



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 30133
Title : Solution Structure of Antibiotic-Resistance Factor ANT(2'')-Ia Reveals
Substrate-Regulated Conformation Dynamics
Authors : Bacot-Davis, V.R.; Berghuis, A.M.
Deposited on : 2016-07-06

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 ⓘ 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

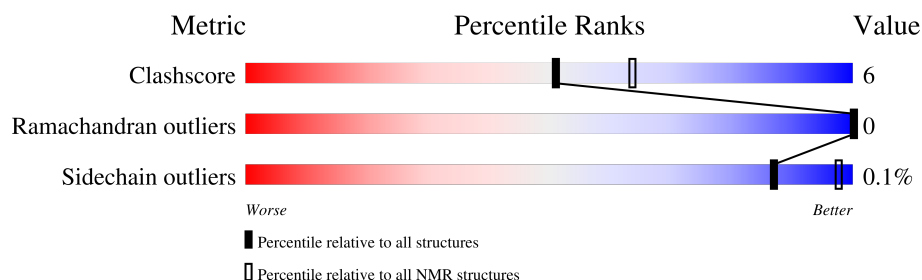
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	185	

2 Ensemble composition and analysis

This entry contains 15 models. Model 6 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:9-A:128 (120)	1.01	6
2	A:145-A:180 (36)	0.34	7

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10
2	11, 12, 13, 14, 15

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2857 atoms, of which 1379 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 2''-aminoglycoside nucleotidyltransferase.

Mol	Chain	Residues	Atoms						Trace
1	A	185	Total	C	H	N	O	S	0
			2857	937	1379	257	277	7	

There are 8 discrepancies between the modelled and reference sequences:

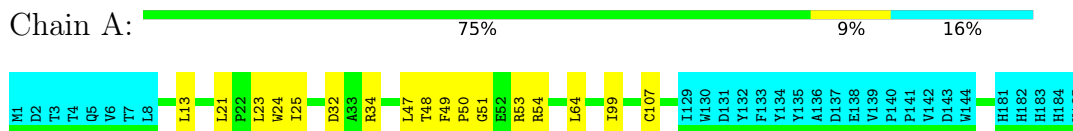
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	LEU	-	expression tag	UNP P0AE05
A	179	GLU	-	expression tag	UNP P0AE05
A	180	HIS	-	expression tag	UNP P0AE05
A	181	HIS	-	expression tag	UNP P0AE05
A	182	HIS	-	expression tag	UNP P0AE05
A	183	HIS	-	expression tag	UNP P0AE05
A	184	HIS	-	expression tag	UNP P0AE05
A	185	HIS	-	expression tag	UNP P0AE05

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.

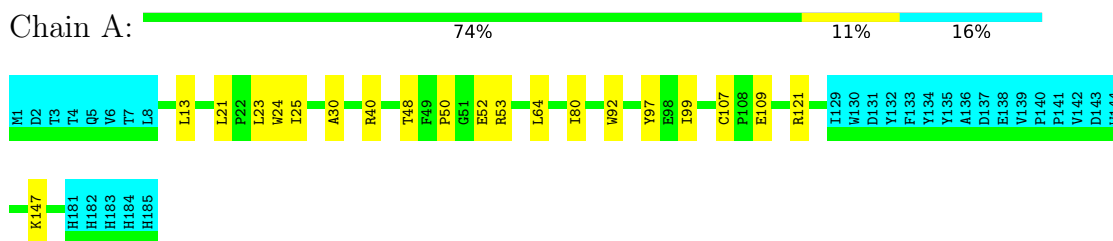
- Molecule 1: 2'-aminoglycoside nucleotidyltransferase



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

The representative model is number 6. Colouring as in section 4.1 above.

- Molecule 1: 2'-aminoglycoside nucleotidyltransferase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 15 calculated structures, 15 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	

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	2015
Number of shifts mapped to atoms	2015
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1217	1170	1179	13±2
All	All	18255	17550	17685	198

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 6.

5 of 65 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ILE:HG13	1:A:107:CYS:SG	0.92	2.04	14	9
1:A:23:LEU:H	1:A:121:ARG:HH21	0.79	1.20	2	2
1:A:99:ILE:CG1	1:A:107:CYS:SG	0.71	2.78	15	5
1:A:21:LEU:HD13	1:A:53:ARG:HD3	0.71	1.62	5	1
1:A:13:LEU:HD23	1:A:23:LEU:HD13	0.70	1.64	7	5

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	156/185 (84%)	154±1 (99±1%)	2±1 (1±1%)	0±0 (0±0%)	100	100
All	All	2340/2775 (84%)	2310 (99%)	30 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	120/148 (81%)	120±0 (100±0%)	0±0 (0±0%)	87	98
All	All	1800/2220 (81%)	1798 (100%)	2 (0%)	87	98

All 2 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	163	LYS	1
1	A	44	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no 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 81% 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: *ANT2_June2016_BMRB31_final.str*

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	2015
Number of shifts mapped to atoms	2015
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	54

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
$^{13}\text{C}_\alpha$	176	-0.32 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	162	-0.21 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	164	-0.15 ± 0.17	None needed (< 0.5 ppm)
^{15}N	165	0.02 ± 0.30	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 81%, i.e. 1687 atoms were assigned a chemical shift out of a possible 2095. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	731/780 (94%)	300/319 (94%)	290/312 (93%)	141/149 (95%)
Sidechain	912/1164 (78%)	626/758 (83%)	285/360 (79%)	1/46 (2%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	44/151 (29%)	0/77 (0%)	44/68 (65%)	0/6 (0%)
Overall	1687/2095 (81%)	926/1154 (80%)	619/740 (84%)	142/201 (71%)

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	11	LYS	HB3	5.68	0.46 – 3.04	15.2
1	A	119	PRO	CD	36.27	45.11 – 55.58	-13.4
1	A	82	ASP	H	14.79	5.52 – 11.08	11.7
1	A	38	VAL	H	0.71	4.98 – 11.56	-11.5
1	A	159	LEU	H	1.71	5.09 – 11.34	-10.4
1	A	34	ARG	CD	34.02	38.57 – 47.75	-9.9
1	A	40	ARG	H	2.34	5.25 – 11.22	-9.9
1	A	146	THR	H	2.71	5.19 – 11.27	-9.1
1	A	167	LEU	CG	36.28	21.37 – 32.19	8.8
1	A	123	ASN	H	3.12	5.28 – 11.36	-8.6
1	A	84	LEU	CD1	12.15	16.71 – 32.55	-7.9
1	A	84	LEU	CD2	11.77	15.73 – 32.47	-7.4
1	A	141	PRO	CG	19.24	21.69 – 32.72	-7.2
1	A	178	LEU	HD11	2.65	-0.61 – 2.12	6.9
1	A	178	LEU	HD12	2.65	-0.61 – 2.12	6.9
1	A	178	LEU	HD13	2.65	-0.61 – 2.12	6.9
1	A	41	LYS	CG	17.22	19.35 – 30.45	-6.9
1	A	150	GLU	CG	28.01	30.20 – 42.01	-6.9
1	A	12	ILE	CD1	24.60	5.18 – 21.60	6.8
1	A	178	LEU	HD21	2.60	-0.65 – 2.13	6.7
1	A	178	LEU	HD22	2.60	-0.65 – 2.13	6.7
1	A	178	LEU	HD23	2.60	-0.65 – 2.13	6.7
1	A	41	LYS	CE	36.23	37.57 – 46.21	-6.5
1	A	19	ARG	CD	49.09	38.57 – 47.75	6.5
1	A	172	ARG	HD2	1.64	1.97 – 4.26	-6.5
1	A	100	ALA	CB	7.72	10.19 – 27.75	-6.4
1	A	128	ILE	HG21	2.48	-0.56 – 2.11	6.4
1	A	128	ILE	HG22	2.48	-0.56 – 2.11	6.4
1	A	128	ILE	HG23	2.48	-0.56 – 2.11	6.4
1	A	172	ARG	HD3	1.50	1.81 – 4.39	-6.2
1	A	178	LEU	CD1	14.95	16.71 – 32.55	-6.1
1	A	23	LEU	CG	20.36	21.37 – 32.19	-5.9

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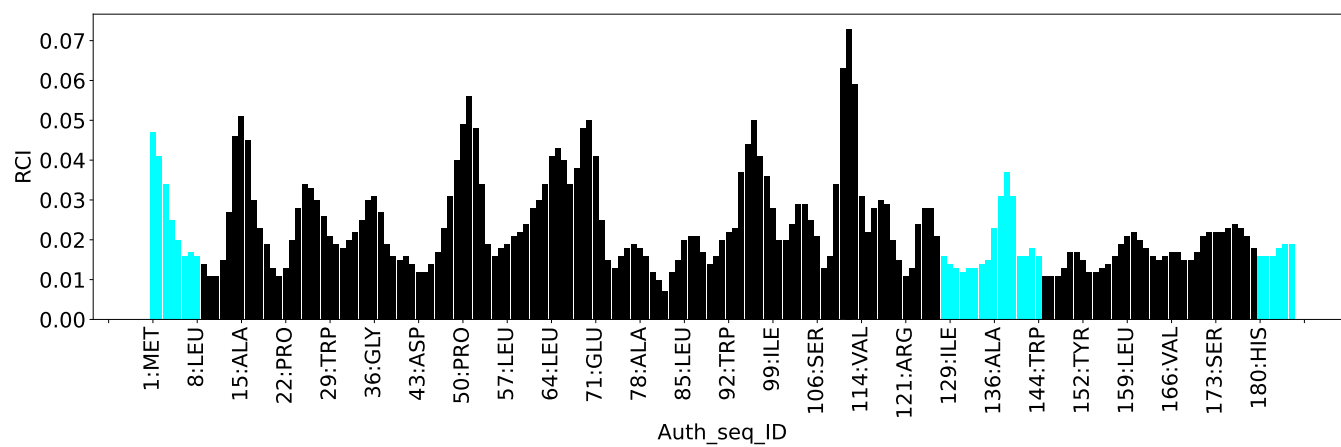
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	178	LEU	CD2	14.63	15.73 – 32.47	-5.7
1	A	12	ILE	CG2	24.96	10.93 – 24.12	5.6
1	A	129	ILE	HG21	2.25	-0.56 – 2.11	5.5
1	A	129	ILE	HG22	2.25	-0.56 – 2.11	5.5
1	A	129	ILE	HG23	2.25	-0.56 – 2.11	5.5
1	A	41	LYS	CD	23.00	23.50 – 34.42	-5.5
1	A	22	PRO	CA	55.22	55.85 – 70.84	-5.4
1	A	129	ILE	HD11	2.20	-0.72 – 2.09	5.4
1	A	129	ILE	HD12	2.20	-0.72 – 2.09	5.4
1	A	129	ILE	HD13	2.20	-0.72 – 2.09	5.4
1	A	80	ILE	CD1	22.11	5.18 – 21.60	5.3
1	A	80	ILE	CG2	24.52	10.93 – 24.12	5.3
1	A	29	TRP	CB	40.32	20.06 – 39.75	5.3
1	A	33	ALA	HB1	2.64	0.14 – 2.58	5.3
1	A	33	ALA	HB2	2.64	0.14 – 2.58	5.3
1	A	33	ALA	HB3	2.64	0.14 – 2.58	5.3
1	A	76	PHE	CZ	121.47	121.82 – 136.66	-5.2
1	A	40	ARG	HG2	0.21	0.26 – 2.87	-5.2
1	A	133	PHE	CZ	121.58	121.82 – 136.66	-5.2
1	A	61	VAL	CG1	28.46	14.71 – 28.29	5.1
1	A	115	ILE	CD1	21.73	5.18 – 21.60	5.1
1	A	35	LEU	CG	32.21	21.37 – 32.19	5.0

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:



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	760
Intra-residue ($ i-j =0$)	44
Sequential ($ i-j =1$)	411
Medium range ($ i-j >1$ and $ i-j <5$)	84
Long range ($ i-j \geq 5$)	58
Inter-chain	0
Hydrogen bond restraints	163
Disulfide bond restraints	0
Total dihedral-angle restraints	214
Number of unmapped restraints	0
Number of restraints per residue	5.3
Number of long range restraints per residue ¹	0.6

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)	33.8	0.2
0.2-0.5 (Medium)	34.5	0.5
>0.5 (Large)	196.9	41.44

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)	48.3	9.99
10.0-20.0 (Medium)	31.3	20.0
>20.0 (Large)	41.4	165.19

9 Distance violation analysis ⓘ

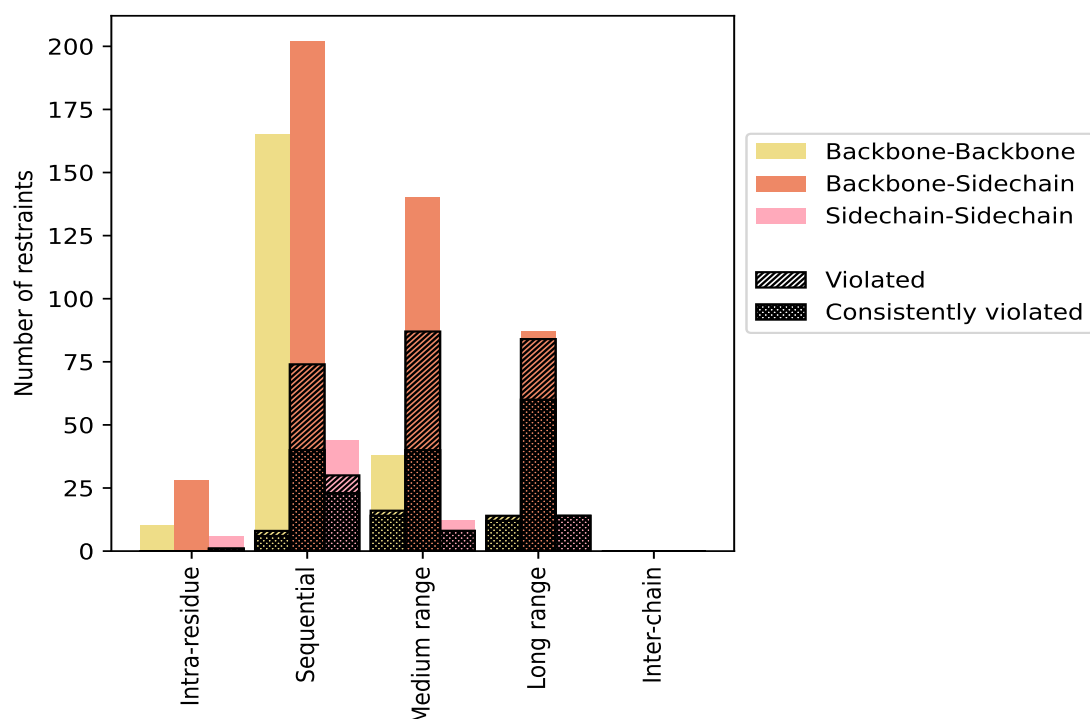
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	44	5.8	1	2.3	0.1	1	2.3	0.1
Backbone-Backbone	10	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	28	3.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	6	0.8	1	16.7	0.1	1	16.7	0.1
Sequential (i-j =1)	411	54.1	112	27.3	14.7	69	16.8	9.1
Backbone-Backbone	165	21.7	8	4.8	1.1	6	3.6	0.8
Backbone-Sidechain	202	26.6	74	36.6	9.7	40	19.8	5.3
Sidechain-Sidechain	44	5.8	30	68.2	3.9	23	52.3	3.0
Medium range (i-j >1 & i-j <5)	84	11.1	46	54.8	6.1	40	47.6	5.3
Backbone-Backbone	38	5.0	16	42.1	2.1	14	36.8	1.8
Backbone-Sidechain	34	4.5	22	64.7	2.9	18	52.9	2.4
Sidechain-Sidechain	12	1.6	8	66.7	1.1	8	66.7	1.1
Long range (i-j ≥5)	58	7.6	58	100.0	7.6	55	94.8	7.2
Backbone-Backbone	14	1.8	14	100.0	1.8	12	85.7	1.6
Backbone-Sidechain	30	3.9	30	100.0	3.9	29	96.7	3.8
Sidechain-Sidechain	14	1.8	14	100.0	1.8	14	100.0	1.8
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	163	21.4	119	73.0	15.7	53	32.5	7.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	760	100.0	336	44.2	44.2	218	28.7	28.7
Backbone-Backbone	227	29.9	38	16.7	5.0	32	14.1	4.2
Backbone-Sidechain	457	60.1	245	53.6	32.2	140	30.6	18.4
Sidechain-Sidechain	76	10.0	53	69.7	7.0	46	60.5	6.1

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	1	79	76	99	0	255	7.6	40.14	9.73	2.09
2	1	79	78	99	0	257	7.6	40.76	9.75	1.86
3	1	85	77	102	0	265	7.37	40.4	9.64	1.59
4	1	85	80	99	0	265	7.42	40.5	9.76	1.51
5	1	81	80	101	0	263	7.34	39.93	9.62	1.69
6	1	85	80	95	0	261	7.54	40.58	9.86	1.59
7	1	91	82	98	0	272	7.26	40.54	9.78	1.49
8	1	87	84	97	0	269	7.37	41.26	9.87	1.5
9	1	87	83	98	0	269	7.34	40.77	9.82	1.49
10	1	87	81	97	0	266	7.45	41.44	9.87	1.61

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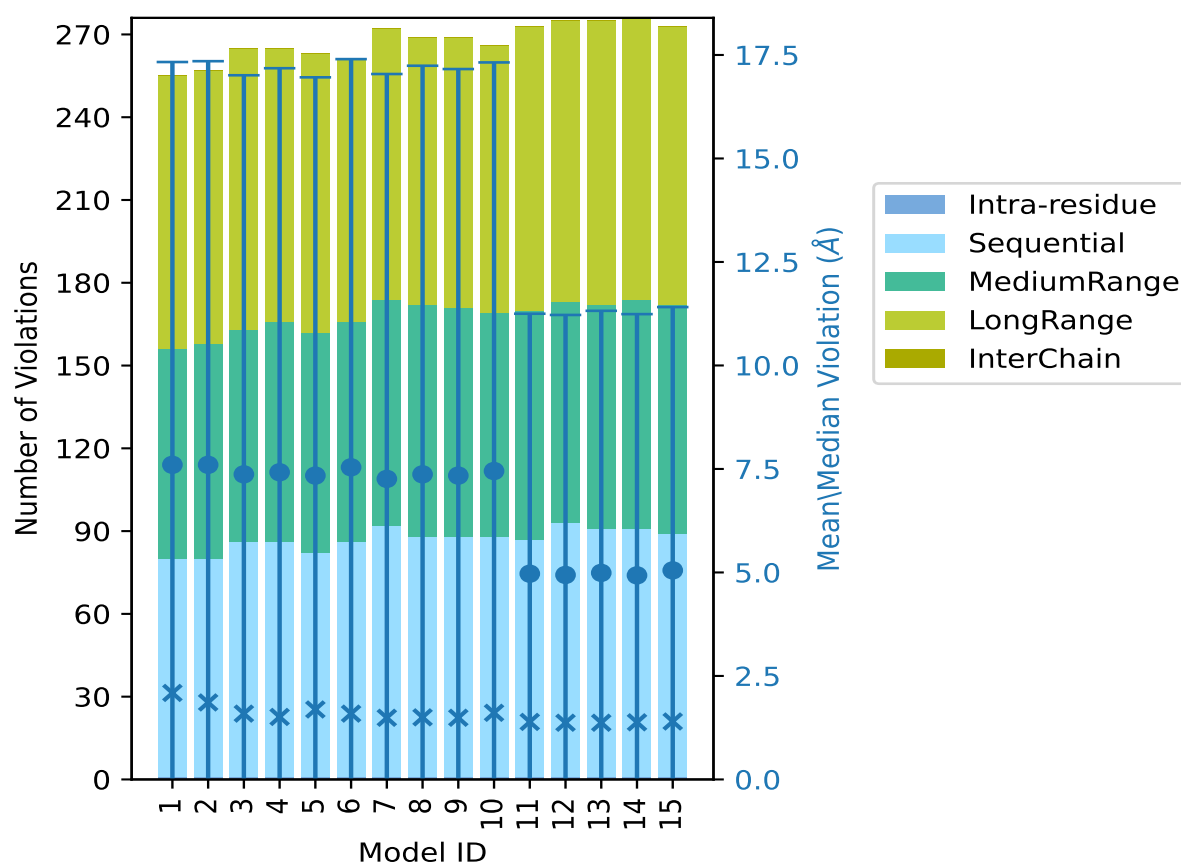
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	86	83	103	0	273	4.97	22.26	6.28	1.39
12	1	92	80	102	0	275	4.94	22.42	6.28	1.37
13	1	90	81	103	0	275	4.99	22.54	6.33	1.37
14	1	90	83	102	0	276	4.93	22.3	6.31	1.38
15	1	88	83	101	0	273	5.05	22.52	6.36	1.4

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 ⓘ

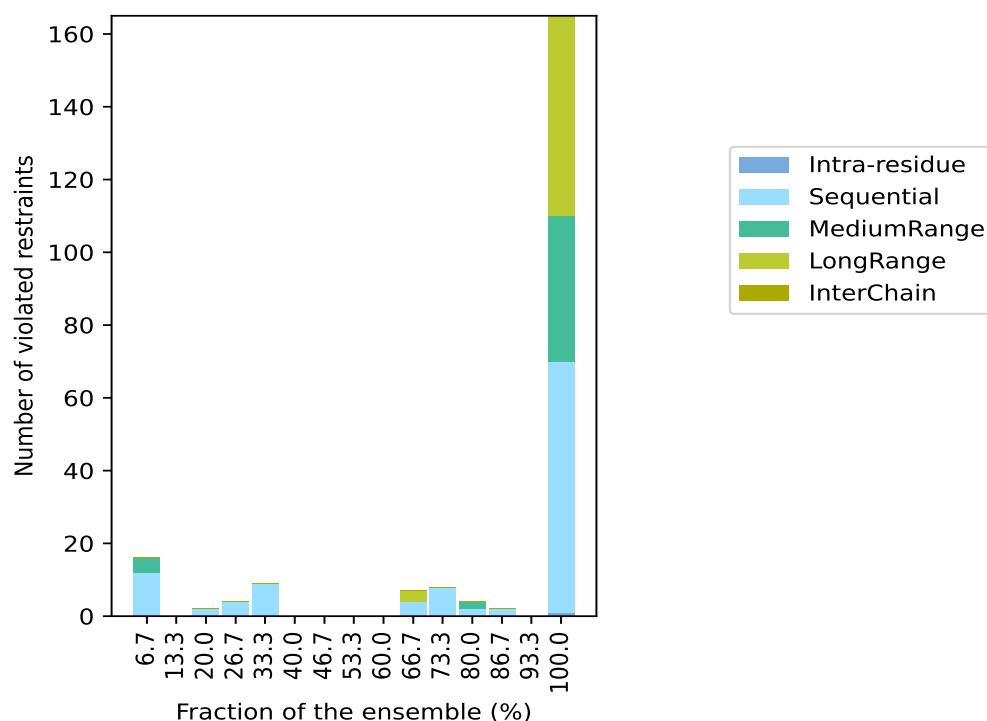
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 380(IR:43, SQ:299, MR:38, LR:0, IC:0) restraints are not 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	12	4	0	0	16	1	6.7
0	0	0	0	0	0	2	13.3
0	2	0	0	0	2	3	20.0
0	4	0	0	0	4	4	26.7
0	9	0	0	0	9	5	33.3
0	0	0	0	0	0	6	40.0
0	0	0	0	0	0	7	46.7
0	0	0	0	0	0	8	53.3
0	0	0	0	0	0	9	60.0
0	4	0	3	0	7	10	66.7
0	8	0	0	0	8	11	73.3
0	2	2	0	0	4	12	80.0
0	2	0	0	0	2	13	86.7
0	0	0	0	0	0	14	93.3
1	69	40	55	0	165	15	100.0

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

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

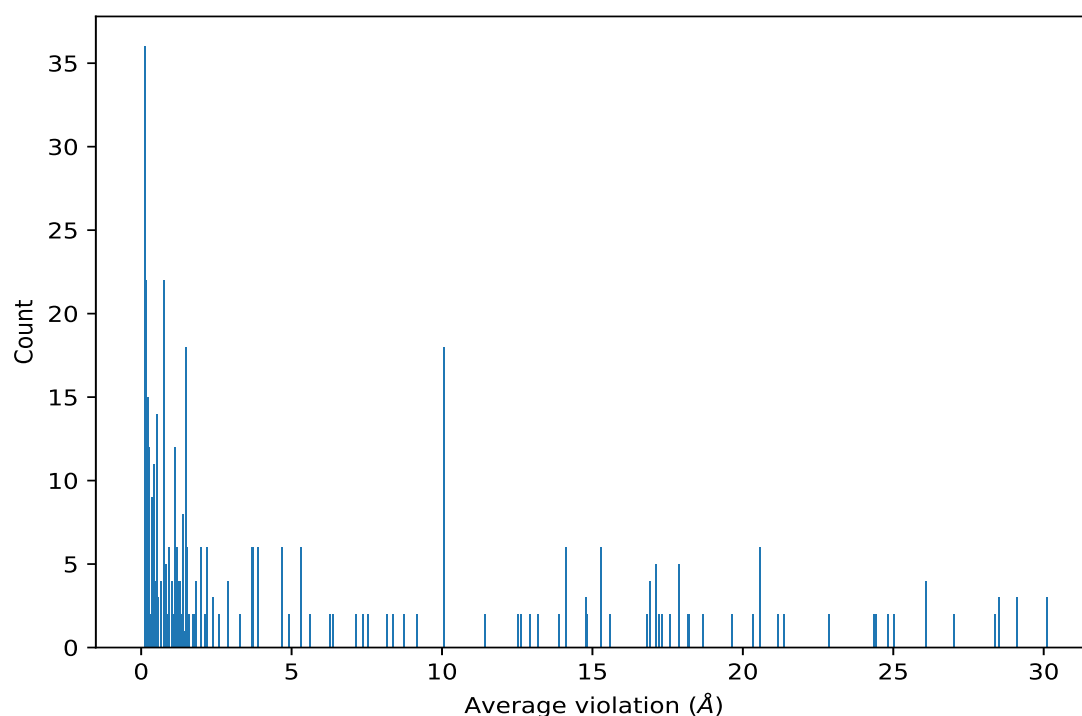
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

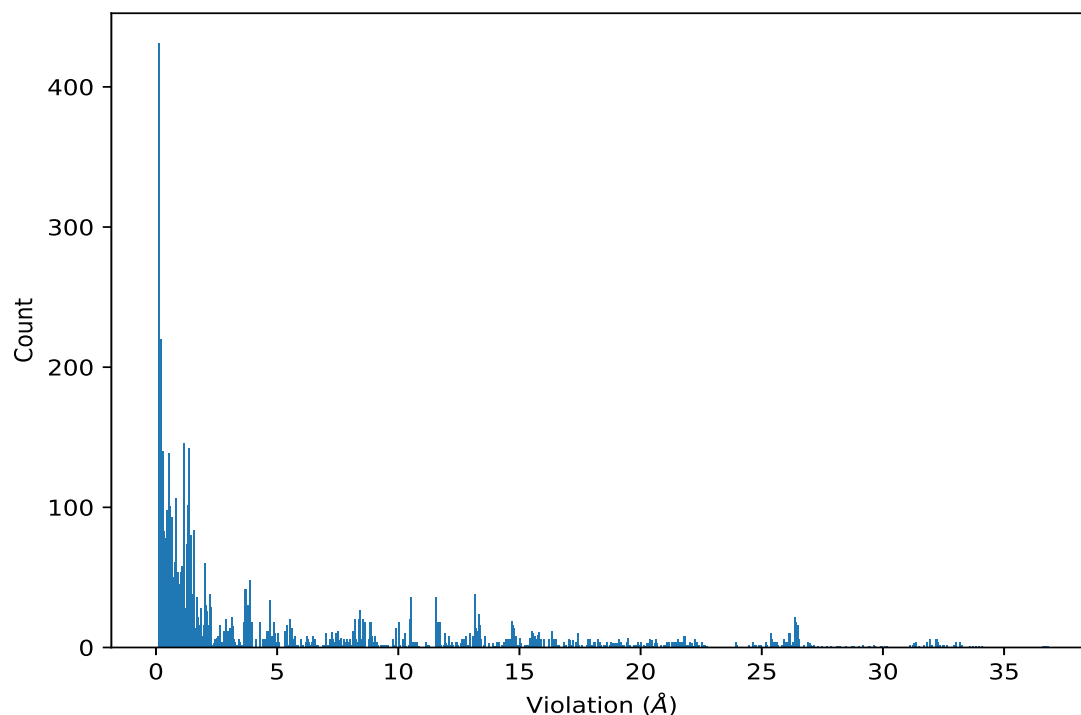
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,9)	1:62:A:GLU:H	1:141:A:PRO:O	15	28.38	6.35	32.53
(5,9)	1:62:A:GLU:H	1:141:A:PRO:O	15	28.38	6.35	32.53
(4,10)	1:62:A:GLU:N	1:141:A:PRO:O	15	27.0	6.54	31.29
(5,10)	1:62:A:GLU:N	1:141:A:PRO:O	15	27.0	6.54	31.29
(6,14)	1:1:A:MET:HE2	1:180:A:HIS:H	15	26.05	13.12	33.83
(6,14)	1:1:A:MET:HE1	1:180:A:HIS:H	15	26.05	13.12	33.83
(6,14)	1:1:A:MET:HG2	1:180:A:HIS:H	15	26.05	13.12	33.83
(6,14)	1:1:A:MET:HB2	1:180:A:HIS:H	15	26.05	13.12	33.83
(2,64)	1:33:A:ALA:H	1:183:A:HIS:H	15	25.02	10.15	32.18
(6,71)	1:33:A:ALA:H	1:183:A:HIS:H	15	25.02	10.15	32.18
(2,84)	1:41:A:LYS:HE2	1:51:A:GLY:HA3	15	24.84	1.82	26.04
(6,93)	1:41:A:LYS:HE2	1:51:A:GLY:HA3	15	24.84	1.82	26.04
(2,83)	1:41:A:LYS:HE2	1:51:A:GLY:H	15	24.41	1.69	25.46

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)
(6,14)	1:1:A:MET:HG2	1:180:A:HIS:H	9	36.85
(6,14)	1:1:A:MET:HG2	1:180:A:HIS:H	10	36.78
(6,14)	1:1:A:MET:HG2	1:180:A:HIS:H	6	36.73
(6,14)	1:1:A:MET:HG2	1:180:A:HIS:H	7	36.67
(6,14)	1:1:A:MET:HG2	1:180:A:HIS:H	8	36.62
(6,14)	1:1:A:MET:HE2	1:180:A:HIS:H	2	34.08
(6,14)	1:1:A:MET:HE2	1:180:A:HIS:H	3	33.98
(6,14)	1:1:A:MET:HE1	1:180:A:HIS:H	4	33.83
(6,14)	1:1:A:MET:HE2	1:180:A:HIS:H	1	33.73
(6,14)	1:1:A:MET:HE1	1:180:A:HIS:H	5	33.58

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

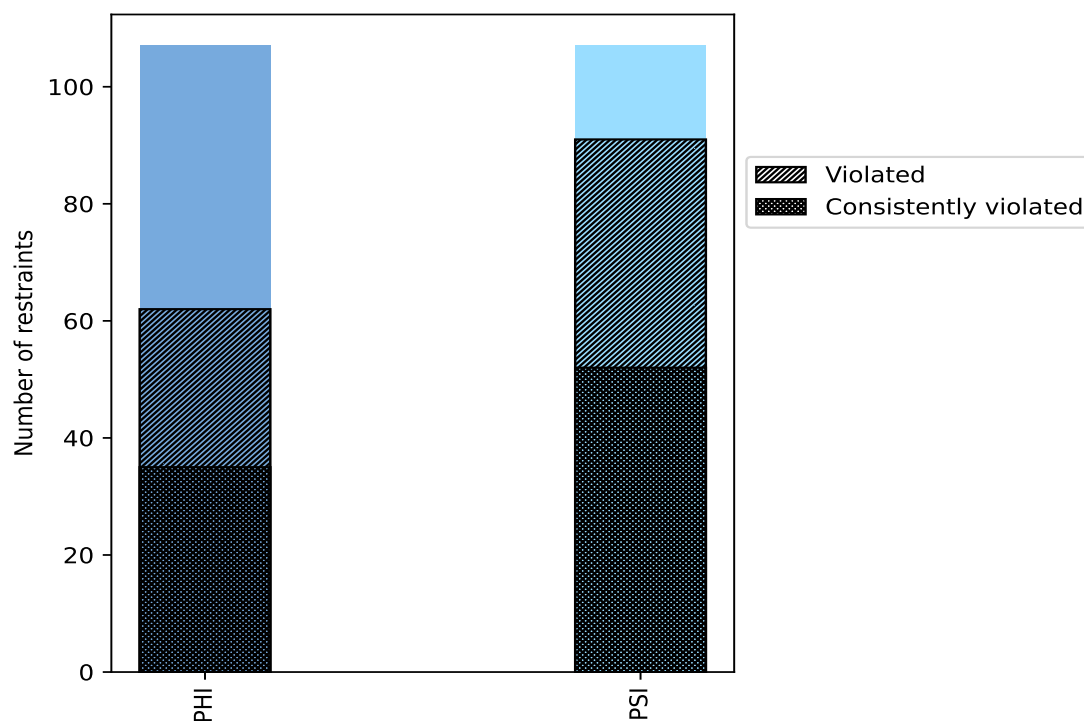
10.1 Summary of dihedral-angle violations [i](#)

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	107	50.0	62	57.9	29.0	35	32.7	16.4
PSI	107	50.0	91	85.0	42.5	52	48.6	24.3
Total	214	100.0	153	71.5	71.5	87	40.7	40.7

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 [i](#)



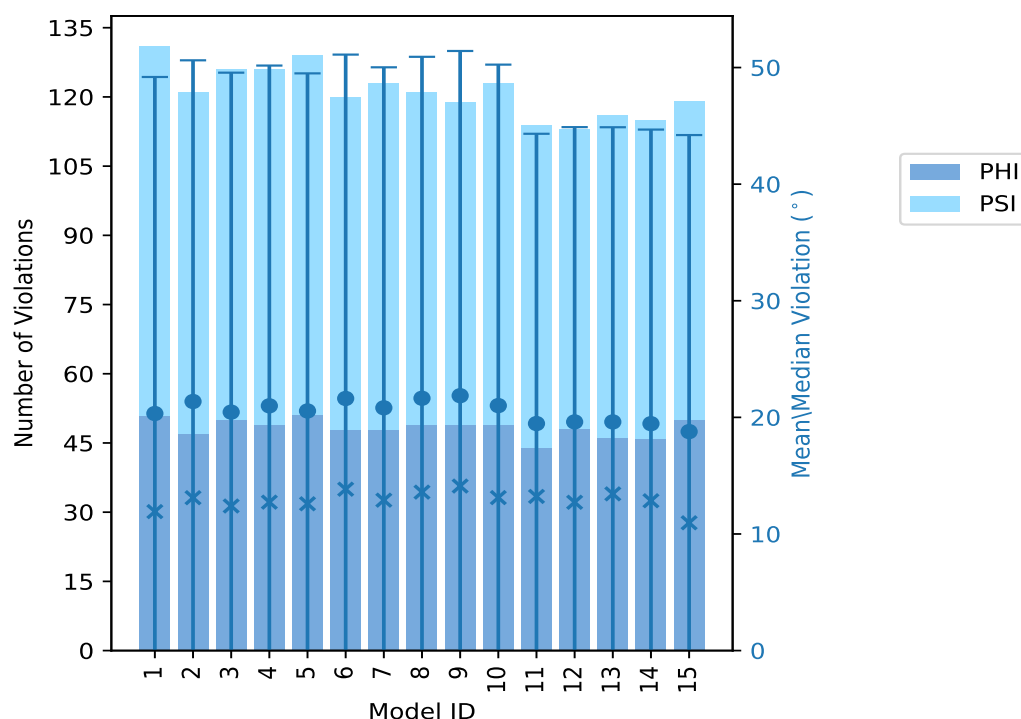
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	51	80	131	20.33	163.84	28.86	11.92
2	47	74	121	21.36	162.27	29.26	13.11
3	50	76	126	20.45	164.41	29.11	12.4
4	49	77	126	20.99	165.19	29.18	12.73
5	51	78	129	20.55	164.01	28.95	12.59
6	48	72	120	21.62	162.62	29.49	13.84
7	48	75	123	20.82	163.09	29.2	12.9
8	49	72	121	21.64	163.25	29.28	13.59
9	49	70	119	21.86	162.81	29.56	14.11
10	49	74	123	21.01	163.19	29.24	13.12
11	44	70	114	19.47	158.57	24.85	13.22
12	48	65	113	19.61	157.53	25.28	12.72
13	46	70	116	19.61	159.07	25.27	13.44
14	46	69	115	19.46	157.28	25.22	12.85
15	50	69	119	18.78	160.32	25.43	10.96

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

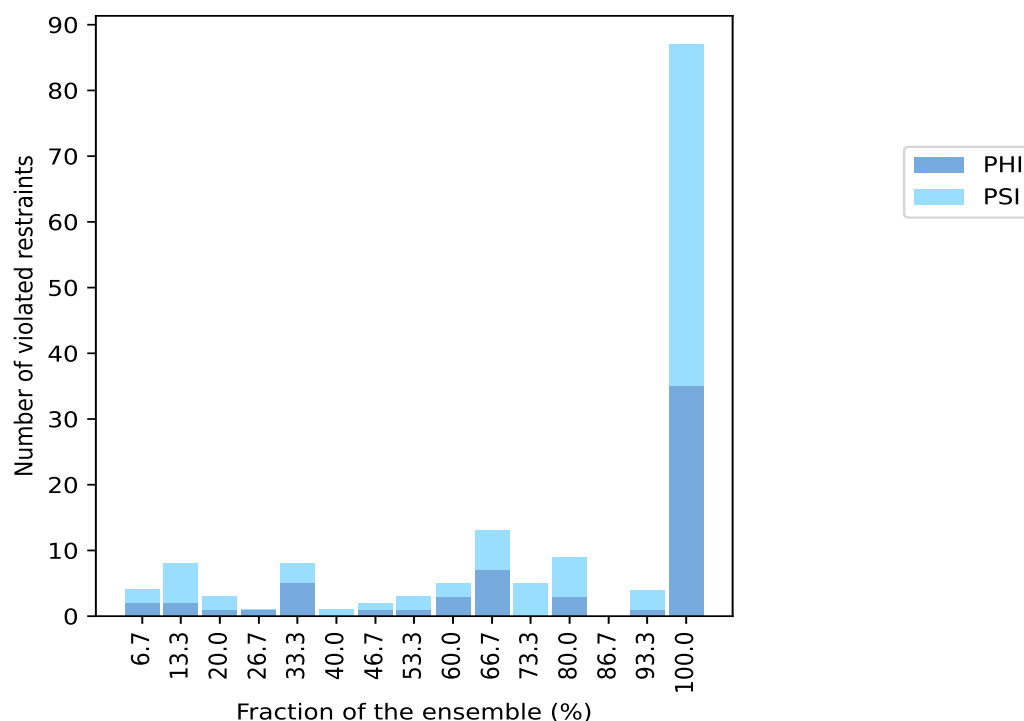
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
2	2	4	1	6.7
2	6	8	2	13.3
1	2	3	3	20.0
1	0	1	4	26.7
5	3	8	5	33.3
0	1	1	6	40.0
1	1	2	7	46.7
1	2	3	8	53.3
3	2	5	9	60.0
7	6	13	10	66.7
0	5	5	11	73.3
3	6	9	12	80.0
0	0	0	13	86.7
1	3	4	14	93.3
35	52	87	15	100.0

¹ Number of models with violations

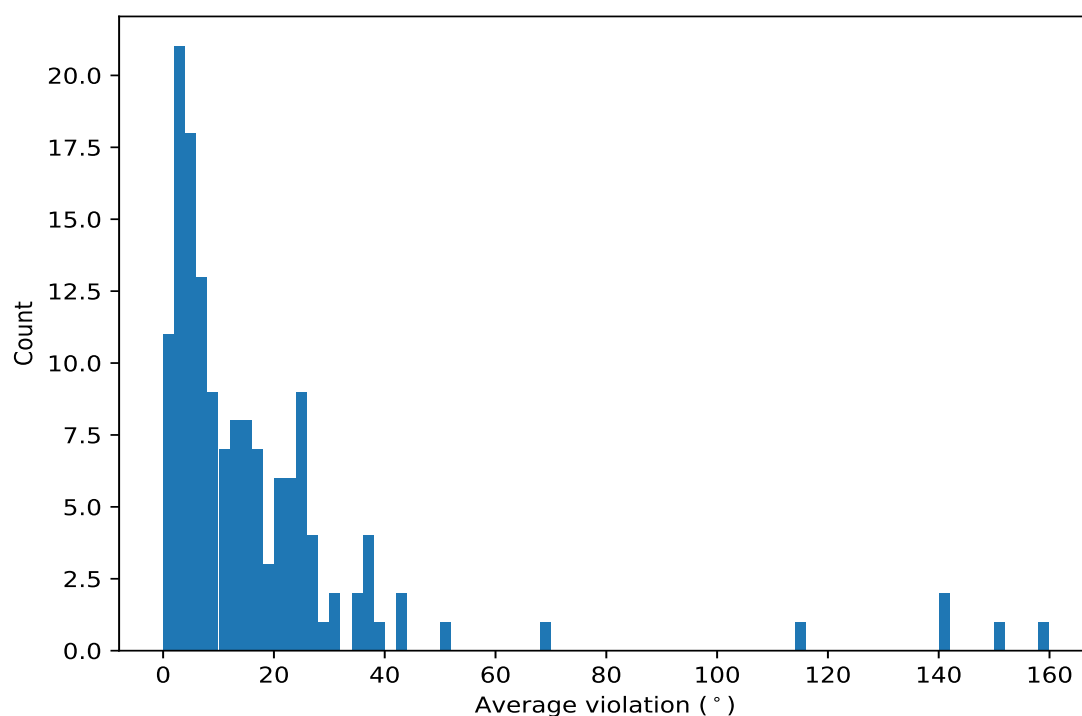
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

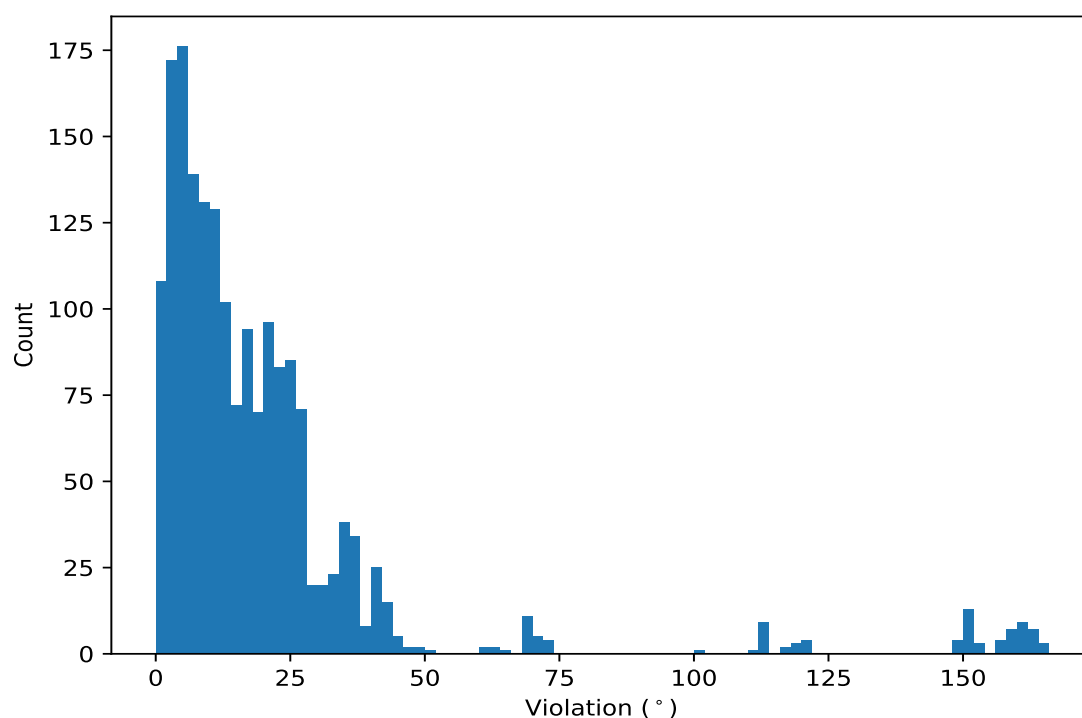
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,4)	1:3:A:THR:N	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:THR:N	15	159.86	1.23	160.32
(2,2)	1:3:A:THR:N	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:THR:N	15	151.11	1.23	151.57
(2,15)	1:26:A:GLY:C	1:27:A:GLY:N	1:27:A:GLY:CA	1:27:A:GLY:C	15	141.23	19.49	150.61
(2,107)	1:179:A:GLU:C	1:180:A:HIS:N	1:180:A:HIS:CA	1:180:A:HIS:C	15	115.38	3.62	113.19
(2,108)	1:180:A:HIS:N	1:180:A:HIS:CA	1:180:A:HIS:C	1:181:A:HIS:N	15	69.7	1.74	68.56
(2,16)	1:27:A:GLY:N	1:27:A:GLY:CA	1:27:A:GLY:C	1:28:A:GLY:N	15	51.15	22.53	62.97
(2,29)	1:40:A:ARG:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	15	43.1	4.79	42.81
(1,2)	1:2:A:ASP:N	1:2:A:ASP:CA	1:2:A:ASP:C	1:3:A:THR:N	15	42.03	2.52	42.87
(2,65)	1:124:A:SER:C	1:125:A:TRP:N	1:125:A:TRP:CA	1:125:A:TRP:C	15	39.12	2.98	40.92
(1,65)	1:138:A:GLU:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	15	36.52	3.16	35.31

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 (°)
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	4	165.19
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	3	164.41
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	5	164.01
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	1	163.84
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	8	163.25
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	10	163.19
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	7	163.09
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	9	162.81
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	6	162.62
(2,112)	1:184:A:HIS:N	1:184:A:HIS:CA	1:184:A:HIS:C	1:185:A:HIS:N	2	162.27