



# wwPDB NMR Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:22 PM UTC

PDB ID : 2LBV / pdb\_00002lbv  
BMRB ID : 17577  
Title : Siderocalin Q83 reveals a dual ligand binding mode  
Authors : Coudeville, N.; Hoetzing, M.; Geist, L.; Kontaxis, G.; Bister, K.; Konrat, R.  
Deposited on : 2011-04-07

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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 : 4-5-2 with Phenix2.0  
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

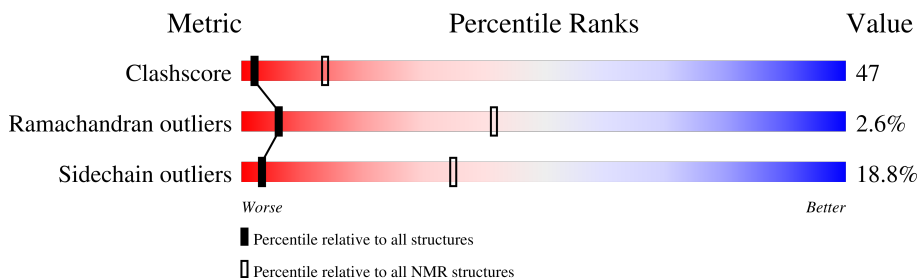
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 70%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	157	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:5-A:66, A:75-A:155 (143)	0.69	13

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

### 3 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2650 atoms, of which 1313 are hydrogens and 0 are deuteriums.

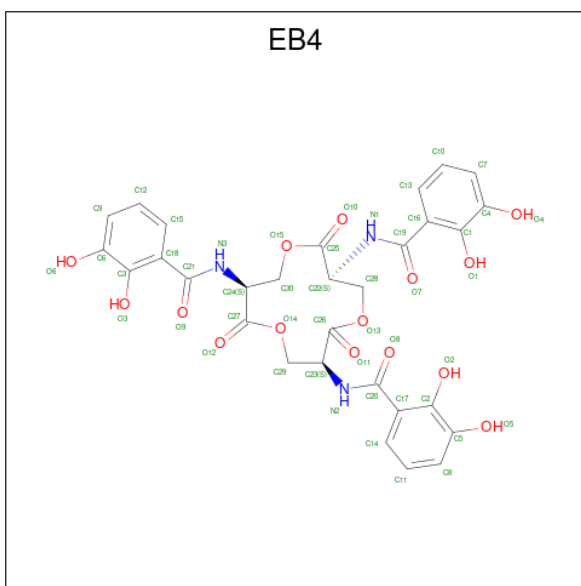
- Molecule 1 is a protein called Extracellular fatty acid-binding protein.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	157	2527	799	1261	213	244	10	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9I9P7

- Molecule 2 is N,N',N''-[(3S,7S,11S)-2,6,10-trioxo-1,5,9-trioxacyclododecane-3,7,11-triyl]tris(2,3-dihydroxybenzamide) (CCD ID: EB4) (formula: C<sub>30</sub>H<sub>27</sub>N<sub>3</sub>O<sub>15</sub>).

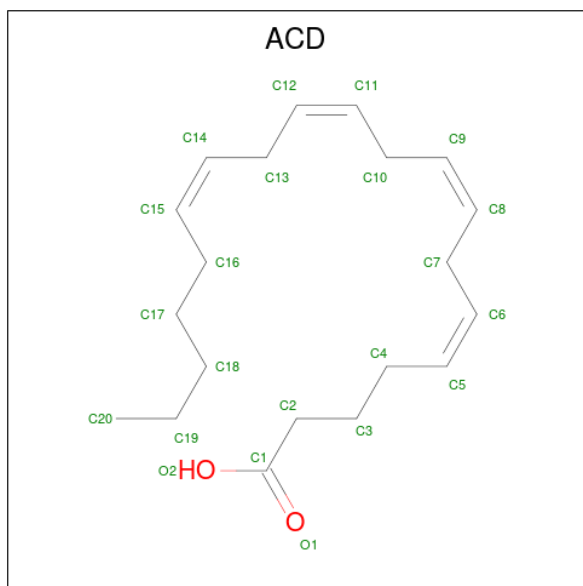


Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	69	30	21	3	15

- Molecule 3 is GALLIUM (III) ION (CCD ID: GA) (formula: Ga).

Mol	Chain	Residues	Atoms	
3	A	1	Total	Ga
			1	1

- Molecule 4 is ARACHIDONIC ACID (CCD ID: ACD) (formula:  $C_{20}H_{32}O_2$ ).



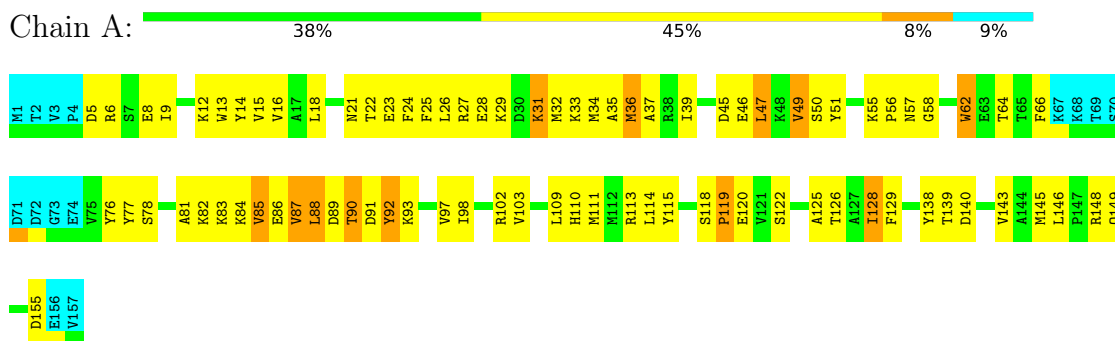
Mol	Chain	Residues	Atoms			
			Total	C	H	O
4	A	1	53	20	31	2

## 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.

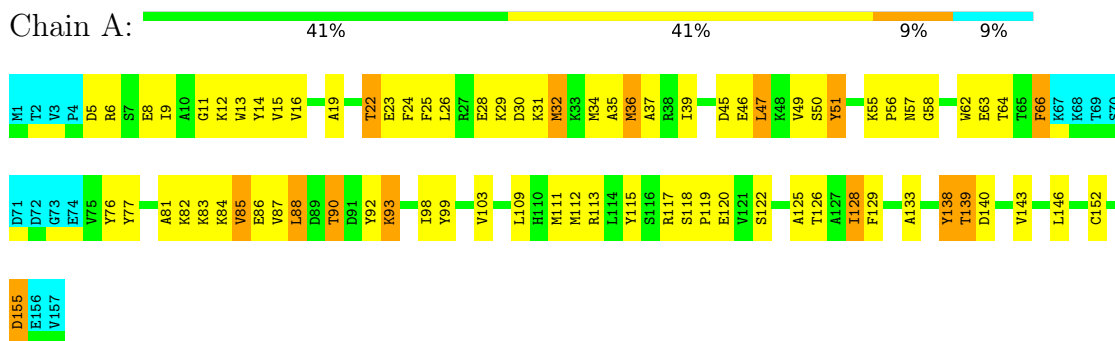
- Molecule 1: Extracellular fatty acid-binding protein



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

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

- Molecule 1: Extracellular fatty acid-binding protein



## 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 least restraint violations*.

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

Software name	Classification	Version
NMRPipe	refinement	

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	1485
Number of shifts mapped to atoms	1485
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	70%

## 6 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: EB4, ACD, GA

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	0.65±0.01	0±0/1184 ( 0.0± 0.0%)	1.02±0.01	0±0/1595 ( 0.0± 0.0%)
All	All	0.65	0/23680 ( 0.0%)	1.02	9/31900 ( 0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	129	PHE	CA-CB-CG	-5.94	107.86	113.80	7	9

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	1160	1157	1157	107±16
2	A	48	21	21	7±2
4	A	22	31	31	26±3
All	All	24620	24180	24180	2279

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 47.

5 of 510 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:VAL:HG21	4:A:300:ACD:H192	1.00	1.34	15	7
1:A:39:ILE:HD12	4:A:300:ACD:H201	0.96	1.35	7	20
4:A:300:ACD:C9	4:A:300:ACD:H191	0.92	1.95	15	7
1:A:33:LYS:C	1:A:146:LEU:HD23	0.90	1.92	2	7
1:A:46:GLU:O	1:A:47:LEU:HD23	0.85	1.72	14	4

## 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	143/157 (91%)	128±1 (90±1%)	11±1 (8±1%)	4±1 (3±1%)	6	42
All	All	2860/3140 (91%)	2570 (90%)	217 (8%)	73 (3%)	6	42

5 of 9 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	119	PRO	20
1	A	87	VAL	14
1	A	56	PRO	13
1	A	92	TYR	7
1	A	5	ASP	7

### 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	124/137 (91%)	101±3 (81±3%)	23±3 (19±3%)	3	35
All	All	2480/2740 (91%)	2013 (81%)	467 (19%)	3	35

5 of 62 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	36	MET	20
1	A	49	VAL	20
1	A	85	VAL	20
1	A	88	LEU	20
1	A	90	THR	20

### 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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	EB4	A	200	3	51,51,51	0.99±0.00	1±0 (1±0%)
4	ACD	A	300	-	21,21,21	1.78±0.00	4±0 (19±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard

deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	EB4	A	200	3	72,72,72	1.02±0.00	5±0 (6±0%)
4	ACD	A	300	-	21,21,21	0.90±0.02	0±0 (1±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EB4	A	200	3	-	0±0,51,51,51	0±0,3,4,4
4	ACD	A	300	-	-	0±0,19,19,19	-

All 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
2	A	200	EB4	C17-C20	5.41	1.39	1.50	3	20
4	A	300	ACD	C9-C8	3.86	1.53	1.31	16	20
4	A	300	ACD	C12-C11	3.85	1.53	1.31	18	20
4	A	300	ACD	C15-C14	3.85	1.53	1.31	8	20
4	A	300	ACD	C6-C5	3.85	1.53	1.31	15	20

5 of 6 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

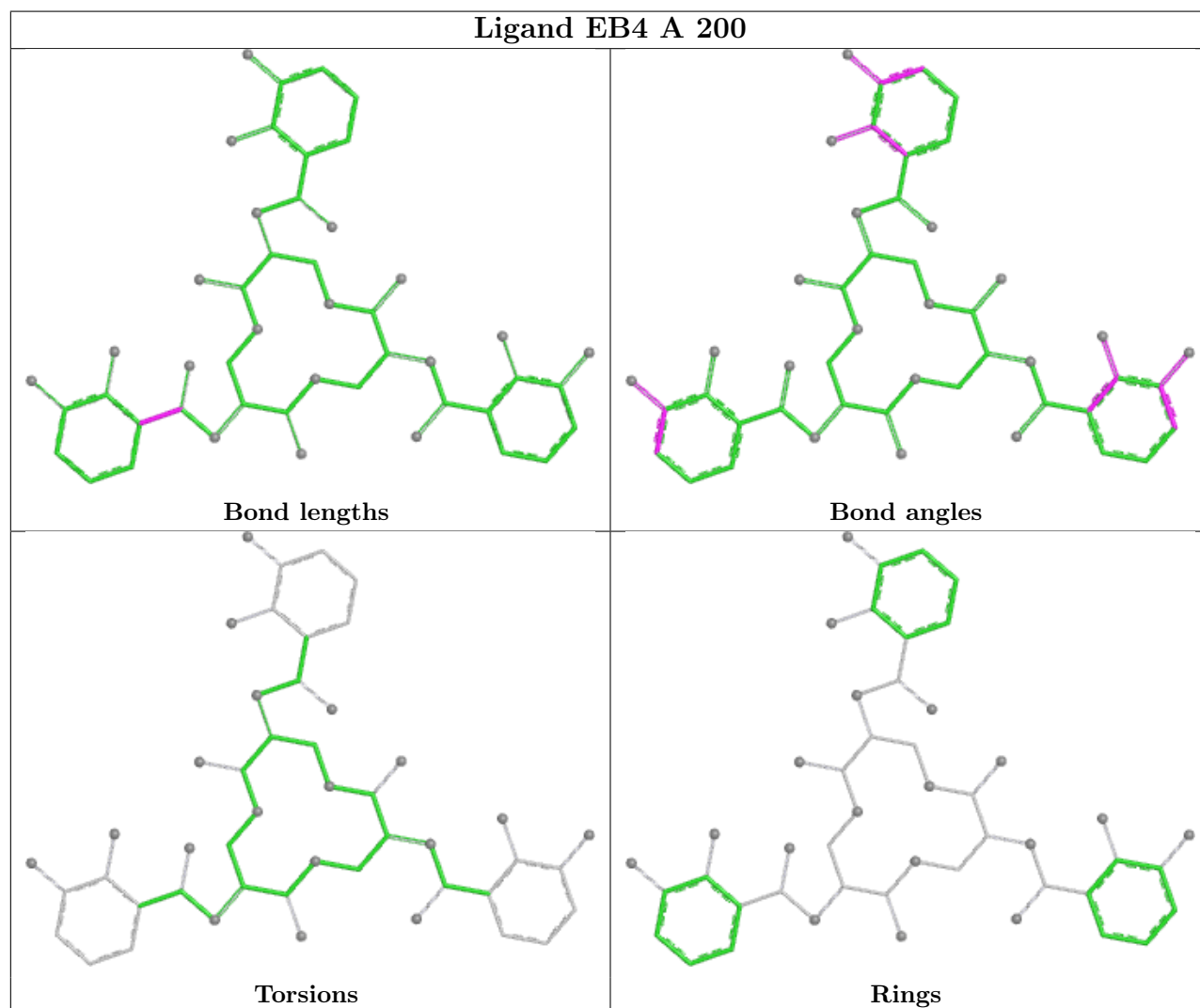
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	200	EB4	O4-C4-C7	2.51	126.08	119.36	12	20
2	A	200	EB4	O1-C1-C16	2.50	125.57	121.11	11	20
4	A	300	ACD	C3-C2-C1	2.29	108.53	114.51	15	7
2	A	200	EB4	O3-C3-C18	2.21	125.04	121.11	13	20
2	A	200	EB4	O5-C5-C8	2.14	125.10	119.36	20	20

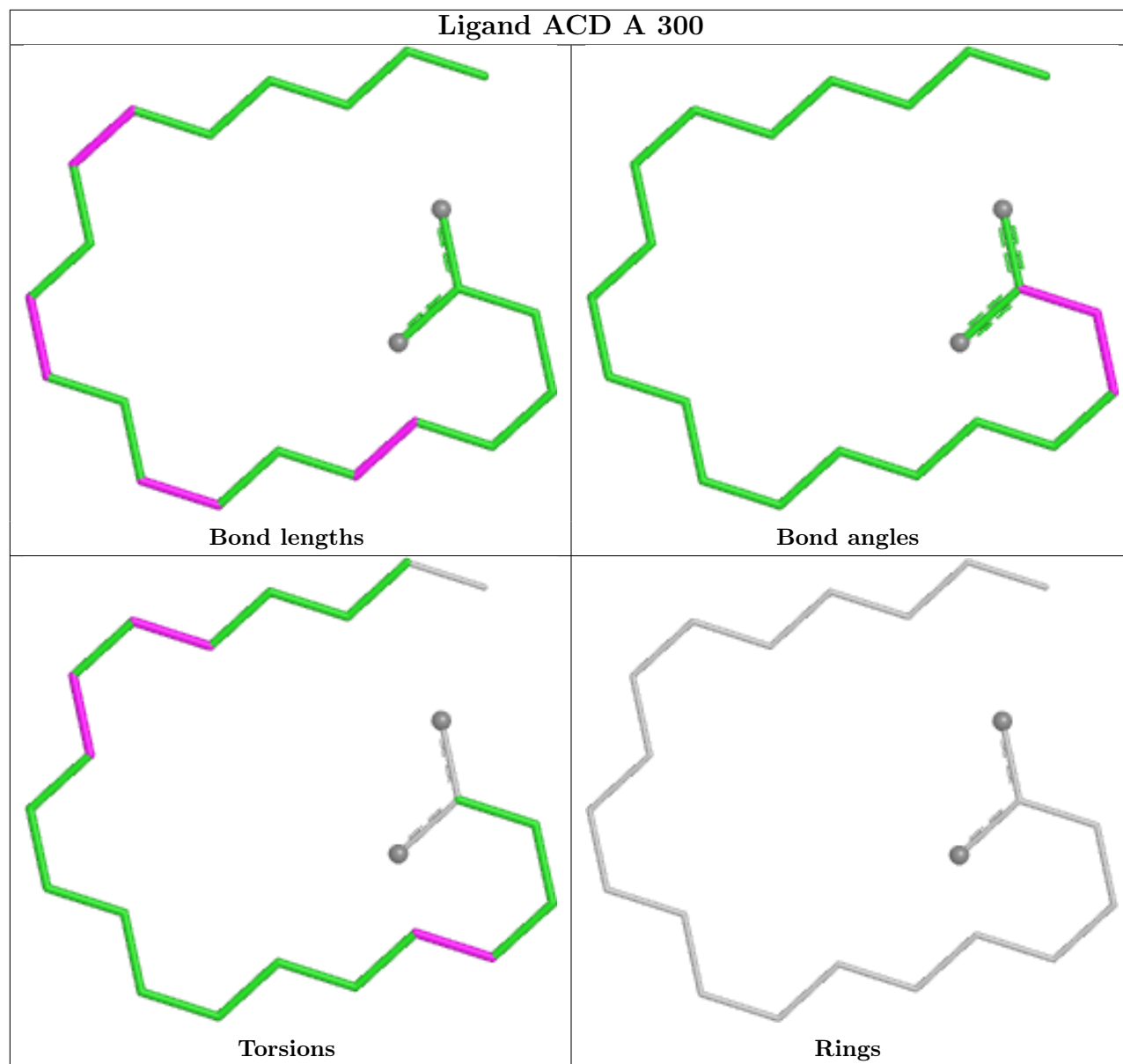
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 i

The completeness of assignment taking into account all chemical shift lists is 70% for the well-defined parts and 68% 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 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	1485
Number of shifts mapped to atoms	1485
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	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
$^{13}\text{C}_\alpha$	152	-1.20 $\pm$ 0.10	Should be applied
$^{13}\text{C}_\beta$	145	-0.97 $\pm$ 0.16	Should be applied
$^{13}\text{C}'$	144	0.28 $\pm$ 0.09	None needed (< 0.5 ppm)
$^{15}\text{N}$	146	0.38 $\pm$ 0.38	None needed (< 0.5 ppm)

#### 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 70%, i.e. 1393 atoms were assigned a chemical shift out of a possible 1998. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	683/710 (96%)	273/286 (95%)	274/286 (96%)	136/138 (99%)
Sidechain	683/1126 (61%)	400/729 (55%)	280/347 (81%)	3/50 (6%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	27/162 (17%)	8/77 (10%)	17/82 (21%)	2/3 (67%)
Overall	1393/1998 (70%)	681/1092 (62%)	571/715 (80%)	141/191 (74%)

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

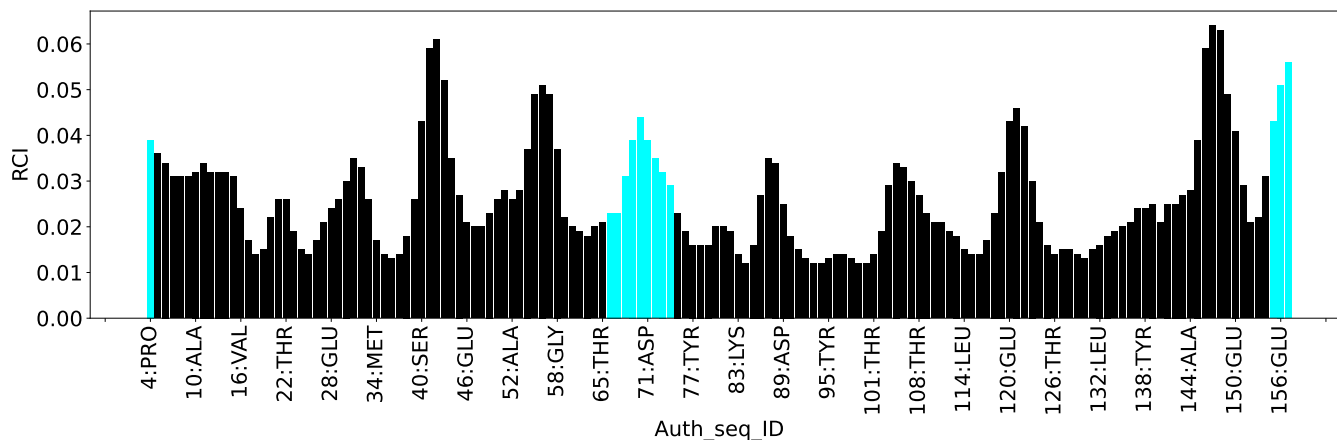
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	94	SER	H	11.42	5.45 – 11.10	5.6
1	A	90	THR	HG21	0.04	0.08 – 2.19	-5.2
1	A	90	THR	HG22	0.04	0.08 – 2.19	-5.2
1	A	90	THR	HG23	0.04	0.08 – 2.19	-5.2

### 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	1368
Intra-residue ( $ i-j =0$ )	189
Sequential ( $ i-j =1$ )	484
Medium range ( $ i-j >1$ and $ i-j <5$ )	145
Long range ( $ i-j \geq 5$ )	377
Inter-chain	36
Hydrogen bond restraints	130
Disulfide bond restraints	1
Total dihedral-angle restraints	230
Number of unmapped restraints	0
Number of restraints per residue	10.0
Number of long range restraints per residue <sup>1</sup>	2.9

<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)	2.0	0.2
0.2-0.5 (Medium)	None	None
>0.5 (Large)	2.0	2.25

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	57.5	9.91
10.0-20.0 (Medium)	3.0	20.0
>20.0 (Large)	None	None

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

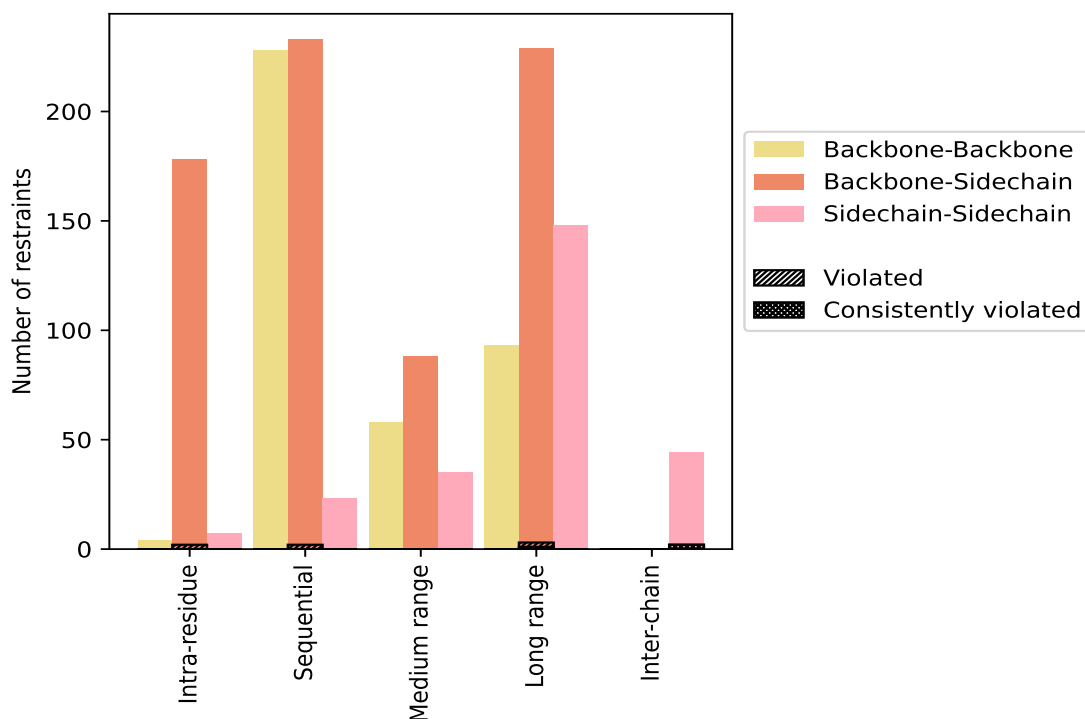
### 9.1 Summary of distance violations [i](#)

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>189</b>	<b>13.8</b>	<b>2</b>	<b>1.1</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	178	13.0	2	1.1	0.1	0	0.0	0.0
Sidechain-Sidechain	7	0.5	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>484</b>	<b>35.4</b>	<b>2</b>	<b>0.4</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	228	16.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	233	17.0	2	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	23	1.7	0	0.0	0.0	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>145</b>	<b>10.6</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	58	4.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	52	3.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	35	2.6	0	0.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>377</b>	<b>27.6</b>	<b>1</b>	<b>0.3</b>	<b>0.1</b>	<b>1</b>	<b>0.3</b>	<b>0.1</b>
Backbone-Backbone	93	6.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	137	10.0	1	0.7	0.1	1	0.7	0.1
Sidechain-Sidechain	147	10.7	0	0.0	0.0	0	0.0	0.0
<b>Inter-chain</b>	<b>36</b>	<b>2.6</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	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	36	2.6	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>130</b>	<b>9.5</b>	<b>4</b>	<b>3.1</b>	<b>0.3</b>	<b>2</b>	<b>1.5</b>	<b>0.1</b>
<b>Disulfide bond</b>	<b>1</b>	<b>0.1</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>1368</b>	<b>100.0</b>	<b>9</b>	<b>0.7</b>	<b>0.7</b>	<b>3</b>	<b>0.2</b>	<b>0.2</b>
Backbone-Backbone	383	28.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	728	53.2	7	1.0	0.5	1	0.1	0.1
Sidechain-Sidechain	257	18.8	2	0.8	0.1	2	0.8	0.1

<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	0	0	0	2	2	4	0.87	1.63	0.72	0.88
2	1	1	0	1	2	5	0.69	1.7	0.71	0.15
3	1	1	0	1	2	5	0.71	1.81	0.73	0.14
4	1	1	0	1	2	5	0.72	1.83	0.73	0.16
5	1	0	0	1	2	4	0.87	1.83	0.75	0.76
6	1	0	0	1	2	4	0.85	1.7	0.71	0.78
7	2	0	0	1	2	5	0.71	1.75	0.71	0.14
8	1	0	0	1	2	4	0.9	1.98	0.8	0.76
9	1	1	0	1	2	5	0.71	1.8	0.73	0.14
10	1	1	0	1	2	5	0.72	1.88	0.74	0.15

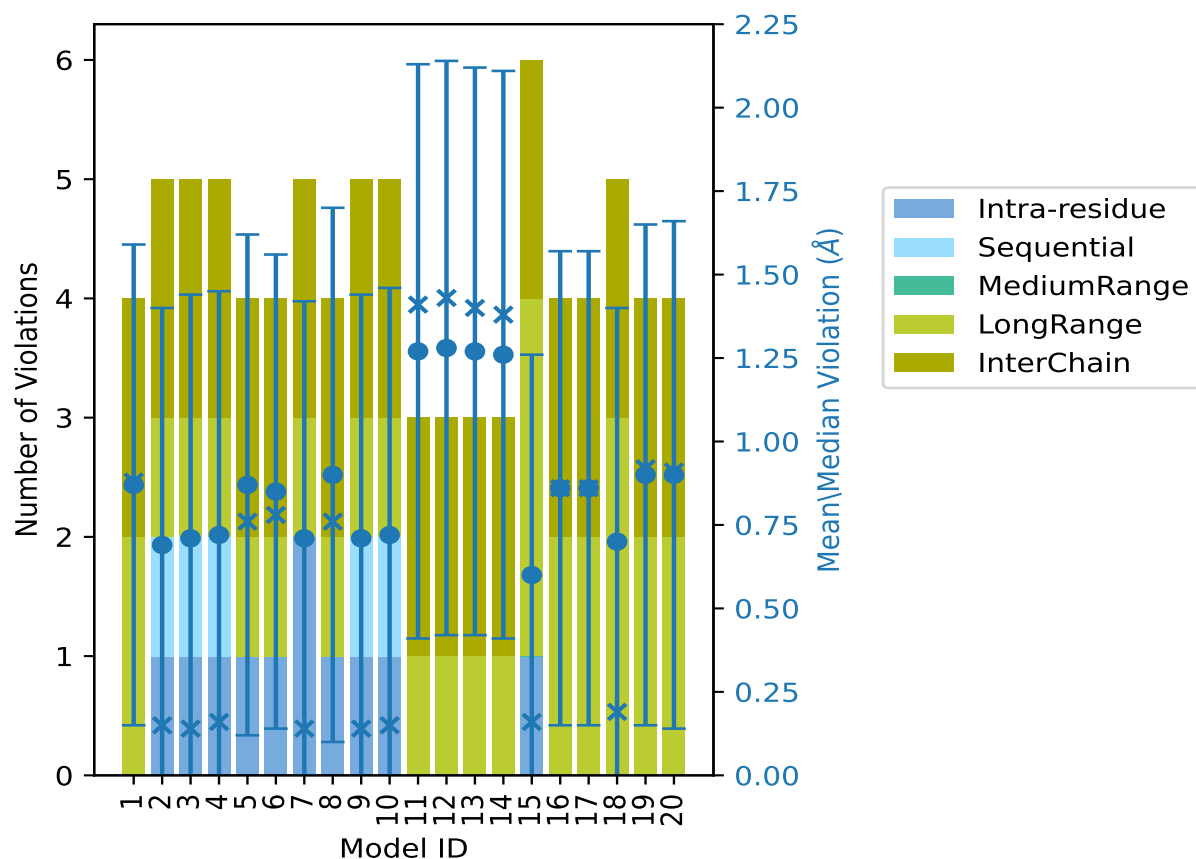
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	0	0	0	1	2	3	1.27	2.25	0.86	1.41
12	0	0	0	1	2	3	1.28	2.25	0.86	1.43
13	0	0	0	1	2	3	1.27	2.23	0.85	1.4
14	0	0	0	1	2	3	1.26	2.23	0.85	1.38
15	1	0	0	3	2	6	0.6	1.57	0.66	0.16
16	0	0	0	2	2	4	0.86	1.61	0.71	0.86
17	0	0	0	2	2	4	0.86	1.61	0.71	0.86
18	0	0	0	3	2	5	0.7	1.61	0.7	0.19
19	0	0	0	2	2	4	0.9	1.67	0.75	0.92
20	0	0	0	2	2	4	0.9	1.69	0.76	0.91

<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

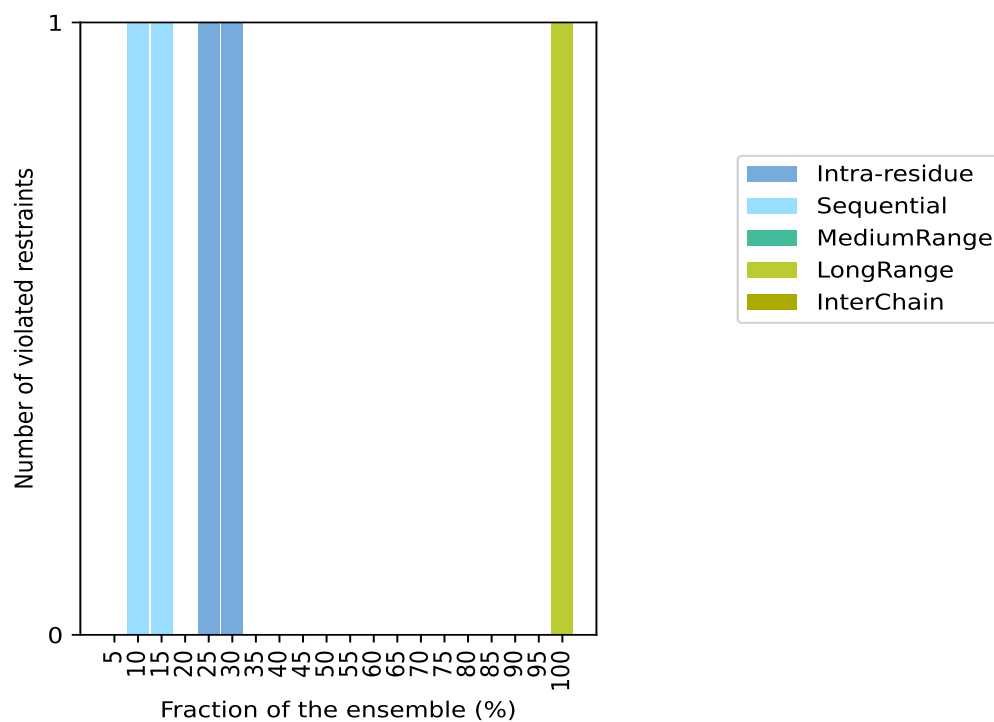
### 9.3 Distance violation statistics for the ensemble

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, 1226(IR:187, SQ:482, MR:145, LR:376, IC:36) 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	0	0	0	0	1	5.0
0	1	0	0	0	1	2	10.0
0	1	0	0	0	1	3	15.0
0	0	0	0	0	0	4	20.0
1	0	0	0	0	1	5	25.0
1	0	0	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	1	0	1	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

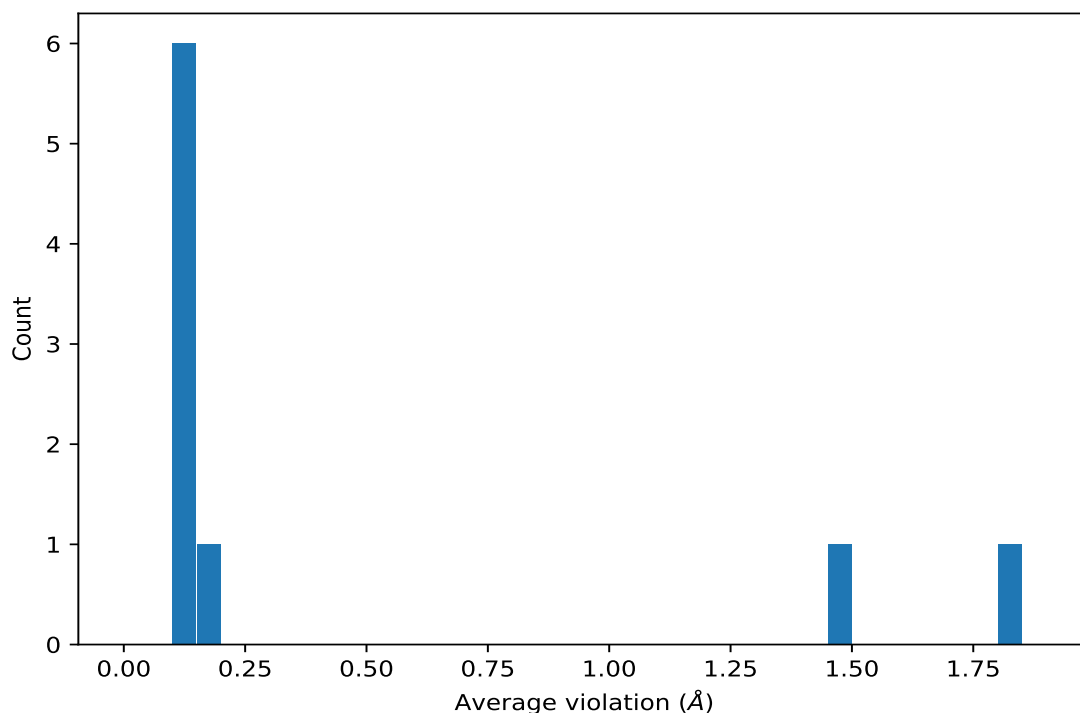
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 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.

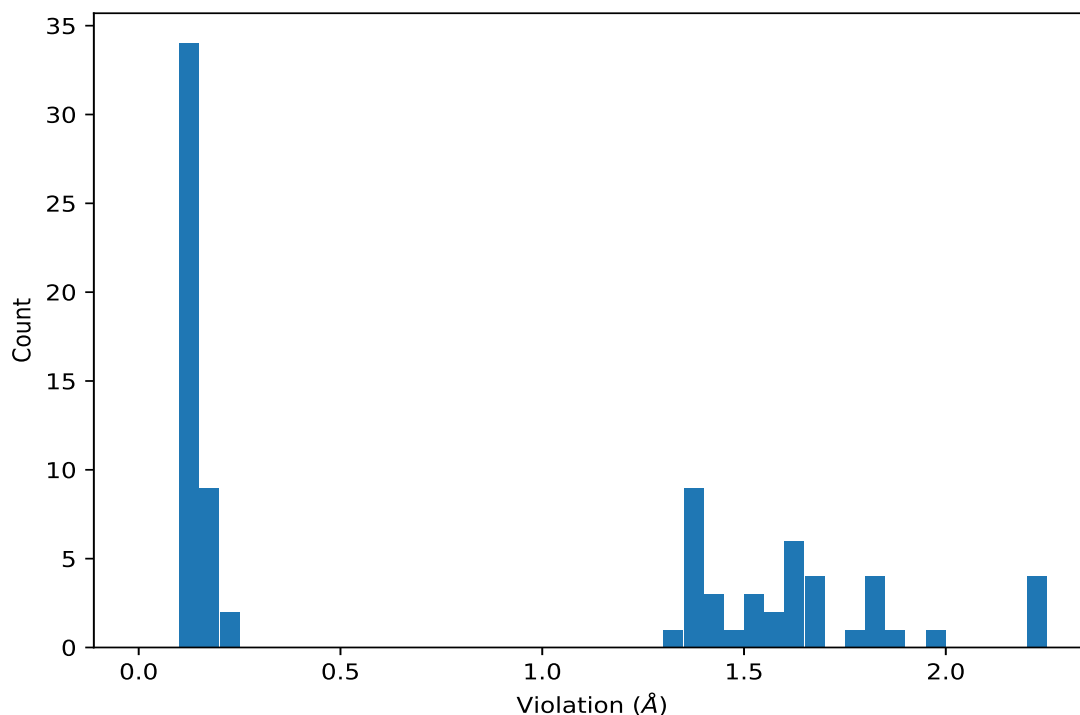
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	20	1.83	0.23	1.78
(2,343)	1:90:A:THR:OG1	4:300:A:ACD:H71	20	1.45	0.1	1.4
(1,269)	1:13:A:TRP:HZ2	1:39:A:ILE:HA	20	0.16	0.02	0.16
(3,59)	1:67:A:LYS:O	1:77:A:TYR:H	7	0.11	0.01	0.11
(1,803)	1:145:A:MET:H	1:145:A:MET:HG3	6	0.14	0.02	0.13
(1,807)	1:146:A:LEU:H	1:146:A:LEU:HG	5	0.13	0.01	0.13
(1,675)	1:109:A:LEU:HB3	1:110:A:HIS:HA	3	0.11	0.0	0.11
(3,5)	1:17:A:ALA:H	1:114:A:LEU:O	2	0.11	0.01	0.11
(1,674)	1:109:A:LEU:HB2	1:110:A:HIS:HA	2	0.11	0.0	0.11

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

## 9.5 All violated distance restraints [i](#)

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

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



### 9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	11	2.25
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	12	2.25
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	13	2.23
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	14	2.23
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	8	1.98
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	10	1.88
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	4	1.83
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	5	1.83
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	3	1.81
(2,342)	1:92:A:TYR:OH	4:300:A:ACD:H71	9	1.8

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

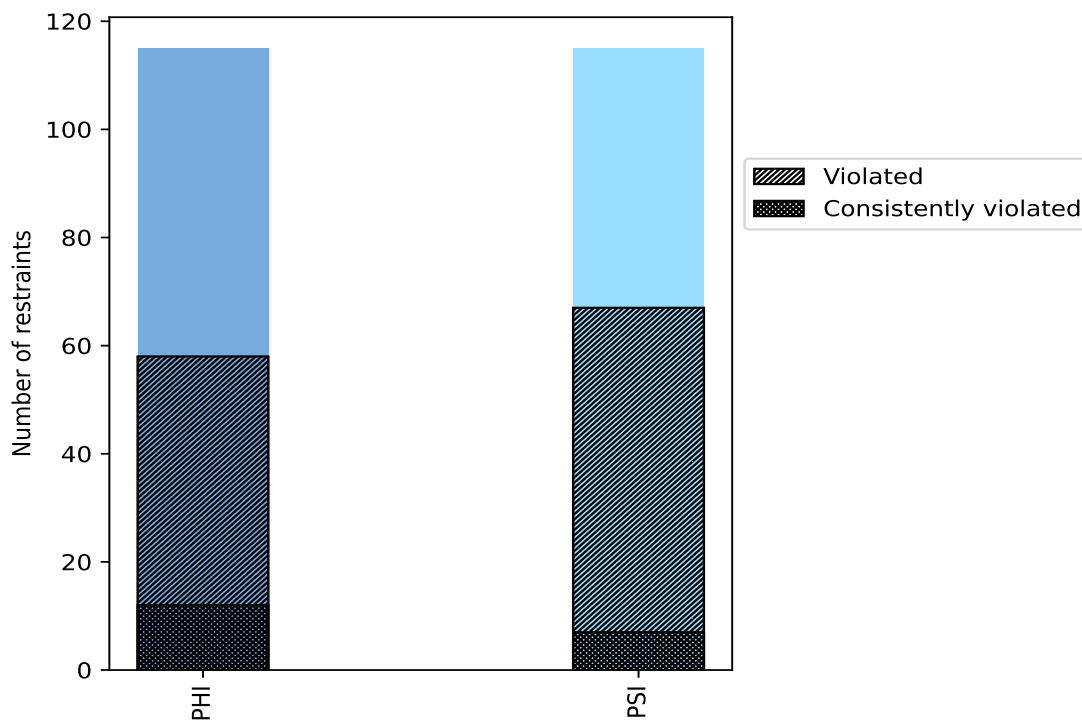
### 10.1 Summary of dihedral-angle violations [i](#)

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	115	50.0	58	50.4	25.2	12	10.4	5.2
PSI	115	50.0	67	58.3	29.1	7	6.1	3.0
Total	230	100.0	125	54.3	54.3	19	8.3	8.3

<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](#)



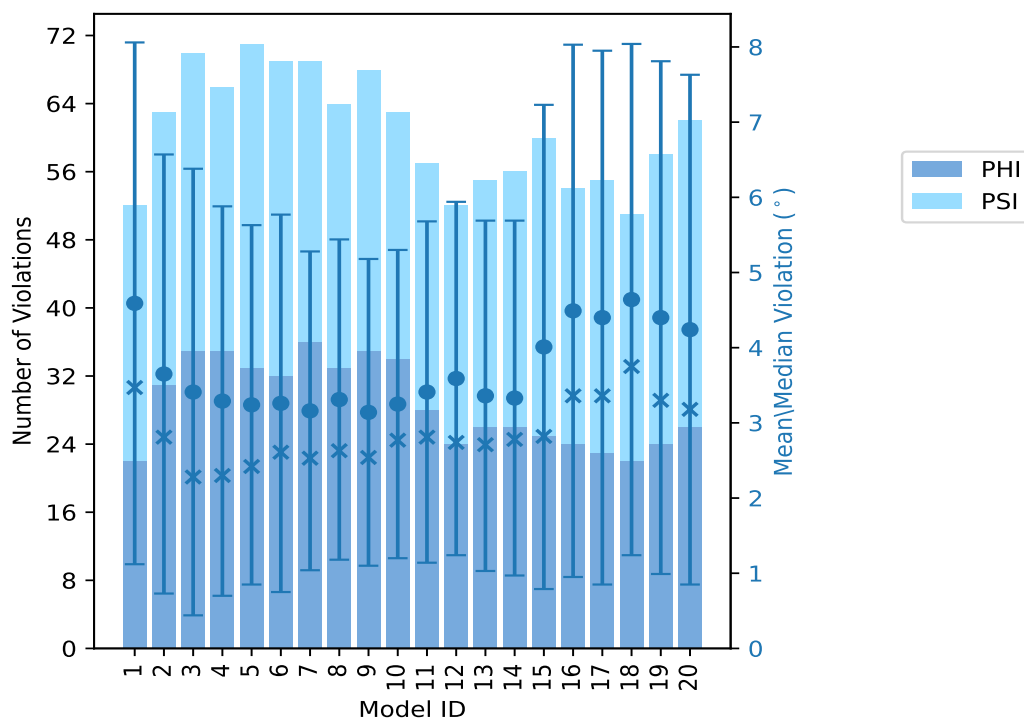
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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	22	30	52	4.59	13.78	3.47	3.47
2	31	32	63	3.65	19.71	2.92	2.81
3	35	35	70	3.41	20.0	2.97	2.28
4	35	31	66	3.29	16.74	2.59	2.3
5	33	38	71	3.24	14.47	2.39	2.42
6	32	37	69	3.26	16.2	2.51	2.61
7	36	33	69	3.16	10.7	2.12	2.53
8	33	31	64	3.31	10.87	2.13	2.63
9	35	33	68	3.14	10.7	2.04	2.54
10	34	29	63	3.25	11.02	2.05	2.77
11	28	29	57	3.41	11.11	2.27	2.81
12	24	28	52	3.59	11.18	2.35	2.74
13	26	29	55	3.36	10.76	2.33	2.71
14	26	30	56	3.33	11.37	2.36	2.78
15	25	35	60	4.01	13.91	3.22	2.82
16	24	30	54	4.49	16.07	3.54	3.36
17	23	32	55	4.4	16.31	3.55	3.36
18	22	29	51	4.64	14.18	3.4	3.75
19	24	34	58	4.4	16.11	3.41	3.3
20	26	36	62	4.24	14.74	3.39	3.18

### 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	6	13	1	5.0
3	4	7	2	10.0
3	3	6	3	15.0
1	3	4	4	20.0
1	4	5	5	25.0
6	4	10	6	30.0
7	10	17	7	35.0
2	2	4	8	40.0
4	3	7	9	45.0
2	1	3	10	50.0
0	3	3	11	55.0

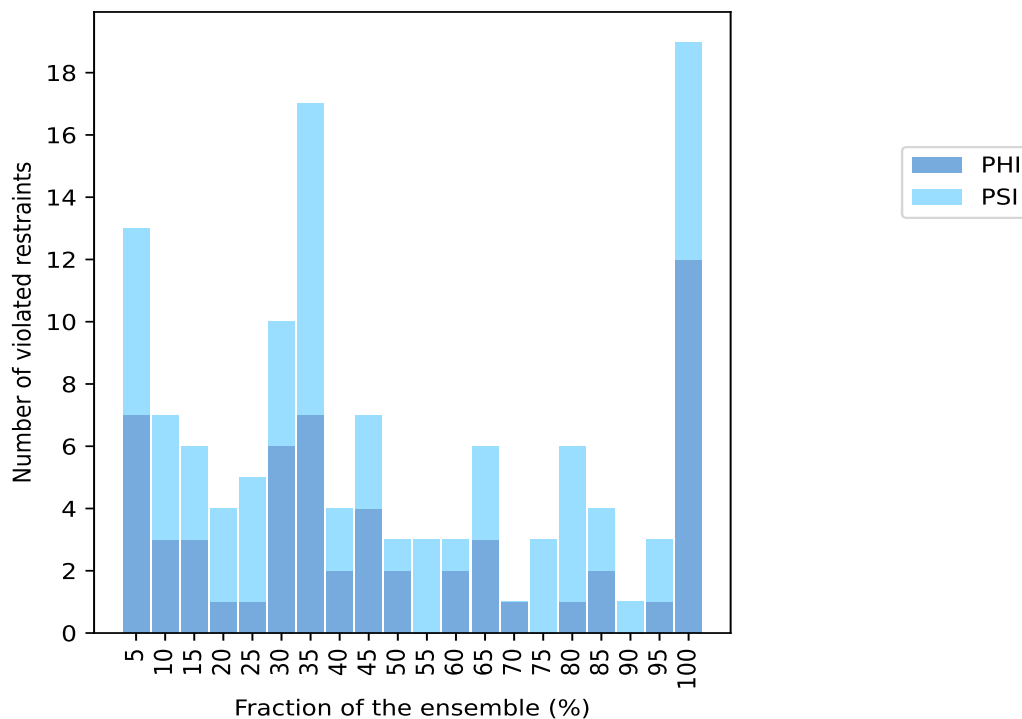
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
2	1	3	12	60.0
3	3	6	13	65.0
1	0	1	14	70.0
0	3	3	15	75.0
1	5	6	16	80.0
2	2	4	17	85.0
0	1	1	18	90.0
1	2	3	19	95.0
12	7	19	20	100.0

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

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

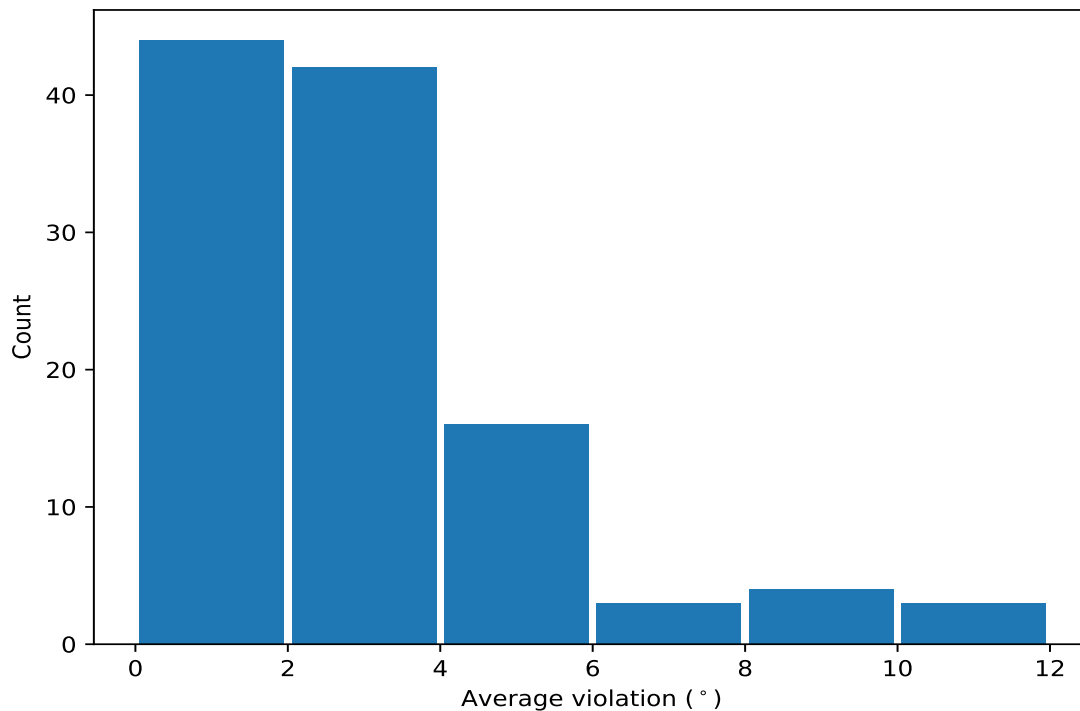


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

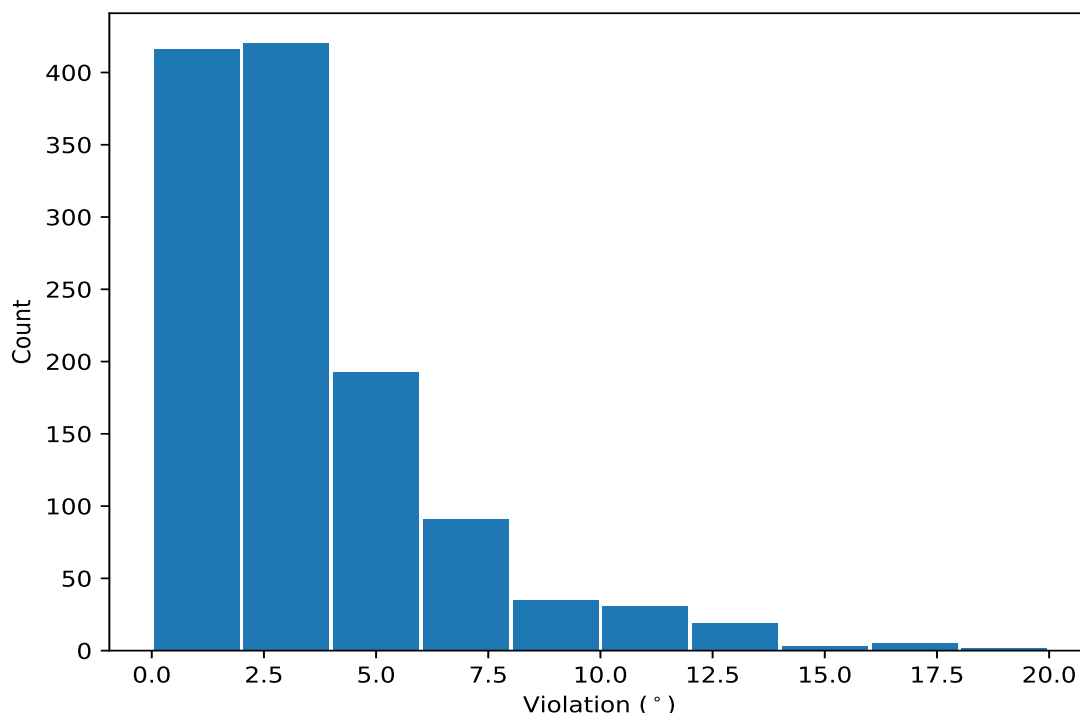
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	20	11.91	5.06	13.68
(1,14)	1:13:A:TRP:N	1:13:A:TRP:CA	1:13:A:TRP:C	1:14:A:TYR:N	20	10.32	0.61	10.5
(1,101)	1:75:A:VAL:C	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	20	9.04	3.76	10.93
(1,100)	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	1:76:A:TYR:N	20	8.5	1.19	8.66
(1,97)	1:73:A:GLY:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	20	6.5	3.12	4.62
(1,54)	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	1:40:A:SER:N	20	5.41	1.05	5.82
(1,117)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:GLU:N	20	5.36	2.36	4.8
(1,206)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:GLU:N	20	5.03	1.23	4.86
(1,47)	1:35:A:ALA:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	20	4.76	0.84	4.9
(1,160)	1:110:A:HIS:C	1:111:A:MET:N	1:111:A:MET:CA	1:111:A:MET:C	20	4.45	0.6	4.52

<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 (°)
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	3	20.0
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	2	19.71
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	4	16.74
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	17	16.31
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	6	16.2
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	19	16.11
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	16	16.07
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	20	14.74
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	5	14.47
(1,43)	1:33:A:LYS:C	1:34:A:MET:N	1:34:A:MET:CA	1:34:A:MET:C	18	14.18