Full wwPDB NMR Structure Validation Report (i)

Dec 24, 2024 – 08:58 PM EST

PDB ID	:	2M9X
BMRB ID	:	19314
Title	:	Solution NMR Structure of Microtubule-associated serine/threonine-protein kinase 1 from Homo sapiens, Northeast Structural Genomics Consortium (NESG) Target HR9151A
Authors	:	Xu, X.; Eletsky, A.; Shastry, R.; Lee, D.; Hamilton, K.; Xiao, R.; Acton, T.B.; Everett, J.K.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2013-06-20

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:

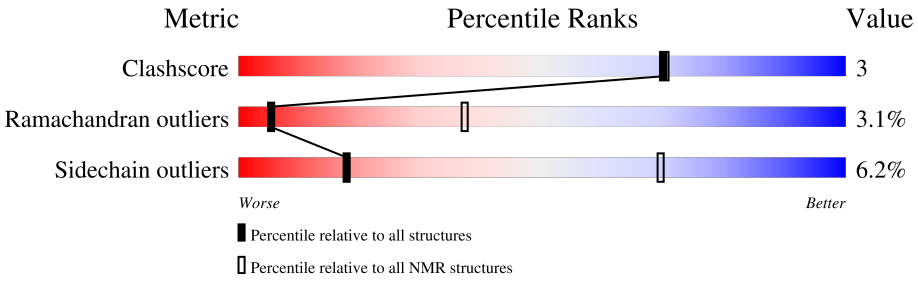
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 89%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	112	81% · 15%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 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:14-A:108 (95)	1.23	18

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1844 atoms, of which 927 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Microtubule-associated serine/threonine-protein kinase 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	112	1844	582	927	163	168	4	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9Y2H9
A	2	GLY	-	expression tag	UNP Q9Y2H9
A	3	HIS	-	expression tag	UNP Q9Y2H9
A	4	HIS	-	expression tag	UNP Q9Y2H9
A	5	HIS	-	expression tag	UNP Q9Y2H9
A	6	HIS	-	expression tag	UNP Q9Y2H9
A	7	HIS	-	expression tag	UNP Q9Y2H9
A	8	HIS	-	expression tag	UNP Q9Y2H9
A	9	SER	-	expression tag	UNP Q9Y2H9
A	10	HIS	-	expression tag	UNP Q9Y2H9
A	11	MET	-	expression tag	UNP Q9Y2H9

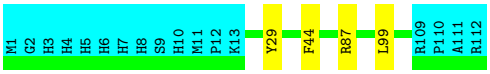
4 Residue-property plots

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: Microtubule-associated serine/threonine-protein kinase 1

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

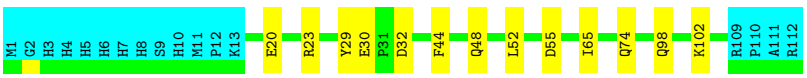
• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

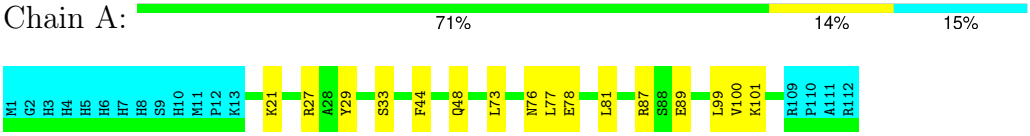
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

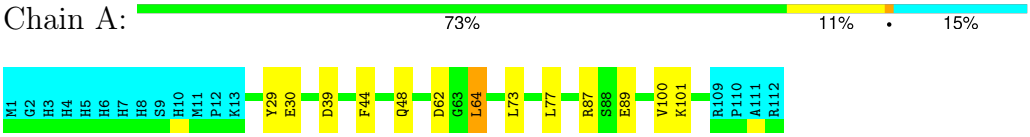
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

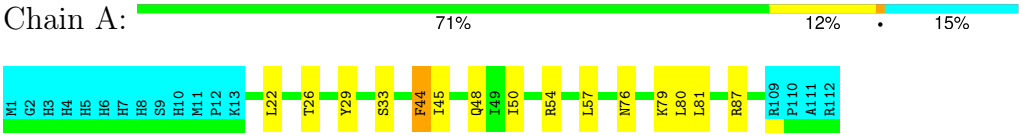
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

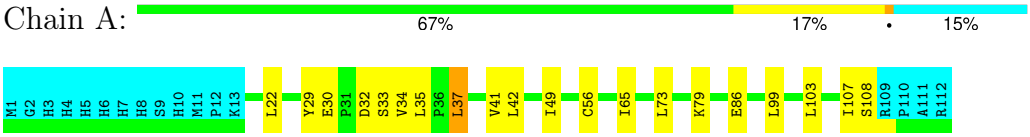
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

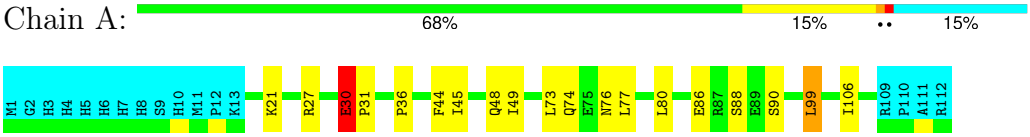
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

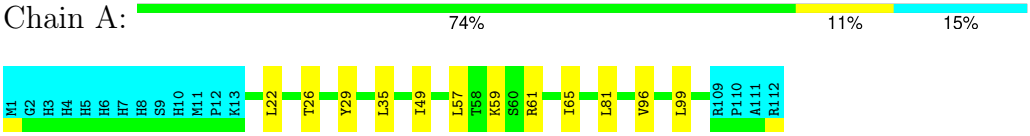
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

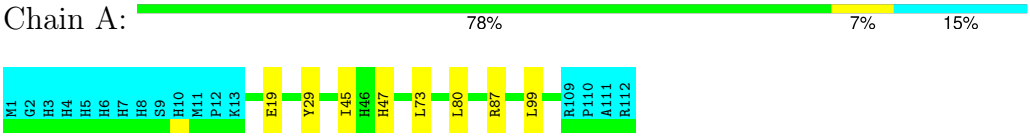
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

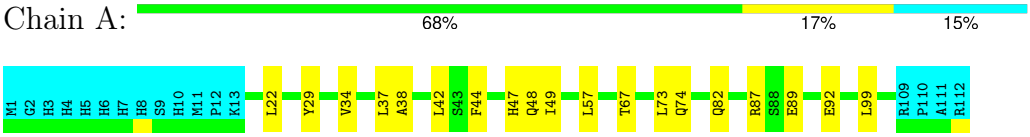
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

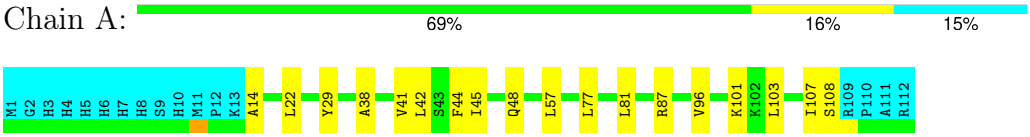
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

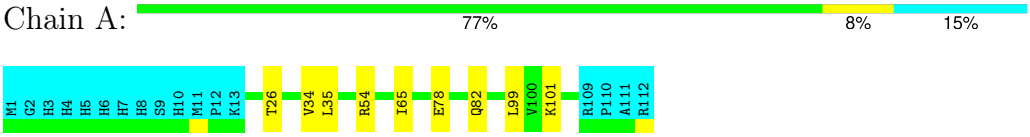
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

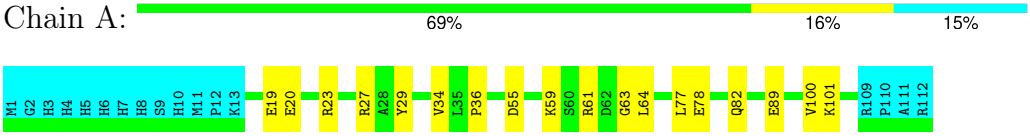
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

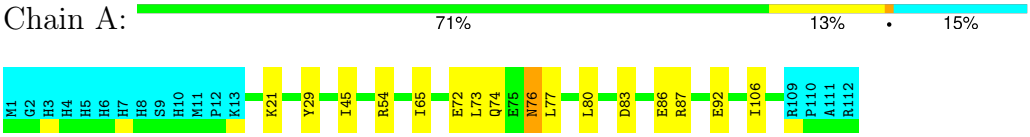
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

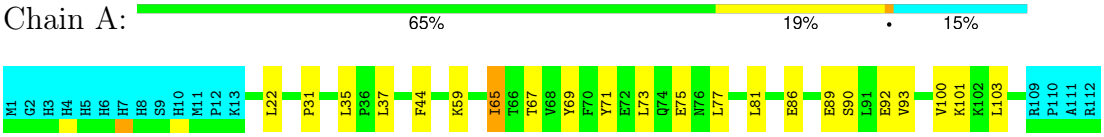
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

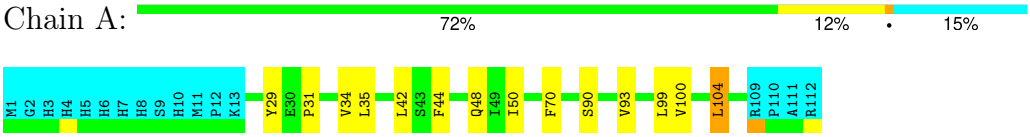
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

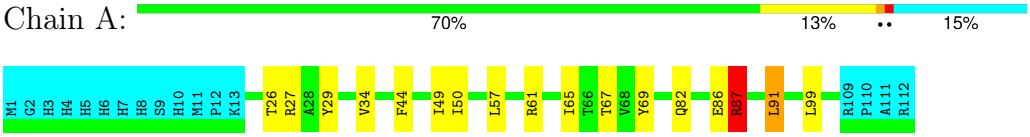
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

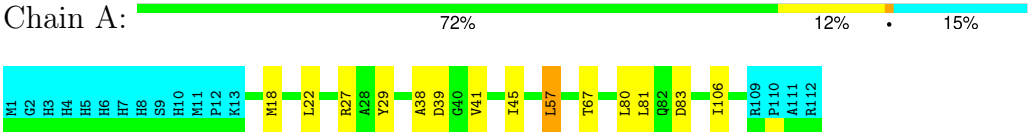
Chain A:



4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

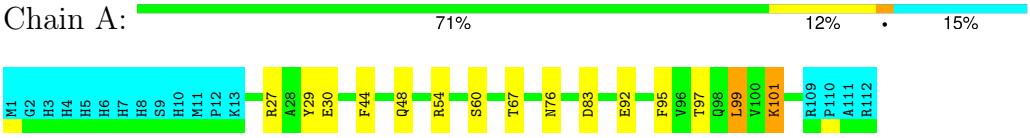
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

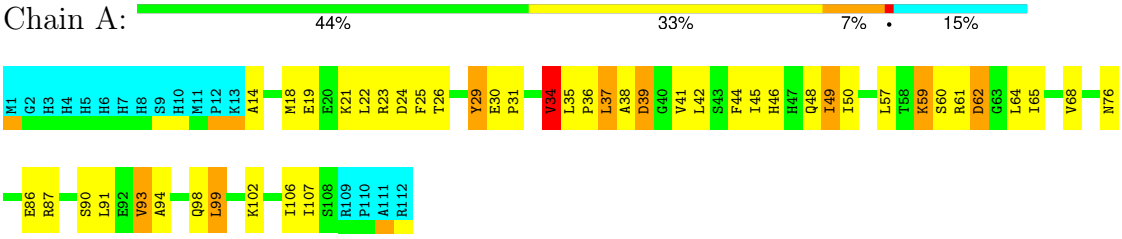
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Microtubule-associated serine/threonine-protein kinase 1

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	refinement	1.3
CNS	structure solution	1.3
CNS	geometry optimization	1.3
CYANA	refinement	3.0
CYANA	geometry optimization	3.0
CYANA	structure solution	3.0
AutoStructure	refinement	2.1
TALOS+	geometry optimization	

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	1294
Number of shifts mapped to atoms	1294
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.94±0.03	0±1/782 (0.0± 0.1%)	0.68±0.05	0±1/1059 (0.0± 0.1%)
All	All	0.95	5/15640 (0.0%)	0.69	3/21180 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.4
All	All	0	4

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	93	VAL	CB-CG2	10.00	1.73	1.52	20	1
1	A	68	VAL	CB-CG2	8.66	1.71	1.52	20	1
1	A	93	VAL	CB-CG1	6.51	1.66	1.52	20	1
1	A	34	VAL	CB-CG2	6.32	1.66	1.52	20	1
1	A	49	ILE	CB-CG2	-6.15	1.33	1.52	20	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(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	VAL	CA-CB-CG2	7.93	122.79	110.90	20	1
1	A	68	VAL	CA-CB-CG1	-6.65	100.93	110.90	20	1
1	A	94	ALA	CB-CA-C	-5.59	101.71	110.10	20	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	35	LEU	Peptide	2
1	A	30	GLU	Peptide	1
1	A	34	VAL	Peptide	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	770	785	783	5±6
All	All	15400	15700	15660	106

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ILE:HD13	1:A:99:LEU:HB3	0.78	1.56	20	1
1:A:49:ILE:HD13	1:A:99:LEU:CB	0.66	2.21	20	1
1:A:29:TYR:HB2	1:A:34:VAL:HG22	0.61	1.73	20	1
1:A:60:SER:HA	1:A:65:ILE:HD11	0.61	1.72	20	1
1:A:26:THR:HG23	1:A:50:ILE:HG23	0.60	1.73	17	2
1:A:45:ILE:HG23	1:A:80:LEU:HB3	0.57	1.77	7	2
1:A:49:ILE:HG21	1:A:99:LEU:HD23	0.57	1.75	6	1
1:A:41:VAL:O	1:A:45:ILE:HG12	0.57	1.98	20	1
1:A:26:THR:HG22	1:A:54:ARG:HH11	0.54	1.62	12	1
1:A:30:GLU:HB3	1:A:31:PRO:HD2	0.54	1.78	20	1
1:A:30:GLU:H	1:A:33:SER:HB3	0.54	1.63	6	1
1:A:37:LEU:HB2	1:A:42:LEU:HB3	0.54	1.80	6	2
1:A:64:LEU:O	1:A:64:LEU:HD23	0.54	2.02	20	1
1:A:62:ASP:HB2	1:A:64:LEU:HD22	0.54	1.80	4	1
1:A:49:ILE:HG21	1:A:99:LEU:HB3	0.52	1.80	10	3
1:A:37:LEU:HB3	1:A:92:GLU:HG3	0.52	1.82	15	1
1:A:22:LEU:HD22	1:A:57:LEU:HB2	0.52	1.82	8	1
1:A:59:LYS:HB2	1:A:59:LYS:NZ	0.52	2.20	20	1
1:A:86:GLU:HG3	1:A:87:ARG:HE	0.51	1.65	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:VAL:O	1:A:35:LEU:HG	0.51	2.06	20	1
1:A:21:LYS:HG3	1:A:106:ILE:HG12	0.51	1.83	14	1
1:A:19:GLU:HG2	1:A:57:LEU:HD12	0.51	1.83	20	1
1:A:30:GLU:HA	1:A:50:ILE:HG21	0.51	1.83	20	1
1:A:45:ILE:O	1:A:49:ILE:HG13	0.50	2.07	20	1
1:A:37:LEU:HD12	1:A:46:HIS:HB2	0.49	1.83	20	1
1:A:107:ILE:HD12	1:A:107:ILE:C	0.49	2.28	20	1
1:A:21:LYS:HB3	1:A:106:ILE:HD13	0.49	1.83	20	1
1:A:76:ASN:HD22	1:A:77:LEU:N	0.49	2.06	14	1
1:A:73:LEU:HD23	1:A:107:ILE:HG12	0.49	1.84	6	1
1:A:49:ILE:HD11	1:A:96:VAL:HG13	0.49	1.84	8	1
1:A:45:ILE:HG21	1:A:96:VAL:HG13	0.48	1.83	11	1
1:A:18:MET:O	1:A:22:LEU:HB2	0.48	2.08	20	1
1:A:44:PHE:O	1:A:48:GLN:HG2	0.48	2.09	5	10
1:A:22:LEU:HB3	1:A:57:LEU:HD13	0.48	1.86	11	3
1:A:77:LEU:HB3	1:A:100:VAL:HB	0.47	1.85	4	1
1:A:103:LEU:O	1:A:107:ILE:HG13	0.46	2.10	6	1
1:A:59:LYS:HB3	1:A:65:ILE:HG12	0.46	1.87	8	1
1:A:57:LEU:O	1:A:61:ARG:HG3	0.46	2.09	17	2
1:A:42:LEU:HD11	1:A:93:VAL:HG12	0.46	1.86	16	1
1:A:41:VAL:HG13	1:A:42:LEU:HD22	0.46	1.88	11	1
1:A:38:ALA:O	1:A:39:ASP:HB3	0.45	2.10	20	1
1:A:20:GLU:HA	1:A:23:ARG:HG2	0.45	1.89	2	1
1:A:22:LEU:HD22	1:A:57:LEU:HD22	0.45	1.89	5	1
1:A:77:LEU:HD11	1:A:103:LEU:HD23	0.45	1.87	11	1
1:A:77:LEU:HB3	1:A:100:VAL:HG13	0.45	1.87	13	2
1:A:65:ILE:HG23	1:A:69:TYR:HB3	0.45	1.88	15	1
1:A:76:ASN:O	1:A:80:LEU:HG	0.45	2.12	7	2
1:A:23:ARG:HG3	1:A:24:ASP:N	0.45	2.27	20	1
1:A:45:ILE:HG12	1:A:80:LEU:HB3	0.45	1.89	18	1
1:A:30:GLU:HB2	1:A:31:PRO:HD3	0.44	1.88	7	1
1:A:98:GLN:O	1:A:102:LYS:HG2	0.44	2.13	20	2
1:A:41:VAL:HG23	1:A:42:LEU:HD22	0.44	1.89	6	1
1:A:38:ALA:O	1:A:39:ASP:CB	0.44	2.65	20	1
1:A:38:ALA:HB3	1:A:42:LEU:HD23	0.43	1.89	11	1
1:A:41:VAL:HG11	1:A:87:ARG:HD2	0.43	1.89	11	1
1:A:87:ARG:NE	1:A:87:ARG:HA	0.43	2.27	17	1
1:A:20:GLU:HG2	1:A:23:ARG:NH2	0.43	2.28	13	1
1:A:41:VAL:HG21	1:A:83:ASP:HB3	0.43	1.91	18	1
1:A:89:GLU:HA	1:A:93:VAL:HB	0.43	1.89	15	1
1:A:42:LEU:HD21	1:A:93:VAL:HG12	0.43	1.91	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:GLU:HA	1:A:81:LEU:HB3	0.43	1.90	3	1
1:A:37:LEU:HB3	1:A:92:GLU:HB3	0.43	1.91	10	1
1:A:78:GLU:HG2	1:A:82:GLN:HE22	0.43	1.74	12	1
1:A:22:LEU:HD11	1:A:56:CYS:SG	0.43	2.53	6	1
1:A:45:ILE:HG12	1:A:80:LEU:HD22	0.42	1.90	5	1
1:A:97:THR:O	1:A:101:LYS:HD2	0.42	2.14	19	1
1:A:100:VAL:O	1:A:104:LEU:HB2	0.42	2.14	16	1
1:A:95:PHE:O	1:A:99:LEU:HB2	0.42	2.14	19	1
1:A:52:LEU:HA	1:A:55:ASP:HB3	0.42	1.91	2	1
1:A:42:LEU:HD13	1:A:92:GLU:HB2	0.42	1.91	10	1
1:A:29:TYR:O	1:A:30:GLU:HG2	0.42	2.15	20	1
1:A:21:LYS:HE2	1:A:106:ILE:HA	0.41	1.92	7	1
1:A:31:PRO:HD3	1:A:50:ILE:HG21	0.41	1.90	16	1
1:A:77:LEU:HB3	1:A:100:VAL:HG22	0.41	1.92	3	1
1:A:78:GLU:O	1:A:82:GLN:HG2	0.41	2.15	13	1
1:A:55:ASP:O	1:A:59:LYS:HG2	0.41	2.16	13	1
1:A:73:LEU:O	1:A:77:LEU:HG	0.41	2.16	7	1
1:A:22:LEU:HD22	1:A:57:LEU:HD23	0.41	1.93	18	1
1:A:23:ARG:O	1:A:27:ARG:HG3	0.41	2.16	13	1
1:A:46:HIS:O	1:A:50:ILE:HG12	0.41	2.15	20	1
1:A:26:THR:O	1:A:29:TYR:O	0.41	2.39	20	1
1:A:30:GLU:HB3	1:A:31:PRO:CD	0.41	2.46	20	1
1:A:45:ILE:HA	1:A:80:LEU:HD13	0.40	1.92	9	1
1:A:90:SER:O	1:A:91:LEU:HB2	0.40	2.15	20	1
1:A:18:MET:HG2	1:A:106:ILE:HG22	0.40	1.93	18	1
1:A:61:ARG:O	1:A:62:ASP:CB	0.40	2.70	20	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	95/112 (85%)	83±3 (87±3%)	9±2 (10±2%)	3±1 (3±1%)	5	37
All	All	1900/2240 (85%)	1653 (87%)	188 (10%)	59 (3%)	5	37

All 23 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	65	ILE	6
1	A	34	VAL	6
1	A	87	ARG	5
1	A	67	THR	5
1	A	35	LEU	4
1	A	30	GLU	4
1	A	37	LEU	3
1	A	36	PRO	3
1	A	90	SER	3
1	A	33	SER	2
1	A	89	GLU	2
1	A	108	SER	2
1	A	38	ALA	2
1	A	92	GLU	2
1	A	39	ASP	2
1	A	32	ASP	1
1	A	88	SER	1
1	A	14	ALA	1
1	A	107	ILE	1
1	A	63	GLY	1
1	A	31	PRO	1
1	A	91	LEU	1
1	A	62	ASP	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	86/101 (85%)	81±2 (94±3%)	5±2 (6±3%)	18	69
All	All	1720/2020 (85%)	1614 (94%)	106 (6%)	18	69

All 37 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	29	TYR	17

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Mol	Chain	Res	Type	Models (Total)
1	A	99	LEU	8
1	A	73	LEU	7
1	A	101	LYS	7
1	A	27	ARG	5
1	A	76	ASN	5
1	A	81	LEU	5
1	A	86	GLU	5
1	A	74	GLN	4
1	A	87	ARG	3
1	A	44	PHE	3
1	A	54	ARG	3
1	A	21	LYS	2
1	A	89	GLU	2
1	A	64	LEU	2
1	A	79	LYS	2
1	A	19	GLU	2
1	A	47	HIS	2
1	A	82	GLN	2
1	A	83	ASP	2
1	A	59	LYS	2
1	A	39	ASP	1
1	A	32	ASP	1
1	A	26	THR	1
1	A	61	ARG	1
1	A	72	GLU	1
1	A	22	LEU	1
1	A	71	TYR	1
1	A	75	GLU	1
1	A	103	LEU	1
1	A	70	PHE	1
1	A	104	LEU	1
1	A	69	TYR	1
1	A	91	LEU	1
1	A	57	LEU	1
1	A	60	SER	1
1	A	25	PHE	1

6.3.3 RNA

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 89% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *hr9151a.str*

7.1.1 Bookkeeping

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

Total number of shifts	1294
Number of shifts mapped to atoms	1294
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	99	-0.40 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	95	0.36 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	86	-0.38 ± 0.20	None needed (< 0.5 ppm)
^{15}N	92	0.26 ± 0.20	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 89%, i.e. 1211 atoms were assigned a chemical shift out of a possible 1360. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	442/473 (93%)	179/190 (94%)	176/190 (93%)	87/93 (94%)
Sidechain	701/795 (88%)	479/519 (92%)	216/250 (86%)	6/26 (23%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	68/92 (74%)	34/44 (77%)	34/44 (77%)	0/4 (0%)
Overall	1211/1360 (89%)	692/753 (92%)	426/484 (88%)	93/123 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1292 atoms were assigned a chemical shift out of a possible 1613. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	467/555 (84%)	190/223 (85%)	185/224 (83%)	92/108 (85%)
Sidechain	757/910 (83%)	517/594 (87%)	234/283 (83%)	6/33 (18%)
Aromatic	68/148 (46%)	34/72 (47%)	34/58 (59%)	0/18 (0%)
Overall	1292/1613 (80%)	741/889 (83%)	453/565 (80%)	98/159 (62%)

7.1.4 Statistically unusual chemical shifts (i)

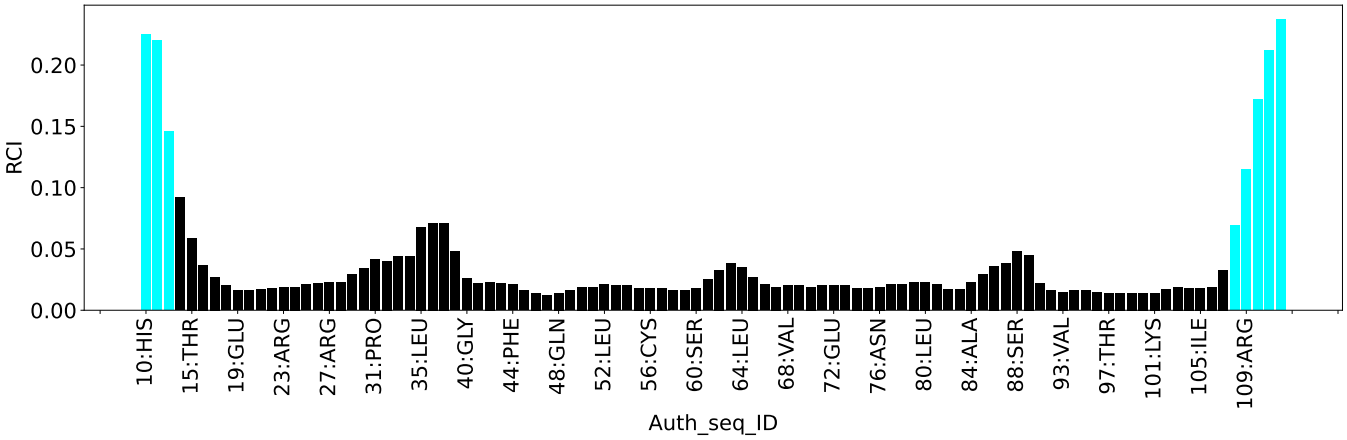
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	26	THR	HG1	4.76	0.08 – 2.19	17.2

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.20
0.15
0.10
0.05
0.00
10:HIS
15:THR
19:GLU
23:ARG
27:ARG
31:PRO
35:LEU
40:GLY
44:PHE
48:GLN
52:LEU
56:CYS
60:SER
64:LEU
68:VAL
72:GLU
76:ASN
80:LEU
84:ALA
88:SER
93:VAL
97:THR
101:LYS
105:ILE
109:ARG
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	961
Intra-residue (|i-j|=0)	259
Sequential (|i-j|=1)	188
Medium range (|i-j|>1 and |i-j|<5)	130
Long range (|i-j|≥5)	192
Inter-chain	0
Hydrogen bond restraints	192
Disulfide bond restraints	0
Total dihedral-angle restraints	130
Number of unmapped restraints	0
Number of restraints per residue	9.7
Number of long range restraints per residue[1]	1.7

[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)	9.3	0.2
0.2-0.5 (Medium)	2.6	0.46
>0.5 (Large)	0.1	1.43

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.6	6.45
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

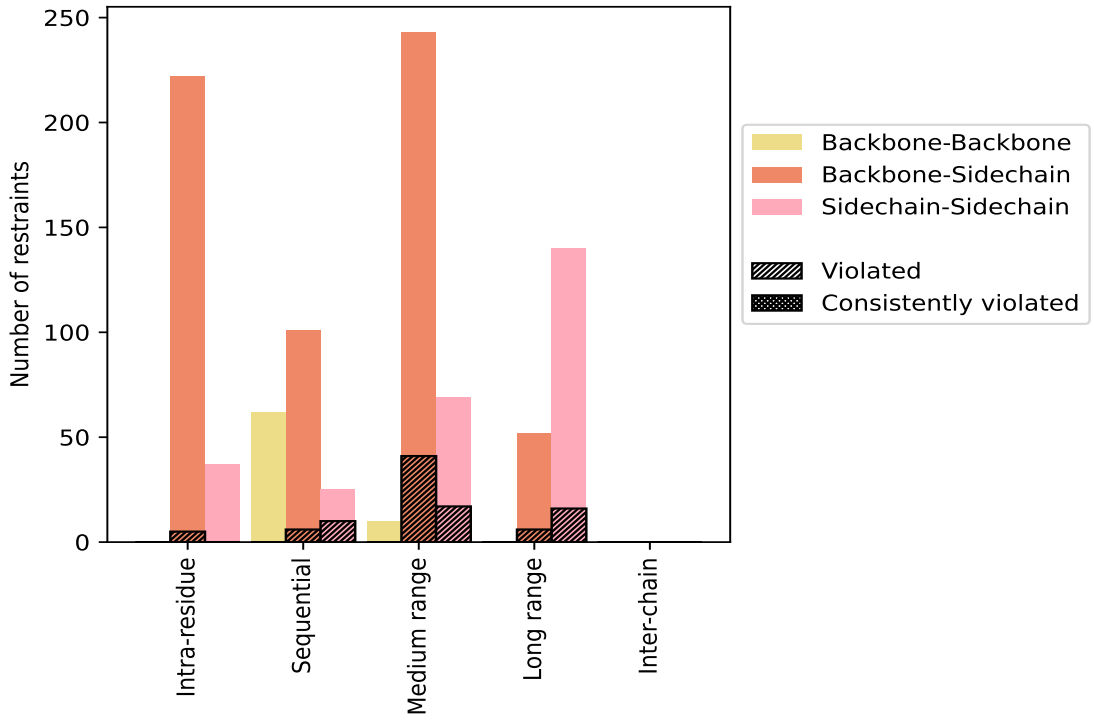
9.1 Summary of distance violations (i)

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)	259	27.0	5	1.9	0.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	222	23.1	5	2.3	0.5	0	0.0	0.0
Sidechain-Sidechain	37	3.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	188	19.6	16	8.5	1.7	0	0.0	0.0
Backbone-Backbone	62	6.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	101	10.5	6	5.9	0.6	0	0.0	0.0
Sidechain-Sidechain	25	2.6	10	40.0	1.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	130	13.5	24	18.5	2.5	0	0.0	0.0
Backbone-Backbone	10	1.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	51	5.3	7	13.7	0.7	0	0.0	0.0
Sidechain-Sidechain	69	7.2	17	24.6	1.8	0	0.0	0.0
Long range (|i-j|≥5)	192	20.0	22	11.5	2.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	52	5.4	6	11.5	0.6	0	0.0	0.0
Sidechain-Sidechain	140	14.6	16	11.4	1.7	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	192	20.0	34	17.7	3.5	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	961	100.0	101	10.5	10.5	0	0.0	0.0
Backbone-Backbone	72	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	618	64.3	58	9.4	6.0	0	0.0	0.0
Sidechain-Sidechain	271	28.2	43	15.9	4.5	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	2	1	8	4	0	15	0.13	0.2	0.03	0.12
2	1	3	9	1	0	14	0.14	0.24	0.04	0.12
3	0	4	10	2	0	16	0.16	0.31	0.06	0.15
4	1	3	8	4	0	16	0.17	0.35	0.08	0.14
5	2	0	6	2	0	10	0.14	0.22	0.04	0.15
6	2	1	8	5	0	16	0.18	0.46	0.09	0.16
7	0	4	6	2	0	12	0.16	0.29	0.05	0.14
8	2	2	7	1	0	12	0.15	0.29	0.05	0.13
9	2	1	6	2	0	11	0.18	0.33	0.07	0.16
10	3	3	8	2	0	16	0.24	1.43	0.32	0.12

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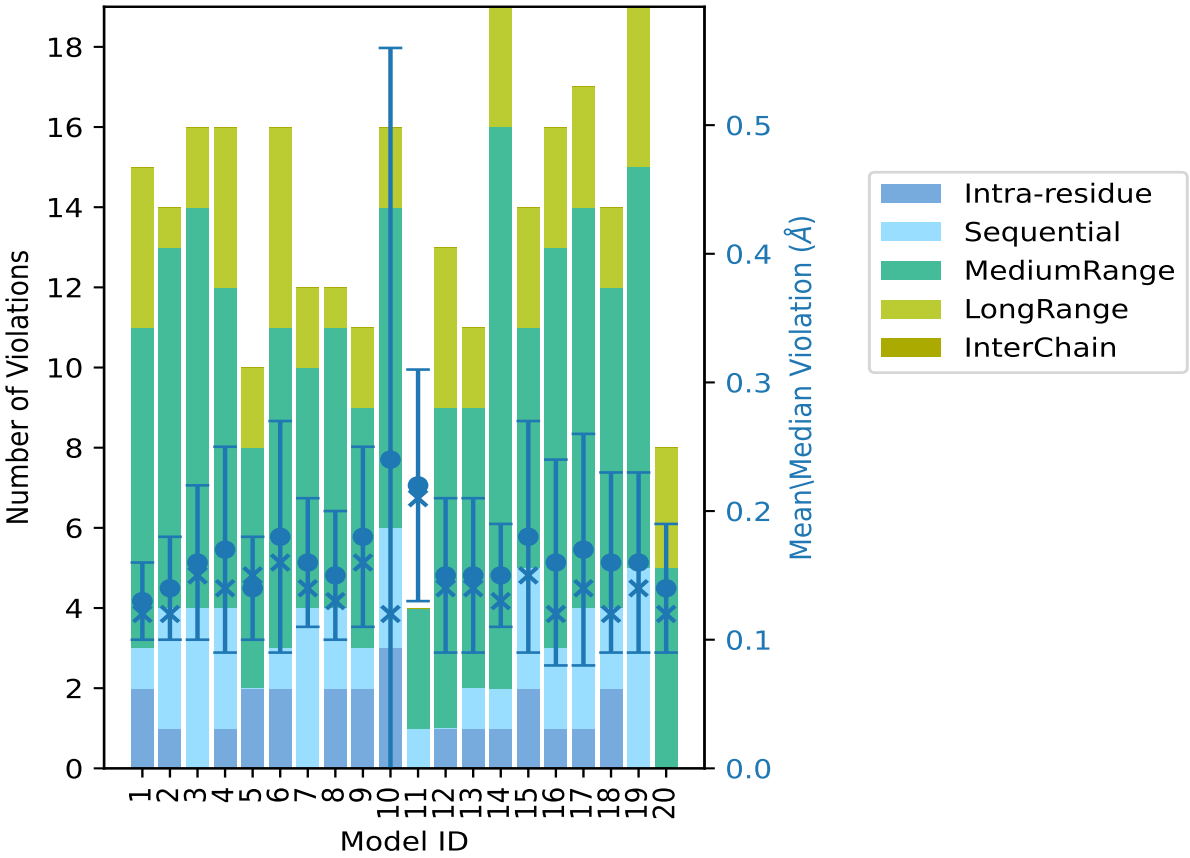
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	1	3	0	0	4	0.22	0.34	0.09	0.21
12	1	0	8	4	0	13	0.15	0.3	0.06	0.14
13	1	1	7	2	0	11	0.15	0.32	0.06	0.14
14	1	1	14	3	0	19	0.15	0.24	0.04	0.13
15	2	3	6	3	0	14	0.18	0.39	0.09	0.15
16	1	2	10	3	0	16	0.16	0.38	0.08	0.12
17	1	3	10	3	0	17	0.17	0.38	0.09	0.14
18	2	2	8	2	0	14	0.16	0.32	0.07	0.12
19	0	5	10	4	0	19	0.16	0.39	0.07	0.14
20	0	0	5	3	0	8	0.14	0.28	0.05	0.12

[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

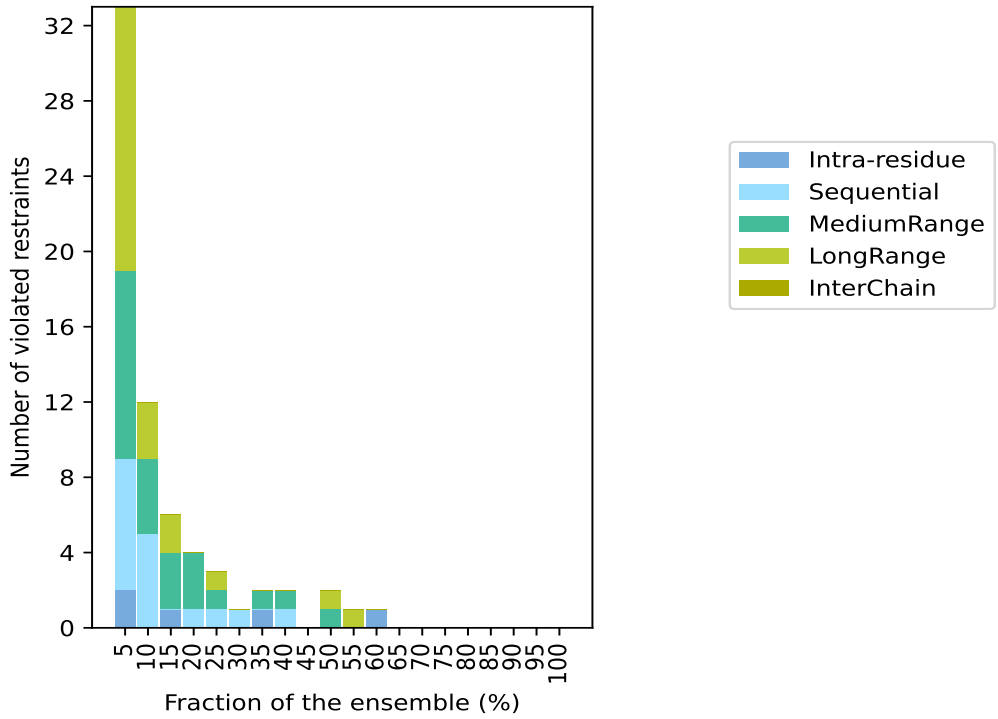
9.3 Distance violation statistics for the ensemble (i)

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, 702(IR:254, SQ:172, MR:106, LR:170, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
2	7	10	14	0	33	1	5.0
0	5	4	3	0	12	2	10.0
1	0	3	2	0	6	3	15.0
0	1	3	0	0	4	4	20.0
0	1	1	1	0	3	5	25.0
0	1	0	0	0	1	6	30.0
1	0	1	0	0	2	7	35.0
0	1	1	0	0	2	8	40.0
0	0	0	0	0	0	9	45.0
0	0	1	1	0	2	10	50.0
0	0	0	1	0	1	11	55.0
1	0	0	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	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
0	0	0	0	0	0	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

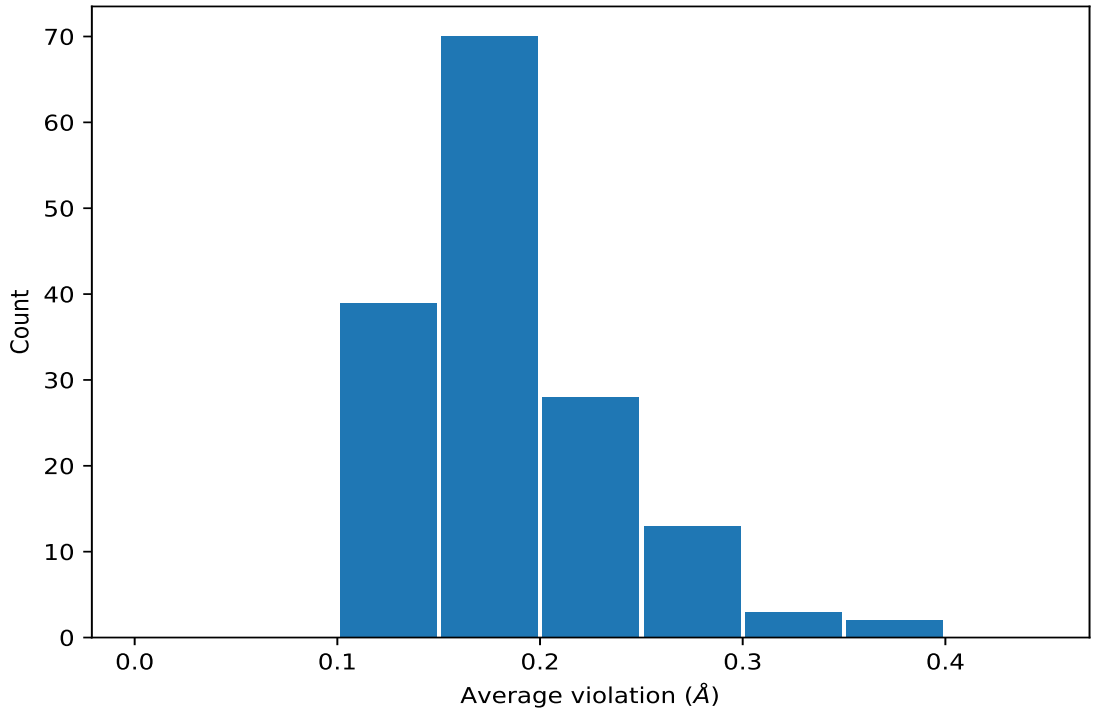
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

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)
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	15	0.12	0.01	0.12
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	12	0.19	0.07	0.2
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	11	0.34	0.36	0.21
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	11	0.34	0.36	0.21
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	11	0.34	0.36	0.21
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	10	0.2	0.09	0.16
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	10	0.2	0.09	0.16
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	10	0.2	0.09	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	10	0.18	0.07	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	10	0.18	0.07	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	10	0.18	0.07	0.16
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	8	0.2	0.07	0.18
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	8	0.2	0.07	0.18
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	8	0.18	0.05	0.15
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	8	0.18	0.05	0.15
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD1	7	0.18	0.06	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD2	7	0.18	0.06	0.17
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD1	7	0.18	0.06	0.17
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD2	7	0.18	0.06	0.17
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD1	7	0.18	0.06	0.17
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD2	7	0.18	0.06	0.17
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE1	7	0.13	0.02	0.12
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE2	7	0.13	0.02	0.12
(2,131)	1:49:A:ILE:O	1:53:A:ALA:H	7	0.12	0.01	0.12
(2,181)	1:97:A:THR:O	1:101:A:LYS:H	7	0.12	0.01	0.11
(2,126)	1:46:A:HIS:O	1:50:A:ILE:N	7	0.11	0.01	0.11
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE2	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE3	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE2	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE3	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE2	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE3	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE2	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE3	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE2	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE3	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE2	6	0.19	0.06	0.2
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE3	6	0.19	0.06	0.2
(2,187)	1:100:A:VAL:O	1:104:A:LEU:H	6	0.12	0.01	0.12
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE2	5	0.21	0.04	0.19
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE3	5	0.21	0.04	0.19
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE2	5	0.21	0.04	0.19
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE3	5	0.21	0.04	0.19
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD11	5	0.16	0.07	0.13
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD12	5	0.16	0.07	0.13
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD13	5	0.16	0.07	0.13
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD1	5	0.15	0.04	0.14
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD2	5	0.15	0.04	0.14
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD1	5	0.15	0.04	0.14
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD2	5	0.15	0.04	0.14
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD21	4	0.19	0.06	0.17
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD22	4	0.19	0.06	0.17
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD23	4	0.19	0.06	0.17
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD21	4	0.19	0.06	0.17
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD22	4	0.19	0.06	0.17
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD23	4	0.19	0.06	0.17
(1,147)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	4	0.17	0.05	0.18
(1,147)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	4	0.17	0.05	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG2	4	0.16	0.03	0.17
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG3	4	0.16	0.03	0.17
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG2	4	0.16	0.03	0.17
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG3	4	0.16	0.03	0.17
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG2	4	0.16	0.03	0.17
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG3	4	0.16	0.03	0.17
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE1	4	0.16	0.01	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE2	4	0.16	0.01	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE3	4	0.16	0.01	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE1	4	0.16	0.01	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE2	4	0.16	0.01	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE3	4	0.16	0.01	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE1	4	0.16	0.01	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE2	4	0.16	0.01	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE3	4	0.16	0.01	0.16
(2,99)	1:16:A:ALA:O	1:20:A:GLU:H	4	0.13	0.01	0.13
(2,175)	1:94:A:ALA:O	1:98:A:GLN:H	4	0.11	0.01	0.11
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD21	3	0.2	0.13	0.11
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD22	3	0.2	0.13	0.11
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD23	3	0.2	0.13	0.11
(1,660)	1:22:A:LEU:HD21	1:54:A:ARG:HG2	3	0.19	0.05	0.17
(1,660)	1:22:A:LEU:HD21	1:54:A:ARG:HG3	3	0.19	0.05	0.17
(1,660)	1:22:A:LEU:HD22	1:54:A:ARG:HG2	3	0.19	0.05	0.17
(1,660)	1:22:A:LEU:HD22	1:54:A:ARG:HG3	3	0.19	0.05	0.17
(1,660)	1:22:A:LEU:HD23	1:54:A:ARG:HG2	3	0.19	0.05	0.17
(1,660)	1:22:A:LEU:HD23	1:54:A:ARG:HG3	3	0.19	0.05	0.17
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG21	3	0.17	0.03	0.15
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG22	3	0.17	0.03	0.15
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG23	3	0.17	0.03	0.15
(1,432)	1:98:A:GLN:HA	1:101:A:LYS:HE2	3	0.17	0.03	0.15
(1,432)	1:98:A:GLN:HA	1:101:A:LYS:HE3	3	0.17	0.03	0.15
(1,643)	1:34:A:VAL:HG21	1:46:A:HIS:HE1	3	0.16	0.01	0.16
(1,643)	1:34:A:VAL:HG22	1:46:A:HIS:HE1	3	0.16	0.01	0.16
(1,643)	1:34:A:VAL:HG23	1:46:A:HIS:HE1	3	0.16	0.01	0.16
(2,159)	1:74:A:GLN:O	1:78:A:GLU:H	3	0.12	0.01	0.12
(2,107)	1:20:A:GLU:O	1:24:A:ASP:H	3	0.11	0.01	0.11
(1,671)	1:44:A:PHE:HD1	1:48:A:GLN:HE21	3	0.1	0.0	0.1
(1,671)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	3	0.1	0.0	0.1
(1,671)	1:44:A:PHE:HD2	1:48:A:GLN:HE21	3	0.1	0.0	0.1
(1,671)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	3	0.1	0.0	0.1
(1,557)	1:101:A:LYS:HE2	1:102:A:LYS:H	2	0.36	0.03	0.36
(1,557)	1:101:A:LYS:HE3	1:102:A:LYS:H	2	0.36	0.03	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG21	2	0.3	0.01	0.3
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG22	2	0.3	0.01	0.3
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG23	2	0.3	0.01	0.3
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG21	2	0.3	0.01	0.3
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG22	2	0.3	0.01	0.3
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG23	2	0.3	0.01	0.3
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG21	2	0.3	0.01	0.3
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG22	2	0.3	0.01	0.3
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG23	2	0.3	0.01	0.3
(1,725)	1:76:A:ASN:HD21	1:77:A:LEU:HB2	2	0.29	0.05	0.29
(1,725)	1:76:A:ASN:HD21	1:77:A:LEU:HB3	2	0.29	0.05	0.29
(1,725)	1:76:A:ASN:HD22	1:77:A:LEU:HB2	2	0.29	0.05	0.29
(1,725)	1:76:A:ASN:HD22	1:77:A:LEU:HB3	2	0.29	0.05	0.29
(1,705)	1:64:A:LEU:H	1:65:A:ILE:HG12	2	0.24	0.14	0.24
(1,705)	1:64:A:LEU:H	1:65:A:ILE:HG13	2	0.24	0.14	0.24
(1,640)	1:25:A:PHE:HD1	1:26:A:THR:HB	2	0.23	0.12	0.23
(1,640)	1:25:A:PHE:HD2	1:26:A:THR:HB	2	0.23	0.12	0.23
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD11	2	0.22	0.1	0.22
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD12	2	0.22	0.1	0.22
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD13	2	0.22	0.1	0.22
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD11	2	0.21	0.01	0.21
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD12	2	0.21	0.01	0.21
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD13	2	0.21	0.01	0.21
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG11	2	0.2	0.03	0.2
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG12	2	0.2	0.03	0.2
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG13	2	0.2	0.03	0.2
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG11	2	0.2	0.03	0.2
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG12	2	0.2	0.03	0.2
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG13	2	0.2	0.03	0.2
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD11	2	0.18	0.06	0.18
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD12	2	0.18	0.06	0.18
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD13	2	0.18	0.06	0.18
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD11	2	0.18	0.06	0.18
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD12	2	0.18	0.06	0.18
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD13	2	0.18	0.06	0.18
(1,462)	1:18:A:MET:HE1	1:107:A:ILE:HA	2	0.15	0.02	0.15
(1,462)	1:18:A:MET:HE2	1:107:A:ILE:HA	2	0.15	0.02	0.15
(1,462)	1:18:A:MET:HE3	1:107:A:ILE:HA	2	0.15	0.02	0.15
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD21	2	0.14	0.0	0.14
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD22	2	0.14	0.0	0.14
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD23	2	0.14	0.0	0.14
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD21	2	0.14	0.0	0.14

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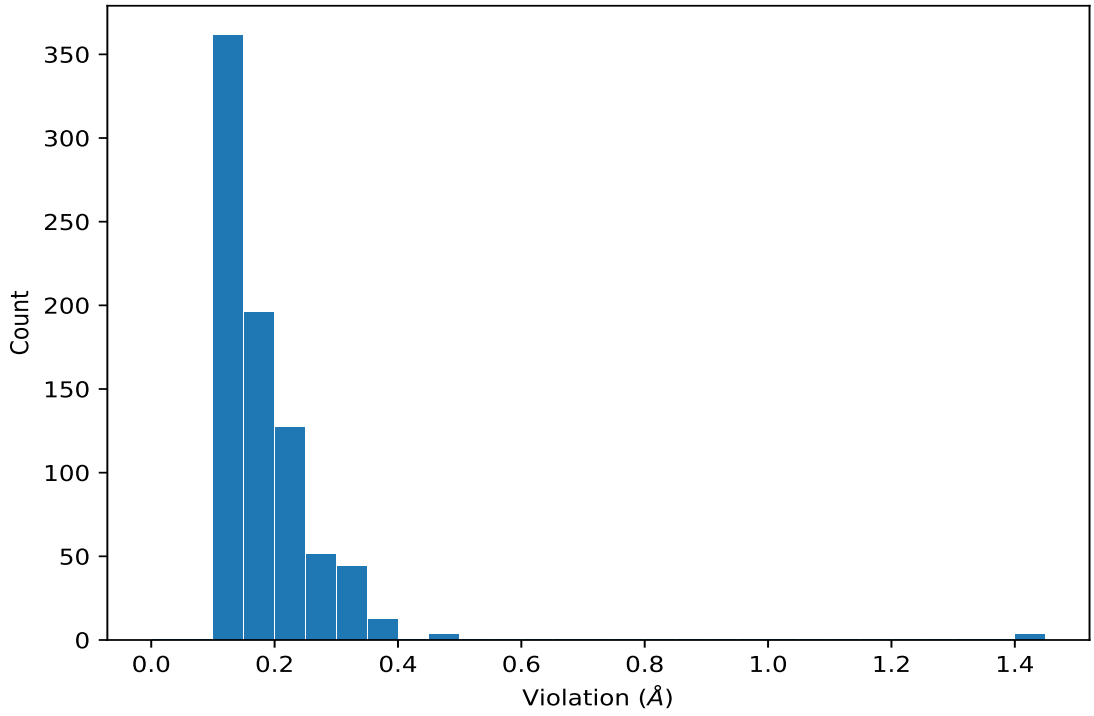
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD22	2	0.14	0.0	0.14
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD23	2	0.14	0.0	0.14
(1,707)	1:65:A:ILE:HG12	1:69:A:TYR:HD1	2	0.12	0.01	0.12
(1,707)	1:65:A:ILE:HG12	1:69:A:TYR:HD2	2	0.12	0.01	0.12
(1,707)	1:65:A:ILE:HG13	1:69:A:TYR:HD1	2	0.12	0.01	0.12
(1,707)	1:65:A:ILE:HG13	1:69:A:TYR:HD2	2	0.12	0.01	0.12
(2,189)	1:101:A:LYS:O	1:105:A:ILE:H	2	0.12	0.01	0.12
(2,101)	1:17:A:GLN:O	1:21:A:LYS:H	2	0.12	0.02	0.12
(2,173)	1:81:A:LEU:O	1:85:A:TYR:H	2	0.12	0.0	0.12
(2,129)	1:48:A:GLN:O	1:52:A:LEU:H	2	0.11	0.0	0.11
(2,97)	1:15:A:THR:O	1:19:A:GLU:H	2	0.11	0.0	0.11
(2,143)	1:55:A:ASP:O	1:59:A:LYS:H	2	0.11	0.0	0.11
(2,151)	1:70:A:PHE:O	1:74:A:GLN:H	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 (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	10	1.43
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	10	1.43
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	10	1.43
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	6	0.46
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	6	0.46
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	6	0.46
(1,557)	1:101:A:LYS:HE2	1:102:A:LYS:H	19	0.39
(1,557)	1:101:A:LYS:HE3	1:102:A:LYS:H	19	0.39
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD21	15	0.39
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD22	15	0.39
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD23	15	0.39
(1,705)	1:64:A:LEU:H	1:65:A:ILE:HG12	16	0.38
(1,705)	1:64:A:LEU:H	1:65:A:ILE:HG13	16	0.38
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	17	0.38
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	17	0.38
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	17	0.38
(1,640)	1:25:A:PHE:HD1	1:26:A:THR:HB	4	0.35
(1,640)	1:25:A:PHE:HD2	1:26:A:THR:HB	4	0.35
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	11	0.34
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	11	0.34
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	11	0.34
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	15	0.34
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	15	0.34
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	15	0.34
(1,725)	1:76:A:ASN:HD21	1:77:A:LEU:HB2	10	0.33
(1,725)	1:76:A:ASN:HD21	1:77:A:LEU:HB3	10	0.33
(1,725)	1:76:A:ASN:HD22	1:77:A:LEU:HB2	10	0.33
(1,725)	1:76:A:ASN:HD22	1:77:A:LEU:HB3	10	0.33
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	9	0.33
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	9	0.33
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	9	0.33
(1,557)	1:101:A:LYS:HE2	1:102:A:LYS:H	4	0.33
(1,557)	1:101:A:LYS:HE3	1:102:A:LYS:H	4	0.33
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	17	0.33
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD11	13	0.32
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD12	13	0.32
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD13	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	18	0.32
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	18	0.32
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	18	0.32
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD1	9	0.31
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD2	9	0.31
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD1	9	0.31
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD2	9	0.31
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD1	9	0.31
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD2	9	0.31
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG21	3	0.31
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG22	3	0.31
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG23	3	0.31
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG21	3	0.31
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG22	3	0.31
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG23	3	0.31
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG21	3	0.31
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG22	3	0.31
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG23	3	0.31
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	4	0.3
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	4	0.3
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	10	0.3
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	10	0.3
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	17	0.3
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	17	0.3
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	12	0.3
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE2	17	0.29
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE3	17	0.29
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE2	17	0.29
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE3	17	0.29
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE2	17	0.29
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE3	17	0.29
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE2	17	0.29
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE3	17	0.29
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE2	17	0.29
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE3	17	0.29
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE2	17	0.29
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE3	17	0.29
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD21	8	0.29
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD22	8	0.29
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD23	8	0.29
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD21	8	0.29
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD22	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD23	8	0.29
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD11	7	0.29
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD12	7	0.29
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD13	7	0.29
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE2	6	0.29
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE3	6	0.29
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE2	6	0.29
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE3	6	0.29
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	16	0.28
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	16	0.28
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	16	0.28
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG21	11	0.28
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG22	11	0.28
(1,382)	1:64:A:LEU:HD21	1:65:A:ILE:HG23	11	0.28
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG21	11	0.28
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG22	11	0.28
(1,382)	1:64:A:LEU:HD22	1:65:A:ILE:HG23	11	0.28
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG21	11	0.28
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG22	11	0.28
(1,382)	1:64:A:LEU:HD23	1:65:A:ILE:HG23	11	0.28
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	20	0.28
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	20	0.28
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	20	0.28
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	12	0.28
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	12	0.28
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	12	0.28
(1,660)	1:22:A:LEU:HD21	1:54:A:ARG:HG2	10	0.26
(1,660)	1:22:A:LEU:HD21	1:54:A:ARG:HG3	10	0.26
(1,660)	1:22:A:LEU:HD22	1:54:A:ARG:HG2	10	0.26
(1,660)	1:22:A:LEU:HD22	1:54:A:ARG:HG3	10	0.26
(1,660)	1:22:A:LEU:HD23	1:54:A:ARG:HG2	10	0.26
(1,660)	1:22:A:LEU:HD23	1:54:A:ARG:HG3	10	0.26
(1,570)	1:98:A:GLN:HA	1:101:A:LYS:HD2	18	0.25
(1,570)	1:98:A:GLN:HA	1:101:A:LYS:HD3	18	0.25
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE2	9	0.24
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE3	9	0.24
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE2	9	0.24
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE3	9	0.24
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE2	9	0.24
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE3	9	0.24
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE2	9	0.24
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE3	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE2	9	0.24
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE3	9	0.24
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE2	9	0.24
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE3	9	0.24
(1,725)	1:76:A:ASN:HD21	1:77:A:LEU:HB2	16	0.24
(1,725)	1:76:A:ASN:HD21	1:77:A:LEU:HB3	16	0.24
(1,725)	1:76:A:ASN:HD22	1:77:A:LEU:HB2	16	0.24
(1,725)	1:76:A:ASN:HD22	1:77:A:LEU:HB3	16	0.24
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD11	14	0.24
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD12	14	0.24
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD13	14	0.24
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD11	14	0.24
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD12	14	0.24
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD13	14	0.24
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	2	0.24
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	2	0.24
(1,559)	1:33:A:SER:H	1:34:A:VAL:HG21	19	0.24
(1,559)	1:33:A:SER:H	1:34:A:VAL:HG22	19	0.24
(1,559)	1:33:A:SER:H	1:34:A:VAL:HG23	19	0.24
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	10	0.24
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG11	4	0.23
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG12	4	0.23
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG13	4	0.23
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG11	4	0.23
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG12	4	0.23
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG13	4	0.23
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE2	15	0.23
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE3	15	0.23
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE2	15	0.23
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE3	15	0.23
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD1	2	0.22
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD2	2	0.22
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD1	2	0.22
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD2	2	0.22
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	16	0.22
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	16	0.22
(1,629)	1:34:A:VAL:HG21	1:95:A:PHE:HE1	5	0.22
(1,629)	1:34:A:VAL:HG21	1:95:A:PHE:HE2	5	0.22
(1,629)	1:34:A:VAL:HG22	1:95:A:PHE:HE1	5	0.22
(1,629)	1:34:A:VAL:HG22	1:95:A:PHE:HE2	5	0.22
(1,629)	1:34:A:VAL:HG23	1:95:A:PHE:HE1	5	0.22
(1,629)	1:34:A:VAL:HG23	1:95:A:PHE:HE2	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:65:A:ILE:HD11	1:69:A:TYR:HE1	14	0.22
(1,607)	1:65:A:ILE:HD11	1:69:A:TYR:HE2	14	0.22
(1,607)	1:65:A:ILE:HD12	1:69:A:TYR:HE1	14	0.22
(1,607)	1:65:A:ILE:HD12	1:69:A:TYR:HE2	14	0.22
(1,607)	1:65:A:ILE:HD13	1:69:A:TYR:HE1	14	0.22
(1,607)	1:65:A:ILE:HD13	1:69:A:TYR:HE2	14	0.22
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD11	14	0.22
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD12	14	0.22
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD13	14	0.22
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG21	15	0.22
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG22	15	0.22
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG23	15	0.22
(1,374)	1:57:A:LEU:HD11	1:60:A:SER:HB2	19	0.22
(1,374)	1:57:A:LEU:HD11	1:60:A:SER:HB3	19	0.22
(1,374)	1:57:A:LEU:HD12	1:60:A:SER:HB2	19	0.22
(1,374)	1:57:A:LEU:HD12	1:60:A:SER:HB3	19	0.22
(1,374)	1:57:A:LEU:HD13	1:60:A:SER:HB2	19	0.22
(1,374)	1:57:A:LEU:HD13	1:60:A:SER:HB3	19	0.22
(1,147)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	6	0.22
(1,147)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	6	0.22
(1,147)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	18	0.22
(1,147)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	18	0.22
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE2	6	0.21
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE3	6	0.21
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE2	6	0.21
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE3	6	0.21
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE2	6	0.21
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE3	6	0.21
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE2	6	0.21
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE3	6	0.21
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE2	6	0.21
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE3	6	0.21
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE2	6	0.21
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE3	6	0.21
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD1	19	0.21
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD2	19	0.21
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD1	19	0.21
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD2	19	0.21
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD1	19	0.21
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD2	19	0.21
(1,432)	1:98:A:GLN:HA	1:101:A:LYS:HE2	3	0.21
(1,432)	1:98:A:GLN:HA	1:101:A:LYS:HE3	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	7	0.21
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	7	0.21
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	7	0.21
(1,218)	1:37:A:LEU:HD21	1:92:A:GLU:HG2	19	0.21
(1,218)	1:37:A:LEU:HD22	1:92:A:GLU:HG2	19	0.21
(1,218)	1:37:A:LEU:HD23	1:92:A:GLU:HG2	19	0.21
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	18	0.21
(1,768)	1:110:A:PRO:HB2	1:111:A:ALA:HB1	3	0.2
(1,768)	1:110:A:PRO:HB2	1:111:A:ALA:HB2	3	0.2
(1,768)	1:110:A:PRO:HB2	1:111:A:ALA:HB3	3	0.2
(1,768)	1:110:A:PRO:HB3	1:111:A:ALA:HB1	3	0.2
(1,768)	1:110:A:PRO:HB3	1:111:A:ALA:HB2	3	0.2
(1,768)	1:110:A:PRO:HB3	1:111:A:ALA:HB3	3	0.2
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD21	3	0.2
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD22	3	0.2
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD23	3	0.2
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD21	3	0.2
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD22	3	0.2
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD23	3	0.2
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	18	0.2
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	18	0.2
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD11	16	0.2
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD12	16	0.2
(1,575)	1:78:A:GLU:HG2	1:81:A:LEU:HD13	16	0.2
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	6	0.2
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	6	0.2
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	6	0.2
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG2	3	0.2
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG3	3	0.2
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG2	3	0.2
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG3	3	0.2
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG2	3	0.2
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG3	3	0.2
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	1	0.2
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	9	0.2
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE2	14	0.19
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE3	14	0.19
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE2	14	0.19
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE3	14	0.19
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE2	14	0.19
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE3	14	0.19
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE2	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE3	14	0.19
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE2	14	0.19
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE3	14	0.19
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE2	14	0.19
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE3	14	0.19
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE2	7	0.19
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE3	7	0.19
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE2	7	0.19
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE3	7	0.19
(1,239)	1:59:A:LYS:HE2	1:69:A:TYR:HE1	18	0.19
(1,239)	1:59:A:LYS:HE2	1:69:A:TYR:HE2	18	0.19
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	4	0.19
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	4	0.19
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	4	0.19
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	6	0.19
(1,679)	1:48:A:GLN:HE21	1:52:A:LEU:HD21	9	0.18
(1,679)	1:48:A:GLN:HE21	1:52:A:LEU:HD22	9	0.18
(1,679)	1:48:A:GLN:HE21	1:52:A:LEU:HD23	9	0.18
(1,679)	1:48:A:GLN:HE22	1:52:A:LEU:HD21	9	0.18
(1,679)	1:48:A:GLN:HE22	1:52:A:LEU:HD22	9	0.18
(1,679)	1:48:A:GLN:HE22	1:52:A:LEU:HD23	9	0.18
(1,643)	1:34:A:VAL:HG21	1:46:A:HIS:HE1	13	0.18
(1,643)	1:34:A:VAL:HG22	1:46:A:HIS:HE1	13	0.18
(1,643)	1:34:A:VAL:HG23	1:46:A:HIS:HE1	13	0.18
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG11	17	0.18
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG12	17	0.18
(1,560)	1:29:A:TYR:HE1	1:34:A:VAL:HG13	17	0.18
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG11	17	0.18
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG12	17	0.18
(1,560)	1:29:A:TYR:HE2	1:34:A:VAL:HG13	17	0.18
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE2	1	0.18
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE3	1	0.18
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE2	1	0.18
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE3	1	0.18
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG2	4	0.18
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG3	4	0.18
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG2	4	0.18
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG3	4	0.18
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG2	4	0.18
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG3	4	0.18
(1,474)	1:93:A:VAL:HB	1:94:A:ALA:HB1	19	0.18
(1,474)	1:93:A:VAL:HB	1:94:A:ALA:HB2	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:93:A:VAL:HB	1:94:A:ALA:HB3	19	0.18
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	8	0.18
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	8	0.18
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	8	0.18
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	10	0.17
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	10	0.17
(1,660)	1:22:A:LEU:HD21	1:54:A:ARG:HG2	6	0.17
(1,660)	1:22:A:LEU:HD21	1:54:A:ARG:HG3	6	0.17
(1,660)	1:22:A:LEU:HD22	1:54:A:ARG:HG2	6	0.17
(1,660)	1:22:A:LEU:HD22	1:54:A:ARG:HG3	6	0.17
(1,660)	1:22:A:LEU:HD23	1:54:A:ARG:HG2	6	0.17
(1,660)	1:22:A:LEU:HD23	1:54:A:ARG:HG3	6	0.17
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE1	2	0.17
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE2	2	0.17
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD1	3	0.17
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD2	3	0.17
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD1	3	0.17
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD2	3	0.17
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD1	3	0.17
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD2	3	0.17
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD1	14	0.17
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD2	14	0.17
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD1	14	0.17
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD2	14	0.17
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD1	14	0.17
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD2	14	0.17
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	15	0.17
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	15	0.17
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD11	13	0.17
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD12	13	0.17
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD13	13	0.17
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE2	14	0.17
(1,558)	1:85:A:TYR:HE1	1:101:A:LYS:HE3	14	0.17
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE2	14	0.17
(1,558)	1:85:A:TYR:HE2	1:101:A:LYS:HE3	14	0.17
(1,462)	1:18:A:MET:HE1	1:107:A:ILE:HA	14	0.17
(1,462)	1:18:A:MET:HE2	1:107:A:ILE:HA	14	0.17
(1,462)	1:18:A:MET:HE3	1:107:A:ILE:HA	14	0.17
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	5	0.17
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	5	0.17
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	5	0.17
(1,332)	1:41:A:VAL:HG11	1:87:A:ARG:HD2	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	1:41:A:VAL:HG11	1:87:A:ARG:HD3	1	0.17
(1,332)	1:41:A:VAL:HG12	1:87:A:ARG:HD2	1	0.17
(1,332)	1:41:A:VAL:HG12	1:87:A:ARG:HD3	1	0.17
(1,332)	1:41:A:VAL:HG13	1:87:A:ARG:HD2	1	0.17
(1,332)	1:41:A:VAL:HG13	1:87:A:ARG:HD3	1	0.17
(1,227)	1:44:A:PHE:HD1	1:48:A:GLN:HG3	14	0.17
(1,227)	1:44:A:PHE:HD2	1:48:A:GLN:HG3	14	0.17
(1,209)	1:35:A:LEU:H	1:35:A:LEU:HD21	6	0.17
(1,209)	1:35:A:LEU:H	1:35:A:LEU:HD22	6	0.17
(1,209)	1:35:A:LEU:H	1:35:A:LEU:HD23	6	0.17
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	15	0.16
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	15	0.16
(1,643)	1:34:A:VAL:HG21	1:46:A:HIS:HE1	1	0.16
(1,643)	1:34:A:VAL:HG22	1:46:A:HIS:HE1	1	0.16
(1,643)	1:34:A:VAL:HG23	1:46:A:HIS:HE1	1	0.16
(1,633)	1:82:A:GLN:HG2	1:85:A:TYR:HD1	20	0.16
(1,633)	1:82:A:GLN:HG2	1:85:A:TYR:HD2	20	0.16
(1,633)	1:82:A:GLN:HG3	1:85:A:TYR:HD1	20	0.16
(1,633)	1:82:A:GLN:HG3	1:85:A:TYR:HD2	20	0.16
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD1	12	0.16
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD2	12	0.16
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD1	12	0.16
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD2	12	0.16
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD1	12	0.16
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD2	12	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	12	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	12	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	12	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	13	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	13	0.16
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	13	0.16
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG2	7	0.16
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG3	7	0.16
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG2	7	0.16
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG3	7	0.16
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG2	7	0.16
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG3	7	0.16
(1,365)	1:104:A:LEU:HD21	1:105:A:ILE:HA	8	0.16
(1,365)	1:104:A:LEU:HD22	1:105:A:ILE:HA	8	0.16
(1,365)	1:104:A:LEU:HD23	1:105:A:ILE:HA	8	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE1	2	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE2	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE3	2	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE1	2	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE2	2	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE3	2	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE1	2	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE2	2	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE3	2	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE1	9	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE2	9	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE3	9	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE1	9	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE2	9	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE3	9	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE1	9	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE2	9	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE3	9	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE1	12	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE2	12	0.16
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE3	12	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE1	12	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE2	12	0.16
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE3	12	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE1	12	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE2	12	0.16
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE3	12	0.16
(1,660)	1:22:A:LEU:HD21	1:54:A:ARG:HG2	16	0.15
(1,660)	1:22:A:LEU:HD21	1:54:A:ARG:HG3	16	0.15
(1,660)	1:22:A:LEU:HD22	1:54:A:ARG:HG2	16	0.15
(1,660)	1:22:A:LEU:HD22	1:54:A:ARG:HG3	16	0.15
(1,660)	1:22:A:LEU:HD23	1:54:A:ARG:HG2	16	0.15
(1,660)	1:22:A:LEU:HD23	1:54:A:ARG:HG3	16	0.15
(1,643)	1:34:A:VAL:HG21	1:46:A:HIS:HE1	12	0.15
(1,643)	1:34:A:VAL:HG22	1:46:A:HIS:HE1	12	0.15
(1,643)	1:34:A:VAL:HG23	1:46:A:HIS:HE1	12	0.15
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE1	5	0.15
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE2	5	0.15
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE1	14	0.15
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE2	14	0.15
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	1	0.15
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	1	0.15
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	1	0.15
(1,544)	1:59:A:LYS:HD2	1:69:A:TYR:HE1	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:59:A:LYS:HD2	1:69:A:TYR:HE2	6	0.15
(1,544)	1:59:A:LYS:HD3	1:69:A:TYR:HE1	6	0.15
(1,544)	1:59:A:LYS:HD3	1:69:A:TYR:HE2	6	0.15
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG21	5	0.15
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG22	5	0.15
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG23	5	0.15
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG21	17	0.15
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG22	17	0.15
(1,504)	1:91:A:LEU:HA	1:93:A:VAL:HG23	17	0.15
(1,432)	1:98:A:GLN:HA	1:101:A:LYS:HE2	5	0.15
(1,432)	1:98:A:GLN:HA	1:101:A:LYS:HE3	5	0.15
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	3	0.15
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	3	0.15
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	3	0.15
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	9	0.15
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	9	0.15
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	9	0.15
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	3	0.15
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	3	0.15
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	3	0.15
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	15	0.15
(2,187)	1:100:A:VAL:O	1:104:A:LEU:H	19	0.14
(2,181)	1:97:A:THR:O	1:101:A:LYS:H	19	0.14
(2,159)	1:74:A:GLN:O	1:78:A:GLU:H	7	0.14
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	13	0.14
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	16	0.14
(2,99)	1:16:A:ALA:O	1:20:A:GLU:H	7	0.14
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD1	3	0.14
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD2	3	0.14
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD1	3	0.14
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD2	3	0.14
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD1	15	0.14
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD2	15	0.14
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD1	15	0.14
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD2	15	0.14
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	2	0.14
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	2	0.14
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	5	0.14
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	5	0.14
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	19	0.14
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	19	0.14
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD21	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD22	10	0.14
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD23	10	0.14
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD21	10	0.14
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD22	10	0.14
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD23	10	0.14
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD21	17	0.14
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD22	17	0.14
(1,654)	1:19:A:GLU:HG2	1:22:A:LEU:HD23	17	0.14
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD21	17	0.14
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD22	17	0.14
(1,654)	1:19:A:GLU:HG3	1:22:A:LEU:HD23	17	0.14
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD1	13	0.14
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD2	13	0.14
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD1	13	0.14
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD2	13	0.14
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD1	13	0.14
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD2	13	0.14
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD21	17	0.14
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD22	17	0.14
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD23	17	0.14
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD21	17	0.14
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD22	17	0.14
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD23	17	0.14
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD21	19	0.14
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD22	19	0.14
(1,601)	1:44:A:PHE:HD1	1:80:A:LEU:HD23	19	0.14
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD21	19	0.14
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD22	19	0.14
(1,601)	1:44:A:PHE:HD2	1:80:A:LEU:HD23	19	0.14
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	8	0.14
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	8	0.14
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	4	0.14
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	4	0.14
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	4	0.14
(1,432)	1:98:A:GLN:HA	1:101:A:LYS:HE2	4	0.14
(1,432)	1:98:A:GLN:HA	1:101:A:LYS:HE3	4	0.14
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	12	0.14
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	12	0.14
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	12	0.14
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE1	11	0.14
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE2	11	0.14
(1,180)	1:14:A:ALA:HB1	1:18:A:MET:HE3	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE1	11	0.14
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE2	11	0.14
(1,180)	1:14:A:ALA:HB2	1:18:A:MET:HE3	11	0.14
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE1	11	0.14
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE2	11	0.14
(1,180)	1:14:A:ALA:HB3	1:18:A:MET:HE3	11	0.14
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	17	0.14
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	17	0.14
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	17	0.14
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	4	0.14
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	8	0.14
(2,189)	1:101:A:LYS:O	1:105:A:ILE:H	8	0.13
(2,181)	1:97:A:THR:O	1:101:A:LYS:H	2	0.13
(2,167)	1:78:A:GLU:O	1:82:A:GLN:H	4	0.13
(2,131)	1:49:A:ILE:O	1:53:A:ALA:H	9	0.13
(2,131)	1:49:A:ILE:O	1:53:A:ALA:H	13	0.13
(2,131)	1:49:A:ILE:O	1:53:A:ALA:H	18	0.13
(2,126)	1:46:A:HIS:O	1:50:A:ILE:N	14	0.13
(2,126)	1:46:A:HIS:O	1:50:A:ILE:N	16	0.13
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	1	0.13
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	8	0.13
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	14	0.13
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	19	0.13
(2,101)	1:17:A:GLN:O	1:21:A:LYS:H	15	0.13
(2,99)	1:16:A:ALA:O	1:20:A:GLU:H	14	0.13
(2,99)	1:16:A:ALA:O	1:20:A:GLU:H	17	0.13
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE2	7	0.13
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE3	7	0.13
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE2	7	0.13
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE3	7	0.13
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE2	7	0.13
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE3	7	0.13
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE2	7	0.13
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE3	7	0.13
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE2	7	0.13
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE3	7	0.13
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE2	7	0.13
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE3	7	0.13
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD1	7	0.13
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD2	7	0.13
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD1	7	0.13
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:65:A:ILE:HG12	1:69:A:TYR:HD1	20	0.13
(1,707)	1:65:A:ILE:HG12	1:69:A:TYR:HD2	20	0.13
(1,707)	1:65:A:ILE:HG13	1:69:A:TYR:HD1	20	0.13
(1,707)	1:65:A:ILE:HG13	1:69:A:TYR:HD2	20	0.13
(1,690)	1:53:A:ALA:HB1	1:54:A:ARG:HG2	7	0.13
(1,690)	1:53:A:ALA:HB1	1:54:A:ARG:HG3	7	0.13
(1,690)	1:53:A:ALA:HB2	1:54:A:ARG:HG2	7	0.13
(1,690)	1:53:A:ALA:HB2	1:54:A:ARG:HG3	7	0.13
(1,690)	1:53:A:ALA:HB3	1:54:A:ARG:HG2	7	0.13
(1,690)	1:53:A:ALA:HB3	1:54:A:ARG:HG3	7	0.13
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE21	6	0.13
(1,674)	1:45:A:ILE:HA	1:48:A:GLN:HE22	6	0.13
(1,617)	1:81:A:LEU:HG	1:85:A:TYR:HE1	20	0.13
(1,617)	1:81:A:LEU:HG	1:85:A:TYR:HE2	20	0.13
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD1	6	0.13
(1,616)	1:81:A:LEU:HD21	1:85:A:TYR:HD2	6	0.13
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD1	6	0.13
(1,616)	1:81:A:LEU:HD22	1:85:A:TYR:HD2	6	0.13
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD1	6	0.13
(1,616)	1:81:A:LEU:HD23	1:85:A:TYR:HD2	6	0.13
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	19	0.13
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	19	0.13
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD11	6	0.13
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD12	6	0.13
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD13	6	0.13
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	8	0.13
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	8	0.13
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	8	0.13
(1,492)	1:49:A:ILE:HD11	1:99:A:LEU:HG	15	0.13
(1,492)	1:49:A:ILE:HD12	1:99:A:LEU:HG	15	0.13
(1,492)	1:49:A:ILE:HD13	1:99:A:LEU:HG	15	0.13
(1,462)	1:18:A:MET:HE1	1:107:A:ILE:HA	3	0.13
(1,462)	1:18:A:MET:HE2	1:107:A:ILE:HA	3	0.13
(1,462)	1:18:A:MET:HE3	1:107:A:ILE:HA	3	0.13
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	19	0.13
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	19	0.13
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	19	0.13
(1,147)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	10	0.13
(1,147)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	10	0.13
(2,191)	1:102:A:LYS:O	1:106:A:ILE:H	12	0.12
(2,187)	1:100:A:VAL:O	1:104:A:LEU:H	1	0.12
(2,187)	1:100:A:VAL:O	1:104:A:LEU:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:100:A:VAL:O	1:104:A:LEU:H	18	0.12
(2,182)	1:97:A:THR:O	1:101:A:LYS:N	19	0.12
(2,181)	1:97:A:THR:O	1:101:A:LYS:H	20	0.12
(2,175)	1:94:A:ALA:O	1:98:A:GLN:H	4	0.12
(2,173)	1:81:A:LEU:O	1:85:A:TYR:H	16	0.12
(2,159)	1:74:A:GLN:O	1:78:A:GLU:H	2	0.12
(2,157)	1:73:A:LEU:O	1:77:A:LEU:H	17	0.12
(2,131)	1:49:A:ILE:O	1:53:A:ALA:H	1	0.12
(2,131)	1:49:A:ILE:O	1:53:A:ALA:H	16	0.12
(2,126)	1:46:A:HIS:O	1:50:A:ILE:N	8	0.12
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	9	0.12
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	11	0.12
(2,115)	1:41:A:VAL:O	1:45:A:ILE:H	1	0.12
(2,109)	1:21:A:LYS:O	1:25:A:PHE:H	7	0.12
(2,107)	1:20:A:GLU:O	1:24:A:ASP:H	7	0.12
(2,102)	1:17:A:GLN:O	1:21:A:LYS:N	15	0.12
(2,99)	1:16:A:ALA:O	1:20:A:GLU:H	6	0.12
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE1	10	0.12
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE2	10	0.12
(1,604)	1:65:A:ILE:HG21	1:69:A:TYR:HD1	16	0.12
(1,604)	1:65:A:ILE:HG21	1:69:A:TYR:HD2	16	0.12
(1,604)	1:65:A:ILE:HG22	1:69:A:TYR:HD1	16	0.12
(1,604)	1:65:A:ILE:HG22	1:69:A:TYR:HD2	16	0.12
(1,604)	1:65:A:ILE:HG23	1:69:A:TYR:HD1	16	0.12
(1,604)	1:65:A:ILE:HG23	1:69:A:TYR:HD2	16	0.12
(1,598)	1:29:A:TYR:HD1	1:30:A:GLU:HA	1	0.12
(1,598)	1:29:A:TYR:HD2	1:30:A:GLU:HA	1	0.12
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	14	0.12
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	14	0.12
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	14	0.12
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD11	2	0.12
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD12	2	0.12
(1,430)	1:96:A:VAL:HA	1:99:A:LEU:HD13	2	0.12
(1,337)	1:37:A:LEU:HD11	1:43:A:SER:HA	4	0.12
(1,337)	1:37:A:LEU:HD12	1:43:A:SER:HA	4	0.12
(1,337)	1:37:A:LEU:HD13	1:43:A:SER:HA	4	0.12
(1,187)	1:35:A:LEU:H	1:35:A:LEU:HG	1	0.12
(2,189)	1:101:A:LYS:O	1:105:A:ILE:H	12	0.11
(2,187)	1:100:A:VAL:O	1:104:A:LEU:H	4	0.11
(2,181)	1:97:A:THR:O	1:101:A:LYS:H	8	0.11
(2,181)	1:97:A:THR:O	1:101:A:LYS:H	14	0.11
(2,177)	1:95:A:PHE:O	1:99:A:LEU:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,176)	1:94:A:ALA:O	1:98:A:GLN:N	4	0.11
(2,175)	1:94:A:ALA:O	1:98:A:GLN:H	1	0.11
(2,173)	1:81:A:LEU:O	1:85:A:TYR:H	8	0.11
(2,159)	1:74:A:GLN:O	1:78:A:GLU:H	12	0.11
(2,151)	1:70:A:PHE:O	1:74:A:GLN:H	10	0.11
(2,143)	1:55:A:ASP:O	1:59:A:LYS:H	17	0.11
(2,141)	1:54:A:ARG:O	1:58:A:THR:H	16	0.11
(2,133)	1:50:A:ILE:O	1:54:A:ARG:H	17	0.11
(2,131)	1:49:A:ILE:O	1:53:A:ALA:H	14	0.11
(2,129)	1:48:A:GLN:O	1:52:A:LEU:H	2	0.11
(2,129)	1:48:A:GLN:O	1:52:A:LEU:H	18	0.11
(2,126)	1:46:A:HIS:O	1:50:A:ILE:N	1	0.11
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	2	0.11
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	3	0.11
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	5	0.11
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	12	0.11
(2,117)	1:42:A:LEU:O	1:46:A:HIS:H	17	0.11
(2,107)	1:20:A:GLU:O	1:24:A:ASP:H	17	0.11
(2,105)	1:19:A:GLU:O	1:23:A:ARG:H	5	0.11
(2,100)	1:16:A:ALA:O	1:20:A:GLU:N	14	0.11
(2,98)	1:15:A:THR:O	1:19:A:GLU:N	20	0.11
(2,97)	1:15:A:THR:O	1:19:A:GLU:H	18	0.11
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE2	2	0.11
(1,753)	1:100:A:VAL:HG11	1:101:A:LYS:HE3	2	0.11
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE2	2	0.11
(1,753)	1:100:A:VAL:HG12	1:101:A:LYS:HE3	2	0.11
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE2	2	0.11
(1,753)	1:100:A:VAL:HG13	1:101:A:LYS:HE3	2	0.11
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE2	2	0.11
(1,753)	1:100:A:VAL:HG21	1:101:A:LYS:HE3	2	0.11
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE2	2	0.11
(1,753)	1:100:A:VAL:HG22	1:101:A:LYS:HE3	2	0.11
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE2	2	0.11
(1,753)	1:100:A:VAL:HG23	1:101:A:LYS:HE3	2	0.11
(1,707)	1:65:A:ILE:HG12	1:69:A:TYR:HD1	14	0.11
(1,707)	1:65:A:ILE:HG12	1:69:A:TYR:HD2	14	0.11
(1,707)	1:65:A:ILE:HG13	1:69:A:TYR:HD1	14	0.11
(1,707)	1:65:A:ILE:HG13	1:69:A:TYR:HD2	14	0.11
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD11	16	0.11
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD12	16	0.11
(1,703)	1:62:A:ASP:HB2	1:64:A:LEU:HD13	16	0.11
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD11	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD12	16	0.11
(1,703)	1:62:A:ASP:HB3	1:64:A:LEU:HD13	16	0.11
(1,688)	1:52:A:LEU:HD21	1:76:A:ASN:HB2	19	0.11
(1,688)	1:52:A:LEU:HD21	1:76:A:ASN:HB3	19	0.11
(1,688)	1:52:A:LEU:HD22	1:76:A:ASN:HB2	19	0.11
(1,688)	1:52:A:LEU:HD22	1:76:A:ASN:HB3	19	0.11
(1,688)	1:52:A:LEU:HD23	1:76:A:ASN:HB2	19	0.11
(1,688)	1:52:A:LEU:HD23	1:76:A:ASN:HB3	19	0.11
(1,640)	1:25:A:PHE:HD1	1:26:A:THR:HB	19	0.11
(1,640)	1:25:A:PHE:HD2	1:26:A:THR:HB	19	0.11
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE1	9	0.11
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE2	9	0.11
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE1	16	0.11
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE2	16	0.11
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD11	1	0.11
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD12	1	0.11
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD13	1	0.11
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD21	20	0.11
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD22	20	0.11
(1,573)	1:19:A:GLU:HA	1:57:A:LEU:HD23	20	0.11
(1,555)	1:21:A:LYS:HE2	1:106:A:ILE:HG21	12	0.11
(1,555)	1:21:A:LYS:HE2	1:106:A:ILE:HG22	12	0.11
(1,555)	1:21:A:LYS:HE2	1:106:A:ILE:HG23	12	0.11
(1,555)	1:21:A:LYS:HE3	1:106:A:ILE:HG21	12	0.11
(1,555)	1:21:A:LYS:HE3	1:106:A:ILE:HG22	12	0.11
(1,555)	1:21:A:LYS:HE3	1:106:A:ILE:HG23	12	0.11
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG2	18	0.11
(1,477)	1:81:A:LEU:HD21	1:82:A:GLN:HG3	18	0.11
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG2	18	0.11
(1,477)	1:81:A:LEU:HD22	1:82:A:GLN:HG3	18	0.11
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG2	18	0.11
(1,477)	1:81:A:LEU:HD23	1:82:A:GLN:HG3	18	0.11
(1,423)	1:45:A:ILE:HD11	1:84:A:ALA:HB1	20	0.11
(1,423)	1:45:A:ILE:HD11	1:84:A:ALA:HB2	20	0.11
(1,423)	1:45:A:ILE:HD11	1:84:A:ALA:HB3	20	0.11
(1,423)	1:45:A:ILE:HD12	1:84:A:ALA:HB1	20	0.11
(1,423)	1:45:A:ILE:HD12	1:84:A:ALA:HB2	20	0.11
(1,423)	1:45:A:ILE:HD12	1:84:A:ALA:HB3	20	0.11
(1,423)	1:45:A:ILE:HD13	1:84:A:ALA:HB1	20	0.11
(1,423)	1:45:A:ILE:HD13	1:84:A:ALA:HB2	20	0.11
(1,423)	1:45:A:ILE:HD13	1:84:A:ALA:HB3	20	0.11
(1,402)	1:73:A:LEU:HA	1:76:A:ASN:HB2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD21	8	0.11
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD22	8	0.11
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD23	8	0.11
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD21	10	0.11
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD22	10	0.11
(1,381)	1:64:A:LEU:HA	1:64:A:LEU:HD23	10	0.11
(1,306)	1:18:A:MET:HE1	1:65:A:ILE:HD11	2	0.11
(1,306)	1:18:A:MET:HE1	1:65:A:ILE:HD12	2	0.11
(1,306)	1:18:A:MET:HE1	1:65:A:ILE:HD13	2	0.11
(1,306)	1:18:A:MET:HE2	1:65:A:ILE:HD11	2	0.11
(1,306)	1:18:A:MET:HE2	1:65:A:ILE:HD12	2	0.11
(1,306)	1:18:A:MET:HE2	1:65:A:ILE:HD13	2	0.11
(1,306)	1:18:A:MET:HE3	1:65:A:ILE:HD11	2	0.11
(1,306)	1:18:A:MET:HE3	1:65:A:ILE:HD12	2	0.11
(1,306)	1:18:A:MET:HE3	1:65:A:ILE:HD13	2	0.11
(1,213)	1:35:A:LEU:HD21	1:36:A:PRO:HD3	17	0.11
(1,213)	1:35:A:LEU:HD22	1:36:A:PRO:HD3	17	0.11
(1,213)	1:35:A:LEU:HD23	1:36:A:PRO:HD3	17	0.11
(1,175)	1:30:A:GLU:H	1:46:A:HIS:HE1	15	0.11
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	10	0.11
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	10	0.11
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	10	0.11
(1,166)	1:18:A:MET:HE1	1:22:A:LEU:H	14	0.11
(1,166)	1:18:A:MET:HE2	1:22:A:LEU:H	14	0.11
(1,166)	1:18:A:MET:HE3	1:22:A:LEU:H	14	0.11
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	13	0.11
(1,19)	1:34:A:VAL:HB	1:35:A:LEU:H	15	0.11
(2,187)	1:100:A:VAL:O	1:104:A:LEU:H	14	0.1
(2,183)	1:98:A:GLN:O	1:102:A:LYS:H	19	0.1
(2,181)	1:97:A:THR:O	1:101:A:LYS:H	4	0.1
(2,181)	1:97:A:THR:O	1:101:A:LYS:H	15	0.1
(2,175)	1:94:A:ALA:O	1:98:A:GLN:H	13	0.1
(2,175)	1:94:A:ALA:O	1:98:A:GLN:H	17	0.1
(2,155)	1:72:A:GLU:O	1:76:A:ASN:H	2	0.1
(2,151)	1:70:A:PHE:O	1:74:A:GLN:H	6	0.1
(2,143)	1:55:A:ASP:O	1:59:A:LYS:H	13	0.1
(2,131)	1:49:A:ILE:O	1:53:A:ALA:H	3	0.1
(2,126)	1:46:A:HIS:O	1:50:A:ILE:N	3	0.1
(2,126)	1:46:A:HIS:O	1:50:A:ILE:N	5	0.1
(2,126)	1:46:A:HIS:O	1:50:A:ILE:N	9	0.1
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	6	0.1
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:46:A:HIS:O	1:50:A:ILE:H	18	0.1
(2,108)	1:20:A:GLU:O	1:24:A:ASP:N	7	0.1
(2,107)	1:20:A:GLU:O	1:24:A:ASP:H	18	0.1
(2,101)	1:17:A:GLN:O	1:21:A:LYS:H	10	0.1
(2,97)	1:15:A:THR:O	1:19:A:GLU:H	1	0.1
(1,764)	1:104:A:LEU:HD11	1:107:A:ILE:HG12	12	0.1
(1,764)	1:104:A:LEU:HD11	1:107:A:ILE:HG13	12	0.1
(1,764)	1:104:A:LEU:HD12	1:107:A:ILE:HG12	12	0.1
(1,764)	1:104:A:LEU:HD12	1:107:A:ILE:HG13	12	0.1
(1,764)	1:104:A:LEU:HD13	1:107:A:ILE:HG12	12	0.1
(1,764)	1:104:A:LEU:HD13	1:107:A:ILE:HG13	12	0.1
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD1	10	0.1
(1,709)	1:69:A:TYR:HB2	1:70:A:PHE:HD2	10	0.1
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD1	10	0.1
(1,709)	1:69:A:TYR:HB3	1:70:A:PHE:HD2	10	0.1
(1,705)	1:64:A:LEU:H	1:65:A:ILE:HG12	13	0.1
(1,705)	1:64:A:LEU:H	1:65:A:ILE:HG13	13	0.1
(1,671)	1:44:A:PHE:HD1	1:48:A:GLN:HE21	2	0.1
(1,671)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	2	0.1
(1,671)	1:44:A:PHE:HD2	1:48:A:GLN:HE21	2	0.1
(1,671)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	2	0.1
(1,671)	1:44:A:PHE:HD1	1:48:A:GLN:HE21	6	0.1
(1,671)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	6	0.1
(1,671)	1:44:A:PHE:HD2	1:48:A:GLN:HE21	6	0.1
(1,671)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	6	0.1
(1,671)	1:44:A:PHE:HD1	1:48:A:GLN:HE21	16	0.1
(1,671)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	16	0.1
(1,671)	1:44:A:PHE:HD2	1:48:A:GLN:HE21	16	0.1
(1,671)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	16	0.1
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE1	18	0.1
(1,618)	1:29:A:TYR:H	1:29:A:TYR:HE2	18	0.1
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD11	3	0.1
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD12	3	0.1
(1,577)	1:78:A:GLU:HG3	1:81:A:LEU:HD13	3	0.1
(1,563)	1:60:A:SER:HA	1:65:A:ILE:HG21	4	0.1
(1,563)	1:60:A:SER:HA	1:65:A:ILE:HG22	4	0.1
(1,563)	1:60:A:SER:HA	1:65:A:ILE:HG23	4	0.1
(1,371)	1:23:A:ARG:HA	1:57:A:LEU:HD21	19	0.1
(1,371)	1:23:A:ARG:HA	1:57:A:LEU:HD22	19	0.1
(1,371)	1:23:A:ARG:HA	1:57:A:LEU:HD23	19	0.1
(1,354)	1:49:A:ILE:HG21	1:95:A:PHE:HZ	16	0.1
(1,354)	1:49:A:ILE:HG22	1:95:A:PHE:HZ	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:49:A:ILE:HG23	1:95:A:PHE:HZ	16	0.1
(1,159)	1:76:A:ASN:H	1:76:A:ASN:HD22	5	0.1
(1,147)	1:44:A:PHE:HD1	1:48:A:GLN:HE22	3	0.1
(1,147)	1:44:A:PHE:HD2	1:48:A:GLN:HE22	3	0.1

10 Dihedral-angle violation analysis

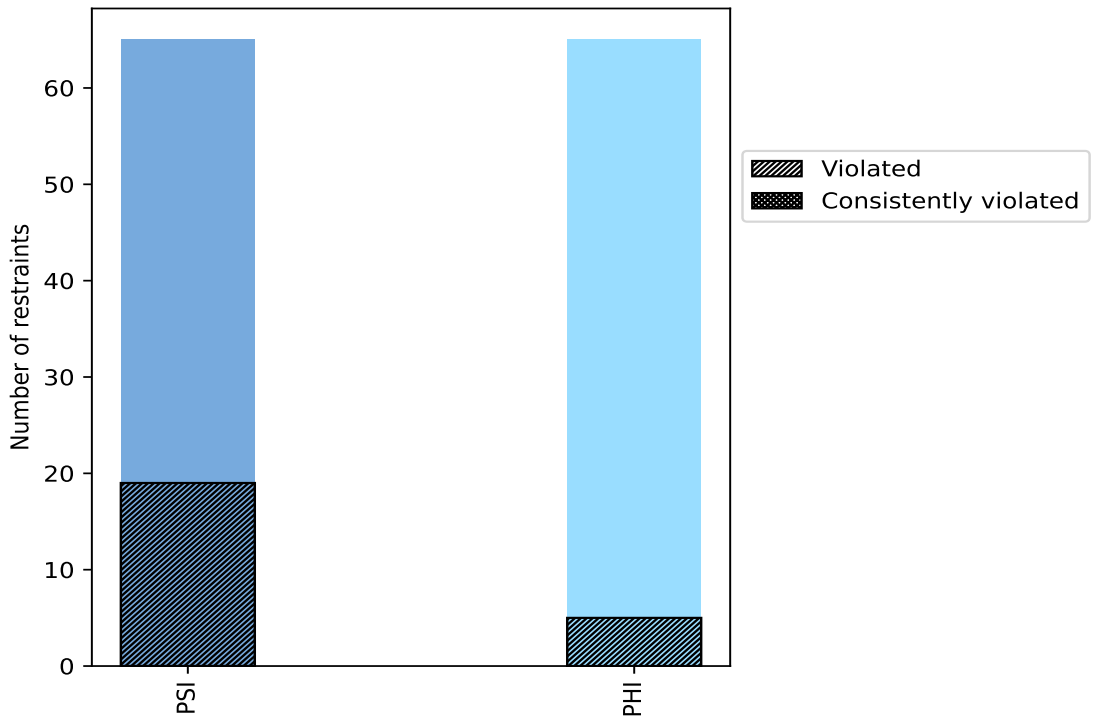
10.1 Summary of dihedral-angle violations

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	65	50.0	19	29.2	14.6	0	0.0	0.0
PHI	65	50.0	5	7.7	3.8	0	0.0	0.0
Total	130	100.0	24	18.5	18.5	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



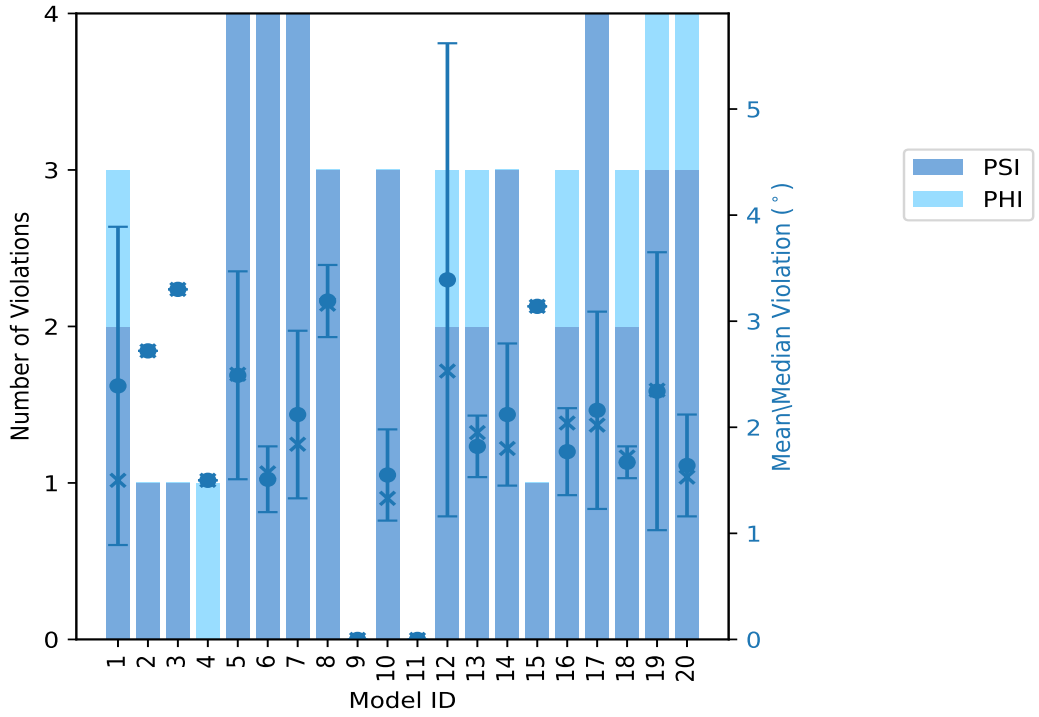
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	1	3	2.39	4.5	1.5	1.5
2	1	0	1	2.72	2.72	0.0	2.72
3	1	0	1	3.3	3.3	0.0	3.3
4	0	1	1	1.5	1.5	0.0	1.5
5	4	0	4	2.49	3.47	0.98	2.5
6	4	0	4	1.51	1.8	0.31	1.57
7	4	0	4	2.12	3.43	0.79	1.84
8	3	0	3	3.19	3.61	0.34	3.16
9	0	0	0	0.0	0.0	0.0	0.0
10	3	0	3	1.55	2.16	0.43	1.33
11	0	0	0	0.0	0.0	0.0	0.0
12	2	1	3	3.39	6.45	2.23	2.53
13	2	1	3	1.82	2.09	0.29	1.95
14	3	0	3	2.12	3.05	0.67	1.8
15	1	0	1	3.14	3.14	0.0	3.14
16	2	1	3	1.77	2.08	0.41	2.04
17	4	0	4	2.16	3.61	0.93	2.02
18	2	1	3	1.67	1.82	0.15	1.72
19	3	1	4	2.34	3.65	1.31	2.35
20	3	1	4	1.64	2.35	0.48	1.53

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]	%
7	3	10	1	5.0
6	1	7	2	10.0
3	1	4	3	15.0
2	0	2	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
1	0	1	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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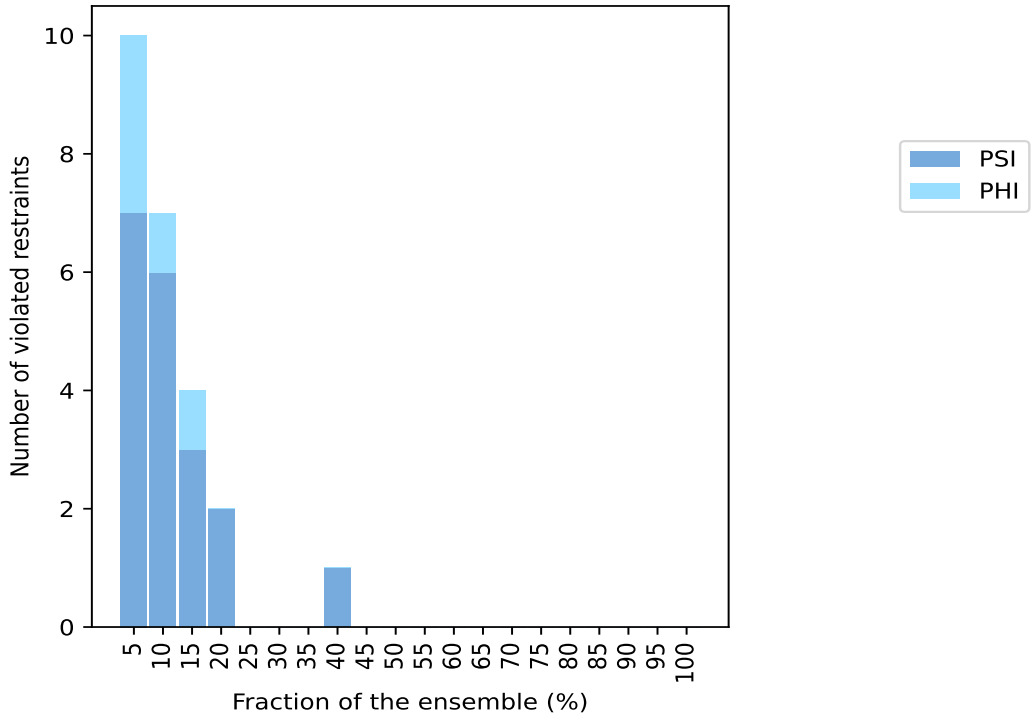
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

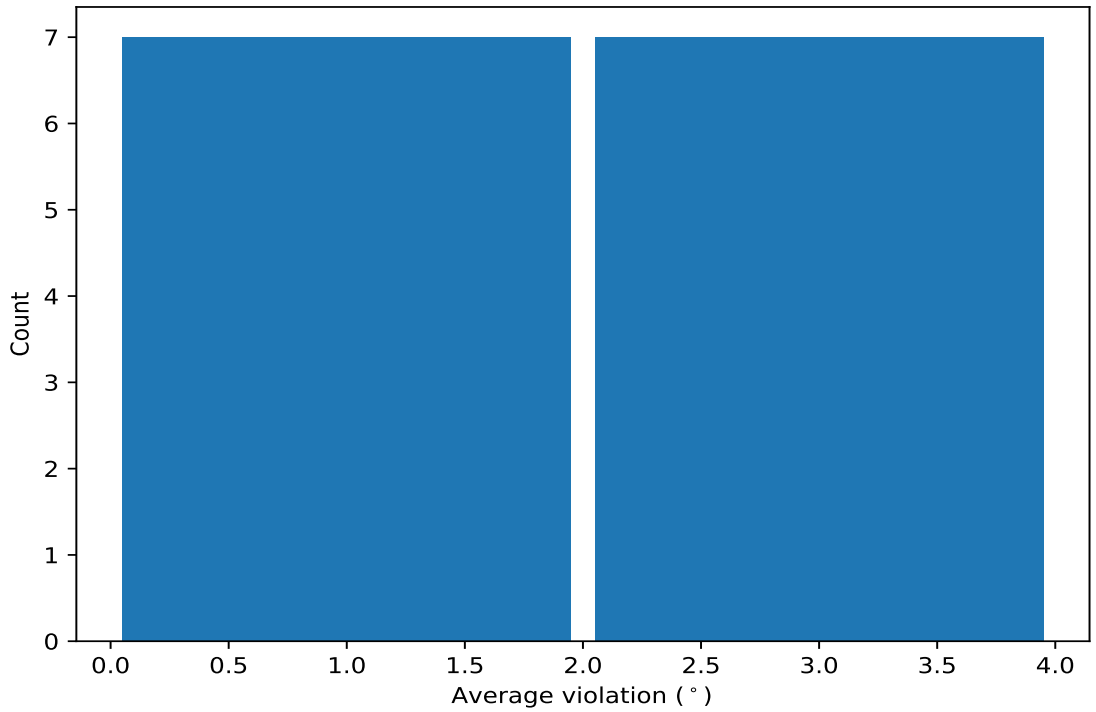


10.4 Most violated dihedral-angle restraints in the ensemble

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.

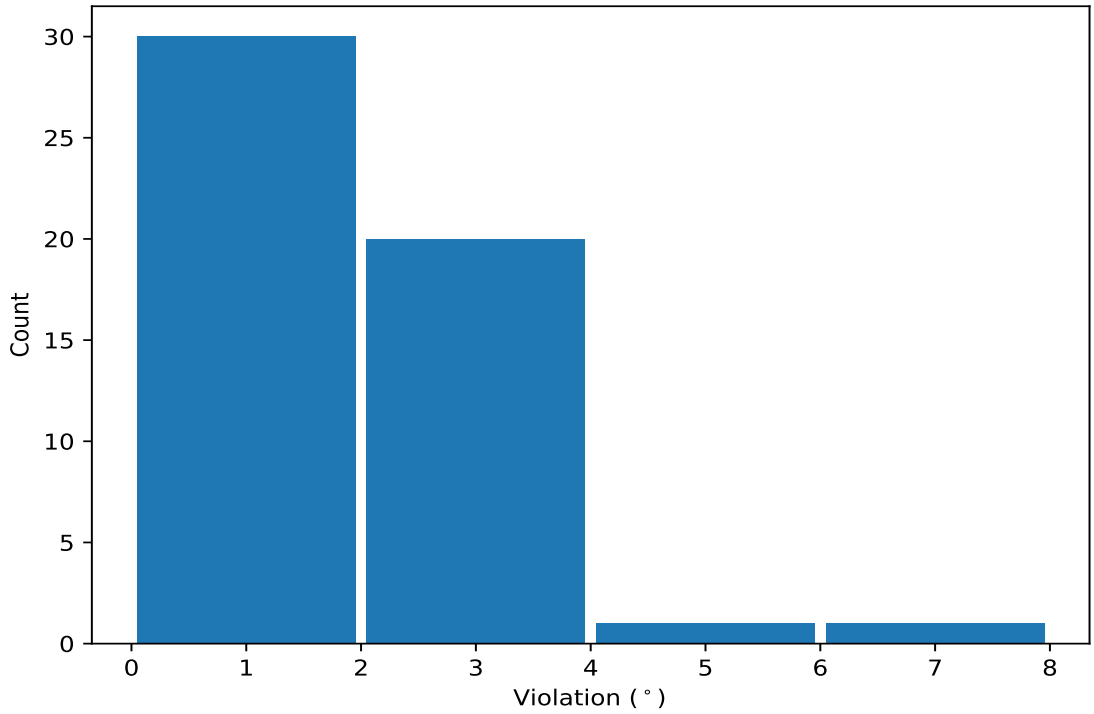
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	8	2.26	1.69	1.52
(1,4)	1:16:A:ALA:N	1:16:A:ALA:CA	1:16:A:ALA:C	1:17:A:GLN:N	4	1.8	0.28	1.88
(1,66)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:ARG:N	4	1.56	0.26	1.61
(1,130)	1:106:A:ILE:N	1:106:A:ILE:CA	1:106:A:ILE:C	1:107:A:ILE:N	3	2.53	1.0	2.79
(1,24)	1:26:A:THR:N	1:26:A:THR:CA	1:26:A:THR:C	1:27:A:ARG:N	3	2.15	0.78	2.04
(1,52)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:ARG:N	3	1.84	0.62	1.47
(1,1)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	3	1.77	0.24	1.72
(1,104)	1:93:A:VAL:N	1:93:A:VAL:CA	1:93:A:VAL:C	1:94:A:ALA:N	2	3.39	0.25	3.39
(1,30)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	2	2.99	1.51	2.99
(1,22)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:THR:N	2	2.39	1.22	2.39
(1,28)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:LEU:N	2	2.24	1.23	2.24
(1,50)	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	1:53:A:ALA:N	2	1.76	0.06	1.76
(1,63)	1:58:A:THR:C	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	2	1.76	0.59	1.76
(1,128)	1:105:A:ILE:N	1:105:A:ILE:CA	1:105:A:ILE:C	1:106:A:ILE:N	2	1.34	0.17	1.34

[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

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 (°)
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	12	6.45
(1,30)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	1	4.5
(1,112)	1:97:A:THR:N	1:97:A:THR:CA	1:97:A:THR:C	1:98:A:GLN:N	19	3.65
(1,104)	1:93:A:VAL:N	1:93:A:VAL:CA	1:93:A:VAL:C	1:94:A:ALA:N	19	3.64
(1,130)	1:106:A:ILE:N	1:106:A:ILE:CA	1:106:A:ILE:C	1:107:A:ILE:N	17	3.61
(1,22)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:THR:N	8	3.61
(1,28)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:LEU:N	5	3.47
(1,12)	1:20:A:GLU:N	1:20:A:GLU:CA	1:20:A:GLU:C	1:21:A:LYS:N	5	3.45
(1,26)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ALA:N	7	3.43
(1,6)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:MET:N	3	3.3
(1,24)	1:26:A:THR:N	1:26:A:THR:CA	1:26:A:THR:C	1:27:A:ARG:N	8	3.16
(1,104)	1:93:A:VAL:N	1:93:A:VAL:CA	1:93:A:VAL:C	1:94:A:ALA:N	15	3.14
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	14	3.05
(1,130)	1:106:A:ILE:N	1:106:A:ILE:CA	1:106:A:ILE:C	1:107:A:ILE:N	8	2.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,52)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:ARG:N	2	2.72
(1,23)	1:25:A:PHE:C	1:26:A:THR:N	1:26:A:THR:CA	1:26:A:THR:C	12	2.53
(1,63)	1:58:A:THR:C	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	20	2.35
(1,70)	1:69:A:TYR:N	1:69:A:TYR:CA	1:69:A:TYR:C	1:70:A:PHE:N	10	2.16
(1,4)	1:16:A:ALA:N	1:16:A:ALA:CA	1:16:A:ALA:C	1:17:A:GLN:N	13	2.09
(1,1)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	16	2.08
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	17	2.04
(1,24)	1:26:A:THR:N	1:26:A:THR:CA	1:26:A:THR:C	1:27:A:ARG:N	16	2.04
(1,60)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:THR:N	17	1.99
(1,4)	1:16:A:ALA:N	1:16:A:ALA:CA	1:16:A:ALA:C	1:17:A:GLN:N	7	1.97
(1,65)	1:59:A:LYS:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	13	1.95
(1,50)	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	1:53:A:ALA:N	18	1.82
(1,66)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:ARG:N	20	1.81
(1,122)	1:102:A:LYS:N	1:102:A:LYS:CA	1:102:A:LYS:C	1:103:A:LEU:N	6	1.8
(1,66)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:ARG:N	6	1.8
(1,4)	1:16:A:ALA:N	1:16:A:ALA:CA	1:16:A:ALA:C	1:17:A:GLN:N	14	1.8
(1,1)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	18	1.72
(1,50)	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	1:53:A:ALA:N	7	1.7
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	5	1.54
(1,128)	1:105:A:ILE:N	1:105:A:ILE:CA	1:105:A:ILE:C	1:106:A:ILE:N	14	1.51
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	1	1.5
(1,1)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	4	1.5
(1,30)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	5	1.48
(1,52)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:ARG:N	18	1.47
(1,66)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:ARG:N	13	1.42
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	7	1.37
(1,4)	1:16:A:ALA:N	1:16:A:ALA:CA	1:16:A:ALA:C	1:17:A:GLN:N	6	1.34
(1,52)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:ARG:N	10	1.33
(1,24)	1:26:A:THR:N	1:26:A:THR:CA	1:26:A:THR:C	1:27:A:ARG:N	20	1.25
(1,66)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:ARG:N	12	1.2
(1,130)	1:106:A:ILE:N	1:106:A:ILE:CA	1:106:A:ILE:C	1:107:A:ILE:N	16	1.19
(1,128)	1:105:A:ILE:N	1:105:A:ILE:CA	1:105:A:ILE:C	1:106:A:ILE:N	20	1.17
(1,63)	1:58:A:THR:C	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1	1.17
(1,22)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:THR:N	10	1.17
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	6	1.09
(1,64)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:SER:N	19	1.06
(1,28)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:LEU:N	17	1.02
(1,47)	1:50:A:ILE:C	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	19	1.01