



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:02 PM UTC

PDB ID : 2XV9 / pdb_00002xv9
BMRB ID : 6333
Title : The solution structure of ABA-1A saturated with oleic acid
Authors : Smith, B.O.; Kennedy, M.W.; Cooper, A.; Meenan, N.A.G.; Bromek, K.
Deposited on : 2010-10-25

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

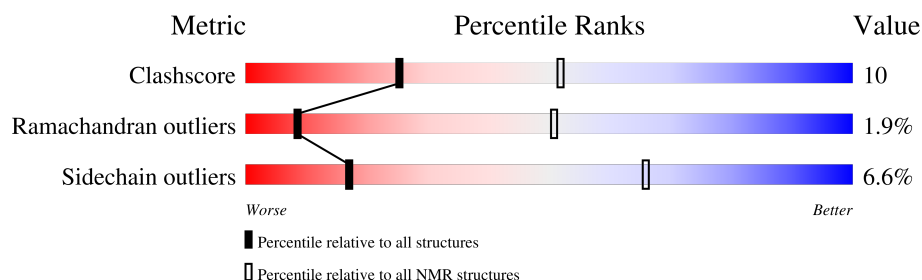
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	134	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 11 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:3-A:126 (124)	0.70	16

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2141 atoms, of which 1074 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ABA-1A1 REPEAT UNIT.

Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2141	672	1074	181	211	3	

There are 5 discrepancies between the modelled and reference sequences:

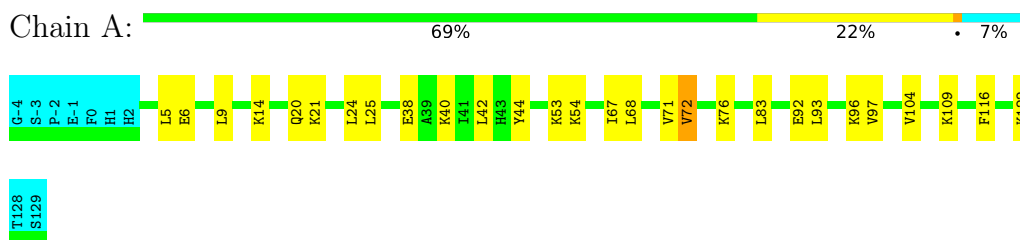
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q06811
A	-3	SER	-	expression tag	UNP Q06811
A	-2	PRO	-	expression tag	UNP Q06811
A	-1	GLU	-	expression tag	UNP Q06811
A	0	PHE	-	expression tag	UNP Q06811

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.

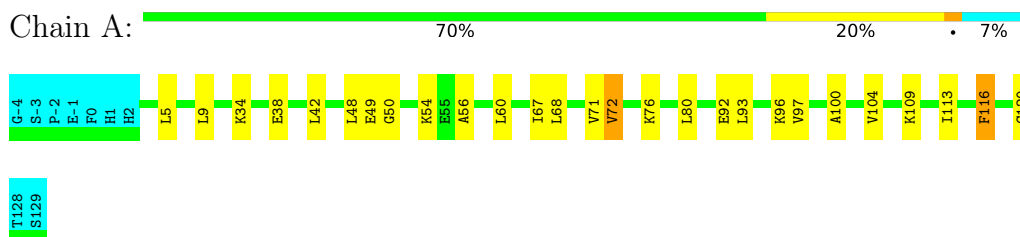
- Molecule 1: ABA-1A1 REPEAT UNIT



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

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: ABA-1A1 REPEAT UNIT



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DEFAULT*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *EXPERIMENTALLY DERIVED RESTRAINT ENERGY*.

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

Software name	Classification	Version
ARIA2.3/CNS	refinement	
DANGLE	structure solution	1.1
CcpNmr Analysis	structure solution	2.1
CNS	structure solution	1.21
ARIA	structure solution	2.3
ANSIG	structure solution	
PALES	structure solution	1

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1432
Number of shifts mapped to atoms	1432
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	0.49±0.01	0±0/1000 (0.0± 0.0%)	0.80±0.01	0±0/1333 (0.0± 0.0%)
All	All	0.49	0/20000 (0.0%)	0.80	1/26660 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.4
All	All	0	19

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	9	LEU	N-CA-C	5.03	118.19	111.75	20	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	124	TYR	Peptide	17
1	A	45	TYR	Sidechain	1
1	A	125	GLY	Peptide	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	986	1007	1002	21±3
All	All	19720	20140	20040	415

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 10.

5 of 135 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LEU:O	1:A:97:VAL:HB	0.78	1.79	8	7
1:A:122:LYS:HA	1:A:126:VAL:O	0.72	1.83	10	1
1:A:67:ILE:O	1:A:71:VAL:HB	0.70	1.87	5	4
1:A:96:LYS:O	1:A:99:GLU:HG3	0.70	1.87	6	1
1:A:92:GLU:O	1:A:96:LYS:HB2	0.67	1.90	20	14

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	124/134 (93%)	113±2 (91±2%)	9±2 (7±1%)	2±1 (2±1%)	8	51
All	All	2480/2680 (93%)	2259 (91%)	175 (7%)	46 (2%)	8	51

5 of 11 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	125	GLY	19
1	A	50	GLY	7
1	A	48	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	126	VAL	5
1	A	69	LYS	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	104/113 (92%)	93±17 (89±16%)	7±3 (6±3%)	18	67
All	All	1988/2260 (88%)	1856 (93%)	132 (7%)	17	66

5 of 35 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	72	VAL	13
1	A	116	PHE	13
1	A	54	LYS	12
1	A	83	LEU	11
1	A	104	VAL	9

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 oligosaccharides 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 80% for the well-defined parts and 79% 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	1432
Number of shifts mapped to atoms	1432
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	134	-0.57 ± 0.07	Should be checked
$^{13}\text{C}_\beta$	125	0.16 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	124	-0.10 ± 0.35	None needed (< 0.5 ppm)

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 80%, i.e. 1361 atoms were assigned a chemical shift out of a possible 1698. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	497/626 (79%)	252/255 (99%)	124/248 (50%)	121/123 (98%)
Sidechain	814/964 (84%)	540/618 (87%)	270/316 (85%)	4/30 (13%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	50/108 (46%)	25/52 (48%)	24/45 (53%)	1/11 (9%)
Overall	1361/1698 (80%)	817/925 (88%)	418/609 (69%)	126/164 (77%)

7.1.4 Statistically unusual chemical shifts [i](#)

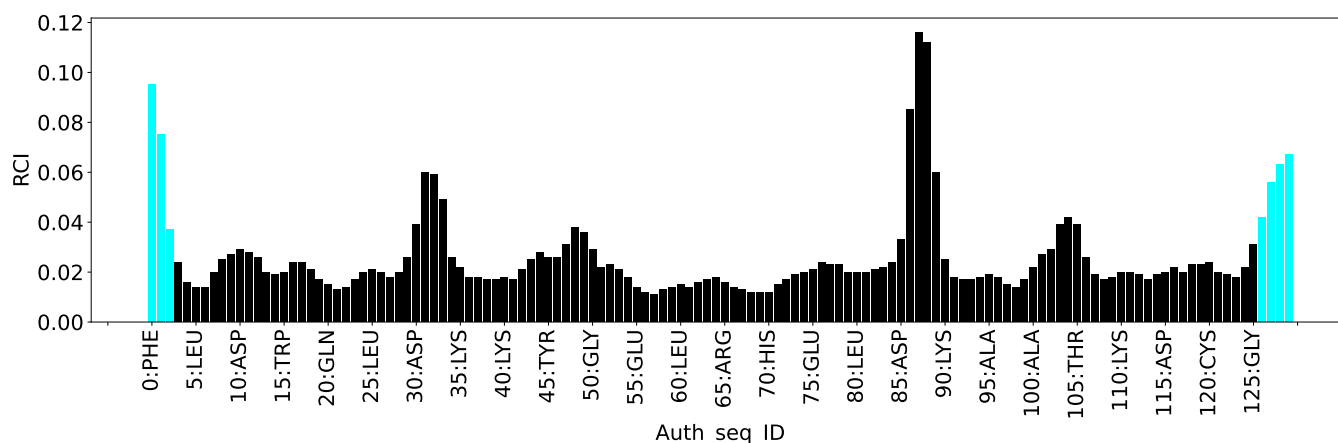
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	67	ILE	HG12	-0.86	-0.69 – 3.24	-5.4
1	A	61	LYS	HG2	0.13	0.13 – 2.61	-5.0

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	74404
Intra-residue ($ i-j =0$)	4006
Sequential ($ i-j =1$)	3682
Medium range ($ i-j >1$ and $ i-j <5$)	6486
Long range ($ i-j \geq 5$)	60177
Inter-chain	0
Hydrogen bond restraints	52
Disulfide bond restraints	1
Total dihedral-angle restraints	194
Number of unmapped restraints	0
Number of restraints per residue	556.7
Number of long range restraints per residue ¹	449.1

¹Long 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)	552.3	0.2
0.2-0.5 (Medium)	1410.8	0.5
>0.5 (Large)	63703.0	46.58

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)	7.2	9.98
10.0-20.0 (Medium)	1.9	19.57
>20.0 (Large)	2.8	26.44

9 Distance violation analysis ⓘ

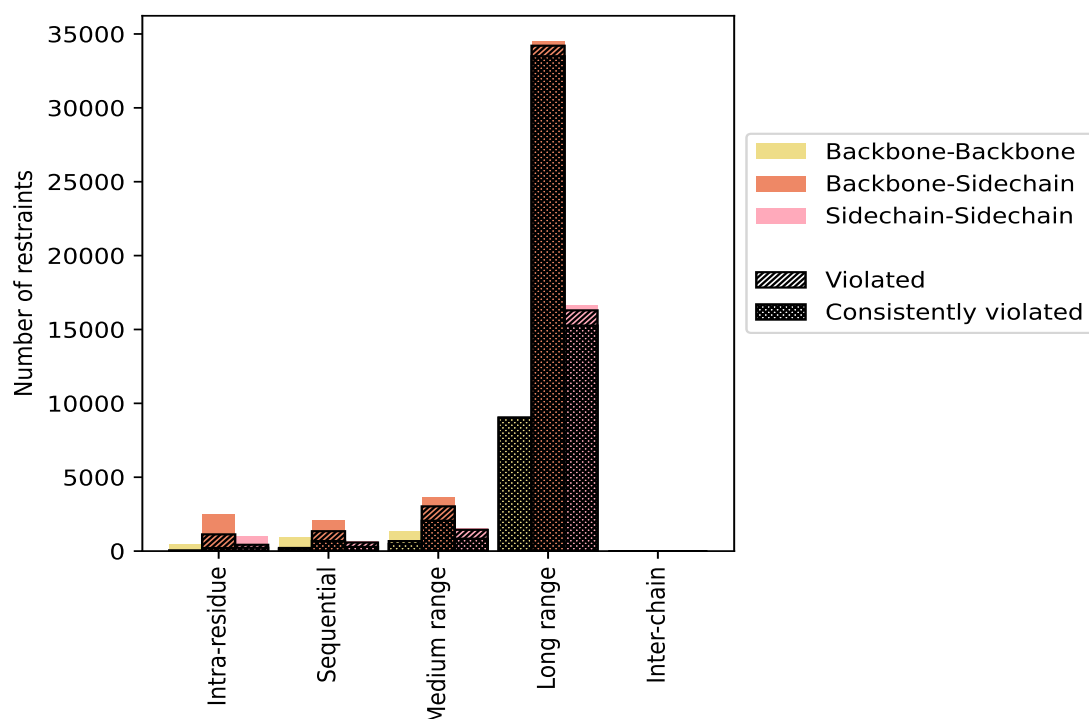
9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	4006	5.4	1598	39.9	2.1	460	11.5	0.6
Backbone-Backbone	477	0.6	39	8.2	0.1	27	5.7	0.0
Backbone-Sidechain	2508	3.4	1132	45.1	1.5	209	8.3	0.3
Sidechain-Sidechain	1021	1.4	427	41.8	0.6	224	21.9	0.3
Sequential ($ i-j =1$)	3682	4.9	2139	58.1	2.9	1124	30.5	1.5
Backbone-Backbone	948	1.3	211	22.3	0.3	158	16.7	0.2
Backbone-Sidechain	2090	2.8	1346	64.4	1.8	681	32.6	0.9
Sidechain-Sidechain	644	0.9	582	90.4	0.8	285	44.3	0.4
Medium range ($ i-j >1$ & $ i-j <5$)	6486	8.7	5139	79.2	6.9	3379	52.1	4.5
Backbone-Backbone	1306	1.8	677	51.8	0.9	482	36.9	0.6
Backbone-Sidechain	3618	4.9	3021	83.5	4.1	2055	56.8	2.8
Sidechain-Sidechain	1562	2.1	1441	92.3	1.9	842	53.9	1.1
Long range ($ i-j \geq 5$)	60177	80.9	59542	98.9	80.0	57776	96.0	77.7
Backbone-Backbone	9060	12.2	9046	99.8	12.2	9019	99.5	12.1
Backbone-Sidechain	34503	46.4	34204	99.1	46.0	33492	97.1	45.0
Sidechain-Sidechain	16614	22.3	16292	98.1	21.9	15265	91.9	20.5
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	52	0.1	7	13.5	0.0	0	0.0	0.0
Disulfide bond	1	0.0	1	100.0	0.0	0	0.0	0.0
Total	74404	100.0	68426	92.0	92.0	62739	84.3	84.3
Backbone-Backbone	11791	15.8	9973	84.6	13.4	9686	82.1	13.0
Backbone-Sidechain	42771	57.5	39710	92.8	53.4	36437	85.2	49.0
Sidechain-Sidechain	19842	26.7	18743	94.5	25.2	16616	83.7	22.3

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	962	1647	4333	58747	0	65689	13.61	42.79	8.75	12.94
2	968	1663	4322	58735	0	65688	13.83	46.58	8.88	13.18
3	949	1678	4320	58717	0	65664	13.72	42.71	8.8	13.09
4	945	1663	4347	58781	0	65736	14.02	43.29	9.05	13.31
5	943	1660	4354	58769	0	65726	13.83	44.19	8.98	13.05
6	992	1679	4309	58726	0	65706	13.48	43.16	8.65	12.87
7	984	1662	4364	58715	0	65725	13.88	44.1	8.95	13.21
8	963	1622	4309	58746	0	65640	13.79	43.86	8.84	13.15
9	958	1652	4335	58756	0	65701	13.62	41.91	8.72	13.02
10	946	1676	4334	58723	0	65679	13.62	42.55	8.7	13.01

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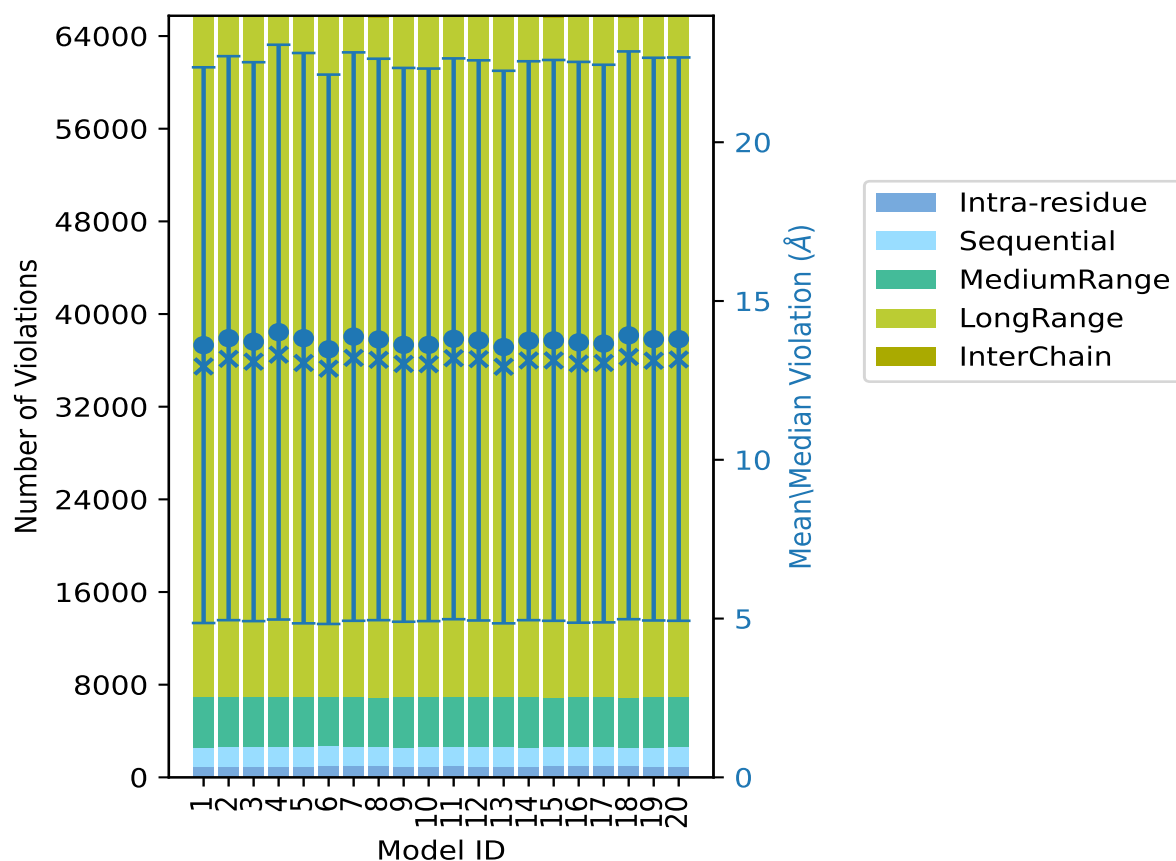
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	968	1672	4348	58762	0	65750	13.81	44.12	8.83	13.2
12	966	1657	4321	58766	0	65710	13.76	41.66	8.82	13.17
13	940	1684	4324	58727	0	65675	13.55	41.45	8.7	12.93
14	952	1658	4330	58796	0	65736	13.75	42.85	8.8	13.13
15	956	1633	4308	58715	0	65612	13.76	44.12	8.83	13.13
16	993	1648	4317	58749	0	65707	13.7	43.65	8.83	13.03
17	965	1678	4330	58738	0	65711	13.66	43.38	8.78	13.05
18	962	1622	4264	58780	0	65628	13.92	42.45	8.94	13.24
19	952	1645	4330	58763	0	65690	13.8	43.28	8.86	13.12
20	944	1684	4316	58791	0	65735	13.8	43.26	8.87	13.16

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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 ⓘ

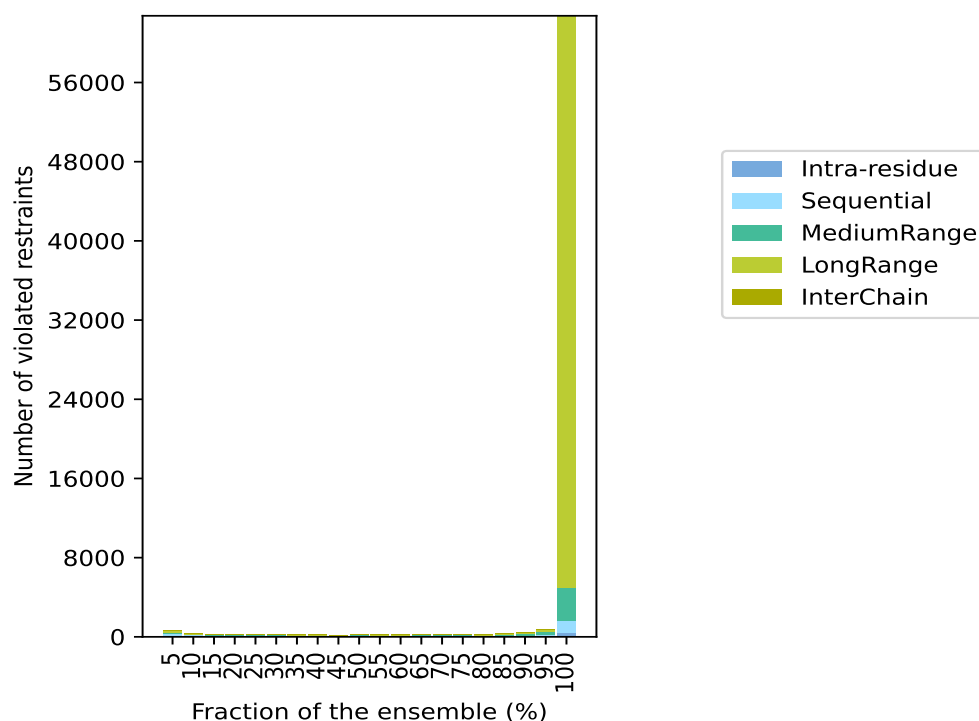
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5933(IR:2408, SQ:1543, MR:1347, LR:635, IC:0) restraints 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	%
155	111	186	150	0	602	1	5.0
104	69	98	115	0	386	2	10.0
46	41	86	77	0	250	3	15.0
48	46	69	76	0	239	4	20.0
61	30	70	74	0	235	5	25.0
85	43	74	63	0	265	6	30.0
53	31	63	64	0	211	7	35.0
62	38	49	58	0	207	8	40.0
42	30	50	63	0	185	9	45.0
42	51	64	65	0	222	10	50.0
47	35	60	59	0	201	11	55.0
43	41	62	55	0	201	12	60.0
48	42	79	60	0	229	13	65.0
39	47	89	68	0	243	14	70.0
34	41	83	81	0	239	15	75.0
31	43	107	104	0	285	16	80.0
41	55	87	111	0	294	17	85.0
54	80	138	167	0	439	18	90.0
103	141	246	256	0	746	19	95.0
460	1124	3379	57776	0	62739	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

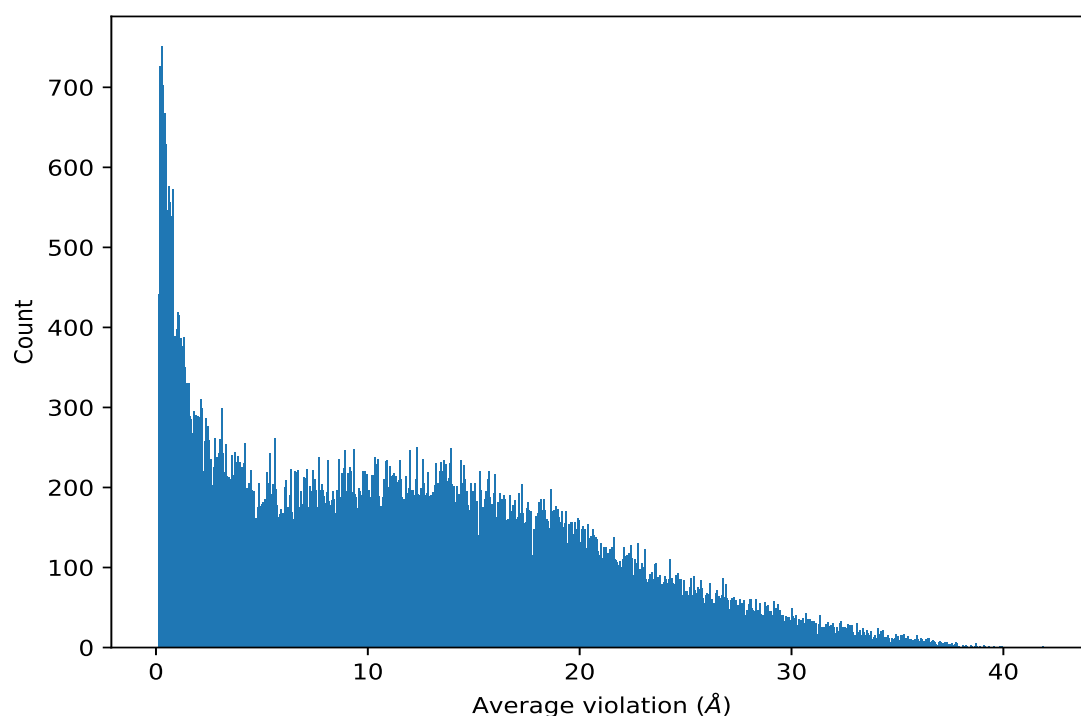
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 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.

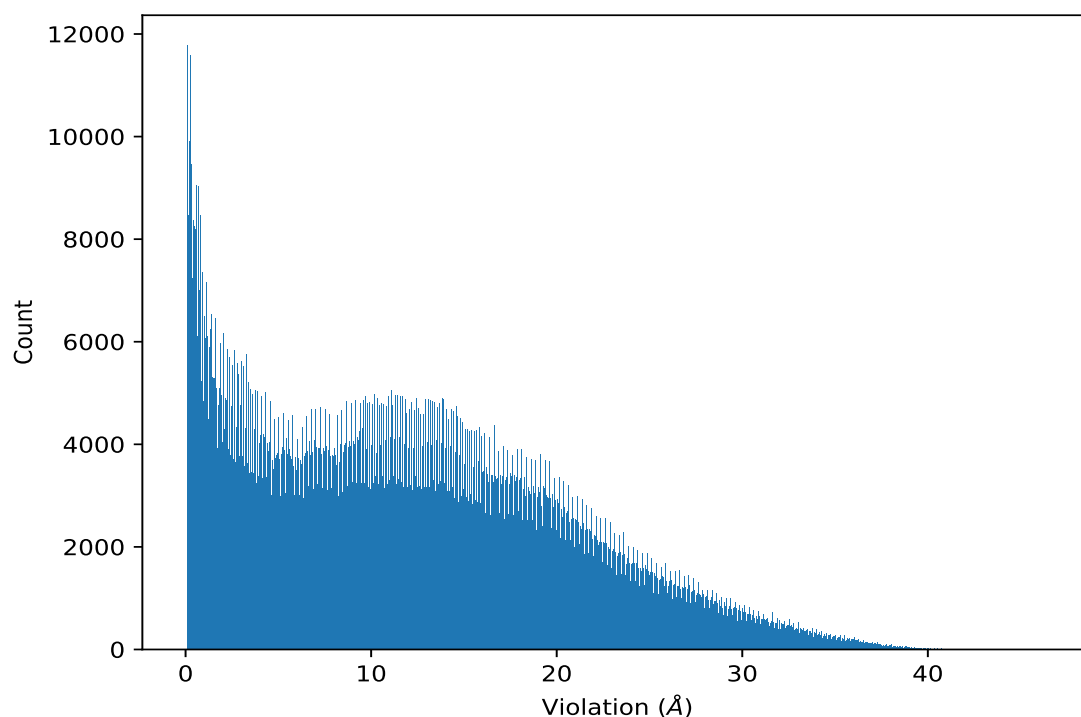
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(9,27685)	1:86:A:SER:HB3	1:30:A:ASP:HB2	20	42.09	0.76	42.38
(9,27691)	1:86:A:SER:HB2	1:30:A:ASP:HB2	20	41.89	1.11	41.77
(9,27715)	1:86:A:SER:HB3	1:30:A:ASP:HB3	20	41.86	1.21	41.9
(9,27688)	1:86:A:SER:HB2	1:30:A:ASP:HB3	20	41.66	1.12	41.74
(9,18615)	1:30:A:ASP:HB2	1:86:A:SER:HA	20	41.64	0.79	41.66
(9,18613)	1:30:A:ASP:HB3	1:86:A:SER:HA	20	41.46	0.95	41.16
(9,36420)	1:31:A:GLY:H	1:86:A:SER:HA	20	40.33	0.62	40.11
(7,12347)	1:31:A:GLY:H	1:86:A:SER:HB3	20	40.21	0.78	40.08
(7,5471)	1:30:A:ASP:H	1:86:A:SER:HB3	20	40.12	0.78	40.02
(7,12359)	1:31:A:GLY:H	1:86:A:SER:HB2	20	40.01	0.99	39.83

¹Number of violated models, ²Standard 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)
(7,17274)	1:87:A:GLY:H	1:-4:A:GLY:HA3	2	46.58
(7,17287)	1:87:A:GLY:H	1:-4:A:GLY:HA2	2	46.54
(7,15703)	1:88:A:ALA:H	1:-4:A:GLY:HA3	2	45.66
(7,15717)	1:88:A:ALA:H	1:-4:A:GLY:HA2	2	45.55
(9,27691)	1:86:A:SER:HB2	1:30:A:ASP:HB2	5	44.19
(9,27715)	1:86:A:SER:HB3	1:30:A:ASP:HB3	11	44.12
(9,27715)	1:86:A:SER:HB3	1:30:A:ASP:HB3	15	44.12
(7,15811)	1:-4:A:GLY:HA3	1:129:A:SER:H	7	44.1
(7,22029)	1:86:A:SER:H	1:-4:A:GLY:HA2	2	44.05
(7,22040)	1:86:A:SER:H	1:-4:A:GLY:HA3	2	44.04

10 Dihedral-angle violation analysis [i](#)

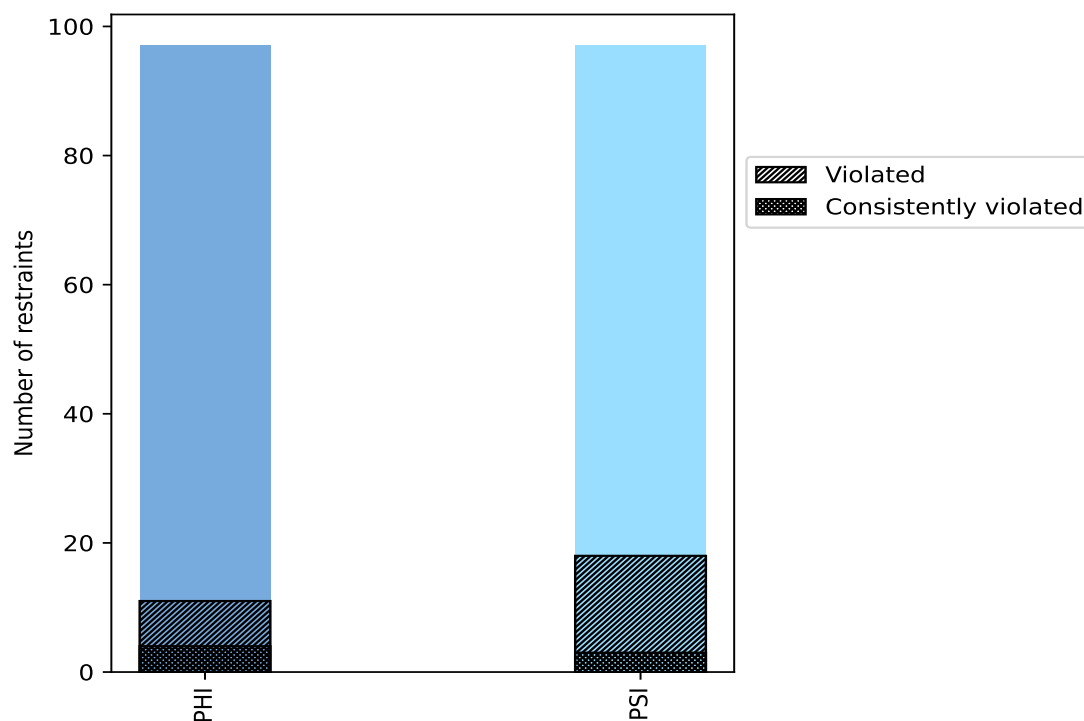
10.1 Summary of dihedral-angle violations [i](#)

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
PHI	97	50.0	11	11.3	5.7	4	4.1	2.1
PSI	97	50.0	18	18.6	9.3	3	3.1	1.5
Total	194	100.0	29	14.9	14.9	7	3.6	3.6

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](#)



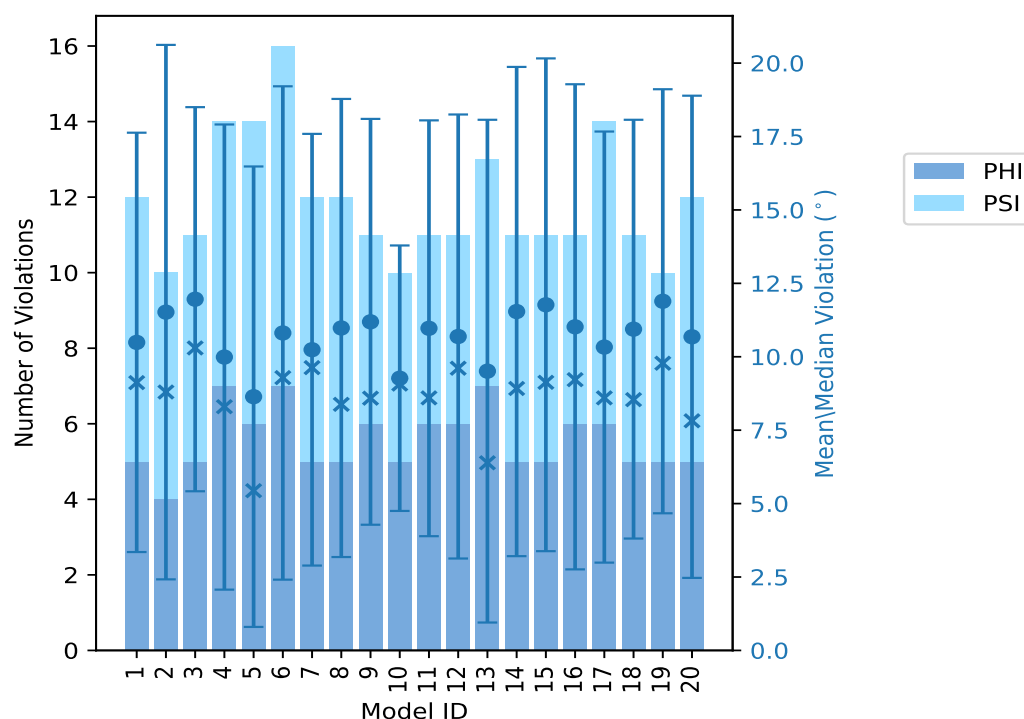
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	5	7	12	10.49	23.27	7.14	9.12
2	4	6	10	11.52	26.44	9.1	8.8
3	5	6	11	11.96	23.32	6.54	10.3
4	7	7	14	9.99	26.44	7.92	8.3
5	6	8	14	8.64	24.14	7.84	5.44
6	7	9	16	10.81	25.3	8.4	9.29
7	5	7	12	10.24	22.66	7.35	9.63
8	5	7	12	10.98	25.15	7.8	8.38
9	6	5	11	11.19	21.76	6.91	8.59
10	5	5	10	9.27	17.16	4.52	9.07
11	6	5	11	10.97	22.85	7.08	8.6
12	6	5	11	10.69	22.75	7.56	9.61
13	7	6	13	9.51	25.49	8.56	6.39
14	5	6	11	11.54	25.75	8.33	8.92
15	5	6	11	11.77	26.24	8.39	9.13
16	6	5	11	11.02	24.96	8.26	9.22
17	6	8	14	10.33	25.71	7.34	8.6
18	5	6	11	10.94	24.91	7.13	8.54
19	5	5	10	11.89	23.54	7.22	9.78
20	5	7	12	10.68	25.5	8.21	7.82

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

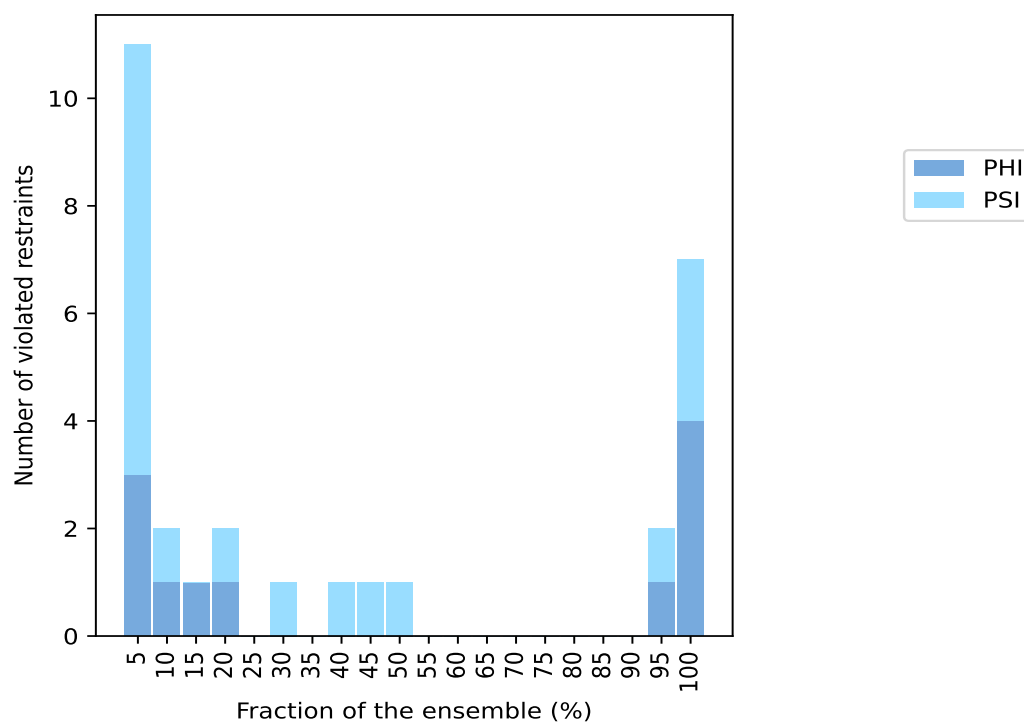
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
1	1	2	19	95.0
4	3	7	20	100.0

¹ Number of models with violations

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

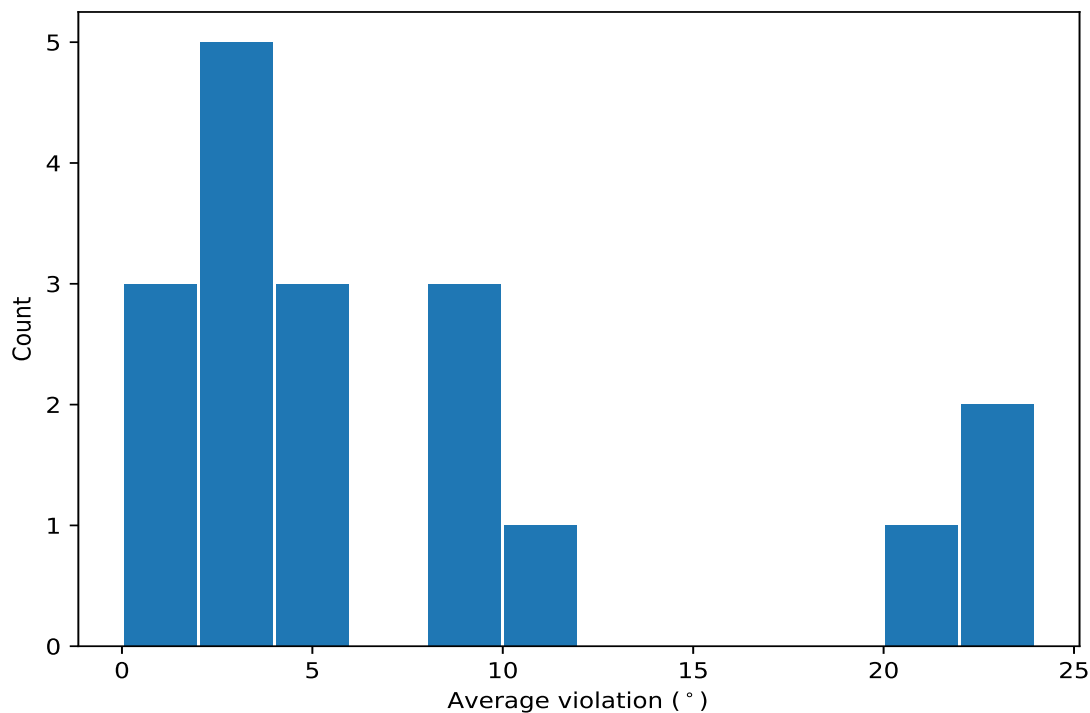


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 [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.

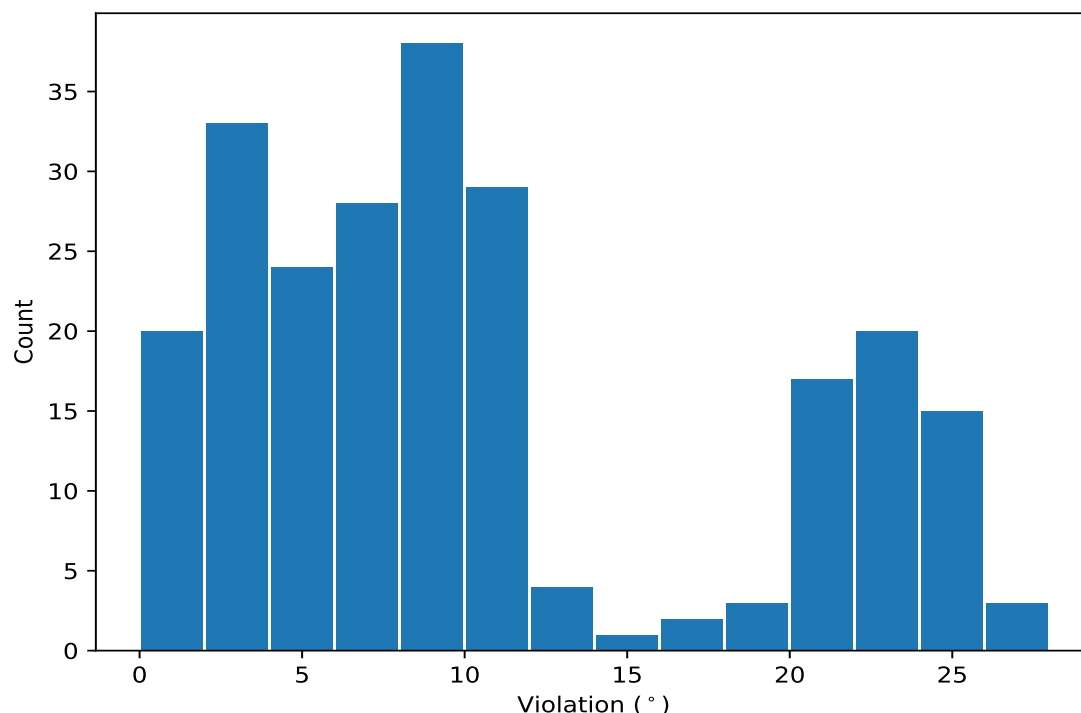
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	20	23.83	2.3	24.55
(1,192)	1:124:A:TYR:N	1:124:A:TYR:CA	1:124:A:TYR:C	1:125:A:GLY:N	20	23.12	1.84	23.26
(1,43)	1:38:A:GLU:C	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	20	10.2	0.88	10.06
(1,99)	1:69:A:LYS:C	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	20	9.41	2.89	10.32
(1,175)	1:115:A:ASP:C	1:116:A:PHE:N	1:116:A:PHE:CA	1:116:A:PHE:C	20	8.46	1.29	8.52
(1,98)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:HIS:N	20	5.93	1.96	6.16
(1,164)	1:110:A:LYS:N	1:110:A:LYS:CA	1:110:A:LYS:C	1:111:A:GLN:N	20	5.76	1.76	5.79
(1,194)	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	1:126:A:VAL:N	19	21.35	1.24	21.35
(1,7)	1:7:A:SER:C	1:8:A:SER:N	1:8:A:SER:CA	1:8:A:SER:C	19	9.14	0.68	9.1
(1,6)	1:7:A:SER:N	1:7:A:SER:CA	1:7:A:SER:C	1:8:A:SER:N	10	3.89	3.14	2.58

¹ Number of violated models, ²Standard 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 provides the list of violations for 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 (°)
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	2	26.44
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	4	26.44
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	15	26.24
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	14	25.75
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	17	25.71
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	20	25.5
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	13	25.49
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	6	25.3
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	8	25.15
(1,193)	1:124:A:TYR:C	1:125:A:GLY:N	1:125:A:GLY:CA	1:125:A:GLY:C	16	24.96