



# Full wwPDB NMR Structure Validation Report ⓘ

Jul 4, 2024 – 12:31 PM JST

PDB ID : 5Z5R  
BMRB ID : 36158  
Title : Nukacin ISK-1 in inactive state  
Authors : Kohda, D.; Fujinami, D.  
Deposited on : 2018-01-19

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.37.1

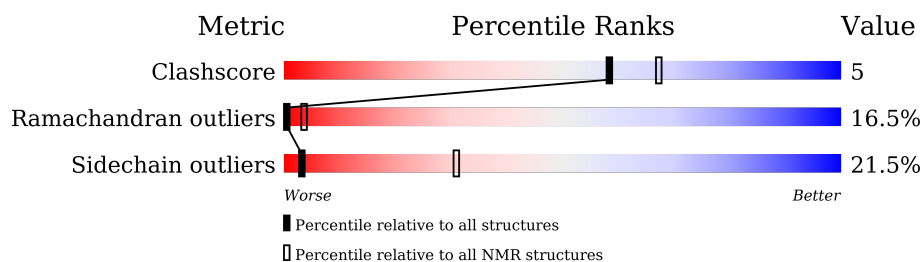
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 50%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	27	

## 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: *target function*.

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:8, A:10-A:10, A:12-A:17, A:19-A:23, A:25-A:26 (17)	1.04	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 5 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 401 atoms, of which 196 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lantibiotic nukacin.

Mol	Chain	Residues	Atoms							Trace
1	A	27	Total	C	H	N	O	S		0
			401	132	196	36	33	4		

There are 3 discrepancies between the modelled and reference sequences:

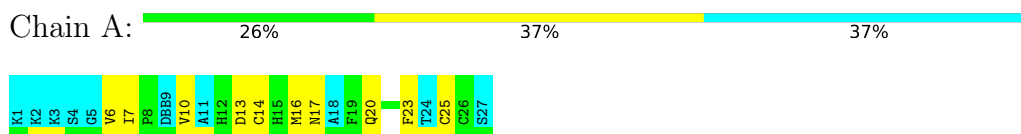
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	DBB	THR	see sequence details	UNP Q9KWM4
A	11	DAL	SER	see sequence details	UNP Q9KWM4
A	18	DAL	SER	see sequence details	UNP Q9KWM4

## 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: Lantibiotic nukacin

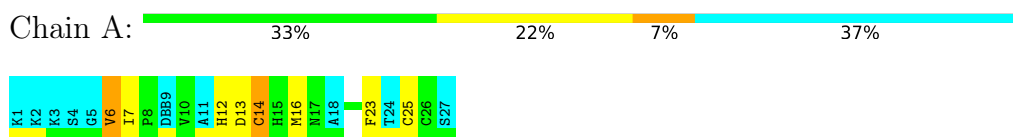


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

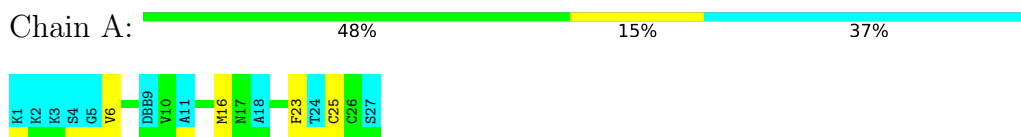
#### 4.2.1 Score per residue for model 1

- Molecule 1: Lantibiotic nukacin



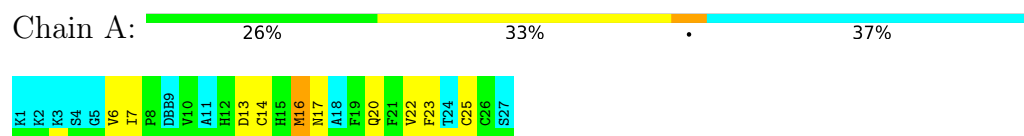
#### 4.2.2 Score per residue for model 2

- Molecule 1: Lantibiotic nukacin



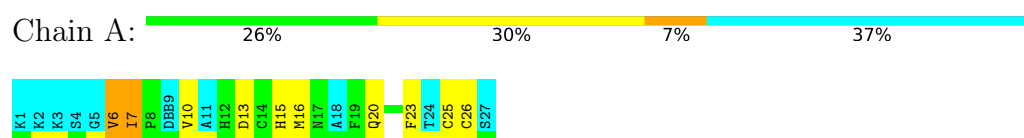
### 4.2.3 Score per residue for model 3

- Molecule 1: Lantibiotic nukacin



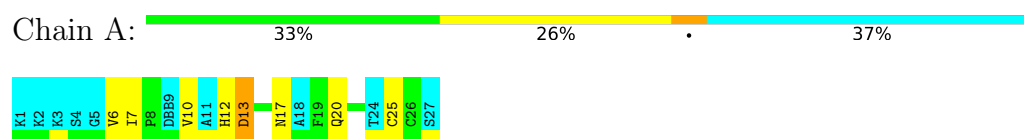
### 4.2.4 Score per residue for model 4

- Molecule 1: Lantibiotic nukacin



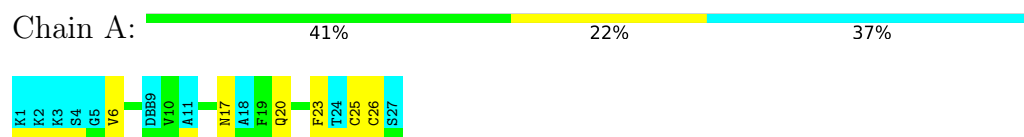
### 4.2.5 Score per residue for model 5

- Molecule 1: Lantibiotic nukacin



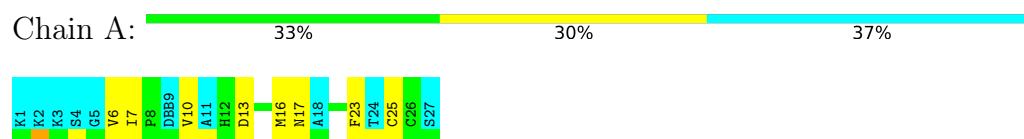
### 4.2.6 Score per residue for model 6

- Molecule 1: Lantibiotic nukacin



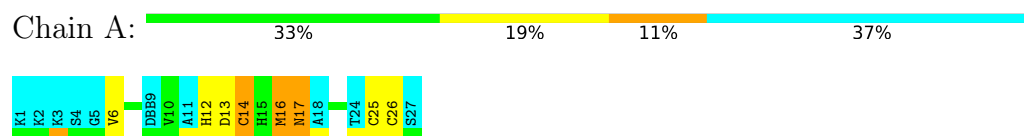
### 4.2.7 Score per residue for model 7

- Molecule 1: Lantibiotic nukacin



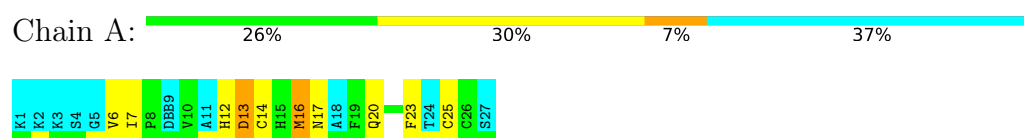
#### 4.2.8 Score per residue for model 8

- Molecule 1: Lantibiotic nukacin



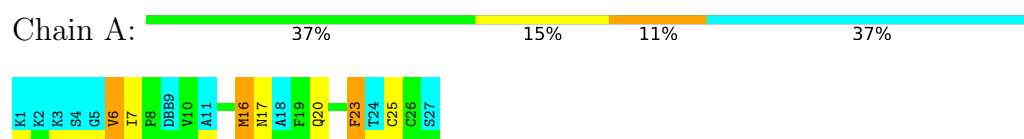
#### 4.2.9 Score per residue for model 9

- Molecule 1: Lantibiotic nukacin



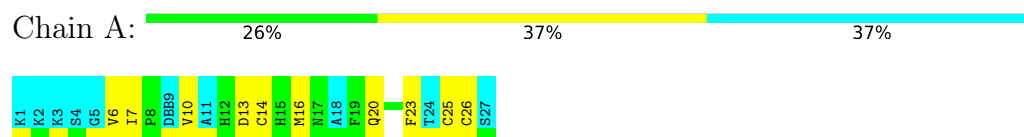
#### 4.2.10 Score per residue for model 10

- Molecule 1: Lantibiotic nukacin



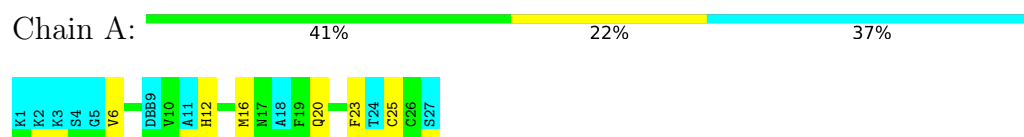
#### 4.2.11 Score per residue for model 11

- Molecule 1: Lantibiotic nukacin



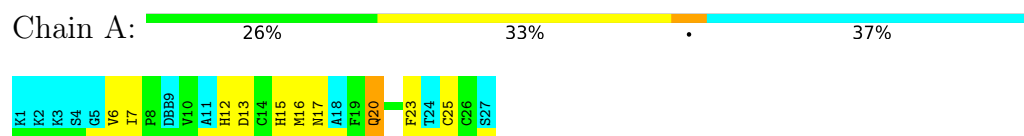
#### 4.2.12 Score per residue for model 12

- Molecule 1: Lantibiotic nukacin



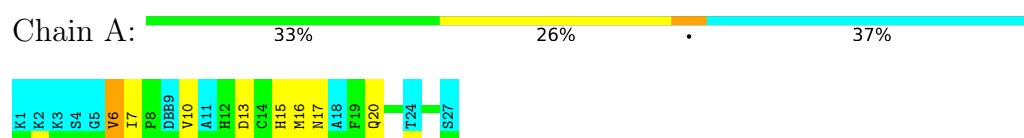
#### 4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Lantibiotic nukacin



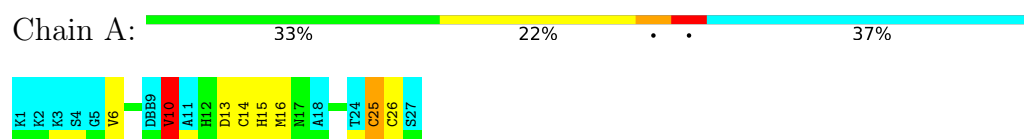
#### 4.2.14 Score per residue for model 14

- Molecule 1: Lantibiotic nukacin



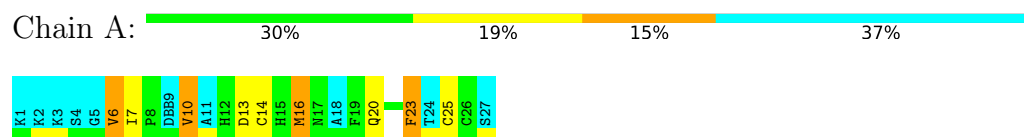
#### 4.2.15 Score per residue for model 15

- Molecule 1: Lantibiotic nukacin



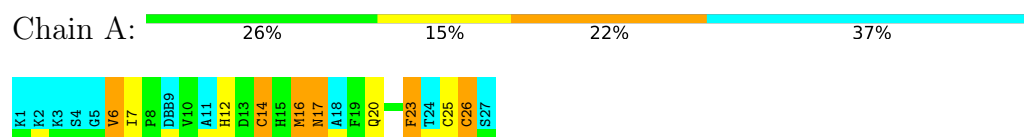
#### 4.2.16 Score per residue for model 16

- Molecule 1: Lantibiotic nukacin



#### 4.2.17 Score per residue for model 17

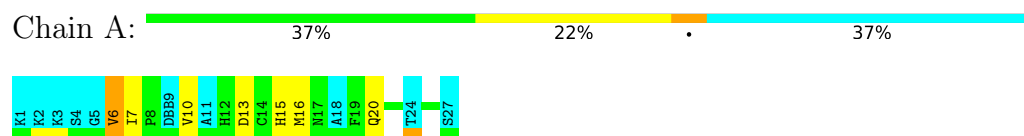
- Molecule 1: Lantibiotic nukacin





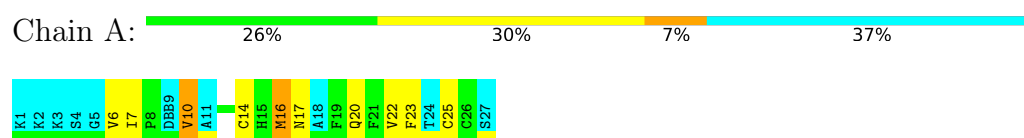
#### 4.2.18 Score per residue for model 18

- Molecule 1: Lantibiotic nukacin



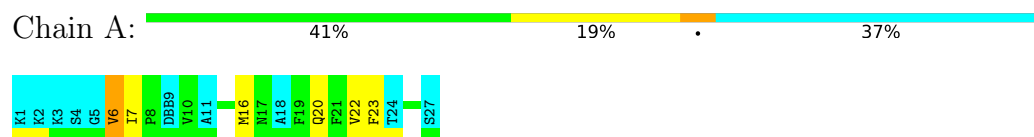
#### 4.2.19 Score per residue for model 19

- Molecule 1: Lantibiotic nukacin



#### 4.2.20 Score per residue for model 20

- Molecule 1: Lantibiotic nukacin



## 5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	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	176
Number of shifts mapped to atoms	175
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	50%

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, DBU, DBB

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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	140	125	125	1±1
All	All	2800	2500	2520	26

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 5.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:ILE:HD12	1:A:10:VAL:HG11	0.86	1.46	4	1
1:A:6:VAL:HG12	1:A:7:ILE:HG12	0.74	1.57	4	7
1:A:22:VAL:HG23	1:A:23:PHE:CD2	0.61	2.31	19	1
1:A:7:ILE:O	1:A:10:VAL:HG22	0.57	1.99	14	2
1:A:7:ILE:CD1	1:A:10:VAL:HG11	0.55	2.28	4	1
1:A:6:VAL:HG12	1:A:7:ILE:HG13	0.54	1.78	1	4
1:A:6:VAL:HG12	1:A:7:ILE:CG1	0.53	2.30	4	1
1:A:10:VAL:O	1:A:10:VAL:HG23	0.50	2.06	14	1
1:A:7:ILE:O	1:A:10:VAL:HG13	0.48	2.08	11	2
1:A:7:ILE:HD12	1:A:10:VAL:CG1	0.47	2.30	4	1
1:A:22:VAL:HG12	1:A:23:PHE:CD1	0.45	2.45	20	1
1:A:22:VAL:O	1:A:23:PHE:CB	0.43	2.65	3	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:HIS:O	1:A:13:ASP:CB	0.42	2.68	9	1
1:A:6:VAL:O	1:A:7:ILE:HD13	0.41	2.16	13	1
1:A:7:ILE:O	1:A:10:VAL:HG12	0.40	2.15	5	1

## 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	17/27 (63%)	9±2 (51±10%)	6±2 (32±10%)	3±1 (16±7%)	0	3
All	All	340/540 (63%)	174 (51%)	110 (32%)	56 (16%)	0	3

All 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	23	PHE	12
1	A	6	VAL	11
1	A	16	MET	11
1	A	14	CYS	7
1	A	17	ASN	7
1	A	13	ASP	3
1	A	10	VAL	3
1	A	25	CYS	1
1	A	20	GLN	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	17/22 (77%)	13±1 (79±8%)	4±1 (21±8%)	3	31
All	All	340/440 (77%)	267 (79%)	73 (21%)	3	31

All 13 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	20	GLN	15
1	A	16	MET	14
1	A	13	ASP	11
1	A	12	HIS	6
1	A	15	HIS	5
1	A	26	CYS	5
1	A	6	VAL	5
1	A	17	ASN	4
1	A	23	PHE	3
1	A	14	CYS	2
1	A	7	ILE	1
1	A	10	VAL	1
1	A	25	CYS	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	DBU	A	24	1	4,5,6	1.54±0.01	1±0 (25±0%)
1	DBB	A	9	1	4,5,6	0.53±0.00	0±0 (0±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	Counts	Bond angles	
						RMSZ	#Z>2
1	DBU	A	24	1	2,5,7	2.53±0.02	1±0 (50±0%)
1	DBB	A	9	1	1,5,7	1.71±0.01	0±0 (0±0%)

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
1	DBU	A	24	1	-	0±0,1,4,6	-
1	DBB	A	9	1	-	0±0,3,4,6	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	24	DBU	C-CA	2.96	1.49	1.45	3	20

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	DBU	O-C-CA	3.62	120.79	125.39	17	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates

There are no monosaccharides in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 50% for the well-defined parts and 50% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *nukacin\_STARch.bmrB*

#### 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	176
Number of shifts mapped to atoms	175
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	DAL	HB3	2.875	0.015	.

#### 7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 50%, i.e. 116 atoms were assigned a chemical shift out of a possible 234. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	33/83 (40%)	33/33 (100%)	0/34 (0%)	0/16 (0%)
Sidechain	66/107 (62%)	66/71 (93%)	0/34 (0%)	0/2 (0%)
Aromatic	17/44 (39%)	17/23 (74%)	0/19 (0%)	0/2 (0%)
Overall	116/234 (50%)	116/127 (91%)	0/87 (0%)	0/20 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 156 atoms were assigned a chemical shift out of a possible 310. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	45/114 (39%)	45/46 (98%)	0/46 (0%)	0/22 (0%)
Sidechain	94/152 (62%)	94/99 (95%)	0/48 (0%)	0/5 (0%)
Aromatic	17/44 (39%)	17/23 (74%)	0/19 (0%)	0/2 (0%)
Overall	156/310 (50%)	156/168 (93%)	0/113 (0%)	0/29 (0%)

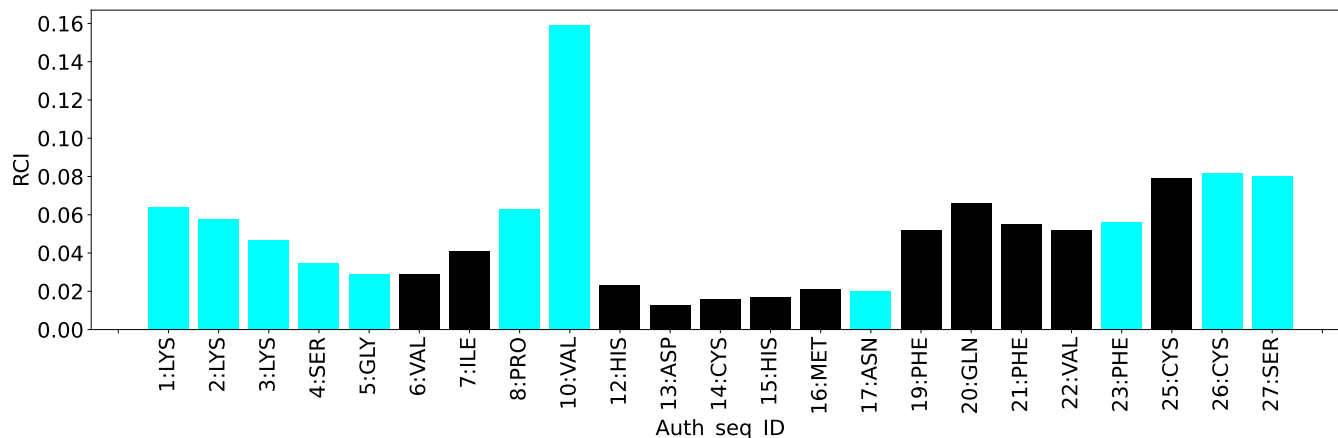
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 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	146
Intra-residue ( $ i-j =0$ )	44
Sequential ( $ i-j =1$ )	42
Medium range ( $ i-j >1$ and $ i-j <5$ )	12
Long range ( $ i-j \geq 5$ )	48
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	7
Number of unmapped restraints	0
Number of restraints per residue	5.7
Number of long range restraints per residue <sup>1</sup>	1.8

<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)	6.5	0.2
0.2-0.5 (Medium)	3.9	0.5
>0.5 (Large)	0.6	0.91

### 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)	1.4	6.48
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

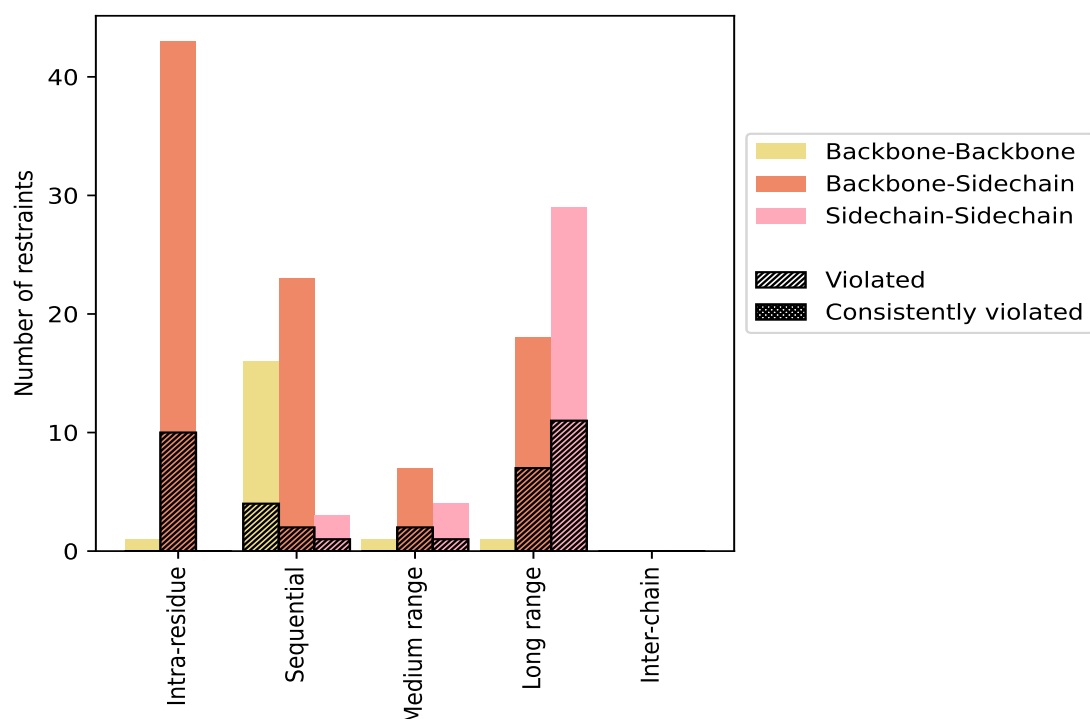
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">44</a>	<a href="#">30.1</a>	<a href="#">10</a>	<a href="#">22.7</a>	<a href="#">6.8</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	1	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	43	29.5	10	23.3	6.8	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<a href="#">Sequential ( i-j =1)</a>	<a href="#">42</a>	<a href="#">28.8</a>	<a href="#">7</a>	<a href="#">16.7</a>	<a href="#">4.8</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	16	11.0	4	25.0	2.7	0	0.0	0.0
Backbone-Sidechain	23	15.8	2	8.7	1.4	0	0.0	0.0
Sidechain-Sidechain	3	2.1	1	33.3	0.7	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">12</a>	<a href="#">8.2</a>	<a href="#">3</a>	<a href="#">25.0</a>	<a href="#">2.1</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	1	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	4.8	2	28.6	1.4	0	0.0	0.0
Sidechain-Sidechain	4	2.7	1	25.0	0.7	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">48</a>	<a href="#">32.9</a>	<a href="#">18</a>	<a href="#">37.5</a>	<a href="#">12.3</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	1	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	12.3	7	38.9	4.8	0	0.0	0.0
Sidechain-Sidechain	29	19.9	11	37.9	7.5	0	0.0	0.0
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
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
<a href="#">Hydrogen bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">146</a>	<a href="#">100.0</a>	<a href="#">38</a>	<a href="#">26.0</a>	<a href="#">26.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	19	13.0	4	21.1	2.7	0	0.0	0.0
Backbone-Sidechain	91	62.3	21	23.1	14.4	0	0.0	0.0
Sidechain-Sidechain	36	24.7	13	36.1	8.9	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 [i](#)



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	1	1	1	6	0	9	0.22	0.49	0.12	0.17
2	4	2	1	3	0	10	0.22	0.55	0.12	0.17
3	3	3	2	4	0	12	0.22	0.47	0.09	0.19
4	1	1	1	6	0	9	0.21	0.41	0.09	0.17
5	3	4	1	3	0	11	0.2	0.5	0.1	0.18
6	3	1	0	5	0	9	0.25	0.5	0.15	0.18
7	3	2	1	5	0	11	0.26	0.47	0.12	0.27
8	4	2	0	4	0	10	0.26	0.49	0.12	0.26
9	3	3	1	5	0	12	0.2	0.54	0.11	0.16
10	4	3	1	4	0	12	0.24	0.64	0.15	0.16

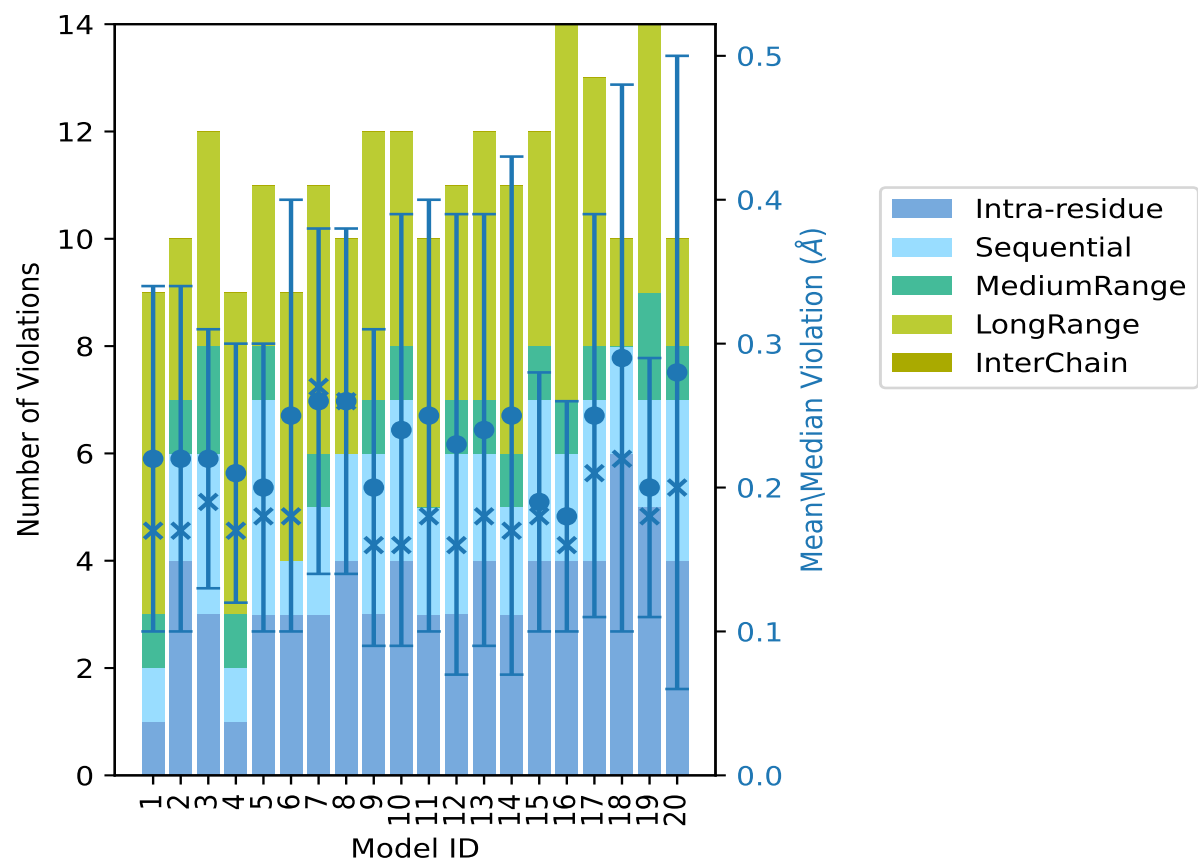
*Continued on next page...*

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	3	2	0	5	0	10	0.25	0.56	0.15	0.18
12	3	3	1	4	0	11	0.23	0.67	0.16	0.16
13	4	2	1	5	0	12	0.24	0.61	0.15	0.18
14	3	2	1	5	0	11	0.25	0.79	0.18	0.17
15	4	3	1	4	0	12	0.19	0.42	0.09	0.18
16	4	2	1	7	0	14	0.18	0.44	0.08	0.16
17	4	3	1	5	0	13	0.25	0.58	0.14	0.21
18	6	2	0	2	0	10	0.29	0.81	0.19	0.22
19	5	2	2	5	0	14	0.2	0.46	0.09	0.18
20	4	3	1	2	0	10	0.28	0.91	0.22	0.2

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

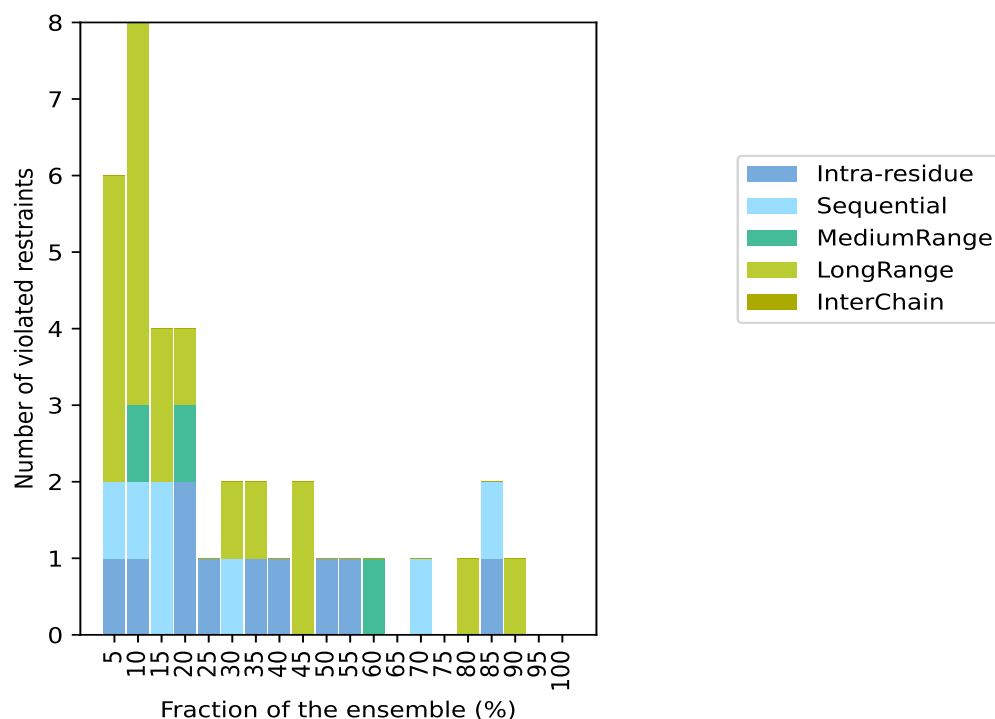
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 108(IR:34, SQ:35, MR:9, LR:30, IC:0) restraints are not violated 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>	%
1	1	0	4	0	6	1	5.0
1	1	1	5	0	8	2	10.0
0	2	0	2	0	4	3	15.0
2	0	1	1	0	4	4	20.0
1	0	0	0	0	1	5	25.0
0	1	0	1	0	2	6	30.0
1	0	0	1	0	2	7	35.0
1	0	0	0	0	1	8	40.0
0	0	0	2	0	2	9	45.0
1	0	0	0	0	1	10	50.0
1	0	0	0	0	1	11	55.0
0	0	1	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	1	0	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	1	0	1	16	80.0
1	1	0	0	0	2	17	85.0
0	0	0	1	0	1	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 [i](#)

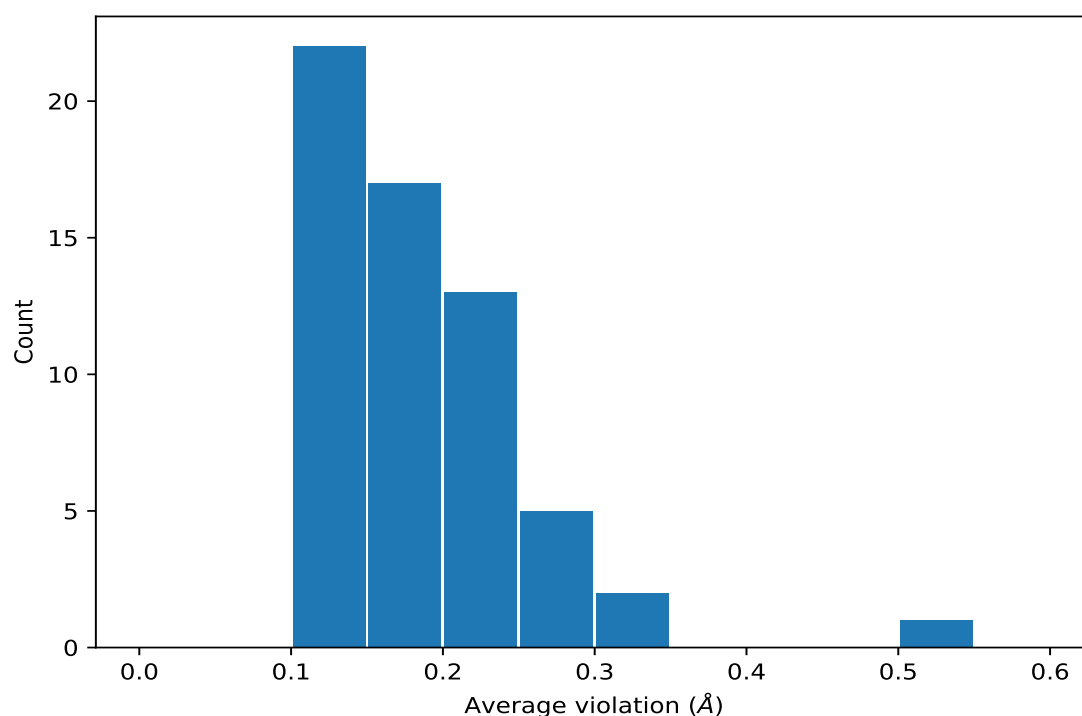


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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)
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	18	0.54	0.18	0.52
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	17	0.27	0.14	0.26
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	17	0.27	0.14	0.26
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	17	0.25	0.05	0.27
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	16	0.23	0.12	0.18
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	14	0.16	0.04	0.16
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	12	0.18	0.05	0.17
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	11	0.21	0.1	0.16
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	10	0.24	0.03	0.25
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	9	0.21	0.06	0.2
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	9	0.15	0.04	0.12
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	8	0.3	0.1	0.32
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB2	7	0.16	0.02	0.16
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB3	7	0.16	0.02	0.16
(2,19)	1:6:A:VAL:HB	1:21:A:PHE:HZ	7	0.13	0.01	0.13
(2,29)	1:22:A:VAL:HA	1:23:A:PHE:H	6	0.15	0.04	0.16

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE1	6	0.14	0.04	0.13
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE2	6	0.14	0.04	0.13
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE1	6	0.14	0.04	0.13
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE2	6	0.14	0.04	0.13
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE1	6	0.14	0.04	0.13
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE2	6	0.14	0.04	0.13
(2,32)	1:11:A:DAL:H	1:11:A:DAL:HB2	5	0.29	0.16	0.27
(2,69)	1:12:A:HIS:HA	1:12:A:HIS:HD2	4	0.29	0.1	0.29
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG1	4	0.21	0.06	0.22
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG2	4	0.21	0.06	0.22
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG3	4	0.21	0.06	0.22
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB2	4	0.2	0.02	0.2
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB3	4	0.2	0.02	0.2
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB2	4	0.2	0.02	0.2
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB3	4	0.2	0.02	0.2
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB2	4	0.2	0.02	0.2
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB3	4	0.2	0.02	0.2
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB2	4	0.12	0.0	0.12
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB3	4	0.12	0.0	0.12
(2,1)	1:9:A:DBB:HB2	1:14:A:CYS:HB2	3	0.15	0.01	0.15
(2,1)	1:9:A:DBB:HB2	1:14:A:CYS:HB3	3	0.15	0.01	0.15
(2,84)	1:18:A:DAL:HB2	1:19:A:PHE:HD1	3	0.14	0.03	0.13
(2,84)	1:18:A:DAL:HB2	1:19:A:PHE:HD2	3	0.14	0.03	0.13
(1,1)	1:9:A:DBB:HB2	1:14:A:CYS:SG	3	0.13	0.02	0.13
(2,63)	1:6:A:VAL:HA	1:7:A:ILE:H	3	0.11	0.0	0.11
(1,2)	1:9:A:DBB:CG	1:14:A:CYS:SG	2	0.33	0.05	0.33
(2,44)	1:21:A:PHE:HD1	1:26:A:CYS:H	2	0.18	0.0	0.18
(2,44)	1:21:A:PHE:HD2	1:26:A:CYS:H	2	0.18	0.0	0.18
(2,21)	1:10:A:VAL:HG21	1:21:A:PHE:HE1	2	0.16	0.02	0.16
(2,21)	1:10:A:VAL:HG21	1:21:A:PHE:HE2	2	0.16	0.02	0.16
(2,21)	1:10:A:VAL:HG22	1:21:A:PHE:HE1	2	0.16	0.02	0.16
(2,21)	1:10:A:VAL:HG22	1:21:A:PHE:HE2	2	0.16	0.02	0.16
(2,21)	1:10:A:VAL:HG23	1:21:A:PHE:HE1	2	0.16	0.02	0.16
(2,21)	1:10:A:VAL:HG23	1:21:A:PHE:HE2	2	0.16	0.02	0.16
(2,27)	1:18:A:DAL:HB2	1:21:A:PHE:HZ	2	0.16	0.05	0.16
(2,70)	1:6:A:VAL:HG11	1:21:A:PHE:HD1	2	0.14	0.02	0.14
(2,70)	1:6:A:VAL:HG11	1:21:A:PHE:HD2	2	0.14	0.02	0.14
(2,70)	1:6:A:VAL:HG12	1:21:A:PHE:HD1	2	0.14	0.02	0.14
(2,70)	1:6:A:VAL:HG12	1:21:A:PHE:HD2	2	0.14	0.02	0.14
(2,70)	1:6:A:VAL:HG13	1:21:A:PHE:HD1	2	0.14	0.02	0.14
(2,70)	1:6:A:VAL:HG13	1:21:A:PHE:HD2	2	0.14	0.02	0.14
(2,64)	1:10:A:VAL:H	1:10:A:VAL:HB	2	0.14	0.04	0.14

*Continued on next page...*

*Continued from previous page...*

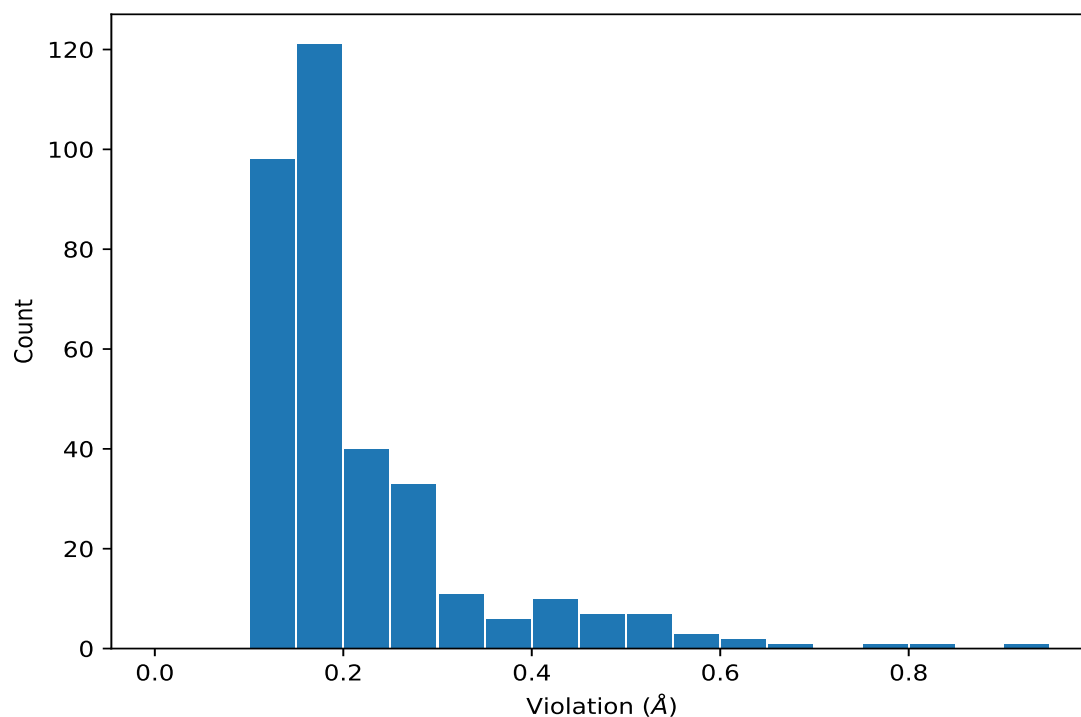
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,87)	1:10:A:VAL:HB	1:11:A:DAL:H	2	0.12	0.01	0.12
(3,1)	1:9:A:DBB:CB	1:14:A:CYS:SG	2	0.12	0.0	0.12

<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 lists the 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)
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	20	0.91
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	18	0.81

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	14	0.79
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	12	0.67
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	10	0.64
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	13	0.61
(2,32)	1:11:A:DAL:H	1:11:A:DAL:HB2	17	0.58
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	11	0.56
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	2	0.55
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	9	0.54
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	11	0.51
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	11	0.51
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	6	0.5
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	6	0.5
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	5	0.5
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	6	0.5
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	8	0.49
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	8	0.49
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	1	0.49
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	13	0.47
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	3	0.47
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	7	0.47
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	19	0.46
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	16	0.44
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	8	0.44
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	15	0.42
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	17	0.42
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	7	0.42
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	7	0.42
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	10	0.42
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	4	0.41
(2,69)	1:12:A:HIS:HA	1:12:A:HIS:HD2	18	0.4
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	7	0.4
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	20	0.39
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	12	0.38
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	12	0.38
(2,69)	1:12:A:HIS:HA	1:12:A:HIS:HD2	14	0.38
(1,2)	1:9:A:DBB:CG	1:14:A:CYS:SG	1	0.38
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	17	0.36
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	17	0.33
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	10	0.33
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	7	0.32
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	8	0.31
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	3	0.31

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	18	0.3
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	18	0.3
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	10	0.3
(2,38)	1:12:A:HIS:H	1:13:A:ASP:H	9	0.3
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	7	0.3
(2,32)	1:11:A:DAL:H	1:11:A:DAL:HB2	20	0.3
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	6	0.29
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	12	0.29
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	4	0.29
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	2	0.29
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	8	0.28
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	13	0.28
(1,2)	1:9:A:DBB:CG	1:14:A:CYS:SG	11	0.28
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	4	0.27
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	15	0.27
(2,32)	1:11:A:DAL:H	1:11:A:DAL:HB2	18	0.27
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG1	7	0.27
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG2	7	0.27
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG3	7	0.27
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG1	17	0.27
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG2	17	0.27
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG3	17	0.27
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	10	0.26
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	10	0.26
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	14	0.26
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	14	0.26
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	20	0.26
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	20	0.26
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	8	0.26
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	15	0.26
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	19	0.26
(2,93)	1:21:A:PHE:HD1	1:26:A:CYS:HA	17	0.25
(2,93)	1:21:A:PHE:HD2	1:26:A:CYS:HA	17	0.25
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	19	0.25
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	1	0.25
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	8	0.25
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	3	0.25
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	16	0.25
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	18	0.25
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	11	0.24
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	19	0.24
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	3	0.24

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	6	0.24
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	16	0.23
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	3	0.23
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	5	0.23
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	5	0.23
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	9	0.23
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB2	4	0.22
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB3	4	0.22
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB2	4	0.22
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB3	4	0.22
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB2	4	0.22
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB3	4	0.22
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB2	14	0.22
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB3	14	0.22
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB2	14	0.22
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB3	14	0.22
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB2	14	0.22
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB3	14	0.22
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	19	0.22
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE1	16	0.22
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE2	16	0.22
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE1	16	0.22
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE2	16	0.22
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE1	16	0.22
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE2	16	0.22
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	15	0.22
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	2	0.22
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	13	0.22
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	20	0.21
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	13	0.21
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	17	0.21
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	2	0.2
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	16	0.2
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	5	0.2
(2,29)	1:22:A:VAL:HA	1:23:A:PHE:H	18	0.2
(2,27)	1:18:A:DAL:HB2	1:21:A:PHE:HZ	3	0.2
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	18	0.2
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	5	0.19
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	12	0.19
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB2	18	0.19
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB3	18	0.19
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB2	19	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB3	19	0.19
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB2	19	0.19
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB3	19	0.19
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB2	19	0.19
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB3	19	0.19
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	11	0.19
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	15	0.19
(2,69)	1:12:A:HIS:HA	1:12:A:HIS:HD2	19	0.19
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	18	0.19
(2,29)	1:22:A:VAL:HA	1:23:A:PHE:H	14	0.19
(2,29)	1:22:A:VAL:HA	1:23:A:PHE:H	20	0.19
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	1	0.18
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	15	0.18
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	15	0.18
(2,84)	1:18:A:DAL:HB2	1:19:A:PHE:HD1	13	0.18
(2,84)	1:18:A:DAL:HB2	1:19:A:PHE:HD2	13	0.18
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	17	0.18
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	5	0.18
(2,69)	1:12:A:HIS:HA	1:12:A:HIS:HD2	15	0.18
(2,44)	1:21:A:PHE:HD1	1:26:A:CYS:H	3	0.18
(2,44)	1:21:A:PHE:HD2	1:26:A:CYS:H	3	0.18
(2,44)	1:21:A:PHE:HD1	1:26:A:CYS:H	13	0.18
(2,44)	1:21:A:PHE:HD2	1:26:A:CYS:H	13	0.18
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	6	0.18
(2,21)	1:10:A:VAL:HG21	1:21:A:PHE:HE1	12	0.18
(2,21)	1:10:A:VAL:HG21	1:21:A:PHE:HE2	12	0.18
(2,21)	1:10:A:VAL:HG22	1:21:A:PHE:HE1	12	0.18
(2,21)	1:10:A:VAL:HG22	1:21:A:PHE:HE2	12	0.18
(2,21)	1:10:A:VAL:HG23	1:21:A:PHE:HE1	12	0.18
(2,21)	1:10:A:VAL:HG23	1:21:A:PHE:HE2	12	0.18
(2,8)	1:18:A:DAL:HB1	1:26:A:CYS:HA	16	0.18
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	2	0.17
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	8	0.17
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB2	8	0.17
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB3	8	0.17
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB2	14	0.17
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB3	14	0.17
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	1	0.17
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	2	0.17
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	4	0.17
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	7	0.17
(2,64)	1:10:A:VAL:H	1:10:A:VAL:HB	14	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	14	0.17
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	19	0.17
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	1	0.17
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG1	10	0.17
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG2	10	0.17
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG3	10	0.17
(2,4)	1:9:A:DBB:HA	1:9:A:DBB:HB2	9	0.17
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	9	0.16
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB2	11	0.16
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB3	11	0.16
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB2	12	0.16
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB3	12	0.16
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB2	16	0.16
(2,119)	1:9:A:DBB:HG1	1:25:A:CYS:HB3	16	0.16
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB2	16	0.16
(2,119)	1:9:A:DBB:HG2	1:25:A:CYS:HB3	16	0.16
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB2	16	0.16
(2,119)	1:9:A:DBB:HG3	1:25:A:CYS:HB3	16	0.16
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	2	0.16
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	2	0.16
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	9	0.16
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	9	0.16
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	2	0.16
(2,70)	1:6:A:VAL:HG11	1:21:A:PHE:HD1	15	0.16
(2,70)	1:6:A:VAL:HG11	1:21:A:PHE:HD2	15	0.16
(2,70)	1:6:A:VAL:HG12	1:21:A:PHE:HD1	15	0.16
(2,70)	1:6:A:VAL:HG12	1:21:A:PHE:HD2	15	0.16
(2,70)	1:6:A:VAL:HG13	1:21:A:PHE:HD1	15	0.16
(2,70)	1:6:A:VAL:HG13	1:21:A:PHE:HD2	15	0.16
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	9	0.16
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	16	0.16
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	20	0.16
(2,42)	1:11:A:DAL:HA	1:11:A:DAL:HB1	11	0.16
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	10	0.16
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	5	0.16
(2,22)	1:15:A:HIS:HA	1:15:A:HIS:HD2	11	0.16
(2,1)	1:9:A:DBB:HB2	1:14:A:CYS:HB2	7	0.16
(2,1)	1:9:A:DBB:HB2	1:14:A:CYS:HB3	7	0.16
(1,1)	1:9:A:DBB:HB2	1:14:A:CYS:SG	13	0.16
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	6	0.15
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	13	0.15
(2,136)	1:23:A:PHE:HA	1:23:A:PHE:HB2	3	0.15

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,136)	1:23:A:PHE:HA	1:23:A:PHE:HB3	3	0.15
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB2	6	0.15
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB3	6	0.15
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	4	0.15
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	4	0.15
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	17	0.15
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	17	0.15
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	3	0.15
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	9	0.15
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	9	0.15
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE1	3	0.15
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE2	3	0.15
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE1	3	0.15
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE2	3	0.15
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE1	3	0.15
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE2	3	0.15
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE1	19	0.15
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE2	19	0.15
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE1	19	0.15
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE2	19	0.15
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE1	19	0.15
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE2	19	0.15
(2,32)	1:11:A:DAL:H	1:11:A:DAL:HB2	19	0.15
(2,21)	1:10:A:VAL:HG21	1:21:A:PHE:HE1	20	0.15
(2,21)	1:10:A:VAL:HG21	1:21:A:PHE:HE2	20	0.15
(2,21)	1:10:A:VAL:HG22	1:21:A:PHE:HE1	20	0.15
(2,21)	1:10:A:VAL:HG22	1:21:A:PHE:HE2	20	0.15
(2,21)	1:10:A:VAL:HG23	1:21:A:PHE:HE1	20	0.15
(2,21)	1:10:A:VAL:HG23	1:21:A:PHE:HE2	20	0.15
(2,19)	1:6:A:VAL:HB	1:21:A:PHE:HZ	13	0.15
(2,1)	1:9:A:DBB:HB2	1:14:A:CYS:HB2	14	0.15
(2,1)	1:9:A:DBB:HB2	1:14:A:CYS:HB3	14	0.15
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	10	0.14
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	3	0.14
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	3	0.14
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	1	0.14
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	12	0.14
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	10	0.14
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	11	0.14
(2,19)	1:6:A:VAL:HB	1:21:A:PHE:HZ	2	0.14
(2,19)	1:6:A:VAL:HB	1:21:A:PHE:HZ	9	0.14
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG1	12	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG2	12	0.14
(2,10)	1:9:A:DBB:HA	1:9:A:DBB:HG3	12	0.14
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB2	20	0.13
(2,131)	1:21:A:PHE:H	1:21:A:PHE:HB3	20	0.13
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	5	0.13
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	5	0.13
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB2	16	0.13
(2,110)	1:7:A:ILE:H	1:8:A:PRO:HB3	16	0.13
(2,87)	1:10:A:VAL:HB	1:11:A:DAL:H	10	0.13
(2,84)	1:18:A:DAL:HB2	1:19:A:PHE:HD1	17	0.13
(2,84)	1:18:A:DAL:HB2	1:19:A:PHE:HD2	17	0.13
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	14	0.13
(2,36)	1:11:A:DAL:HB1	1:26:A:CYS:H	9	0.13
(2,32)	1:11:A:DAL:H	1:11:A:DAL:HB2	16	0.13
(2,19)	1:6:A:VAL:HB	1:21:A:PHE:HZ	4	0.13
(2,19)	1:6:A:VAL:HB	1:21:A:PHE:HZ	19	0.13
(2,1)	1:9:A:DBB:HB2	1:14:A:CYS:HB2	4	0.13
(2,1)	1:9:A:DBB:HB2	1:14:A:CYS:HB3	4	0.13
(1,1)	1:9:A:DBB:HB2	1:14:A:CYS:SG	9	0.13
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	7	0.12
(3,1)	1:9:A:DBB:CB	1:14:A:CYS:SG	1	0.12
(3,1)	1:9:A:DBB:CB	1:14:A:CYS:SG	17	0.12
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB2	15	0.12
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB3	15	0.12
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB2	16	0.12
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB3	16	0.12
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB2	17	0.12
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB3	17	0.12
(2,84)	1:18:A:DAL:HB2	1:19:A:PHE:HD1	19	0.12
(2,84)	1:18:A:DAL:HB2	1:19:A:PHE:HD2	19	0.12
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	7	0.12
(2,70)	1:6:A:VAL:HG11	1:21:A:PHE:HD1	16	0.12
(2,70)	1:6:A:VAL:HG11	1:21:A:PHE:HD2	16	0.12
(2,70)	1:6:A:VAL:HG12	1:21:A:PHE:HD1	16	0.12
(2,70)	1:6:A:VAL:HG12	1:21:A:PHE:HD2	16	0.12
(2,70)	1:6:A:VAL:HG13	1:21:A:PHE:HD1	16	0.12
(2,70)	1:6:A:VAL:HG13	1:21:A:PHE:HD2	16	0.12
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	2	0.12
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	7	0.12
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	16	0.12
(2,29)	1:22:A:VAL:HA	1:23:A:PHE:H	5	0.12
(2,19)	1:6:A:VAL:HB	1:21:A:PHE:HZ	1	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:6:A:VAL:HB	1:21:A:PHE:HZ	12	0.12
(2,5)	1:11:A:DAL:HB2	1:25:A:CYS:HA	14	0.12
(2,5)	1:11:A:DAL:HB1	1:25:A:CYS:HA	14	0.12
(2,133)	1:21:A:PHE:HE1	1:26:A:CYS:HB2	16	0.11
(2,133)	1:21:A:PHE:HE1	1:26:A:CYS:HB3	16	0.11
(2,133)	1:21:A:PHE:HE2	1:26:A:CYS:HB2	16	0.11
(2,133)	1:21:A:PHE:HE2	1:26:A:CYS:HB3	16	0.11
(2,87)	1:10:A:VAL:HB	1:11:A:DAL:H	12	0.11
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB2	19	0.11
(2,85)	1:11:A:DAL:H	1:14:A:CYS:HB3	19	0.11
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	5	0.11
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	12	0.11
(2,78)	1:10:A:VAL:HA	1:11:A:DAL:H	13	0.11
(2,73)	1:21:A:PHE:HB2	1:25:A:CYS:H	20	0.11
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE1	6	0.11
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE2	6	0.11
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE1	6	0.11
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE2	6	0.11
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE1	6	0.11
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE2	6	0.11
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE1	8	0.11
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE2	8	0.11
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE1	8	0.11
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE2	8	0.11
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE1	8	0.11
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE2	8	0.11
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE1	11	0.11
(2,72)	1:10:A:VAL:HG11	1:21:A:PHE:HE2	11	0.11
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE1	11	0.11
(2,72)	1:10:A:VAL:HG12	1:21:A:PHE:HE2	11	0.11
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE1	11	0.11
(2,72)	1:10:A:VAL:HG13	1:21:A:PHE:HE2	11	0.11
(2,66)	1:18:A:DAL:H	1:18:A:DAL:HB1	18	0.11
(2,63)	1:6:A:VAL:HA	1:7:A:ILE:H	3	0.11
(2,63)	1:6:A:VAL:HA	1:7:A:ILE:H	5	0.11
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	10	0.11
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	15	0.11
(2,47)	1:11:A:DAL:HB2	1:26:A:CYS:H	17	0.11
(2,29)	1:22:A:VAL:HA	1:23:A:PHE:H	8	0.11
(2,29)	1:22:A:VAL:HA	1:23:A:PHE:H	15	0.11
(2,27)	1:18:A:DAL:HB2	1:21:A:PHE:HZ	19	0.11
(1,1)	1:9:A:DBB:HB2	1:14:A:CYS:SG	6	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:11:A:DAL:CB	1:25:A:CYS:SG	4	0.1
(2,64)	1:10:A:VAL:H	1:10:A:VAL:HB	13	0.1
(2,63)	1:6:A:VAL:HA	1:7:A:ILE:H	10	0.1
(2,59)	1:11:A:DAL:HB1	1:25:A:CYS:H	15	0.1

## 10 Dihedral-angle violation analysis ⓘ

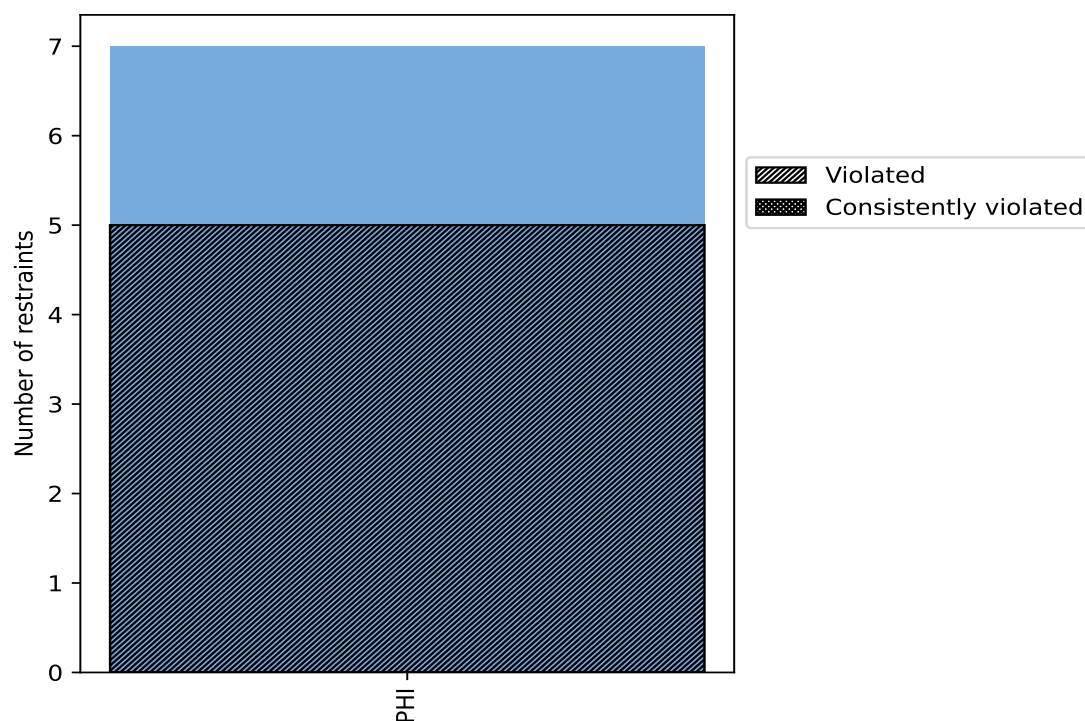
### 10.1 Summary of dihedral-angle violations ⓘ

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	7	100.0	5	71.4	71.4	0	0.0	0.0
Total	7	100.0	5	71.4	71.4	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 ⓘ



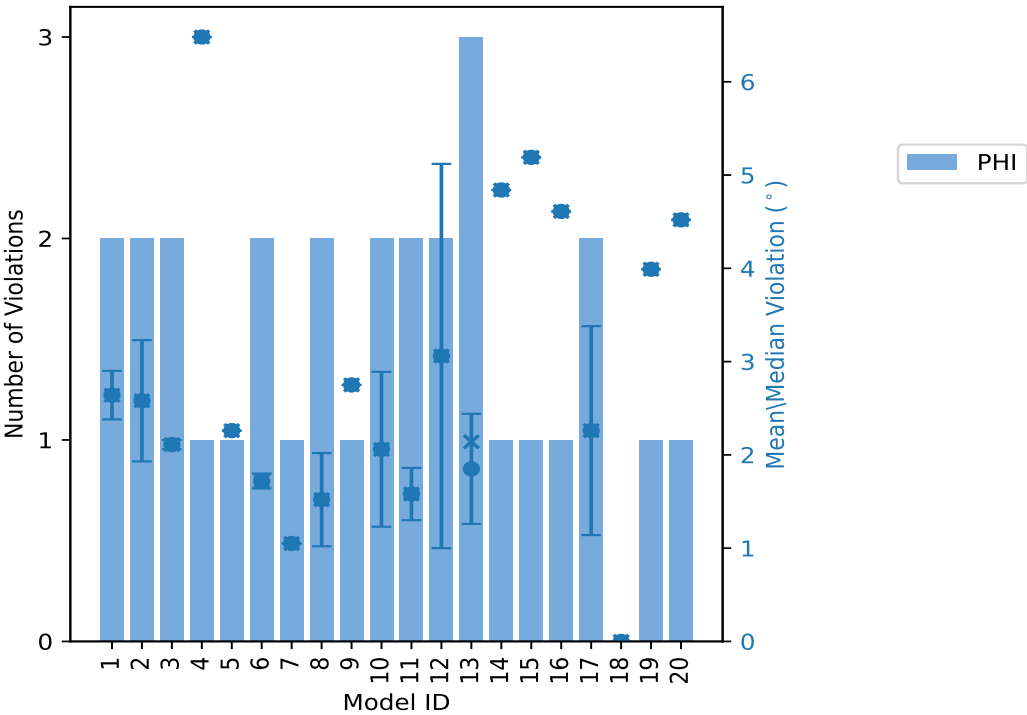
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations		Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	Total				
1	2	2	2.64	2.89	0.26	2.64
2	2	2	2.58	3.22	0.65	2.58
3	2	2	2.11	2.16	0.05	2.11
4	1	1	6.48	6.48	0.0	6.48
5	1	1	2.26	2.26	0.0	2.26
6	2	2	1.72	1.8	0.08	1.72
7	1	1	1.05	1.05	0.0	1.05
8	2	2	1.52	2.03	0.5	1.52
9	1	1	2.75	2.75	0.0	2.75
10	2	2	2.06	2.89	0.83	2.06
11	2	2	1.58	1.86	0.28	1.58
12	2	2	3.06	5.12	2.06	3.06
13	3	3	1.85	2.38	0.59	2.14
14	1	1	4.84	4.84	0.0	4.84
15	1	1	5.19	5.19	0.0	5.19
16	1	1	4.61	4.61	0.0	4.61
17	2	2	2.26	3.38	1.12	2.26
18	0	0	0.0	0.0	0.0	0.0
19	1	1	3.99	3.99	0.0	3.99
20	1	1	4.52	4.52	0.0	4.52

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

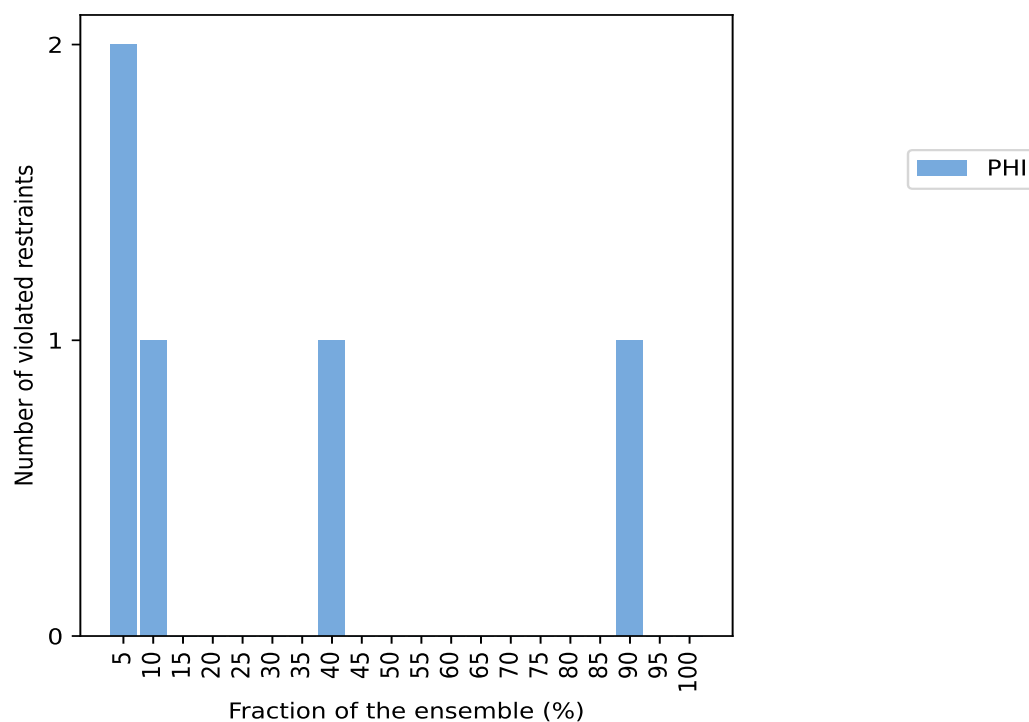
Continued on next page...

*Continued from previous page...*

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

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

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



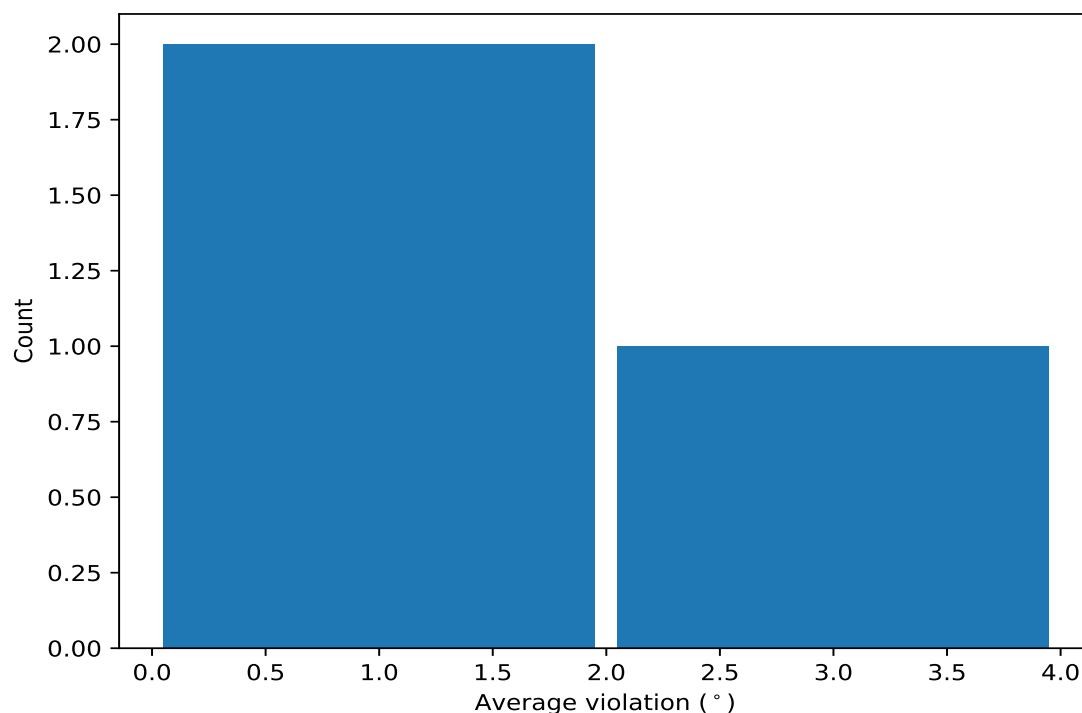
## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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

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



in the ensemble



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

The following table provides the mean and the standard deviation of the 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.

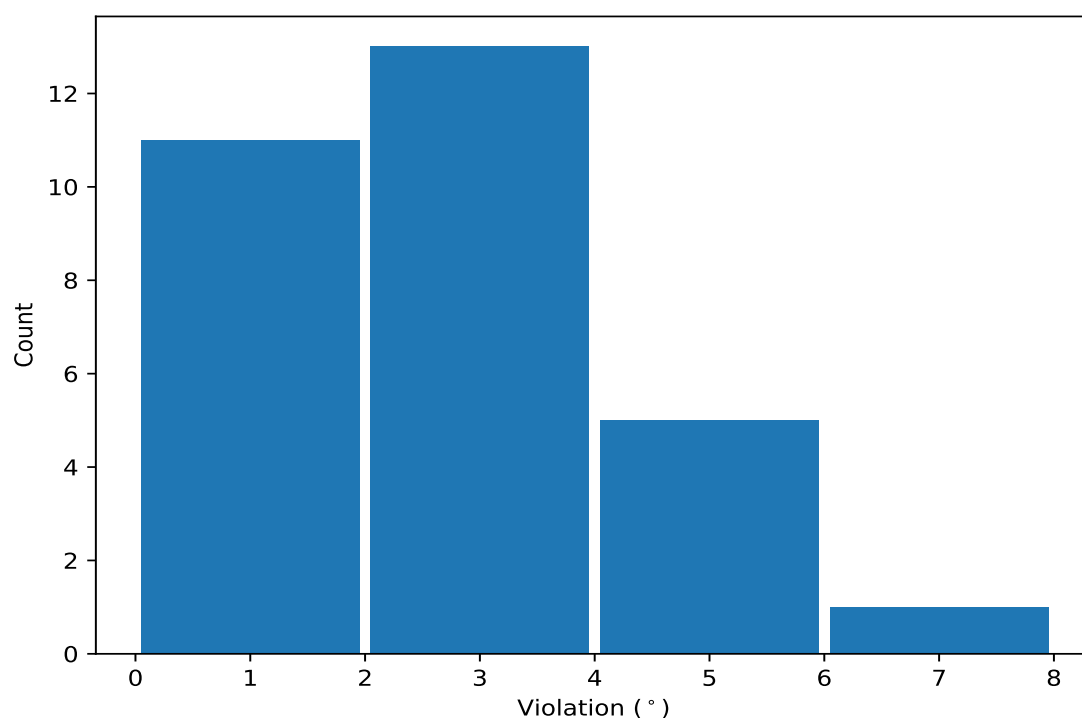
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	18	3.42	1.37	3.06
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	8	1.78	0.61	1.86
(1,7)	1:21:A:PHE:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	2	1.04	0.01	1.04

<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 lists the 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	4	6.48
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	15	5.19
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	12	5.12
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	14	4.84
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	16	4.61
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	20	4.52
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	19	3.99
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	17	3.38
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	2	3.22
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	1	2.89
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	10	2.89
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	9	2.75
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	1	2.38
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	13	2.38
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	5	2.26
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	3	2.16
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	13	2.14
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	3	2.06
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	8	2.03
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	2	1.93
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	11	1.86

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	6	1.8
(1,1)	1:6:A:VAL:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	6	1.64
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	11	1.31
(1,4)	1:14:A:CYS:C	1:15:A:HIS:N	1:15:A:HIS:CA	1:15:A:HIS:C	10	1.23
(1,6)	1:20:A:GLN:C	1:21:A:PHE:N	1:21:A:PHE:CA	1:21:A:PHE:C	17	1.15
(1,7)	1:21:A:PHE:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	7	1.05
(1,7)	1:21:A:PHE:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	13	1.03
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	8	1.02
(1,3)	1:11:A:DAL:C	1:12:A:HIS:N	1:12:A:HIS:CA	1:12:A:HIS:C	12	1.0