wwPDB NMR Structure Validation Summary Report

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Title	:	Solution structure of TRIM28 RING domain
Authors	:	Stevens, R.V.; Esposito, D.; Rittinger, K.
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

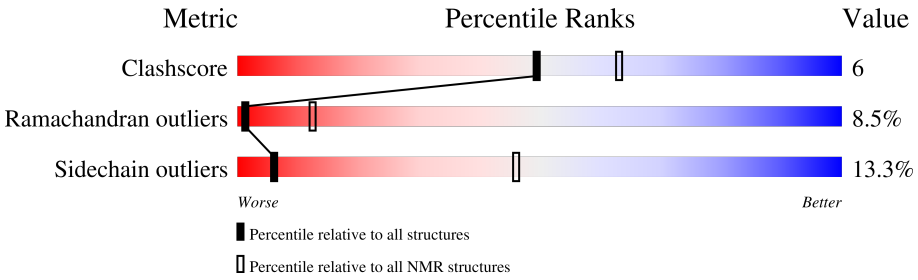
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 91%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	94	59% 12% • • 23% •

2 Ensemble composition and analysis

This entry contains 18 models. Model 10 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:56-A:96, A:110-A:138 (70)	0.63	10

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 7, 9, 11, 12, 14, 17, 18
2	4, 5, 6, 8, 10, 13, 15, 16
3	1, 2

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1285 atoms, of which 624 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription intermediary factor 1-beta.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1283	396	624	121	133	9	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLY	-	expression tag	UNP Q13263
A	53	PRO	-	expression tag	UNP Q13263

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

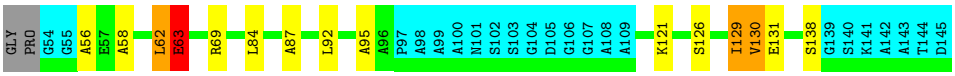
4 Residue-property plots

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: Transcription intermediary factor 1-beta

Chain A:



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

The representative model is number 10. Colouring as in section 4.1 above.

• Molecule 1: Transcription intermediary factor 1-beta

Chain A:

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 18 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
ARIA	structure calculation	
Xplor-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	1038
Number of shifts mapped to atoms	1026
Number of unparsed shifts	0
Number of shifts with mapping errors	12
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	534	515	515	6±2
All	All	9648	9270	9270	108

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ALA:HB3	1:A:92:LEU:HD21	0.59	1.72	16	11
1:A:95:ALA:HB1	1:A:116:ASP:O	0.58	1.98	17	1
1:A:87:ALA:HB3	1:A:92:LEU:CD1	0.54	2.32	14	7
1:A:96:ALA:HB2	1:A:115:VAL:HG22	0.54	1.78	17	1
1:A:58:ALA:HB3	1:A:63:GLU:HA	0.54	1.78	11	18

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	70/94 (74%)	56±2 (80±2%)	8±1 (12±2%)	6±1 (8±1%)	1	12
All	All	1260/1692 (74%)	1003 (80%)	150 (12%)	107 (8%)	1	12

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	62	LEU	18
1	A	63	GLU	18
1	A	130	VAL	18
1	A	131	GLU	18
1	A	129	ILE	14

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	60/70 (86%)	52±2 (87±3%)	8±2 (13±3%)	6	46
All	All	1080/1260 (86%)	936 (87%)	144 (13%)	6	46

5 of 24 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	62	LEU	18
1	A	63	GLU	18
1	A	84	LEU	17
1	A	69	ARG	12
1	A	126	SER	11

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 oligosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 91% for the well-defined parts and 92% 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	1038
Number of shifts mapped to atoms	1026
Number of unparsed shifts	0
Number of shifts with mapping errors	12
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 12) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	PRO	HA	4.485	0.002	1
1	A	53	PRO	HB2	2.311	0.002	2
1	A	53	PRO	HB3	1.955	0.019	2
1	A	53	PRO	HD2	3.576	0.007	2
1	A	53	PRO	HD3	3.598	0.009	2
1	A	53	PRO	HG2	2.151	0.003	2
1	A	53	PRO	HG3	1.857	0.002	2
1	A	53	PRO	C	177.453	0.000	1
1	A	53	PRO	CA	63.43	0.056	1
1	A	53	PRO	CB	32.262	0.000	1
1	A	53	PRO	CD	49.706	0.000	1
1	A	53	PRO	CG	27.789	0.054	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	91	-0.18 ± 0.28	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	83	0.09 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	92	-0.09 ± 0.18	None needed (< 0.5 ppm)
^{15}N	86	-0.37 ± 0.44	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 91%, i.e. 837 atoms were assigned a chemical shift out of a possible 916. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	342/344 (99%)	139/139 (100%)	138/140 (99%)	65/65 (100%)
Sidechain	459/529 (87%)	313/343 (91%)	143/163 (88%)	3/23 (13%)
Aromatic	36/43 (84%)	18/22 (82%)	18/19 (95%)	0/2 (0%)
Overall	837/916 (91%)	470/504 (93%)	299/322 (93%)	68/90 (76%)

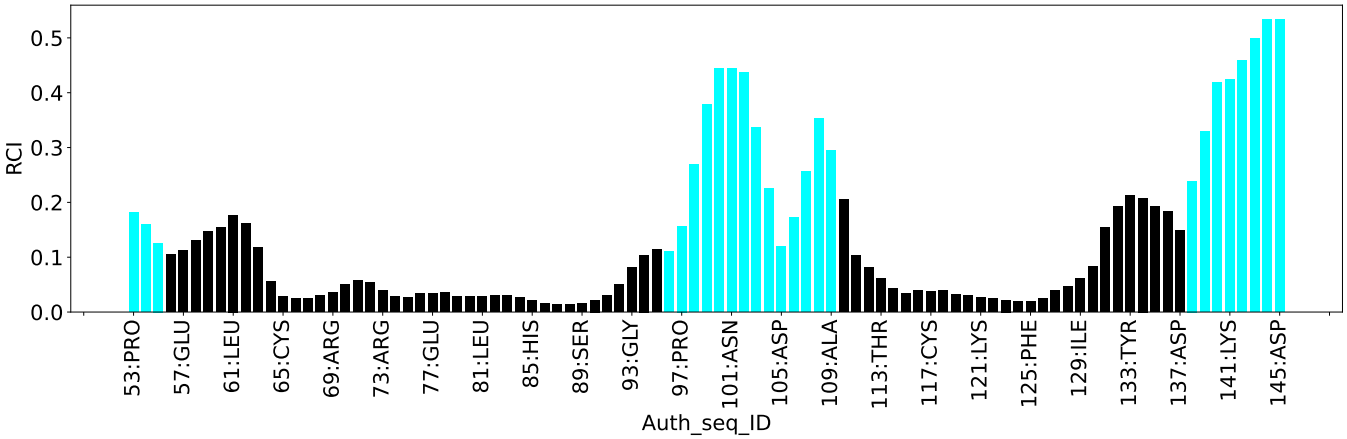
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
53:PRO
57:GLU
61:LEU
65:CYS
69:ARG
73:ARG
77:GLU
81:LEU
85:HIS
89:SER
93:GLY
97:PRO
101:ASN
105:ASP
109:ALA
113:THR
117:CYS
121:LYS
125:PHE
129:ILE
133:TYR
137:ASP
141:LYS
145:ASP
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1495
Intra-residue (|i-j|=0)	684
Sequential (|i-j|=1)	347
Medium range (|i-j|>1 and |i-j|<5)	188
Long range (|i-j|≥5)	276
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	92
Number of unmapped restraints	0
Number of restraints per residue	16.5
Number of long range restraints per residue[1]	2.9

[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)	65.1	0.2
0.2-0.5 (Medium)	122.7	0.5
>0.5 (Large)	71.3	1.88

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)	11.8	4.86
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

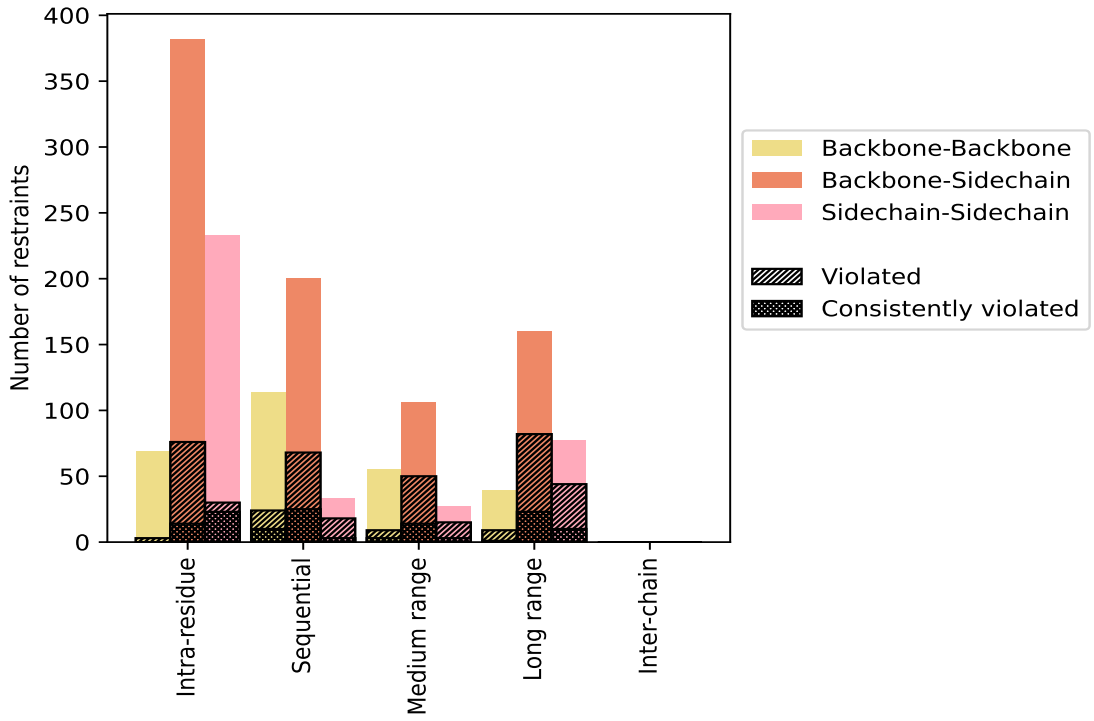
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	684	45.8	109	15.9	7.3	37	5.4	2.5
Backbone-Backbone	69	4.6	3	4.3	0.2	0	0.0	0.0
Backbone-Sidechain	382	25.6	76	19.9	5.1	14	3.7	0.9
Sidechain-Sidechain	233	15.6	30	12.9	2.0	23	9.9	1.5
Sequential (|i-j|=1)	347	23.2	110	31.7	7.4	38	11.0	2.5
Backbone-Backbone	114	7.6	24	21.1	1.6	10	8.8	0.7
Backbone-Sidechain	200	13.4	68	34.0	4.5	25	12.5	1.7
Sidechain-Sidechain	33	2.2	18	54.5	1.2	3	9.1	0.2
Medium range (|i-j|>1 & |i-j|<5)	188	12.6	74	39.4	4.9	20	10.6	1.3
Backbone-Backbone	55	3.7	9	16.4	0.6	3	5.5	0.2
Backbone-Sidechain	106	7.1	50	47.2	3.3	14	13.2	0.9
Sidechain-Sidechain	27	1.8	15	55.6	1.0	3	11.1	0.2
Long range (|i-j|≥5)	276	18.5	135	48.9	9.0	34	12.3	2.3
Backbone-Backbone	39	2.6	9	23.1	0.6	1	2.6	0.1
Backbone-Sidechain	160	10.7	82	51.2	5.5	23	14.4	1.5
Sidechain-Sidechain	77	5.2	44	57.1	2.9	10	13.0	0.7
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1495	100.0	428	28.6	28.6	129	8.6	8.6
Backbone-Backbone	277	18.5	45	16.2	3.0	14	5.1	0.9
Backbone-Sidechain	848	56.7	276	32.5	18.5	76	9.0	5.1
Sidechain-Sidechain	370	24.7	107	28.9	7.2	39	10.5	2.6

[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	66	67	51	72	0	256	0.41	1.5	0.29	0.32
2	67	66	51	78	0	262	0.41	1.67	0.28	0.34
3	65	71	47	78	0	261	0.42	1.41	0.28	0.33
4	70	69	40	83	0	262	0.4	1.77	0.29	0.32
5	69	68	44	82	0	263	0.4	1.69	0.28	0.33
6	72	70	47	81	0	270	0.42	1.66	0.28	0.34
7	67	66	47	82	0	262	0.41	1.29	0.27	0.32
8	76	63	47	81	0	267	0.4	1.49	0.27	0.33
9	69	73	41	82	0	265	0.4	1.49	0.27	0.31
10	68	67	44	74	0	253	0.42	1.55	0.29	0.33

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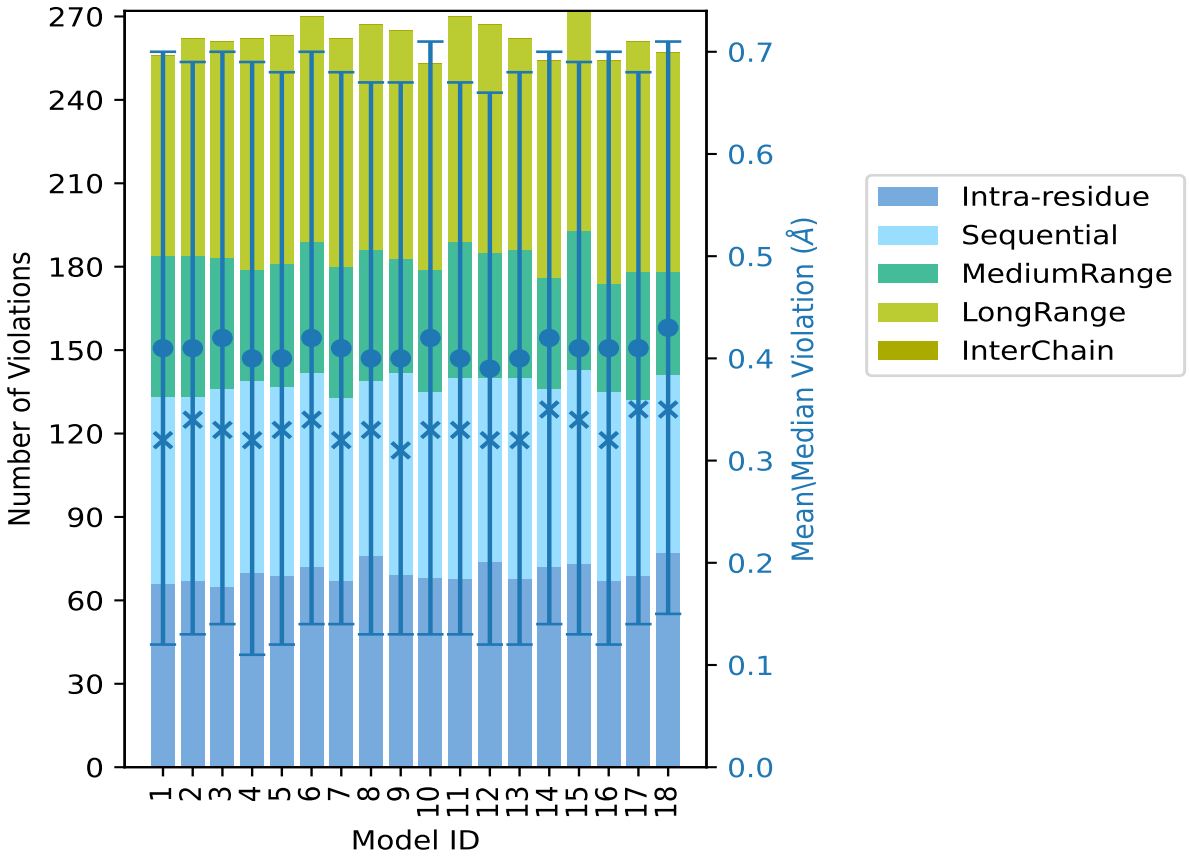
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	68	72	49	81	0	270	0.4	1.37	0.27	0.33
12	74	66	45	82	0	267	0.39	1.37	0.27	0.32
13	68	72	46	76	0	262	0.4	1.88	0.28	0.32
14	72	64	40	78	0	254	0.42	1.47	0.28	0.35
15	73	70	50	79	0	272	0.41	1.53	0.28	0.34
16	67	68	39	80	0	254	0.41	1.48	0.29	0.32
17	69	63	46	83	0	261	0.41	1.46	0.27	0.35
18	77	64	37	79	0	257	0.43	1.53	0.28	0.35

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

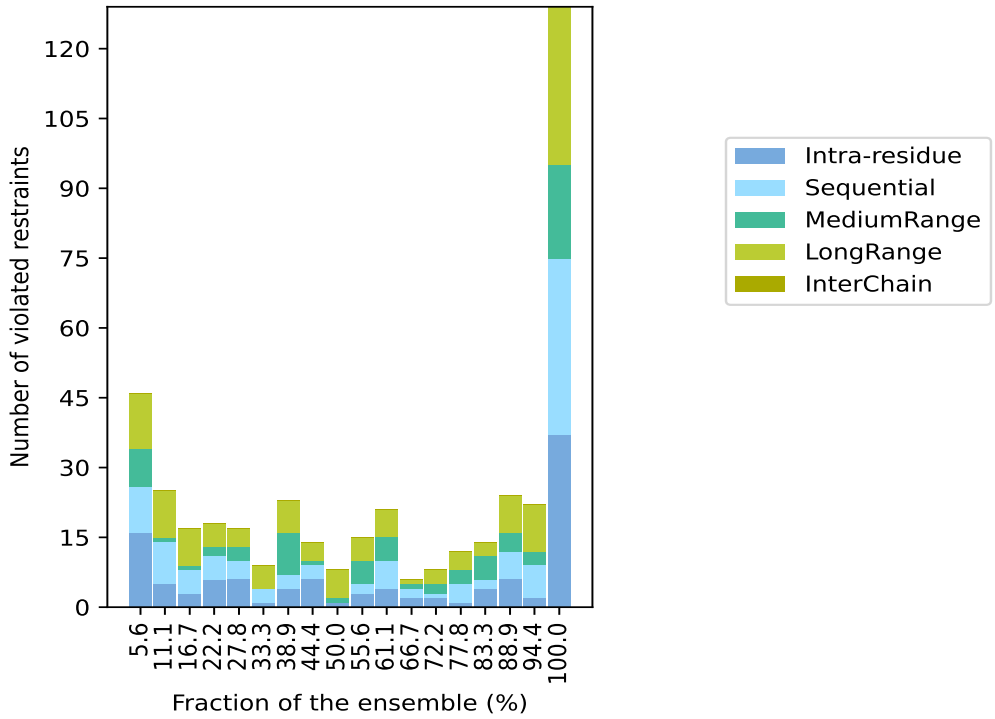
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1067(IR:575, SQ:237, MR:114, LR:141, 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]	%
16	10	8	12	0	46	1	5.6
5	9	1	10	0	25	2	11.1
3	5	1	8	0	17	3	16.7
6	5	2	5	0	18	4	22.2
6	4	3	4	0	17	5	27.8
1	3	0	5	0	9	6	33.3
4	3	9	7	0	23	7	38.9
6	3	1	4	0	14	8	44.4
1	0	1	6	0	8	9	50.0
3	2	5	5	0	15	10	55.6
4	6	5	6	0	21	11	61.1
2	2	1	1	0	6	12	66.7
2	1	2	3	0	8	13	72.2
1	4	3	4	0	12	14	77.8
4	2	5	3	0	14	15	83.3
6	6	4	8	0	24	16	88.9
2	7	3	10	0	22	17	94.4
37	38	20	34	0	129	18	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

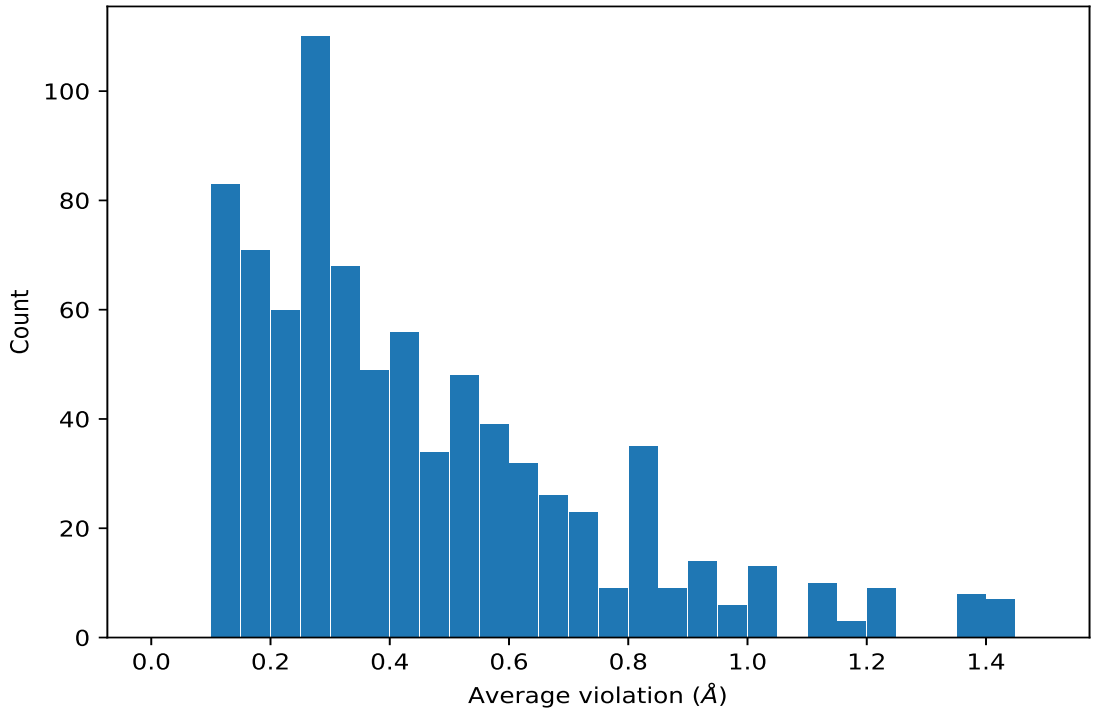
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(1,1489)	1:87:A:ALA:HB1	1:72:A:LEU:HD23	18	1.41	0.08	1.42
(1,1489)	1:87:A:ALA:HB2	1:72:A:LEU:HD21	18	1.41	0.08	1.42
(1,1489)	1:87:A:ALA:HB1	1:72:A:LEU:HD22	18	1.41	0.08	1.42
(1,1489)	1:87:A:ALA:HB3	1:72:A:LEU:HD22	18	1.41	0.08	1.42
(1,1489)	1:87:A:ALA:HB3	1:72:A:LEU:HD23	18	1.41	0.08	1.42
(1,1489)	1:87:A:ALA:HB2	1:72:A:LEU:HD22	18	1.41	0.08	1.42
(1,1489)	1:87:A:ALA:HB2	1:72:A:LEU:HD23	18	1.41	0.08	1.42
(1,1292)	1:134:A:PHE:H	1:80:A:LEU:HD21	18	1.38	0.23	1.28
(1,1292)	1:135:A:MET:H	1:72:A:LEU:HD13	18	1.38	0.23	1.28
(1,1292)	1:134:A:PHE:H	1:72:A:LEU:HD11	18	1.38	0.23	1.28
(1,1292)	1:135:A:MET:H	1:72:A:LEU:HD12	18	1.38	0.23	1.28
(1,1292)	1:134:A:PHE:H	1:80:A:LEU:HD23	18	1.38	0.23	1.28
(1,1292)	1:134:A:PHE:H	1:72:A:LEU:HD12	18	1.38	0.23	1.28
(1,1292)	1:134:A:PHE:H	1:80:A:LEU:HD22	18	1.38	0.23	1.28
(1,1425)	1:115:A:VAL:HG22	1:110:A:GLY:HA2	18	1.21	0.25	1.27
(1,1425)	1:115:A:VAL:HG22	1:110:A:GLY:HA3	18	1.21	0.25	1.27

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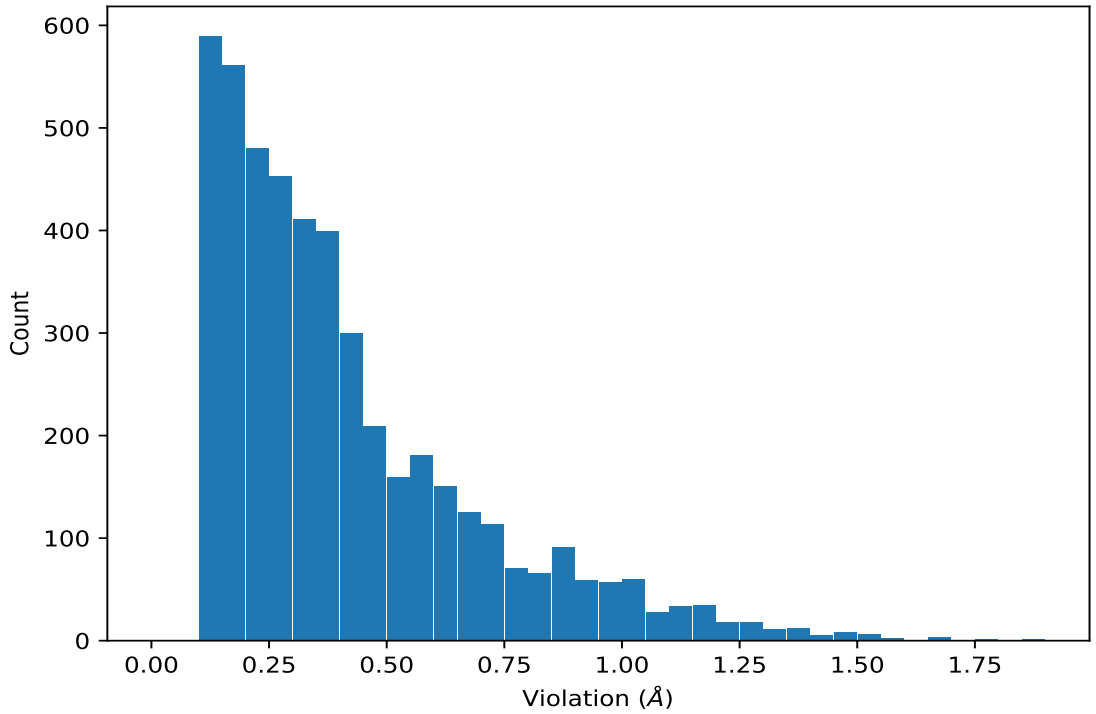
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1425)	1:115:A:VAL:HG21	1:110:A:GLY:HA3	18	1.21	0.25	1.27
(1,1425)	1:115:A:VAL:HG23	1:110:A:GLY:HA2	18	1.21	0.25	1.27
(1,1425)	1:115:A:VAL:HG23	1:110:A:GLY:HA3	18	1.21	0.25	1.27
(1,1425)	1:115:A:VAL:HG21	1:110:A:GLY:HA2	18	1.21	0.25	1.27
(1,381)	1:66:A:GLY:H	1:67:A:VAL:HG11	18	1.16	0.05	1.17
(1,381)	1:66:A:GLY:H	1:67:A:VAL:HG13	18	1.16	0.05	1.17
(1,381)	1:66:A:GLY:H	1:67:A:VAL:HG12	18	1.16	0.05	1.17
(1,882)	1:87:A:ALA:HB1	1:72:A:LEU:HD23	18	1.13	0.08	1.14
(1,882)	1:87:A:ALA:HB2	1:72:A:LEU:HD21	18	1.13	0.08	1.14
(1,882)	1:87:A:ALA:HB1	1:72:A:LEU:HD22	18	1.13	0.08	1.14
(1,882)	1:87:A:ALA:HB3	1:72:A:LEU:HD22	18	1.13	0.08	1.14
(1,882)	1:87:A:ALA:HB3	1:72:A:LEU:HD23	18	1.13	0.08	1.14
(1,882)	1:87:A:ALA:HB2	1:72:A:LEU:HD22	18	1.13	0.08	1.14
(1,882)	1:87:A:ALA:HB2	1:72:A:LEU:HD23	18	1.13	0.08	1.14
(1,1448)	1:74:A:PRO:HB3	1:56:A:ALA:HB1	18	1.02	0.23	1.02
(1,1448)	1:74:A:PRO:HB3	1:56:A:ALA:HB3	18	1.02	0.23	1.02
(1,1448)	1:74:A:PRO:HB3	1:56:A:ALA:HB2	18	1.02	0.23	1.02
(1,1351)	1:76:A:ARG:HD2	1:78:A:PRO:HA	18	1.02	0.09	1.04
(1,710)	1:59:A:LEU:HD11	1:59:A:LEU:HA	18	1.01	0.01	1.01
(1,710)	1:59:A:LEU:HD12	1:59:A:LEU:HA	18	1.01	0.01	1.01
(1,710)	1:59:A:LEU:HD13	1:59:A:LEU:HA	18	1.01	0.01	1.01
(1,1147)	1:88:A:CYS:HB2	1:72:A:LEU:HD21	18	1.0	0.08	1.02
(1,1147)	1:88:A:CYS:HB2	1:72:A:LEU:HD22	18	1.0	0.08	1.02
(1,1147)	1:88:A:CYS:HB2	1:72:A:LEU:HD23	18	1.0	0.08	1.02
(1,1373)	1:63:A:GLU:HG3	1:72:A:LEU:HD13	18	0.99	0.06	0.98

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:134:A:PHE:H	1:72:A:LEU:HD12	13	1.88
(1,1292)	1:135:A:MET:H	1:72:A:LEU:HD13	4	1.77
(1,1292)	1:134:A:PHE:H	1:72:A:LEU:HD11	5	1.69
(1,1292)	1:135:A:MET:H	1:72:A:LEU:HD13	2	1.67
(1,1425)	1:115:A:VAL:HG23	1:110:A:GLY:HA2	6	1.66
(1,1319)	1:123:A:GLN:HB2	1:111:A:ASP:H	10	1.55
(1,1292)	1:134:A:PHE:H	1:80:A:LEU:HD21	6	1.55
(1,1287)	1:131:A:GLU:H	1:92:A:LEU:HD12	4	1.54
(1,1489)	1:87:A:ALA:HB1	1:72:A:LEU:HD22	4	1.53
(1,1489)	1:87:A:ALA:HB3	1:72:A:LEU:HD22	18	1.53

10 Dihedral-angle violation analysis

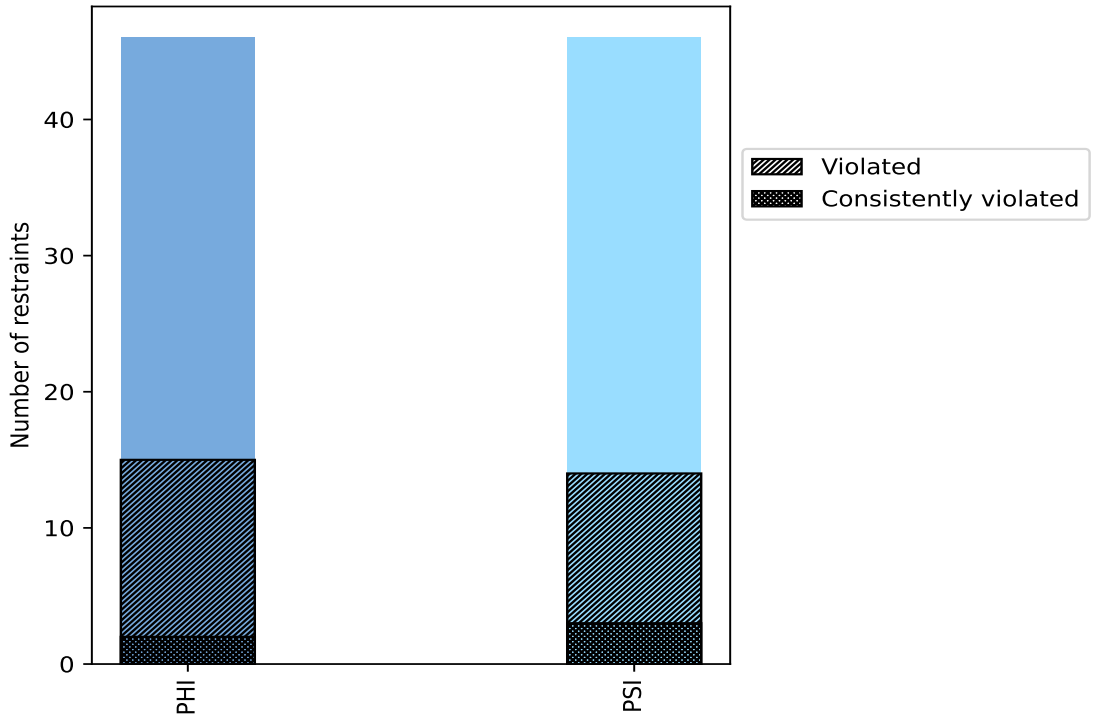
10.1 Summary of dihedral-angle violations

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	46	50.0	15	32.6	16.3	2	4.3	2.2
PSI	46	50.0	14	30.4	15.2	3	6.5	3.3
Total	92	100.0	29	31.5	31.5	5	5.4	5.4

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



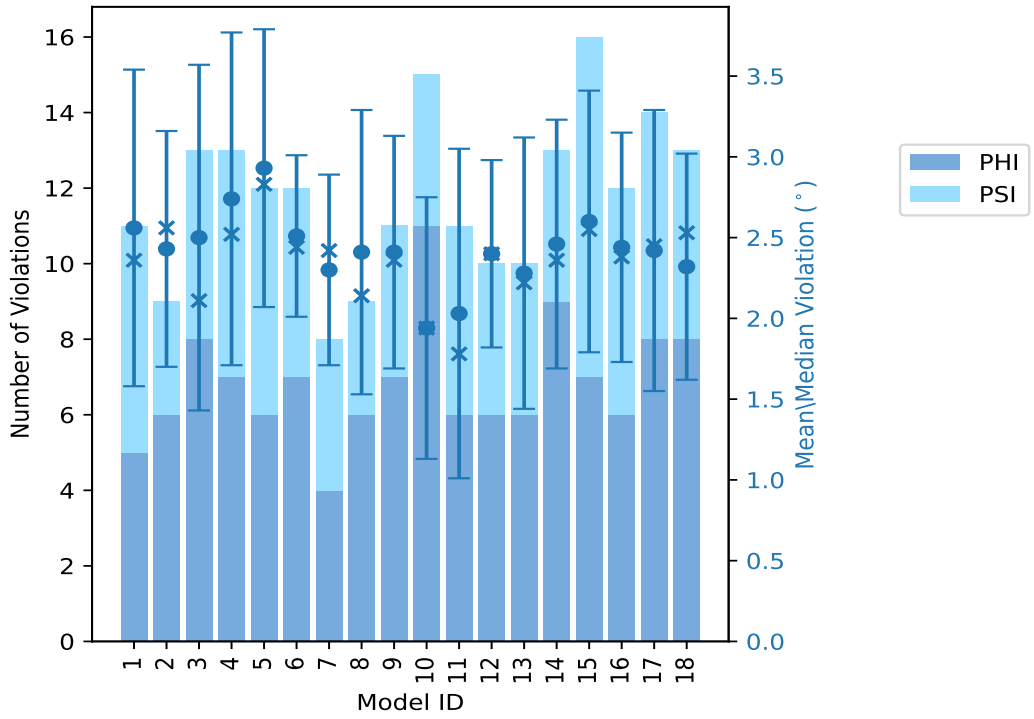
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	5	6	11	2.56	4.52	0.98	2.36
2	6	3	9	2.43	3.3	0.73	2.56
3	8	5	13	2.5	4.3	1.07	2.11
4	7	6	13	2.74	4.86	1.03	2.52
5	6	6	12	2.93	4.12	0.86	2.83
6	7	5	12	2.51	3.45	0.5	2.44
7	4	4	8	2.3	3.08	0.59	2.42
8	6	3	9	2.41	4.21	0.88	2.14
9	7	4	11	2.41	3.42	0.72	2.36
10	11	4	15	1.94	3.4	0.81	1.94
11	6	5	11	2.03	4.73	1.02	1.78
12	6	4	10	2.4	3.16	0.58	2.4
13	6	4	10	2.28	3.85	0.84	2.22
14	9	4	13	2.46	3.66	0.77	2.36
15	7	9	16	2.6	3.88	0.81	2.55
16	6	6	12	2.44	3.51	0.71	2.38
17	8	6	14	2.42	3.94	0.87	2.45
18	8	5	13	2.32	3.54	0.7	2.53

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]	%
2	2	4	1	5.6
2	3	5	2	11.1
1	2	3	3	16.7
0	2	2	4	22.2
1	0	1	5	27.8
2	1	3	6	33.3
1	1	2	7	38.9
0	0	0	8	44.4
0	0	0	9	50.0
0	0	0	10	55.6
1	0	1	11	61.1

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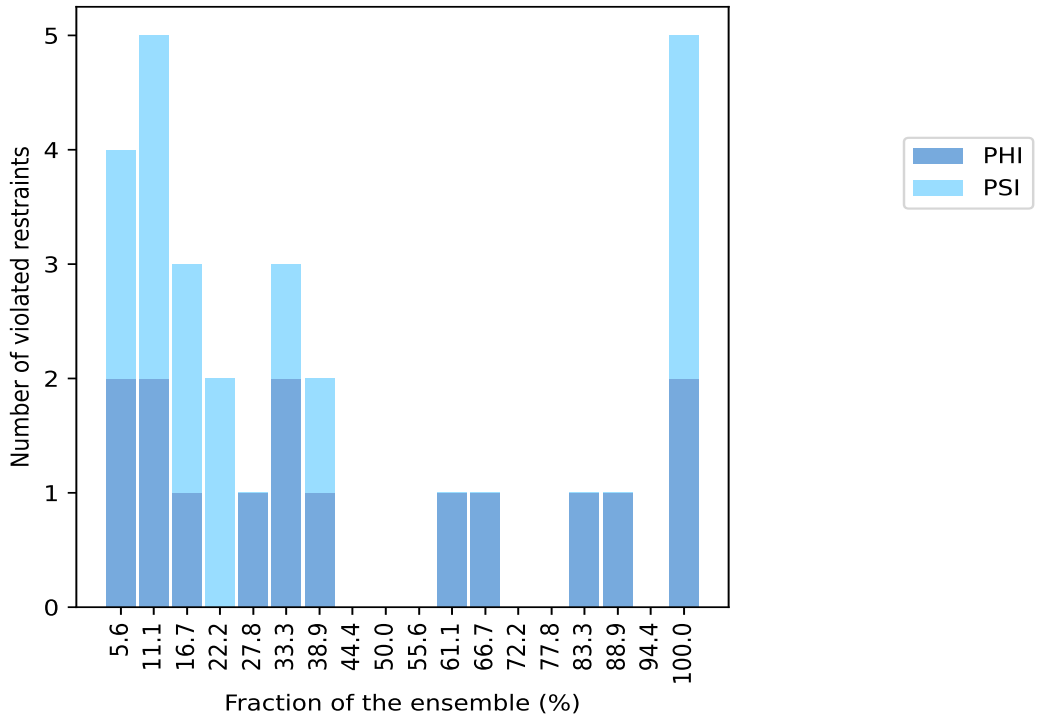
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	0	1	12	66.7
0	0	0	13	72.2
0	0	0	14	77.8
1	0	1	15	83.3
1	0	1	16	88.9
0	0	0	17	94.4
2	3	5	18	100.0

[1] Number of models with violations

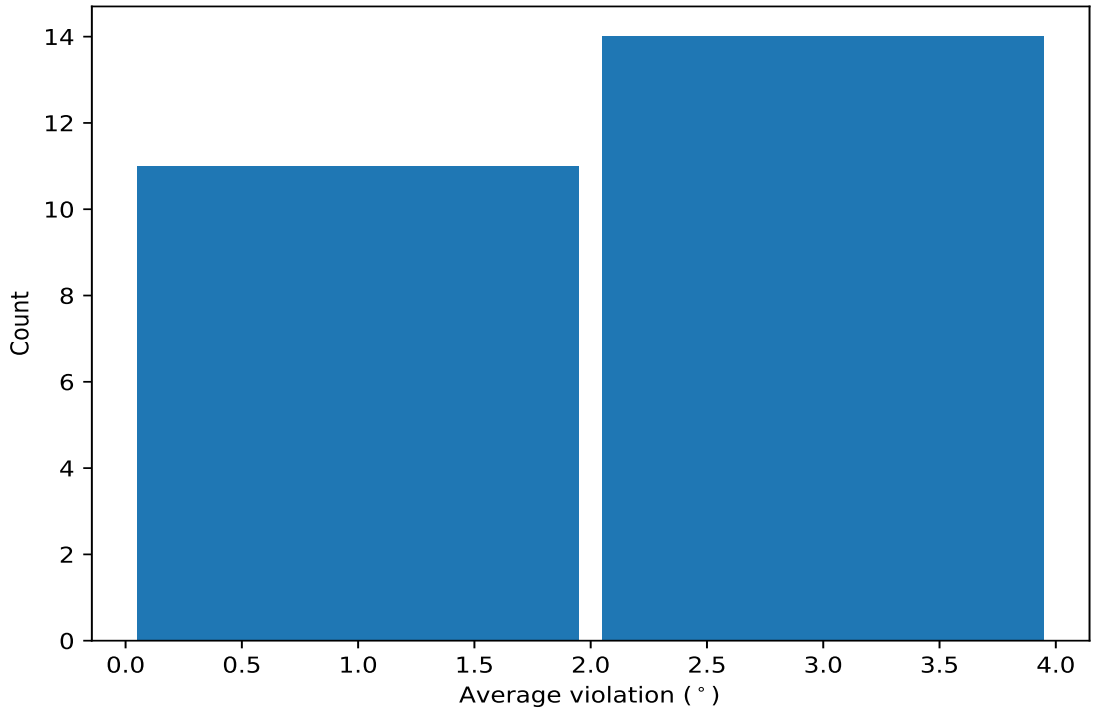
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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.

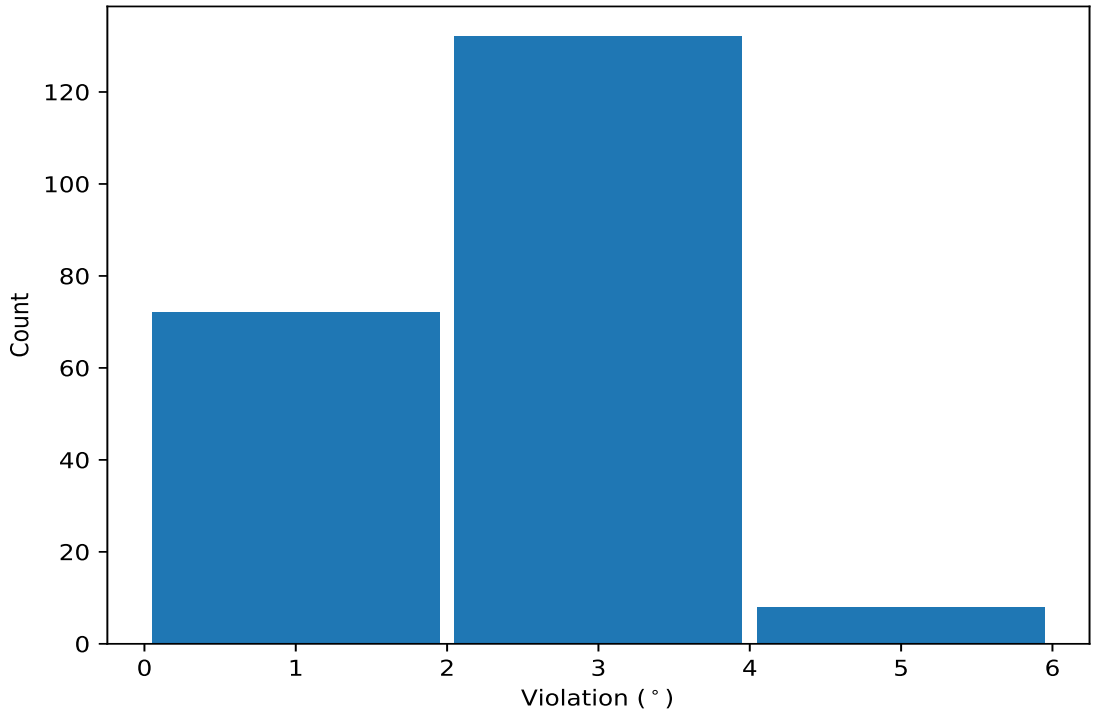
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,86)	1:58:A:ALA:N	1:58:A:ALA:CA	1:58:A:ALA:C	1:59:A:LEU:N	18	3.29	0.42	3.28
(1,14)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:GLU:N	18	3.12	0.64	3.12
(1,92)	1:61:A:LEU:N	1:61:A:LEU:CA	1:61:A:LEU:C	1:62:A:LEU:N	18	3.02	0.73	2.97
(1,91)	1:60:A:GLU:C	1:61:A:LEU:N	1:61:A:LEU:CA	1:61:A:LEU:C	18	2.87	0.33	2.9
(1,27)	1:85:A:HIS:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	18	2.38	0.62	2.36
(1,83)	1:112:A:GLY:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	16	2.19	0.71	2.11
(1,13)	1:75:A:GLU:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	15	2.14	1.04	1.91
(1,65)	1:124:A:CYS:C	1:125:A:PHE:N	1:125:A:PHE:CA	1:125:A:PHE:C	12	2.77	0.91	3.01
(1,67)	1:126:A:SER:C	1:127:A:LYS:N	1:127:A:LYS:CA	1:127:A:LYS:C	11	2.27	0.79	2.33
(1,84)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:VAL:N	7	2.1	0.53	2.09

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

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 (°)
(1,13)	1:75:A:GLU:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	4	4.86
(1,92)	1:61:A:LEU:N	1:61:A:LEU:CA	1:61:A:LEU:C	1:62:A:LEU:N	11	4.73
(1,14)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:GLU:N	1	4.52
(1,65)	1:124:A:CYS:C	1:125:A:PHE:N	1:125:A:PHE:CA	1:125:A:PHE:C	3	4.3
(1,86)	1:58:A:ALA:N	1:58:A:ALA:CA	1:58:A:ALA:C	1:59:A:LEU:N	8	4.21
(1,14)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:GLU:N	4	4.16
(1,13)	1:75:A:GLU:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	5	4.12
(1,14)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:GLU:N	5	4.06
(1,27)	1:85:A:HIS:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	17	3.94
(1,92)	1:61:A:LEU:N	1:61:A:LEU:CA	1:61:A:LEU:C	1:62:A:LEU:N	5	3.93