wwPDB NMR Structure Validation Summary Report

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BMRB ID	:	25712
Title	:	Solution structure of the dehydroascorbate reductase 3A from Populus trichocarpa
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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:

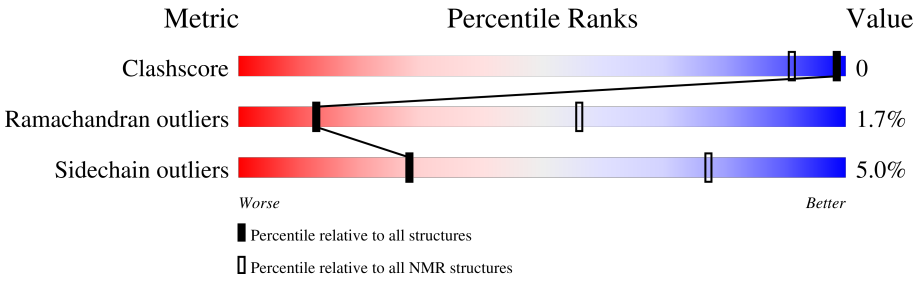
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 63%.

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	218	91%

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:3-A:208 (206)	0.95	11

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

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

The models can be grouped into 4 clusters and 11 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3352 atoms, of which 1691 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dehydroascorbate reductase family protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	212	3352	1085	1691	272	300	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	HIS	TYR	conflict	UNP B9HM36
A	171	PRO	THR	conflict	UNP B9HM36
A	213	HIS	-	expression tag	UNP B9HM36
A	214	HIS	-	expression tag	UNP B9HM36
A	215	HIS	-	expression tag	UNP B9HM36
A	216	HIS	-	expression tag	UNP B9HM36
A	217	HIS	-	expression tag	UNP B9HM36
A	218	HIS	-	expression tag	UNP B9HM36

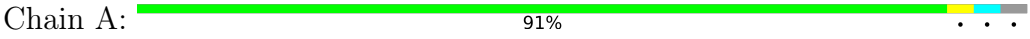
4 Residue-property plots

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: Dehydroascorbate reductase family protein

Chain A:

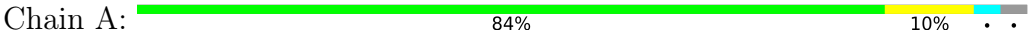


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 11. Colouring as in section 4.1 above.

- Molecule 1: Dehydroascorbate reductase family protein

Chain A:



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
ARIA	structure solution	v 2.3
ARIA	refinement	v 2.3
CNS	refinement	v 1.21
CNS	structure solution	v 1.21

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	1854
Number of shifts mapped to atoms	1836
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	63%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.59±0.02	0±0/1665 (0.0± 0.0%)	0.95±0.03	5±1/2266 (0.2± 0.1%)
All	All	0.59	0/33300 (0.0%)	0.95	100/45320 (0.2%)

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	1.8±1.3
All	All	0	35

There are no bond-length outliers.

5 of 20 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	25	ARG	NE-CZ-NH1	10.35	125.47	120.30	6	20
1	A	189	ARG	NE-CZ-NH1	9.84	125.22	120.30	1	20
1	A	196	ARG	NE-CZ-NH1	9.62	125.11	120.30	14	19
1	A	174	ASP	CB-CG-OD1	8.35	125.81	118.30	6	5
1	A	114	ASP	CB-CG-OD1	6.54	124.18	118.30	16	1

There are no chirality outliers.

5 of 18 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	140	PHE	Peptide	7
1	A	19	ASP	Peptide	4
1	A	114	ASP	Peptide	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	182	TYR	Sidechain	3
1	A	158	TYR	Sidechain	2

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	1619	1642	1651	0±1
All	All	32380	32840	33006	6

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:SER:OG	1:A:60:VAL:HG22	0.47	2.10	20	1
1:A:90:ALA:HA	1:A:148:ALA:HB2	0.45	1.89	19	1
1:A:199:GLU:H	1:A:199:GLU:CD	0.43	2.16	11	1
1:A:134:LEU:HD13	1:A:178:HIS:CD2	0.43	2.48	1	1
1:A:178:HIS:CD2	1:A:178:HIS:C	0.42	2.92	6	2

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	206/218 (94%)	186±3 (90±1%)	17±2 (8±1%)	4±1 (2±1%)	13	56
All	All	4120/4360 (94%)	3719 (90%)	331 (8%)	70 (2%)	13	56

5 of 17 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	93	PRO	19
1	A	92	PRO	15
1	A	139	PRO	9
1	A	48	PRO	5
1	A	189	ARG	4

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	179/189 (95%)	170±2 (95±1%)	9±2 (5±1%)	28 77
All	All	3580/3780 (95%)	3401 (95%)	179 (5%)	28 77

5 of 72 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	178	HIS	12
1	A	30	LEU	10
1	A	17	LEU	8
1	A	177	THR	7
1	A	134	LEU	7

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 63% for the well-defined parts and 63% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1854
Number of shifts mapped to atoms	1836
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. First 5 (of 18) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	HIS	HE2	7.054	0.008	1
1	A	159	HIS	HD1	3.31	0.000	1
1	A	213	HIS	H	8.333	0.005	1
1	A	213	HIS	HA	4.502	0.007	1
1	A	213	HIS	HB2	2.964	0.000	2
1	A	213	HIS	HB3	3.025	0.000	2
1	A	213	HIS	HD1	4.698	0.010	1
1	A	213	HIS	N	117.683	0.049	1
1	A	214	HIS	HA	4.676	0.017	1
1	A	215	HIS	H	8.176	0.012	1
1	A	215	HIS	HA	4.356	0.022	1
1	A	215	HIS	HB2	3.0	0.019	2
1	A	215	HIS	HB3	3.133	0.000	2
1	A	215	HIS	N	125.321	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	217	HIS	H	6.957	0.005	1
1	A	217	HIS	HA	3.691	1.017	1
1	A	217	HIS	HB2	2.663	0.024	1
1	A	217	HIS	N	117.038	0.013	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	196	-0.23 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	160	0.38 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	186	-0.15 ± 0.14	None needed (< 0.5 ppm)
^{15}N	192	0.66 ± 0.20	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 63%, i.e. 1787 atoms were assigned a chemical shift out of a possible 2832. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	956/1006 (95%)	395/406 (97%)	375/412 (91%)	186/188 (99%)
Sidechain	767/1609 (48%)	600/1053 (57%)	157/516 (30%)	10/40 (25%)
Aromatic	64/217 (29%)	61/114 (54%)	0/99 (0%)	3/4 (75%)
Overall	1787/2832 (63%)	1056/1573 (67%)	532/1027 (52%)	199/232 (86%)

7.1.4 Statistically unusual chemical shifts (i)

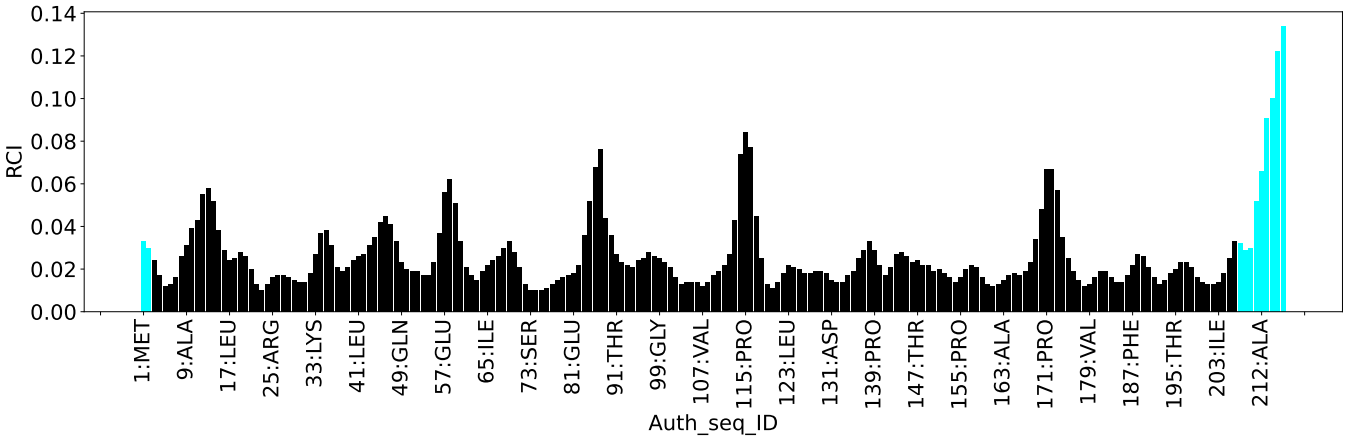
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	209	LYS	NZ	113.12	19.79 – 46.09	30.5
1	A	73	SER	CB	29.93	56.28 – 71.32	-22.5
1	A	120	GLU	HA	2.22	2.24 – 6.23	-5.1

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:



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	186
Intra-residue (|i-j|=0)	1
Sequential (|i-j|=1)	2
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	0
Inter-chain	0
Hydrogen bond restraints	183
Disulfide bond restraints	0
Total dihedral-angle restraints	410
Number of unmapped restraints	9
Number of restraints per residue	2.7
Number of long range restraints per residue[1]	0.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	7.7	0.2
0.2-0.5 (Medium)	15.3	0.5
>0.5 (Large)	37.0	8.93

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)	22.0	10.0
10.0-20.0 (Medium)	12.3	20.0
>20.0 (Large)	26.0	139.9

9 Distance violation analysis (i)

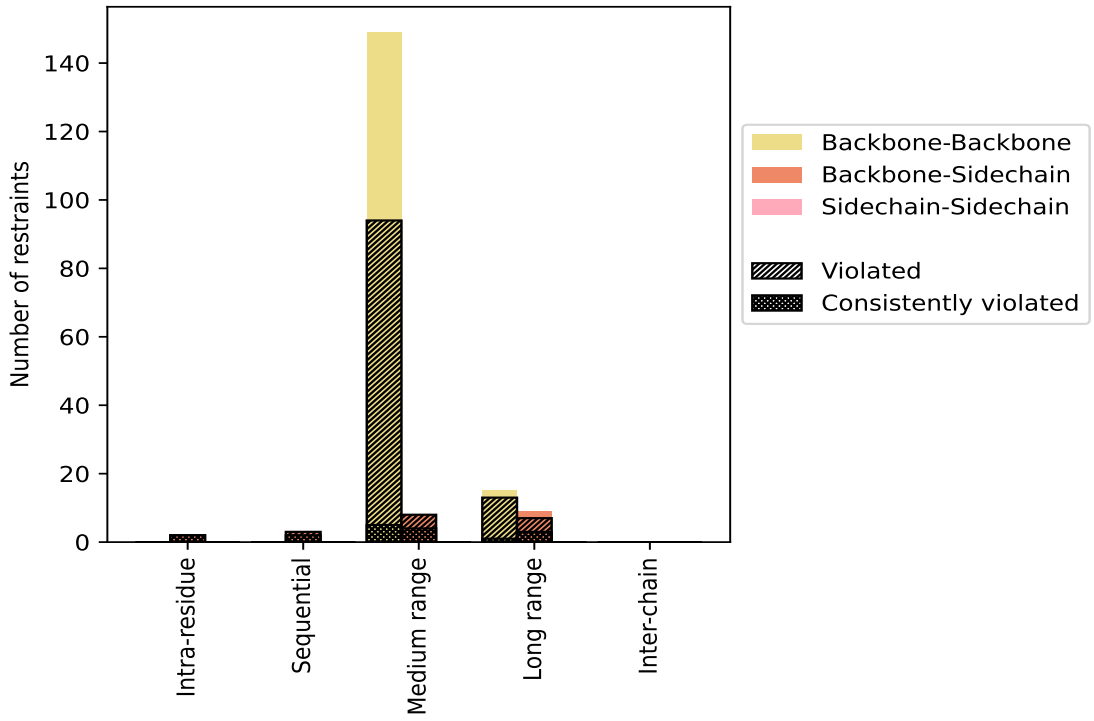
9.1 Summary of distance violations (i)

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)	1	0.5	1	100.0	0.5	1	100.0	0.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.5	1	100.0	0.5	1	100.0	0.5
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	2	1.1	2	100.0	1.1	1	50.0	0.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	1.1	2	100.0	1.1	1	50.0	0.5
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	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
Long range (|i-j|≥5)	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
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	183	98.4	124	67.8	66.7	15	8.2	8.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	186	100.0	127	68.3	68.3	17	9.1	9.1
Backbone-Backbone	164	88.2	107	65.2	57.5	6	3.7	3.2
Backbone-Sidechain	22	11.8	20	90.9	10.8	11	50.0	5.9
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	2	3	44	17	0	66	1.19	5.98	1.28	0.69
2	2	3	44	8	0	57	1.42	7.19	1.54	0.82
3	2	3	53	10	0	68	1.13	6.34	1.28	0.74
4	2	3	42	9	0	56	1.15	5.82	1.31	0.5
5	2	3	49	10	0	64	1.06	5.84	1.2	0.6
6	2	3	47	8	0	60	1.18	6.08	1.23	0.75
7	2	3	45	9	0	59	1.0	5.1	1.03	0.62
8	2	2	38	10	0	52	1.48	8.5	1.76	0.72
9	2	3	39	8	0	52	1.24	5.31	1.19	0.7
10	2	3	49	14	0	68	1.27	8.38	1.57	0.66
11	2	3	43	9	0	57	1.23	7.61	1.37	0.9

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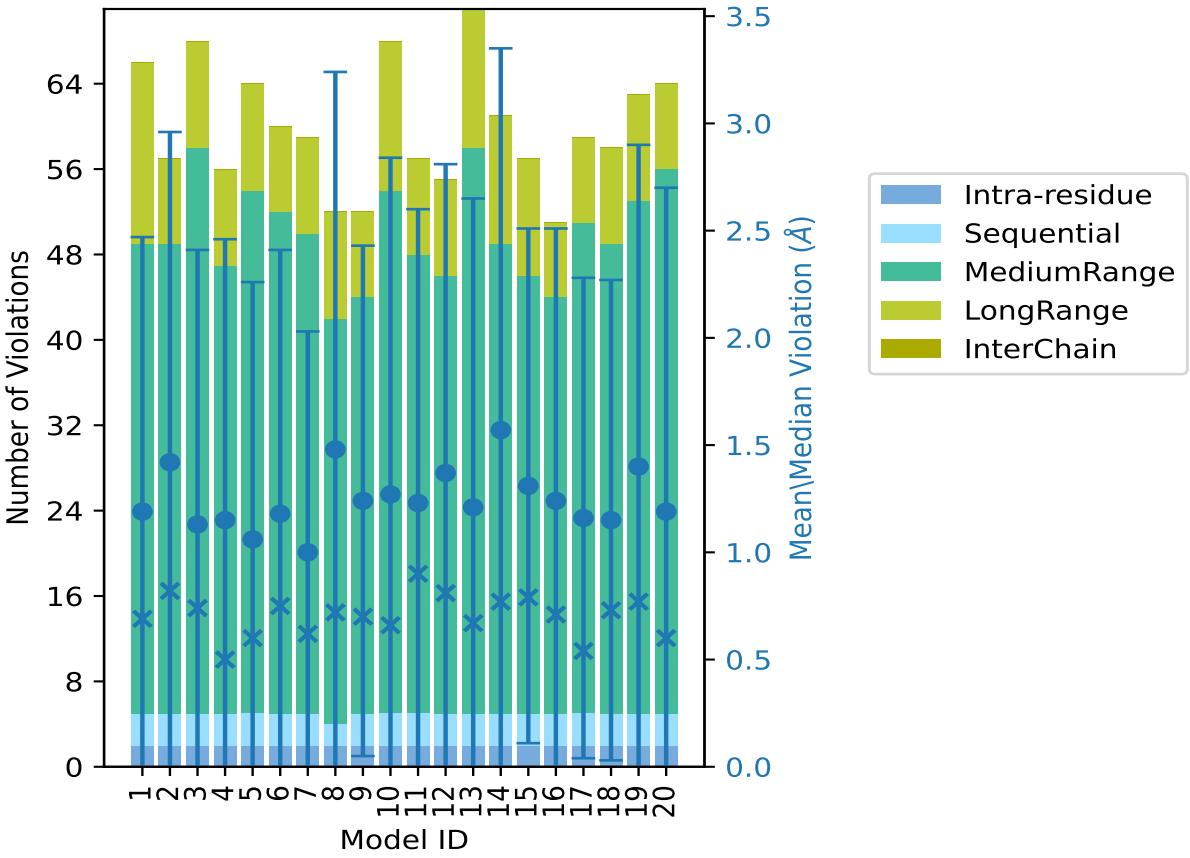
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	3	41	9	0	55	1.37	6.18	1.44	0.81
13	2	3	53	13	0	71	1.21	6.57	1.44	0.67
14	2	3	44	12	0	61	1.57	8.93	1.78	0.77
15	2	3	41	11	0	57	1.31	5.28	1.2	0.79
16	2	3	39	7	0	51	1.24	6.02	1.27	0.71
17	2	3	46	8	0	59	1.16	4.56	1.12	0.54
18	2	3	44	9	0	58	1.15	5.24	1.12	0.73
19	2	3	48	10	0	63	1.4	7.72	1.5	0.77
20	2	3	51	8	0	64	1.19	7.75	1.51	0.6

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

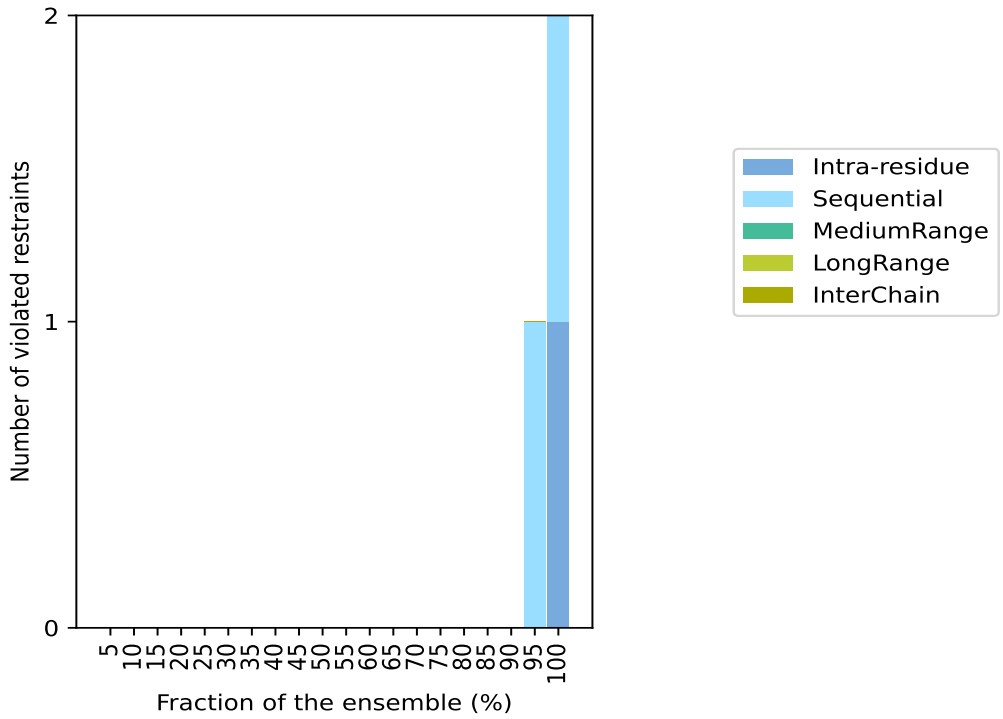
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 0(IR:0, SQ:0, MR:0, LR:0, 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	0	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	1	0	0	0	1	19	95.0
1	1	0	0	0	2	20	100.0

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

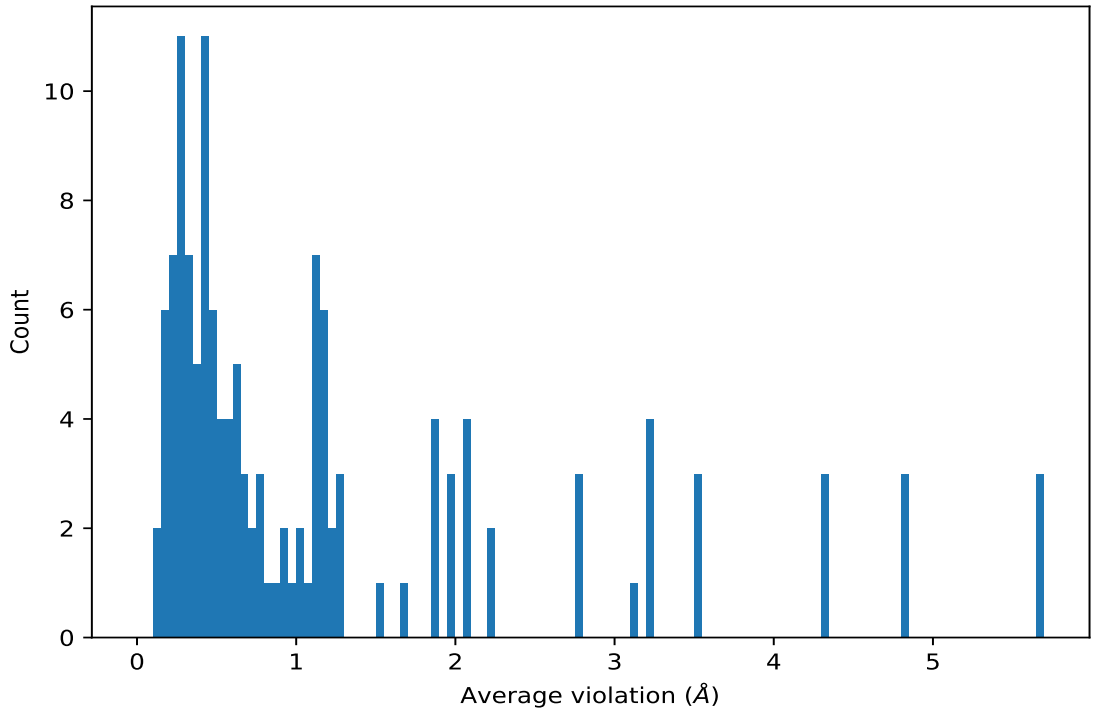
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of 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)
(1,176)	1:A:34:LYS:HZ1	1:A:35:ILE:O	20	5.65	0.68	5.85
(1,176)	1:A:34:LYS:HZ2	1:A:35:ILE:O	20	5.65	0.68	5.85
(1,176)	1:A:34:LYS:HZ3	1:A:35:ILE:O	20	5.65	0.68	5.85
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	20	4.85	2.66	4.4
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	20	4.85	2.66	4.4
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	20	4.85	2.66	4.4
(1,170)	1:A:34:LYS:HZ1	1:A:30:LEU:O	20	4.35	0.95	4.9
(1,170)	1:A:34:LYS:HZ2	1:A:30:LEU:O	20	4.35	0.95	4.9
(1,170)	1:A:34:LYS:HZ3	1:A:30:LEU:O	20	4.35	0.95	4.9
(1,172)	1:A:33:LYS:HZ1	1:A:84:ASN:O	20	3.5	1.12	3.96
(1,172)	1:A:33:LYS:HZ2	1:A:84:ASN:O	20	3.5	1.12	3.96
(1,172)	1:A:33:LYS:HZ3	1:A:84:ASN:O	20	3.5	1.12	3.96
(1,151)	1:A:140:PHE:H	1:A:143:GLY:O	20	3.2	0.44	3.2
(1,180)	1:A:50:TRP:H	1:A:49:GLN:OE1	20	3.15	0.41	3.28
(1,175)	1:A:88:PRO:O	1:A:33:LYS:HZ1	20	2.78	0.6	2.63
(1,175)	1:A:88:PRO:O	1:A:33:LYS:HZ2	20	2.78	0.6	2.63

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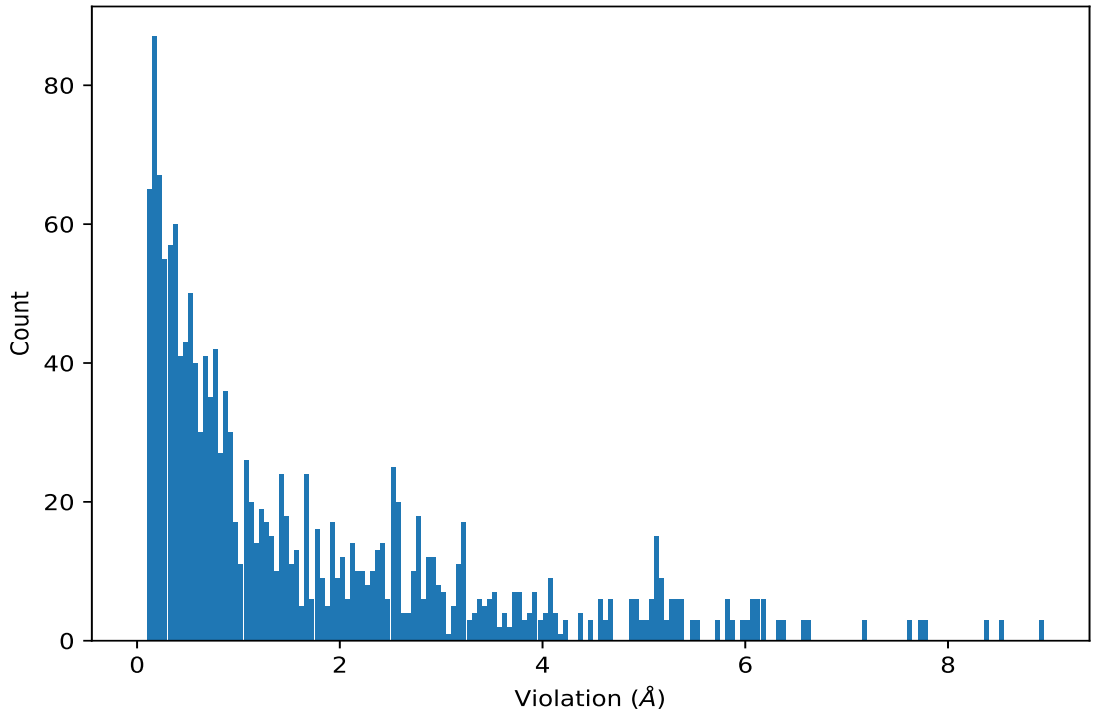
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,175)	1:A:88:PRO:O	1:A:33:LYS:HZ3	20	2.78	0.6	2.63
(1,53)	1:A:119:THR:H	1:A:115:PRO:O	20	2.23	0.53	2.13
(1,165)	1:A:5:ILE:O	1:A:39:SER:HG	20	2.2	0.67	2.21
(1,181)	1:A:55:SER:HG	1:A:59:LYS:O	20	2.08	0.36	2.16

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations

The following table 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)
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	14	8.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	14	8.93
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	14	8.93
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	8	8.5
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	8	8.5
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	8	8.5
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	10	8.38
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	10	8.38
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	10	8.38
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	20	7.75
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	20	7.75
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	20	7.75
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	19	7.72
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	19	7.72
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	19	7.72
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	11	7.61
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	11	7.61
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	11	7.61
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	2	7.19
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	2	7.19
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	2	7.19
(1,176)	1:A:34:LYS:HZ1	1:A:35:ILE:O	14	6.62
(1,176)	1:A:34:LYS:HZ2	1:A:35:ILE:O	14	6.62
(1,176)	1:A:34:LYS:HZ3	1:A:35:ILE:O	14	6.62
(1,177)	1:A:47:LYS:HZ1	1:A:44:LEU:O	13	6.57
(1,177)	1:A:47:LYS:HZ2	1:A:44:LEU:O	13	6.57
(1,177)	1:A:47:LYS:HZ3	1:A:44:LEU:O	13	6.57
(1,176)	1:A:34:LYS:HZ1	1:A:35:ILE:O	8	6.39

10 Dihedral-angle violation analysis

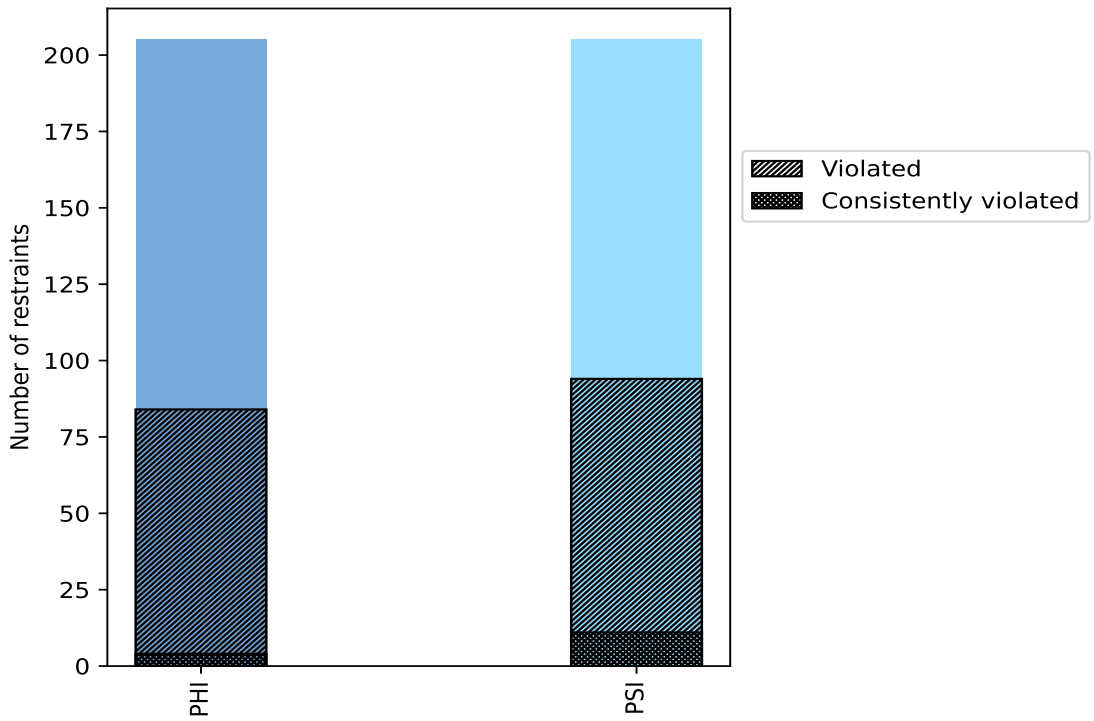
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	205	50.0	84	41.0	20.5	4	2.0	1.0
PSI	205	50.0	94	45.9	22.9	11	5.4	2.7
Total	410	100.0	178	43.4	43.4	15	3.7	3.7

[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



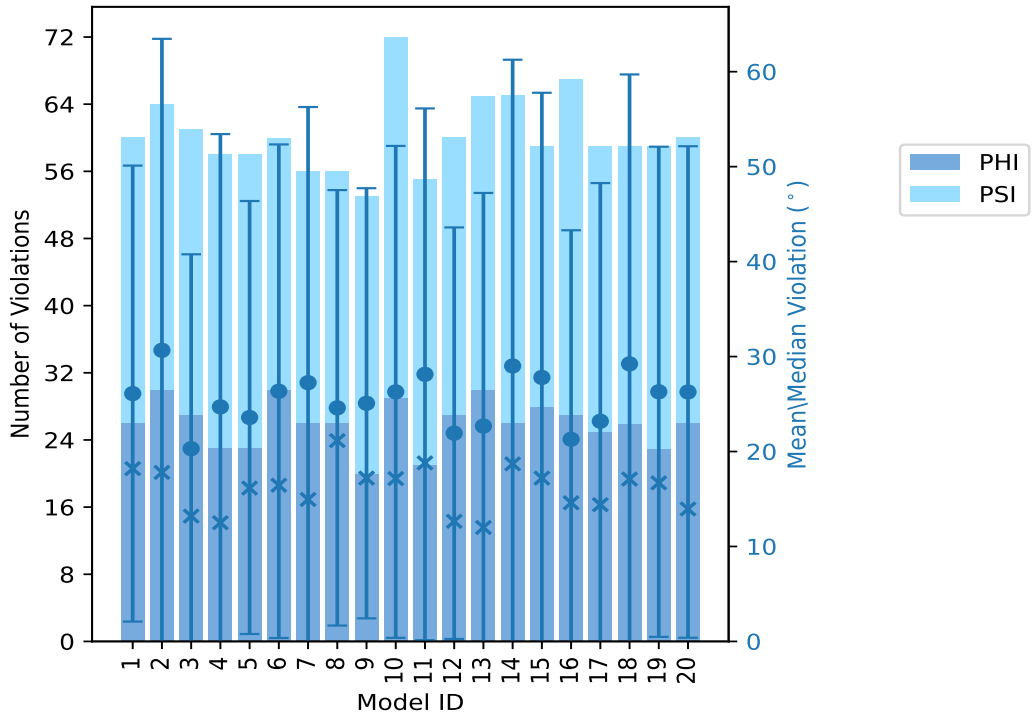
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	26	34	60	26.1	99.7	24.01	18.2
2	30	34	64	30.66	139.9	32.8	17.8
3	27	34	61	20.3	97.4	20.47	13.2
4	23	35	58	24.7	128.3	28.73	12.5
5	23	35	58	23.58	115.3	22.8	16.15
6	30	30	60	26.35	115.1	25.99	16.45
7	26	30	56	27.25	124.9	29.03	14.95
8	26	30	56	24.6	93.4	22.93	21.15
9	20	33	53	25.08	99.3	22.65	17.2
10	29	43	72	26.28	112.3	25.9	17.15
11	21	34	55	28.13	121.5	28.0	18.8
12	27	33	60	21.93	100.4	21.67	12.65
13	30	35	65	22.68	127.6	24.55	12.0
14	26	39	65	29.01	120.1	32.25	18.7
15	28	31	59	27.8	124.8	29.98	17.2
16	27	40	67	21.29	122.2	22.01	14.6
17	25	34	59	23.19	114.8	25.08	14.4
18	26	33	59	29.23	131.0	30.48	17.1
19	23	36	59	26.29	103.8	25.81	16.7
20	26	34	60	26.27	106.5	25.88	13.95

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	
PHI	PSI	Total	Count[1]	%
24	20	44	1	5.0
11	20	31	2	10.0
6	4	10	3	15.0
10	5	15	4	20.0
3	2	5	5	25.0
2	8	10	6	30.0
2	1	3	7	35.0
3	3	6	8	40.0
4	0	4	9	45.0
0	2	2	10	50.0
2	2	4	11	55.0

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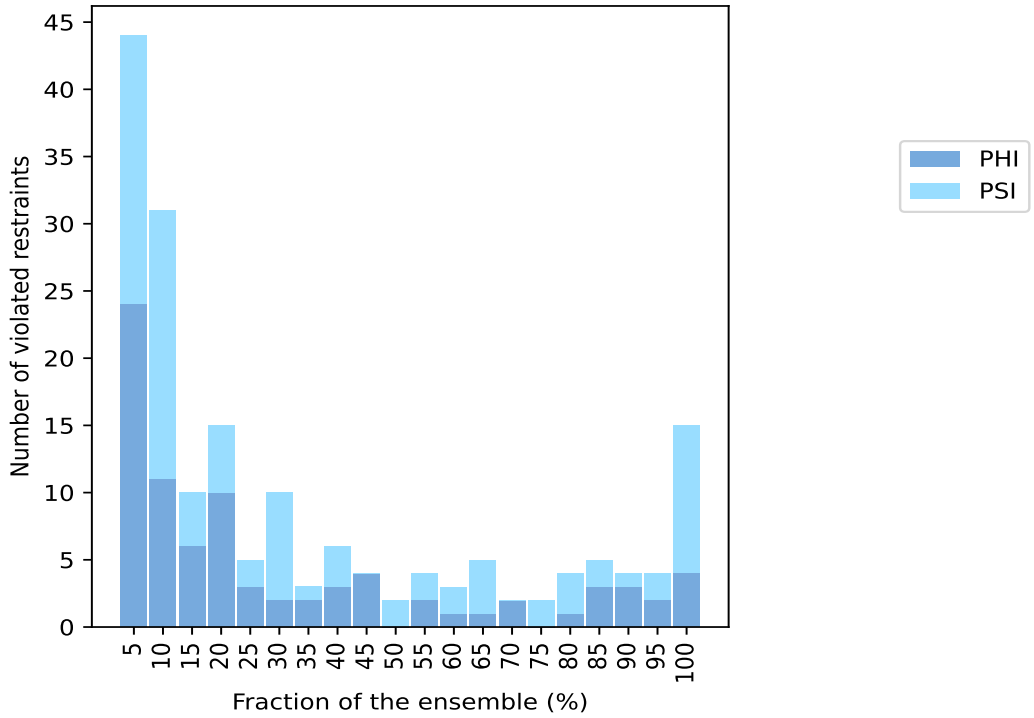
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	2	3	12	60.0
1	4	5	13	65.0
2	0	2	14	70.0
0	2	2	15	75.0
1	3	4	16	80.0
3	2	5	17	85.0
3	1	4	18	90.0
2	2	4	19	95.0
4	11	15	20	100.0

[1] Number of models with violations

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

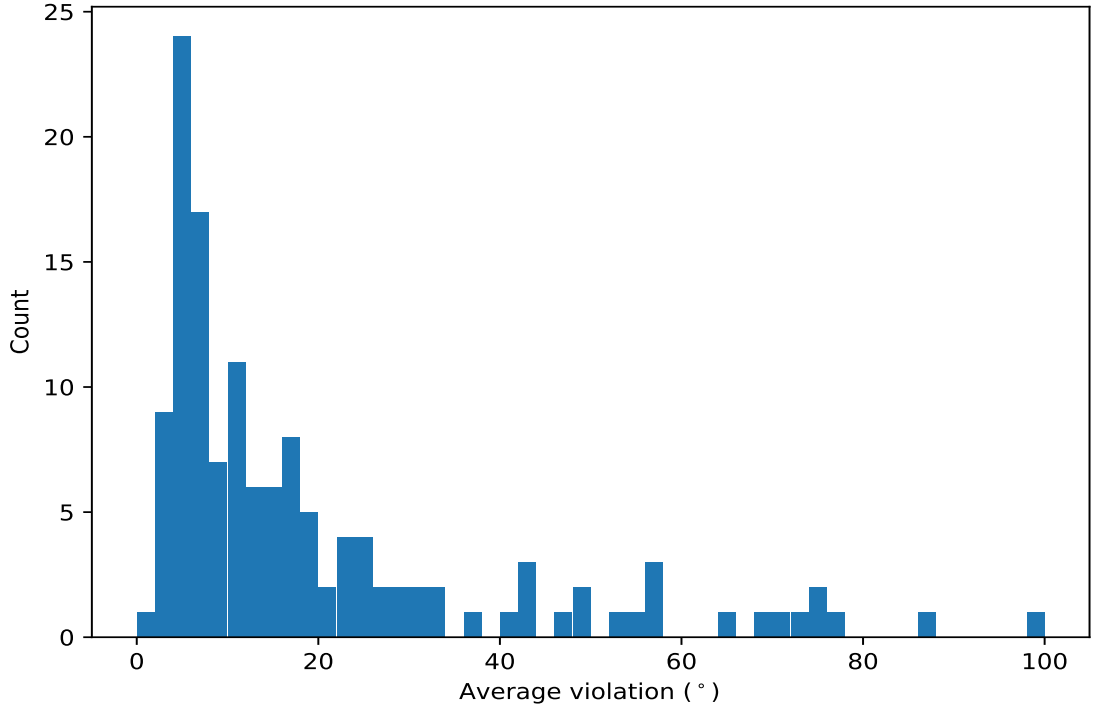


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the 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.

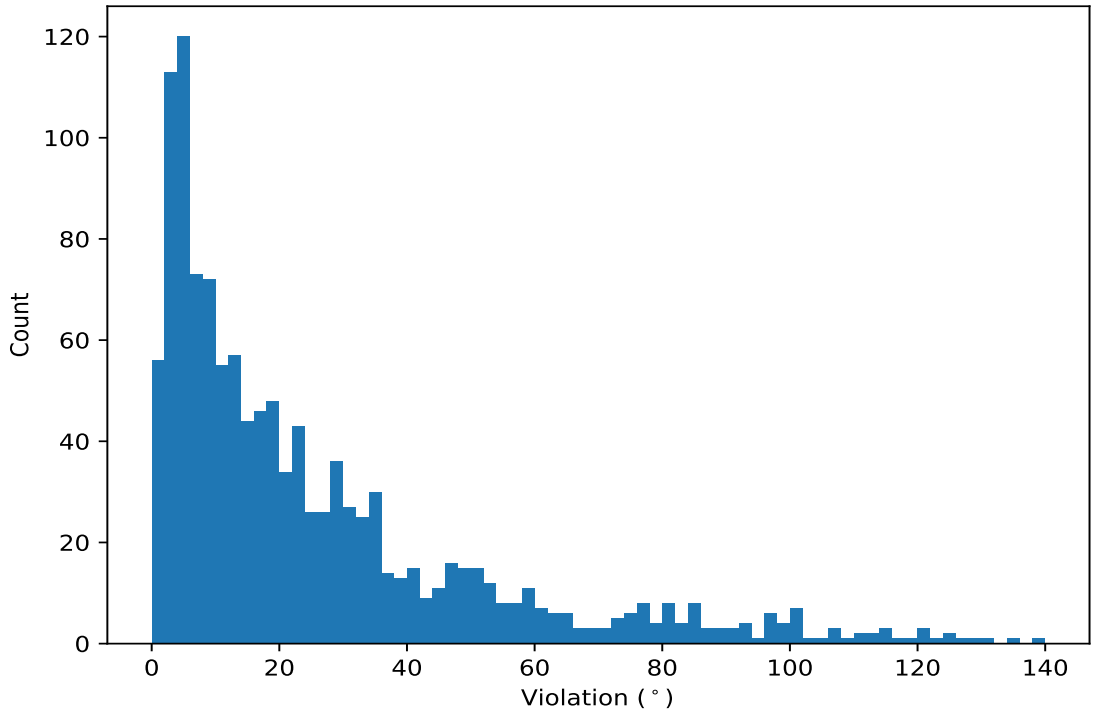
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,100)	1:A:54:ILE:N	1:A:54:ILE:CA	1:A:54:ILE:C	1:A:55:SER:N	20	98.94	17.03	100.45
(1,176)	1:A:93:PRO:N	1:A:93:PRO:CA	1:A:93:PRO:C	1:A:94:GLU:N	20	75.0	14.27	75.05
(1,110)	1:A:59:LYS:N	1:A:59:LYS:CA	1:A:59:LYS:C	1:A:60:VAL:N	20	68.6	29.38	75.4
(1,396)	1:A:207:GLU:N	1:A:207:GLU:CA	1:A:207:GLU:C	1:A:208:PRO:N	20	57.52	10.48	58.45
(1,220)	1:A:115:PRO:N	1:A:115:PRO:CA	1:A:115:PRO:C	1:A:116:ASN:N	20	56.84	20.0	49.55
(1,22)	1:A:14:PRO:N	1:A:14:PRO:CA	1:A:14:PRO:C	1:A:15:ASN:N	20	54.11	26.37	53.4
(1,216)	1:A:113:LYS:N	1:A:113:LYS:CA	1:A:113:LYS:C	1:A:114:ASP:N	20	43.12	9.22	46.05
(1,174)	1:A:92:PRO:N	1:A:92:PRO:CA	1:A:92:PRO:C	1:A:93:PRO:N	20	41.58	11.16	40.0
(1,170)	1:A:90:ALA:N	1:A:90:ALA:CA	1:A:90:ALA:C	1:A:91:THR:N	20	36.22	13.37	33.45
(1,395)	1:A:206:TRP:C	1:A:207:GLU:N	1:A:207:GLU:CA	1:A:207:GLU:C	20	32.37	9.04	34.75

[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 (°)
(1,110)	1:A:59:LYS:N	1:A:59:LYS:CA	1:A:59:LYS:C	1:A:60:VAL:N	2	139.9
(1,132)	1:A:71:ALA:N	1:A:71:ALA:CA	1:A:71:ALA:C	1:A:72:ASP:N	2	135.0
(1,69)	1:A:38:LYS:C	1:A:39:SER:N	1:A:39:SER:CA	1:A:39:SER:C	18	131.0
(1,132)	1:A:71:ALA:N	1:A:71:ALA:CA	1:A:71:ALA:C	1:A:72:ASP:N	4	128.3
(1,69)	1:A:38:LYS:C	1:A:39:SER:N	1:A:39:SER:CA	1:A:39:SER:C	13	127.6
(1,358)	1:A:188:SER:N	1:A:188:SER:CA	1:A:188:SER:C	1:A:189:ARG:N	7	124.9
(1,4)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:ILE:N	15	124.8
(1,132)	1:A:71:ALA:N	1:A:71:ALA:CA	1:A:71:ALA:C	1:A:72:ASP:N	16	122.2
(1,358)	1:A:188:SER:N	1:A:188:SER:CA	1:A:188:SER:C	1:A:189:ARG:N	11	121.5
(1,358)	1:A:188:SER:N	1:A:188:SER:CA	1:A:188:SER:C	1:A:189:ARG:N	14	120.1