



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 9CCH / pdb_00009cch
BMRB ID : 16492
Title : Solution structure of the Bsu Anti-TRAP trimer
Authors : Foster, M.P.; McElroy, C.A.; Ihms, E.C.; Kumar Yadav, D.
Deposited on : 2024-06-21

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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.44

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 31%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:2-A:53, B:2-B:53, C:2-C:53 (156)	0.42	13

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2370 atoms, of which 1185 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Anti-TRAP regulator.

Mol	Chain	Residues	Atoms						Trace
1	A	53	Total	C	H	N	O	S	0
			789	246	395	65	78	5	
1	B	53	Total	C	H	N	O	S	0
			789	246	395	65	78	5	
1	C	53	Total	C	H	N	O	S	0
			789	246	395	65	78	5	

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

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1
2	C	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

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: Anti-TRAP regulator

Chain A:  98% .



- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



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

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .



- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
X-PLOR NIH	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	629
Number of shifts mapped to atoms	629
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	31%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

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6.5 Carbohydrates [i](#)

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6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

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 31% for the well-defined parts and 31% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	629
Number of shifts mapped to atoms	629
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 \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	52	-0.63 ± 0.13	Should be applied
$^{13}\text{C}_\beta$	47	-0.27 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	48	-0.18 ± 0.25	None needed (< 0.5 ppm)
^{15}N	49	0.69 ± 0.64	None needed (imprecise)

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 31%, i.e. 614 atoms were assigned a chemical shift out of a possible 1995. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	255/777 (33%)	106/318 (33%)	100/312 (32%)	49/147 (33%)
Sidechain	345/1137 (30%)	232/744 (31%)	110/363 (30%)	3/30 (10%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	14/81 (17%)	7/39 (18%)	7/36 (19%)	0/6 (0%)
Overall	614/1995 (31%)	345/1101 (31%)	217/711 (31%)	52/183 (28%)

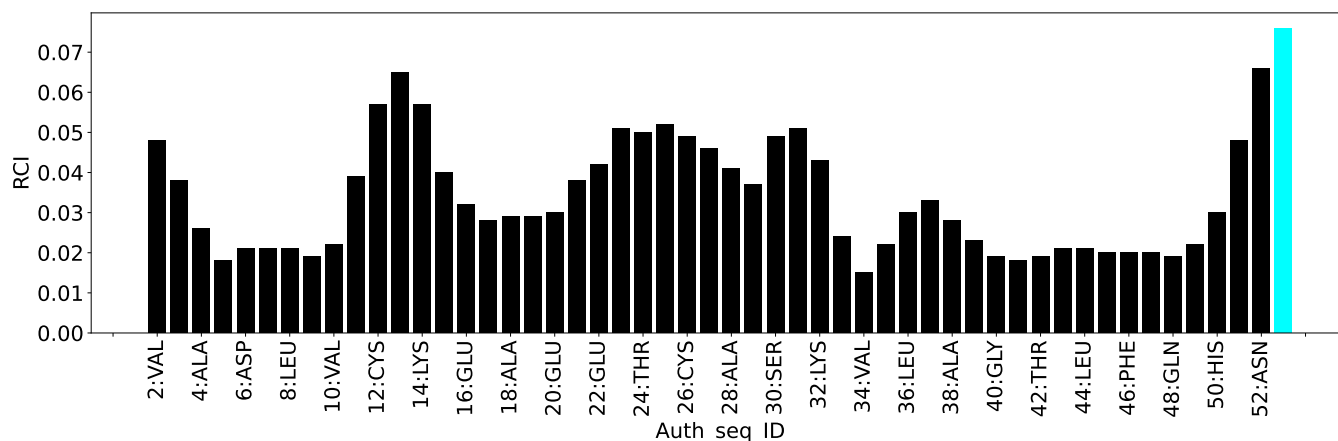
7.1.4 Statistically unusual chemical shifts [i](#)

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:



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	7065
Intra-residue ($ i-j =0$)	2198
Sequential ($ i-j =1$)	1748
Medium range ($ i-j >1$ and $ i-j <5$)	1327
Long range ($ i-j \geq 5$)	1201
Inter-chain	591
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	317
Number of unmapped restraints	10
Number of restraints per residue	45.6
Number of long range restraints per residue ¹	7.4

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)	69.5	0.2
0.2-0.5 (Medium)	47.6	0.5
>0.5 (Large)	34.6	1.74

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)	57.5	10.0
10.0-20.0 (Medium)	14.5	18.88
>20.0 (Large)	0.1	20.56

9 Distance violation analysis ⓘ

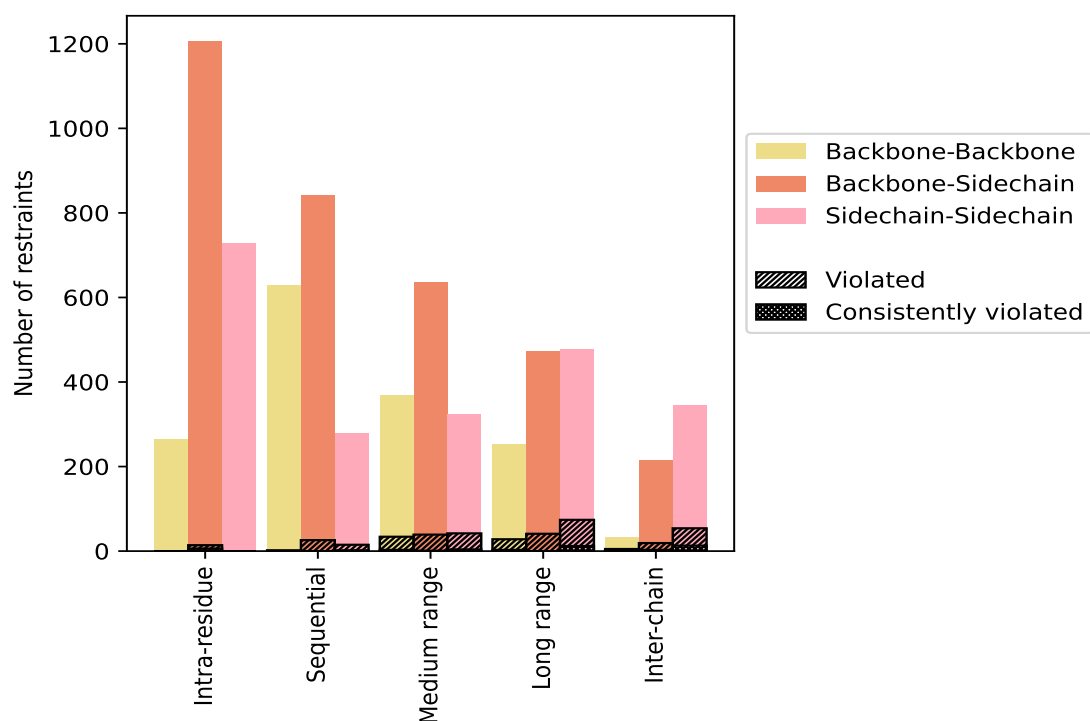
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	2198	31.1	14	0.6	0.2	6	0.3	0.1
Backbone-Backbone	264	3.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1206	17.1	14	1.2	0.2	6	0.5	0.1
Sidechain-Sidechain	728	10.3	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	1748	24.7	43	2.5	0.6	2	0.1	0.0
Backbone-Backbone	628	8.9	2	0.3	0.0	0	0.0	0.0
Backbone-Sidechain	842	11.9	26	3.1	0.4	0	0.0	0.0
Sidechain-Sidechain	278	3.9	15	5.4	0.2	2	0.7	0.0
Medium range ($i-j >1$ & $i-j <5$)	1327	18.8	115	8.7	1.6	8	0.6	0.1
Backbone-Backbone	369	5.2	34	9.2	0.5	3	0.8	0.0
Backbone-Sidechain	635	9.0	39	6.1	0.6	1	0.2	0.0
Sidechain-Sidechain	323	4.6	42	13.0	0.6	4	1.2	0.1
Long range ($i-j \geq 5$)	1201	17.0	143	11.9	2.0	15	1.2	0.2
Backbone-Backbone	252	3.6	28	11.1	0.4	3	1.2	0.0
Backbone-Sidechain	473	6.7	41	8.7	0.6	0	0.0	0.0
Sidechain-Sidechain	476	6.7	74	15.5	1.0	12	2.5	0.2
Inter-chain	591	8.4	78	13.2	1.1	19	3.2	0.3
Backbone-Backbone	33	0.5	5	15.2	0.1	3	9.1	0.0
Backbone-Sidechain	214	3.0	19	8.9	0.3	3	1.4	0.0
Sidechain-Sidechain	344	4.9	54	15.7	0.8	13	3.8	0.2
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	7065	100.0	393	5.6	5.6	50	0.7	0.7
Backbone-Backbone	1546	21.9	69	4.5	1.0	9	0.6	0.1
Backbone-Sidechain	3370	47.7	139	4.1	2.0	10	0.3	0.1
Sidechain-Sidechain	2149	30.4	185	8.6	2.6	31	1.4	0.4

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 disulfid 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	10	26	53	44	25	158	0.32	1.31	0.29	0.19
2	8	20	43	57	24	152	0.34	1.6	0.3	0.22
3	6	16	46	56	30	154	0.34	1.21	0.31	0.21
4	8	15	45	59	25	152	0.36	1.62	0.32	0.21
5	8	23	40	61	27	159	0.34	1.28	0.29	0.21
6	8	25	50	62	25	170	0.34	1.35	0.31	0.22
7	8	17	43	63	25	156	0.33	1.24	0.29	0.21
8	8	21	42	52	25	148	0.35	1.2	0.29	0.22
9	8	16	47	57	28	156	0.38	1.53	0.34	0.22
10	8	14	42	49	31	144	0.38	1.56	0.32	0.24

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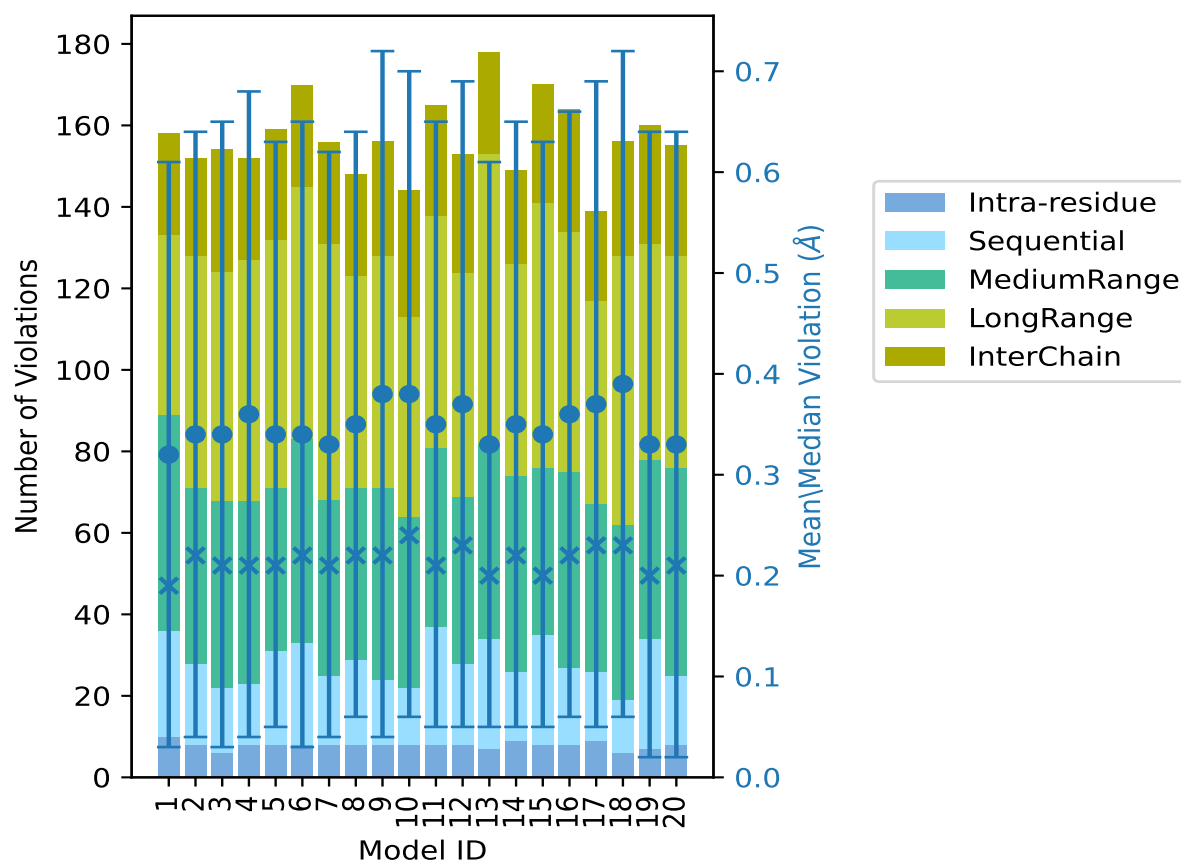
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	8	29	44	57	27	165	0.35	1.22	0.3	0.21
12	8	20	41	55	29	153	0.37	1.59	0.32	0.23
13	7	27	48	71	25	178	0.33	1.2	0.28	0.2
14	9	17	48	52	23	149	0.35	1.33	0.3	0.22
15	8	27	41	65	29	170	0.34	1.18	0.29	0.2
16	8	19	48	59	30	164	0.36	1.21	0.3	0.22
17	9	17	41	50	22	139	0.37	1.56	0.32	0.23
18	6	13	43	66	28	156	0.39	1.32	0.33	0.23
19	7	27	44	53	29	160	0.33	1.28	0.31	0.2
20	8	17	51	52	27	155	0.33	1.74	0.31	0.21

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 ⓘ



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

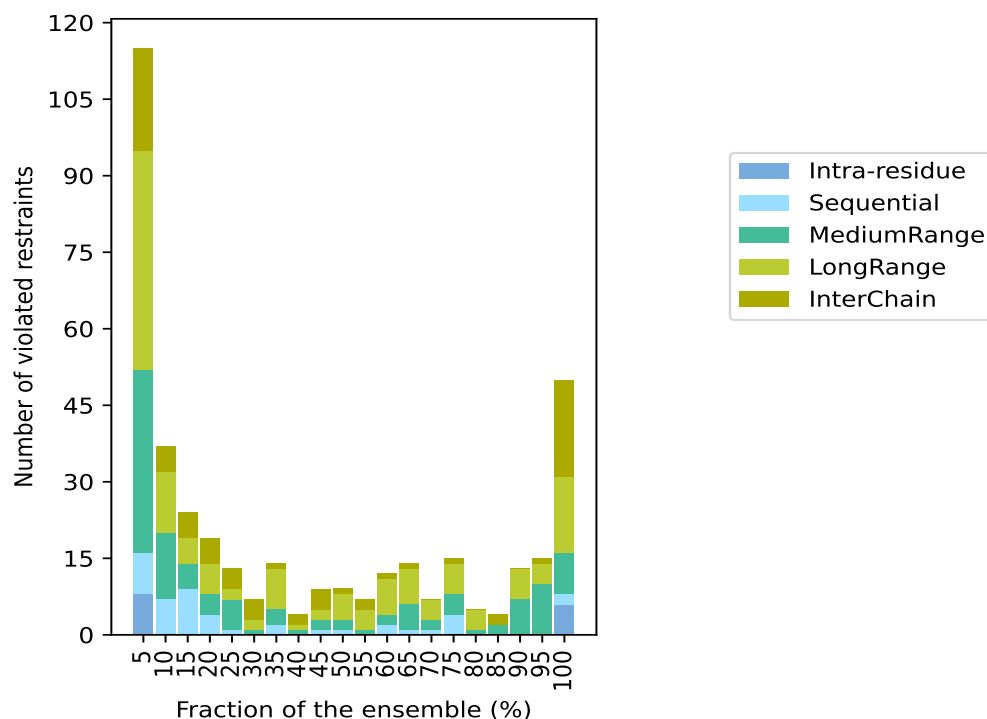
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 6672(IR:2184, SQ:1705, MR:1212, LR:1058, IC:513) restraints 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	%
8	8	36	43	20	115	1	5.0
0	7	13	12	5	37	2	10.0
0	9	5	5	5	24	3	15.0
0	4	4	6	5	19	4	20.0
0	1	6	2	4	13	5	25.0
0	0	1	2	4	7	6	30.0
0	2	3	8	1	14	7	35.0
0	0	1	1	2	4	8	40.0
0	1	2	2	4	9	9	45.0
0	1	2	5	1	9	10	50.0
0	0	1	4	2	7	11	55.0
0	2	2	7	1	12	12	60.0
0	1	5	7	1	14	13	65.0
0	1	2	4	0	7	14	70.0
0	4	4	6	1	15	15	75.0
0	0	1	4	0	5	16	80.0
0	0	2	0	2	4	17	85.0
0	0	7	6	0	13	18	90.0
0	0	10	4	1	15	19	95.0
6	2	8	15	19	50	20	100.0

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

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

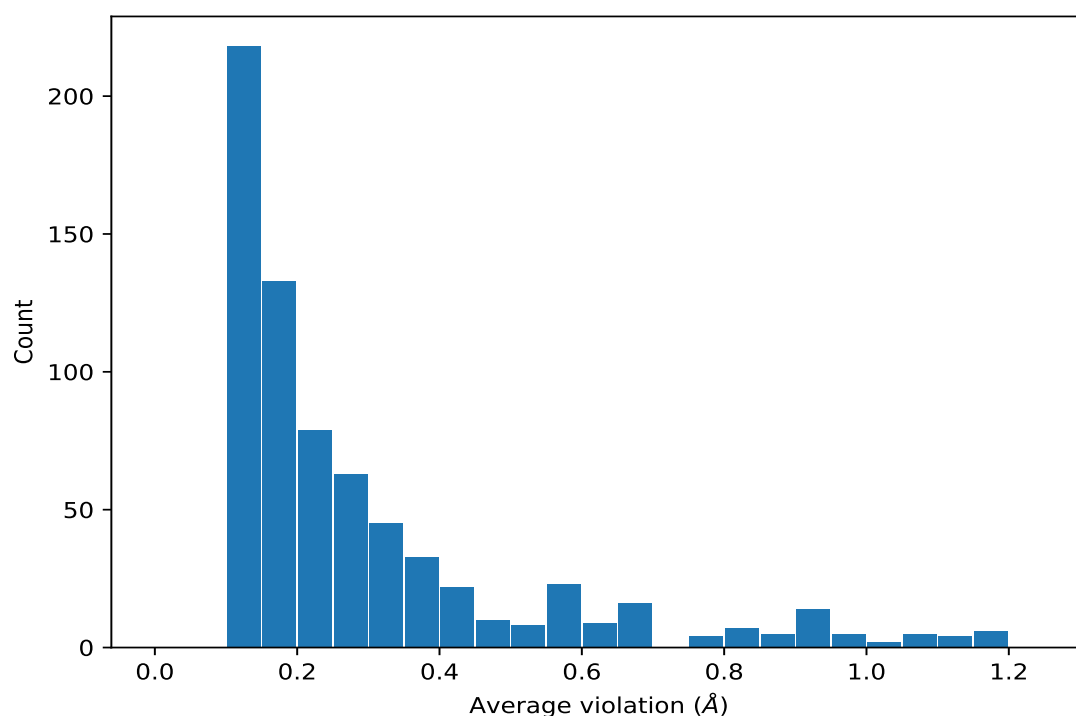
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

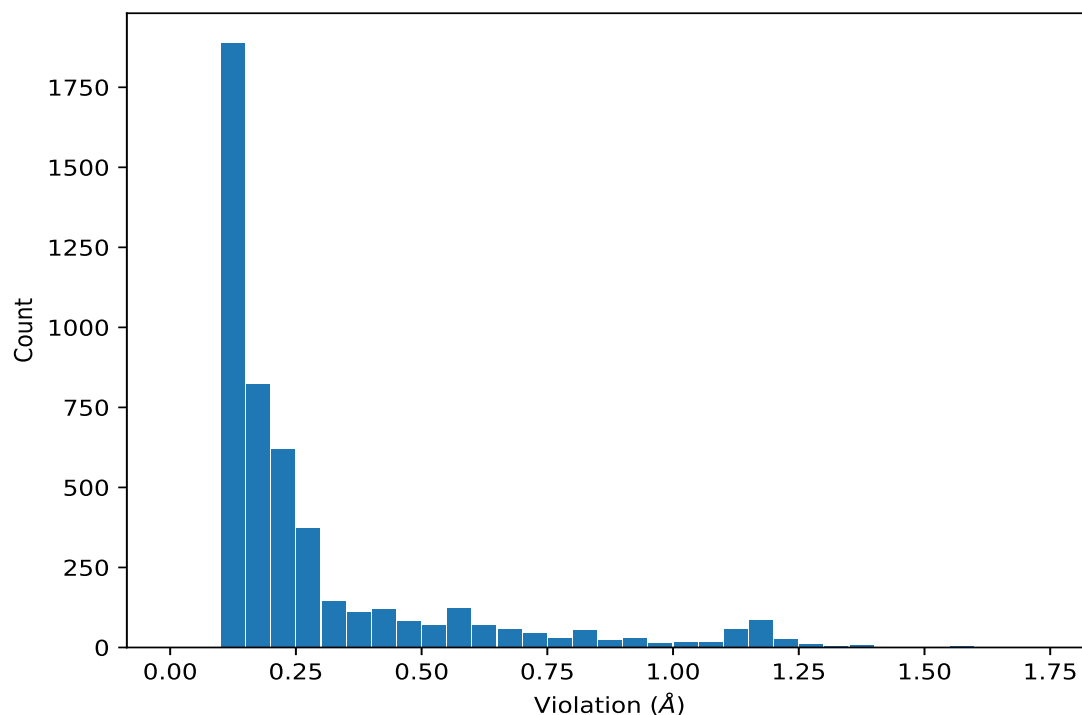
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,396)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	20	1.2	0.06	1.19
(2,1193)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	20	1.2	0.06	1.19
(2,397)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.2	0.1	1.18
(2,1194)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.2	0.1	1.18
(2,395)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	20	1.18	0.03	1.18
(2,1192)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	20	1.18	0.03	1.18
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	20	1.11	0.08	1.12
(2,277)	1:21:C:ILE:HB	1:13:C:PRO:HB2	20	1.11	0.08	1.12
(2,276)	1:21:B:ILE:HB	1:13:B:PRO:HB2	20	1.1	0.25	1.13
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	20	1.1	0.25	1.13
(2,275)	1:21:A:ILE:HB	1:13:A:PRO:HB2	20	1.09	0.2	1.13
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	20	1.09	0.2	1.13
(2,1168)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	20	0.95	0.34	1.04

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)
(2,1168)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	20	1.74
(2,1170)	1:35:C:ILE:HG12	1:13:C:PRO:HG3	4	1.62
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	2	1.6
(2,1170)	1:35:C:ILE:HG12	1:16:C:GLU:HG3	12	1.59
(2,1194)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	17	1.56
(2,1170)	1:35:C:ILE:HG12	1:13:C:PRO:HG3	10	1.56
(2,397)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	17	1.56
(2,353)	1:14:A:LYS:HD3	1:21:A:ILE:HA	9	1.53
(2,354)	1:14:B:LYS:HD2	1:21:B:ILE:HA	9	1.38
(2,1194)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.37

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

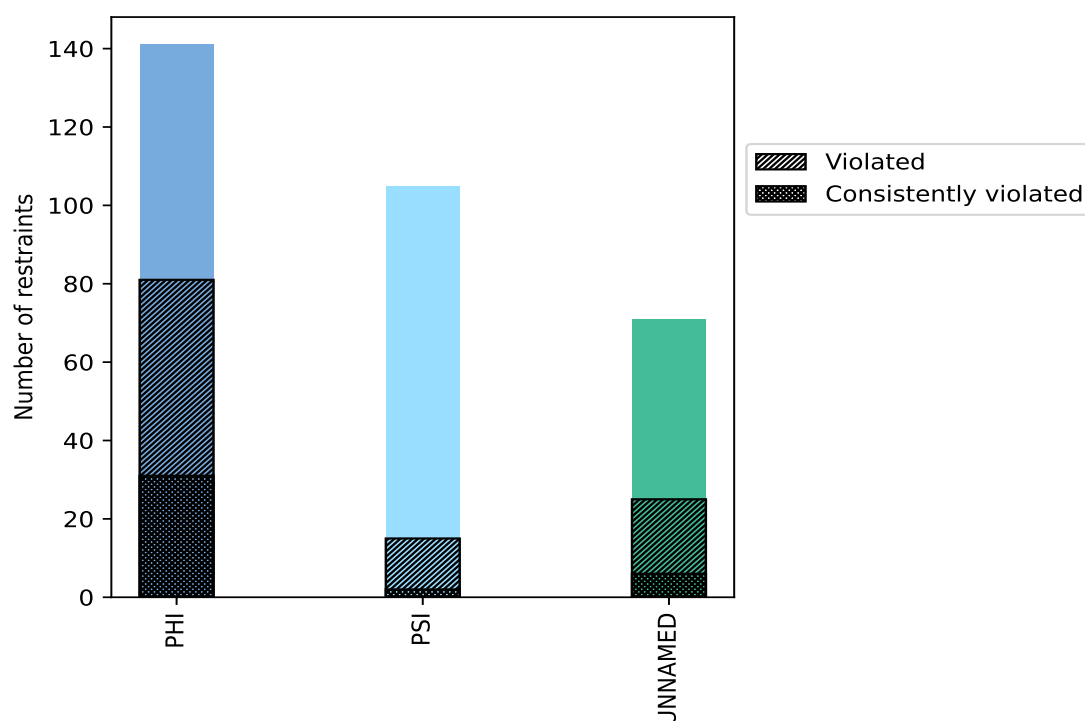
10.1 Summary of dihedral-angle violations [i](#)

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	141	44.5	81	57.4	25.6	31	22.0	9.8
PSI	105	33.1	15	14.3	4.7	2	1.9	0.6
UNNAMED	71	22.4	25	35.2	7.9	6	8.5	1.9
Total	317	100.0	121	38.2	38.2	39	12.3	12.3

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



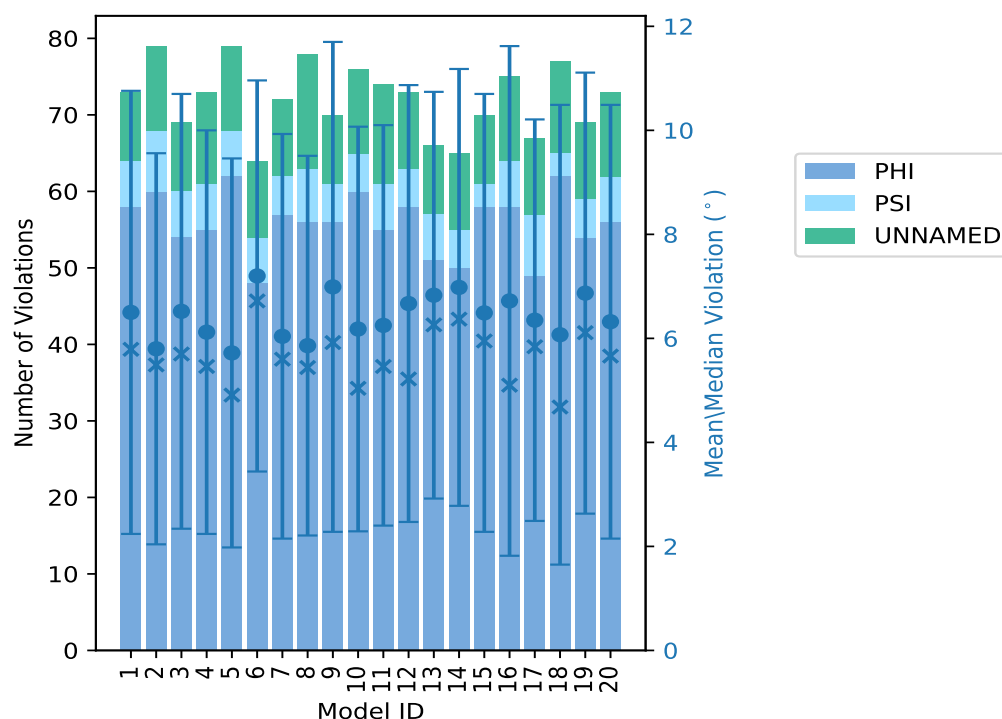
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	UNNAMED	Total				
1	58	6	9	73	6.5	18.88	4.26	5.79
2	60	8	11	79	5.8	15.66	3.76	5.49
3	54	6	9	69	6.52	16.99	4.18	5.7
4	55	6	12	73	6.12	15.25	3.88	5.46
5	62	6	11	79	5.72	16.37	3.74	4.91
6	48	6	10	64	7.2	17.04	3.76	6.72
7	57	5	10	72	6.04	16.28	3.89	5.6
8	56	7	15	78	5.86	14.88	3.65	5.44
9	56	5	9	70	6.99	18.23	4.71	5.92
10	60	5	11	76	6.18	15.08	3.89	5.04
11	55	6	13	74	6.25	15.34	3.85	5.46
12	58	5	10	73	6.67	17.1	4.2	5.22
13	51	6	9	66	6.83	17.25	3.91	6.26
14	50	5	10	65	6.98	17.62	4.2	6.37
15	58	3	9	70	6.49	15.8	4.21	5.95
16	58	6	11	75	6.72	20.56	4.9	5.1
17	49	8	10	67	6.35	16.68	3.86	5.84
18	62	3	12	77	6.07	17.0	4.42	4.68
19	54	5	10	69	6.87	18.53	4.24	6.11
20	56	6	11	73	6.32	18.35	4.17	5.66

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	UNNAMED	Total	Count ¹	%
6	6	6	18	1	5.0
7	1	1	9	2	10.0
2	1	8	11	3	15.0
1	0	0	1	4	20.0
2	1	1	4	5	25.0
1	0	0	1	6	30.0
3	0	0	3	7	35.0
1	0	0	1	8	40.0
1	0	0	1	9	45.0
1	0	0	1	10	50.0
0	1	0	1	11	55.0

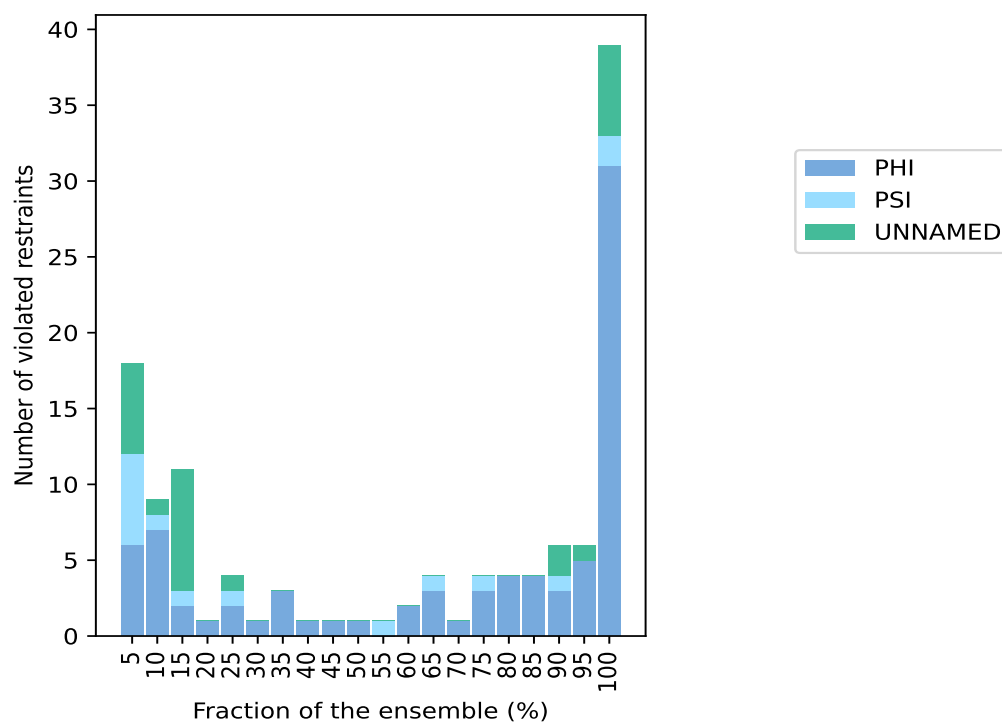
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Number of violated restraints				Fraction of the ensemble	
PHI	PSI	UNNAMED	Total	Count ¹	%
2	0	0	2	12	60.0
3	1	0	4	13	65.0
1	0	0	1	14	70.0
3	1	0	4	15	75.0
4	0	0	4	16	80.0
4	0	0	4	17	85.0
3	1	2	6	18	90.0
5	0	1	6	19	95.0
31	2	6	39	20	100.0

¹ Number of models with violations

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

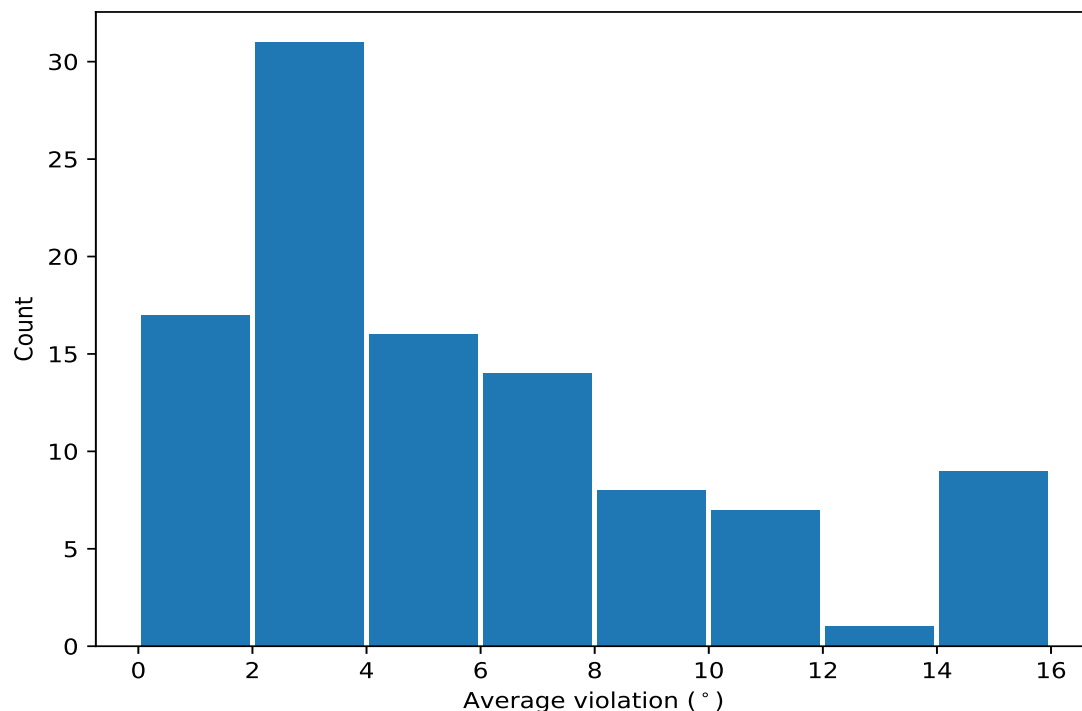


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

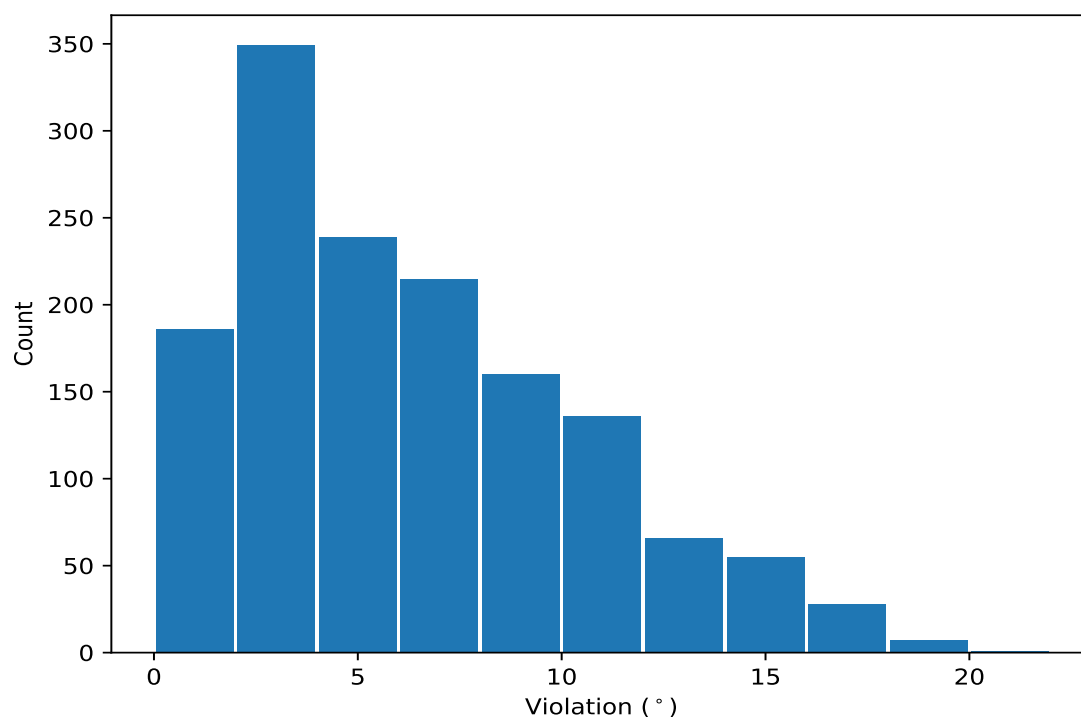
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	20	15.61	1.8	15.4
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	20	15.31	2.36	15.7
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	20	14.9	2.19	15.4
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	20	14.59	0.86	14.66
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	20	14.49	1.27	14.76
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	20	14.48	0.96	14.33
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	20	11.11	0.71	11.0
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	20	10.99	0.66	11.08
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	20	10.93	0.77	10.84
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	20	10.92	1.3	10.75

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	16	20.56
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	1	18.88
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	19	18.53
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	20	18.35
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	9	18.23
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	16	18.2
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	19	18.11
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	16	18.02
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	9	17.94
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	9	17.85