wwPDB NMR Structure Validation Summary Report

Jun 6, 2023 – 06:19 pm BST

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

This is a wwPDB NMR Structure Validation Summary 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:

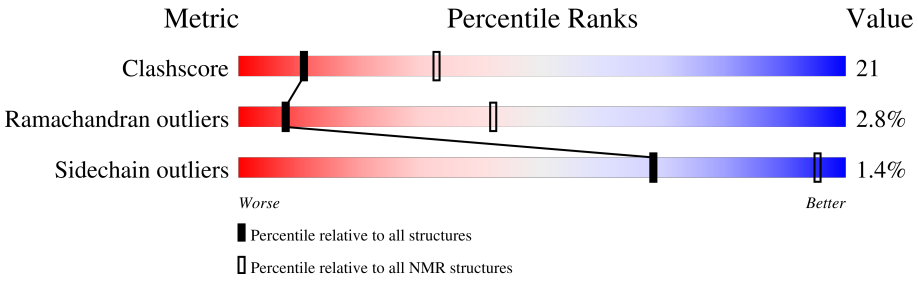
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 88%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	108	69% 24% • • 5%

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:106 (103)	0.21	31

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

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

The models can be grouped into 7 clusters and 9 single-model clusters were found.

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

3 Entry composition (i)

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

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

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

There is a discrepancy between the modelled and reference sequences:

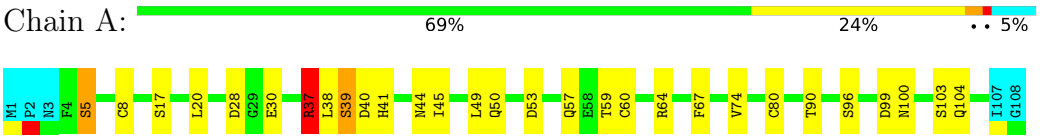
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ARG	HIS	conflict	UNP Q2MDE2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

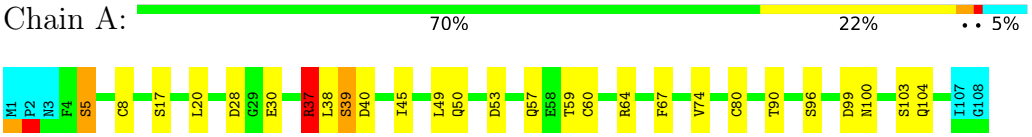
- Molecule 1: Mannan-binding lectin



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 31. Colouring as in section 4.1 above.

- Molecule 1: Mannan-binding lectin



5 Refinement protocol and experimental data overview

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

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

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

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1206
Number of shifts mapped to atoms	1205
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.20±0.00	0±0/829 (0.0± 0.0%)	0.93±0.00	1±0/1126 (0.1± 0.0%)
All	All	1.20	0/33160 (0.0%)	0.93	40/45040 (0.1%)

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

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

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	64	ARG	NE-CZ-NH1	-5.57	117.51	120.30	18	40

There are no chirality outliers.

All unique planar outliers are listed below.

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

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	814	724	724	32±3
All	All	32560	28960	28960	1277

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 21.

5 of 82 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ARG:HH21	1:A:37:ARG:CG	0.75	1.94	37	40
1:A:45:ILE:HG23	1:A:45:ILE:O	0.74	1.82	18	37
1:A:82:THR:HG22	1:A:88:LYS:NZ	0.72	2.00	4	1
1:A:37:ARG:NH2	1:A:39:SER:OG	0.68	2.27	2	40
1:A:8:CYS:SG	1:A:100:ASN:ND2	0.67	2.67	2	39

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	103/108 (95%)	92±1 (89±1%)	8±1 (8±1%)	3±0 (3±0%)	8	42
All	All	4120/4320 (95%)	3674 (89%)	330 (8%)	116 (3%)	8	42

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	39	SER	40
1	A	96	SER	40
1	A	5	SER	36

6.3.2 Protein sidechains (i)

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	94/98 (96%)	93±0 (99±1%)	1±0 (1±1%)	68 95
All	All	3760/3920 (96%)	3709 (99%)	51 (1%)	68 95

All 5 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	37	ARG	40
1	A	6	HIS	4
1	A	14	ASP	3
1	A	32	LEU	2
1	A	39	SER	2

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no 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

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

7.1 Chemical shift list 1

File name: working_cs.cif

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

7.1.1 Bookkeeping

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

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

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

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

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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	108	-0.22 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	100	-0.03 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	106	0.33 ± 0.10	None needed (< 0.5 ppm)
^{15}N	102	-0.03 ± 0.43	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 88%, i.e. 1154 atoms were assigned a chemical shift out of a possible 1314. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

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

7.1.4 Statistically unusual chemical shifts

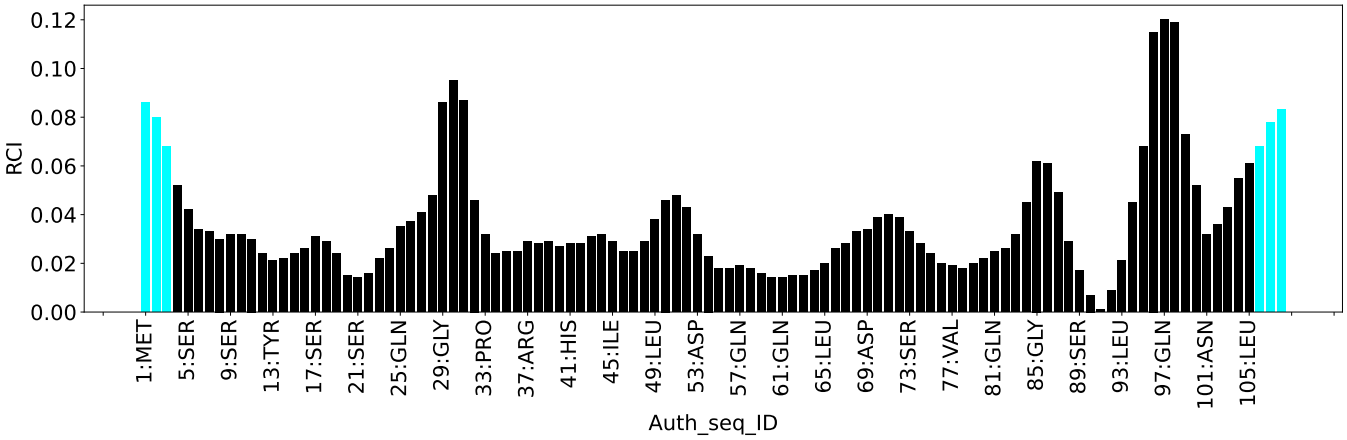
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

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

7.1.5 Random Coil Index (RCI) plots

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
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1:MET
5:SER
9:SER
13:TYR
17:SER
21:SER
25:GLN
29:GLY
33:PRO
37:ARG
41:HIS
45:ILE
49:LEU
53:ASP
57:GLN
61:GLN
65:LEU
69:ASP
73:SER
77:VAL
81:GLN
85:GLY
89:SER
93:LEU
97:GLN
101:ASN
105:LEU
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	1344
Intra-residue (|i-j|=0)	362
Sequential (|i-j|=1)	432
Medium range (|i-j|>1 and |i-j|<5)	118
Long range (|i-j|≥5)	395
Inter-chain	0
Hydrogen bond restraints	34
Disulfide bond restraints	3
Total dihedral-angle restraints	141
Number of unmapped restraints	0
Number of restraints per residue	13.8
Number of long range restraints per residue[1]	4.0

[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)	11.9	0.2
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.1	9.2
10.0-20.0 (Medium)	0.1	13.6
>20.0 (Large)	0.5	139.9

9 Distance violation analysis (i)

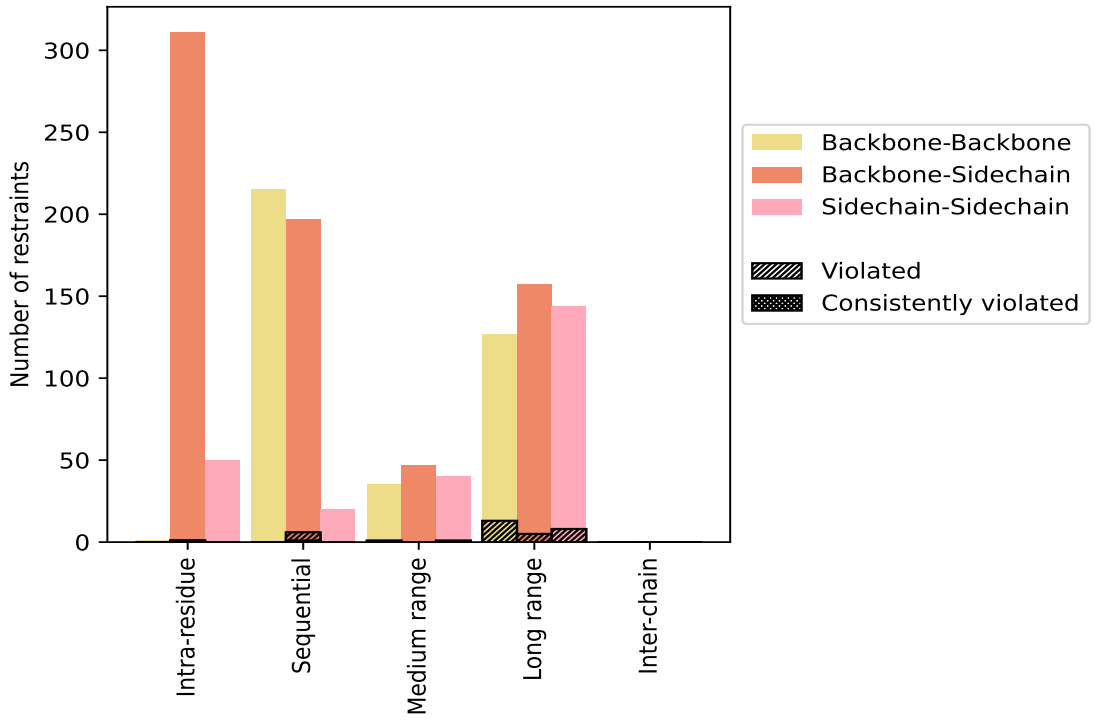
9.1 Summary of distance violations (i)

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)	362	26.9	1	0.3	0.1	1	0.3	0.1
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	311	23.1	1	0.3	0.1	1	0.3	0.1
Sidechain-Sidechain	50	3.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	432	32.1	6	1.4	0.4	1	0.2	0.1
Backbone-Backbone	215	16.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	197	14.7	6	3.0	0.4	1	0.5	0.1
Sidechain-Sidechain	20	1.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	118	8.8	2	1.7	0.1	0	0.0	0.0
Backbone-Backbone	31	2.3	1	3.2	0.1	0	0.0	0.0
Backbone-Sidechain	47	3.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	40	3.0	1	2.5	0.1	0	0.0	0.0
Long range (|i-j|≥5)	395	29.4	21	5.3	1.6	0	0.0	0.0
Backbone-Backbone	97	7.2	8	8.2	0.6	0	0.0	0.0
Backbone-Sidechain	157	11.7	5	3.2	0.4	0	0.0	0.0
Sidechain-Sidechain	141	10.5	8	5.7	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	34	2.5	5	14.7	0.4	0	0.0	0.0
Disulfide bond	3	0.2	0	0.0	0.0	0	0.0	0.0
Total	1344	100.0	35	2.6	2.6	2	0.1	0.1
Backbone-Backbone	378	28.1	14	3.7	1.0	0	0.0	0.0
Backbone-Sidechain	712	53.0	12	1.7	0.9	2	0.3	0.1
Sidechain-Sidechain	254	18.9	9	3.5	0.7	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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	1	2	0	9	0	12	0.13	0.16	0.02	0.13
2	1	3	1	7	0	12	0.14	0.17	0.02	0.14
3	1	3	0	12	0	16	0.13	0.18	0.02	0.12
4	1	4	0	7	0	12	0.13	0.17	0.02	0.12
5	1	2	0	9	0	12	0.13	0.17	0.02	0.12
6	1	4	0	6	0	11	0.13	0.15	0.02	0.12
7	1	4	0	8	0	13	0.13	0.15	0.01	0.13
8	1	3	0	7	0	11	0.13	0.16	0.02	0.13
9	1	4	0	5	0	10	0.12	0.14	0.01	0.12
10	1	3	0	10	0	14	0.13	0.16	0.02	0.14
11	1	5	1	9	0	16	0.12	0.15	0.01	0.12

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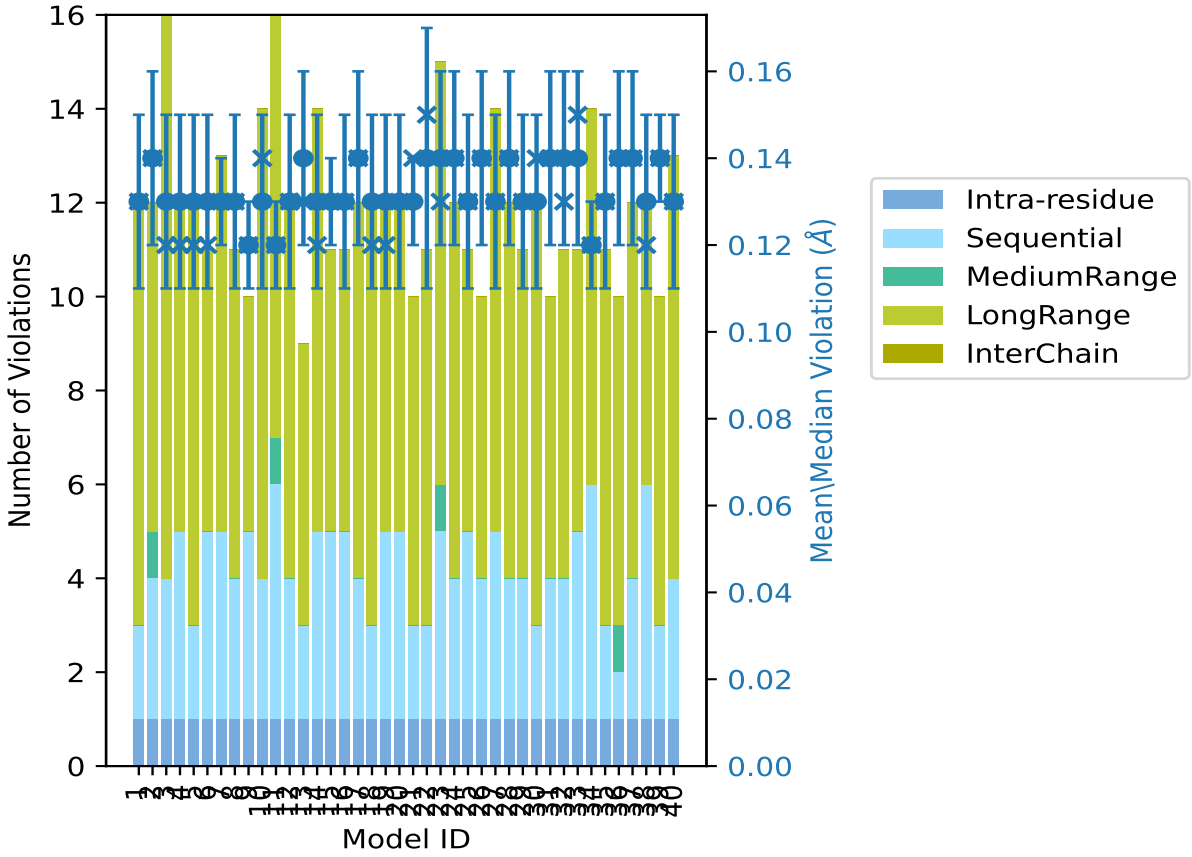
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	3	0	8	0	12	0.13	0.16	0.02	0.13
13	1	2	0	6	0	9	0.14	0.19	0.02	0.13
14	1	4	0	9	0	14	0.13	0.17	0.02	0.12
15	1	4	0	6	0	11	0.13	0.16	0.01	0.13
16	1	4	0	6	0	11	0.13	0.16	0.02	0.13
17	1	3	0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

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

9.2.1 Bar graph : Distance Violation statistics for each model (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, 1277(IR:361, SQ:426, MR:116, LR:374, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	1	1	3	0	5	1	2.5
0	0	0	3	0	3	2	5.0
0	0	1	1	0	2	3	7.5
0	0	0	1	0	1	4	10.0
0	0	0	1	0	1	5	12.5
0	0	0	1	0	1	6	15.0

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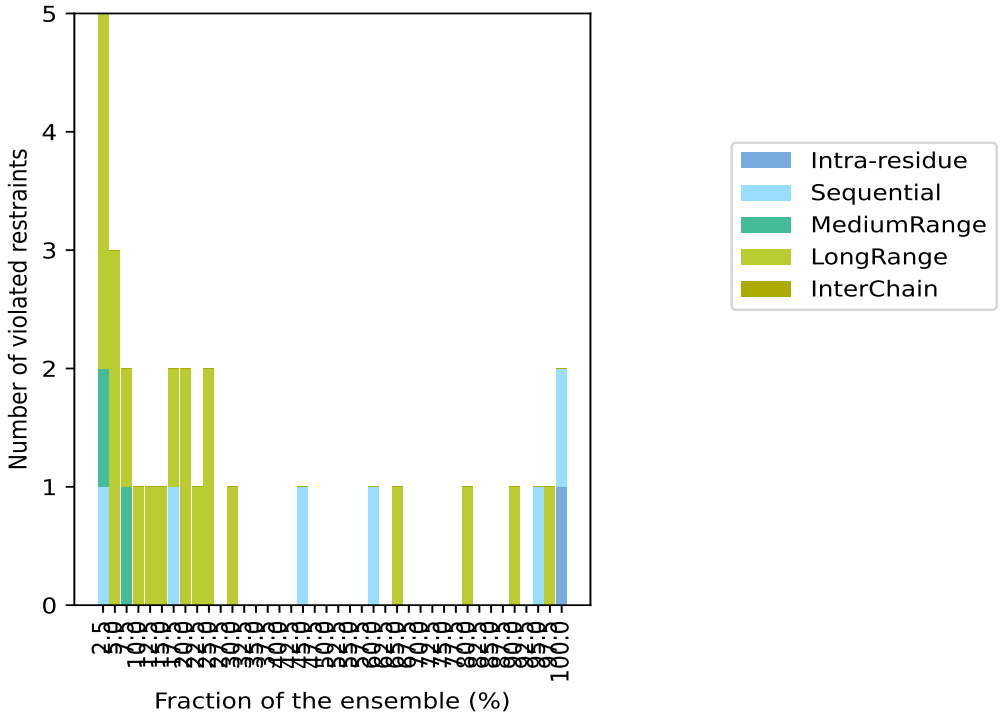
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	1	0	1	0	2	7	17.5
0	0	0	2	0	2	8	20.0
0	0	0	1	0	1	9	22.5
0	0	0	2	0	2	10	25.0
0	0	0	0	0	0	11	27.5
0	0	0	1	0	1	12	30.0
0	0	0	0	0	0	13	32.5
0	0	0	0	0	0	14	35.0
0	0	0	0	0	0	15	37.5
0	0	0	0	0	0	16	40.0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

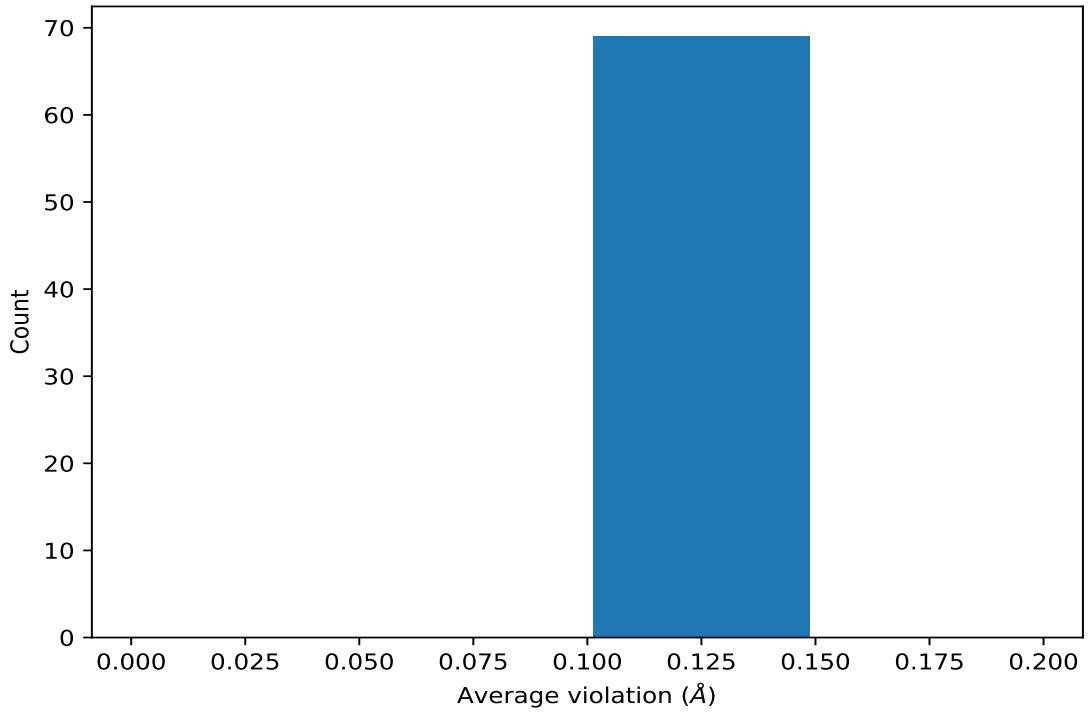
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,111)	1:A:21:SER:HB2	1:A:22:ALA:H	40	0.15	0.02	0.16
(1,111)	1:A:21:SER:HB3	1:A:22:ALA:H	40	0.15	0.02	0.16
(1,551)	1:A:90:THR:HB	1:A:90:THR:H	40	0.14	0.01	0.14
(1,270)	1:A:46:ASP:H	1:A:83:MET:HG2	39	0.13	0.01	0.14
(1,270)	1:A:46:ASP:H	1:A:83:MET:HG3	39	0.13	0.01	0.14
(1,417)	1:A:66:GLU:HG2	1:A:67:PHE:H	38	0.13	0.01	0.13
(1,417)	1:A:66:GLU:HG3	1:A:67:PHE:H	38	0.13	0.01	0.13
(1,311)	1:A:51:PHE:H	1:A:92:ILE:HD11	36	0.13	0.02	0.13
(1,311)	1:A:51:PHE:H	1:A:92:ILE:HD12	36	0.13	0.02	0.13
(1,311)	1:A:51:PHE:H	1:A:92:ILE:HD13	36	0.13	0.02	0.13
(1,792)	1:A:21:SER:HB2	1:A:35:GLU:HA	32	0.13	0.02	0.12
(1,792)	1:A:21:SER:HB3	1:A:35:GLU:HA	32	0.13	0.02	0.12
(1,1017)	1:A:49:LEU:HD11	1:A:91:GLN:HA	26	0.13	0.02	0.13
(1,1017)	1:A:49:LEU:HD12	1:A:91:GLN:HA	26	0.13	0.02	0.13
(1,1017)	1:A:49:LEU:HD13	1:A:91:GLN:HA	26	0.13	0.02	0.13
(1,1017)	1:A:49:LEU:HD21	1:A:91:GLN:HA	26	0.13	0.02	0.13

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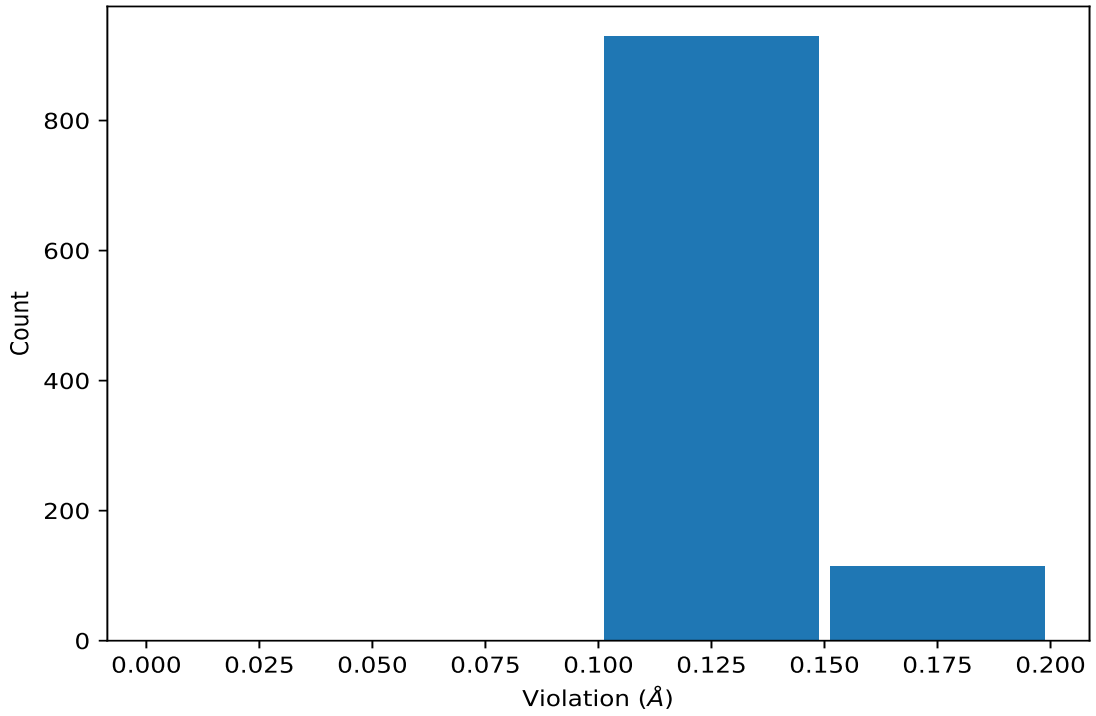
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1017)	1:A:49:LEU:HD22	1:A:91:GLN:HA	26	0.13	0.02	0.13
(1,1017)	1:A:49:LEU:HD23	1:A:91:GLN:HA	26	0.13	0.02	0.13
(2,14)	1:A:43:GLY:O	1:A:50:GLN:H	25	0.14	0.02	0.15
(1,873)	1:A:34:THR:HG21	1:A:35:GLU:HA	24	0.14	0.02	0.15
(1,873)	1:A:34:THR:HG22	1:A:35:GLU:HA	24	0.14	0.02	0.15
(1,873)	1:A:34:THR:HG23	1:A:35:GLU:HA	24	0.14	0.02	0.15
(2,29)	1:A:99:ASP:H	1:A:106:GLU:O	23	0.14	0.02	0.14

[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 provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:A:14:ASP:O	1:A:19:ILE:H	28	0.2
(2,5)	1:A:14:ASP:O	1:A:19:ILE:H	22	0.19
(2,5)	1:A:14:ASP:O	1:A:19:ILE:H	26	0.19
(1,111)	1:A:21:SER:HB2	1:A:22:ALA:H	13	0.19
(1,111)	1:A:21:SER:HB3	1:A:22:ALA:H	13	0.19
(1,111)	1:A:21:SER:HB2	1:A:22:ALA:H	23	0.19
(1,111)	1:A:21:SER:HB3	1:A:22:ALA:H	23	0.19
(2,5)	1:A:14:ASP:O	1:A:19:ILE:H	17	0.18
(2,29)	1:A:99:ASP:H	1:A:106:GLU:O	32	0.18
(2,14)	1:A:43:GLY:O	1:A:50:GLN:H	36	0.18
(1,311)	1:A:51:PHE:H	1:A:92:ILE:HD11	32	0.18
(1,311)	1:A:51:PHE:H	1:A:92:ILE:HD12	32	0.18
(1,311)	1:A:51:PHE:H	1:A:92:ILE:HD13	32	0.18
(1,111)	1:A:21:SER:HB2	1:A:22:ALA:H	3	0.18

10 Dihedral-angle violation analysis

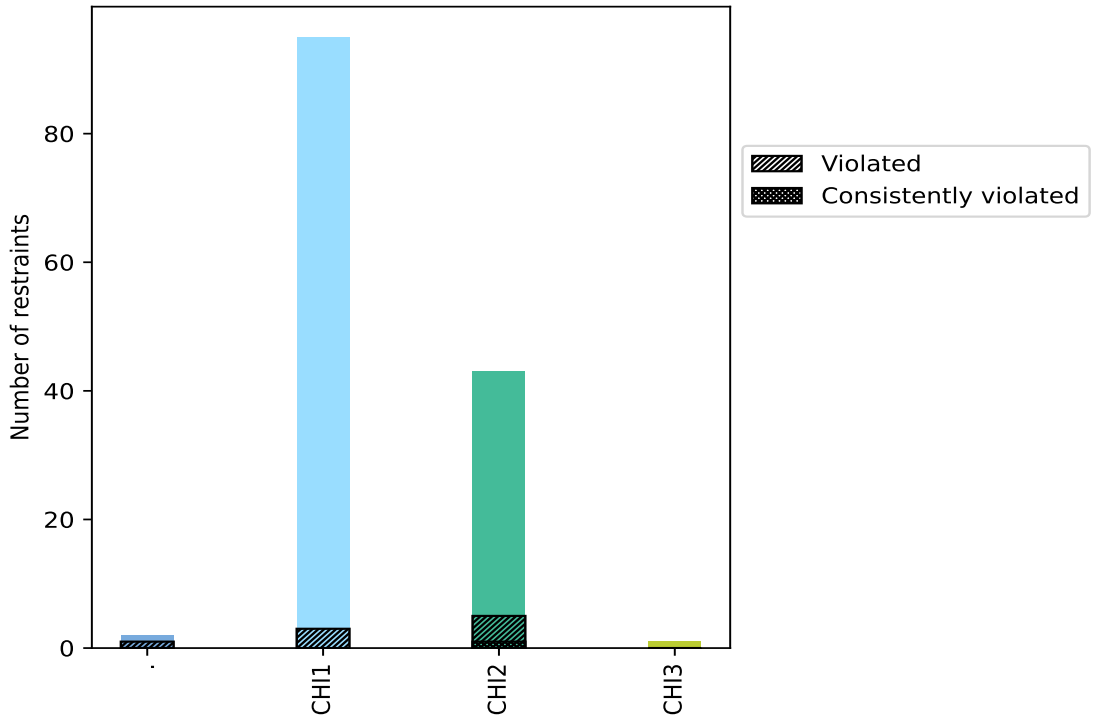
10.1 Summary of dihedral-angle violations

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]
.	2	1.4	1	50.0	0.7	0	0.0	0.0
CHI1	95	67.4	3	3.2	2.1	0	0.0	0.0
CHI2	43	30.5	5	11.6	3.5	1	2.3	0.7
CHI3	1	0.7	0	0.0	0.0	0	0.0	0.0
Total	141	100.0	9	6.4	6.4	1	0.7	0.7

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



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

10.2 Dihedral-angle violation statistics for each model (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 (°)
	.	CHI1	CHI2	CHI3	Total				
1	0	0	2	0	2	39.15	69.8	30.65	39.15
2	0	2	1	0	3	4.2	9.2	3.55	2.1
3	0	1	2	0	3	25.8	67.6	29.72	8.7
4	0	1	2	0	3	37.13	69.8	28.05	40.3
5	0	1	1	0	2	6.6	12.1	5.5	6.6
6	0	1	2	0	3	5.83	9.0	3.23	7.1
7	0	1	1	0	2	11.8	22.5	10.7	11.8
8	0	2	2	0	4	4.32	7.9	3.01	4.1
9	0	1	2	0	3	49.77	139.4	63.45	8.6
10	0	1	3	0	4	4.82	12.8	4.75	2.7
11	0	2	1	0	3	10.8	29.2	13.01	1.9
12	0	1	2	0	3	3.7	8.6	3.47	1.3
13	0	1	2	0	3	5.47	9.0	3.18	6.1
14	0	1	1	0	2	5.0	8.6	3.6	5.0
15	0	1	2	0	3	5.5	8.6	3.08	6.6
16	0	0	1	0	1	45.1	45.1	0.0	45.1
17	1	1	2	0	4	4.38	9.1	3.08	3.5
18	0	1	2	0	3	15.43	37.7	15.91	7.1
19	0	1	2	0	3	13.93	35.2	15.13	5.3
20	0	0	1	0	1	33.1	33.1	0.0	33.1
21	0	0	2	0	2	20.45	34.7	14.25	20.45
22	1	1	1	0	3	3.93	8.6	3.32	2.1
23	0	2	1	0	3	4.17	8.9	3.36	2.1
24	0	0	1	0	1	38.7	38.7	0.0	38.7
25	0	1	1	0	2	4.9	8.4	3.5	4.9
26	1	1	1	0	3	13.4	37.7	17.18	1.4
27	0	1	1	0	2	24.65	48.1	23.45	24.65
28	0	1	3	0	4	4.5	8.7	3.24	4.05
29	1	0	1	0	2	4.95	8.5	3.55	4.95
30	0	1	1	0	2	5.1	8.8	3.7	5.1
31	0	1	2	0	3	26.97	66.1	28.13	13.6
32	0	1	1	0	2	12.25	23.4	11.15	12.25
33	0	1	2	0	3	5.5	8.6	3.2	6.8
34	0	1	2	0	3	5.3	8.6	3.07	6.1
35	0	1	1	0	2	5.0	8.8	3.8	5.0
36	0	1	2	0	3	50.2	139.9	63.5	9.0
37	0	1	1	0	2	4.85	8.6	3.75	4.85
38	0	1	1	0	2	23.85	46.2	22.35	23.85

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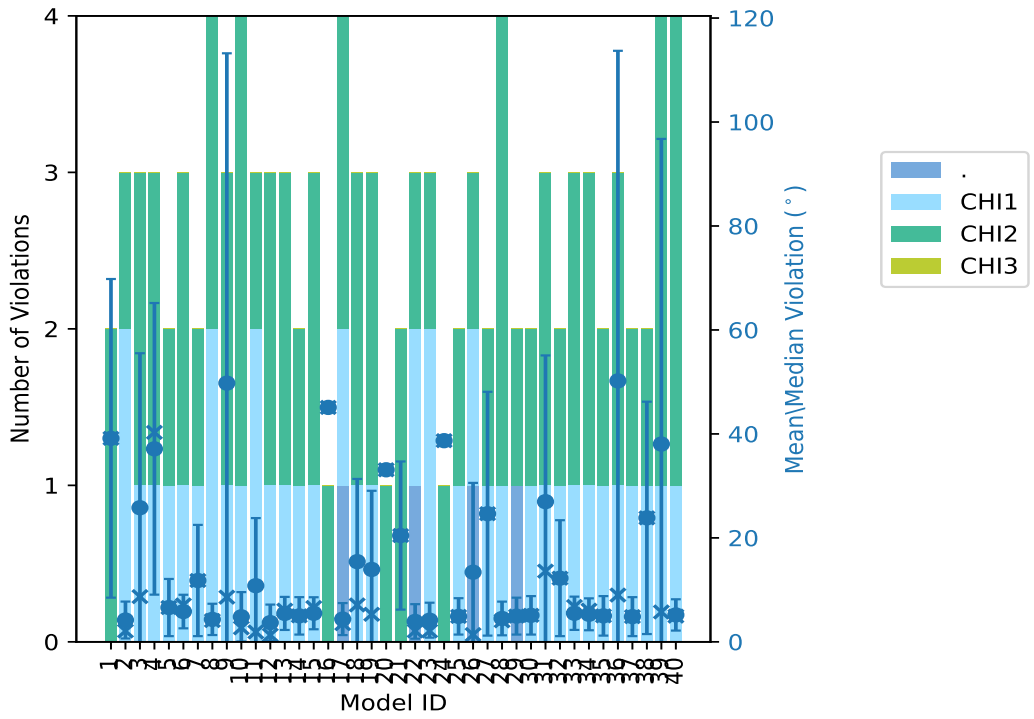
Model ID	Number of violations					Mean (°)	Max (°)	SD (°)	Median (°)
	.	CHI1	CHI2	CHI3	Total				
39	0	1	3	0	4	38.05	139.6	58.7	5.75
40	0	1	3	0	4	5.18	9.0	3.01	4.95

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	
.	CHI1	CHI2	CHI3	Total	Count[1]	%
0	0	0	0	0	1	2.5
0	1	2	0	3	2	5.0
0	1	1	0	2	3	7.5
1	0	0	0	1	4	10.0

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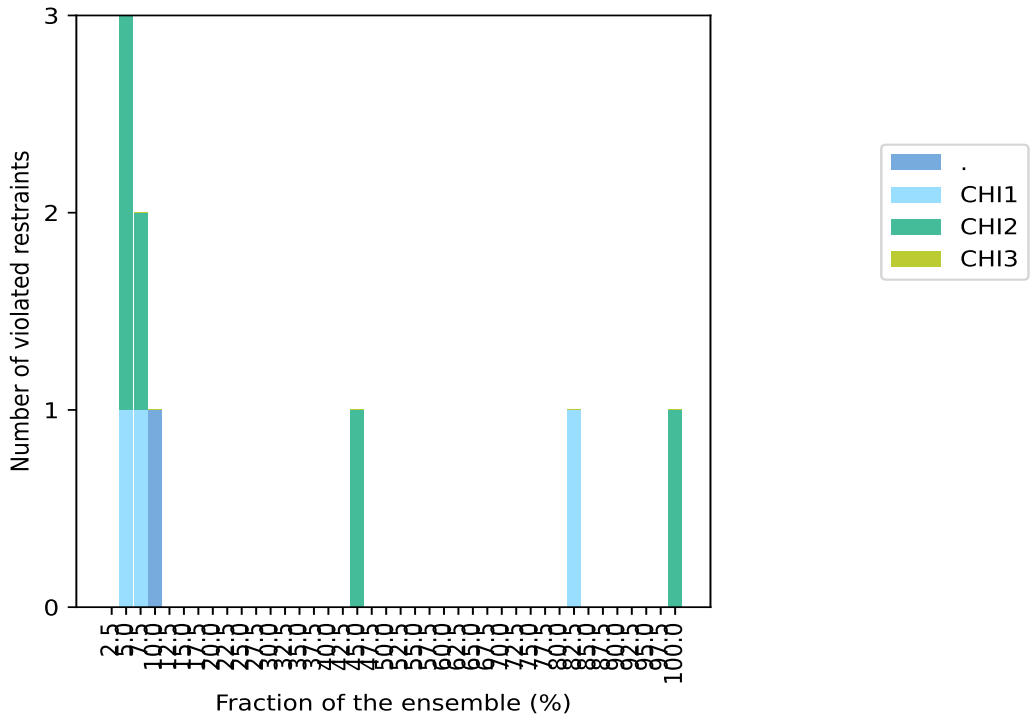
Number of violated restraints					Fraction of the ensemble	
.	CHI1	CHI2	CHI3	Total	Count[1]	%
0	0	0	0	0	5	12.5
0	0	0	0	0	6	15.0
0	0	0	0	0	7	17.5
0	0	0	0	0	8	20.0
0	0	0	0	0	9	22.5
0	0	0	0	0	10	25.0
0	0	0	0	0	11	27.5
0	0	0	0	0	12	30.0
0	0	0	0	0	13	32.5
0	0	0	0	0	14	35.0
0	0	0	0	0	15	37.5
0	0	0	0	0	16	40.0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

[1] Number of models with violations

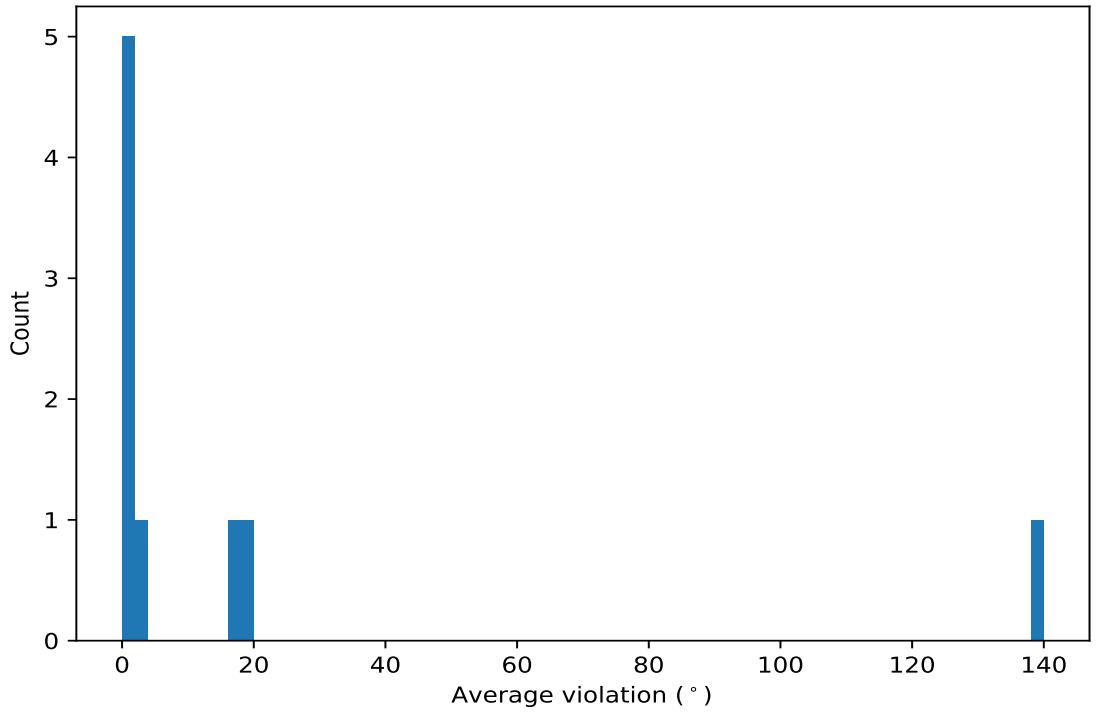
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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

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

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



10.4.2 Table: Most violated dihedral-angle restraints

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

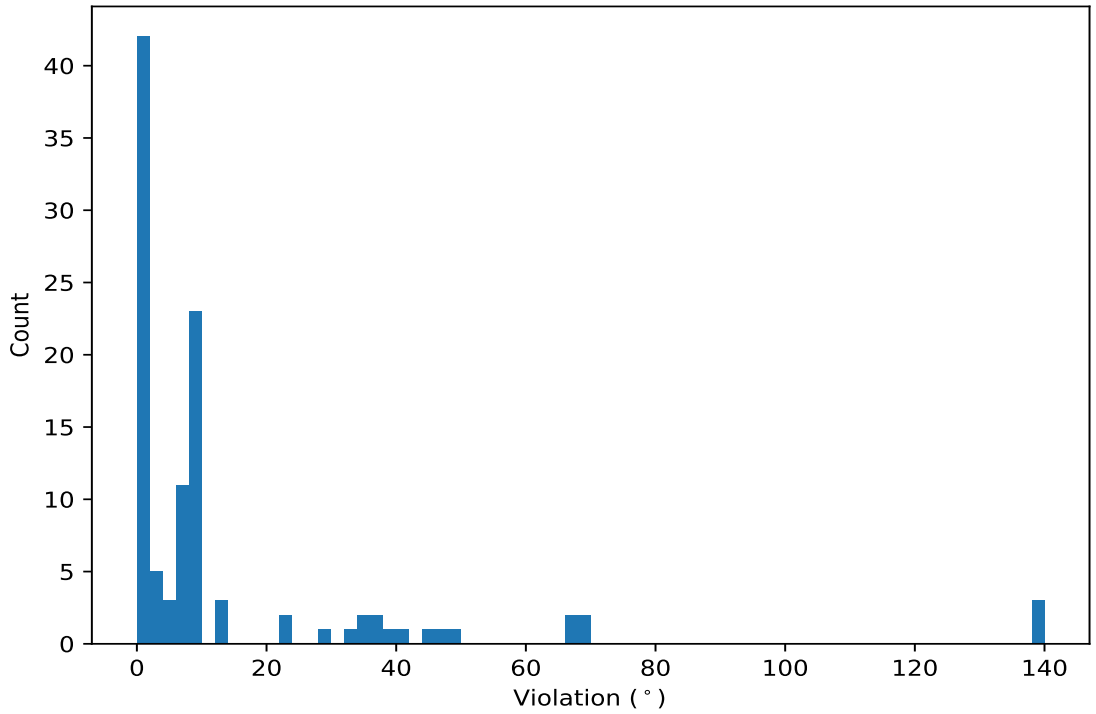
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,7)	1:A:6:HIS:CA	1:A:6:HIS:CB	1:A:6:HIS:CG	1:A:6:HIS:ND1	40	17.98	13.48	9.0
(1,79)	1:A:63:CYS:N	1:A:63:CYS:CA	1:A:63:CYS:CB	1:A:63:CYS:SG	33	1.35	0.24	1.3
(1,36)	1:A:32:LEU:CA	1:A:32:LEU:CB	1:A:32:LEU:CG	1:A:32:LEU:CD1	18	19.76	26.01	6.65
(1,118)	1:A:91:GLN:CB	1:A:91:GLN:CG	1:A:91:GLN:CD	1:A:91:GLN:NE2	4	1.25	0.15	1.25
(1,4)	1:A:4:PHE:CA	1:A:4:PHE:CB	1:A:4:PHE:CG	1:A:4:PHE:CD1	3	139.63	0.21	139.6
(1,46)	1:A:39:SER:N	1:A:39:SER:CA	1:A:39:SER:CB	1:A:39:SER:OG	3	1.83	0.38	2.1
(1,41)	1:A:36:LEU:CA	1:A:36:LEU:CB	1:A:36:LEU:CG	1:A:36:LEU:CD1	2	2.75	0.05	2.75
(1,22)	1:A:20:LEU:N	1:A:20:LEU:CA	1:A:20:LEU:CB	1:A:20:LEU:CG	2	1.7	0.2	1.7
(1,49)	1:A:41:HIS:CA	1:A:41:HIS:CB	1:A:41:HIS:CG	1:A:41:HIS:ND1	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

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 provides the list of violationsfor the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:A:4:PHE:CA	1:A:4:PHE:CB	1:A:4:PHE:CG	1:A:4:PHE:CD1	36	139.9
(1,4)	1:A:4:PHE:CA	1:A:4:PHE:CB	1:A:4:PHE:CG	1:A:4:PHE:CD1	39	139.6
(1,4)	1:A:4:PHE:CA	1:A:4:PHE:CB	1:A:4:PHE:CG	1:A:4:PHE:CD1	9	139.4
(1,36)	1:A:32:LEU:CA	1:A:32:LEU:CB	1:A:32:LEU:CG	1:A:32:LEU:CD1	1	69.8
(1,36)	1:A:32:LEU:CA	1:A:32:LEU:CB	1:A:32:LEU:CG	1:A:32:LEU:CD1	4	69.8
(1,36)	1:A:32:LEU:CA	1:A:32:LEU:CB	1:A:32:LEU:CG	1:A:32:LEU:CD1	3	67.6
(1,36)	1:A:32:LEU:CA	1:A:32:LEU:CB	1:A:32:LEU:CG	1:A:32:LEU:CD1	31	66.1
(1,7)	1:A:6:HIS:CA	1:A:6:HIS:CB	1:A:6:HIS:CG	1:A:6:HIS:ND1	27	48.1
(1,7)	1:A:6:HIS:CA	1:A:6:HIS:CB	1:A:6:HIS:CG	1:A:6:HIS:ND1	38	46.2
(1,7)	1:A:6:HIS:CA	1:A:6:HIS:CB	1:A:6:HIS:CG	1:A:6:HIS:ND1	16	45.1