



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:49 AM UTC

PDB ID : 2LTQ / pdb\_00002ltq  
BMRB ID : 18493  
Title : High resolution structure of DsbB C41S by joint calculation with solid-state NMR and X-ray data  
Authors : Tang, M.; Sperling, L.J.; Schwieters, C.D.; Nesbitt, A.E.; Gennis, R.B.; Rienstra, C.M.  
Deposited on : 2012-05-30

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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>.

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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)  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 2%.

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 10 models. Model 4 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:15-A:29, A:53-A:55, A:73-A:93, A:151-A:152, B:21-B:132, B:134-B:239, C:1-C:100, C:105-C:119, C:121-C:221, D:53-D:62, D:72-D:91, E:21-E:132, E:134-E:239, F:1-F:119, F:121-F:215 (937)	0.13	4

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

### 3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17810 atoms, of which 8819 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Disulfide bond formation protein B.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2387	794	1212	183	189	9	
1	D	148	Total	C	H	N	O	S	0
			2387	794	1212	183	189	9	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	CYS	engineered mutation	UNP P0A6M2
A	41	SER	CYS	engineered mutation	UNP P0A6M2
A	49	VAL	CYS	engineered mutation	UNP P0A6M2
D	8	ALA	CYS	engineered mutation	UNP P0A6M2
D	41	SER	CYS	engineered mutation	UNP P0A6M2
D	49	VAL	CYS	engineered mutation	UNP P0A6M2

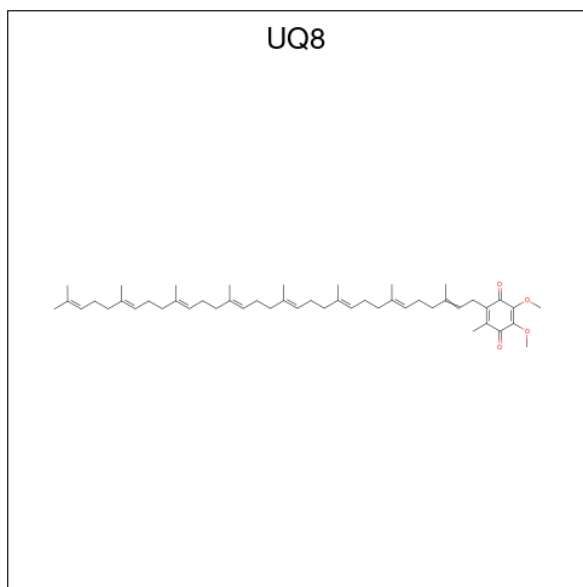
- Molecule 2 is a protein called Fab fragment light chain.

Mol	Chain	Residues	Atoms						Trace
2	B	218	Total	C	H	N	O	S	0
			3319	1052	1629	283	347	8	
2	E	218	Total	C	H	N	O	S	0
			3319	1052	1629	283	347	8	

- Molecule 3 is a protein called Fab fragment heavy chain.

Mol	Chain	Residues	Atoms						Trace
3	C	216	Total	C	H	N	O	S	0
			3189	1017	1574	264	325	9	
3	F	214	Total	C	H	N	O	S	0
			3173	1015	1563	262	324	9	

- Molecule 4 is Ubiquinone-8 (CCD ID: UQ8) (formula:  $C_{49}H_{74}O_4$ ).



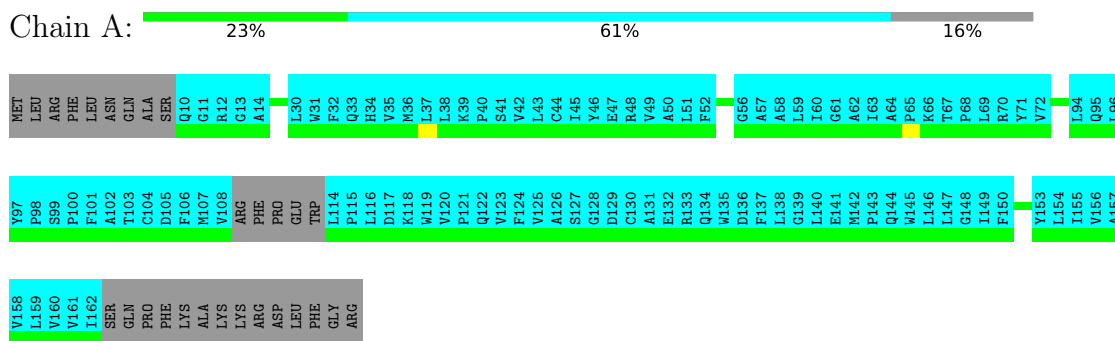
Mol	Chain	Residues	Atoms		
4	A	1	Total	C	O
			18	14	4
4	D	1	Total	C	O
			18	14	4

## 4 Residue-property plots [i](#)

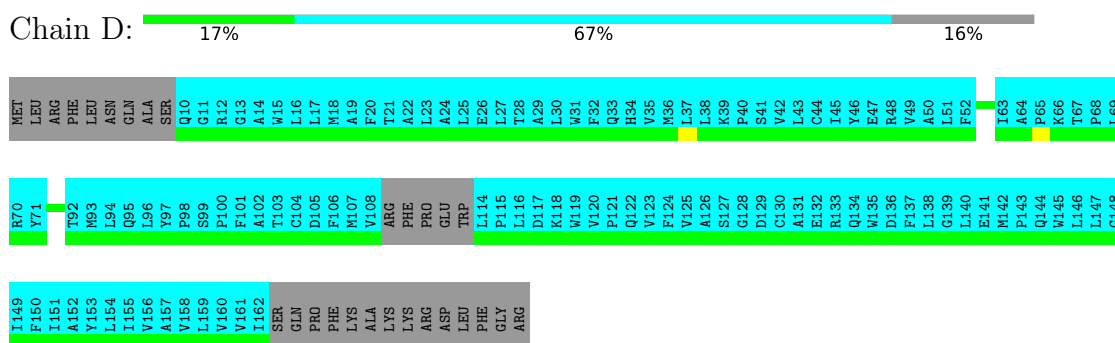
### 4.1 Average score per residue in the NMR ensemble

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.

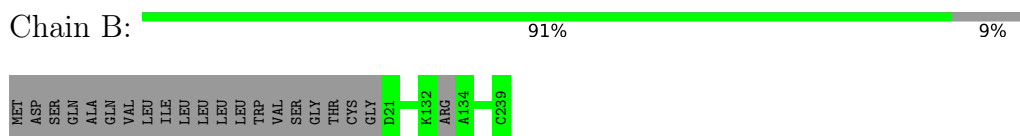
- Molecule 1: Disulfide bond formation protein B



- Molecule 1: Disulfide bond formation protein B

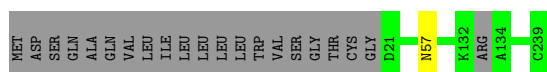


- Molecule 2: Fab fragment light chain



- Molecule 2: Fab fragment light chain





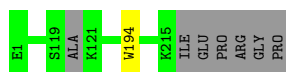
- Molecule 3: Fab fragment heavy chain

Chain C: 97%



- Molecule 3: Fab fragment heavy chain

Chain F: 96%

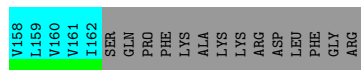
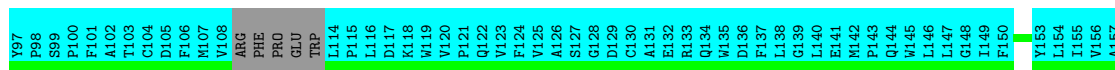
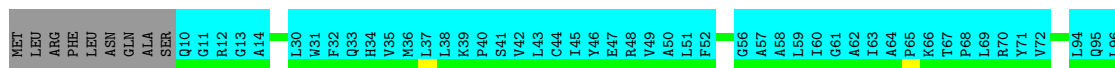


## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

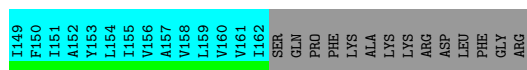
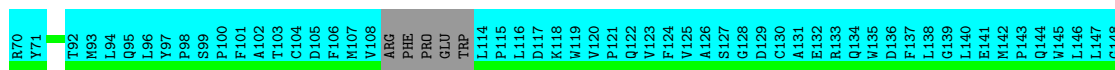
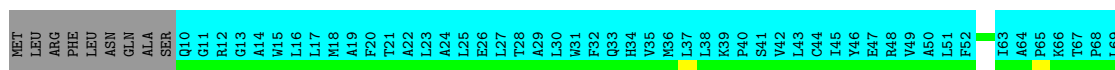
- Molecule 1: Disulfide bond formation protein B

Chain A: 23% 61% 16%



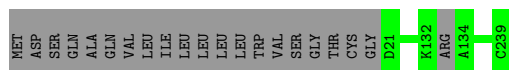
- Molecule 1: Disulfide bond formation protein B

Chain D: 17% 67% 16%



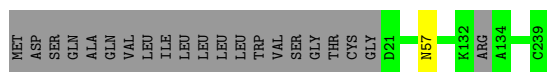
- Molecule 2: Fab fragment light chain

Chain B:  91% 9%



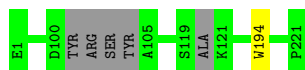
- Molecule 2: Fab fragment light chain

Chain E:  91% 9%



- Molecule 3: Fab fragment heavy chain

Chain C:  97% .



- Molecule 3: Fab fragment heavy chain

Chain F:  96% .



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 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	
X-PLOR NIH	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	744
Number of shifts mapped to atoms	671
Number of unparsed shifts	0
Number of shifts with mapping errors	73
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	2%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 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](#)

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

### 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 i

The completeness of assignment taking into account all chemical shift lists is 2% for the well-defined parts and 4% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts\_list\_DsbB*

#### 7.1.1 Bookkeeping i

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	744
Number of shifts mapped to atoms	671
Number of unparsed shifts	0
Number of shifts with mapping errors	73
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 73) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	ASN	C	179.258	0.145	1
1	A	6	ASN	CA	57.564	0.300	1
1	A	6	ASN	CB	38.167	0.300	1
1	A	7	GLN	H	9.338	0.026	1
1	A	7	GLN	C	180.404	0.092	1
1	A	7	GLN	CA	57.611	0.012	1
1	A	7	GLN	CB	26.649	0.210	1
1	A	7	GLN	CG	31.228	0.300	1
1	A	7	GLN	N	120.525	0.189	1
1	A	8	ALA	H	9.436	0.052	1
1	A	8	ALA	C	179.313	0.300	1
1	A	8	ALA	CA	54.645	0.300	1
1	A	8	ALA	CB	17.967	0.300	1
1	A	8	ALA	N	123.894	0.176	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	SER	C	173.894	0.126	1
1	A	9	SER	CA	60.565	0.137	1
1	A	9	SER	CB	63.79	0.070	1
1	A	109	ARG	N	112.15	0.050	1
1	A	110	PHE	CA	58.681	0.114	1
1	A	111	PRO	CA	65.848	0.300	1
1	A	111	PRO	CD	51.081	0.220	1
1	A	112	GLU	C	177.165	0.300	1
1	A	113	TRP	H	9.706	0.060	1
1	A	113	TRP	CA	53.381	0.091	1
1	A	113	TRP	N	111.82	0.076	1
1	A	163	SER	H	9.427	0.022	1
1	A	163	SER	CA	60.441	0.222	1
1	A	163	SER	CB	63.788	0.300	1
1	A	163	SER	N	112.832	0.300	1
1	A	165	PRO	CA	62.249	0.011	1
1	A	165	PRO	CD	51.723	0.128	1
1	A	165	PRO	N	134.035	0.022	1
1	A	168	ALA	CA	51.195	0.007	1
1	A	168	ALA	CB	18.891	0.003	1
1	B	201	SER	C1	135.534	0.060	1
1	B	201	SER	C10	20.609	0.118	4
1	B	201	SER	C11	43.4	0.643	4
1	B	201	SER	C12	30.3	0.643	4
1	B	201	SER	C15	20.7	0.643	4
1	B	201	SER	C16	43.0	0.643	4
1	B	201	SER	C17	29.8	0.643	4
1	B	201	SER	C1M	15.859	0.061	4
1	B	201	SER	C2	154.709	0.300	1
1	B	201	SER	C20	20.2	0.643	4
1	B	201	SER	C21	42.6	0.643	4
1	B	201	SER	C22	29.3	0.643	4
1	B	201	SER	C25	19.7	0.643	4
1	B	201	SER	C26	42.2	0.643	4
1	B	201	SER	C27	28.8	0.643	4
1	B	201	SER	C3	142.41	0.300	4
1	B	201	SER	C30	19.2	0.643	4
1	B	201	SER	C31	41.8	0.643	4
1	B	201	SER	C32	28.3	0.643	4
1	B	201	SER	C35	18.7	0.643	4
1	B	201	SER	C36	41.4	0.643	4

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	201	SER	C37	27.8	0.643	4
1	B	201	SER	C38	124.75	0.300	4
1	B	201	SER	C39	136.254	0.051	4
1	B	201	SER	C3M	63.804	0.193	4
1	B	201	SER	C4	142.41	0.300	1
1	B	201	SER	C40	18.2	0.643	4
1	B	201	SER	C41	41.517	0.095	4
1	B	201	SER	C42	28.26	0.020	4
1	B	201	SER	C43	126.157	0.271	4
1	B	201	SER	C44	135.212	0.112	4
1	B	201	SER	C45	17.92	0.069	4
1	B	201	SER	C46	28.177	0.074	4
1	B	201	SER	C4M	63.804	0.193	4
1	B	201	SER	C5	154.709	0.300	4
1	B	201	SER	C6	127.427	0.300	1
1	B	201	SER	C7	26.58	0.011	4
1	B	201	SER	C8	123.68	0.098	4
1	B	201	SER	C9	140.1	0.117	4

### 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
$^{13}\text{C}_\alpha$	130	$-0.89 \pm 0.21$	Should be checked
$^{13}\text{C}_\beta$	114	$0.43 \pm 0.09$	None needed (< 0.5 ppm)
$^{13}\text{C}'$	116	$-0.45 \pm 0.25$	None needed (< 0.5 ppm)
$^{15}\text{N}$	125	$1.12 \pm 0.38$	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 2%, i.e. 225 atoms were assigned a chemical shift out of a possible 12014. 0 out of 143 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	140/4666 (3%)	21/1899 (1%)	78/1874 (4%)	41/893 (5%)
Sidechain	82/6296 (1%)	0/4124 (0%)	82/1972 (4%)	0/200 (0%)
Aromatic	3/1052 (0%)	0/501 (0%)	3/510 (1%)	0/41 (0%)
Overall	225/12014 (2%)	21/6524 (0%)	163/4356 (4%)	41/1134 (4%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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

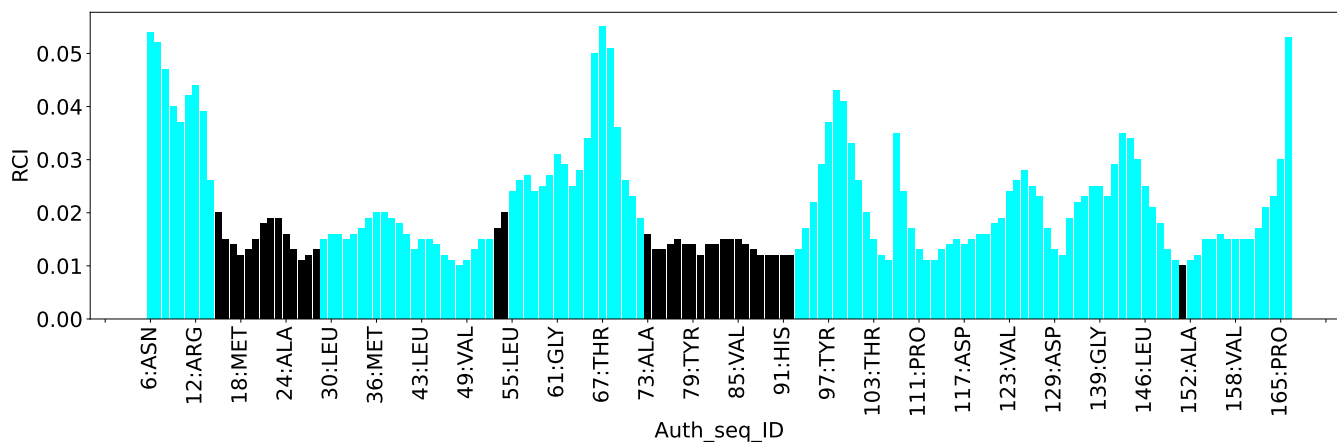
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	92	THR	CG2	27.48	16.06 – 27.03	5.4

### 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:



Random coil index (RCI) for chain B:



## 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	1318
Intra-residue ( $ i-j =0$ )	374
Sequential ( $ i-j =1$ )	516
Medium range ( $ i-j >1$ and $ i-j <5$ )	420
Long range ( $ i-j \geq 5$ )	8
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	372
Number of unmapped restraints	6
Number of restraints per residue	1.3
Number of long range restraints per residue <sup>1</sup>	0.0

<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)	42.0	0.2
0.2-0.5 (Medium)	47.0	0.33
>0.5 (Large)	0.6	0.85

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	11.4	6.17
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis [i](#)

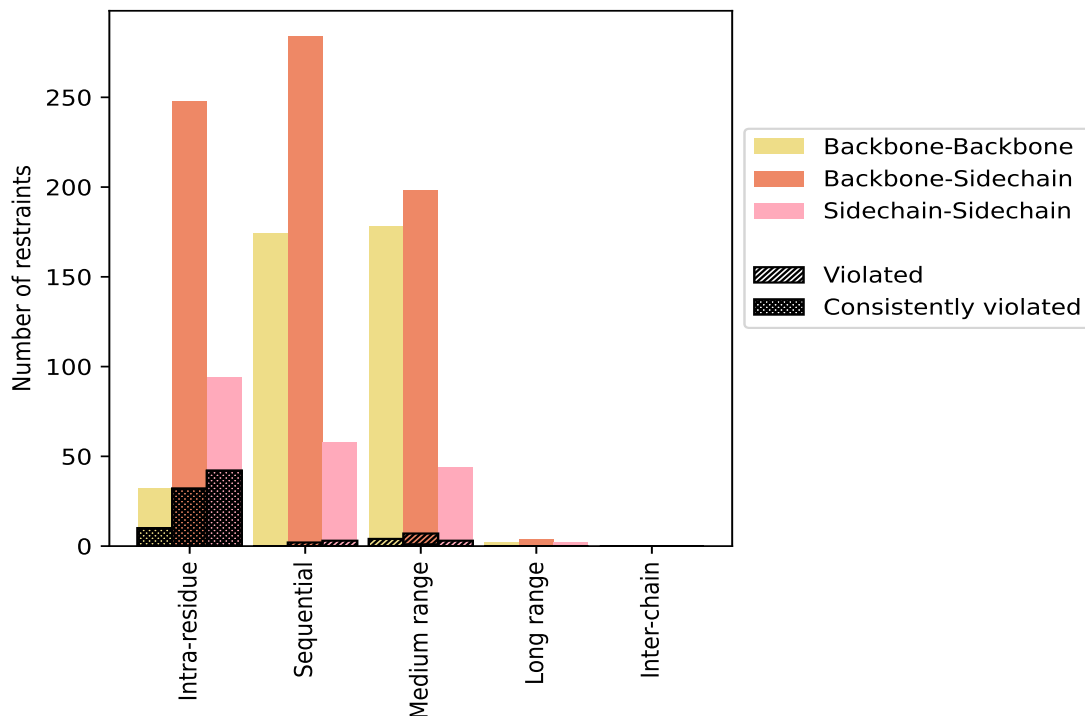
### 9.1 Summary of distance violations [i](#)

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

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>374</b>	<b>28.4</b>	<b>84</b>	<b>22.5</b>	<b>6.4</b>	<b>84</b>	<b>22.5</b>	<b>6.4</b>
Backbone-Backbone	32	2.4	10	31.2	0.8	10	31.2	0.8
Backbone-Sidechain	248	18.8	32	12.9	2.4	32	12.9	2.4
Sidechain-Sidechain	94	7.1	42	44.7	3.2	42	44.7	3.2
<b>Sequential (<math> i-j =1</math>)</b>	<b>516</b>	<b>39.2</b>	<b>5</b>	<b>1.0</b>	<b>0.4</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	174	13.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	284	21.5	2	0.7	0.2	0	0.0	0.0
Sidechain-Sidechain	58	4.4	3	5.2	0.2	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>420</b>	<b>31.9</b>	<b>14</b>	<b>3.3</b>	<b>1.1</b>	<b>1</b>	<b>0.2</b>	<b>0.1</b>
Backbone-Backbone	178	13.5	4	2.2	0.3	0	0.0	0.0
Backbone-Sidechain	198	15.0	7	3.5	0.5	1	0.5	0.1
Sidechain-Sidechain	44	3.3	3	6.8	0.2	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>8</b>	<b>0.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	0.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	2	0.2	0	0.0	0.0	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1318</b>	<b>100.0</b>	<b>103</b>	<b>7.8</b>	<b>7.8</b>	<b>85</b>	<b>6.4</b>	<b>6.4</b>
Backbone-Backbone	386	29.3	14	3.6	1.1	10	2.6	0.8
Backbone-Sidechain	734	55.7	41	5.6	3.1	33	4.5	2.5
Sidechain-Sidechain	198	15.0	48	24.2	3.6	42	21.2	3.2

<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 disulfid bonds are counted in their appropriate category on the x-axis

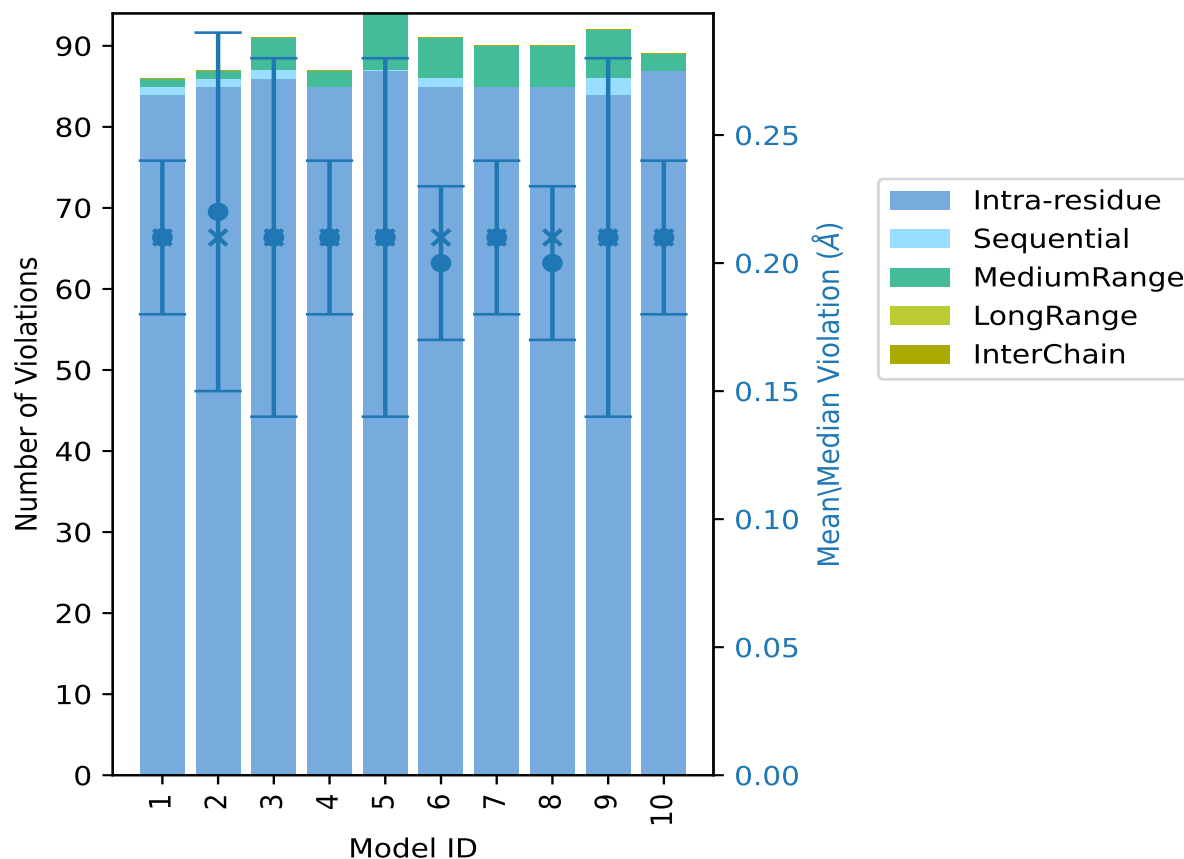
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <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	84	1	1	0	0	86	0.21	0.24	0.03	0.21
2	85	1	1	0	0	87	0.22	0.85	0.07	0.21
3	86	1	4	0	0	91	0.21	0.83	0.07	0.21
4	85	0	2	0	0	87	0.21	0.24	0.03	0.21
5	87	0	7	0	0	94	0.21	0.79	0.07	0.21
6	85	1	5	0	0	91	0.2	0.25	0.03	0.21
7	85	0	5	0	0	90	0.21	0.28	0.03	0.21
8	85	0	5	0	0	90	0.2	0.24	0.03	0.21
9	84	2	6	0	0	92	0.21	0.7	0.07	0.21
10	87	0	2	0	0	89	0.21	0.32	0.03	0.21

<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 [i](#)



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

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1215(IR:290, SQ:511, MR:406, LR:8, 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>	%
0	0	5	0	0	5	1	10.0
0	3	3	0	0	6	2	20.0
0	1	2	0	0	3	3	30.0

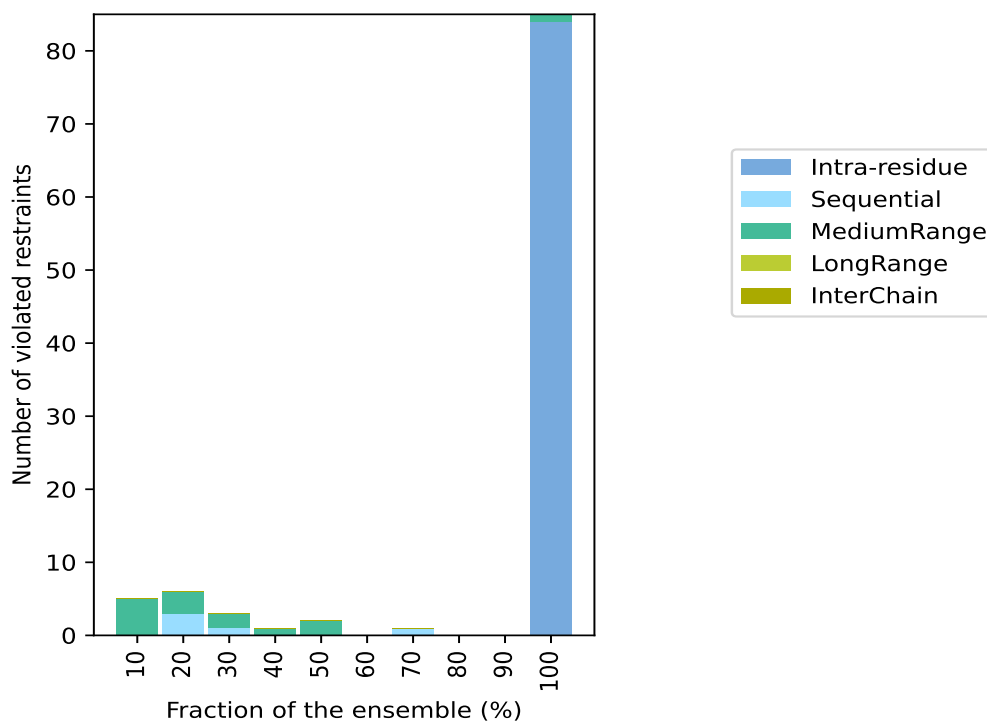
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	1	0	0	1	4	40.0
0	0	2	0	0	2	5	50.0
0	0	0	0	0	0	6	60.0
0	1	0	0	0	1	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
84	0	1	0	0	85	10	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](#)

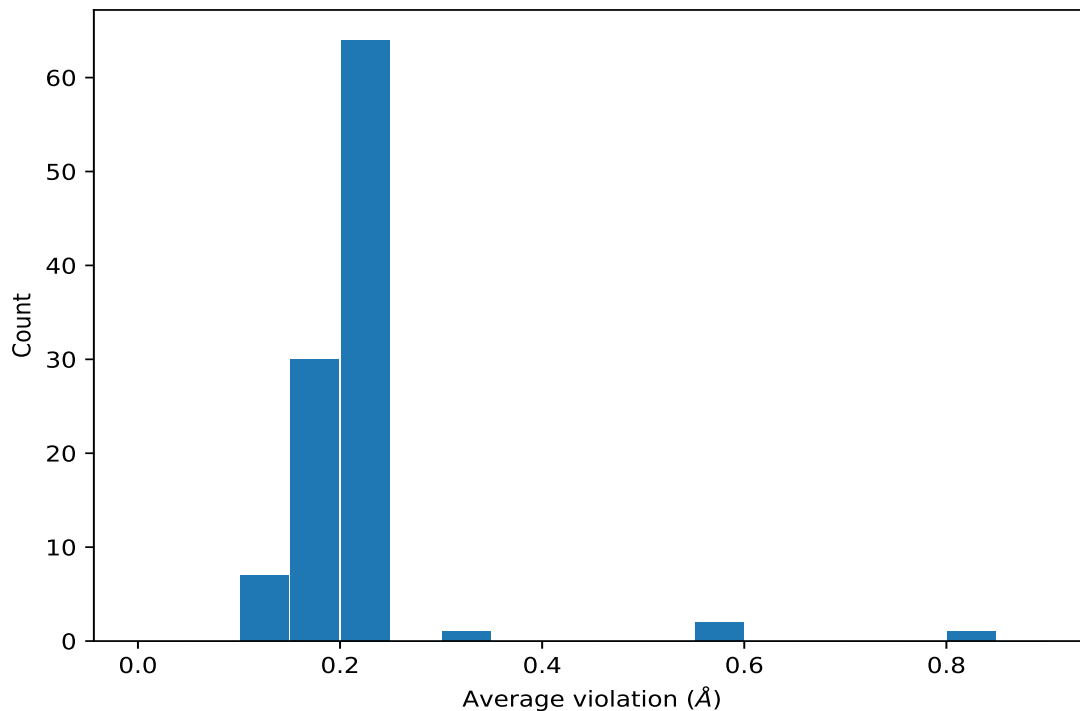


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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.

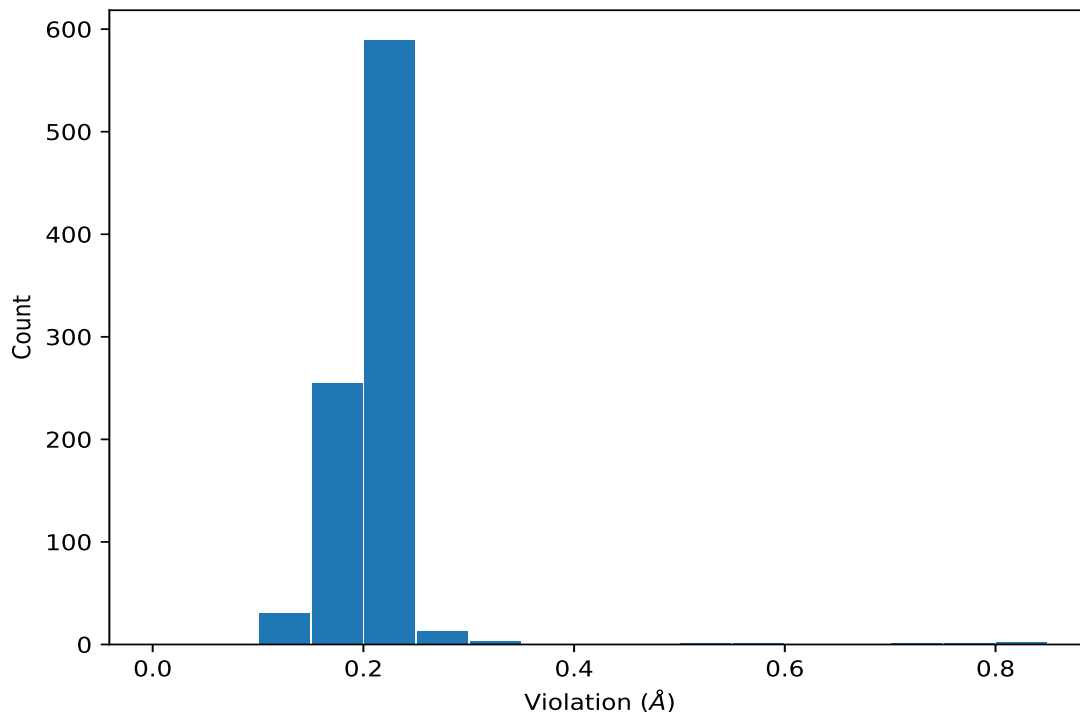
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1311)	1:151:D:ILE:CD1	1:151:D:ILE:CG1	10	0.24	0.0	0.24
(1,743)	1:68:D:PRO:CB	1:68:D:PRO:CA	10	0.24	0.01	0.24
(1,767)	1:68:D:PRO:CB	1:68:D:PRO:CA	10	0.24	0.01	0.24
(1,782)	1:48:D:ARG:CB	1:48:D:ARG:CA	10	0.24	0.0	0.24
(1,1205)	1:68:D:PRO:CB	1:70:D:ARG:C	10	0.24	0.06	0.24
(1,644)	1:151:A:ILE:CD1	1:151:A:ILE:CG1	10	0.24	0.0	0.24
(1,168)	1:48:A:ARG:CG	1:48:A:ARG:CD	10	0.24	0.01	0.24
(1,483)	1:115:A:PRO:CG	1:115:A:PRO:CB	10	0.24	0.0	0.24
(1,484)	1:115:A:PRO:CG	1:115:A:PRO:CB	10	0.24	0.0	0.24
(1,97)	1:93:A:MET:CB	1:93:A:MET:CA	10	0.23	0.0	0.23

<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)
(1,1260)	1:75:D:VAL:CG1	1:76:D:ILE:CG1	2	0.85
(1,1260)	1:75:D:VAL:CG1	1:76:D:ILE:CG1	3	0.83
(1,1206)	1:155:D:ILE:CG1	1:151:D:ILE:C	5	0.79
(1,593)	1:75:A:VAL:CG1	1:76:A:ILE:CG1	9	0.7
(1,161)	1:49:A:VAL:CB	1:48:A:ARG:CD	9	0.55
(1,593)	1:158:A:VAL:CG1	1:162:A:ILE:CG1	5	0.51
(1,1205)	1:68:D:PRO:CB	1:70:D:ARG:C	3	0.33
(1,1205)	1:68:D:PRO:CB	1:70:D:ARG:C	10	0.32
(1,1205)	1:68:D:PRO:CB	1:70:D:ARG:C	2	0.31
(1,671)	1:68:D:PRO:CA	1:65:D:PRO:CA	7	0.28

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

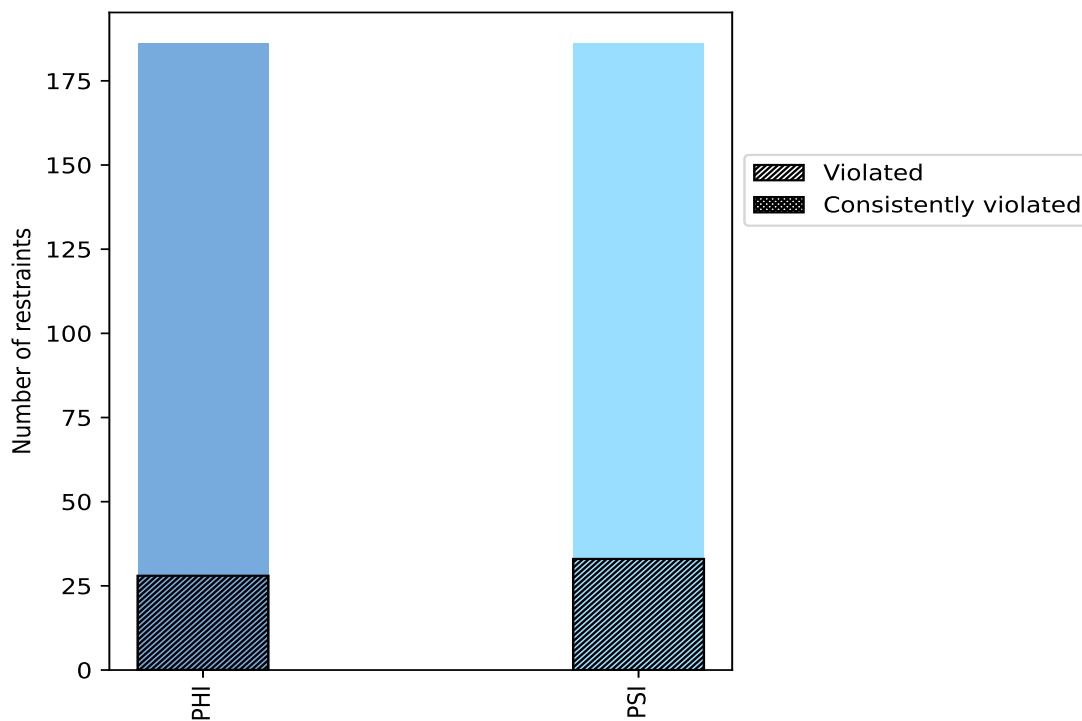
### 10.1 Summary of dihedral-angle violations [i](#)

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	186	50.0	28	15.1	7.5	0	0.0	0.0
PSI	186	50.0	33	17.7	8.9	0	0.0	0.0
Total	372	100.0	61	16.4	16.4	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](#)



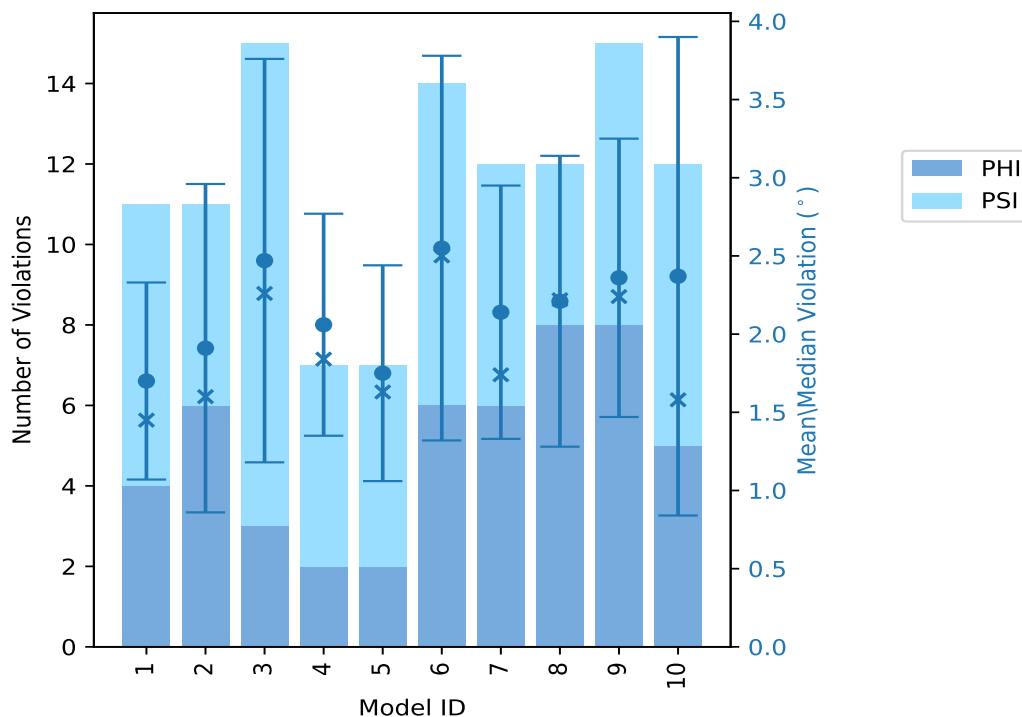
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	4	7	11	1.7	3.01	0.63	1.45
2	6	5	11	1.91	4.89	1.05	1.6
3	3	12	15	2.47	5.61	1.29	2.26
4	2	5	7	2.06	3.49	0.71	1.84
5	2	5	7	1.75	3.19	0.69	1.63
6	6	8	14	2.55	5.35	1.23	2.5
7	6	6	12	2.14	3.77	0.81	1.74
8	8	4	12	2.21	3.93	0.93	2.22
9	8	7	15	2.36	3.77	0.89	2.24
10	5	7	12	2.37	6.17	1.53	1.58

### 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

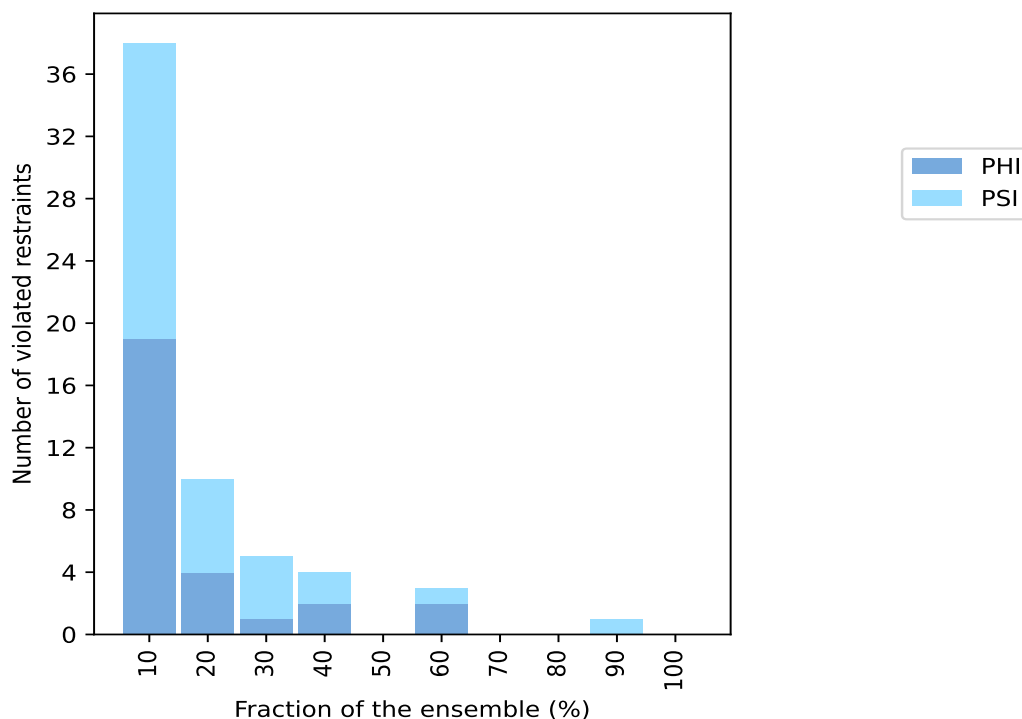
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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>	%
19	19	38	1	10.0
4	6	10	2	20.0
1	4	5	3	30.0
2	2	4	4	40.0
0	0	0	5	50.0
2	1	3	6	60.0
0	0	0	7	70.0
0	0	0	8	80.0
0	1	1	9	90.0
0	0	0	10	100.0

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

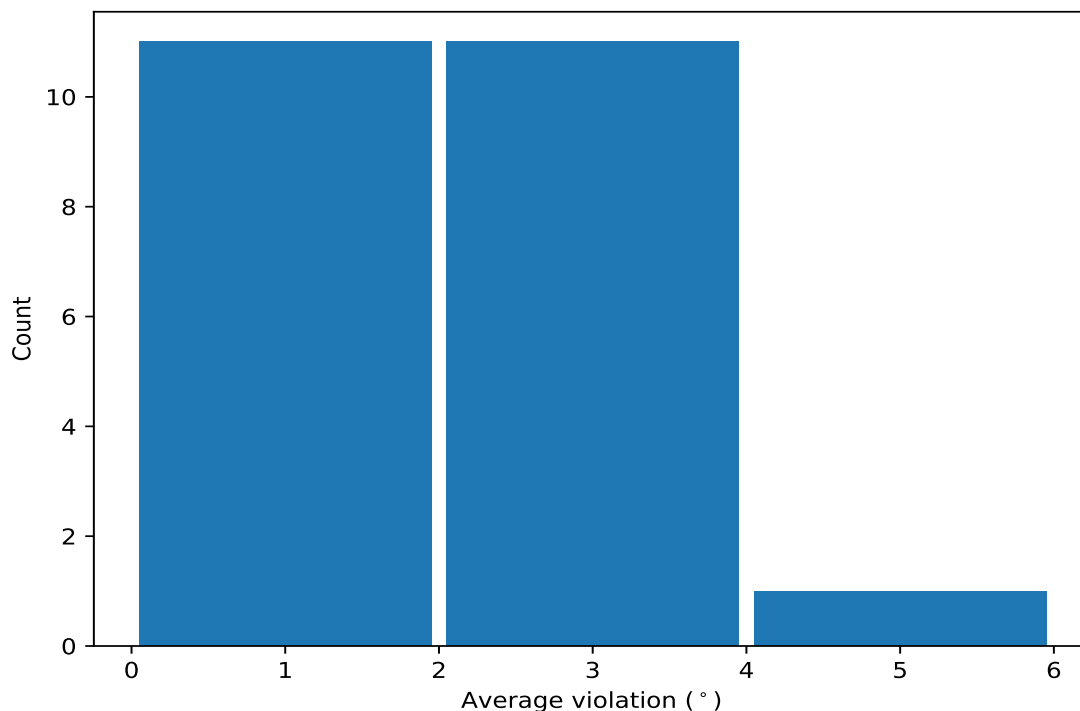
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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.

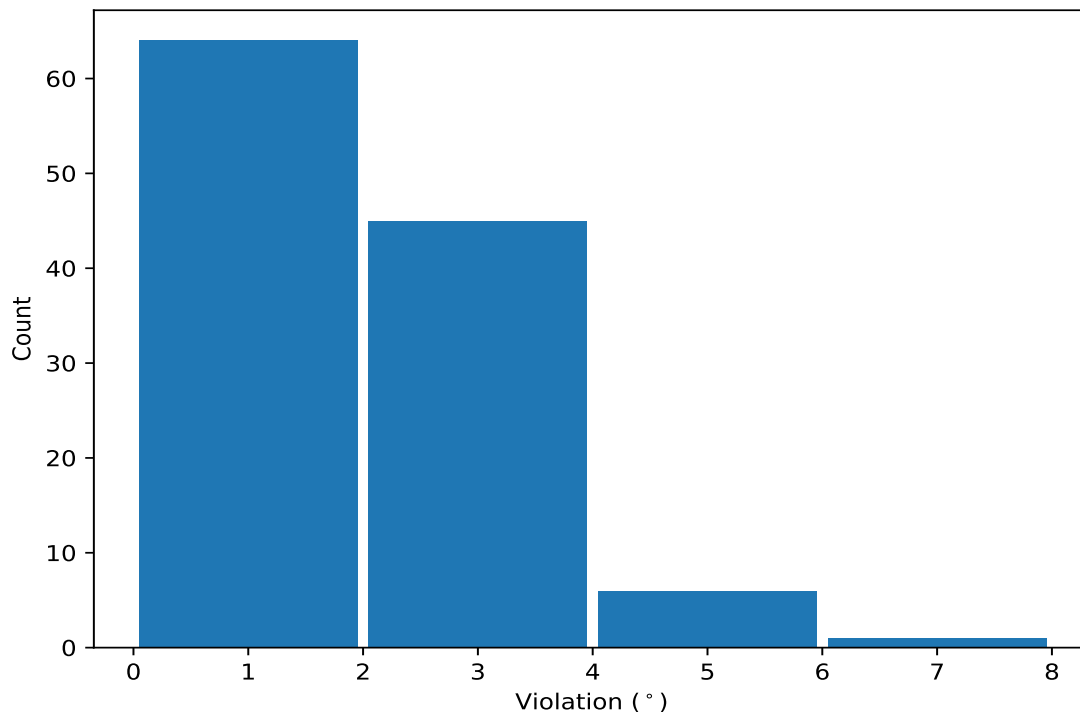
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,140)	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	1:121:A:PRO:N	9	2.58	0.68	2.69
(1,237)	1:43:D:LEU:C	1:44:D:CYS:N	1:44:D:CYS:CA	1:44:D:CYS:C	6	2.88	0.79	2.84
(1,238)	1:44:D:CYS:N	1:44:D:CYS:CA	1:44:D:CYS:C	1:45:D:ILE:N	6	2.84	0.46	3.0
(1,135)	1:103:A:THR:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	6	1.66	0.52	1.51
(1,150)	1:130:A:CYS:N	1:130:A:CYS:CA	1:130:A:CYS:C	1:131:A:ALA:N	4	4.97	1.02	5.12
(1,321)	1:103:D:THR:C	1:104:D:CYS:N	1:104:D:CYS:CA	1:104:D:CYS:C	4	2.64	0.67	2.34
(1,362)	1:156:D:VAL:N	1:156:D:VAL:CA	1:156:D:VAL:C	1:157:D:ALA:N	4	2.0	0.81	2.01
(1,341)	1:145:D:TRP:C	1:146:D:LEU:N	1:146:D:LEU:CA	1:146:D:LEU:C	4	1.79	0.78	1.54
(1,368)	1:159:D:LEU:N	1:159:D:LEU:CA	1:159:D:LEU:C	1:160:D:VAL:N	3	2.42	0.59	2.78
(1,138)	1:105:A:ASP:N	1:105:A:ASP:CA	1:105:A:ASP:C	1:106:A:PHE:N	3	1.52	0.21	1.63

<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 (°)
(1,150)	1:130:A:CYS:N	1:130:A:CYS:CA	1:130:A:CYS:C	1:131:A:ALA:N	10	6.17
(1,150)	1:130:A:CYS:N	1:130:A:CYS:CA	1:130:A:CYS:C	1:131:A:ALA:N	3	5.61
(1,367)	1:158:D:VAL:C	1:159:D:LEU:N	1:159:D:LEU:CA	1:159:D:LEU:C	6	5.35
(1,151)	1:130:A:CYS:C	1:131:A:ALA:N	1:131:A:ALA:CA	1:131:A:ALA:C	2	4.89
(1,150)	1:130:A:CYS:N	1:130:A:CYS:CA	1:130:A:CYS:C	1:131:A:ALA:N	6	4.62
(1,139)	1:119:A:TRP:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	10	4.53
(1,237)	1:43:D:LEU:C	1:44:D:CYS:N	1:44:D:CYS:CA	1:44:D:CYS:C	3	4.15
(1,320)	1:103:D:THR:N	1:103:D:THR:CA	1:103:D:THR:C	1:104:D:CYS:N	8	3.93
(1,336)	1:130:D:CYS:N	1:130:D:CYS:CA	1:130:D:CYS:C	1:131:D:ALA:N	3	3.81
(1,321)	1:103:D:THR:C	1:104:D:CYS:N	1:104:D:CYS:CA	1:104:D:CYS:C	7	3.77