



# 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  
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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](mailto:validation@mail.wwpdb.org)

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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>.

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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 : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR, 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](#)

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

#### 6.3.2 Protein sidechains [i](#)

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

#### 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](#)

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

### 6.5 Carbohydrates [i](#)

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

### 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	$-0.63 \pm 0.13$	Should be applied
$^{13}\text{C}_\beta$	47	$-0.27 \pm 0.18$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	48	$-0.18 \pm 0.25$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	49	$0.69 \pm 0.64$	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	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
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	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
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%)

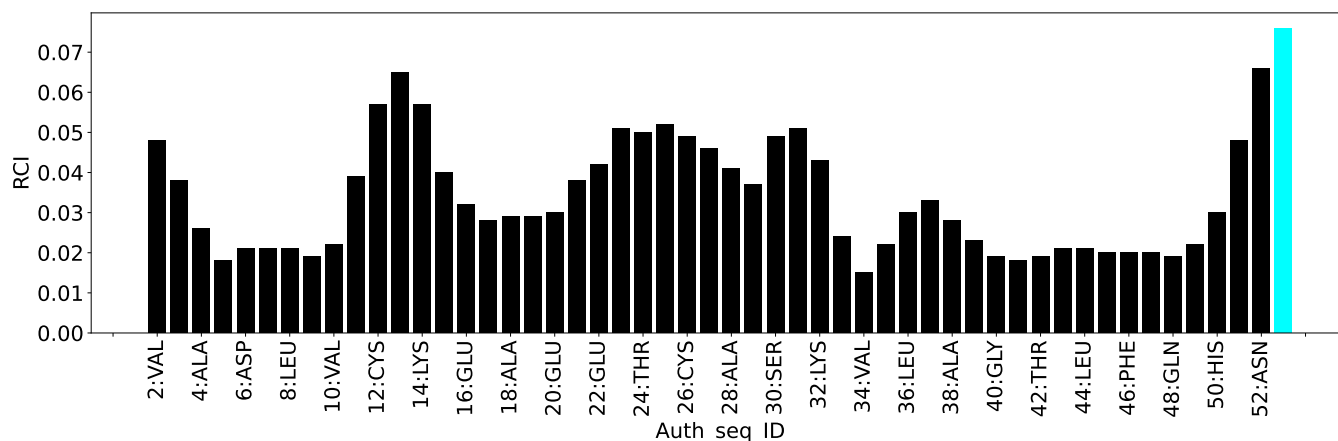
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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 [i](#)

### 8.1 Conformationally restricting restraints [i](#)

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	6897
Intra-residue ( $ i-j =0$ )	2154
Sequential ( $ i-j =1$ )	1730
Medium range ( $ i-j >1$ and $ i-j <5$ )	1303
Long range ( $ i-j \geq 5$ )	1183
Inter-chain	527
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	315
Number of unmapped restraints	0
Number of restraints per residue	44.5
Number of long range restraints per residue <sup>1</sup>	7.3

<sup>1</sup>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 [i](#)

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 [i](#)

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)	68.2	0.2
0.2-0.5 (Medium)	42.3	0.5
>0.5 (Large)	33.9	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 ⓘ

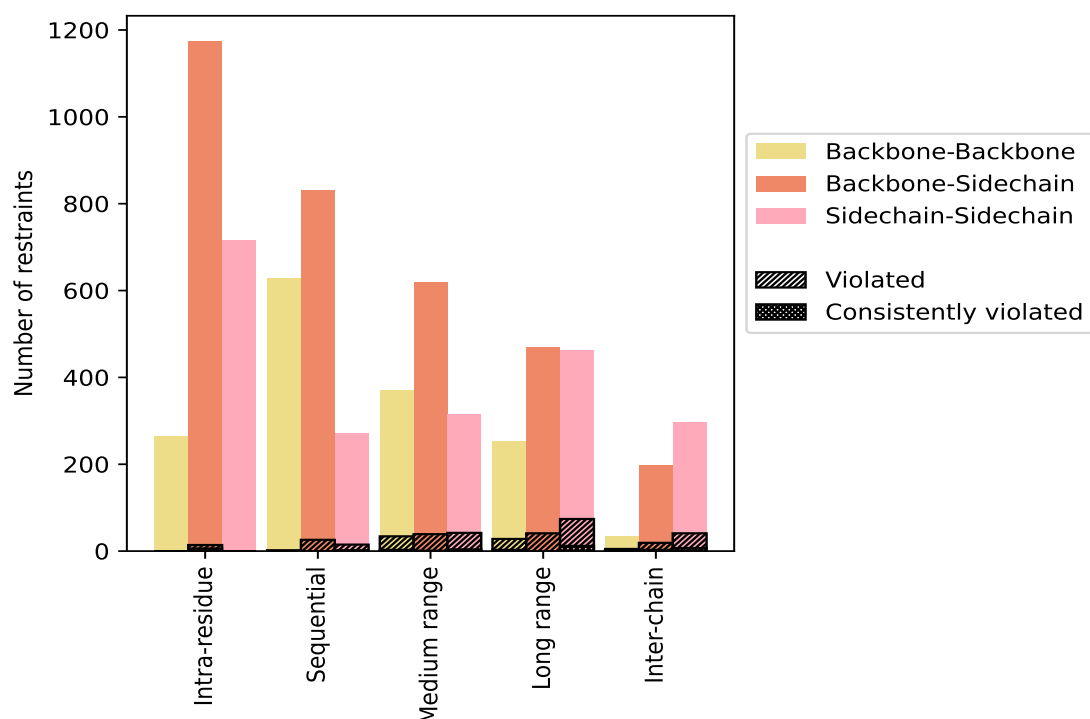
### 9.1 Summary of distance violations ⓘ

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>2154</b>	<b>31.2</b>	<b>14</b>	<b>0.6</b>	<b>0.2</b>	<b>6</b>	<b>0.3</b>	<b>0.1</b>
Backbone-Backbone	264	3.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1174	17.0	14	1.2	0.2	6	0.5	0.1
Sidechain-Sidechain	716	10.4	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>1730</b>	<b>25.1</b>	<b>43</b>	<b>2.5</b>	<b>0.6</b>	<b>2</b>	<b>0.1</b>	<b>0.0</b>
Backbone-Backbone	628	9.1	2	0.3	0.0	0	0.0	0.0
Backbone-Sidechain	830	12.0	26	3.1	0.4	0	0.0	0.0
Sidechain-Sidechain	272	3.9	15	5.5	0.2	2	0.7	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>1303</b>	<b>18.9</b>	<b>115</b>	<b>8.8</b>	<b>1.7</b>	<b>8</b>	<b>0.6</b>	<b>0.1</b>
Backbone-Backbone	369	5.4	34	9.2	0.5	3	0.8	0.0
Backbone-Sidechain	619	9.0	39	6.3	0.6	1	0.2	0.0
Sidechain-Sidechain	315	4.6	42	13.3	0.6	4	1.3	0.1
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>1183</b>	<b>17.2</b>	<b>143</b>	<b>12.1</b>	<b>2.1</b>	<b>15</b>	<b>1.3</b>	<b>0.2</b>
Backbone-Backbone	252	3.7	28	11.1	0.4	3	1.2	0.0
Backbone-Sidechain	469	6.8	41	8.7	0.6	0	0.0	0.0
Sidechain-Sidechain	462	6.7	74	16.0	1.1	12	2.6	0.2
<b>Inter-chain</b>	<b>527</b>	<b>7.6</b>	<b>65</b>	<b>12.3</b>	<b>0.9</b>	<b>13</b>	<b>2.5</b>	<b>0.2</b>
Backbone-Backbone	33	0.5	5	15.2	0.1	3	9.1	0.0
Backbone-Sidechain	198	2.9	19	9.6	0.3	3	1.5	0.0
Sidechain-Sidechain	296	4.3	41	13.9	0.6	7	2.4	0.1
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
<b>Total</b>	<b>6897</b>	<b>100.0</b>	<b>380</b>	<b>5.5</b>	<b>5.5</b>	<b>44</b>	<b>0.6</b>	<b>0.6</b>
Backbone-Backbone	1546	22.4	69	4.5	1.0	9	0.6	0.1
Backbone-Sidechain	3290	47.7	139	4.2	2.0	10	0.3	0.1
Sidechain-Sidechain	2061	29.9	172	8.3	2.5	25	1.2	0.4

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

## 9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	10	26	53	44	17	150	0.32	1.31	0.3	0.19
2	8	20	43	57	17	145	0.34	1.6	0.31	0.21
3	6	16	46	56	23	147	0.35	1.21	0.31	0.2
4	8	15	45	59	18	145	0.36	1.62	0.33	0.21
5	8	23	40	61	21	153	0.34	1.28	0.29	0.21
6	8	25	50	62	18	163	0.34	1.35	0.31	0.21
7	8	17	44	63	17	149	0.33	1.24	0.29	0.21
8	8	21	42	52	17	140	0.35	1.2	0.3	0.22
9	8	16	47	57	19	147	0.39	1.53	0.34	0.22
10	8	14	42	49	23	136	0.38	1.56	0.33	0.24

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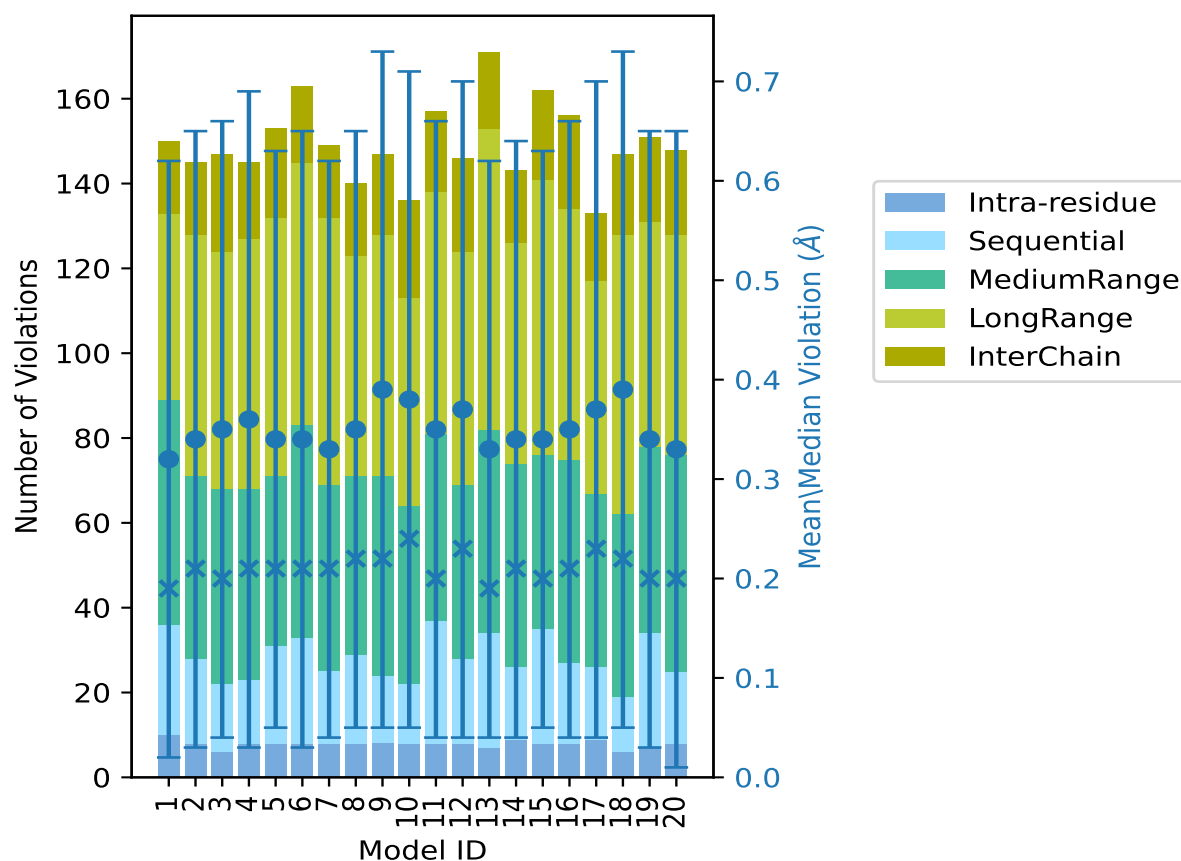
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	8	29	44	57	19	157	0.35	1.22	0.31	0.2
12	8	20	41	55	22	146	0.37	1.59	0.33	0.23
13	7	27	48	71	18	171	0.33	1.2	0.29	0.19
14	9	17	48	52	17	143	0.34	1.33	0.3	0.21
15	8	27	41	65	21	162	0.34	1.18	0.29	0.2
16	8	19	48	59	22	156	0.35	1.21	0.31	0.21
17	9	17	41	50	16	133	0.37	1.56	0.33	0.23
18	6	13	43	66	19	147	0.39	1.32	0.34	0.22
19	7	27	44	53	20	151	0.34	1.28	0.31	0.2
20	8	17	51	52	20	148	0.33	1.74	0.32	0.2

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>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 ⓘ

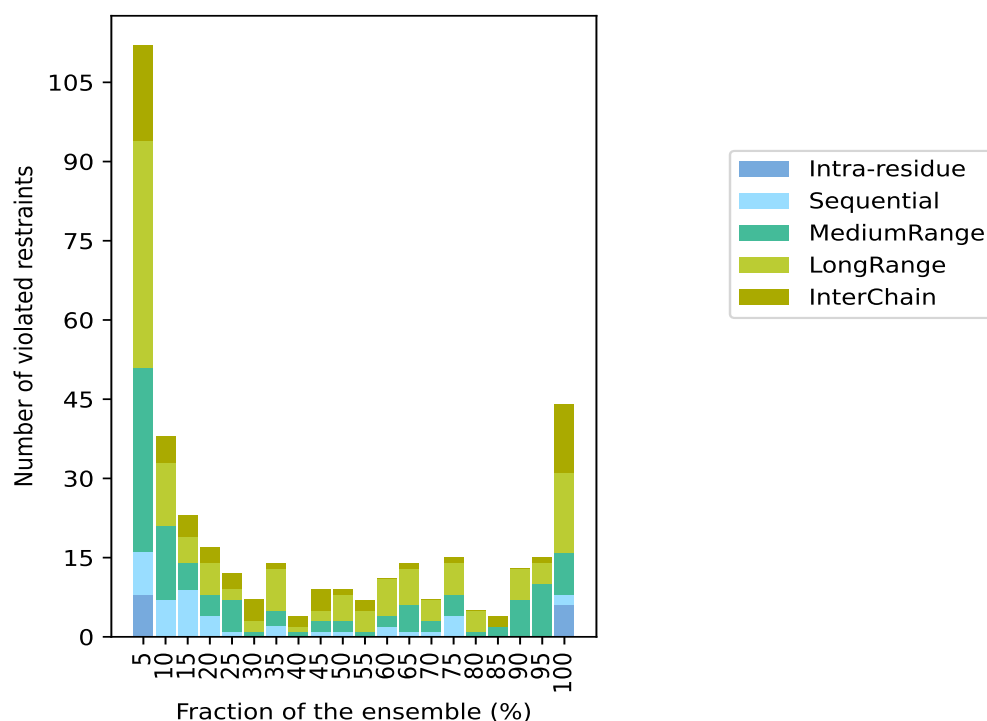
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 6517(IR:2140, SQ:1687, MR:1188, LR:1040, IC:462) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
8	8	35	43	18	112	1	5.0
0	7	14	12	5	38	2	10.0
0	9	5	5	4	23	3	15.0
0	4	4	6	3	17	4	20.0
0	1	6	2	3	12	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	0	11	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	13	44	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

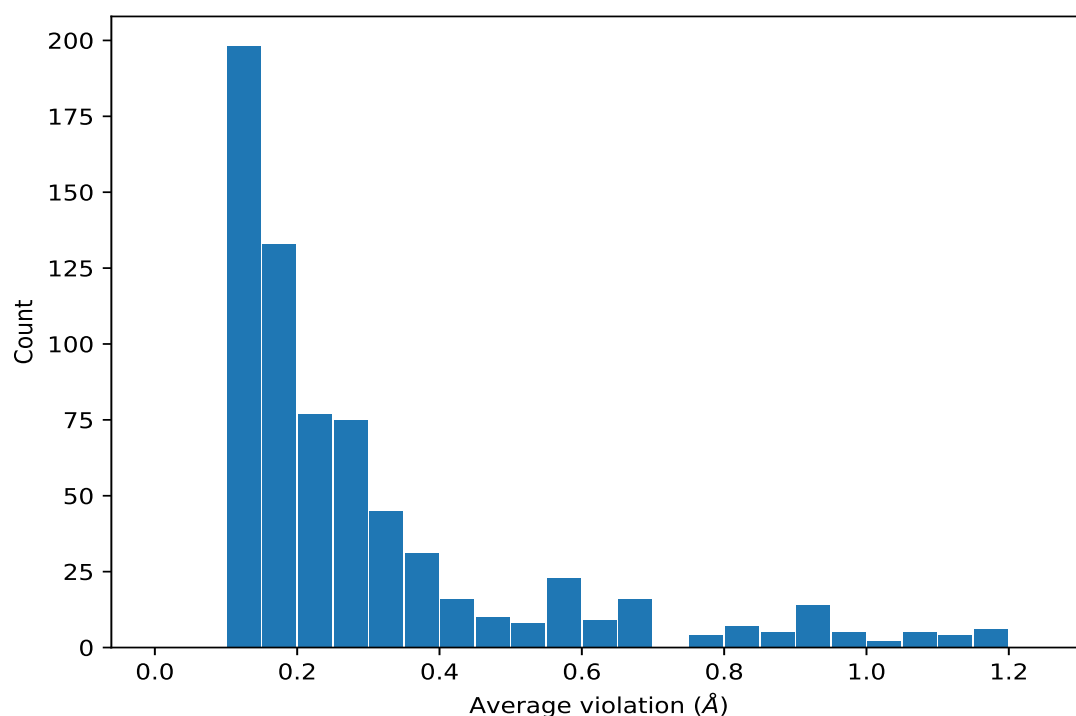
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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.

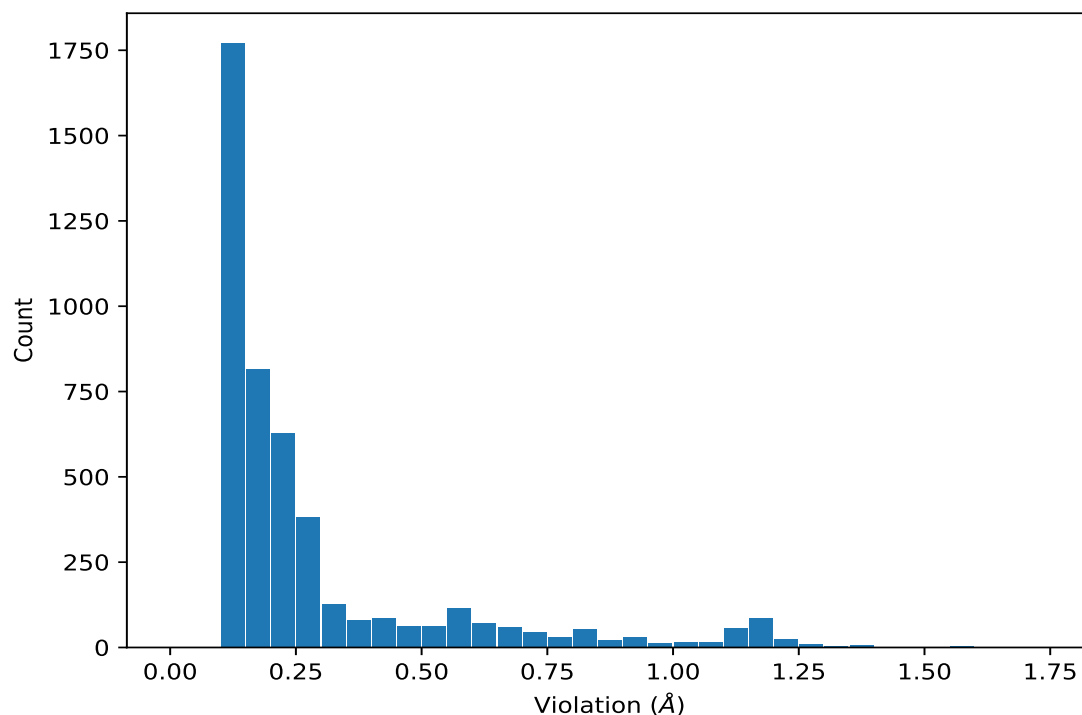
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	20	1.2	0.06	1.19
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	20	1.2	0.06	1.19
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.2	0.1	1.18
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.2	0.1	1.18
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	20	1.18	0.03	1.18
(2,1185)	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
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	20	0.95	0.34	1.04

<sup>1</sup>Number of violated models, <sup>2</sup>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)
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	20	1.74
(2,1163)	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
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG3	12	1.59
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	17	1.56
(2,1163)	1:35:C:ILE:HG12	1:13:C:PRO:HG3	10	1.56
(2,395)	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
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.37

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

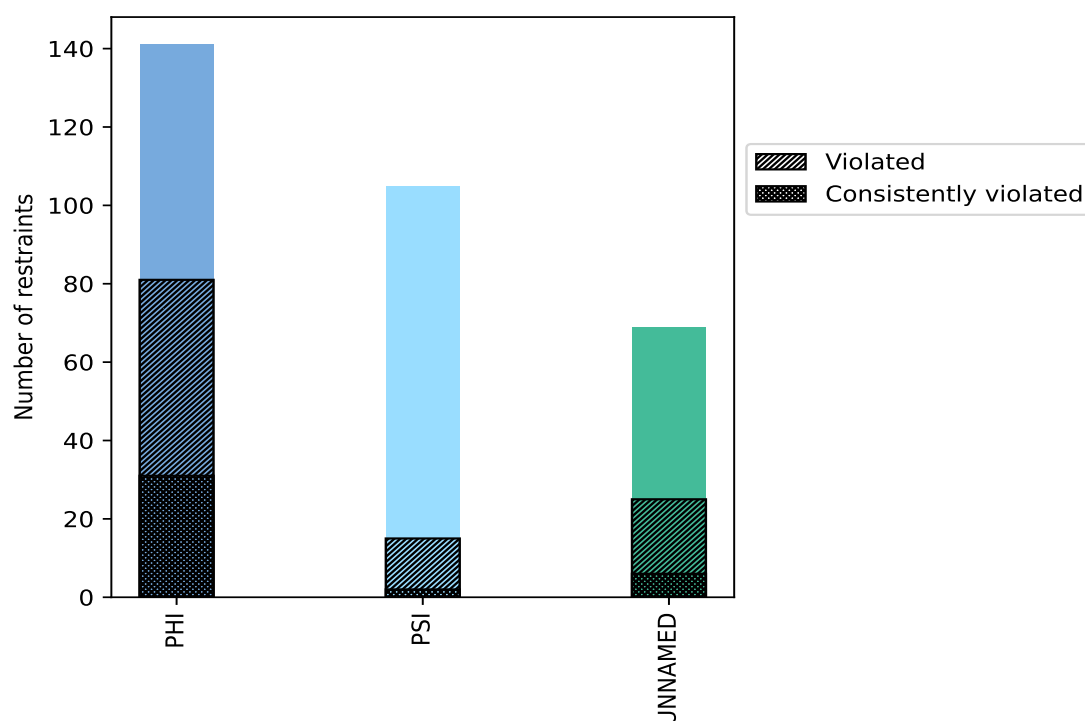
### 10.1 Summary of dihedral-angle violations [i](#)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	141	44.8	81	57.4	25.7	31	22.0	9.8
PSI	105	33.3	15	14.3	4.8	2	1.9	0.6
UNNAMED	69	21.9	25	36.2	7.9	6	8.7	1.9
Total	315	100.0	121	38.4	38.4	39	12.4	12.4

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

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



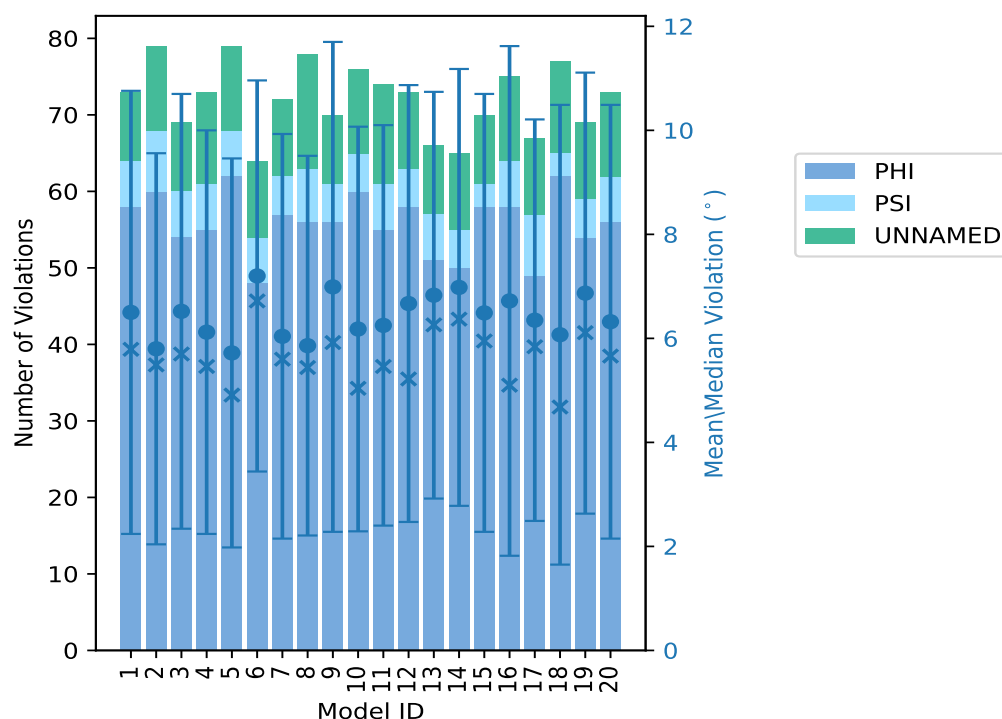
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 <sup>1</sup>	%
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

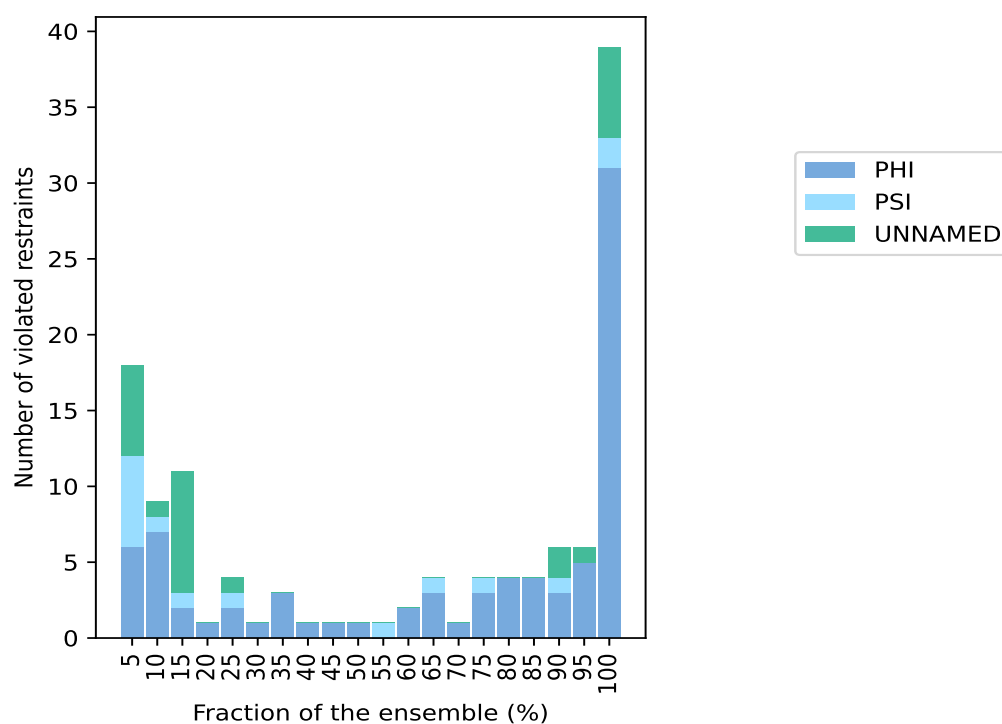
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Number of violated restraints				Fraction of the ensemble	
PHI	PSI	UNNAMED	Total	Count <sup>1</sup>	%
2	0	0	2	12	60.0
3	1	0	4	13	65.0
1	0	0	1	14	70.0
3	1	0	4	15	75.0
4	0	0	4	16	80.0
4	0	0	4	17	85.0
3	1	2	6	18	90.0
5	0	1	6	19	95.0
31	2	6	39	20	100.0

<sup>1</sup> Number of models with violations

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



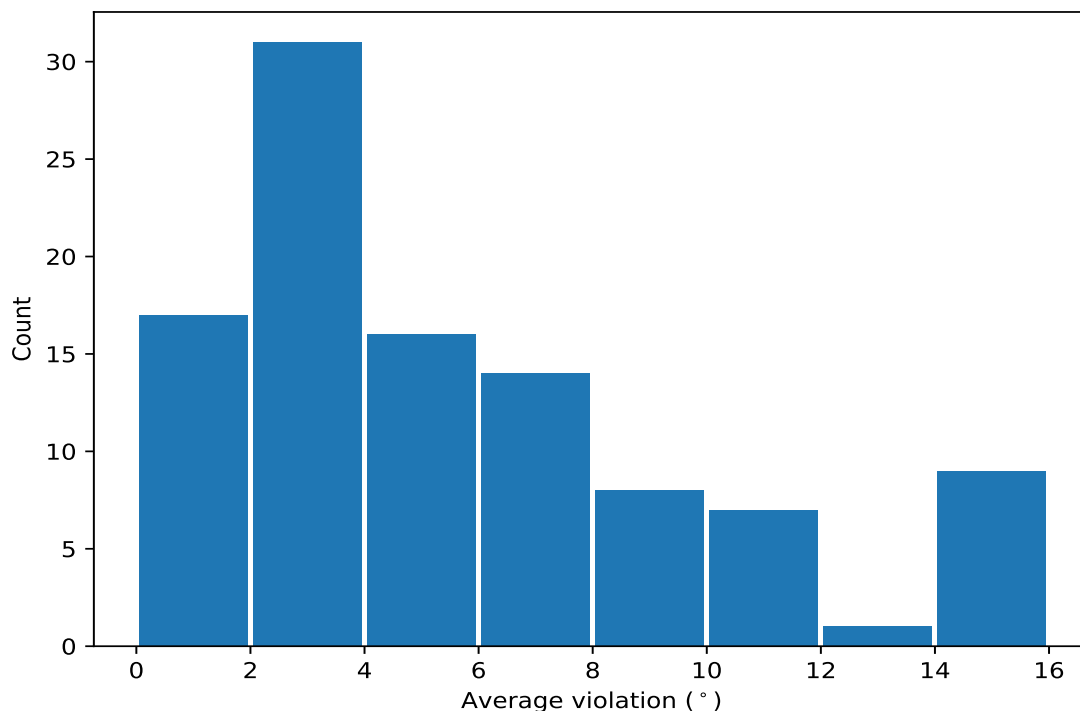
## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

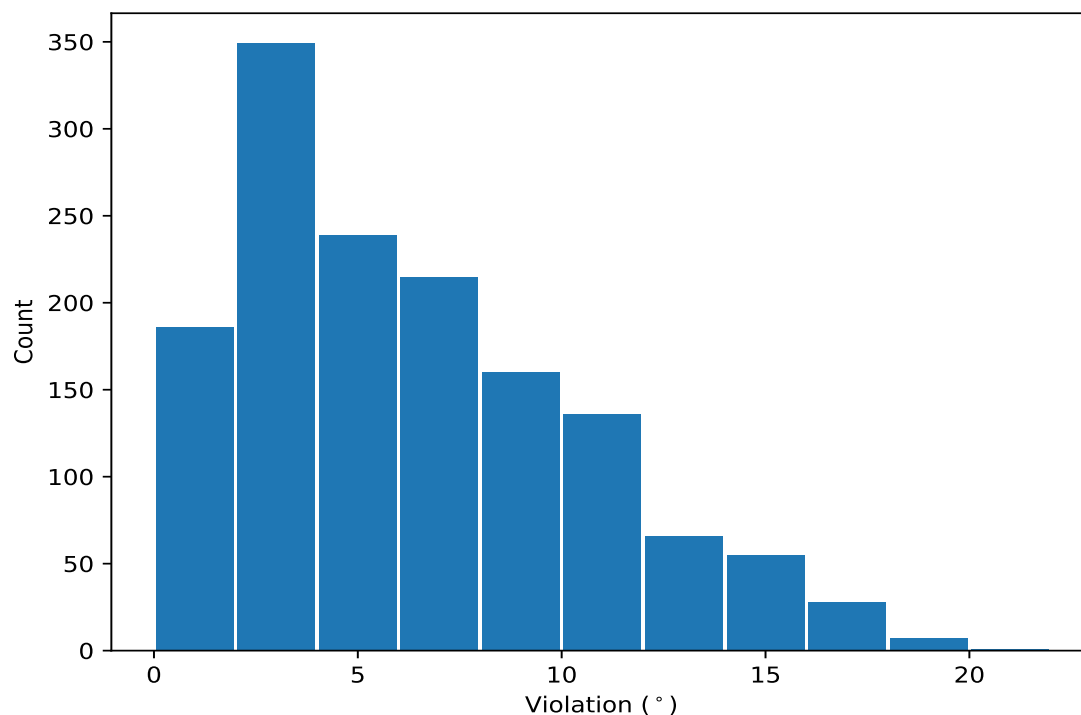
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	20	15.61	1.8	15.4
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	20	15.31	2.36	15.7
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	20	14.9	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

<sup>1</sup> Number of violated models, <sup>2</sup>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 [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