Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2LC1
Title	:	Rv0020c_FHA Structure
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Deposited on	:	2011-04-11

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

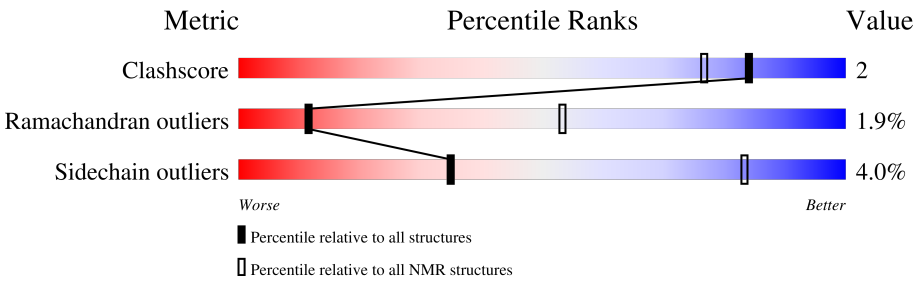
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 81%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	100	89% 5% 6%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 22 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:7-A:100 (94)	0.87	22

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 7, 8, 9, 11, 12, 15, 17, 19, 20, 21, 22, 24, 25, 28, 30
2	2, 4, 5, 14, 18, 23, 26, 27
3	6, 10, 13, 16, 29

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1508 atoms, of which 742 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative uncharacterized protein TB39.8.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	100	1508	464	742	149	152	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P71590
A	2	HIS	-	expression tag	UNP P71590

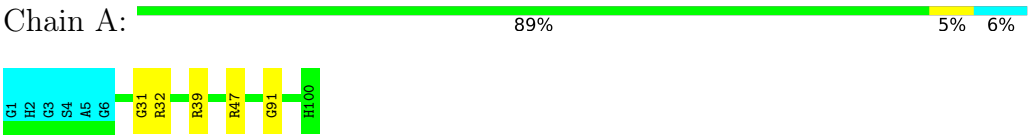
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A:



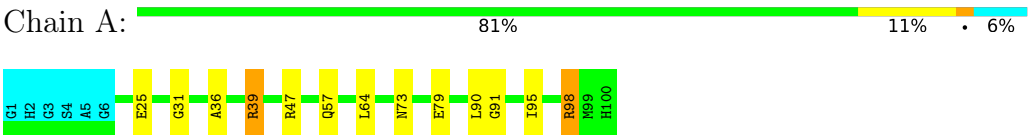
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Putative uncharacterized protein TB39.8

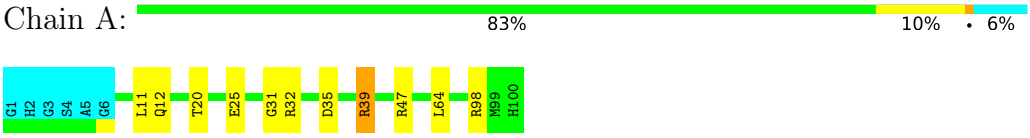
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 81% 13% 6%

4.2.4 Score per residue for model 4

- Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 85% 7% • 6%

4.2.5 Score per residue for model 5

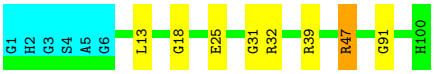
- Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 82% 12% 6%

4.2.6 Score per residue for model 6

- Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 86% 7% • 6%



4.2.7 Score per residue for model 7

- Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 81% 12% • 6%

4.2.8 Score per residue for model 8

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 78% 16% 6%

4.2.9 Score per residue for model 9

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 81% 13% 6%

4.2.10 Score per residue for model 10

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 84% 10% 6%

4.2.11 Score per residue for model 11

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 79% 15% 6%

4.2.12 Score per residue for model 12

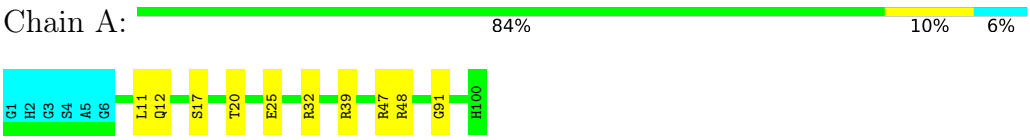
• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 86% 7% • 6%

4.2.13 Score per residue for model 13

• Molecule 1: Putative uncharacterized protein TB39.8

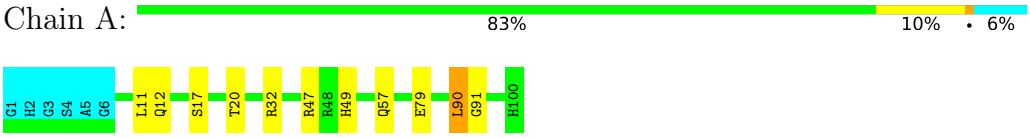
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Putative uncharacterized protein TB39.8

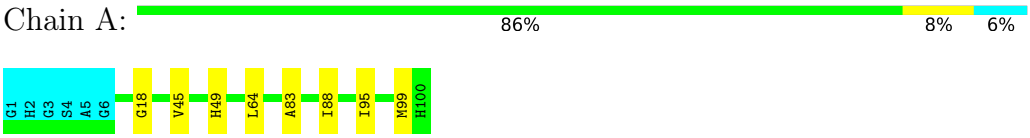
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Putative uncharacterized protein TB39.8

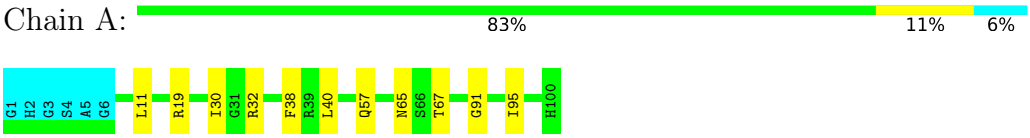
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Putative uncharacterized protein TB39.8

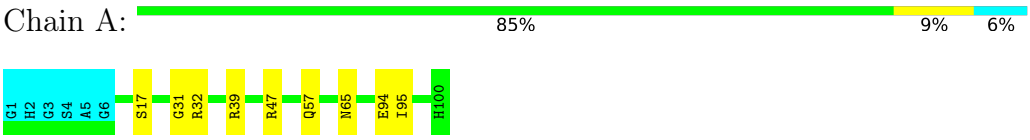
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 88% 5% • 6%

4.2.19 Score per residue for model 19

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 78% 16% 6%

4.2.20 Score per residue for model 20

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 83% 10% • 6%

4.2.21 Score per residue for model 21

• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 86% 7% • 6%

4.2.22 Score per residue for model 22 (medoid)

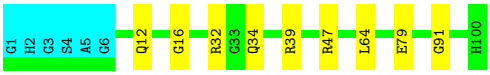
• Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 84% 9% • 6%

4.2.23 Score per residue for model 23

- Molecule 1: Putative uncharacterized protein TB39.8

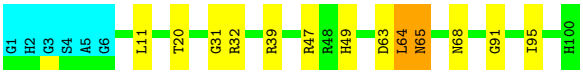
Chain A: 85% 9% 6%



4.2.24 Score per residue for model 24

- Molecule 1: Putative uncharacterized protein TB39.8

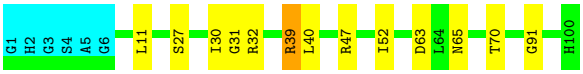
Chain A: 81% 11% • 6%



4.2.25 Score per residue for model 25

- Molecule 1: Putative uncharacterized protein TB39.8

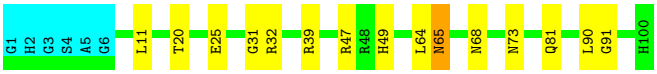
Chain A: 81% 12% • 6%



4.2.26 Score per residue for model 26

- Molecule 1: Putative uncharacterized protein TB39.8

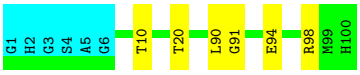
Chain A: 79% 14% • 6%



4.2.27 Score per residue for model 27

- Molecule 1: Putative uncharacterized protein TB39.8

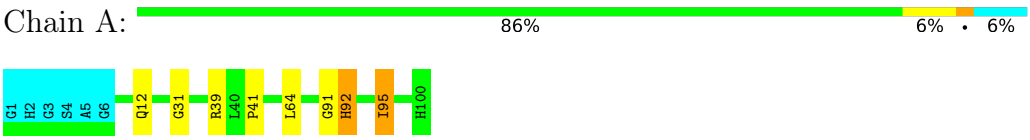
Chain A: 88% 6% 6%



4.2.28 Score per residue for model 28

- Molecule 1: Putative uncharacterized protein TB39.8

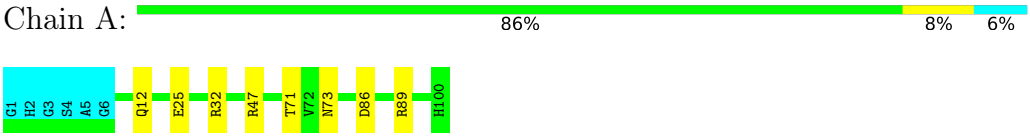
Chain A:



4.2.29 Score per residue for model 29

- Molecule 1: Putative uncharacterized protein TB39.8

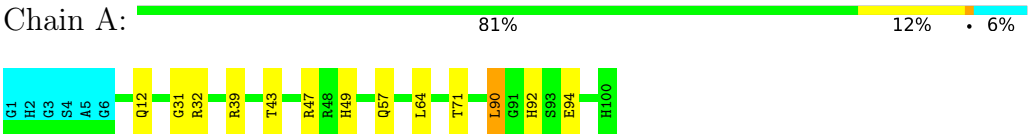
Chain A:



4.2.30 Score per residue for model 30

- Molecule 1: Putative uncharacterized protein TB39.8

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 30 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
CYANA	structure solution	2.1
CNS	refinement	1.2

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	1074
Number of shifts mapped to atoms	1074
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality (i)

6.1 Standard geometry (i)

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

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	0.3±0.4
All	All	0	8

There are no bond-length outliers.

There are no bond-angle outliers.

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	98	ARG	Sidechain	4
1	A	48	ARG	Sidechain	2
1	A	24	ARG	Sidechain	1
1	A	53	ARG	Sidechain	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	733	714	714	3±2
All	All	21990	21420	21420	99

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:GLY:O	1:A:39:ARG:HA	0.63	1.93	20	19
1:A:32:ARG:O	1:A:47:ARG:HA	0.62	1.95	12	21
1:A:63:ASP:OD1	1:A:70:THR:HB	0.55	2.00	7	1
1:A:12:GLN:O	1:A:95:ILE:HA	0.52	2.04	20	2
1:A:71:THR:OG1	1:A:89:ARG:HB2	0.52	2.05	3	2
1:A:35:ASP:OD2	1:A:48:ARG:HD3	0.51	2.05	5	1
1:A:11:LEU:O	1:A:20:THR:HA	0.49	2.08	10	9
1:A:49:HIS:CE1	1:A:68:ASN:HB3	0.47	2.45	7	2
1:A:13:LEU:O	1:A:18:GLY:HA2	0.46	2.11	6	1
1:A:49:HIS:HE2	1:A:90:LEU:HB2	0.45	1.71	14	1
1:A:65:ASN:ND2	1:A:68:ASN:HB2	0.45	2.26	26	3
1:A:30:ILE:HA	1:A:38:PHE:O	0.45	2.12	10	2
1:A:65:ASN:OD1	1:A:67:THR:HB	0.45	2.12	16	1
1:A:25:GLU:H	1:A:25:GLU:CD	0.45	2.15	7	2
1:A:73:ASN:ND2	1:A:86:ASP:HA	0.45	2.27	29	1
1:A:64:LEU:O	1:A:65:ASN:HB2	0.44	2.12	24	1
1:A:11:LEU:HB3	1:A:95:ILE:CG1	0.44	2.42	16	1
1:A:72:VAL:HG21	1:A:80:TRP:CD2	0.44	2.47	20	1
1:A:36:ALA:HB2	1:A:47:ARG:O	0.44	2.12	1	1
1:A:27:SER:HA	1:A:52:ILE:O	0.44	2.12	25	3
1:A:32:ARG:HD3	1:A:40:LEU:O	0.44	2.13	16	1
1:A:19:ARG:HA	1:A:19:ARG:NE	0.43	2.28	16	1
1:A:68:ASN:OD1	1:A:91:GLY:HA3	0.43	2.14	19	1
1:A:30:ILE:HG23	1:A:40:LEU:HD21	0.43	1.89	25	1
1:A:32:ARG:NH1	1:A:43:THR:HA	0.43	2.29	30	1
1:A:32:ARG:C	1:A:47:ARG:HA	0.43	2.34	2	1
1:A:83:ALA:HA	1:A:99:MET:SD	0.43	2.54	10	3
1:A:72:VAL:HA	1:A:87:VAL:O	0.42	2.14	11	1
1:A:24:ARG:HA	1:A:24:ARG:NE	0.42	2.29	8	1
1:A:45:VAL:HG23	1:A:49:HIS:HB2	0.42	1.90	19	2
1:A:49:HIS:NE2	1:A:90:LEU:HB2	0.42	2.29	30	2
1:A:82:LEU:HD22	1:A:88:ILE:HD11	0.42	1.90	11	1
1:A:10:THR:CG2	1:A:20:THR:HB	0.41	2.44	27	1
1:A:63:ASP:OD2	1:A:70:THR:HB	0.41	2.15	25	1
1:A:11:LEU:HB2	1:A:95:ILE:CG1	0.41	2.46	21	1
1:A:28:ASN:HD22	1:A:28:ASN:N	0.41	2.14	21	2
1:A:88:ILE:HB	1:A:95:ILE:CG2	0.40	2.46	15	1
1:A:41:PRO:HD2	1:A:92:HIS:NE2	0.40	2.31	28	1
1:A:32:ARG:HD2	1:A:42:ASP:O	0.40	2.16	8	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	93/100 (93%)	85±1 (91±2%)	6±1 (7±2%)	2±1 (2±1%)	11 53
All	All	2790/3000 (93%)	2552 (91%)	186 (7%)	52 (2%)	11 53

All 7 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	91	GLY	18
1	A	57	GLN	12
1	A	17	SER	7
1	A	65	ASN	6
1	A	92	HIS	5
1	A	16	GLY	3
1	A	18	GLY	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	79/81 (98%)	76±2 (96±2%)	3±2 (4±2%)	35 83
All	All	2370/2430 (98%)	2275 (96%)	95 (4%)	35 83

All 24 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	12	GLN	12
1	A	64	LEU	10
1	A	95	ILE	10

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Mol	Chain	Res	Type	Models (Total)
1	A	39	ARG	8
1	A	25	GLU	7
1	A	90	LEU	6
1	A	28	ASN	6
1	A	81	GLN	5
1	A	79	GLU	4
1	A	98	ARG	4
1	A	94	GLU	4
1	A	73	ASN	3
1	A	71	THR	3
1	A	34	GLN	2
1	A	11	LEU	2
1	A	35	ASP	1
1	A	57	GLN	1
1	A	65	ASN	1
1	A	47	ARG	1
1	A	15	ASP	1
1	A	53	ARG	1
1	A	42	ASP	1
1	A	86	ASP	1
1	A	63	ASP	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1074
Number of shifts mapped to atoms	1074
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	100	-0.34 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	87	-0.15 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	100	-0.04 ± 0.12	None needed (< 0.5 ppm)
^{15}N	97	-1.56 ± 0.32	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1028 atoms were assigned a chemical shift out of a possible 1274. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	474/476 (100%)	195/196 (99%)	188/188 (100%)	91/92 (99%)
Sidechain	524/734 (71%)	426/474 (90%)	84/221 (38%)	14/39 (36%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	30/64 (47%)	27/33 (82%)	0/26 (0%)	3/5 (60%)
Overall	1028/1274 (81%)	648/703 (92%)	272/435 (63%)	108/136 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1072 atoms were assigned a chemical shift out of a possible 1324. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	506/509 (99%)	209/211 (99%)	200/200 (100%)	97/98 (99%)
Sidechain	534/744 (72%)	433/481 (90%)	87/224 (39%)	14/39 (36%)
Aromatic	32/71 (45%)	29/37 (78%)	0/28 (0%)	3/6 (50%)
Overall	1072/1324 (81%)	671/729 (92%)	287/452 (63%)	114/143 (80%)

7.1.4 Statistically unusual chemical shifts (i)

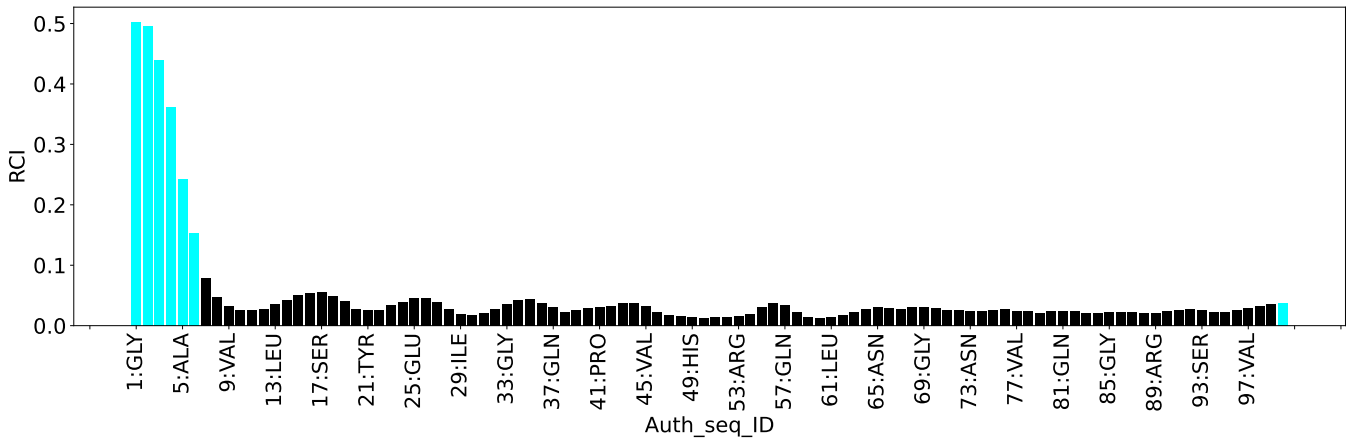
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	70	THR	HG1	7.10	0.08 – 2.19	28.3
1	A	46	SER	H	11.92	5.45 – 11.10	6.5
1	A	72	VAL	HB	0.23	0.43 – 3.54	-5.6

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
0.0
0.1
0.2
0.3
0.4
0.5
1:GLY
5:ALA
9:VAL
13:LEU
17:SER
21:TYR
25:GLU
29:ILE
33:GLY
37:GLN
41:PRO
45:VAL
49:HIS
53:ARG
57:GLN
61:LEU
65:ASN
69:GLY
73:ASN
77:VAL
81:GLN
85:GLY
89:ARG
93:SER
97:VAL
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1363
Intra-residue (|i-j|=0)	328
Sequential (|i-j|=1)	416
Medium range (|i-j|>1 and |i-j|<5)	137
Long range (|i-j|≥5)	420
Inter-chain	0
Hydrogen bond restraints	62
Disulfide bond restraints	0
Total dihedral-angle restraints	152
Number of unmapped restraints	0
Number of restraints per residue	15.2
Number of long range restraints per residue[1]	4.8

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.3	0.18
0.2-0.5 (Medium)	0.1	0.21
>0.5 (Large)	0.2	1.56

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	7.0	4.6
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

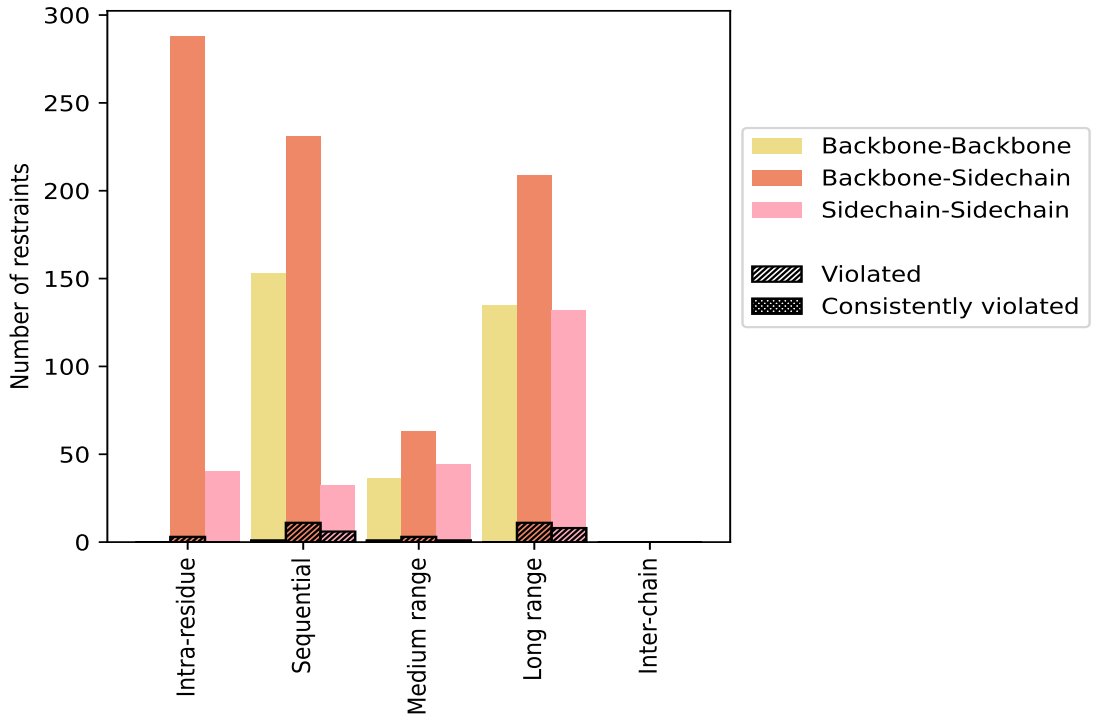
9.1 Summary of distance violations (i)

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)	328	24.1	3	0.9	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	288	21.1	3	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	40	2.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	416	30.5	18	4.3	1.3	0	0.0	0.0
Backbone-Backbone	153	11.2	1	0.7	0.1	0	0.0	0.0
Backbone-Sidechain	231	16.9	11	4.8	0.8	0	0.0	0.0
Sidechain-Sidechain	32	2.3	6	18.8	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	137	10.1	5	3.6	0.4	0	0.0	0.0
Backbone-Backbone	30	2.2	1	3.3	0.1	0	0.0	0.0
Backbone-Sidechain	63	4.6	3	4.8	0.2	0	0.0	0.0
Sidechain-Sidechain	44	3.2	1	2.3	0.1	0	0.0	0.0
Long range (|i-j|≥5)	420	30.8	19	4.5	1.4	0	0.0	0.0
Backbone-Backbone	79	5.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	209	15.3	11	5.3	0.8	0	0.0	0.0
Sidechain-Sidechain	132	9.7	8	6.1	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	62	4.5	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1363	100.0	45	3.3	3.3	0	0.0	0.0
Backbone-Backbone	324	23.8	2	0.6	0.1	0	0.0	0.0
Backbone-Sidechain	791	58.0	28	3.5	2.1	0	0.0	0.0
Sidechain-Sidechain	248	18.2	15	6.0	1.1	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	2	0	1	0	3	0.13	0.13	0.0	0.13
2	0	2	0	1	0	3	0.13	0.15	0.02	0.12
3	1	1	0	0	0	2	0.12	0.12	0.0	0.12
4	0	2	0	3	0	5	0.64	1.48	0.64	0.14
5	0	2	0	0	0	2	0.12	0.12	0.0	0.12
6	1	1	1	1	0	4	0.34	0.96	0.36	0.13
7	1	1	0	2	0	4	0.14	0.16	0.01	0.15
8	0	1	0	1	0	2	0.12	0.12	0.0	0.12
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	1	0	0	1	0.16	0.16	0.0	0.16
11	0	2	0	2	0	4	0.14	0.21	0.04	0.11

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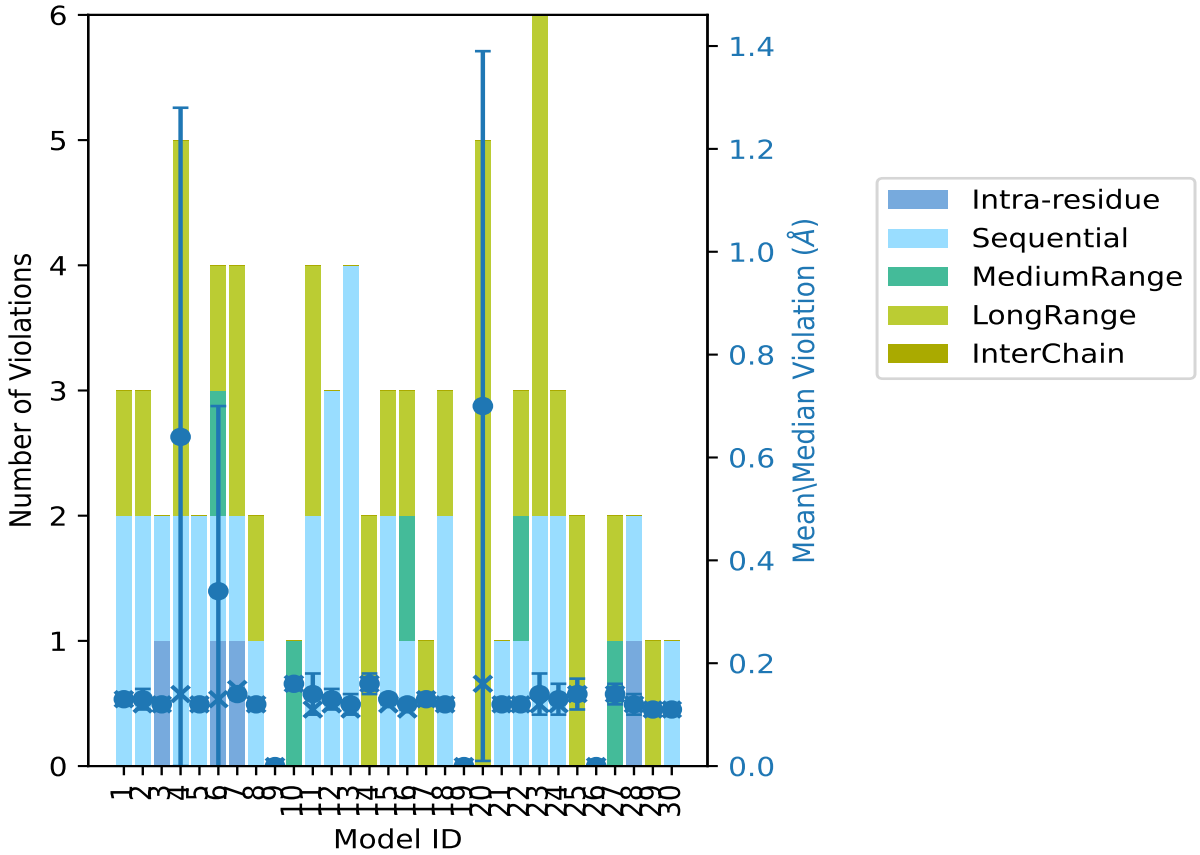
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	3	0	0	0	3	0.13	0.16	0.02	0.12
13	0	4	0	0	0	4	0.12	0.15	0.02	0.11
14	0	0	0	2	0	2	0.16	0.18	0.02	0.16
15	0	2	0	1	0	3	0.13	0.14	0.01	0.12
16	0	1	1	1	0	3	0.12	0.13	0.01	0.11
17	0	0	0	1	0	1	0.13	0.13	0.0	0.13
18	0	2	0	1	0	3	0.12	0.13	0.01	0.12
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	5	0	5	0.7	1.56	0.69	0.16
21	0	1	0	0	0	1	0.12	0.12	0.0	0.12
22	0	1	1	1	0	3	0.12	0.13	0.01	0.12
23	0	2	0	4	0	6	0.14	0.21	0.04	0.12
24	0	2	0	1	0	3	0.13	0.17	0.03	0.12
25	0	0	0	2	0	2	0.14	0.17	0.03	0.14
26	0	0	0	0	0	0	0.0	0.0	0.0	0.0
27	0	0	1	1	0	2	0.14	0.16	0.02	0.14
28	1	1	0	0	0	2	0.12	0.14	0.02	0.12
29	0	0	0	1	0	1	0.11	0.11	0.0	0.11
30	0	1	0	0	0	1	0.11	0.11	0.0	0.11

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

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



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1256(IR:325, SQ:398, MR:132, LR:401, 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	10	5	11	0	28	1	3.3
1	5	0	4	0	10	2	6.7
0	0	0	3	0	3	3	10.0
0	2	0	1	0	3	4	13.3
0	0	0	0	0	0	5	16.7
0	1	0	0	0	1	6	20.0

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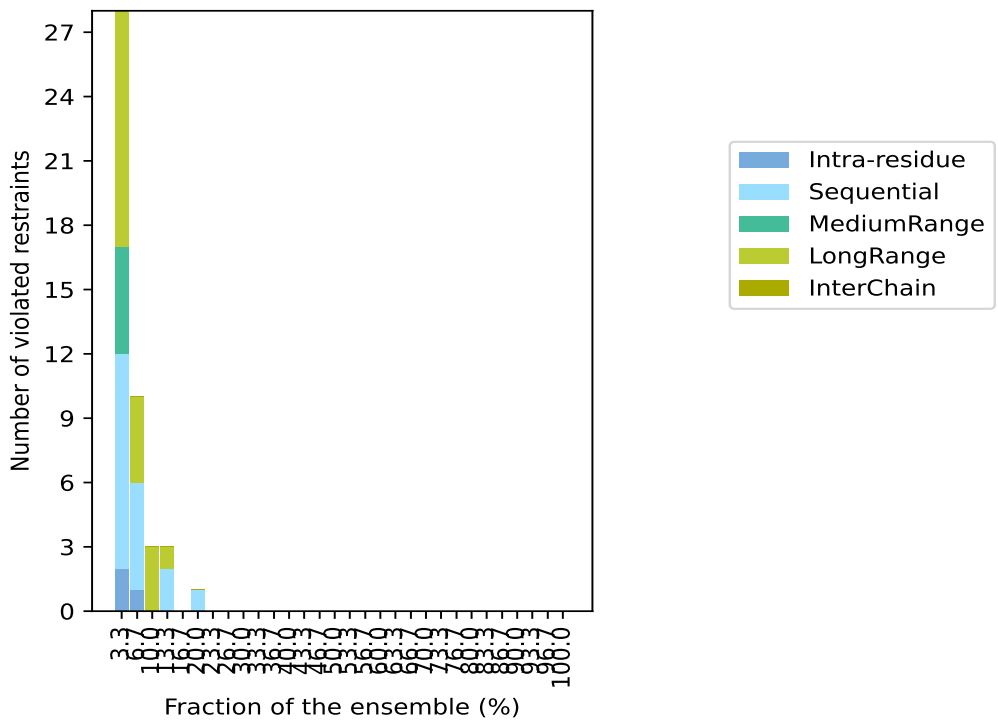
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	0	0	0	0	30	100.0

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

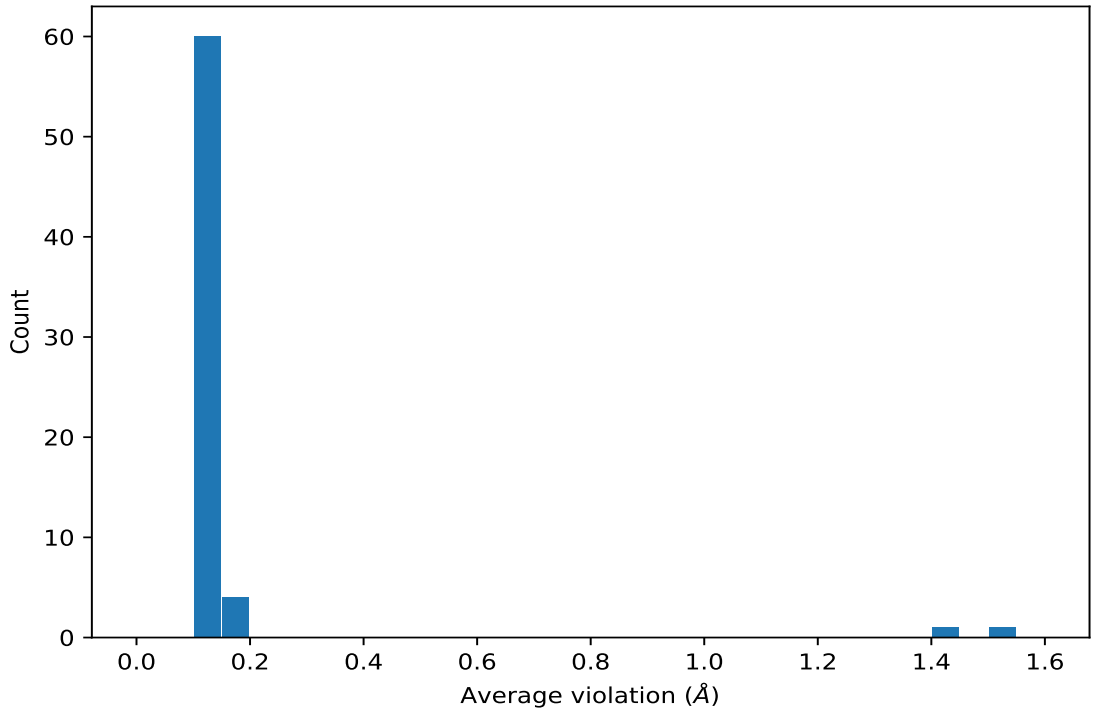
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG21	6	0.12	0.0	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG22	6	0.12	0.0	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG23	6	0.12	0.0	0.12
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD21	4	0.12	0.01	0.12
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD22	4	0.12	0.01	0.12
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD21	4	0.12	0.01	0.12
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD22	4	0.12	0.01	0.12
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD21	4	0.12	0.01	0.12
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD22	4	0.12	0.01	0.12
(1,953)	1:A:72:VAL:HB	1:A:80:TRP:HB3	4	0.12	0.01	0.12
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG11	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG12	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG13	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG21	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG22	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG23	4	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG11	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG12	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG13	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG21	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG22	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG23	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG11	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG12	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG13	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG21	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG22	4	0.11	0.0	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG23	4	0.11	0.0	0.11
(1,959)	1:A:72:VAL:HB	1:A:86:ASP:HB2	3	0.18	0.02	0.17
(1,959)	1:A:72:VAL:HB	1:A:86:ASP:HB3	3	0.18	0.02	0.17
(1,867)	1:A:63:ASP:HB2	1:A:70:THR:HB	3	0.17	0.0	0.17
(1,867)	1:A:63:ASP:HB3	1:A:70:THR:HB	3	0.17	0.0	0.17
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD11	3	0.12	0.01	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD12	3	0.12	0.01	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD13	3	0.12	0.01	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD21	3	0.12	0.01	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD22	3	0.12	0.01	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD23	3	0.12	0.01	0.11
(2,63)	1:A:99:MET:H	1:A:84:ASP:OD1	2	1.52	0.04	1.52
(2,64)	1:A:99:MET:N	1:A:84:ASP:OD1	2	1.44	0.08	1.44
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD11	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD12	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD13	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD21	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD22	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD23	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD11	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD12	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD13	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD21	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD22	2	0.15	0.03	0.15
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD23	2	0.15	0.03	0.15
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB1	2	0.14	0.02	0.14
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB2	2	0.14	0.02	0.14
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB3	2	0.14	0.02	0.14
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB1	2	0.14	0.02	0.14
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB2	2	0.14	0.02	0.14
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB3	2	0.14	0.02	0.14

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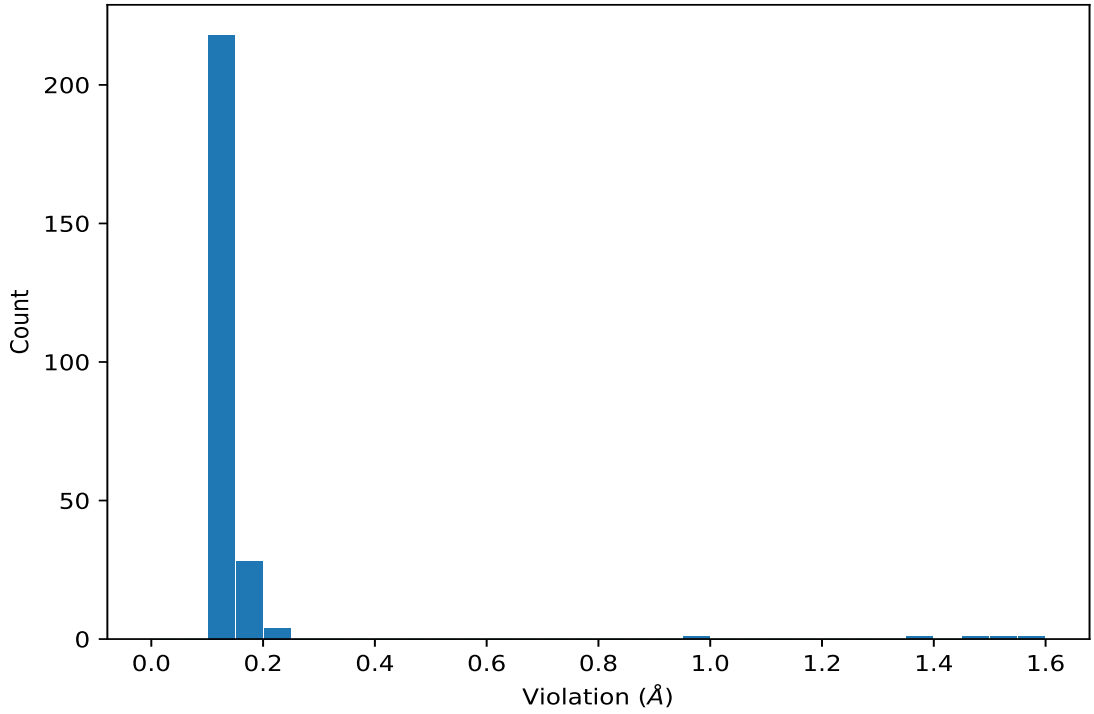
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD11	2	0.14	0.02	0.14
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD12	2	0.14	0.02	0.14
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD13	2	0.14	0.02	0.14
(1,8)	1:A:2:HIS:H	1:A:2:HIS:HD2	2	0.12	0.02	0.12
(1,115)	1:A:11:LEU:HG	1:A:12:GLN:H	2	0.12	0.01	0.12
(1,187)	1:A:14:ASP:H	1:A:15:ASP:HA	2	0.12	0.01	0.12
(1,588)	1:A:42:ASP:HB3	1:A:43:THR:HB	2	0.12	0.0	0.12
(1,1282)	1:A:98:ARG:HG2	1:A:99:MET:H	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,63)	1:A:99:MET:H	1:A:84:ASP:OD1	20	1.56
(2,64)	1:A:99:MET:N	1:A:84:ASP:OD1	20	1.53
(2,63)	1:A:99:MET:H	1:A:84:ASP:OD1	4	1.48
(2,64)	1:A:99:MET:N	1:A:84:ASP:OD1	4	1.36
(1,158)	1:A:12:GLN:H	1:A:95:ILE:HG13	6	0.96
(1,959)	1:A:72:VAL:HB	1:A:86:ASP:HB2	11	0.21
(1,959)	1:A:72:VAL:HB	1:A:86:ASP:HB3	11	0.21
(1,1054)	1:A:80:TRP:HA	1:A:81:GLN:HG2	23	0.21
(1,1054)	1:A:80:TRP:HA	1:A:81:GLN:HG3	23	0.21
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD11	14	0.18
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD12	14	0.18
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD13	14	0.18
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD21	14	0.18
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD22	14	0.18
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD23	14	0.18
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD11	14	0.18
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD12	14	0.18
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD13	14	0.18
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD21	14	0.18
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD22	14	0.18
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD23	14	0.18
(1,959)	1:A:72:VAL:HB	1:A:86:ASP:HB2	23	0.17
(1,959)	1:A:72:VAL:HB	1:A:86:ASP:HB3	23	0.17
(1,867)	1:A:63:ASP:HB2	1:A:70:THR:HB	24	0.17
(1,867)	1:A:63:ASP:HB3	1:A:70:THR:HB	24	0.17
(1,867)	1:A:63:ASP:HB2	1:A:70:THR:HB	25	0.17
(1,867)	1:A:63:ASP:HB3	1:A:70:THR:HB	25	0.17
(1,959)	1:A:72:VAL:HB	1:A:86:ASP:HB2	20	0.16
(1,959)	1:A:72:VAL:HB	1:A:86:ASP:HB3	20	0.16
(1,867)	1:A:63:ASP:HB2	1:A:70:THR:HB	7	0.16
(1,867)	1:A:63:ASP:HB3	1:A:70:THR:HB	7	0.16
(1,815)	1:A:60:LEU:HG	1:A:61:LEU:H	12	0.16
(1,189)	1:A:15:ASP:HB2	1:A:17:SER:H	10	0.16
(1,189)	1:A:15:ASP:HB3	1:A:17:SER:H	10	0.16
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD11	27	0.16
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD12	27	0.16
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD13	27	0.16
(1,484)	1:A:33:GLY:H	1:A:47:ARG:HB2	2	0.15
(1,439)	1:A:31:GLY:HA2	1:A:32:ARG:HG3	13	0.15
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB1	7	0.15
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB2	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB3	7	0.15
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB1	7	0.15
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB2	7	0.15
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB3	7	0.15
(1,953)	1:A:72:VAL:HB	1:A:80:TRP:HB3	14	0.14
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD21	15	0.14
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD22	15	0.14
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD21	15	0.14
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD22	15	0.14
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD21	15	0.14
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD22	15	0.14
(1,8)	1:A:2:HIS:H	1:A:2:HIS:HD2	7	0.14
(1,574)	1:A:40:LEU:HD11	1:A:41:PRO:HD3	28	0.14
(1,574)	1:A:40:LEU:HD12	1:A:41:PRO:HD3	28	0.14
(1,574)	1:A:40:LEU:HD13	1:A:41:PRO:HD3	28	0.14
(1,1225)	1:A:93:SER:HA	1:A:94:GLU:HG2	4	0.14
(1,1225)	1:A:93:SER:HA	1:A:94:GLU:HG3	4	0.14
(1,953)	1:A:72:VAL:HB	1:A:80:TRP:HB3	1	0.13
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD21	16	0.13
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD22	16	0.13
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD21	16	0.13
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD22	16	0.13
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD21	16	0.13
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD22	16	0.13
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD11	17	0.13
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD12	17	0.13
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD13	17	0.13
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD21	17	0.13
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD22	17	0.13
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD23	17	0.13
(1,663)	1:A:49:HIS:H	1:A:64:LEU:HB2	20	0.13
(1,663)	1:A:49:HIS:H	1:A:64:LEU:HB3	20	0.13
(1,327)	1:A:27:SER:HB2	1:A:52:ILE:HG21	23	0.13
(1,327)	1:A:27:SER:HB2	1:A:52:ILE:HG22	23	0.13
(1,327)	1:A:27:SER:HB2	1:A:52:ILE:HG23	23	0.13
(1,214)	1:A:19:ARG:HG2	1:A:20:THR:H	18	0.13
(1,214)	1:A:19:ARG:HG3	1:A:20:THR:H	18	0.13
(1,211)	1:A:19:ARG:HB3	1:A:21:TYR:H	6	0.13
(1,187)	1:A:14:ASP:H	1:A:15:ASP:HA	6	0.13
(1,168)	1:A:13:LEU:HD11	1:A:15:ASP:H	22	0.13
(1,168)	1:A:13:LEU:HD12	1:A:15:ASP:H	22	0.13
(1,168)	1:A:13:LEU:HD13	1:A:15:ASP:H	22	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:A:13:LEU:HD21	1:A:15:ASP:H	22	0.13
(1,168)	1:A:13:LEU:HD22	1:A:15:ASP:H	22	0.13
(1,168)	1:A:13:LEU:HD23	1:A:15:ASP:H	22	0.13
(1,115)	1:A:11:LEU:HG	1:A:12:GLN:H	1	0.13
(1,953)	1:A:72:VAL:HB	1:A:80:TRP:HB3	23	0.12
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG11	15	0.12
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG12	15	0.12
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG13	15	0.12
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG21	15	0.12
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG22	15	0.12
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG23	15	0.12
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG11	15	0.12
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG12	15	0.12
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG13	15	0.12
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG21	15	0.12
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG22	15	0.12
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG23	15	0.12
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG11	15	0.12
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG12	15	0.12
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG13	15	0.12
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG21	15	0.12
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG22	15	0.12
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG23	15	0.12
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD21	12	0.12
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD22	12	0.12
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD21	12	0.12
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD22	12	0.12
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD21	12	0.12
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD22	12	0.12
(1,872)	1:A:63:ASP:HB3	1:A:70:THR:HB	7	0.12
(1,77)	1:A:9:VAL:H	1:A:23:LEU:HB3	15	0.12
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD11	22	0.12
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD12	22	0.12
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD13	22	0.12
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD21	22	0.12
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD22	22	0.12
(1,633)	1:A:48:ARG:HD2	1:A:64:LEU:HD23	22	0.12
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD11	22	0.12
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD12	22	0.12
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD13	22	0.12
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD21	22	0.12
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD22	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:A:48:ARG:HD3	1:A:64:LEU:HD23	22	0.12
(1,588)	1:A:42:ASP:HB3	1:A:43:THR:HB	2	0.12
(1,549)	1:A:39:ARG:H	1:A:39:ARG:HB2	3	0.12
(1,549)	1:A:39:ARG:H	1:A:39:ARG:HB3	3	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG21	4	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG22	4	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG23	4	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG21	5	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG22	5	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG23	5	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG21	21	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG22	21	0.12
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG23	21	0.12
(1,146)	1:A:12:GLN:HG2	1:A:13:LEU:H	24	0.12
(1,146)	1:A:12:GLN:HG3	1:A:13:LEU:H	24	0.12
(1,143)	1:A:12:GLN:HE21	1:A:13:LEU:H	1	0.12
(1,143)	1:A:12:GLN:HE22	1:A:13:LEU:H	1	0.12
(1,142)	1:A:12:GLN:HB2	1:A:96:ILE:H	18	0.12
(1,1246)	1:A:95:ILE:H	1:A:95:ILE:HB	6	0.12
(1,115)	1:A:11:LEU:HG	1:A:12:GLN:H	5	0.12
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB1	8	0.12
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB2	8	0.12
(1,10)	1:A:4:SER:HB2	1:A:5:ALA:HB3	8	0.12
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB1	8	0.12
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB2	8	0.12
(1,10)	1:A:4:SER:HB3	1:A:5:ALA:HB3	8	0.12
(1,956)	1:A:72:VAL:HB	1:A:80:TRP:HH2	23	0.11
(1,953)	1:A:72:VAL:HB	1:A:80:TRP:HB3	29	0.11
(1,943)	1:A:71:THR:HG21	1:A:89:ARG:H	16	0.11
(1,943)	1:A:71:THR:HG22	1:A:89:ARG:H	16	0.11
(1,943)	1:A:71:THR:HG23	1:A:89:ARG:H	16	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG11	11	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG12	11	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG13	11	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG21	11	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG22	11	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG23	11	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG11	11	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG12	11	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG13	11	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG21	11	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG22	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG23	11	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG11	11	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG12	11	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG13	11	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG21	11	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG22	11	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG23	11	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG11	22	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG12	22	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG13	22	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG21	22	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG22	22	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG23	22	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG11	22	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG12	22	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG13	22	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG21	22	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG22	22	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG23	22	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG11	22	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG12	22	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG13	22	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG21	22	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG22	22	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG23	22	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG11	23	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG12	23	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG13	23	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG21	23	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG22	23	0.11
(1,935)	1:A:71:THR:HG21	1:A:72:VAL:HG23	23	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG11	23	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG12	23	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG13	23	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG21	23	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG22	23	0.11
(1,935)	1:A:71:THR:HG22	1:A:72:VAL:HG23	23	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG11	23	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG12	23	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG13	23	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG21	23	0.11
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG22	23	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:A:71:THR:HG23	1:A:72:VAL:HG23	23	0.11
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD21	13	0.11
(1,899)	1:A:67:THR:HG21	1:A:68:ASN:HD22	13	0.11
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD21	13	0.11
(1,899)	1:A:67:THR:HG22	1:A:68:ASN:HD22	13	0.11
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD21	13	0.11
(1,899)	1:A:67:THR:HG23	1:A:68:ASN:HD22	13	0.11
(1,8)	1:A:2:HIS:H	1:A:2:HIS:HD2	28	0.11
(1,798)	1:A:59:ALA:HA	1:A:60:LEU:HB3	12	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD11	8	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD12	8	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD13	8	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD21	8	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD22	8	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD23	8	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD11	20	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD12	20	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD13	20	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD21	20	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD22	20	0.11
(1,746)	1:A:54:TRP:HA	1:A:60:LEU:HD23	20	0.11
(1,588)	1:A:42:ASP:HB3	1:A:43:THR:HB	13	0.11
(1,536)	1:A:38:PHE:HD1	1:A:41:PRO:HD2	16	0.11
(1,536)	1:A:38:PHE:HD1	1:A:41:PRO:HD3	16	0.11
(1,536)	1:A:38:PHE:HD2	1:A:41:PRO:HD2	16	0.11
(1,536)	1:A:38:PHE:HD2	1:A:41:PRO:HD3	16	0.11
(1,409)	1:A:30:ILE:HB	1:A:38:PHE:HE1	25	0.11
(1,409)	1:A:30:ILE:HB	1:A:38:PHE:HE2	25	0.11
(1,321)	1:A:27:SER:HA	1:A:54:TRP:HB3	11	0.11
(1,289)	1:A:24:ARG:HD3	1:A:25:GLU:H	24	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG21	11	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG22	11	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG23	11	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG21	13	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG22	13	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG23	13	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG21	18	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG22	18	0.11
(1,209)	1:A:19:ARG:HB3	1:A:20:THR:HG23	18	0.11
(1,187)	1:A:14:ASP:H	1:A:15:ASP:HA	2	0.11
(1,181)	1:A:14:ASP:HA	1:A:16:GLY:H	27	0.11
(1,1282)	1:A:98:ARG:HG2	1:A:99:MET:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1282)	1:A:98:ARG:HG2	1:A:99:MET:H	30	0.11
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD11	4	0.11
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD12	4	0.11
(1,1082)	1:A:82:LEU:HA	1:A:88:ILE:HD13	4	0.11

10 Dihedral-angle violation analysis (i)

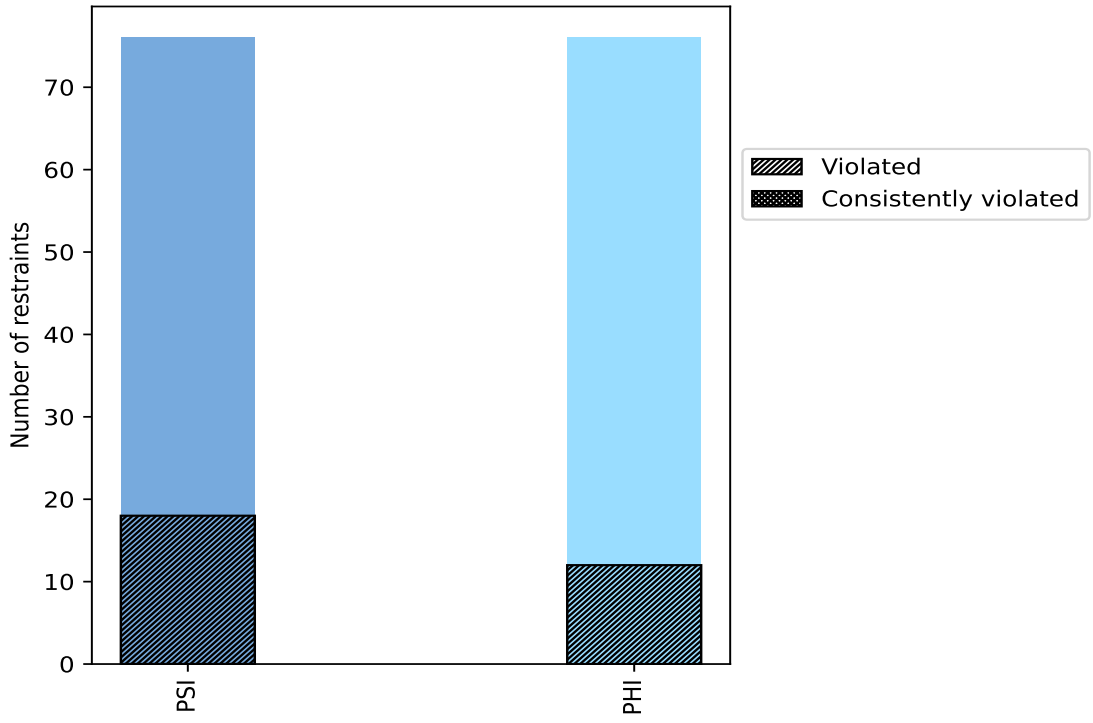
10.1 Summary of dihedral-angle violations (i)

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	76	50.0	18	23.7	11.8	0	0.0	0.0
PHI	76	50.0	12	15.8	7.9	0	0.0	0.0
Total	152	100.0	30	19.7	19.7	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 (i)



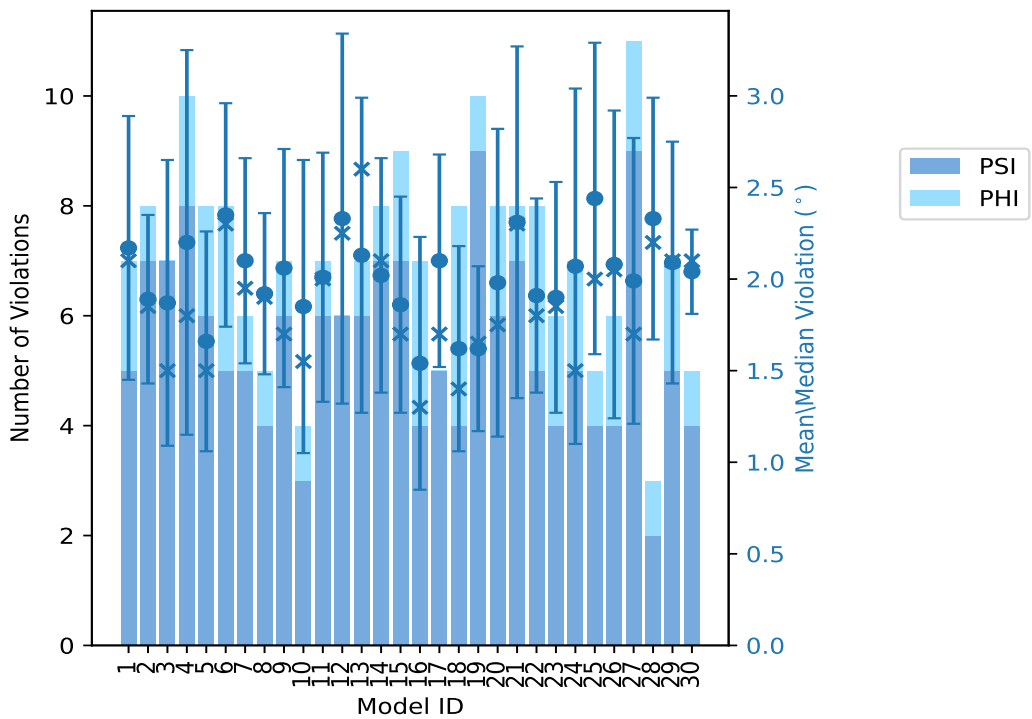
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	5	2	7	2.17	3.4	0.72	2.1
2	7	1	8	1.89	2.7	0.46	1.85
3	7	0	7	1.87	3.4	0.78	1.5
4	8	2	10	2.2	4.6	1.05	1.8
5	6	2	8	1.66	3.0	0.6	1.5
6	5	3	8	2.35	3.2	0.61	2.3
7	5	1	6	2.1	3.3	0.56	1.95
8	4	1	5	1.92	2.5	0.44	1.9
9	6	1	7	2.06	3.1	0.65	1.7
10	3	1	4	1.85	3.2	0.8	1.55
11	6	1	7	2.01	3.3	0.68	2.0
12	6	0	6	2.33	3.8	1.01	2.25
13	6	1	7	2.13	3.5	0.86	2.6
14	7	1	8	2.02	2.9	0.64	2.1
15	7	2	9	1.86	2.9	0.59	1.7
16	4	3	7	1.54	3.2	0.69	1.3
17	5	0	5	2.1	3.1	0.58	1.7
18	4	4	8	1.62	2.6	0.56	1.4
19	9	1	10	1.62	2.7	0.45	1.65
20	6	2	8	1.98	4.0	0.84	1.75
21	7	1	8	2.31	4.1	0.96	2.3
22	5	3	8	1.91	2.9	0.53	1.8
23	4	2	6	1.9	2.9	0.63	1.85
24	5	2	7	2.07	3.9	0.97	1.5
25	4	1	5	2.44	3.6	0.85	2.0
26	4	2	6	2.08	3.2	0.84	2.05
27	9	2	11	1.99	3.7	0.78	1.7
28	2	1	3	2.33	3.2	0.66	2.2
29	5	2	7	2.09	3.2	0.66	2.1
30	4	1	5	2.04	2.4	0.23	2.1

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

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

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
2	3	5	1	3.3
3	2	5	2	6.7
2	5	7	3	10.0
2	0	2	4	13.3
1	0	1	5	16.7
1	1	2	6	20.0
0	0	0	7	23.3
1	0	1	8	26.7
0	0	0	9	30.0
0	0	0	10	33.3
0	0	0	11	36.7

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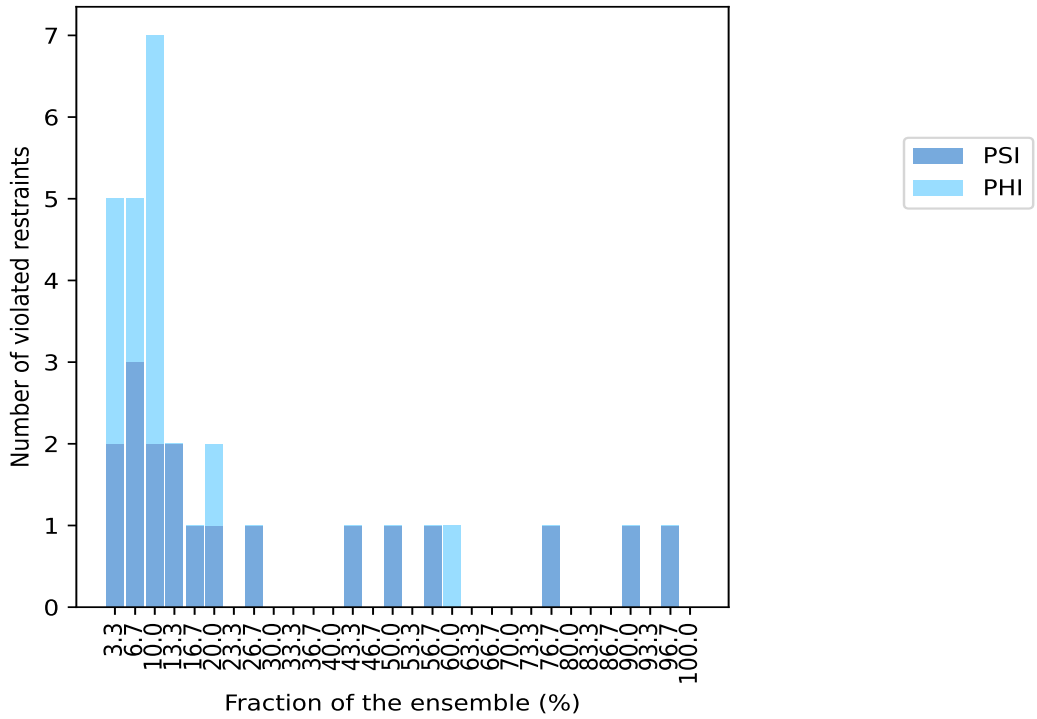
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	40.0
1	0	1	13	43.3
0	0	0	14	46.7
1	0	1	15	50.0
0	0	0	16	53.3
1	0	1	17	56.7
0	1	1	18	60.0
0	0	0	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
0	0	0	22	73.3
1	0	1	23	76.7
0	0	0	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
1	0	1	27	90.0
0	0	0	28	93.3
1	0	1	29	96.7
0	0	0	30	100.0

[1] Number of models with violations

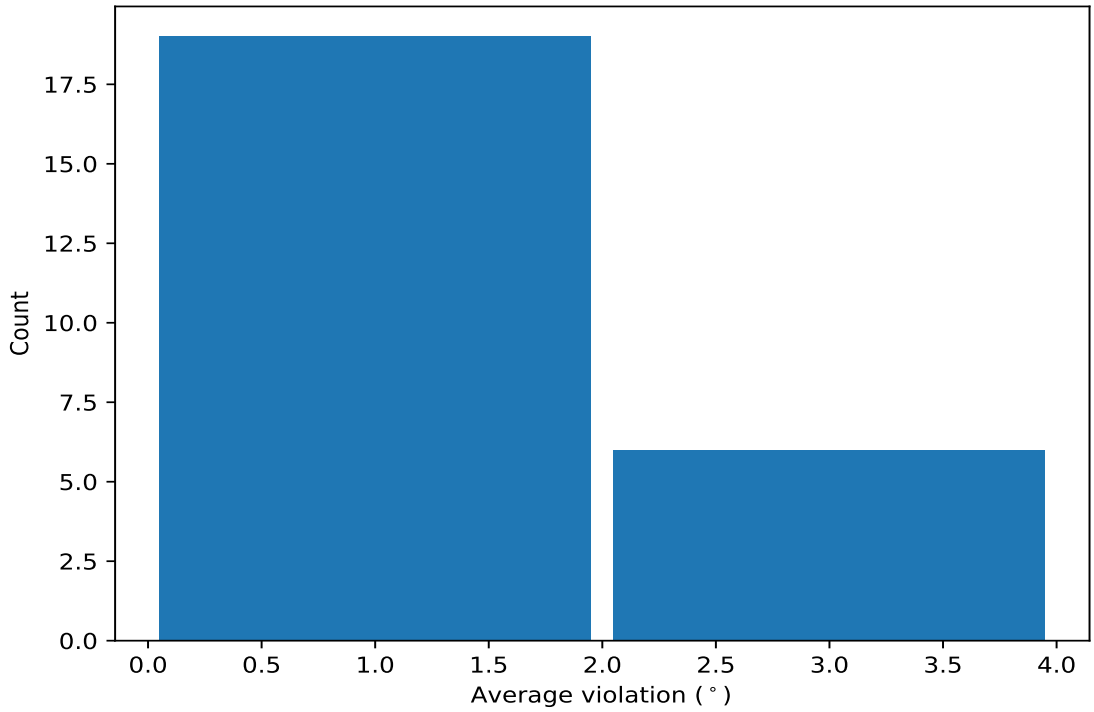
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

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



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	29	2.44	0.88	2.4
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	27	2.68	0.66	2.6
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	23	2.5	0.7	2.6
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	18	1.72	0.5	1.6
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	17	2.04	0.65	1.8
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	15	1.85	0.57	1.6
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	13	1.47	0.36	1.4
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	8	1.51	0.4	1.4
(1,97)	1:A:68:ASN:C	1:A:69:GLY:N	1:A:69:GLY:CA	1:A:69:GLY:C	6	1.82	0.32	1.85
(1,72)	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	1:A:54:TRP:N	6	1.2	0.08	1.2
(1,140)	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	1:A:92:HIS:N	5	2.32	0.52	2.4
(1,92)	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	1:A:67:THR:N	4	1.67	0.31	1.75
(1,120)	1:A:80:TRP:N	1:A:80:TRP:CA	1:A:80:TRP:C	1:A:81:GLN:N	4	1.23	0.08	1.25
(1,139)	1:A:90:LEU:C	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	3	2.5	0.33	2.5
(1,63)	1:A:48:ARG:C	1:A:49:HIS:N	1:A:49:HIS:CA	1:A:49:HIS:C	3	1.67	0.05	1.7
(1,91)	1:A:65:ASN:C	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	3	1.67	0.41	1.6
(1,102)	1:A:71:THR:N	1:A:71:THR:CA	1:A:71:THR:C	1:A:72:VAL:N	3	1.53	0.17	1.6
(1,112)	1:A:76:PRO:N	1:A:76:PRO:CA	1:A:76:PRO:C	1:A:77:VAL:N	3	1.53	0.12	1.5
(1,29)	1:A:26:GLY:C	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	3	1.37	0.12	1.4
(1,71)	1:A:52:ILE:C	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	3	1.27	0.12	1.3
(1,32)	1:A:28:ASN:N	1:A:28:ASN:CA	1:A:28:ASN:C	1:A:29:ILE:N	2	1.75	0.25	1.75

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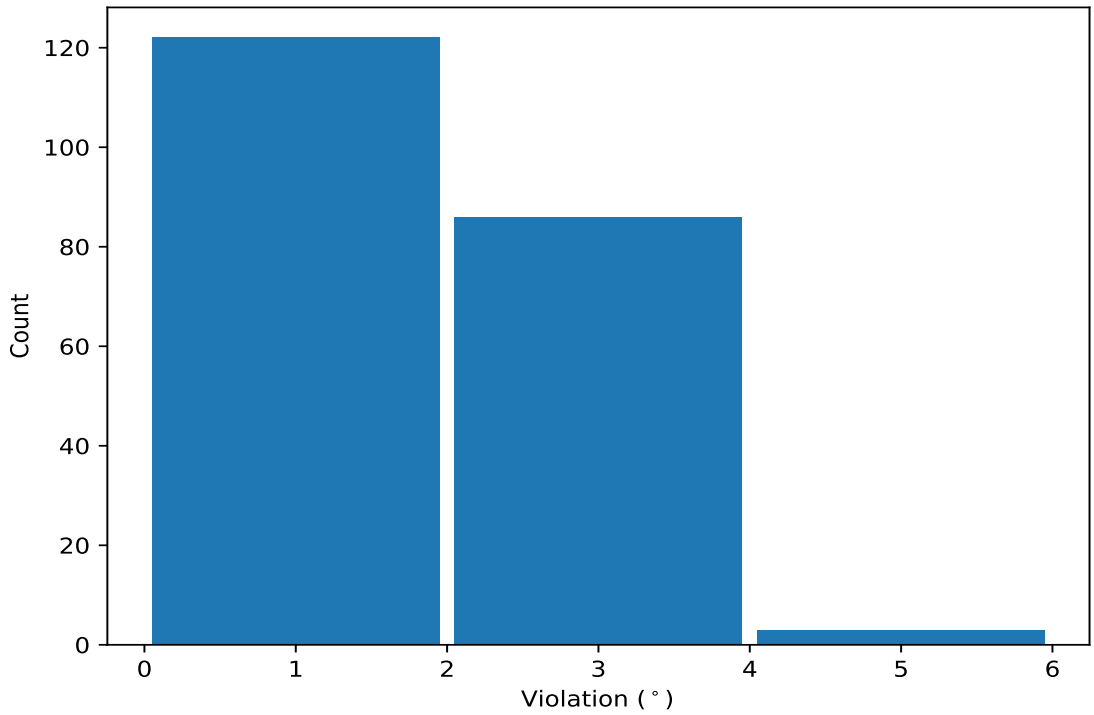
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,78)	1:A:58:VAL:N	1:A:58:VAL:CA	1:A:58:VAL:C	1:A:59:ALA:N	2	1.35	0.25	1.35
(1,95)	1:A:67:THR:C	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	2	1.35	0.15	1.35
(1,4)	1:A:8:SER:N	1:A:8:SER:CA	1:A:8:SER:C	1:A:9:VAL:N	2	1.2	0.0	1.2
(1,93)	1:A:66:SER:C	1:A:67:THR:N	1:A:67:THR:CA	1:A:67:THR:C	2	1.15	0.05	1.15

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	4	4.6
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	21	4.1
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	20	4.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	24	3.9
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	12	3.8
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	27	3.7
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	25	3.6
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	13	3.5
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	3	3.4
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	1	3.4
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	11	3.3
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	12	3.3
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	7	3.3
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	25	3.3
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	28	3.2
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	29	3.2
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	21	3.2
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	26	3.2
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	6	3.2
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	10	3.2
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	16	3.2
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	9	3.1
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	24	3.1
(1,140)	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	1:A:92:HIS:N	4	3.1
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	17	3.1
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	1	3.0
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	4	3.0
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	5	3.0
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	9	3.0
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	6	2.9
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	14	2.9
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	22	2.9
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	23	2.9
(1,139)	1:A:90:LEU:C	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	26	2.9
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	6	2.9
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	15	2.9
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	6	2.8
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	27	2.8
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	12	2.7
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	21	2.7
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	19	2.7
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	27	2.7
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	2	2.7
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	3	2.7
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	14	2.7
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	13	2.6
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	15	2.6
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	18	2.6
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	13	2.6
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	29	2.6
(1,140)	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	1:A:92:HIS:N	26	2.6
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	13	2.6
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	4	2.5
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	14	2.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,139)	1:A:90:LEU:C	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	8	2.5
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	18	2.5
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	21	2.5
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	22	2.4
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	17	2.4
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	23	2.4
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	2	2.4
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	11	2.4
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	27	2.4
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	20	2.4
(1,140)	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	1:A:92:HIS:N	30	2.4
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	29	2.4
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	14	2.4
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	11	2.3
(1,97)	1:A:68:ASN:C	1:A:69:GLY:N	1:A:69:GLY:CA	1:A:69:GLY:C	28	2.2
(1,91)	1:A:65:ASN:C	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	1	2.2
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	5	2.2
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	15	2.2
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	8	2.2
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	22	2.2
(1,97)	1:A:68:ASN:C	1:A:69:GLY:N	1:A:69:GLY:CA	1:A:69:GLY:C	29	2.1
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	7	2.1
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	30	2.1
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	1	2.1
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	15	2.1
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	30	2.1
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	21	2.1
(1,139)	1:A:90:LEU:C	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	24	2.1
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	23	2.1
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	4	2.0
(1,92)	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	1:A:67:THR:N	7	2.0
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	25	2.0
(1,32)	1:A:28:ASN:N	1:A:28:ASN:CA	1:A:28:ASN:C	1:A:29:ILE:N	27	2.0
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	11	2.0
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	9	2.0
(1,97)	1:A:68:ASN:C	1:A:69:GLY:N	1:A:69:GLY:CA	1:A:69:GLY:C	20	1.9
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	2	1.9
(1,92)	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	1:A:67:THR:N	30	1.9
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	2	1.9
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	22	1.9
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	7	1.9
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	19	1.9
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	8	1.9
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	25	1.9
(1,97)	1:A:68:ASN:C	1:A:69:GLY:N	1:A:69:GLY:CA	1:A:69:GLY:C	6	1.8
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	14	1.8
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	8	1.8
(1,57)	1:A:43:THR:C	1:A:44:GLY:N	1:A:44:GLY:CA	1:A:44:GLY:C	2	1.8
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	6	1.8
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	12	1.8
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	19	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	1:A:92:HIS:N	20	1.8
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	2	1.8
(1,97)	1:A:68:ASN:C	1:A:69:GLY:N	1:A:69:GLY:CA	1:A:69:GLY:C	22	1.7
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	15	1.7
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	17	1.7
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	9	1.7
(1,63)	1:A:48:ARG:C	1:A:49:HIS:N	1:A:49:HIS:CA	1:A:49:HIS:C	6	1.7
(1,63)	1:A:48:ARG:C	1:A:49:HIS:N	1:A:49:HIS:CA	1:A:49:HIS:C	20	1.7
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	27	1.7
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	30	1.7
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	17	1.7
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	7	1.7
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	22	1.7
(1,140)	1:A:91:GLY:N	1:A:91:GLY:CA	1:A:91:GLY:C	1:A:92:HIS:N	19	1.7
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	3	1.7
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	29	1.7
(1,112)	1:A:76:PRO:N	1:A:76:PRO:CA	1:A:76:PRO:C	1:A:77:VAL:N	19	1.7
(1,102)	1:A:71:THR:N	1:A:71:THR:CA	1:A:71:THR:C	1:A:72:VAL:N	9	1.7
(1,1)	1:A:6:GLY:C	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	6	1.7
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	27	1.6
(1,92)	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	1:A:67:THR:N	5	1.6
(1,91)	1:A:65:ASN:C	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	23	1.6
(1,78)	1:A:58:VAL:N	1:A:58:VAL:CA	1:A:58:VAL:C	1:A:59:ALA:N	19	1.6
(1,63)	1:A:48:ARG:C	1:A:49:HIS:N	1:A:49:HIS:CA	1:A:49:HIS:C	18	1.6
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	10	1.6
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	28	1.6
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	17	1.6
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	1	1.6
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	7	1.6
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	1	1.6
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	4	1.6
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	4	1.6
(1,102)	1:A:71:THR:N	1:A:71:THR:CA	1:A:71:THR:C	1:A:72:VAL:N	21	1.6
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	18	1.5
(1,95)	1:A:67:THR:C	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	14	1.5
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	9	1.5
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	11	1.5
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	24	1.5
(1,32)	1:A:28:ASN:N	1:A:28:ASN:CA	1:A:28:ASN:C	1:A:29:ILE:N	15	1.5
(1,29)	1:A:26:GLY:C	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	10	1.5
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	2	1.5
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	5	1.5
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	16	1.5
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	5	1.5
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	11	1.5
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	26	1.5
(1,112)	1:A:76:PRO:N	1:A:76:PRO:CA	1:A:76:PRO:C	1:A:77:VAL:N	3	1.5
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	9	1.4
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	20	1.4
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	24	1.4
(1,90)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	29	1.4

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Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,71)	1:A:52:ILE:C	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	27	1.4
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	20	1.4
(1,29)	1:A:26:GLY:C	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	16	1.4
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	25	1.4
(1,112)	1:A:76:PRO:N	1:A:76:PRO:CA	1:A:76:PRO:C	1:A:77:VAL:N	15	1.4
(1,72)	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	1:A:54:TRP:N	4	1.3
(1,72)	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	1:A:54:TRP:N	19	1.3
(1,71)	1:A:52:ILE:C	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	18	1.3
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	16	1.3
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	22	1.3
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	23	1.3
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	13	1.3
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	24	1.3
(1,120)	1:A:80:TRP:N	1:A:80:TRP:CA	1:A:80:TRP:C	1:A:81:GLN:N	1	1.3
(1,120)	1:A:80:TRP:N	1:A:80:TRP:CA	1:A:80:TRP:C	1:A:81:GLN:N	3	1.3
(1,106)	1:A:73:ASN:N	1:A:73:ASN:CA	1:A:73:ASN:C	1:A:74:ASN:N	14	1.3
(1,102)	1:A:71:THR:N	1:A:71:THR:CA	1:A:71:THR:C	1:A:72:VAL:N	3	1.3
(1,97)	1:A:68:ASN:C	1:A:69:GLY:N	1:A:69:GLY:CA	1:A:69:GLY:C	4	1.2
(1,96)	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	1:A:69:GLY:N	13	1.2
(1,95)	1:A:67:THR:C	1:A:68:ASN:N	1:A:68:ASN:CA	1:A:68:ASN:C	16	1.2
(1,93)	1:A:66:SER:C	1:A:67:THR:N	1:A:67:THR:CA	1:A:67:THR:C	18	1.2
(1,92)	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	1:A:67:THR:N	19	1.2
(1,91)	1:A:65:ASN:C	1:A:66:SER:N	1:A:66:SER:CA	1:A:66:SER:C	22	1.2
(1,72)	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	1:A:54:TRP:N	5	1.2
(1,72)	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	1:A:54:TRP:N	27	1.2
(1,58)	1:A:44:GLY:N	1:A:44:GLY:CA	1:A:44:GLY:C	1:A:45:VAL:N	15	1.2
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	5	1.2
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	21	1.2
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	3	1.2
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	26	1.2
(1,4)	1:A:8:SER:N	1:A:8:SER:CA	1:A:8:SER:C	1:A:9:VAL:N	8	1.2
(1,4)	1:A:8:SER:N	1:A:8:SER:CA	1:A:8:SER:C	1:A:9:VAL:N	18	1.2
(1,29)	1:A:26:GLY:C	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	29	1.2
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	19	1.2
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	27	1.2
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	12	1.2
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	20	1.2
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	24	1.2
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	27	1.2
(1,120)	1:A:80:TRP:N	1:A:80:TRP:CA	1:A:80:TRP:C	1:A:81:GLN:N	12	1.2
(1,93)	1:A:66:SER:C	1:A:67:THR:N	1:A:67:THR:CA	1:A:67:THR:C	5	1.1
(1,78)	1:A:58:VAL:N	1:A:58:VAL:CA	1:A:58:VAL:C	1:A:59:ALA:N	21	1.1
(1,72)	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	1:A:54:TRP:N	2	1.1
(1,72)	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	1:A:54:TRP:N	16	1.1
(1,71)	1:A:52:ILE:C	1:A:53:ARG:N	1:A:53:ARG:CA	1:A:53:ARG:C	15	1.1
(1,41)	1:A:32:ARG:C	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	18	1.1
(1,40)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:GLY:N	16	1.1
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	4	1.1
(1,2)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:SER:N	13	1.1
(1,16)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:ASP:N	23	1.1
(1,138)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLY:N	19	1.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	10	1.1
(1,132)	1:A:87:VAL:N	1:A:87:VAL:CA	1:A:87:VAL:C	1:A:88:ILE:N	11	1.1
(1,123)	1:A:81:GLN:C	1:A:82:LEU:N	1:A:82:LEU:CA	1:A:82:LEU:C	26	1.1
(1,120)	1:A:80:TRP:N	1:A:80:TRP:CA	1:A:80:TRP:C	1:A:81:GLN:N	14	1.1