



# wwPDB NMR Structure Validation Summary Report ⓘ

Dec 24, 2024 – 04:35 PM EST

PDB ID : 2LLS  
BMRB ID : 18087  
Title : solution structure of human apo-S100A1 C85M  
Authors : Budzinska, M.; Jaremko, L.; Jaremko, M.; Zdanowski, K.; Zhukov, I.; Bierzynski, A.; Ejchart, A.  
Deposited on : 2011-11-17

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)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
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) : 2.40

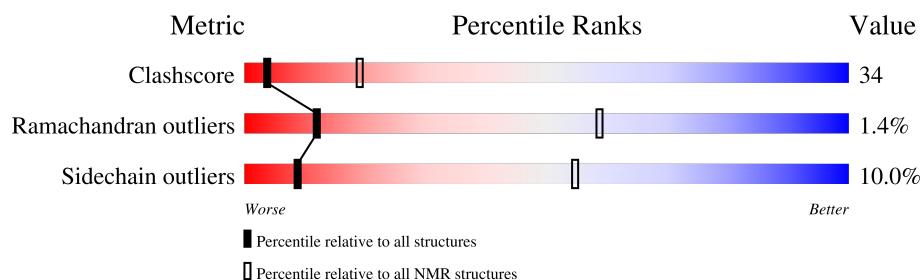
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 47%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	93	
1	B	93	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:2-A:90, B:2-B:89 (177)	0.88	11

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 4 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2888 atoms, of which 1420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A1.

Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1444	463	710	115	153	3	
1	B	93	Total	C	H	N	O	S	0
			1444	463	710	115	153	3	

There are 2 discrepancies between the modelled and reference sequences:

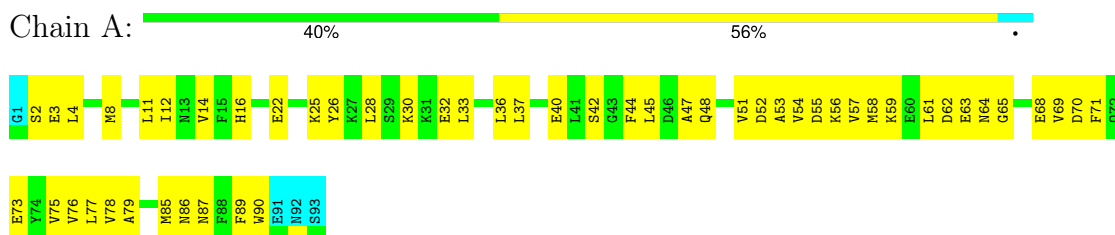
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	MET	CYS	engineered mutation	UNP P23297
B	85	MET	CYS	engineered mutation	UNP P23297

## 4 Residue-property plots

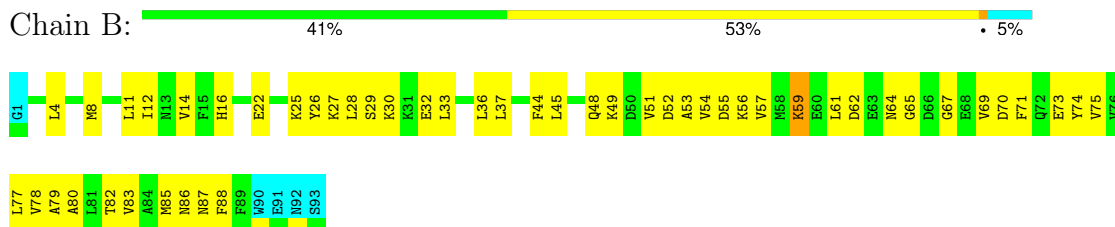
### 4.1 Average score per residue in the NMR ensemble

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: Protein S100-A1



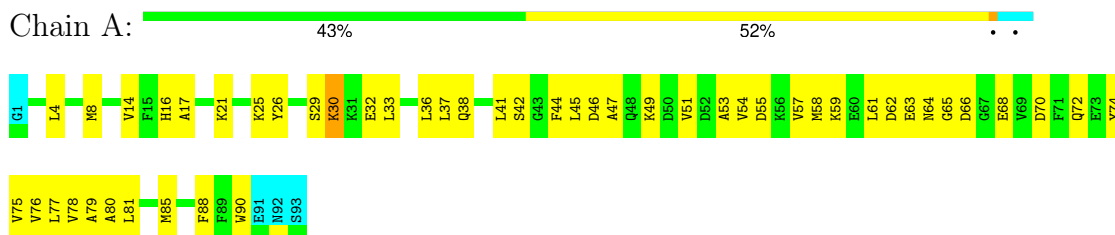
#### • Molecule 1: Protein S100-A1



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

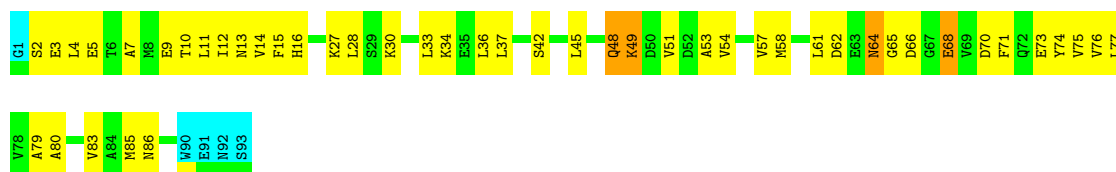
The representative model is number 11. Colouring as in section 4.1 above.

#### • Molecule 1: Protein S100-A1



#### • Molecule 1: Protein S100-A1

Chain B:



## 5 Refinement protocol and experimental data overview

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

Of the 200 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	refinement	2.26
CYANA	structure solution	

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	1148
Number of shifts mapped to atoms	1148
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.91±0.01	0±0/717 ( 0.0± 0.0%)	0.76±0.01	0±0/966 ( 0.0± 0.0%)
1	B	0.91±0.01	0±0/701 ( 0.0± 0.1%)	0.73±0.01	0±0/943 ( 0.0± 0.0%)
All	All	0.91	8/28360 ( 0.0%)	0.74	0/38180 ( 0.0%)

5 of 7 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	9	GLU	CD-OE2	-5.34	1.19	1.25	4	2
1	B	73	GLU	CD-OE1	-5.25	1.19	1.25	16	1
1	B	5	GLU	CD-OE2	-5.24	1.19	1.25	7	1
1	A	73	GLU	CD-OE1	-5.19	1.20	1.25	7	1
1	B	35	GLU	CD-OE1	-5.11	1.20	1.25	2	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	706	690	688	54±7
1	B	692	680	678	53±9
All	All	27960	27400	27320	1863

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 34.

5 of 662 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG21	1:B:4:LEU:HD21	1.00	1.29	1	4
1:A:11:LEU:HD23	1:B:4:LEU:HD22	0.93	1.39	14	9
1:A:14:VAL:HG21	1:B:4:LEU:HD11	0.89	1.42	13	9
1:A:75:VAL:HG21	1:B:79:ALA:CB	0.89	1.96	12	20
1:B:47:ALA:HB3	1:B:85:MET:SD	0.89	2.07	18	8

## 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	89/93 (96%)	83±1 (94±2%)	5±2 (5±2%)	1±1 (1±1%)	14	62
1	B	88/93 (95%)	82±2 (94±2%)	4±1 (5±1%)	1±1 (2±1%)	11	57
All	All	3540/3720 (95%)	3316 (94%)	175 (5%)	49 (1%)	12	59

5 of 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	67	GLY	12
1	A	67	GLY	8
1	B	23	GLY	5
1	B	24	ASP	3
1	B	25	LYS	3

### 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	77/80 (96%)	69±2 (90±3%)	8±2 (10±3%)	8	53
1	B	76/80 (95%)	69±2 (90±3%)	7±2 (10±3%)	9	55
All	All	3060/3200 (96%)	2755 (90%)	305 (10%)	9	55

5 of 69 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	70	ASP	16
1	B	70	ASP	15
1	B	48	GLN	13
1	B	59	LYS	12
1	A	42	SER	11

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 47% for the well-defined parts and 46% 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	1148
Number of shifts mapped to atoms	1148
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	93	$-0.42 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	87	$0.12 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	73	$-0.36 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	86	$0.45 \pm 0.31$	None needed ( $< 0.5$ ppm)

#### 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 47%, i.e. 1115 atoms were assigned a chemical shift out of a possible 2380. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	419/895 (47%)	177/364 (49%)	159/354 (45%)	83/177 (47%)
Sidechain	619/1305 (47%)	423/844 (50%)	189/429 (44%)	7/32 (22%)

*Continued on next page...*

Continued from previous page...

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	77/180 (43%)	39/88 (44%)	37/83 (45%)	1/9 (11%)
Overall	1115/2380 (47%)	639/1296 (49%)	385/866 (44%)	91/218 (42%)

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

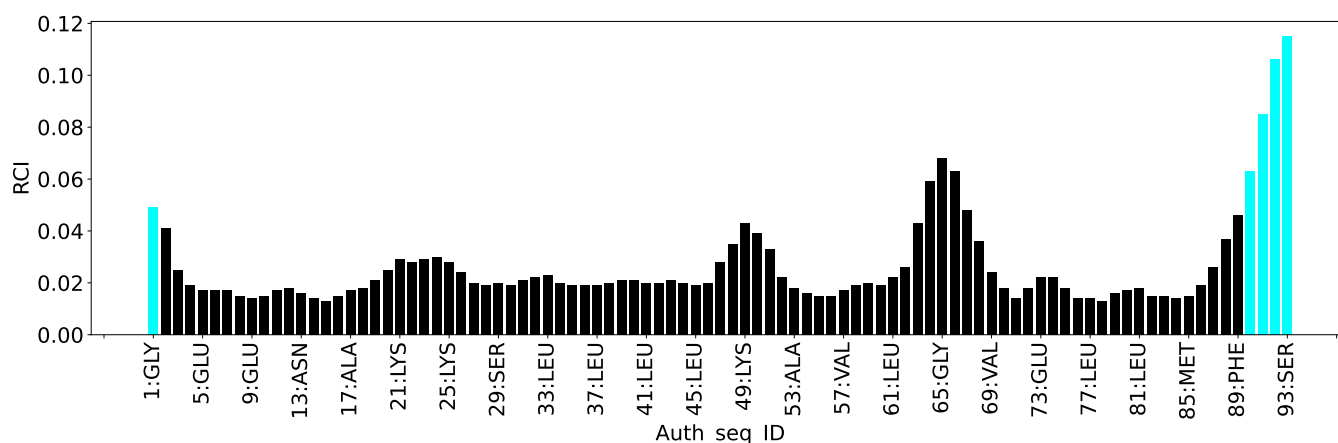
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	19	SER	HB3	2.42	2.49 – 5.20	-5.3

#### 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	3740
Intra-residue ( $ i-j =0$ )	756
Sequential ( $ i-j =1$ )	986
Medium range ( $ i-j >1$ and $ i-j <5$ )	1007
Long range ( $ i-j \geq 5$ )	645
Inter-chain	346
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	292
Number of unmapped restraints	0
Number of restraints per residue	21.7
Number of long range restraints per residue <sup>1</sup>	3.5

<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

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)	64.5	0.2
0.2-0.5 (Medium)	31.2	0.5
>0.5 (Large)	43.8	4.08

### 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)	3.5	4.77
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis

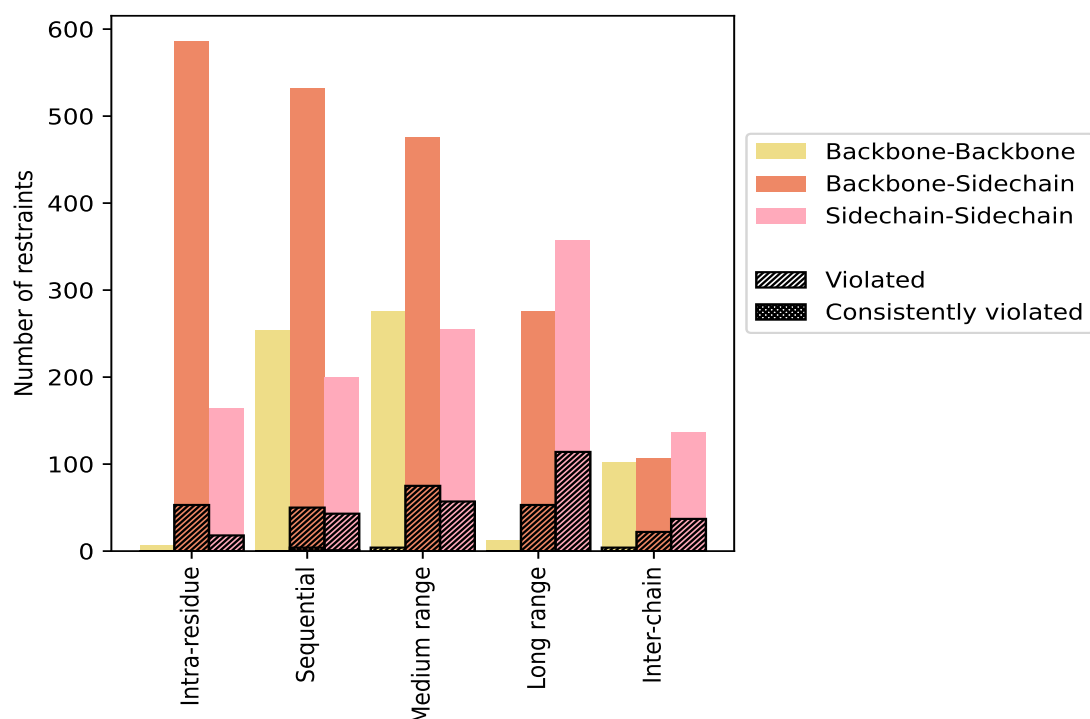
### 9.1 Summary of distance violations

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.

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>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">756</a>	<a href="#">20.2</a>	<a href="#">71</a>	<a href="#">9.4</a>	<a href="#">1.9</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	6	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	586	15.7	53	9.0	1.4	0	0.0	0.0
Sidechain-Sidechain	164	4.4	18	11.0	0.5	0	0.0	0.0
<a href="#">Sequential ( i-j =1)</a>	<a href="#">986</a>	<a href="#">26.4</a>	<a href="#">93</a>	<a href="#">9.4</a>	<a href="#">2.5</a>	<a href="#">5</a>	<a href="#">0.5</a>	<a href="#">0.1</a>
Backbone-Backbone	254	6.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	532	14.2	50	9.4	1.3	4	0.8	0.1
Sidechain-Sidechain	200	5.3	43	21.5	1.1	1	0.5	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">1007</a>	<a href="#">26.9</a>	<a href="#">136</a>	<a href="#">13.5</a>	<a href="#">3.6</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	276	7.4	4	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	476	12.7	75	15.8	2.0	0	0.0	0.0
Sidechain-Sidechain	255	6.8	57	22.4	1.5	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">645</a>	<a href="#">17.2</a>	<a href="#">167</a>	<a href="#">25.9</a>	<a href="#">4.5</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	12	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	276	7.4	53	19.2	1.4	0	0.0	0.0
Sidechain-Sidechain	357	9.5	114	31.9	3.0	0	0.0	0.0
<a href="#">Inter-chain</a>	<a href="#">346</a>	<a href="#">9.3</a>	<a href="#">63</a>	<a href="#">18.2</a>	<a href="#">1.7</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	102	2.7	4	3.9	0.1	0	0.0	0.0
Backbone-Sidechain	107	2.9	22	20.6	0.6	0	0.0	0.0
Sidechain-Sidechain	137	3.7	37	27.0	1.0	0	0.0	0.0
<a href="#">Hydrogen bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">3740</a>	<a href="#">100.0</a>	<a href="#">530</a>	<a href="#">14.2</a>	<a href="#">14.2</a>	<a href="#">5</a>	<a href="#">0.1</a>	<a href="#">0.1</a>
Backbone-Backbone	650	17.4	8	1.2	0.2	0	0.0	0.0
Backbone-Sidechain	1977	52.9	253	12.8	6.8	4	0.2	0.1
Sidechain-Sidechain	1113	29.8	269	24.2	7.2	1	0.1	0.0

<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	19	27	31	38	24	139	0.63	3.2	0.79	0.2
2	15	33	35	52	25	160	0.75	3.26	0.87	0.24
3	22	32	32	27	14	127	0.54	3.16	0.75	0.19
4	17	23	38	39	19	136	0.5	3.07	0.69	0.2
5	18	27	32	29	27	133	0.58	4.05	0.76	0.2
6	20	27	35	39	13	134	0.47	2.61	0.65	0.18
7	21	20	42	75	14	172	0.76	3.16	0.78	0.34
8	14	30	32	40	25	141	0.63	3.38	0.81	0.2
9	22	29	30	37	17	135	0.51	2.74	0.68	0.18
10	17	31	39	35	21	143	0.61	3.01	0.79	0.19

*Continued on next page...*



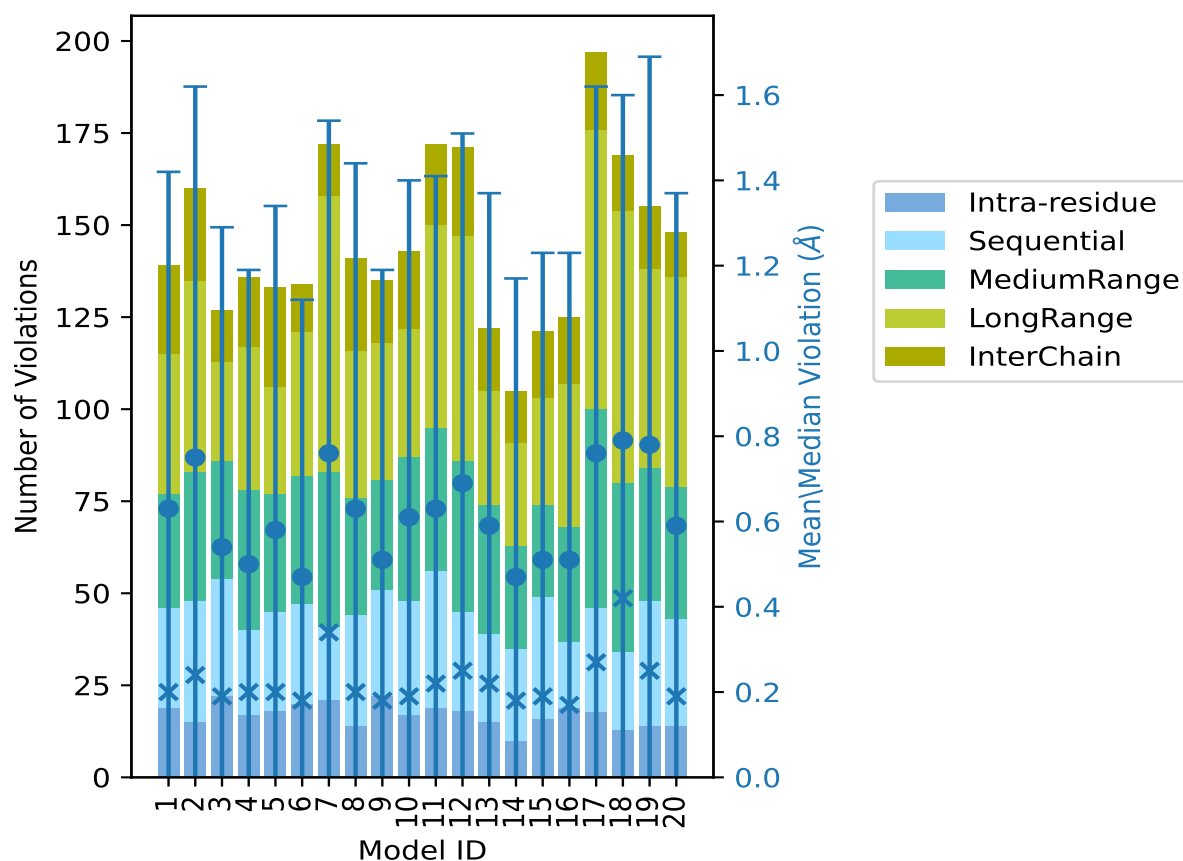
Continued from previous page...

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	19	37	39	55	22	172	0.63	3.53	0.78	0.22
12	18	27	41	61	24	171	0.69	4.08	0.82	0.25
13	15	24	35	31	17	122	0.59	2.8	0.78	0.22
14	10	25	28	28	14	105	0.47	3.21	0.7	0.18
15	16	33	25	29	18	121	0.51	2.99	0.72	0.19
16	19	18	31	39	18	125	0.51	3.01	0.72	0.17
17	18	28	54	76	21	197	0.76	4.02	0.86	0.27
18	13	21	46	74	15	169	0.79	3.72	0.81	0.42
19	14	34	36	54	17	155	0.78	3.73	0.91	0.25
20	14	29	36	57	12	148	0.59	4.02	0.78	0.19

<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 ⓘ

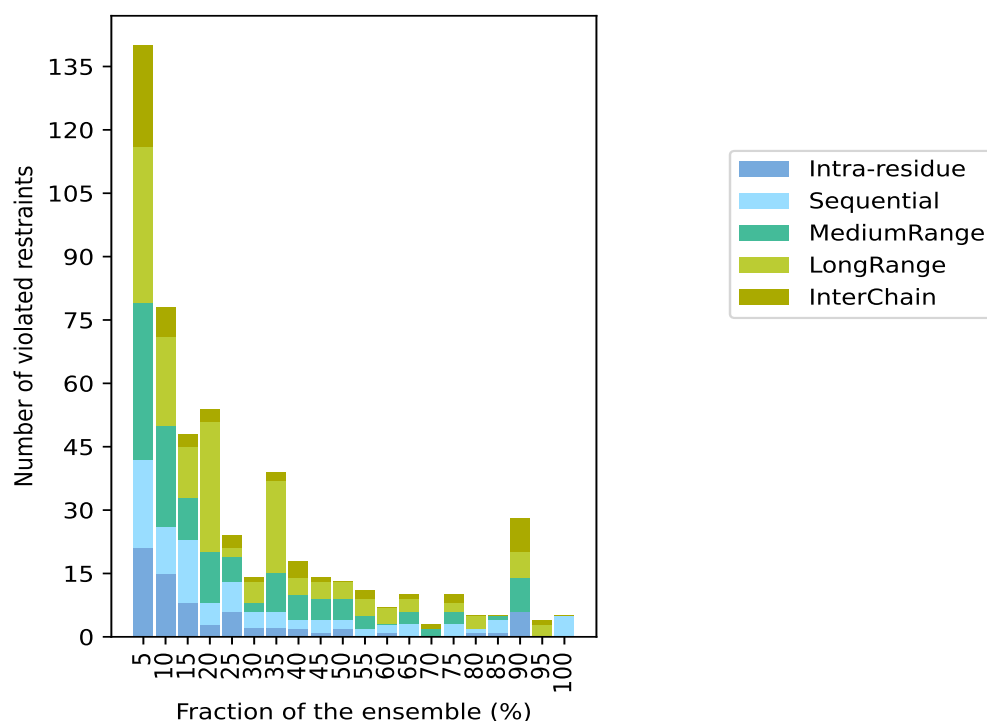
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3210(IR:685, SQ:893, MR:871, LR:478, IC:283) restraints are 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>	%
21	21	37	37	24	140	1	5.0
15	11	24	21	7	78	2	10.0
8	15	10	12	3	48	3	15.0
3	5	12	31	3	54	4	20.0
6	7	6	2	3	24	5	25.0
2	4	2	5	1	14	6	30.0
2	4	9	22	2	39	7	35.0
2	2	6	4	4	18	8	40.0
1	3	5	4	1	14	9	45.0
2	2	5	4	0	13	10	50.0
0	2	3	4	2	11	11	55.0
1	2	0	4	0	7	12	60.0
0	3	3	3	1	10	13	65.0
0	0	2	0	1	3	14	70.0
0	3	3	2	2	10	15	75.0
1	1	0	3	0	5	16	80.0
1	3	1	0	0	5	17	85.0
6	0	8	6	8	28	18	90.0
0	0	0	3	1	4	19	95.0
0	5	0	0	0	5	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

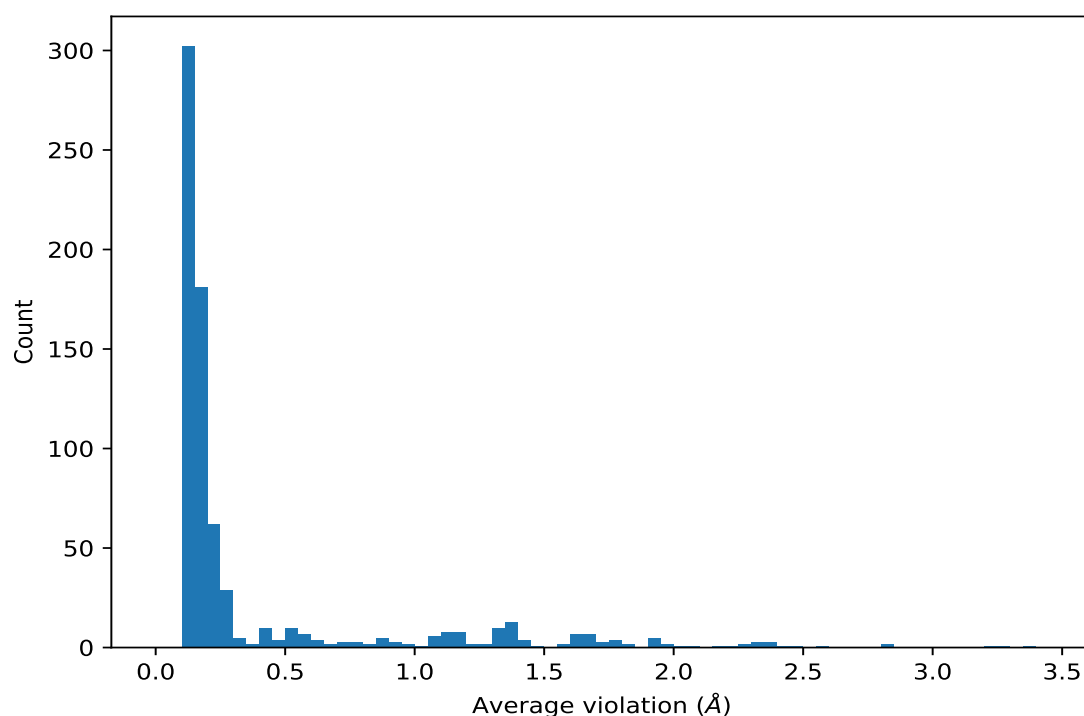
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(1,2824)	1:44:A:PHE:H	1:45:A:LEU:HG	20	0.42	0.04	0.42
(1,1031)	1:45:B:LEU:HD11	1:46:B:ASP:HB2	20	0.25	0.08	0.24
(1,1031)	1:45:B:LEU:HD12	1:46:B:ASP:HB2	20	0.25	0.08	0.24
(1,1031)	1:45:B:LEU:HD13	1:46:B:ASP:HB2	20	0.25	0.08	0.24
(1,2830)	1:44:B:PHE:H	1:45:B:LEU:HG	20	0.24	0.07	0.22
(1,1041)	1:75:A:VAL:HG21	1:76:A:VAL:H	20	0.17	0.04	0.17
(1,1041)	1:75:A:VAL:HG22	1:76:A:VAL:H	20	0.17	0.04	0.17
(1,1041)	1:75:A:VAL:HG23	1:76:A:VAL:H	20	0.17	0.04	0.17
(1,1049)	1:75:B:VAL:HG21	1:76:B:VAL:H	20	0.17	0.03	0.17
(1,1049)	1:75:B:VAL:HG22	1:76:B:VAL:H	20	0.17	0.03	0.17
(1,1049)	1:75:B:VAL:HG23	1:76:B:VAL:H	20	0.17	0.03	0.17
(1,3448)	1:37:A:LEU:HD21	1:44:A:PHE:HD1	19	1.36	0.49	1.39
(1,3448)	1:37:A:LEU:HD22	1:44:A:PHE:HD1	19	1.36	0.49	1.39
(1,3448)	1:37:A:LEU:HD23	1:44:A:PHE:HD1	19	1.36	0.49	1.39
(1,3576)	1:37:B:LEU:HD21	1:44:B:PHE:HD1	19	1.16	0.59	1.09
(1,3576)	1:37:B:LEU:HD22	1:44:B:PHE:HD1	19	1.16	0.59	1.09

*Continued on next page...*

*Continued from previous page...*

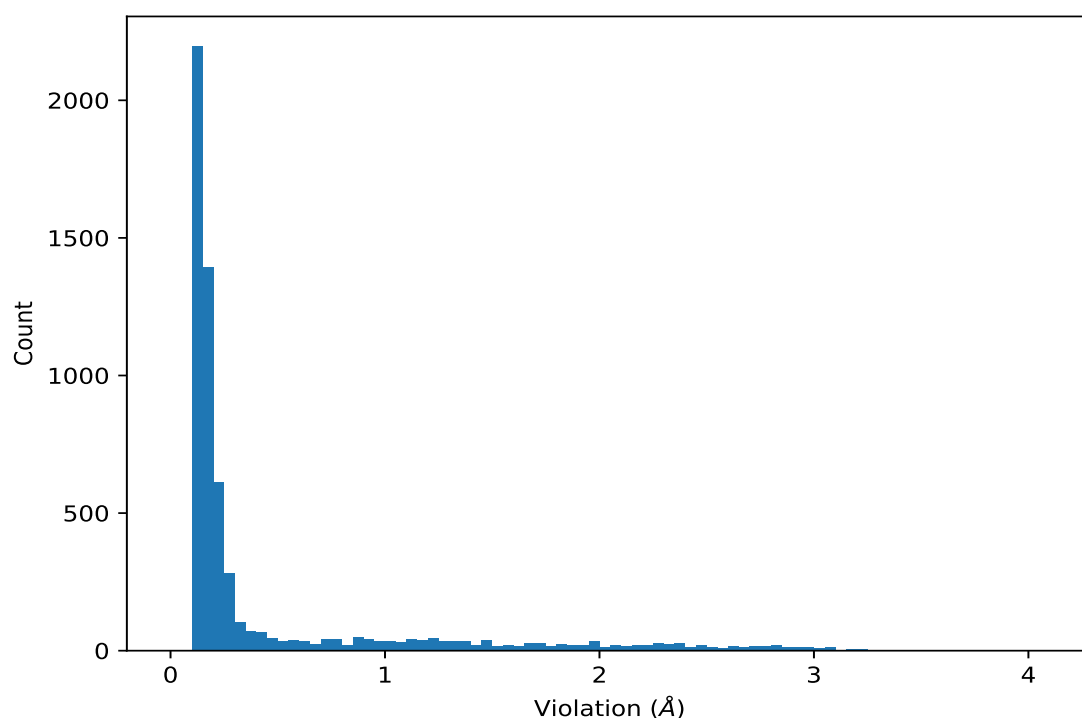
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3576)	1:37:B:LEU:HD23	1:44:B:PHE:HD1	19	1.16	0.59	1.09
(1,988)	1:37:A:LEU:HD21	1:78:A:VAL:HG11	19	0.15	0.03	0.14
(1,988)	1:37:A:LEU:HD21	1:78:A:VAL:HG12	19	0.15	0.03	0.14
(1,988)	1:37:A:LEU:HD21	1:78:A:VAL:HG13	19	0.15	0.03	0.14
(1,988)	1:37:A:LEU:HD22	1:78:A:VAL:HG11	19	0.15	0.03	0.14
(1,988)	1:37:A:LEU:HD22	1:78:A:VAL:HG12	19	0.15	0.03	0.14
(1,988)	1:37:A:LEU:HD22	1:78:A:VAL:HG13	19	0.15	0.03	0.14
(1,988)	1:37:A:LEU:HD23	1:78:A:VAL:HG11	19	0.15	0.03	0.14
(1,988)	1:37:A:LEU:HD23	1:78:A:VAL:HG12	19	0.15	0.03	0.14
(1,988)	1:37:A:LEU:HD23	1:78:A:VAL:HG13	19	0.15	0.03	0.14
(1,104)	1:75:A:VAL:HG21	1:79:B:ALA:HB1	19	0.14	0.02	0.14
(1,104)	1:75:A:VAL:HG21	1:79:B:ALA:HB2	19	0.14	0.02	0.14
(1,104)	1:75:A:VAL:HG21	1:79:B:ALA:HB3	19	0.14	0.02	0.14
(1,104)	1:75:A:VAL:HG22	1:79:B:ALA:HB1	19	0.14	0.02	0.14
(1,104)	1:75:A:VAL:HG22	1:79:B:ALA:HB2	19	0.14	0.02	0.14
(1,104)	1:75:A:VAL:HG22	1:79:B:ALA:HB3	19	0.14	0.02	0.14
(1,104)	1:75:A:VAL:HG23	1:79:B:ALA:HB1	19	0.14	0.02	0.14
(1,104)	1:75:A:VAL:HG23	1:79:B:ALA:HB2	19	0.14	0.02	0.14
(1,104)	1:75:A:VAL:HG23	1:79:B:ALA:HB3	19	0.14	0.02	0.14
(1,887)	1:44:A:PHE:HE2	1:85:A:MET:HB2	18	2.58	0.49	2.76

<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)
(1,1016)	1:16:B:HIS:HE1	1:26:B:TYR:HD1	12	4.08
(1,205)	1:90:A:TRP:HA	1:26:B:TYR:HE1	5	4.05
(1,3540)	1:15:B:PHE:HE2	1:26:B:TYR:H	20	4.02
(1,1010)	1:16:A:HIS:HE1	1:26:A:TYR:HD1	17	4.02
(1,1010)	1:16:A:HIS:HE1	1:26:A:TYR:HD1	19	3.73
(1,3412)	1:15:A:PHE:HE2	1:26:A:TYR:H	18	3.72
(1,1016)	1:16:B:HIS:HE1	1:26:B:TYR:HD1	11	3.53
(1,205)	1:90:A:TRP:HA	1:26:B:TYR:HE1	11	3.5
(1,3540)	1:15:B:PHE:HE2	1:26:B:TYR:H	11	3.48
(1,3540)	1:15:B:PHE:HE2	1:26:B:TYR:H	17	3.48

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

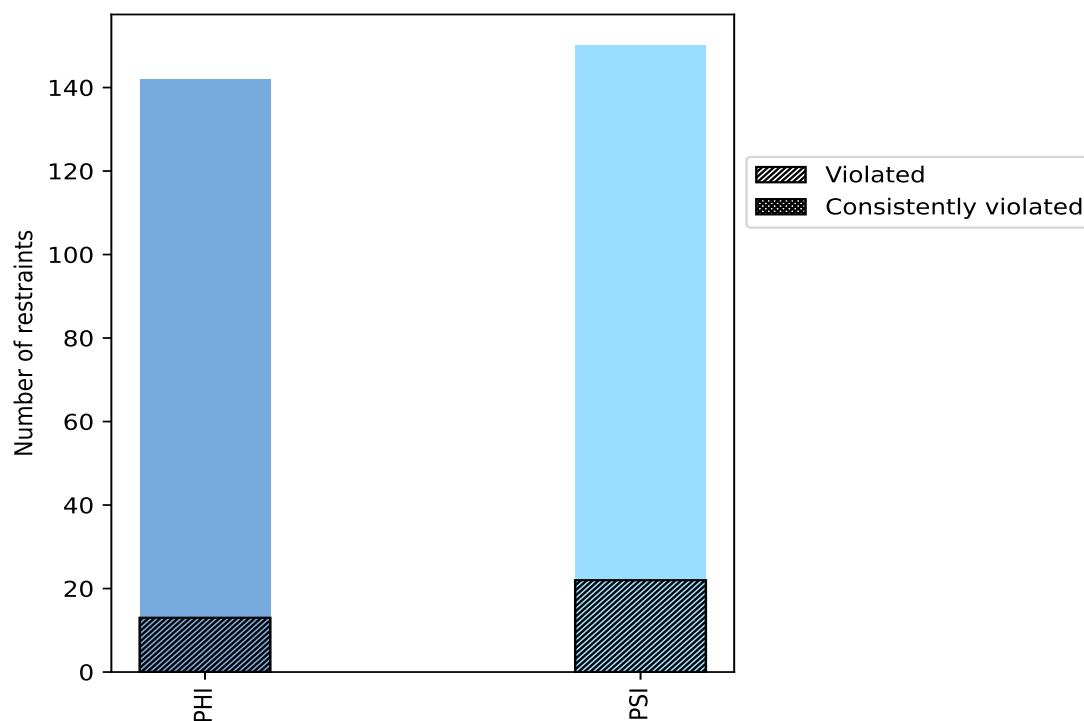
### 10.1 Summary of dihedral-angle violations [i](#)

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	142	48.6	13	9.2	4.5	0	0.0	0.0
PSI	150	51.4	22	14.7	7.5	0	0.0	0.0
Total	292	100.0	35	12.0	12.0	0	0.0	0.0

<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

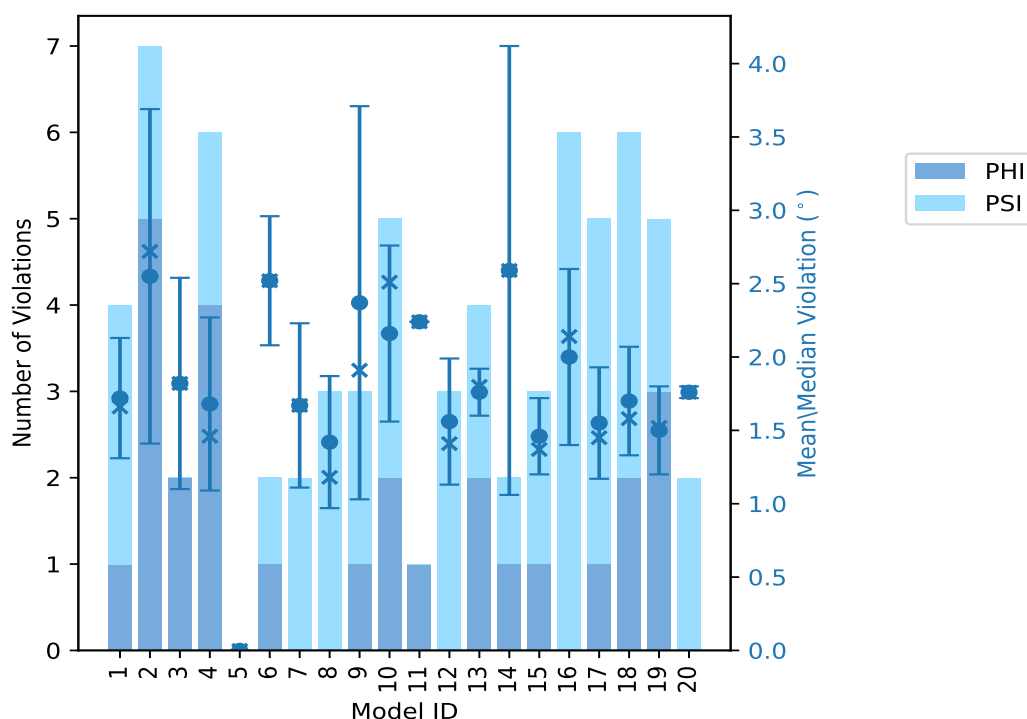
## 10.2 Dihedral-angle violation statistics for each model

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	Total				
1	1	3	4	1.72	2.31	0.41	1.66
2	5	2	7	2.55	4.77	1.14	2.72
3	2	0	2	1.82	2.54	0.72	1.82
4	4	2	6	1.68	2.7	0.59	1.46
5	0	0	0	0.0	0.0	0.0	0.0
6	1	1	2	2.52	2.96	0.44	2.52
7	0	2	2	1.67	2.23	0.56	1.67
8	0	3	3	1.42	2.06	0.45	1.18
9	1	2	3	2.37	4.19	1.34	1.91
10	2	3	5	2.16	2.73	0.6	2.51
11	1	0	1	2.24	2.24	0.0	2.24
12	0	3	3	1.56	2.14	0.43	1.41
13	2	2	4	1.76	1.93	0.16	1.8
14	1	1	2	2.59	4.12	1.53	2.59
15	1	2	3	1.46	1.81	0.26	1.37
16	0	6	6	2.0	2.85	0.6	2.14
17	1	4	5	1.55	2.03	0.38	1.45
18	2	4	6	1.7	2.37	0.37	1.58
19	3	2	5	1.5	1.87	0.3	1.52
20	0	2	2	1.76	1.8	0.04	1.76



### 10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
7	12	19	1	5.0
2	5	7	2	10.0
3	3	6	3	15.0
0	1	1	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
1	0	1	7	35.0
0	0	0	8	40.0
0	1	1	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

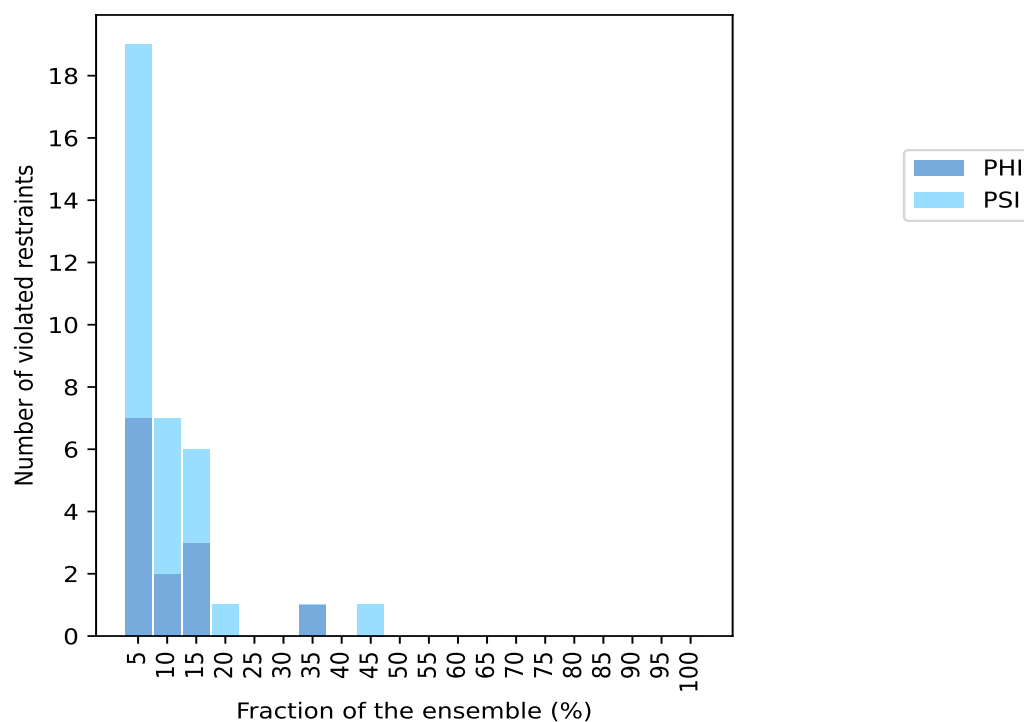
*Continued on next page...*

*Continued from previous page...*

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

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

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

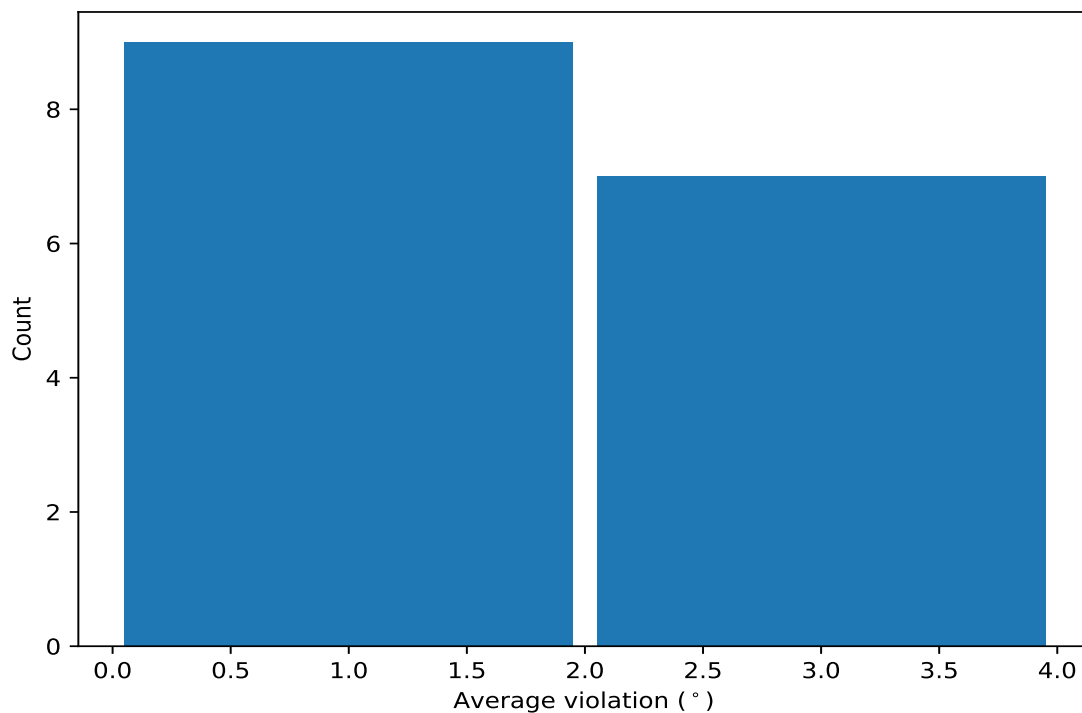


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 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.

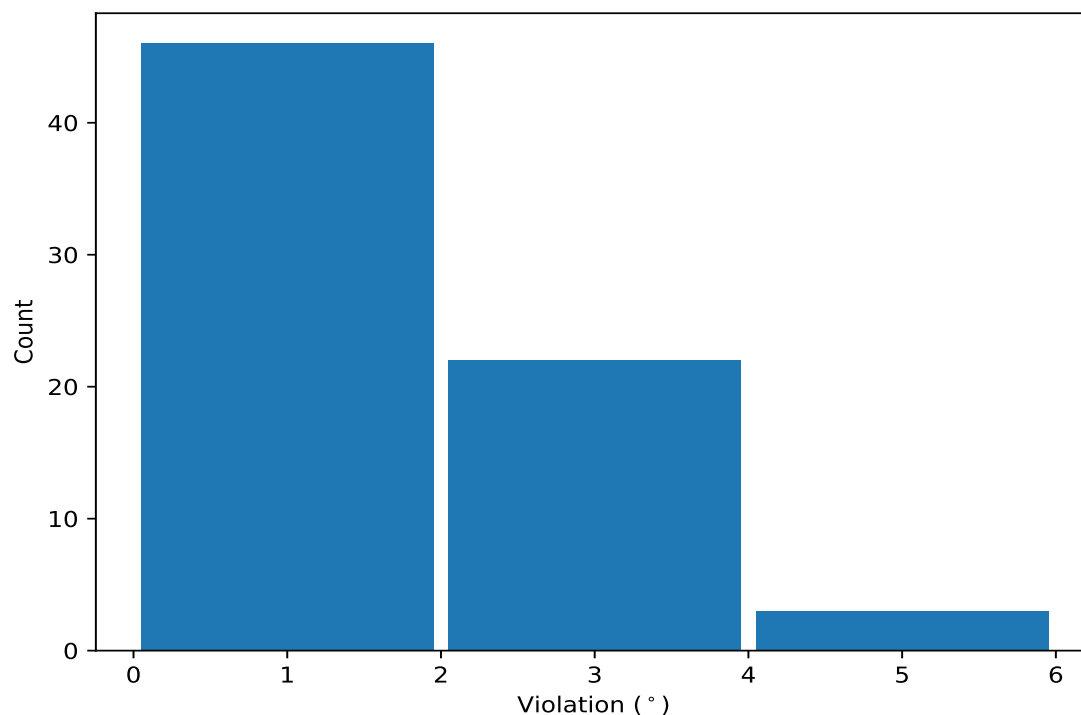
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,146)	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	1:93:A:SER:N	9	1.65	0.91	1.28
(1,19)	1:27:A:LYS:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	7	2.31	0.92	2.24
(1,269)	1:68:B:GLU:N	1:68:B:GLU:CA	1:68:B:GLU:C	1:69:B:VAL:N	4	1.66	0.48	1.56
(1,70)	1:90:A:TRP:C	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	3	2.26	0.84	2.75
(1,255)	1:50:B:ASP:N	1:50:B:ASP:CA	1:50:B:ASP:C	1:51:B:VAL:N	3	2.15	0.41	1.91
(1,165)	1:27:B:LYS:C	1:28:B:LEU:N	1:28:B:LEU:CA	1:28:B:LEU:C	3	2.08	0.45	1.78
(1,292)	1:92:B:ASN:N	1:92:B:ASN:CA	1:92:B:ASN:C	1:93:B:SER:N	3	1.95	0.37	2.01
(1,95)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:LYS:N	3	1.69	0.38	1.72
(1,48)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	3	1.39	0.41	1.11
(1,217)	1:91:B:GLU:C	1:92:B:ASN:N	1:92:B:ASN:CA	1:92:B:ASN:C	2	3.51	1.26	3.51

<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 (°)
(1,217)	1:91:B:GLU:C	1:92:B:ASN:N	1:92:B:ASN:CA	1:92:B:ASN:C	2	4.77
(1,19)	1:27:A:LYS:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	9	4.19
(1,146)	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	1:93:A:SER:N	14	4.12
(1,71)	1:91:A:GLU:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	2	3.2
(1,70)	1:90:A:TRP:C	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	6	2.96
(1,93)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:LEU:N	16	2.85
(1,70)	1:90:A:TRP:C	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	2	2.75
(1,255)	1:50:B:ASP:N	1:50:B:ASP:CA	1:50:B:ASP:C	1:51:B:VAL:N	10	2.73
(1,165)	1:27:B:LYS:C	1:28:B:LEU:N	1:28:B:LEU:CA	1:28:B:LEU:C	2	2.72
(1,19)	1:27:A:LYS:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	4	2.7