W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB NMR Structure Validation Summary Report ⓘ

Jun 3, 2023 – 11:34 AM EDT

PDB ID	:	6OFA
BMRB ID	:	30597
Title	:	Wasabi Receptor Toxin
Authors	:	Lin King, J.V.; Kelly, M.J.S.; Julius, D.
Deposited on	:	2019-03-28

The following versions of software and data (see references ⓘ) were used in the production of this report:
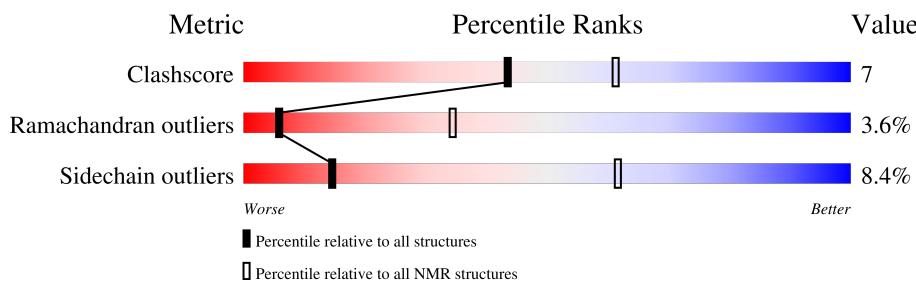
|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
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
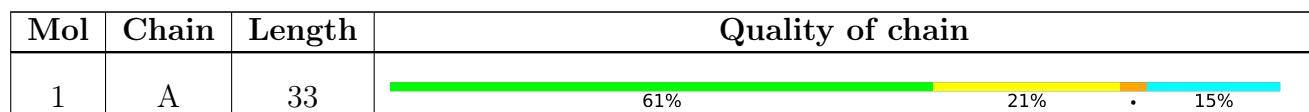
The overall completeness of chemical shifts assignment is 78%.

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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		3.6%
Sidechain outliers		8.4%

Worse .... *Better*

▮ Percentile relative to all structures

◻ Percentile relative to all NMR structures

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	33	61% 21% • 15%

2 Ensemble composition and analysis ⓘ

This entry contains 50 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average.*

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:31 (28)	0.42	8

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 6 clusters and 10 single-model clusters were found.

Cluster number	Models
1	1, 4, 6, 8, 9, 11, 14, 17, 25, 27, 29, 32, 34, 35, 36, 38, 42, 43, 46
2	19, 20, 21, 22, 26, 33, 41, 44, 45
3	5, 7, 23, 24, 28
4	16, 39, 49
5	2, 48
6	12, 50
Single-model clusters	3; 10; 13; 15; 18; 30; 31; 37; 40; 47

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 507 atoms, of which 242 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Wasabi Receptor Toxin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	33	507	164	242	45	51	5	0

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: Wasabi Receptor Toxin

Chain A:

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

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Wasabi Receptor Toxin

Chain A:

5 Refinement protocol and experimental data overview ⓘ

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

Of the 200 calculated structures, 50 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	refinement	
ARIA	structure calculation	

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	331
Number of shifts mapped to atoms	331
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6　Model quality ⓘ

6.1　Standard geometry ⓘ

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 ⓘ

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	231	208	208	3±1
All	All	11550	10400	10400	154

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 7.

5 of 29 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:10:TYR:HA	1:A:23:CYS:SG	0.62	2.34	23	23
1:A:28:SER:OG	1:A:29:PRO:HD3	0.60	1.96	38	32
1:A:14:ASN:HD22	1:A:15:VAL:N	0.58	1.96	49	9
1:A:22:GLN:O	1:A:25:GLN:HG2	0.53	2.04	38	3
1:A:8:TYR:O	1:A:11:GLU:HG2	0.52	2.03	41	3

6.3　Torsion angles ⓘ

6.3.1　Protein backbone ⓘ

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	28/33 (85%)	25±1 (90±3%)	2±1 (6±3%)	1±0 (4±0%)	6	34
All	All	1400/1650 (85%)	1263 (90%)	87 (6%)	50 (4%)	6	34

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	17	LYS	50

6.3.2 Protein sidechains ⓘ

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	27/31 (87%)	25±1 (92±4%)	2±1 (8±4%)	14	61
All	All	1350/1550 (87%)	1236 (92%)	114 (8%)	14	61

5 of 11 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	12	GLN	36
1	A	18	VAL	26
1	A	14	ASN	14
1	A	17	LYS	12
1	A	4	GLN	9

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

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 78% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	331
Number of shifts mapped to atoms	331
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	27	-3.31 ± 0.18	Should be checked
$^{13}C_{\beta}$	33	-2.59 ± 0.21	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 290 atoms were assigned a chemical shift out of a possible 373. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	76/136 (56%)	54/54 (100%)	22/56 (39%)	0/26 (0%)
Sidechain	180/200 (90%)	126/127 (99%)	54/64 (84%)	0/9 (0%)

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|	Total	^{1}H	^{13}C	^{15}N
Aromatic	34/37 (92%)	17/17 (100%)	17/20 (85%)	0/0 (—%)
Overall	290/373 (78%)	197/198 (99%)	93/140 (66%)	0/35 (0%)
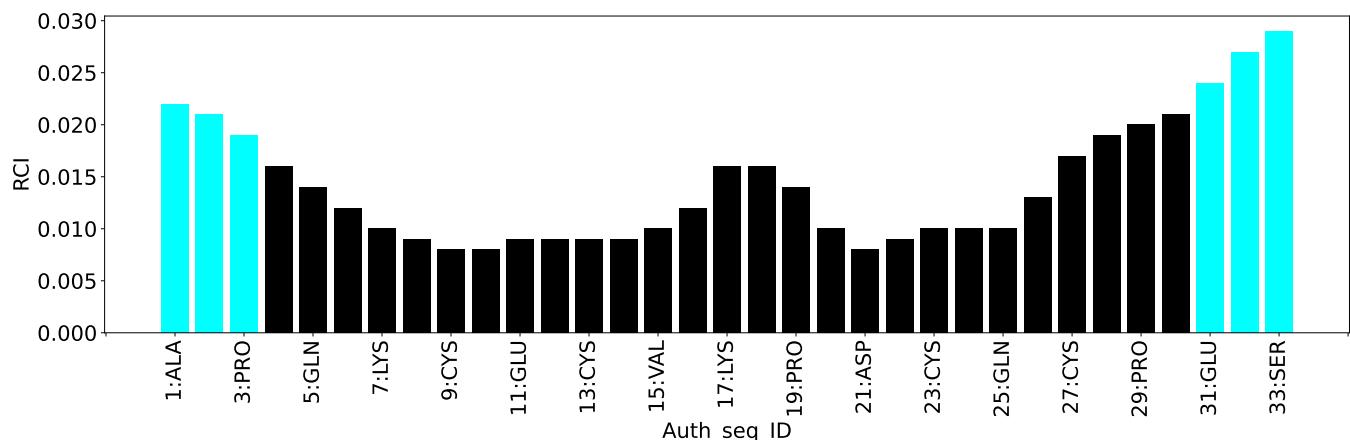
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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	1996
Intra-residue ($|i\text{-}j|$=0)	1222
Sequential ($|i\text{-}j|$=1)	416
Medium range ($|i\text{-}j|$>1 and $|i\text{-}j|$<5)	250
Long range ($|i\text{-}j|$≥5)	106
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	2
Total dihedral-angle restraints	58
Number of unmapped restraints	0
Number of restraints per residue	62.2
Number of long range restraints per residue[1]	3.3

[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)	154.7	0.2
0.2-0.5 (Medium)	242.3	0.5
>0.5 (Large)	59.6	3.15

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8.2.2 Average number of dihedral-angle violations per model ⓘ

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)	4.3	9.6
10.0-20.0 (Medium)	0.0	10.6
>20.0 (Large)	None	None

9   Distance violation analysis ⓘ
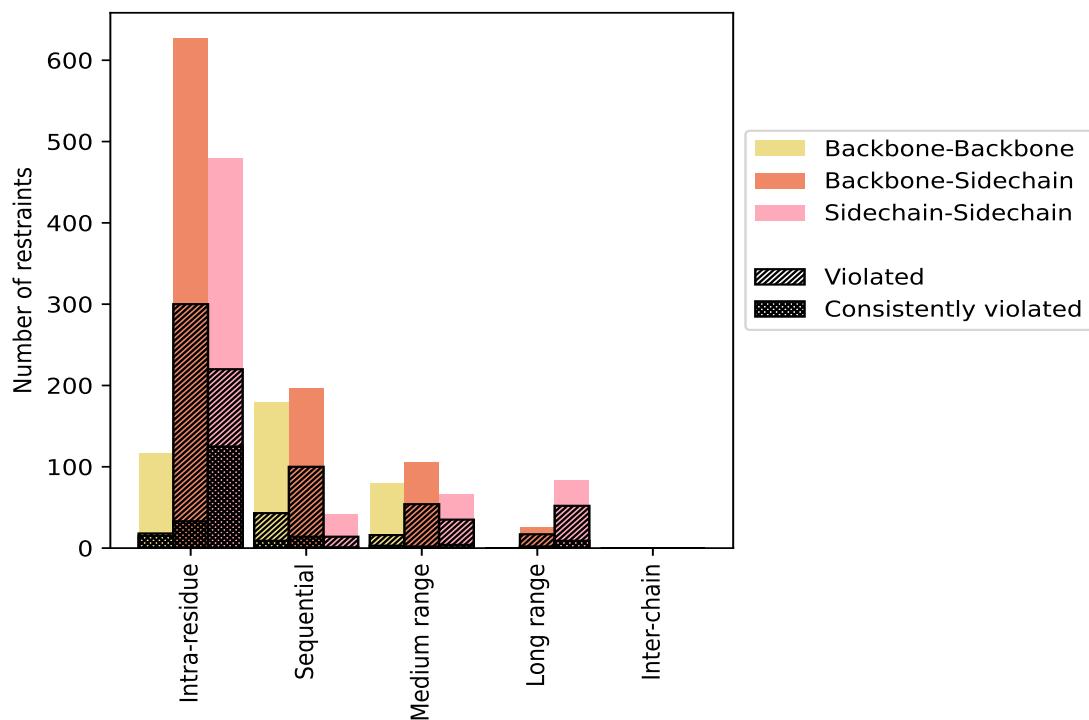
9.1   Summary of distance violations ⓘ

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)	1222	61.2	538	44.0	27.0	173	14.2	8.7
Backbone-Backbone	116	5.8	18	15.5	0.9	15	12.9	0.8
Backbone-Sidechain	627	31.4	300	47.8	15.0	33	5.3	1.7
Sidechain-Sidechain	479	24.0	220	45.9	11.0	125	26.1	6.3
Sequential (|i-j|=1)	416	20.8	157	37.7	7.9	24	5.8	1.2
Backbone-Backbone	179	9.0	43	24.0	2.2	9	5.0	0.5
Backbone-Sidechain	196	9.8	100	51.0	5.0	14	7.1	0.7
Sidechain-Sidechain	41	2.1	14	34.1	0.7	1	2.4	0.1
Medium range (|i-j|>1 & |i-j|<5)	250	12.5	105	42.0	5.3	9	3.6	0.5
Backbone-Backbone	79	4.0	16	20.3	0.8	3	3.8	0.2
Backbone-Sidechain	105	5.3	54	51.4	2.7	2	1.9	0.1
Sidechain-Sidechain	66	3.3	35	53.0	1.8	4	6.1	0.2
Long range (|i-j|≥5)	106	5.3	69	65.1	3.5	11	10.4	0.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	25	1.3	17	68.0	0.9	2	8.0	0.1
Sidechain-Sidechain	81	4.1	52	64.2	2.6	9	11.1	0.5
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	2	0.1	0	0.0	0.0	0	0.0	0.0
Total	1996	100.0	869	43.5	43.5	217	10.9	10.9
Backbone-Backbone	374	18.7	77	20.6	3.9	27	7.2	1.4
Backbone-Sidechain	953	47.7	471	49.4	23.6	51	5.4	2.6
Sidechain-Sidechain	669	33.5	321	48.0	16.1	139	20.8	7.0

[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	310	85	33	22	0	450	0.31	1.75	0.2	0.25
2	336	82	24	19	0	461	0.32	1.86	0.22	0.26
3	329	84	31	24	0	468	0.33	2.37	0.25	0.26
4	330	90	27	32	0	479	0.36	2.46	0.3	0.27
5	338	82	30	38	0	488	0.37	2.45	0.29	0.28
6	323	98	26	29	0	476	0.31	1.86	0.21	0.25
7	311	79	37	23	0	450	0.35	2.25	0.25	0.28
8	320	95	27	26	0	468	0.32	1.82	0.22	0.25
9	315	78	34	25	0	452	0.32	1.81	0.22	0.25
10	318	83	27	25	0	453	0.31	1.84	0.21	0.25
11	312	80	34	22	0	448	0.31	1.66	0.2	0.25

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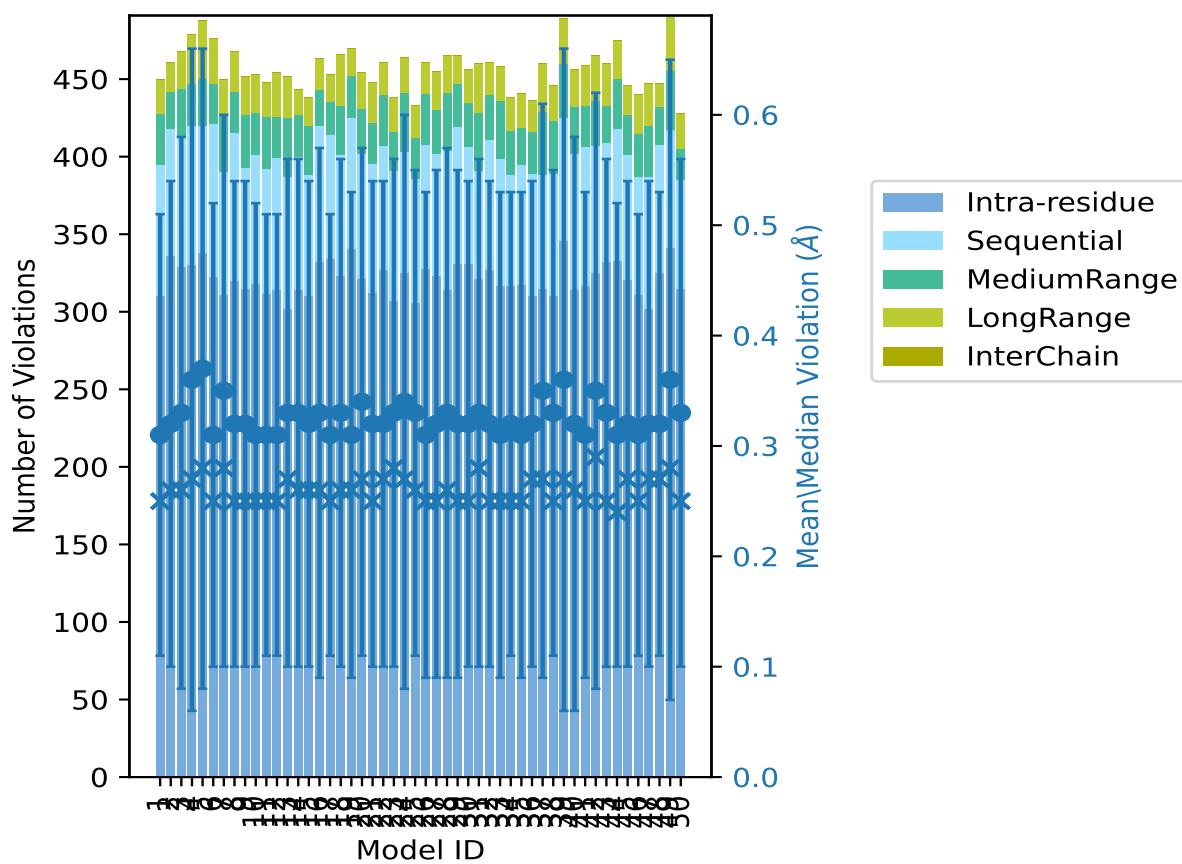
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	314	85	27	28	0	454	0.31	1.89	0.2	0.25
13	302	85	38	27	0	452	0.33	2.17	0.23	0.27
14	314	86	27	16	0	443	0.33	1.84	0.23	0.26
15	310	78	32	18	0	438	0.32	1.99	0.22	0.26
16	332	88	23	20	0	463	0.33	1.88	0.24	0.26
17	334	80	21	18	0	453	0.31	1.76	0.2	0.25
18	323	78	32	33	0	466	0.33	2.12	0.23	0.26
19	341	84	27	18	0	470	0.31	1.79	0.22	0.26
20	321	81	29	23	0	454	0.34	1.86	0.23	0.27
21	312	83	27	26	0	448	0.32	1.79	0.22	0.25
22	327	80	33	21	0	461	0.32	1.62	0.22	0.27
23	307	84	25	22	0	438	0.33	2.34	0.23	0.28
24	325	78	38	23	0	464	0.34	2.51	0.26	0.27
25	306	80	26	21	0	433	0.33	1.83	0.22	0.26
26	328	80	33	20	0	461	0.31	1.8	0.22	0.25
27	323	79	28	25	0	455	0.32	1.94	0.23	0.25
28	314	90	37	24	0	465	0.33	2.36	0.24	0.26
29	331	88	28	18	0	465	0.32	1.98	0.23	0.25
30	331	75	29	21	0	456	0.32	1.85	0.22	0.25
31	321	70	37	32	0	460	0.33	2.12	0.23	0.28
32	327	84	29	21	0	461	0.32	2.03	0.22	0.25
33	317	82	37	22	0	458	0.31	1.79	0.22	0.25
34	317	71	29	21	0	438	0.32	1.8	0.21	0.25
35	317	78	24	22	0	441	0.31	1.94	0.22	0.25
36	310	79	27	20	0	436	0.32	1.84	0.22	0.27
37	315	73	41	31	0	460	0.35	2.28	0.26	0.27
38	310	79	34	23	0	446	0.33	1.79	0.22	0.25
39	346	79	35	29	0	489	0.36	2.54	0.3	0.27
40	314	88	30	24	0	456	0.32	3.15	0.26	0.26
41	317	89	27	26	0	459	0.31	1.88	0.22	0.25
42	325	82	29	29	0	465	0.35	2.28	0.27	0.29
43	332	77	24	27	0	460	0.33	2.0	0.23	0.25
44	333	85	32	25	0	475	0.31	1.67	0.21	0.24
45	321	80	26	19	0	446	0.32	1.89	0.22	0.27
46	311	76	28	25	0	440	0.31	1.6	0.2	0.25
47	302	85	33	27	0	447	0.32	1.92	0.22	0.27
48	325	83	24	15	0	447	0.32	1.9	0.21	0.27
49	341	76	38	36	0	491	0.36	2.36	0.29	0.28
50	315	70	20	23	0	428	0.33	1.9	0.23	0.25

[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 ⓘ

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, 1125(IR:684, SQ:259, MR:145, LR:37, 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]	%
34	12	24	7	0	77	1	2.0
24	4	15	3	0	46	2	4.0
6	4	4	5	0	19	3	6.0
15	10	15	6	0	46	4	8.0
27	3	1	7	0	38	5	10.0
13	6	5	2	0	26	6	12.0

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Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	4	3	0	0	7	7	14.0
9	0	0	0	0	9	8	16.0
3	3	1	4	0	11	9	18.0
10	3	1	0	0	14	10	20.0
10	4	3	3	0	20	11	22.0
5	3	0	0	0	8	12	24.0
9	3	0	6	0	18	13	26.0
3	0	3	3	0	9	14	28.0
7	3	0	0	0	10	15	30.0
4	0	0	0	0	4	16	32.0
15	4	0	1	0	20	17	34.0
4	2	2	0	0	8	18	36.0
6	0	0	0	0	6	19	38.0
6	0	1	4	0	11	20	40.0
2	0	0	0	0	2	21	42.0
3	0	0	0	0	3	22	44.0
4	3	3	0	0	10	23	46.0
6	0	0	0	0	6	24	48.0
0	0	0	0	0	0	25	50.0
4	7	0	0	0	11	26	52.0
7	3	0	0	0	10	27	54.0
10	0	3	0	0	13	28	56.0
4	0	0	0	0	4	29	58.0
7	6	0	0	0	13	30	60.0
3	0	0	0	0	3	31	62.0
12	6	0	0	0	18	32	64.0
10	3	0	0	0	13	33	66.0
0	3	0	4	0	7	34	68.0
0	0	1	0	0	1	35	70.0
0	0	0	0	0	0	36	72.0
1	0	0	0	0	1	37	74.0
0	3	0	0	0	3	38	76.0
13	0	0	1	0	14	39	78.0
4	2	0	0	0	6	40	80.0
0	3	0	0	0	3	41	82.0
7	3	0	0	0	10	42	84.0
5	3	1	0	0	9	43	86.0
6	6	0	0	0	12	44	88.0
3	4	1	1	0	9	45	90.0
8	0	0	0	0	8	46	92.0
7	1	2	0	0	10	47	94.0

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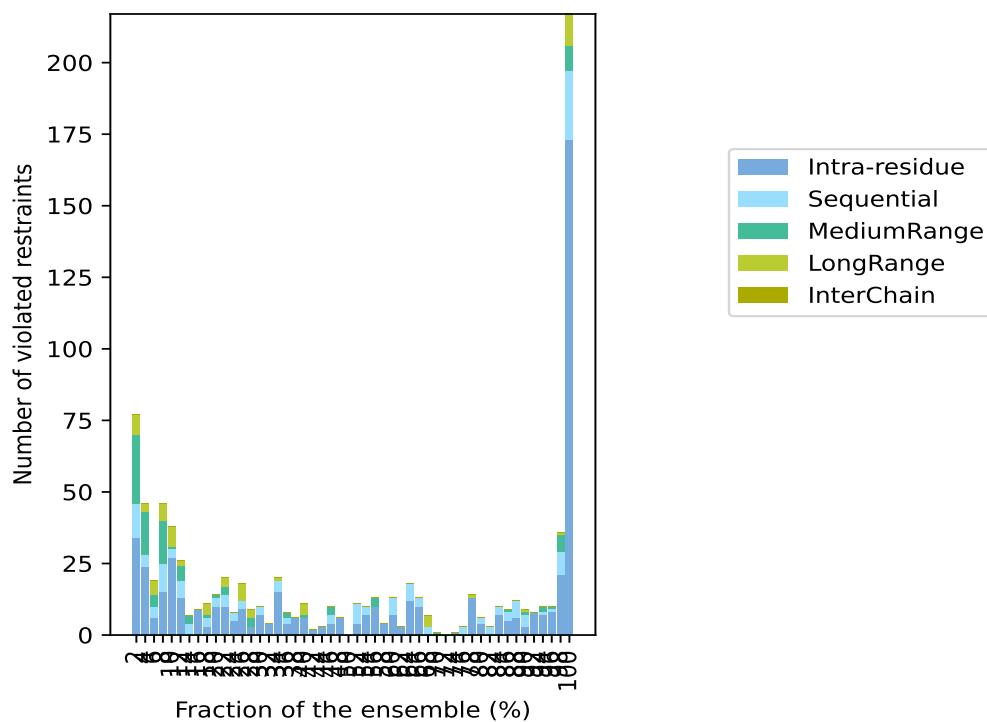
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Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
8	1	1	0	0	10	48	96.0
21	8	6	1	0	36	49	98.0
173	24	9	11	0	217	50	100.0

[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
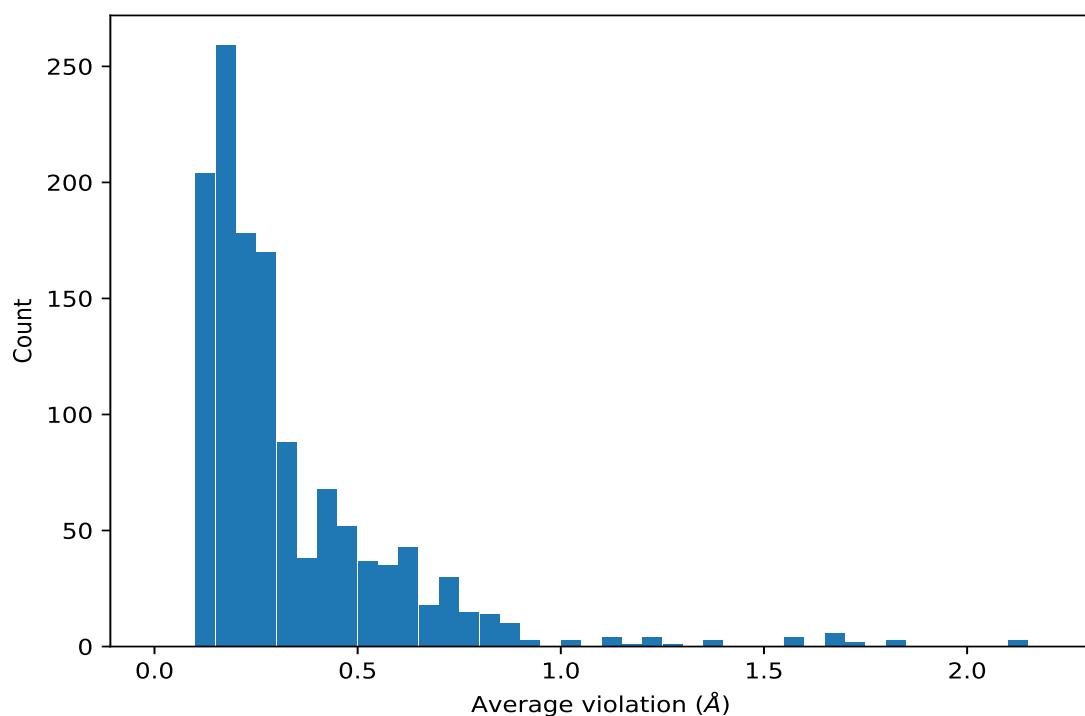
9.3.1   Bar graph : Distance violation statistics for the ensemble ⓘ

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 ⓘ

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)
(1,992)	1:A:5:GLN:HB3	1:A:8:TYR:HA	50	1.73	0.15	1.76
(1,992)	1:A:5:GLN:HB2	1:A:8:TYR:HA	50	1.73	0.15	1.76
(2,817)	1:A:13:CYS:HA	1:A:18:VAL:HB	50	1.57	0.3	1.64
(1,182)	1:A:19:PRO:HD3	1:A:18:VAL:HG22	50	1.02	0.19	1.08
(1,182)	1:A:19:PRO:HD3	1:A:18:VAL:HG21	50	1.02	0.19	1.08
(1,182)	1:A:19:PRO:HD3	1:A:18:VAL:HG23	50	1.02	0.19	1.08
(1,12)	1:A:19:PRO:HD3	1:A:19:PRO:HB2	50	0.79	0.01	0.79
(2,675)	1:A:13:CYS:HB2	1:A:18:VAL:HB	50	0.75	0.83	0.34
(1,1002)	1:A:32:ARG:HB2	1:A:32:ARG:HG2	50	0.72	0.05	0.77
(1,1002)	1:A:29:PRO:HB2	1:A:29:PRO:HG2	50	0.72	0.05	0.77
(1,1002)	1:A:29:PRO:HB2	1:A:32:ARG:HB2	50	0.72	0.05	0.77
(1,1002)	1:A:32:ARG:HB2	1:A:32:ARG:HG3	50	0.72	0.05	0.77
(1,1002)	1:A:29:PRO:HG2	1:A:32:ARG:HG2	50	0.72	0.05	0.77
(1,1002)	1:A:29:PRO:HG2	1:A:32:ARG:HG3	50	0.72	0.05	0.77
(1,990)	1:A:7:LYS:HG2	1:A:7:LYS:HD2	50	0.72	0.02	0.72
(1,990)	1:A:7:LYS:HD2	1:A:17:LYS:HG2	50	0.72	0.02	0.72

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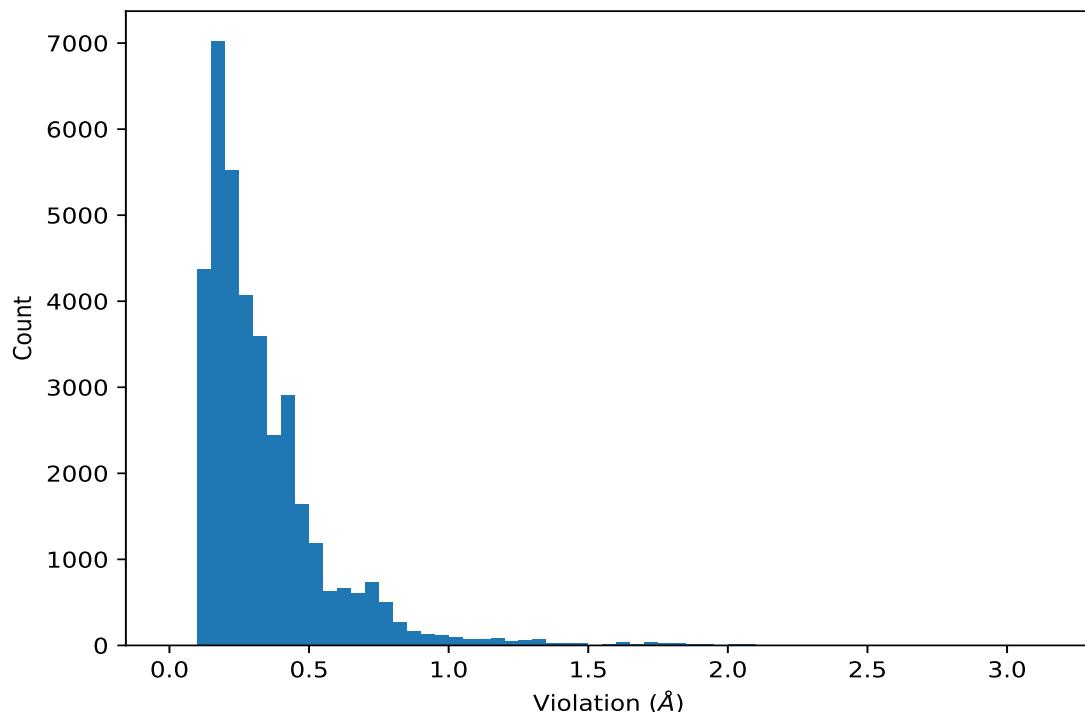
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,990)	1:A:7:LYS:HG2	1:A:17:LYS:HD2	50	0.72	0.02	0.72
(1,990)	1:A:7:LYS:HG2	1:A:7:LYS:HD3	50	0.72	0.02	0.72
(1,990)	1:A:17:LYS:HG3	1:A:17:LYS:HD2	50	0.72	0.02	0.72
(1,990)	1:A:17:LYS:HG2	1:A:17:LYS:HD2	50	0.72	0.02	0.72
(1,990)	1:A:7:LYS:HD3	1:A:17:LYS:HG3	50	0.72	0.02	0.72
(1,990)	1:A:7:LYS:HD2	1:A:17:LYS:HG3	50	0.72	0.02	0.72
(1,990)	1:A:7:LYS:HD3	1:A:17:LYS:HG2	50	0.72	0.02	0.72
(1,815)	1:A:19:PRO:HD2	1:A:22:GLN:HB2	50	0.62	0.14	0.66
(1,815)	1:A:19:PRO:HD2	1:A:22:GLN:HB3	50	0.62	0.14	0.66
(2,269)	1:A:19:PRO:HD2	1:A:22:GLN:HB2	50	0.62	0.14	0.66
(2,269)	1:A:19:PRO:HD2	1:A:22:GLN:HB3	50	0.62	0.14	0.66
(2,841)	1:A:19:PRO:HD2	1:A:22:GLN:HB2	50	0.62	0.14	0.66

[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)
(1,179)	1:A:18:VAL:HG22	1:A:14:ASN:HB3	40	3.15
(1,179)	1:A:18:VAL:HG21	1:A:14:ASN:HB3	40	3.15
(1,179)	1:A:18:VAL:HG23	1:A:14:ASN:HB3	40	3.15
(2,675)	1:A:13:CYS:HB2	1:A:18:VAL:HB	40	2.62
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD11	39	2.54
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD13	39	2.54
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD12	39	2.54
(2,675)	1:A:13:CYS:HB2	1:A:18:VAL:HB	24	2.51
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD11	4	2.46
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD13	4	2.46
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD12	4	2.46
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD11	5	2.45
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD13	5	2.45
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD12	5	2.45
(2,675)	1:A:13:CYS:HB2	1:A:18:VAL:HB	3	2.37
(2,675)	1:A:13:CYS:HB2	1:A:18:VAL:HB	28	2.36
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD11	49	2.36
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD13	49	2.36
(1,165)	1:A:9:CYS:HB3	1:A:30:LEU:HD12	49	2.36
(2,675)	1:A:13:CYS:HB2	1:A:18:VAL:HB	23	2.34

10 Dihedral-angle violation analysis ⓘ
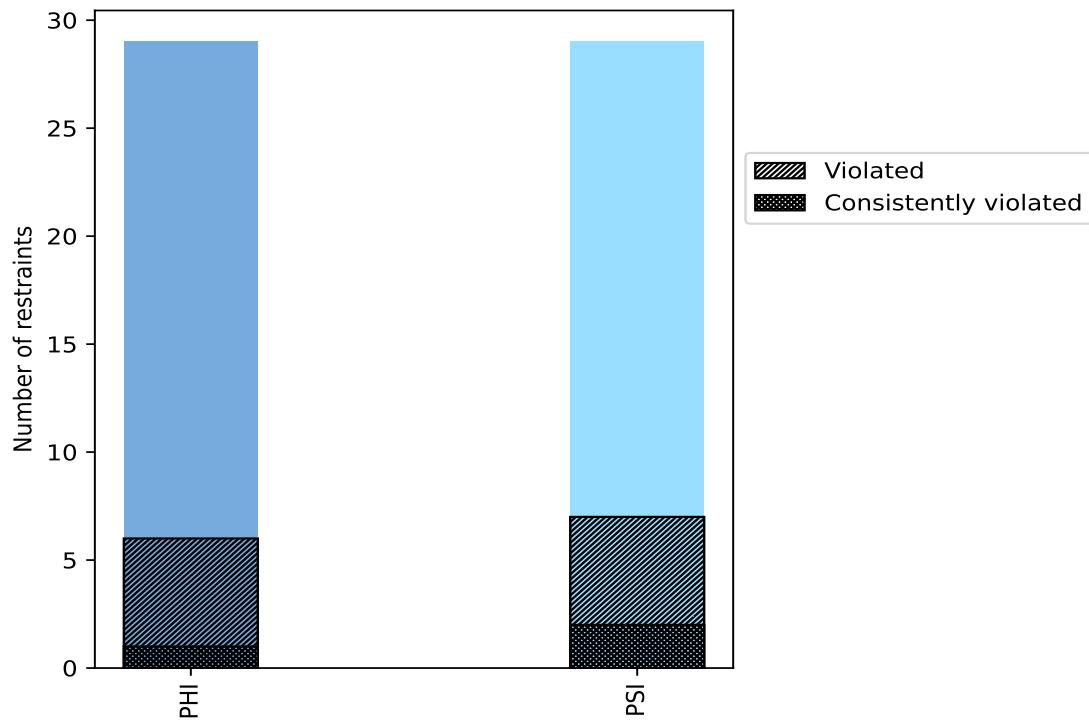
10.1 Summary of dihedral-angle violations ⓘ

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	29	50.0	6	20.7	10.3	1	3.4	1.7
PSI	29	50.0	7	24.1	12.1	2	6.9	3.4
Total	58	100.0	13	22.4	22.4	3	5.2	5.2

[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 ⓘ

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.
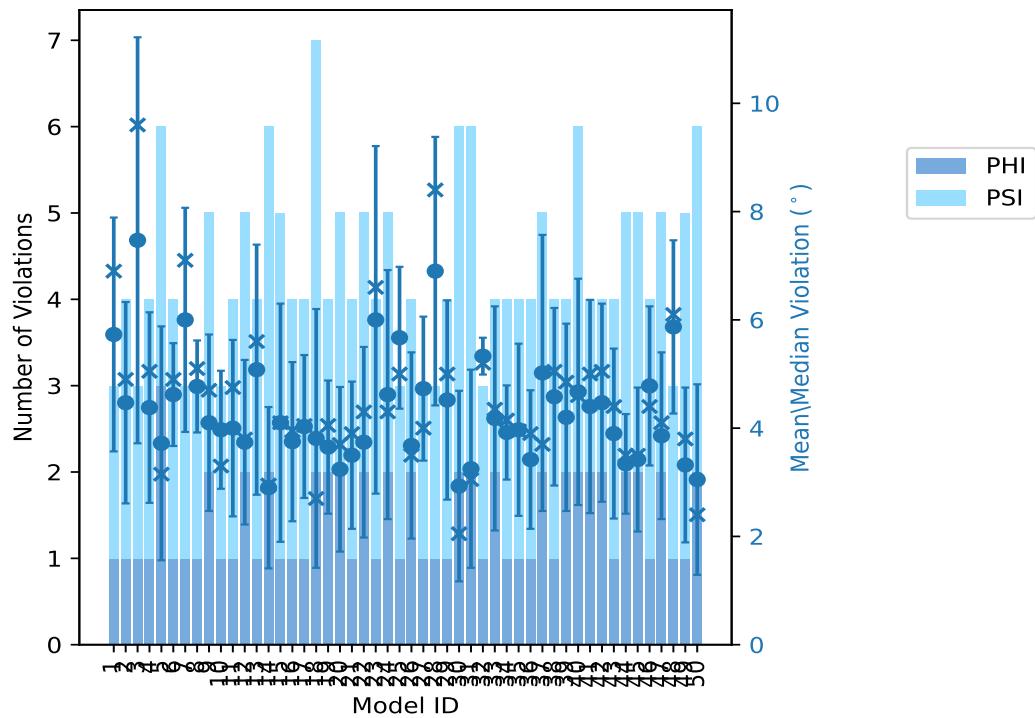
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	1	2	3	5.73	7.6	2.16	6.9
2	1	3	4	4.47	6.6	1.86	4.9
3	1	2	3	7.47	10.6	3.75	9.6
4	1	3	4	4.38	6.0	1.76	5.05
5	3	3	6	3.72	7.1	2.16	3.15
6	1	3	4	4.62	5.6	0.95	4.9
7	1	2	3	6.0	7.8	2.07	7.1
8	1	2	3	4.77	5.6	0.85	5.1
9	2	3	5	4.1	6.4	1.63	4.7
10	1	2	3	3.97	5.5	1.09	3.3
11	1	3	4	4.0	5.3	1.63	4.75
12	2	3	5	3.74	6.1	1.52	3.8
13	1	3	4	5.08	7.4	2.31	5.6
14	2	4	6	2.9	4.7	1.49	2.95
15	1	4	5	4.1	6.7	2.2	4.1
16	1	3	4	3.75	5.5	1.47	3.95
17	1	3	4	4.03	5.6	1.32	4.05
18	2	5	7	3.81	8.3	2.39	2.7
19	2	2	4	3.65	4.9	1.23	4.05
20	2	3	5	3.24	4.8	1.52	3.7
21	1	3	4	3.5	4.8	1.36	3.9
22	2	3	5	3.74	5.6	1.76	4.3
23	1	3	4	6.0	9.1	3.21	6.6
24	2	3	5	4.62	7.6	2.3	4.3
25	1	2	3	5.67	7.5	1.31	5.0
26	2	2	4	3.68	6.1	1.72	3.5
27	1	2	3	4.73	6.6	1.33	4.0
28	1	2	3	6.9	8.9	2.48	8.4
29	1	3	4	4.52	6.4	1.84	5.0
30	2	4	6	2.93	5.7	1.76	2.05
31	2	4	6	3.25	6.1	1.83	3.05
32	1	2	3	5.33	5.8	0.34	5.2
33	2	2	4	4.18	6.9	2.07	4.35
34	1	3	4	3.92	4.8	0.87	4.15
35	1	3	4	3.97	5.8	1.59	3.95
36	1	3	4	3.42	4.6	1.28	3.9
37	2	3	5	5.02	8.3	2.55	3.7
38	1	3	4	4.58	6.3	1.64	5.05

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	2	2	4	4.2	5.8	1.73	4.85
40	2	4	6	4.67	7.4	2.09	4.6
41	2	2	4	4.4	6.3	1.97	5.0
42	2	2	4	4.47	6.3	1.83	5.05
43	1	3	4	3.9	5.5	1.57	4.4
44	2	3	5	3.34	4.6	0.92	3.5
45	2	3	5	3.42	5.4	1.33	3.5
46	1	3	4	4.78	6.9	1.47	4.4
47	2	3	5	3.86	6.3	1.54	4.1
48	1	2	3	5.87	7.7	1.6	6.1
49	1	4	5	3.32	4.9	1.43	3.8
50	2	4	6	3.05	5.7	1.76	2.4

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]	%
0	0	0	1	2.0
2	0	2	2	4.0
0	2	2	3	6.0
0	0	0	4	8.0
2	1	3	5	10.0
0	1	1	6	12.0
0	0	0	7	14.0
0	0	0	8	16.0
1	0	1	9	18.0
0	0	0	10	20.0
0	0	0	11	22.0
0	0	0	12	24.0
0	0	0	13	26.0
0	0	0	14	28.0
0	0	0	15	30.0
0	0	0	16	32.0
0	0	0	17	34.0
0	0	0	18	36.0
0	0	0	19	38.0
0	0	0	20	40.0
0	0	0	21	42.0
0	0	0	22	44.0
0	0	0	23	46.0
0	0	0	24	48.0
0	0	0	25	50.0
0	1	1	26	52.0
0	0	0	27	54.0
0	0	0	28	56.0
0	0	0	29	58.0
0	0	0	30	60.0
0	0	0	31	62.0
0	0	0	32	64.0
0	0	0	33	66.0
0	0	0	34	68.0
0	0	0	35	70.0
0	0	0	36	72.0
0	0	0	37	74.0
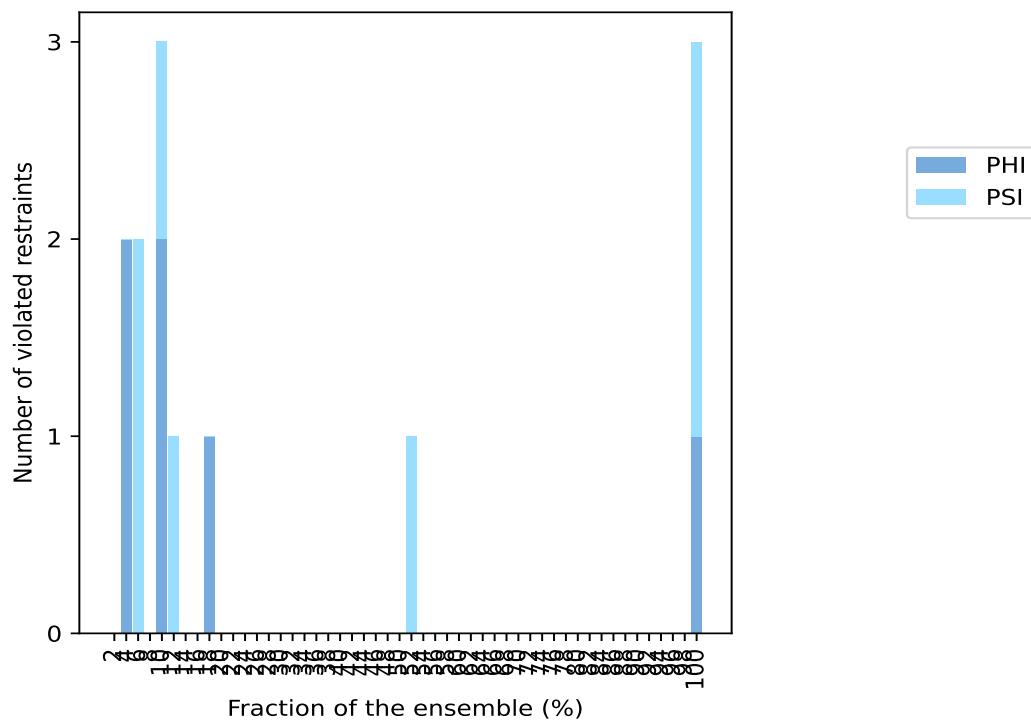
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| Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	38	76.0
0	0	0	39	78.0
0	0	0	40	80.0
0	0	0	41	82.0
0	0	0	42	84.0
0	0	0	43	86.0
0	0	0	44	88.0
0	0	0	45	90.0
0	0	0	46	92.0
0	0	0	47	94.0
0	0	0	48	96.0
0	0	0	49	98.0
1	2	3	50	100.0

[1] Number of models with violations
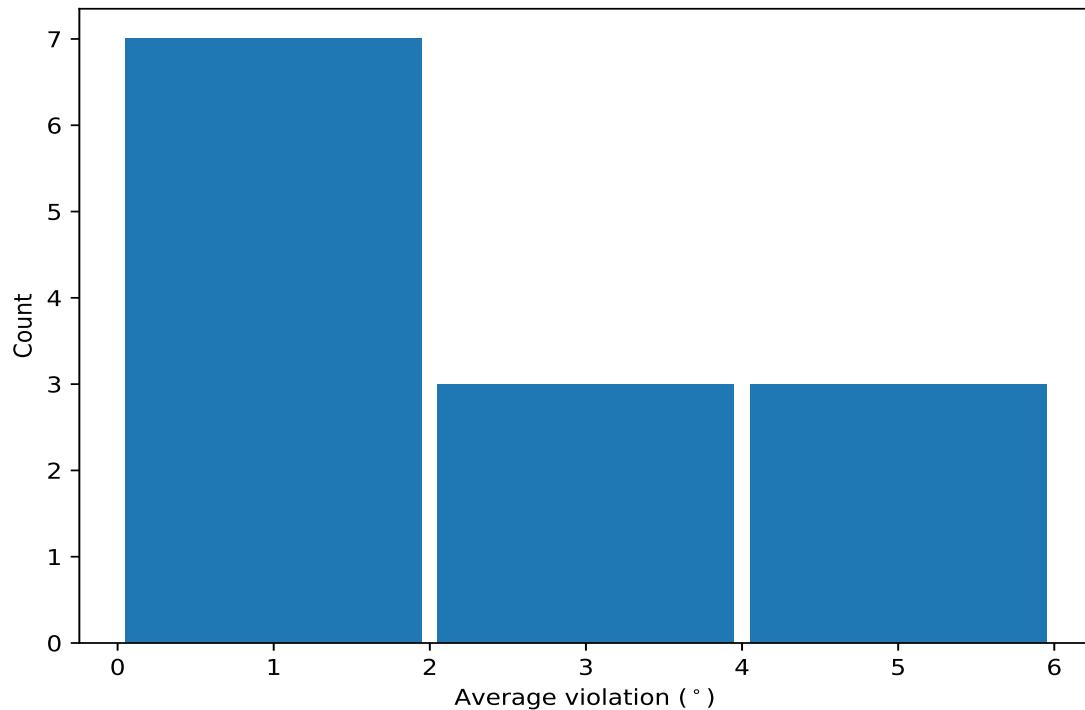
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

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.
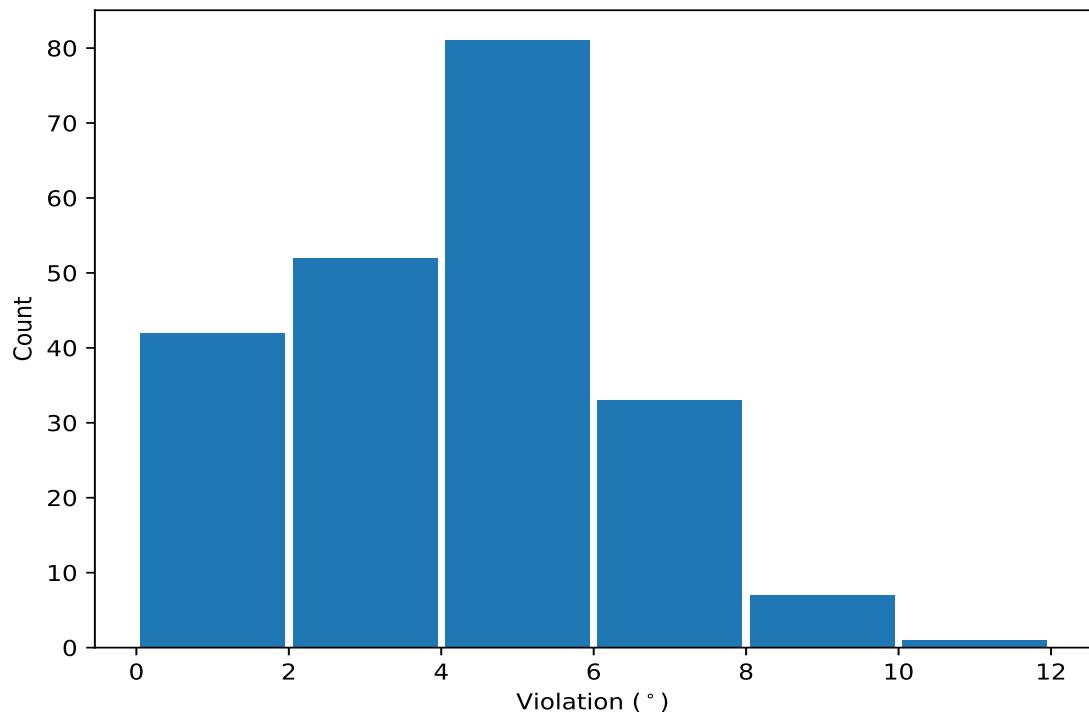
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(2,28)	1:A:16:ASN:N	1:A:16:ASN:CA	1:A:16:ASN:C	1:A:17:LYS:N	50	5.77	1.67	5.45
(2,29)	1:A:16:ASN:C	1:A:17:LYS:N	1:A:17:LYS:CA	1:A:17:LYS:C	50	5.1	1.65	4.8
(2,30)	1:A:17:LYS:N	1:A:17:LYS:CA	1:A:17:LYS:C	1:A:18:VAL:N	50	4.72	1.1	4.65
(2,24)	1:A:14:ASN:N	1:A:14:ASN:CA	1:A:14:ASN:C	1:A:15:VAL:N	26	2.03	0.64	1.9
(2,47)	1:A:25:GLN:C	1:A:26:MET:N	1:A:26:MET:CA	1:A:26:MET:C	9	1.49	0.32	1.6
(2,58)	1:A:31:GLU:N	1:A:31:GLU:CA	1:A:31:GLU:C	1:A:32:ARG:N	6	1.9	0.45	1.8
(2,50)	1:A:27:CYS:N	1:A:27:CYS:CA	1:A:27:CYS:C	1:A:28:SER:N	5	2.72	0.64	2.5
(2,31)	1:A:17:LYS:C	1:A:18:VAL:N	1:A:18:VAL:CA	1:A:18:VAL:C	5	2.46	1.02	2.4
(2,19)	1:A:11:GLU:C	1:A:12:GLN:N	1:A:12:GLN:CA	1:A:12:GLN:C	5	1.48	0.21	1.5
(2,20)	1:A:12:GLN:N	1:A:12:GLN:CA	1:A:12:GLN:C	1:A:13:CYS:N	3	1.43	0.26	1.3

[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 (°)
(2,28)	1:A:16:ASN:N	1:A:16:ASN:CA	1:A:16:ASN:C	1:A:17:LYS:N	3	10.6
(2,29)	1:A:16:ASN:C	1:A:17:LYS:N	1:A:17:LYS:CA	1:A:17:LYS:C	3	9.6
(2,29)	1:A:16:ASN:C	1:A:17:LYS:N	1:A:17:LYS:CA	1:A:17:LYS:C	23	9.1
(2,28)	1:A:16:ASN:N	1:A:16:ASN:CA	1:A:16:ASN:C	1:A:17:LYS:N	23	9.1
(2,28)	1:A:16:ASN:N	1:A:16:ASN:CA	1:A:16:ASN:C	1:A:17:LYS:N	28	8.9
(2,29)	1:A:16:ASN:C	1:A:17:LYS:N	1:A:17:LYS:CA	1:A:17:LYS:C	28	8.4
(2,30)	1:A:17:LYS:N	1:A:17:LYS:CA	1:A:17:LYS:C	1:A:18:VAL:N	37	8.3
(2,28)	1:A:16:ASN:N	1:A:16:ASN:CA	1:A:16:ASN:C	1:A:17:LYS:N	18	8.3
(2,28)	1:A:16:ASN:N	1:A:16:ASN:CA	1:A:16:ASN:C	1:A:17:LYS:N	37	7.9
(2,28)	1:A:16:ASN:N	1:A:16:ASN:CA	1:A:16:ASN:C	1:A:17:LYS:N	7	7.8