:A:8:ASN:HB2	12	0.14
(1,598)	1:A:9:LEU:H	1:A:8:ASN:HB3	12	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	1	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	1	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	1	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	5	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	5	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	5	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	12	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	12	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	12	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	18	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	18	0.14
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	18	0.14
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	11	0.14
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	11	0.14
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	14	0.14
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	14	0.14
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	12	0.14
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	12	0.14
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	12	0.14
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	13	0.14
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	13	0.14
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	13	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	1	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	1	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	1	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	6	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	6	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	6	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	7	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	7	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	8	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	8	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	8	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	10	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	10	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	10	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	11	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	11	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	11	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	13	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	13	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	13	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	14	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	14	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	14	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	15	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	15	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	15	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	17	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	17	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	17	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	18	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	18	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	18	0.14
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	19	0.14
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	19	0.14
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	19	0.14
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	2	0.14
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	3	0.14
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	5	0.14
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	9	0.14
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	11	0.14
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	14	0.14
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	19	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	3	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	3	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	3	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	3	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	3	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	3	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	7	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	7	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	7	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	7	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	7	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	9	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	9	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	9	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	9	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	9	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	9	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	11	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	11	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	11	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	11	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	11	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	11	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	12	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	12	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	12	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	12	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	12	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	12	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	14	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	14	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	14	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	14	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	14	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	14	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	15	0.14
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	15	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	15	0.14
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	15	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	15	0.14
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	15	0.14
(1,187)	1:A:19:GLU:HG2	1:A:47:ASP:H	20	0.14
(1,187)	1:A:19:GLU:HG3	1:A:47:ASP:H	20	0.14
(2,32)	1:A:39:VAL:O	1:A:43:TRP:N	8	0.13
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	7	0.13
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	12	0.13
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	18	0.13
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	1	0.13
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	4	0.13
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	5	0.13
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	7	0.13
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	19	0.13
(1,936)	1:A:53:THR:H	1:A:53:THR:HG21	4	0.13
(1,936)	1:A:53:THR:H	1:A:53:THR:HG22	4	0.13
(1,936)	1:A:53:THR:H	1:A:53:THR:HG23	4	0.13
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	20	0.13
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	16	0.13
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	6	0.13
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	8	0.13
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	9	0.13
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	10	0.13
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	18	0.13
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	20	0.13
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	1	0.13
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	4	0.13
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	7	0.13
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	9	0.13
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	8	0.13
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	8	0.13
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	17	0.13
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	17	0.13
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	4	0.13
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	4	0.13
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG12	11	0.13
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG13	11	0.13
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG12	19	0.13
(1,729)	1:A:25:ILE:H	1:A:25:ILE:HG13	19	0.13
(1,594)	1:A:8:ASN:H	1:A:9:LEU:HB3	9	0.13
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	1	0.13
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	1	0.13
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	1	0.13
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	1	0.13
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	2	0.13
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	2	0.13
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	2	0.13
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	2	0.13
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	7	0.13
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	7	0.13
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	7	0.13
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	19	0.13
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD11	15	0.13
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD12	15	0.13
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD13	15	0.13
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD11	15	0.13
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD12	15	0.13
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD13	15	0.13
(1,510)	1:A:51:THR:HA	1:A:54:VAL:HB	15	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	13	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	13	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	13	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	15	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	15	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	15	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	16	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	16	0.13
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	16	0.13
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	13	0.13
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	20	0.13
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	16	0.13
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	16	0.13
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	19	0.13
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	19	0.13
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	20	0.13
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	20	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	1	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	1	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	1	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	7	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	7	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	7	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	16	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	16	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	16	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	18	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	18	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	18	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	19	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	19	0.13
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	19	0.13
(1,356)	1:A:33:ILE:HD11	1:A:33:ILE:HA	20	0.13
(1,356)	1:A:33:ILE:HD12	1:A:33:ILE:HA	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:A:33:ILE:HD13	1:A:33:ILE:HA	20	0.13
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	1	0.13
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	4	0.13
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	8	0.13
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	15	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	1	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	1	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	1	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	1	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	1	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	1	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	5	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	5	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	5	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	5	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	5	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	5	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	6	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	6	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	6	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	6	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	6	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	6	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	16	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	16	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	16	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	16	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	16	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	16	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	17	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	17	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	17	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	17	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	17	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	17	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG2	19	0.13
(1,251)	1:A:26:ALA:HB1	1:A:28:LYS:HG3	19	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG2	19	0.13
(1,251)	1:A:26:ALA:HB2	1:A:28:LYS:HG3	19	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG2	19	0.13
(1,251)	1:A:26:ALA:HB3	1:A:28:LYS:HG3	19	0.13
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	16	0.13
(1,187)	1:A:19:GLU:HG2	1:A:47:ASP:H	7	0.13
(1,187)	1:A:19:GLU:HG3	1:A:47:ASP:H	7	0.13
(1,187)	1:A:19:GLU:HG2	1:A:47:ASP:H	11	0.13
(1,187)	1:A:19:GLU:HG3	1:A:47:ASP:H	11	0.13
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	5	0.13
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	7	0.13
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	14	0.13
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	17	0.13
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	17	0.13
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	17	0.13
(2,32)	1:A:39:VAL:O	1:A:43:TRP:N	12	0.12
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	2	0.12
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	3	0.12
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	6	0.12
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	8	0.12
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	15	0.12
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	17	0.12
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	9	0.12
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	13	0.12
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	14	0.12
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	18	0.12
(1,940)	1:A:54:VAL:H	1:A:53:THR:H	4	0.12
(1,936)	1:A:53:THR:H	1:A:53:THR:HG21	1	0.12
(1,936)	1:A:53:THR:H	1:A:53:THR:HG22	1	0.12
(1,936)	1:A:53:THR:H	1:A:53:THR:HG23	1	0.12
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	10	0.12
(1,930)	1:A:53:THR:H	1:A:52:PHE:HA	16	0.12
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	2	0.12
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	6	0.12
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	8	0.12
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	15	0.12
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	17	0.12
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	20	0.12
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	1	0.12
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	3	0.12
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	6	0.12
(1,868)	1:A:45:LEU:H	1:A:47:ASP:H	20	0.12
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	5	0.12
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	11	0.12
(1,851)	1:A:44:THR:H	1:A:41:GLY:HA3	13	0.12
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	5	0.12
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	6	0.12
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	11	0.12
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	12	0.12
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	13	0.12
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	16	0.12
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	11	0.12
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	11	0.12
(1,810)	1:A:39:VAL:H	1:A:37:LYS:H	16	0.12
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	12	0.12
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	12	0.12
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	12	0.12
(1,75)	1:A:9:LEU:HD11	1:A:9:LEU:HB2	15	0.12
(1,75)	1:A:9:LEU:HD12	1:A:9:LEU:HB2	15	0.12
(1,75)	1:A:9:LEU:HD13	1:A:9:LEU:HB2	15	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	1	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	1	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	5	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	5	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	18	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	18	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	19	0.12
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	19	0.12
(1,598)	1:A:9:LEU:H	1:A:8:ASN:HB2	20	0.12
(1,598)	1:A:9:LEU:H	1:A:8:ASN:HB3	20	0.12
(1,594)	1:A:8:ASN:H	1:A:9:LEU:HB3	13	0.12
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	3	0.12
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	3	0.12
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	3	0.12
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	3	0.12
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	13	0.12
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	13	0.12
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	13	0.12
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	13	0.12
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	16	0.12
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	16	0.12
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	16	0.12
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	16	0.12
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	20	0.12
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	20	0.12
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	20	0.12
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	8	0.12
(1,525)	1:A:53:THR:HB	1:A:52:PHE:HA	8	0.12
(1,525)	1:A:53:THR:HB	1:A:52:PHE:HA	13	0.12
(1,524)	1:A:53:THR:HB	1:A:50:LEU:HA	7	0.12
(1,510)	1:A:51:THR:HA	1:A:54:VAL:HB	8	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	3	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	3	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	3	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	4	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	4	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	4	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	7	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	7	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	7	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	8	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	8	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	8	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	9	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	9	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	9	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	19	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	19	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	19	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	20	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	20	0.12
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	20	0.12
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	19	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	9	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	9	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	10	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	10	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	15	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	15	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	17	0.12
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	17	0.12
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	9	0.12
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	9	0.12
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	9	0.12
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	6	0.12
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	10	0.12
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	12	0.12
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	18	0.12
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	20	0.12
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	4	0.12
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	13	0.12
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	18	0.12
(1,190)	1:A:20:LEU:HA	1:A:20:LEU:HG	14	0.12
(1,187)	1:A:19:GLU:HG2	1:A:47:ASP:H	6	0.12
(1,187)	1:A:19:GLU:HG3	1:A:47:ASP:H	6	0.12
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG2	15	0.12
(1,161)	1:A:18:LYS:HA	1:A:18:LYS:HG3	15	0.12
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	10	0.12
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	10	0.12
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	11	0.12
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	11	0.12
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	12	0.12
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	12	0.12
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	14	0.12
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	14	0.12
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	15	0.12
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	15	0.12
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	18	0.12
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	18	0.12
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	20	0.12
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	20	0.12
(2,50)	1:A:48:GLU:O	1:A:52:PHE:N	9	0.11
(2,50)	1:A:48:GLU:O	1:A:52:PHE:N	12	0.11
(2,38)	1:A:42:VAL:O	1:A:46:LYS:N	9	0.11
(2,38)	1:A:42:VAL:O	1:A:46:LYS:N	12	0.11
(2,32)	1:A:39:VAL:O	1:A:43:TRP:N	17	0.11
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	1	0.11
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	4	0.11
(2,28)	1:A:29:TYR:O	1:A:33:ILE:N	5	0.11
(2,12)	1:A:14:GLU:O	1:A:18:LYS:N	11	0.11
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG11	6	0.11
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG12	6	0.11
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG13	6	0.11
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG11	13	0.11
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG12	13	0.11
(1,943)	1:A:54:VAL:H	1:A:54:VAL:HG13	13	0.11
(1,935)	1:A:53:THR:H	1:A:53:THR:HB	12	0.11
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	3	0.11
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:A:51:THR:H	1:A:52:PHE:H	13	0.11
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	2	0.11
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	4	0.11
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	12	0.11
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	16	0.11
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	19	0.11
(1,91)	1:A:11:GLN:HA	1:A:13:LYS:H	20	0.11
(1,868)	1:A:45:LEU:H	1:A:47:ASP:H	7	0.11
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	8	0.11
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	18	0.11
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	19	0.11
(1,830)	1:A:41:GLY:H	1:A:42:VAL:H	20	0.11
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	2	0.11
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	2	0.11
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	4	0.11
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	4	0.11
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB2	18	0.11
(1,826)	1:A:41:GLY:H	1:A:40:GLU:HB3	18	0.11
(1,77)	1:A:9:LEU:HD11	1:A:9:LEU:H	16	0.11
(1,77)	1:A:9:LEU:HD12	1:A:9:LEU:H	16	0.11
(1,77)	1:A:9:LEU:HD13	1:A:9:LEU:H	16	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	3	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	3	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	6	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	6	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	7	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	7	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	9	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	9	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	11	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	11	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	12	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	12	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	14	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	14	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	15	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	15	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB2	17	0.11
(1,745)	1:A:28:LYS:H	1:A:28:LYS:HB3	17	0.11
(1,725)	1:A:25:ILE:H	1:A:24:GLY:HA2	6	0.11
(1,676)	1:A:19:GLU:H	1:A:17:ILE:HB	14	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG3	4	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG2	5	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG3	5	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG2	6	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG3	6	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG2	13	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG3	13	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG2	19	0.11
(1,633)	1:A:13:LYS:H	1:A:13:LYS:HG3	19	0.11
(1,594)	1:A:8:ASN:H	1:A:9:LEU:HB3	16	0.11
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB2	10	0.11
(1,559)	1:A:52:PHE:HD1	1:A:52:PHE:HB3	10	0.11
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB2	10	0.11
(1,559)	1:A:52:PHE:HD2	1:A:52:PHE:HB3	10	0.11
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	2	0.11
(1,530)	1:A:54:VAL:HA	1:A:52:PHE:HA	18	0.11
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD11	13	0.11
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD12	13	0.11
(1,516)	1:A:52:PHE:HB2	1:A:49:ILE:HD13	13	0.11
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD11	13	0.11
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD12	13	0.11
(1,516)	1:A:52:PHE:HB3	1:A:49:ILE:HD13	13	0.11
(1,510)	1:A:51:THR:HA	1:A:54:VAL:HB	4	0.11
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	10	0.11
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	10	0.11
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	10	0.11
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD11	11	0.11
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD12	11	0.11
(1,498)	1:A:50:LEU:HB3	1:A:50:LEU:HD13	11	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	1	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	3	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	4	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	6	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	7	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	8	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	11	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	12	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	16	0.11
(1,467)	1:A:46:LYS:HA	1:A:49:ILE:HB	17	0.11
(1,441)	1:A:44:THR:HA	1:A:46:LYS:HG2	20	0.11
(1,441)	1:A:44:THR:HA	1:A:46:LYS:HG3	20	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	1	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	5	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	5	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	7	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	7	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	8	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	8	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD2	12	0.11
(1,423)	1:A:42:VAL:HA	1:A:13:LYS:HD3	12	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG11	9	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG12	9	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG13	9	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG11	13	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG12	13	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG13	13	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG11	18	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG12	18	0.11
(1,384)	1:A:36:ALA:HA	1:A:42:VAL:HG13	18	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	3	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	3	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	3	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	4	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	4	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	4	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD11	8	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD12	8	0.11
(1,364)	1:A:34:ALA:HA	1:A:33:ILE:HD13	8	0.11
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	7	0.11
(1,324)	1:A:32:LEU:HA	1:A:32:LEU:HG	17	0.11
(1,238)	1:A:25:ILE:HA	1:A:27:GLU:H	13	0.11
(1,238)	1:A:25:ILE:HA	1:A:27:GLU:H	20	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	1	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	2	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	3	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	5	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	8	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	12	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	14	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	15	0.11
(1,215)	1:A:22:ASP:HA	1:A:21:VAL:HA	20	0.11
(1,190)	1:A:20:LEU:HA	1:A:20:LEU:HG	13	0.11
(1,187)	1:A:19:GLU:HG2	1:A:47:ASP:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:A:19:GLU:HG3	1:A:47:ASP:H	2	0.11
(1,187)	1:A:19:GLU:HG2	1:A:47:ASP:H	12	0.11
(1,187)	1:A:19:GLU:HG3	1:A:47:ASP:H	12	0.11
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	1	0.11
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	9	0.11
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	12	0.11
(1,177)	1:A:19:GLU:HA	1:A:23:ALA:H	16	0.11
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	13	0.11
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	13	0.11
(1,113)	1:A:13:LYS:HB2	1:A:10:LYS:H	16	0.11
(1,113)	1:A:13:LYS:HB3	1:A:10:LYS:H	16	0.11

10 Dihedral-angle violation analysis

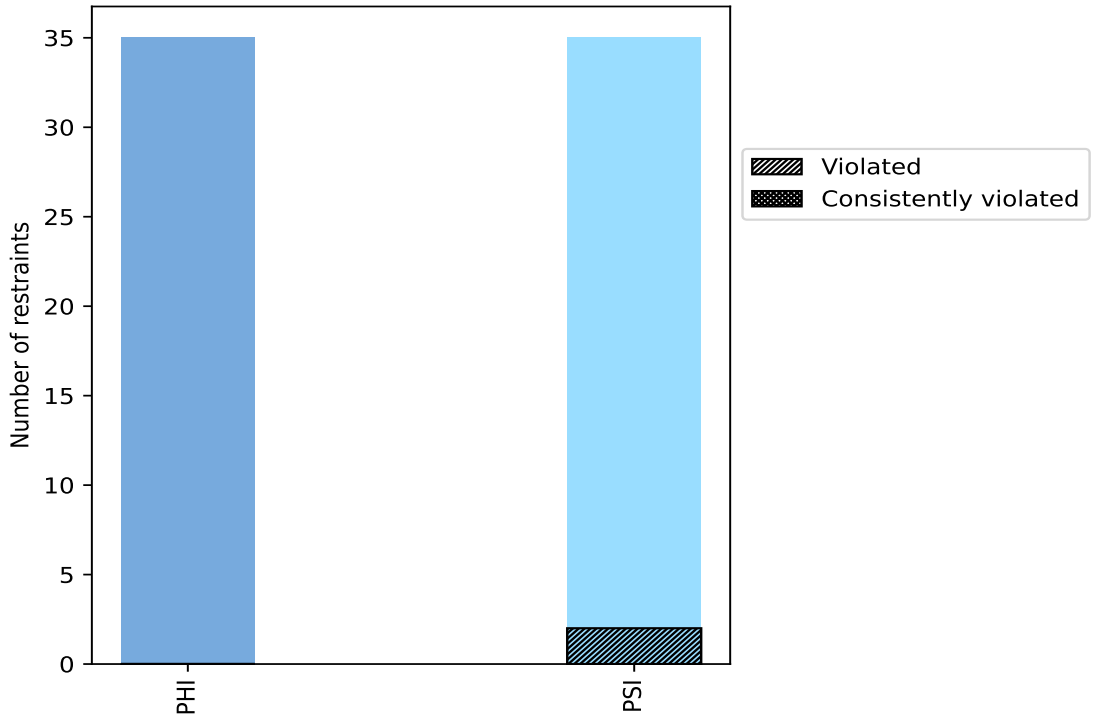
10.1 Summary of dihedral-angle violations

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]
PHI	35	50.0	0	0.0	0.0	0	0.0	0.0
PSI	35	50.0	2	5.7	2.9	0	0.0	0.0
Total	70	100.0	2	2.9	2.9	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



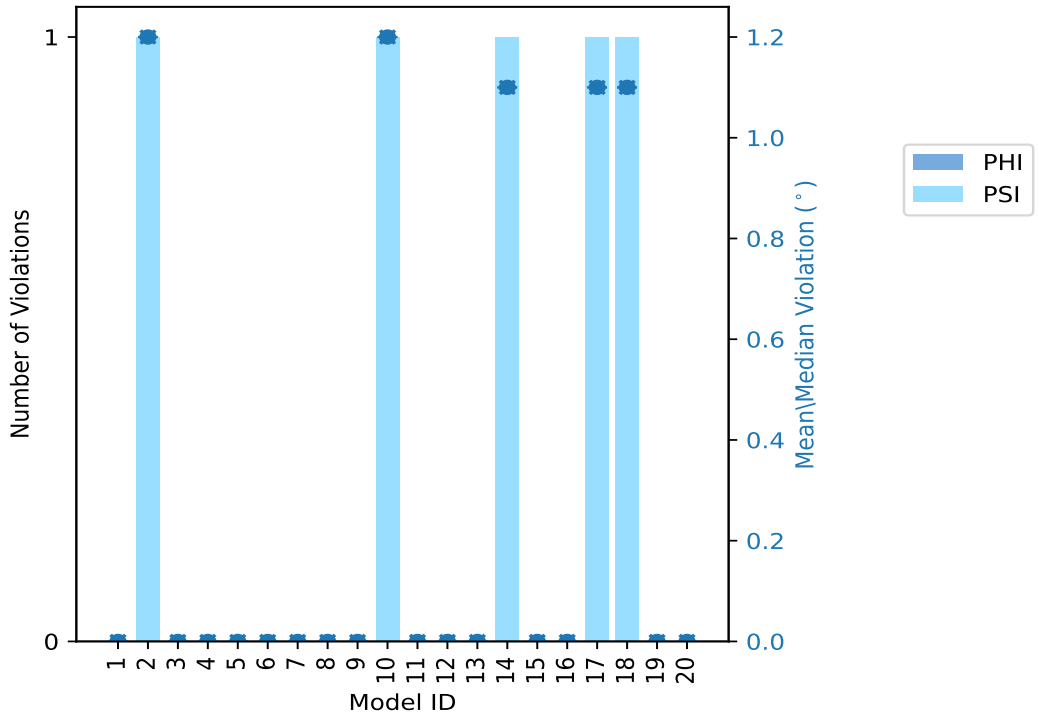
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	1	1	1.2	1.2	0.0	1.2
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	1	1	1.2	1.2	0.0	1.2
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	1	1	1.1	1.1	0.0	1.1
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	1	1	1.1	1.1	0.0	1.1
18	0	1	1	1.1	1.1	0.0	1.1
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

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

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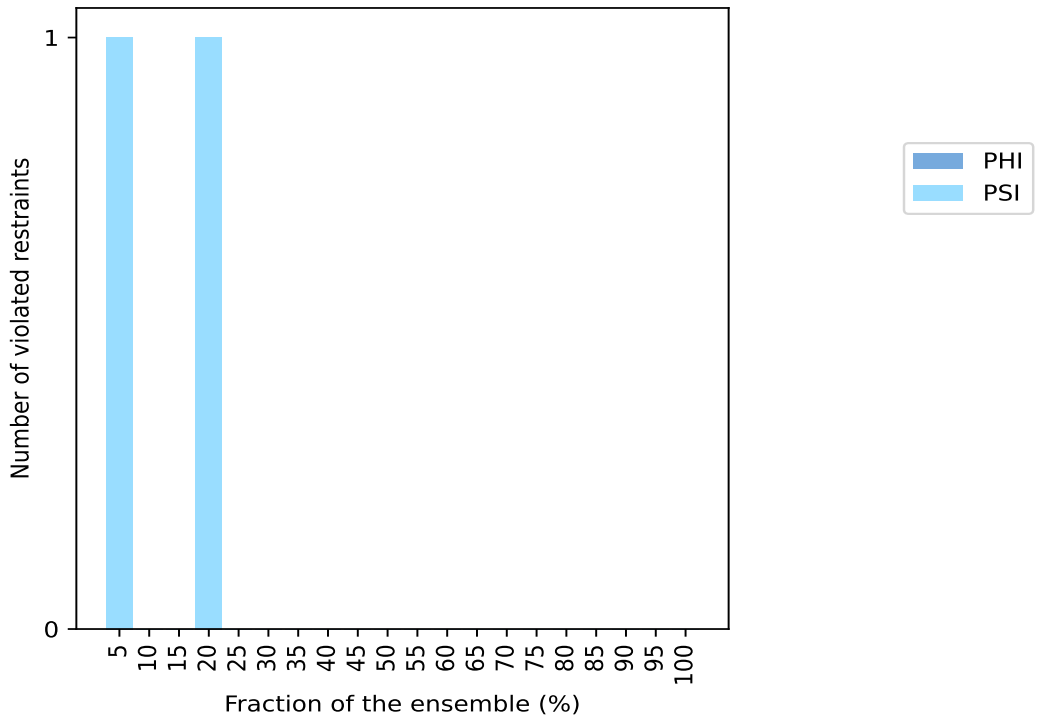
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

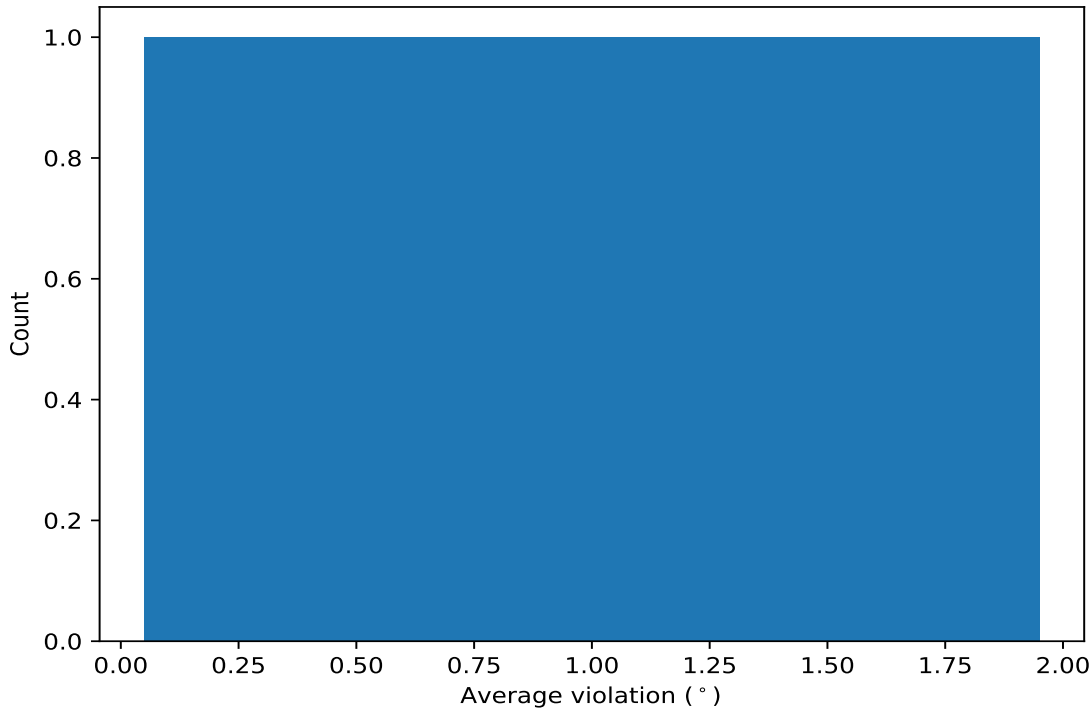


10.4 Most violated dihedral-angle restraints in the ensemble

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
(1,20)	1:A:18:LYS:N	1:A:18:LYS:CA	1:A:18:LYS:C	1:A:19:GLU:N	4	1.12	0.04	1.1

[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.
Data insufficient to plot histogram

10.5.2 Table: All violated dihedral-angle restraints

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 (°)
(1,30)	1:A:23:ALA:N	1:A:23:ALA:CA	1:A:23:ALA:C	1:A:24:GLY:N	2	1.2
(1,20)	1:A:18:LYS:N	1:A:18:LYS:CA	1:A:18:LYS:C	1:A:19:GLU:N	10	1.2
(1,20)	1:A:18:LYS:N	1:A:18:LYS:CA	1:A:18:LYS:C	1:A:19:GLU:N	14	1.1
(1,20)	1:A:18:LYS:N	1:A:18:LYS:CA	1:A:18:LYS:C	1:A:19:GLU:N	17	1.1
(1,20)	1:A:18:LYS:N	1:A:18:LYS:CA	1:A:18:LYS:C	1:A:19:GLU:N	18	1.1