



# wwPDB NMR Structure Validation Summary Report ⓘ

Jul 2, 2020 – 12:13 AM CDT

PDB ID : 2KZN  
Title : Solution NMR Structure of Peptide methionine sulfoxide reductase msrB from Bacillus subtilis, Northeast Structural Genomics Consortium Target SR10  
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Deposited on : 2010-06-18

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.6.dev1
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.6.dev1

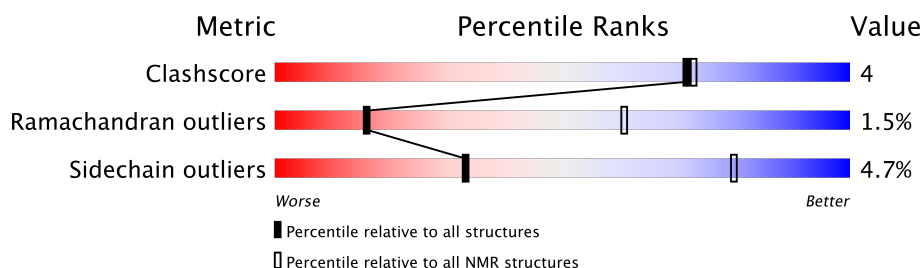
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 41%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

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	151	 78% 7% 13% .

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:6-A:27, A:37-A:142 (128)	0.98	8

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2363 atoms, of which 1156 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptide methionine sulfoxide reductase msrB.

Mol	Chain	Residues	Atoms						Trace
1	A	147	Total	C	H	N	O	S	0
			2363	761	1156	209	232	5	

There are 8 discrepancies between the modelled and reference sequences:

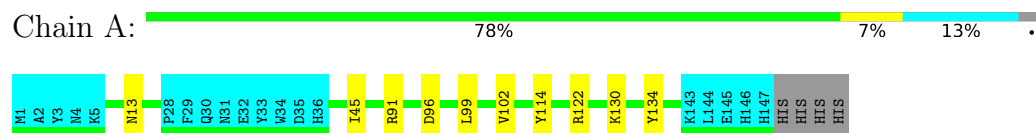
Chain	Residue	Modelled	Actual	Comment	Reference
A	144	LEU	-	EXPRESSION TAG	UNP P54155
A	145	GLU	-	EXPRESSION TAG	UNP P54155
A	146	HIS	-	EXPRESSION TAG	UNP P54155
A	147	HIS	-	EXPRESSION TAG	UNP P54155
A	148	HIS	-	EXPRESSION TAG	UNP P54155
A	149	HIS	-	EXPRESSION TAG	UNP P54155
A	150	HIS	-	EXPRESSION TAG	UNP P54155
A	151	HIS	-	EXPRESSION TAG	UNP P54155

## 4 Residue-property plots

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

These plots are provided for all protein, RNA and DNA 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.

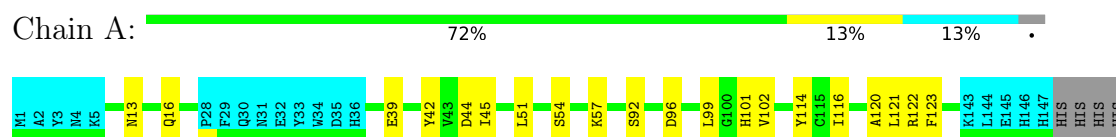
- Molecule 1: Peptide methionine sulfoxide reductase msrB



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

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

- Molecule 1: Peptide methionine sulfoxide reductase msrB



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	3.0
CYANA	geometry optimization	3.0
TALOS+	geometry optimization	
PALES	geometry optimization	
CYANA	refinement	3.0

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)	2kzn_nmr.cif
Number of chemical shift lists	1
Total number of shifts	869
Number of shifts mapped to atoms	732
Number of unparsed shifts	82
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	55
Assignment completeness (well-defined parts)	41%

## 6 Model quality [i](#)

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

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	97	SER	Peptide	1

### 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	1031	999	994	8±2
All	All	20620	19980	19880	154

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

5 of 69 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:VAL:HG12	1:A:114:TYR:HA	0.69	1.65	16	20
1:A:45:ILE:HG12	1:A:122:ARG:HB2	0.66	1.66	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LYS:HB2	1:A:49:LYS:HZ2	0.65	1.52	7	1
1:A:92:SER:HB3	1:A:96:ASP:HB2	0.65	1.67	9	7
1:A:106:GLY:HA3	1:A:113:ARG:HB2	0.64	1.69	5	5

## 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	128/151 (85%)	116±3 (90±2%)	10±3 (8±2%)	2±1 (1±1%)	16	61
All	All	2560/3020 (85%)	2315 (90%)	207 (8%)	38 (1%)	16	61

5 of 15 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	99	LEU	12
1	A	134	TYR	9
1	A	96	ASP	3
1	A	142	ASN	3
1	A	71	ILE	1

### 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	115/137 (84%)	110±2 (95±2%)	5±2 (5±2%)	33	80
All	All	2300/2740 (84%)	2192 (95%)	108 (5%)	33	80

5 of 45 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	13	ASN	15
1	A	77	GLU	6
1	A	87	ARG	5
1	A	57	LYS	5
1	A	42	TYR	4

### 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 carbohydrates 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 41% for the well-defined parts and 39% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2kzn\_nmr.cif

Chemical shift list name: *nef\_chemical\_shift\_list\_2kzn.mr*

#### 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	869
Number of shifts mapped to atoms	732
Number of unparsed shifts	82
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	55
Number of shift outliers (ShiftChecker)	2

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 82) occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
31	A	9	ILE	HD1%	0.822	0.030	1
32	A	9	ILE	HD1%	0.822	0.030	1
50	A	12	LEU	HD1%	0.822	0.030	1
51	A	12	LEU	HD1%	0.822	0.030	1
53	A	12	LEU	HD2%	0.744	0.030	1

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

- No matching atoms found in structure. First 5 (of 55) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	16	GLN	HE2y	7.862	0.03	2
A	22	ASN	HD2y	6.892	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	121	LEU	HD1%	0.626	0.03	1
A	129	LEU	HD2%	0.431	0.03	1
A	99	LEU	HD1%	0.723	0.03	1

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	142	$-0.18 \pm 0.18$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	132	$0.47 \pm 0.23$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	141	$-0.49 \pm 0.18$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	131	$1.13 \pm 0.45$	Should be applied

### 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 41%, i.e. 654 atoms were assigned a chemical shift out of a possible 1608. 17 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	489/626 (78%)	118/249 (47%)	253/256 (99%)	118/121 (98%)
Sidechain	163/836 (19%)	0/495 (0%)	156/302 (52%)	7/39 (18%)
Aromatic	2/146 (1%)	1/76 (1%)	0/59 (0%)	1/11 (9%)
Overall	654/1608 (41%)	119/820 (15%)	409/617 (66%)	126/171 (74%)

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

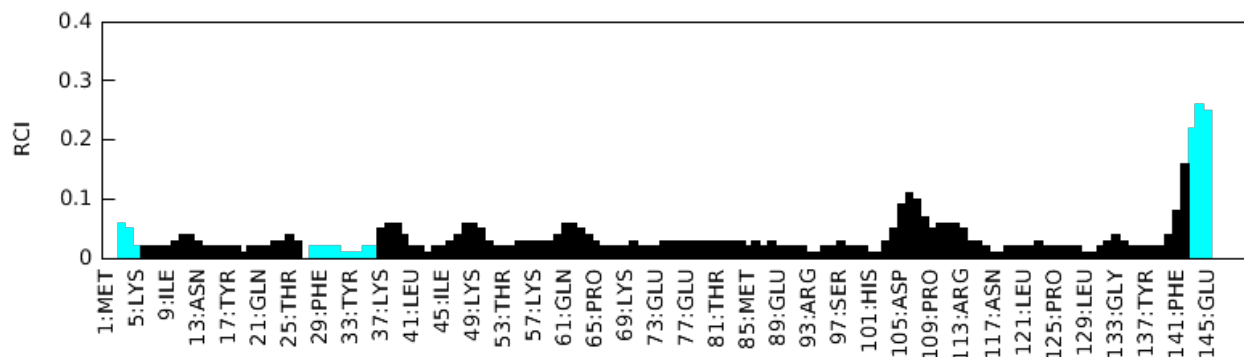
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	118	SER	H	13.13	11.23 – 5.33	8.2
1	A	38	GLU	H	5.26	11.34 – 5.34	-5.1

### 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.

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	624
Intra-residue ( $ i-j =0$ )	46
Sequential ( $ i-j =1$ )	165
Medium range ( $ i-j >1$ and $ i-j <5$ )	133
Long range ( $ i-j \geq 5$ )	280
Inter-chain	0
Total dihedral-angle restraints	470
Total hydrogen bond restraints	0
Total disulfide bond restraints	0
Number of unmapped restraints	0
Number of restraints per residue	4.4
Number of long range restraints per residue	2.0

### 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)	27.9	0.2
0.2-0.5 (Medium)	8.9	0.48
>0.5 (Large)	0.3	1.85

#### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	56.8	10.0
10.0-20.0 (Medium)	2.9	19.7
>20.0 (Large)	0.1	20.8

## 9 Distance violation analysis

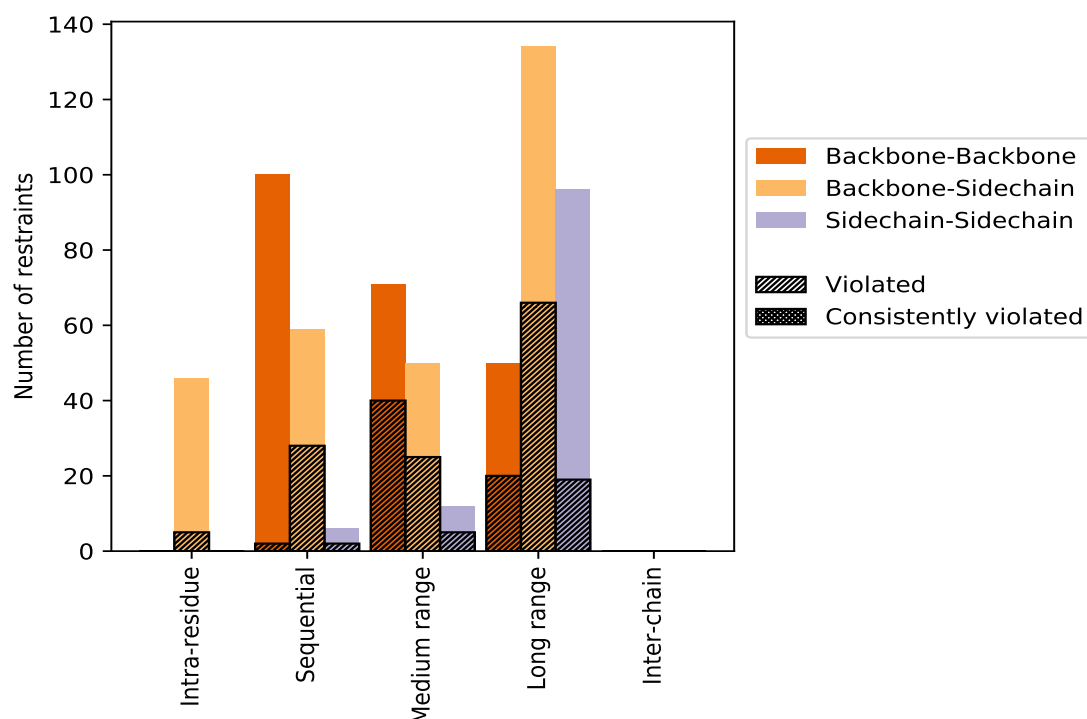
### 9.1 Summary of distance violations

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>
Intra-residue ( $ i-j =0$ )	46	7.4	5	10.9	0.8	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	46	7.4	5	10.9	0.8	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ( $ i-j =1$ )	165	26.4	32	19.4	5.1	0	0.0	0.0
Backbone-Backbone	100	16.0	2	2.0	0.3	0	0.0	0.0
Backbone-Sidechain	59	9.5	28	47.5	4.5	0	0.0	0.0
Sidechain-Sidechain	6	1.0	2	33.3	0.3	0	0.0	0.0
Medium range ( $ i-j >1$ & $ i-j <5$ )	133	21.3	70	52.6	11.2	0	0.0	0.0
Backbone-Backbone	71	11.4	40	56.3	6.4	0	0.0	0.0
Backbone-Sidechain	50	8.0	25	50.0	4.0	0	0.0	0.0
Sidechain-Sidechain	12	1.9	5	41.7	0.8	0	0.0	0.0
Long range ( $ i-j \geq 5$ )	280	44.9	105	37.5	16.8	0	0.0	0.0
Backbone-Backbone	50	8.0	20	40.0	3.2	0	0.0	0.0
Backbone-Sidechain	134	21.5	66	49.3	10.6	0	0.0	0.0
Sidechain-Sidechain	96	15.4	19	19.8	3.0	0	0.0	0.0
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
Total	624	100.0	212	34.0	34.0	0	0.0	0.0
Backbone-Backbone	221	35.4	62	28.1	9.9	0	0.0	0.0
Backbone-Sidechain	289	46.3	124	42.9	19.9	0	0.0	0.0
Sidechain-Sidechain	114	18.3	26	22.8	4.2	0	0.0	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



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

## 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 <sup>6</sup> (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total			
1	0	11	9	25	0	45	0.16	0.28	0.04
2	1	10	8	17	0	36	0.16	0.28	0.05
3	1	3	9	19	0	32	0.22	1.39	0.22
4	1	7	10	20	0	38	0.16	0.34	0.05
5	0	8	10	20	0	38	0.18	0.41	0.07
6	0	7	10	16	0	33	0.19	0.35	0.06
7	1	9	13	14	0	37	0.18	0.42	0.06
8	0	6	14	20	0	40	0.16	0.48	0.07
9	1	10	8	20	0	39	0.17	0.37	0.06
10	1	7	11	23	0	42	0.23	1.82	0.29
11	1	12	5	23	0	41	0.17	0.36	0.05
12	1	5	14	13	0	33	0.19	0.58	0.08

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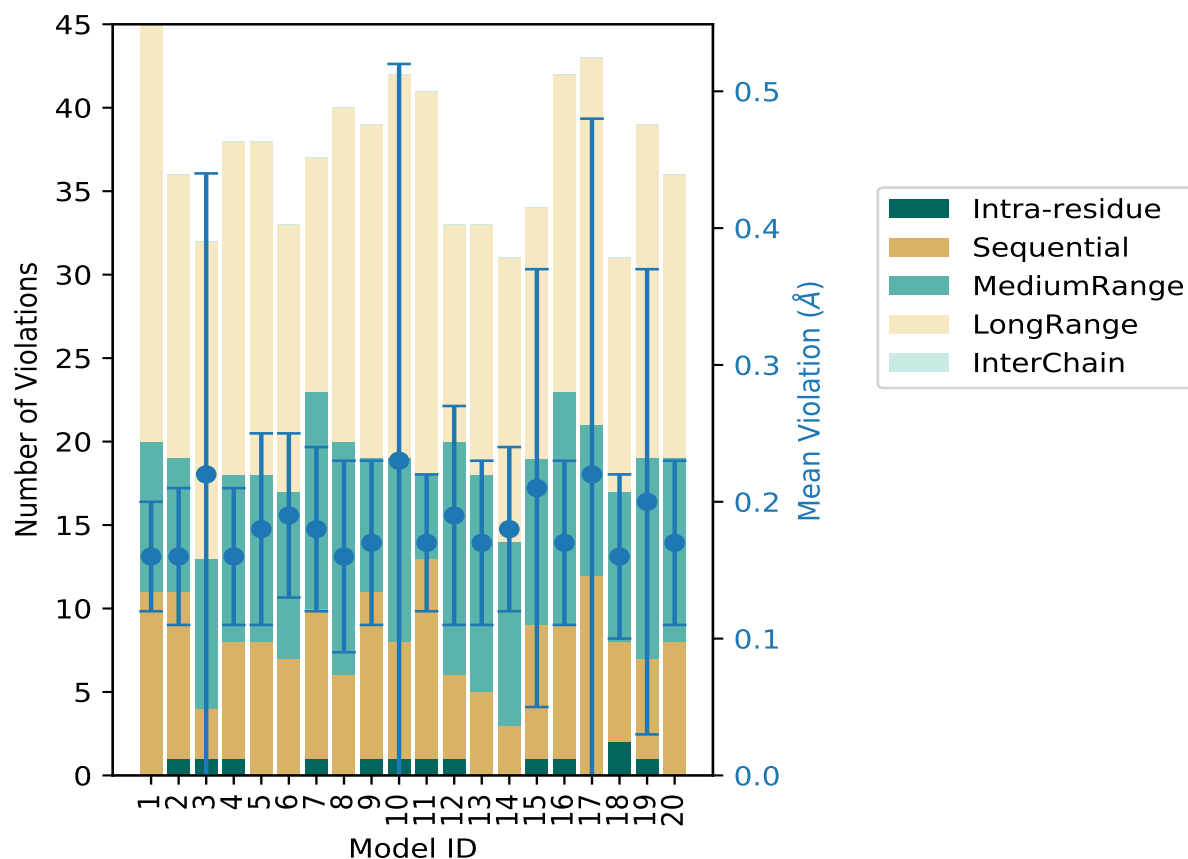


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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total			
13	0	5	13	15	0	33	0.17	0.35	0.06
14	0	3	11	17	0	31	0.18	0.32	0.06
15	1	8	10	15	0	34	0.21	1.04	0.16
16	1	8	14	19	0	42	0.17	0.33	0.06
17	0	12	9	22	0	43	0.22	1.85	0.26
18	2	6	9	14	0	31	0.16	0.39	0.06
19	1	6	12	20	0	39	0.2	1.2	0.17
20	0	8	11	17	0	36	0.17	0.37	0.06

<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 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

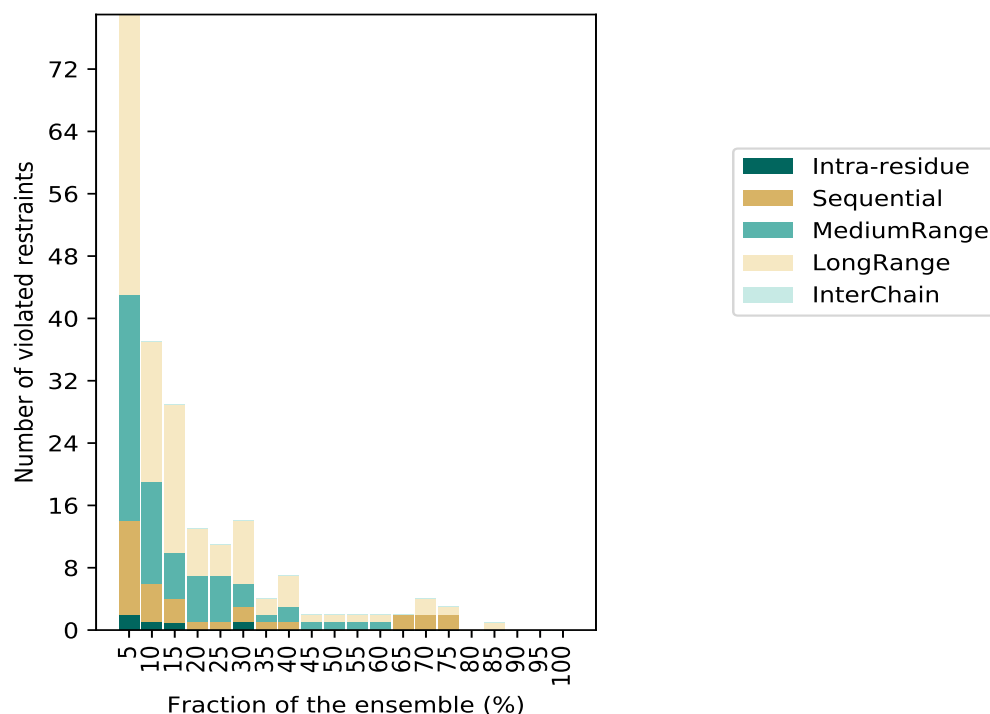
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 412(IR:41, SQ:133, MR:63, LR:175, IC:0) restraints are not 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>	%
2	12	29	36	0	79	1	5.0
1	5	13	18	0	37	2	10.0
1	3	6	19	0	29	3	15.0
0	1	6	6	0	13	4	20.0
0	1	6	4	0	11	5	25.0
1	2	3	8	0	14	6	30.0
0	1	1	2	0	4	7	35.0
0	1	2	4	0	7	8	40.0
0	0	1	1	0	2	9	45.0
0	0	1	1	0	2	10	50.0
0	0	1	1	0	2	11	55.0
0	0	1	1	0	2	12	60.0
0	2	0	0	0	2	13	65.0
0	2	0	2	0	4	14	70.0
0	2	0	1	0	3	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	1	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	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

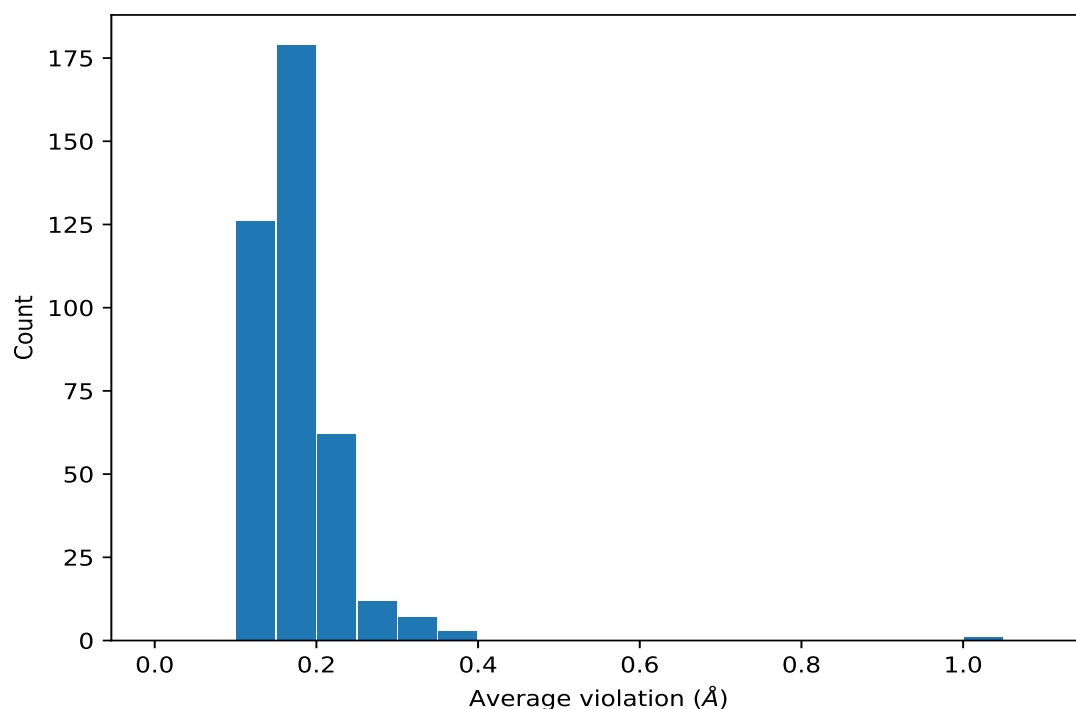
### 9.3.1 Bar graph : Distance violation statistics for the ensemble



## 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 top ten absolute value of the violation for each restraint sorted by number of violated models and the mean 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)
(1,411)	1:A:129:LEU:HD11	1:A:138:LEU:HD21	17	0.21	0.05
(1,411)	1:A:129:LEU:HD11	1:A:138:LEU:HD22	17	0.21	0.05
(1,411)	1:A:129:LEU:HD11	1:A:138:LEU:HD23	17	0.21	0.05
(1,411)	1:A:129:LEU:HD12	1:A:138:LEU:HD21	17	0.21	0.05
(1,411)	1:A:129:LEU:HD12	1:A:138:LEU:HD22	17	0.21	0.05
(1,411)	1:A:129:LEU:HD12	1:A:138:LEU:HD23	17	0.21	0.05
(1,411)	1:A:129:LEU:HD13	1:A:138:LEU:HD21	17	0.21	0.05
(1,411)	1:A:129:LEU:HD13	1:A:138:LEU:HD22	17	0.21	0.05
(1,411)	1:A:129:LEU:HD13	1:A:138:LEU:HD23	17	0.21	0.05
(1,616)	1:A:90:VAL:HG11	1:A:99:LEU:HD21	15	0.17	0.06
(1,616)	1:A:90:VAL:HG11	1:A:99:LEU:HD22	15	0.17	0.06
(1,616)	1:A:90:VAL:HG11	1:A:99:LEU:HD23	15	0.17	0.06
(1,616)	1:A:90:VAL:HG12	1:A:99:LEU:HD21	15	0.17	0.06
(1,616)	1:A:90:VAL:HG12	1:A:99:LEU:HD22	15	0.17	0.06
(1,616)	1:A:90:VAL:HG12	1:A:99:LEU:HD23	15	0.17	0.06
(1,616)	1:A:90:VAL:HG13	1:A:99:LEU:HD21	15	0.17	0.06

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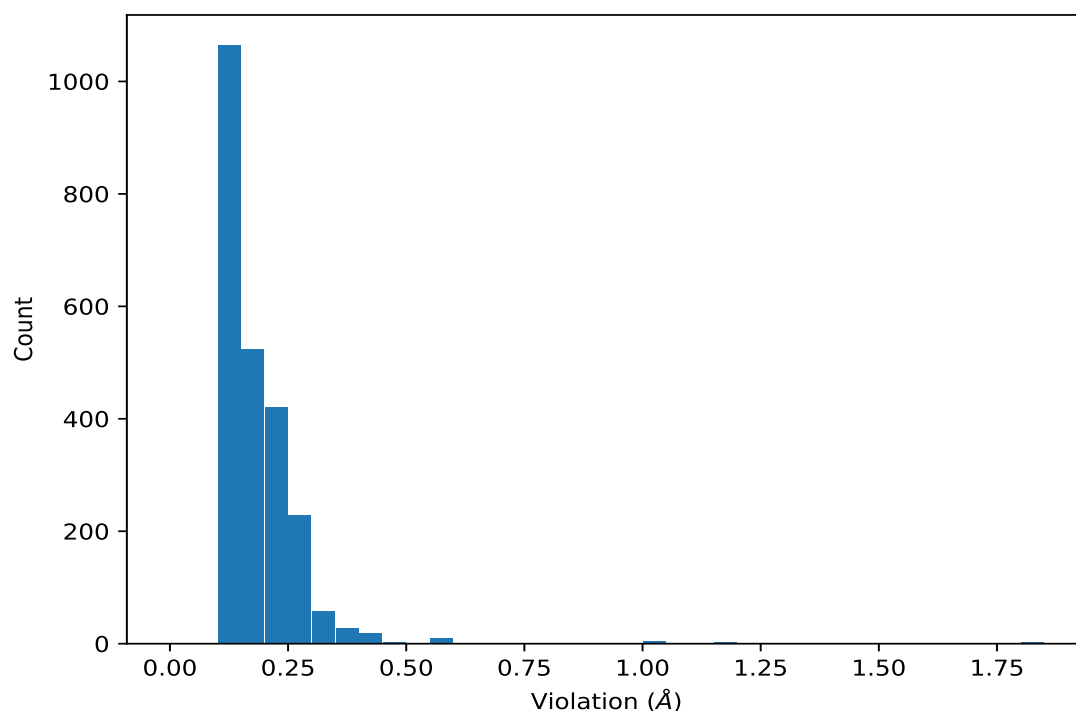
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)
(1,616)	1:A:90:VAL:HG13	1:A:99:LEU:HD22	15	0.17	0.06
(1,616)	1:A:90:VAL:HG13	1:A:99:LEU:HD23	15	0.17	0.06
(1,585)	1:A:74:GLU:H	1:A:75:VAL:HG11	15	0.18	0.04
(1,585)	1:A:74:GLU:H	1:A:75:VAL:HG12	15	0.18	0.04
(1,585)	1:A:74:GLU:H	1:A:75:VAL:HG13	15	0.18	0.04
(1,26)	1:A:128:LYS:H	1:A:129:LEU:HD11	15	0.16	0.04
(1,26)	1:A:128:LYS:H	1:A:129:LEU:HD12	15	0.16	0.04
(1,26)	1:A:128:LYS:H	1:A:129:LEU:HD13	15	0.16	0.04
(1,493)	1:A:43:VAL:HG11	1:A:52:PHE:H	14	0.19	0.06
(1,493)	1:A:43:VAL:HG12	1:A:52:PHE:H	14	0.19	0.06
(1,493)	1:A:43:VAL:HG13	1:A:52:PHE:H	14	0.19	0.06
(1,248)	1:A:120:ALA:H	1:A:121:LEU:HD11	14	0.19	0.06
(1,248)	1:A:120:ALA:H	1:A:121:LEU:HD12	14	0.19	0.06
(1,248)	1:A:120:ALA:H	1:A:121:LEU:HD13	14	0.19	0.06
(1,247)	1:A:121:LEU:HD11	1:A:122:ARG:H	14	0.17	0.06
(1,247)	1:A:121:LEU:HD12	1:A:122:ARG:H	14	0.17	0.06
(1,247)	1:A:121:LEU:HD13	1:A:122:ARG:H	14	0.17	0.06
(1,192)	1:A:19:VAL:HG11	1:A:117:ASN:H	14	0.15	0.03
(1,192)	1:A:19:VAL:HG12	1:A:117:ASN:H	14	0.15	0.03
(1,192)	1:A:19:VAL:HG13	1:A:117:ASN:H	14	0.15	0.03
(1,419)	1:A:120:ALA:H	1:A:121:LEU:HD21	13	0.22	0.06
(1,419)	1:A:120:ALA:H	1:A:121:LEU:HD22	13	0.22	0.06
(1,419)	1:A:120:ALA:H	1:A:121:LEU:HD23	13	0.22	0.06
(1,11)	1:A:128:LYS:H	1:A:129:LEU:HD21	13	0.17	0.04

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All distance violations

### 9.5.1 Histogram : Distribution of distance violations

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



### 9.5.2 Table : All distance violations

The following table lists the top ten absolute value of the violation for each restraint in the ensemble sorted by its 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)
(1,111)	1:A:92:SER:H	1:A:97:SER:H	17	1.85
(1,111)	1:A:92:SER:H	1:A:97:SER:H	10	1.82
(1,111)	1:A:92:SER:H	1:A:97:SER:H	3	1.39
(1,33)	1:A:92:SER:H	1:A:99:LEU:HD11	19	1.2
(1,33)	1:A:92:SER:H	1:A:99:LEU:HD12	19	1.2
(1,33)	1:A:92:SER:H	1:A:99:LEU:HD13	19	1.2
(1,56)	1:A:110:ASN:HD22	1:A:112:LEU:HD11	15	1.04
(1,56)	1:A:110:ASN:HD22	1:A:112:LEU:HD12	15	1.04
(1,56)	1:A:110:ASN:HD22	1:A:112:LEU:HD13	15	1.04
(1,162)	1:A:92:SER:H	1:A:96:ASP:H	10	1.04
(1,408)	1:A:41:LEU:HD11	1:A:138:LEU:HD11	12	0.58
(1,408)	1:A:41:LEU:HD11	1:A:138:LEU:HD12	12	0.58
(1,408)	1:A:41:LEU:HD11	1:A:138:LEU:HD13	12	0.58
(1,408)	1:A:41:LEU:HD12	1:A:138:LEU:HD11	12	0.58
(1,408)	1:A:41:LEU:HD12	1:A:138:LEU:HD12	12	0.58
(1,408)	1:A:41:LEU:HD12	1:A:138:LEU:HD13	12	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,408)	1:A:41:LEU:HD13	1:A:138:LEU:HD11	12	0.58
(1,408)	1:A:41:LEU:HD13	1:A:138:LEU:HD12	12	0.58
(1,408)	1:A:41:LEU:HD13	1:A:138:LEU:HD13	12	0.58
(1,572)	1:A:41:LEU:HD11	1:A:141:PHE:H	8	0.48
(1,572)	1:A:41:LEU:HD12	1:A:141:PHE:H	8	0.48
(1,572)	1:A:41:LEU:HD13	1:A:141:PHE:H	8	0.48
(1,162)	1:A:92:SER:H	1:A:96:ASP:H	17	0.43
(1,111)	1:A:92:SER:H	1:A:97:SER:H	7	0.42

## 10 Dihedral-angle violation analysis

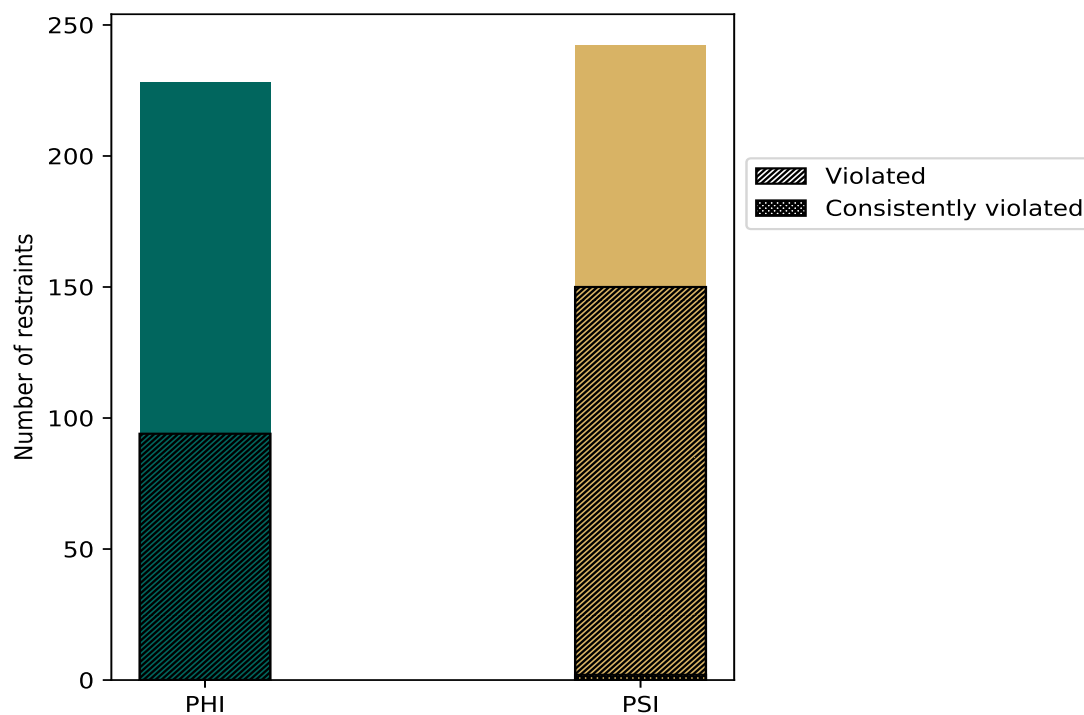
### 10.1 Summary of dihedral-angle violations

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	% <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	228	48.5	94	41.2	20.0	0	0.0	0.0
PSI	242	51.5	150	62.0	31.9	2	0.8	0.4
Total	470	100.0	244	51.9	51.9	2	0.4	0.4

<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



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

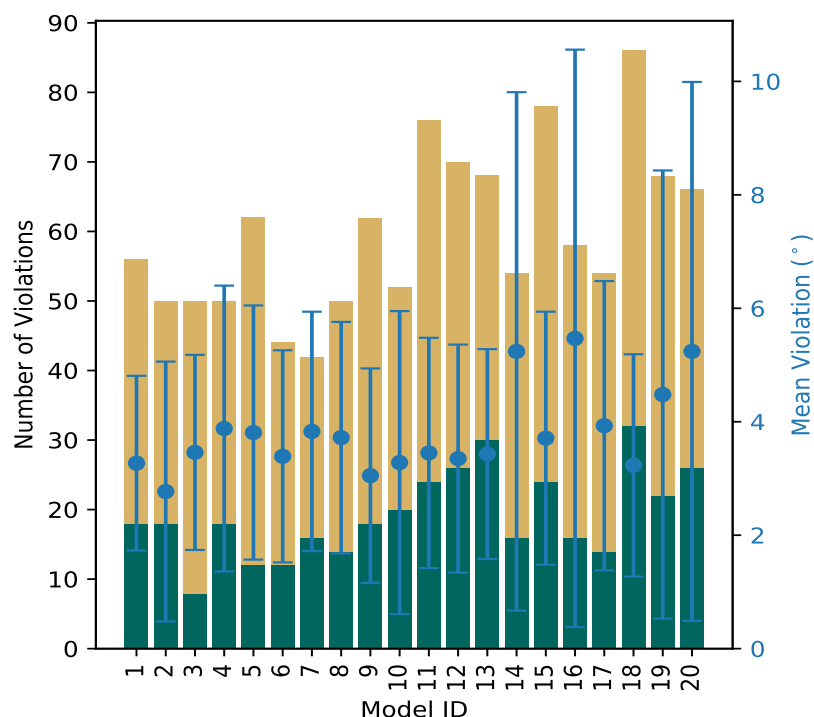


## 10.2 Dihedral-angle violation statistics in each model

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 (°)	Std. deviation (°)
	PHI	PSI	Total			
1	18	38	56	3.27	7.7	1.54
2	18	32	50	2.77	12.3	2.29
3	8	42	50	3.46	8.7	1.72
4	18	32	50	3.88	10.7	2.52
5	12	50	62	3.81	11.3	2.24
6	12	32	44	3.39	6.6	1.87
7	16	26	42	3.83	10.6	2.11
8	14	36	50	3.72	10.2	2.04
9	18	44	62	3.05	10.7	1.89
10	20	32	52	3.28	12.4	2.67
11	24	52	76	3.45	11.0	2.03
12	26	44	70	3.35	10.7	2.01
13	30	38	68	3.43	9.6	1.85
14	16	38	54	5.24	16.0	4.57
15	24	54	78	3.71	10.6	2.23
16	16	42	58	5.47	20.8	5.09
17	14	40	54	3.93	13.1	2.55
18	32	54	86	3.23	9.2	1.96
19	22	46	68	4.48	16.6	3.95
20	26	40	66	5.24	19.7	4.75

### 10.2.1 Bar graph : Dihedral violation statistics for each model



The mean and the standard deviation are shown in blue with respect to the y axis on the right

## 10.3 Violation statistics in 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 <sup>1</sup>	%
32	36	68	1	5.0
14	22	36	2	10.0
8	8	16	3	15.0
2	8	10	4	20.0
14	10	24	5	25.0
2	16	18	6	30.0
4	14	18	7	35.0
8	4	12	8	40.0
2	6	8	9	45.0
0	4	4	10	50.0
4	4	8	11	55.0
2	2	4	12	60.0

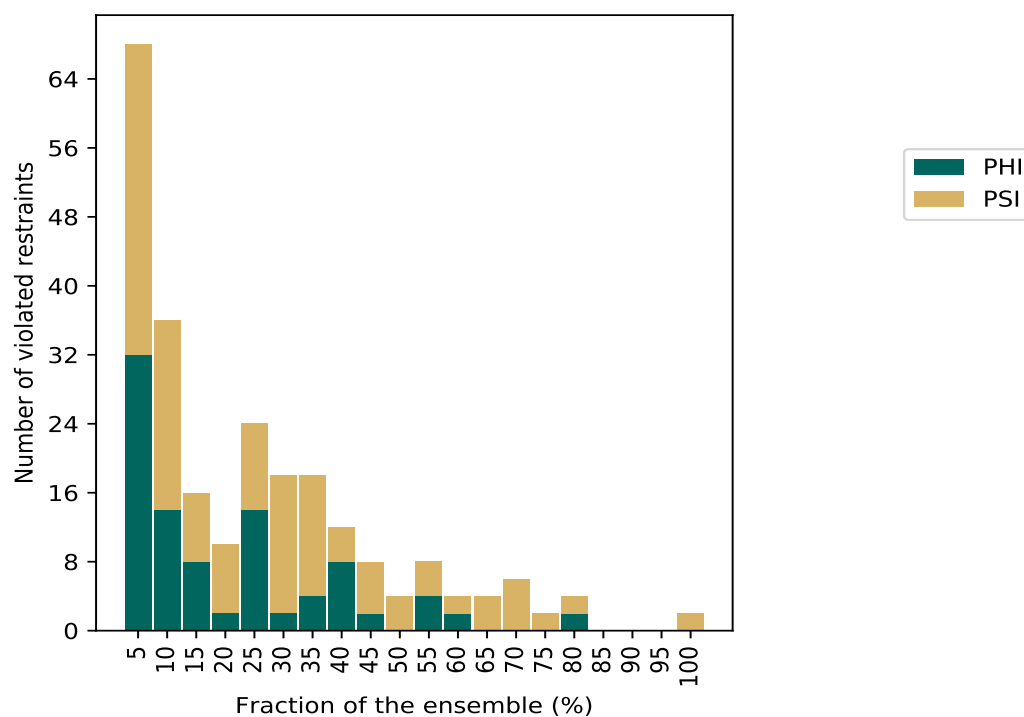
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
0	4	4	13	65.0
0	6	6	14	70.0
0	2	2	15	75.0
2	2	4	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	2	2	20	100.0

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

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

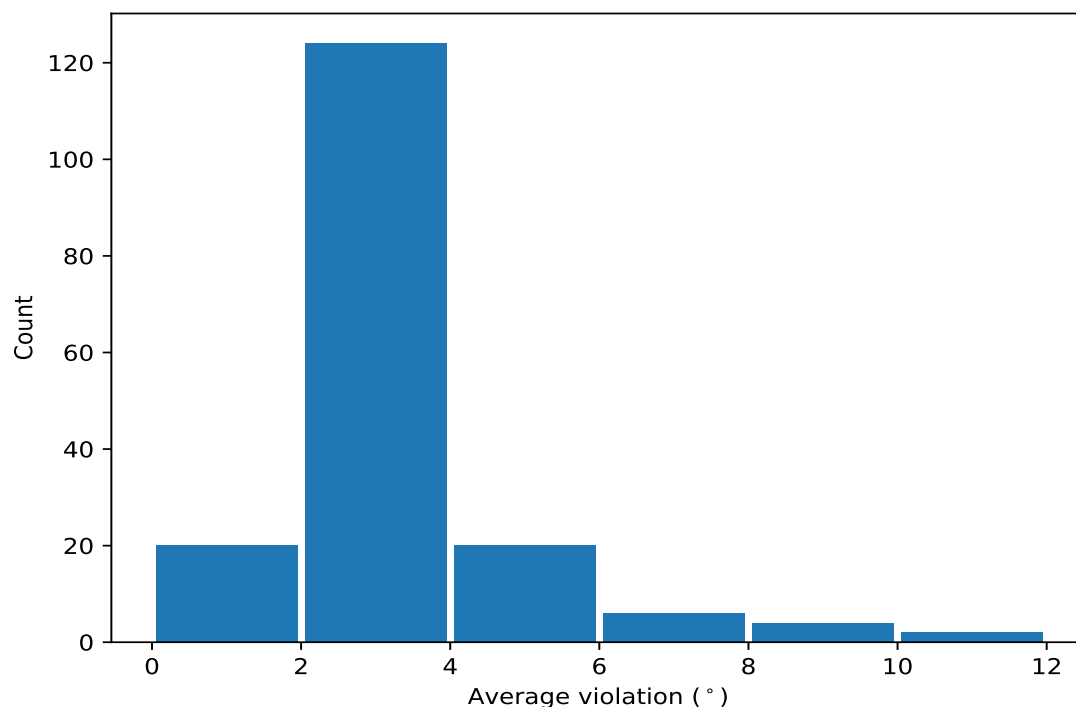


## 10.4 Most violated dihedral-angle restraints

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the top ten absolute value of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

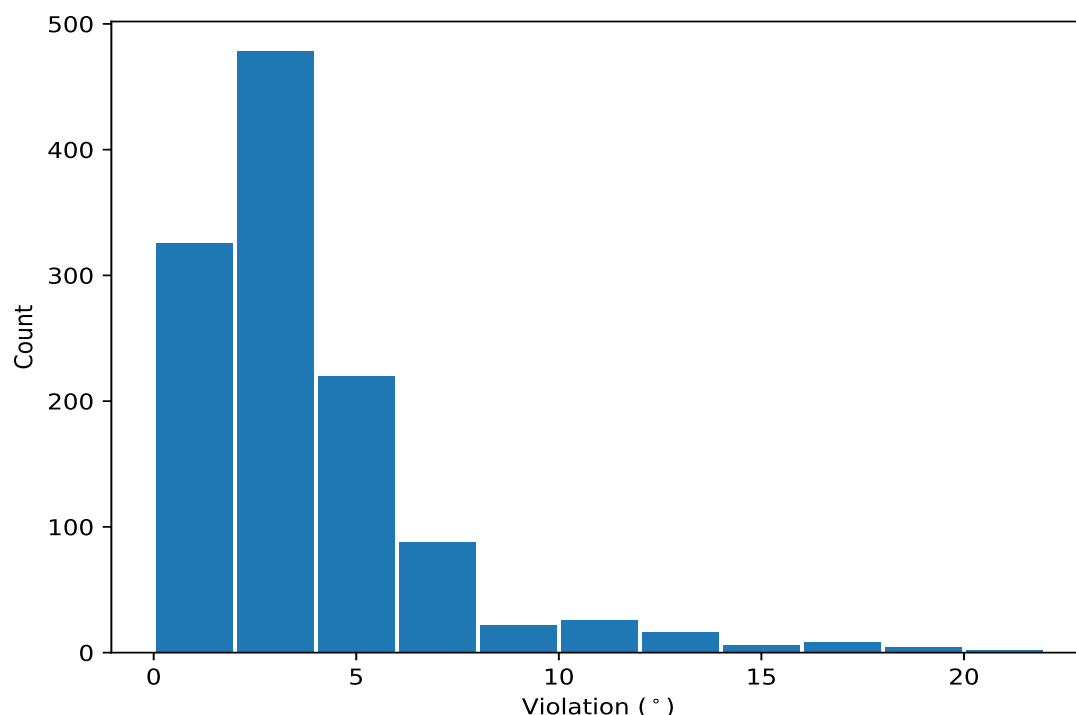
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean (°)	SD <sup>2</sup> (°)
(1,389)	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	1:A:96:ASP:N	9	11.88	5.05
(1,154)	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	1:A:96:ASP:N	9	11.88	5.05
(1,387)	1:A:94:THR:N	1:A:94:THR:CA	1:A:94:THR:C	1:A:95:ALA:N	14	6.42	4.09
(1,152)	1:A:94:THR:N	1:A:94:THR:CA	1:A:94:THR:C	1:A:95:ALA:N	14	6.42	4.09
(1,156)	1:A:96:ASP:N	1:A:96:ASP:CA	1:A:96:ASP:C	1:A:97:SER:N	16	8.28	3.57
(1,391)	1:A:96:ASP:N	1:A:96:ASP:CA	1:A:96:ASP:C	1:A:97:SER:N	16	8.28	3.57
(1,110)	1:A:70:PRO:N	1:A:70:PRO:CA	1:A:70:PRO:C	1:A:71:ILE:N	11	5.03	2.54
(1,345)	1:A:70:PRO:N	1:A:70:PRO:CA	1:A:70:PRO:C	1:A:71:ILE:N	11	5.03	2.54
(1,82)	1:A:53:THR:N	1:A:53:THR:CA	1:A:53:THR:C	1:A:54:SER:N	15	4.44	2.61
(1,317)	1:A:53:THR:N	1:A:53:THR:CA	1:A:53:THR:C	1:A:54:SER:N	15	4.44	2.61

<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation

## 10.5 All violated dihedral-angle restraints

### 10.5.1 Histogram : Distribution of violations

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



### 10.5.2 Table: All violated dihedral-angle restraints

The following table lists the absolute value of the top ten violation for each restraint in the ensemble sorted by its 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 (°)
(1,389)	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	1:A:96:ASP:N	16	20.8
(1,154)	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	1:A:96:ASP:N	16	20.8
(1,388)	1:A:94:THR:C	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	20	19.7
(1,153)	1:A:94:THR:C	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	20	19.7
(1,389)	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	1:A:96:ASP:N	20	18.9
(1,154)	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	1:A:96:ASP:N	20	18.9
(1,388)	1:A:94:THR:C	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	19	16.6
(1,153)	1:A:94:THR:C	1:A:95:ALA:N	1:A:95:ALA:CA	1:A:95:ALA:C	19	16.6
(1,387)	1:A:94:THR:N	1:A:94:THR:CA	1:A:94:THR:C	1:A:95:ALA:N	19	16.2
(1,152)	1:A:94:THR:N	1:A:94:THR:CA	1:A:94:THR:C	1:A:95:ALA:N	19	16.2