



# wwPDB NMR Structure Validation Summary Report i

Jun 6, 2023 – 06:26 pm BST

PDB ID : 3ZGP  
BMRB ID : 18911  
Title : NMR structure of the catalytic domain from E. faecium L,D- transpeptidase acylated by ertapenem  
Authors : Lecoq, L.; Triboulet, S.; Dubee, V.; Bougault, C.; Hugonnet, J.E.; Arthur, M.; Simorre, J.P.  
Deposited on : 2012-12-18

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>  
with specific help available everywhere you see the i 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](#) ①) were used in the production of this report:

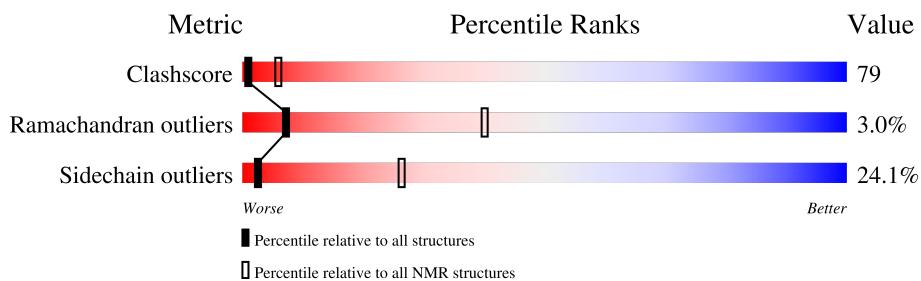
MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*SOLUTION NMR*

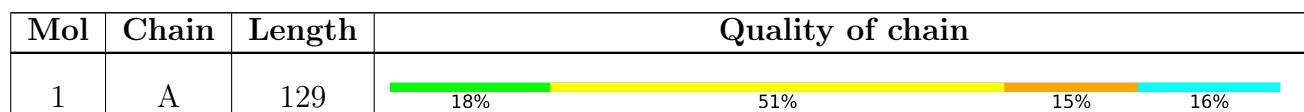
The overall completeness of chemical shifts assignment is 94%.

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  $\leq 5\%$



## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:342-A:394, A:404-A:412, A:418-A:424, A:428-A:466 (108)	0.16	10

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

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

The models can be grouped into 1 clusters and 1 single-model cluster was found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 2040 atoms, of which 980 are hydrogens and 0 are deuteriums.

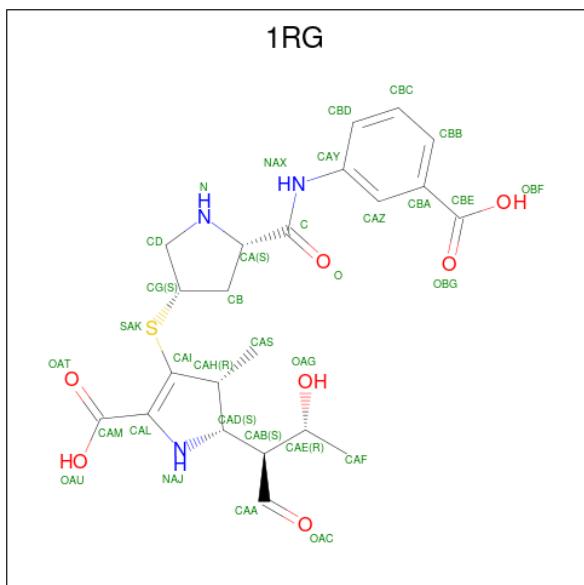
- Molecule 1 is a protein called ERFK/YBIS/YCFS/YNHG.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	129	1982	657	955	161	203	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	338	GLY	-	expression tag	UNP Q3Y185
A	339	HIS	-	expression tag	UNP Q3Y185
A	340	MET	-	expression tag	UNP Q3Y185

- Molecule 2 is (4R,5S)-3-((3S,5S)-5-[(3-carboxyphenyl)carbamoyl]pyrrolidin-3-yl)sulfanyl)-5-[(1S,2R)-1-formyl-2-hydroxypropyl]-4-methyl-4,5-dihydro-1H-pyrrole-2-carboxylic acid (three-letter code: 1RG) (formula: C<sub>22</sub>H<sub>27</sub>N<sub>3</sub>O<sub>7</sub>S).



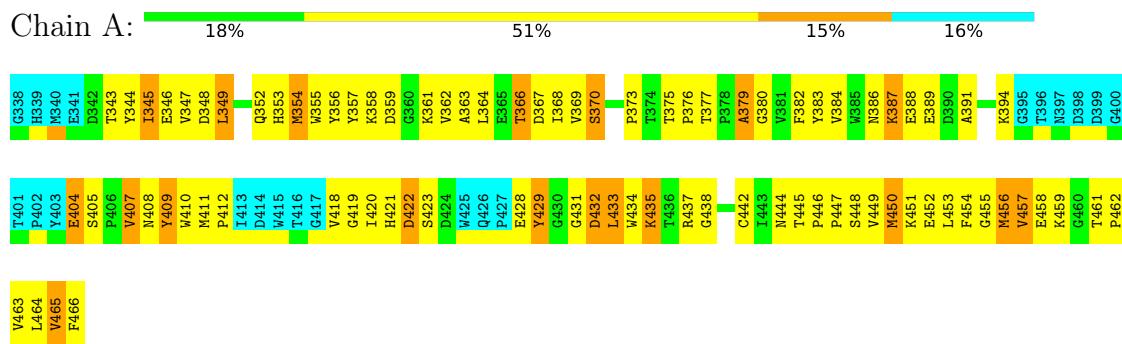
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	58	22	25	3	7	1

## 4 Residue-property plots

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

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

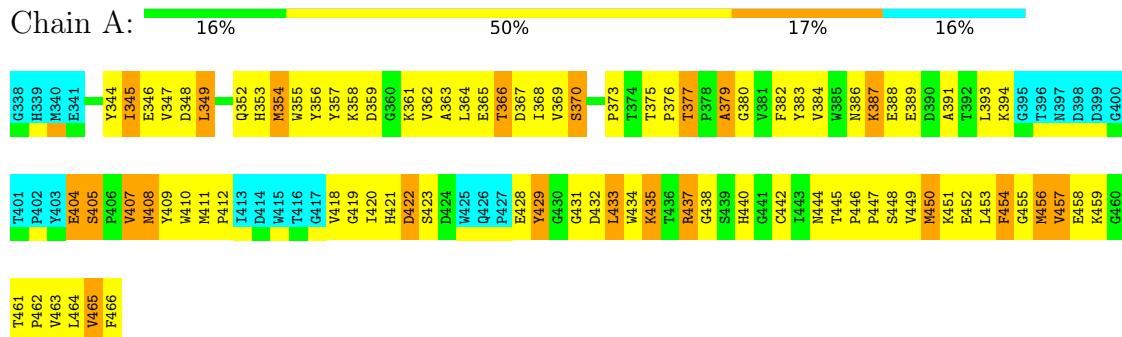
- Molecule 1: ERFK/YBIS/YCFS/YNHG



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

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: ERFK/YBIS/YCFS/YNHG



## 5 Refinement protocol and experimental data overview i

The models were refined using the following method: *ARIA2.3*.

Of the 1700 calculated structures, 20 were deposited, based on the following criterion: *TOTAL ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
UNIO	structure solution	10
TALOS	structure solution	
CcpNmr Analysis	structure solution	ANALYSIS

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	1701
Number of shifts mapped to atoms	1701
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

## 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:  
1RG

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	0.89±0.03	1±1/887 ( 0.1± 0.1%)	0.86±0.01	0±0/1209 ( 0.0± 0.0%)
All	All	0.89	19/17740 ( 0.1%)	0.86	0/24180 ( 0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.8
All	All	0	18

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
1	A	454	PHE	CE2-CZ	7.57	1.51	1.37	20	10
1	A	454	PHE	CE1-CZ	-6.45	1.25	1.37	20	7
1	A	346	GLU	CG-CD	-5.95	1.43	1.51	6	1
1	A	409	TYR	CE1-CZ	5.63	1.45	1.38	8	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	409	TYR	Sidechain	11
1	A	356	TYR	Sidechain	7

## 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	860	817	815	131±4
2	A	33	25	24	7±2
All	All	17860	16840	16780	2723

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 79.

5 of 280 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:349:LEU:HD21	1:A:465:VAL:HG23	0.96	1.33	5	20
1:A:450:MET:SD	1:A:453:LEU:HD23	0.85	2.11	6	20
2:A:130:1RG:CAM	2:A:130:1RG:HBA	0.84	2.02	7	2
1:A:433:LEU:HD22	1:A:437:ARG:HD2	0.84	1.48	5	6
1:A:343:THR:CG2	1:A:356:TYR:OH	0.82	2.27	5	7

## 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	107/129 (83%)	87±1 (81±1%)	17±1 (16±1%)	3±1 (3±0%)	7 40
All	All	2140/2580 (83%)	1741 (81%)	335 (16%)	64 (3%)	7 40

5 of 6 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	379	ALA	20
1	A	431	GLY	20

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Mol	Chain	Res	Type	Models (Total)
1	A	432	ASP	19
1	A	418	VAL	2
1	A	440	HIS	2

### 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	95/112 (85%)	72±2 (76±2%)	23±2 (24±2%)	2 26
All	All	1900/2240 (85%)	1443 (76%)	457 (24%)	2 26

5 of 34 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	345	ILE	20
1	A	349	LEU	20
1	A	354	MET	20
1	A	359	ASP	20
1	A	366	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 monosaccharides in this entry.

## 6.6 Ligand geometry (i)

1 ligand is 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
2	1RG	A	130	1	32,35,35	2.32±0.03	6±0 (19±1%)

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	1RG	A	130	1	28,50,50	1.48±0.03	5±1 (19±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	1RG	A	130	1	-	0±0,27,55,55	0±0,3,3,3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	130	1RG	CAL-CAM	8.94	1.34	1.48	11	20
2	A	130	1RG	CAH-CAI	5.14	1.38	1.52	18	20
2	A	130	1RG	CBA-CBE	4.77	1.39	1.49	12	20
2	A	130	1RG	CAB-CAA	4.55	1.57	1.50	7	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	130	1RG	CG-SAK	3.97	1.77	1.82	13	20

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

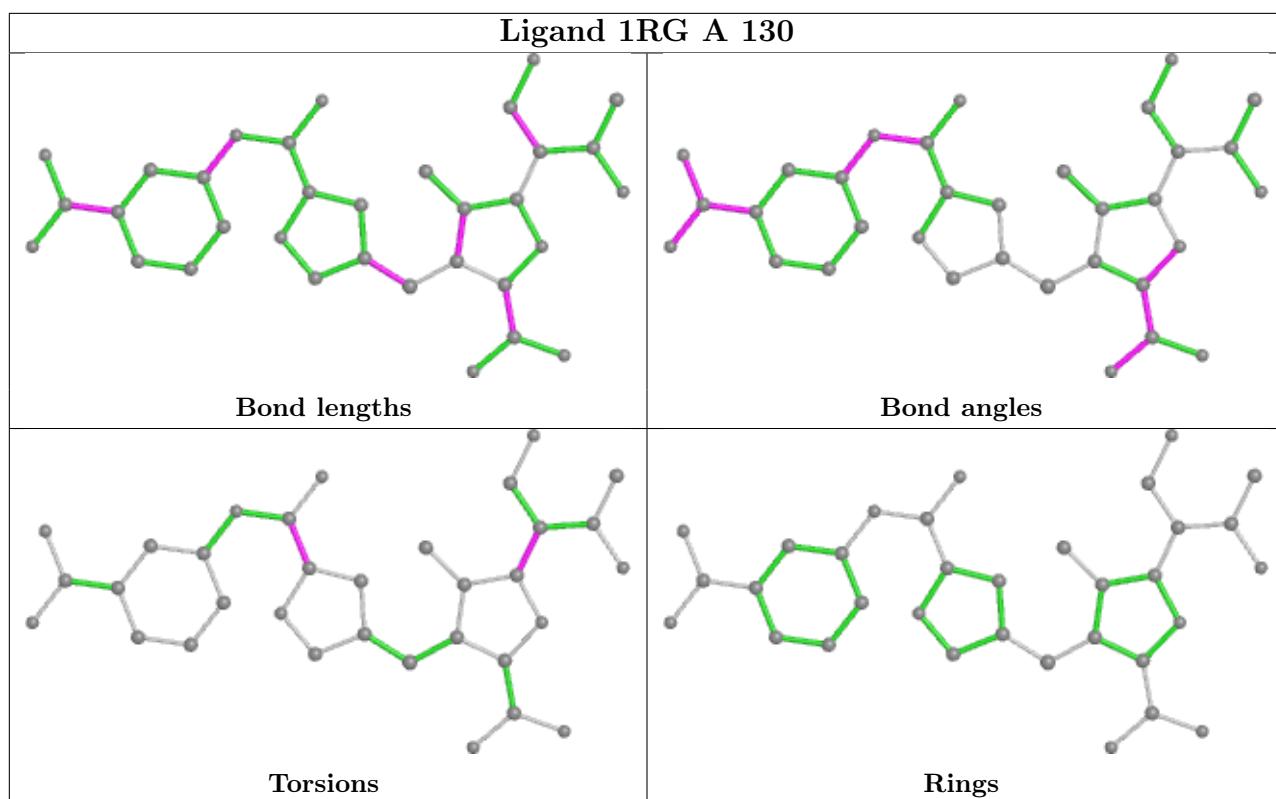
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	130	1RG	CAM-CAL-NAJ	5.37	127.14	120.38	11	20
2	A	130	1RG	CAY-NAX-C	3.09	120.00	127.40	20	20
2	A	130	1RG	OAU-CAM-CAL	3.06	121.80	116.76	9	20
2	A	130	1RG	OBF-CBE-OBG	2.51	117.78	123.35	6	20
2	A	130	1RG	OBF-CBE-CBA	2.48	121.28	114.85	7	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 94% for the well-defined parts and 92% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list*

#### 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	1701
Number of shifts mapped to atoms	1701
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

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

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	340	MET	HE2	1.95	0.005	1
1	A	340	MET	HE3	1.95	0.005	1
1	A	343	THR	HG22	1.581	0.003	1
1	A	343	THR	HG23	1.581	0.003	1
1	A	345	ILE	HD12	0.626	0.003	1
1	A	345	ILE	HD13	0.626	0.003	1
1	A	345	ILE	HG22	0.867	0.007	1
1	A	345	ILE	HG23	0.867	0.007	1
1	A	347	VAL	HG12	0.605	0.006	2
1	A	347	VAL	HG13	0.605	0.006	2
1	A	347	VAL	HG22	0.689	0.002	2
1	A	347	VAL	HG23	0.689	0.002	2
1	A	349	LEU	HD12	0.392	0.005	2
1	A	349	LEU	HD13	0.392	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	349	LEU	HD22	0.547	0.005	2
1	A	349	LEU	HD23	0.547	0.005	2
1	A	354	MET	HE2	1.476	0.002	1
1	A	354	MET	HE3	1.476	0.002	1
1	A	362	VAL	HG12	0.678	0.004	2
1	A	362	VAL	HG13	0.678	0.004	2
1	A	362	VAL	HG22	0.806	0.003	2
1	A	362	VAL	HG23	0.806	0.003	2
1	A	363	ALA	HB2	1.258	0.002	1
1	A	363	ALA	HB3	1.258	0.002	1
1	A	364	LEU	HD12	0.646	0.005	2
1	A	364	LEU	HD13	0.646	0.005	2
1	A	364	LEU	HD22	0.81	0.004	2
1	A	364	LEU	HD23	0.81	0.004	2
1	A	366	THR	HG22	0.553	0.004	1
1	A	366	THR	HG23	0.553	0.004	1
1	A	368	ILE	HD12	0.437	0.004	1
1	A	368	ILE	HD13	0.437	0.004	1
1	A	368	ILE	HG22	0.612	0.001	1
1	A	368	ILE	HG23	0.612	0.001	1
1	A	369	VAL	HG12	1.01	0.003	2
1	A	369	VAL	HG13	1.01	0.003	2
1	A	369	VAL	HG22	1.115	0.005	2
1	A	369	VAL	HG23	1.115	0.005	2
1	A	374	THR	HG22	1.286	0.001	1
1	A	374	THR	HG23	1.286	0.001	1
1	A	375	THR	HG22	1.125	0.004	1
1	A	375	THR	HG23	1.125	0.004	1
1	A	377	THR	HG22	1.12	0.002	1
1	A	377	THR	HG23	1.12	0.002	1
1	A	379	ALA	HB2	1.415	0.003	1
1	A	379	ALA	HB3	1.415	0.003	1
1	A	381	VAL	HG12	0.876	0.002	2
1	A	381	VAL	HG13	0.876	0.002	2
1	A	381	VAL	HG22	0.77	0.002	2
1	A	381	VAL	HG23	0.77	0.002	2
1	A	384	VAL	HG12	0.745	0.002	2
1	A	384	VAL	HG13	0.745	0.002	2
1	A	384	VAL	HG22	0.694	0.002	2
1	A	384	VAL	HG23	0.694	0.002	2
1	A	391	ALA	HB2	0.945	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	391	ALA	HB3	0.945	0.005	1
1	A	392	THR	HG22	0.818	0.002	1
1	A	392	THR	HG23	0.818	0.002	1
1	A	393	LEU	HD12	-0.597	0.007	2
1	A	393	LEU	HD13	-0.597	0.007	2
1	A	393	LEU	HD22	-0.087	0.006	2
1	A	393	LEU	HD23	-0.087	0.006	2
1	A	396	THR	HG22	1.124	0.005	1
1	A	396	THR	HG23	1.124	0.005	1
1	A	401	THR	HG22	1.253	0.003	1
1	A	401	THR	HG23	1.253	0.003	1
1	A	407	VAL	HG12	0.619	0.004	2
1	A	407	VAL	HG13	0.619	0.004	2
1	A	407	VAL	HG22	1.012	0.007	2
1	A	407	VAL	HG23	1.012	0.007	2
1	A	411	MET	HE2	1.634	0.003	1
1	A	411	MET	HE3	1.634	0.003	1
1	A	413	ILE	HD12	0.175	0.006	1
1	A	413	ILE	HD13	0.175	0.006	1
1	A	413	ILE	HG22	0.657	0.004	1
1	A	413	ILE	HG23	0.657	0.004	1
1	A	416	THR	HG22	0.863	0.005	1
1	A	416	THR	HG23	0.863	0.005	1
1	A	418	VAL	HG12	0.757	0.006	2
1	A	418	VAL	HG13	0.757	0.006	2
1	A	418	VAL	HG22	0.587	0.004	2
1	A	418	VAL	HG23	0.587	0.004	2
1	A	420	ILE	HD12	0.646	0.003	1
1	A	420	ILE	HD13	0.646	0.003	1
1	A	420	ILE	HG22	0.719	0.002	1
1	A	420	ILE	HG23	0.719	0.002	1
1	A	433	LEU	HD12	0.721	0.008	2
1	A	433	LEU	HD13	0.721	0.008	2
1	A	433	LEU	HD22	0.619	0.003	2
1	A	433	LEU	HD23	0.619	0.003	2
1	A	436	THR	HG22	1.079	0.005	1
1	A	436	THR	HG23	1.079	0.005	1
1	A	443	ILE	HD12	0.6	0.002	1
1	A	443	ILE	HD13	0.6	0.002	1
1	A	443	ILE	HG22	0.629	0.006	1
1	A	443	ILE	HG23	0.629	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	445	THR	HG22	0.762	0.006	1
1	A	445	THR	HG23	0.762	0.006	1
1	A	449	VAL	HG12	0.878	0.003	2
1	A	449	VAL	HG13	0.878	0.003	2
1	A	449	VAL	HG22	0.665	0.003	2
1	A	449	VAL	HG23	0.665	0.003	2
1	A	450	MET	HE2	2.074	0.003	1
1	A	450	MET	HE3	2.074	0.003	1
1	A	453	LEU	HD12	0.375	0.003	2
1	A	453	LEU	HD13	0.375	0.003	2
1	A	453	LEU	HD22	0.606	0.003	2
1	A	453	LEU	HD23	0.606	0.003	2
1	A	456	MET	HE2	2.074	0.004	1
1	A	456	MET	HE3	2.074	0.004	1
1	A	457	VAL	HG12	0.199	0.002	2
1	A	457	VAL	HG13	0.199	0.002	2
1	A	457	VAL	HG22	0.581	0.005	2
1	A	457	VAL	HG23	0.581	0.005	2
1	A	461	THR	HG22	1.568	0.005	1
1	A	461	THR	HG23	1.568	0.005	1
1	A	463	VAL	HG12	0.836	0.001	2
1	A	463	VAL	HG13	0.836	0.001	2
1	A	463	VAL	HG22	0.669	0.003	2
1	A	463	VAL	HG23	0.669	0.003	2
1	A	464	LEU	HD12	0.8	0.006	2
1	A	464	LEU	HD13	0.8	0.006	2
1	A	464	LEU	HD22	0.823	0.004	2
1	A	464	LEU	HD23	0.823	0.004	2
1	A	465	VAL	HG12	0.801	0.003	2
1	A	465	VAL	HG13	0.801	0.003	2
1	A	465	VAL	HG22	0.807	0.003	2
1	A	465	VAL	HG23	0.807	0.003	2
1	A	130	1RG	HA	0.818	0.001	4
1	A	130	1RG	HA	4.563	0.002	1

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, ppm	Suggested action
<sup>13</sup> C <sub>α</sub>	124	0.04 ± 0.19	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, ppm	Suggested action
$^{13}\text{C}_\beta$	114	-0.05 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	106	0.42 ± 0.19	None needed (< 0.5 ppm)
$^{15}\text{N}$	112	0.24 ± 0.51	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 94%, i.e. 1339 atoms were assigned a chemical shift out of a possible 1428. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	508/534 (95%)	212/218 (97%)	198/216 (92%)	98/100 (98%)
Sidechain	694/739 (94%)	471/481 (98%)	217/242 (90%)	6/16 (38%)
Aromatic	137/155 (88%)	68/75 (91%)	62/71 (87%)	7/9 (78%)
Overall	1339/1428 (94%)	751/774 (97%)	477/529 (90%)	111/125 (89%)

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

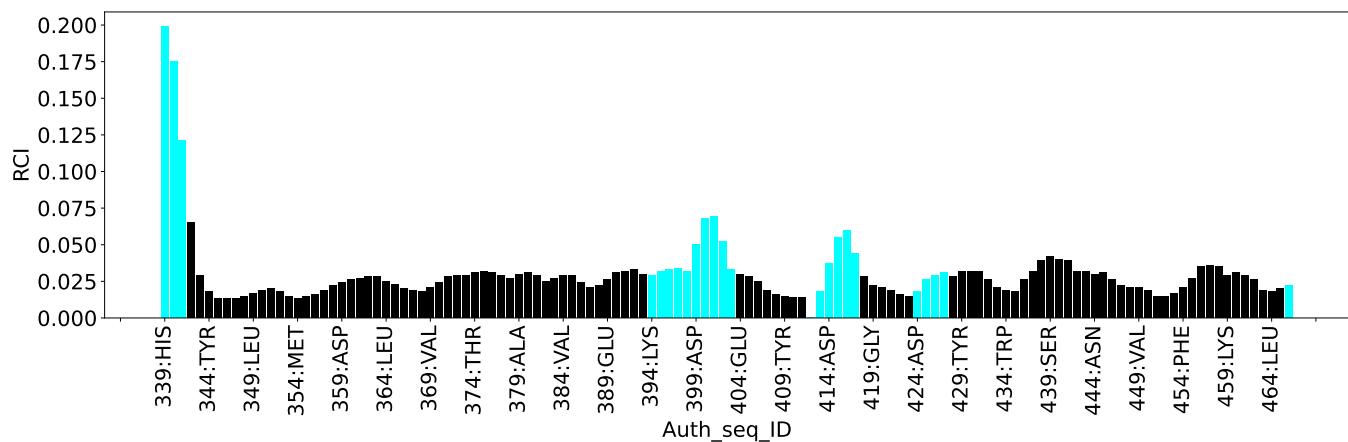
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	366	THR	HG1	5.48	0.08 – 2.19	20.6
1	A	446	PRO	HG2	-0.11	0.41 – 3.45	-6.7
1	A	435	LYS	HG3	-0.33	0.04 – 2.67	-6.4
1	A	435	LYS	HG2	-0.18	0.13 – 2.61	-6.2
1	A	423	SER	HB2	2.35	2.61 – 5.13	-6.0
1	A	423	SER	HB3	2.24	2.49 – 5.20	-5.9
1	A	412	PRO	HD3	1.45	1.76 – 5.48	-5.8
1	A	353	HIS	HD2	4.41	4.65 – 9.35	-5.5

### 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 (i)

### 8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	4226
Intra-residue ( $ i-j =0$ )	2403
Sequential ( $ i-j =1$ )	1191
Medium range ( $ i-j >1$ and $ i-j <5$ )	161
Long range ( $ i-j \geq 5$ )	471
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	214
Number of unmapped restraints	0
Number of restraints per residue	34.4
Number of long range restraints per residue <sup>1</sup>	3.7

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	235.4	0.2
0.2-0.5 (Medium)	612.9	0.5
>0.5 (Large)	1179.0	12.55

### 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)	34.3	10.0
10.0-20.0 (Medium)	8.0	19.9
>20.0 (Large)	0.8	22.2

## 9 Distance violation analysis (i)

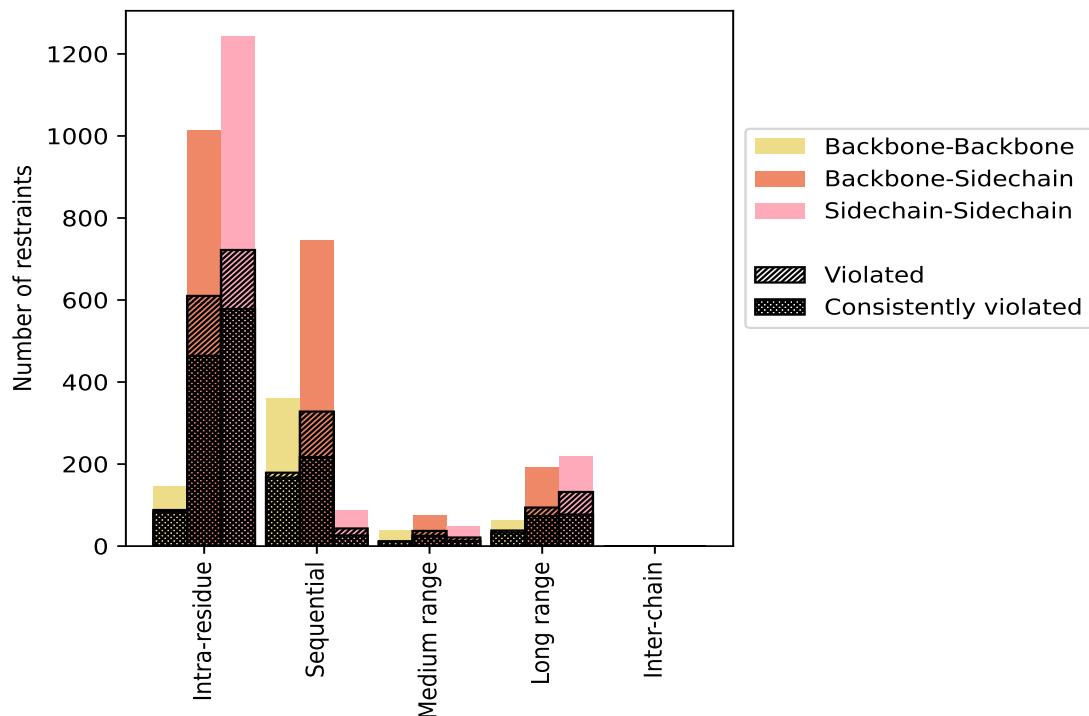
### 9.1 Summary of distance violations (i)

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.

Restraints type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
Intra-residue ( $ i-j =0$ )	2403	56.9	1420	59.1	33.6	1125	46.8	26.6
Backbone-Backbone	146	3.5	88	60.3	2.1	83	56.8	2.0
Backbone-Sidechain	1014	24.0	610	60.2	14.4	464	45.8	11.0
Sidechain-Sidechain	1243	29.4	722	58.1	17.1	578	46.5	13.7
Sequential ( $ i-j =1$ )	1191	28.2	550	46.2	13.0	410	34.4	9.7
Backbone-Backbone	360	8.5	179	49.7	4.2	167	46.4	4.0
Backbone-Sidechain	745	17.6	328	44.0	7.8	217	29.1	5.1
Sidechain-Sidechain	86	2.0	43	50.0	1.0	26	30.2	0.6
Medium range ( $ i-j >1 \text{ & }  i-j <5$ )	161	3.8	70	43.5	1.7	48	29.8	1.1
Backbone-Backbone	39	0.9	12	30.8	0.3	10	25.6	0.2
Backbone-Sidechain	75	1.8	37	49.3	0.9	25	33.3	0.6
Sidechain-Sidechain	47	1.1	21	44.7	0.5	13	27.7	0.3
Long range ( $ i-j \geq 5$ )	471	11.1	264	56.1	6.2	183	38.9	4.3
Backbone-Backbone	62	1.5	38	61.3	0.9	33	53.2	0.8
Backbone-Sidechain	191	4.5	94	49.2	2.2	73	38.2	1.7
Sidechain-Sidechain	218	5.2	132	60.6	3.1	77	35.3	1.8
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4226	100.0	2304	54.5	54.5	1766	41.8	41.8
Backbone-Backbone	607	14.4	317	52.2	7.5	293	48.3	6.9
Backbone-Sidechain	2025	47.9	1069	52.8	25.3	779	38.5	18.4
Sidechain-Sidechain	1594	37.7	918	57.6	21.7	694	43.5	16.4

<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	1270	481	59	222	0	2032	0.76	12.35	0.76	0.59
2	1266	478	61	223	0	2028	0.76	12.27	0.76	0.59
3	1269	482	61	225	0	2037	0.76	12.31	0.75	0.59
4	1270	479	61	223	0	2033	0.76	12.37	0.76	0.6
5	1265	482	58	222	0	2027	0.76	12.55	0.76	0.59
6	1257	478	59	220	0	2014	0.76	12.34	0.76	0.6
7	1275	478	60	221	0	2034	0.76	12.38	0.76	0.59
8	1270	474	61	221	0	2026	0.76	12.28	0.76	0.6
9	1265	482	62	221	0	2030	0.76	12.24	0.76	0.59
10	1270	473	62	221	0	2026	0.76	12.22	0.76	0.59
11	1263	471	58	221	0	2013	0.76	12.31	0.76	0.59

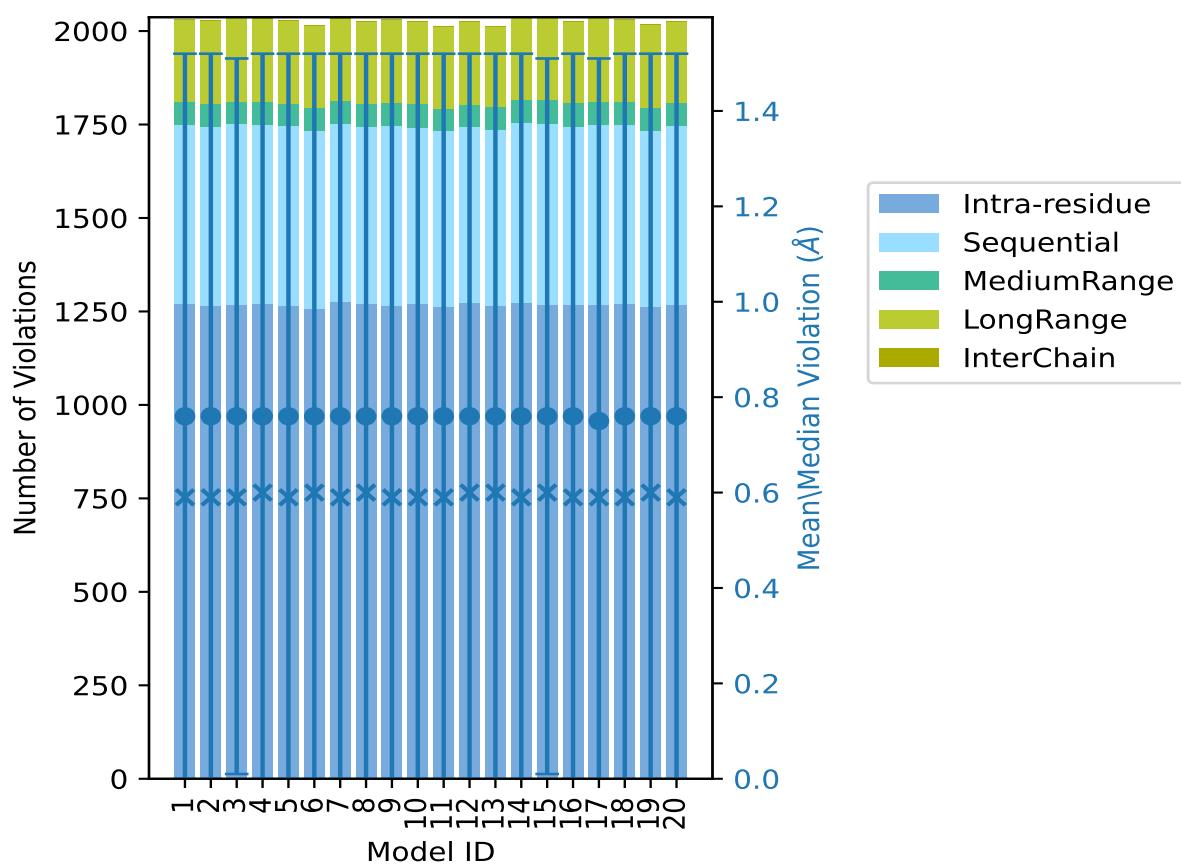
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
12	1272	473	58	222	0	2025	0.76	12.46	0.76	0.6
13	1264	473	60	216	0	2013	0.76	12.26	0.76	0.6
14	1272	483	62	220	0	2037	0.76	12.36	0.76	0.59
15	1268	485	63	219	0	2035	0.76	12.24	0.75	0.6
16	1268	477	62	218	0	2025	0.76	12.4	0.76	0.59
17	1269	480	61	226	0	2036	0.75	12.36	0.76	0.59
18	1270	479	60	222	0	2031	0.76	12.38	0.76	0.59
19	1262	472	61	223	0	2018	0.76	12.31	0.76	0.6
20	1268	478	61	219	0	2026	0.76	12.25	0.76	0.59

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

### 9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



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

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

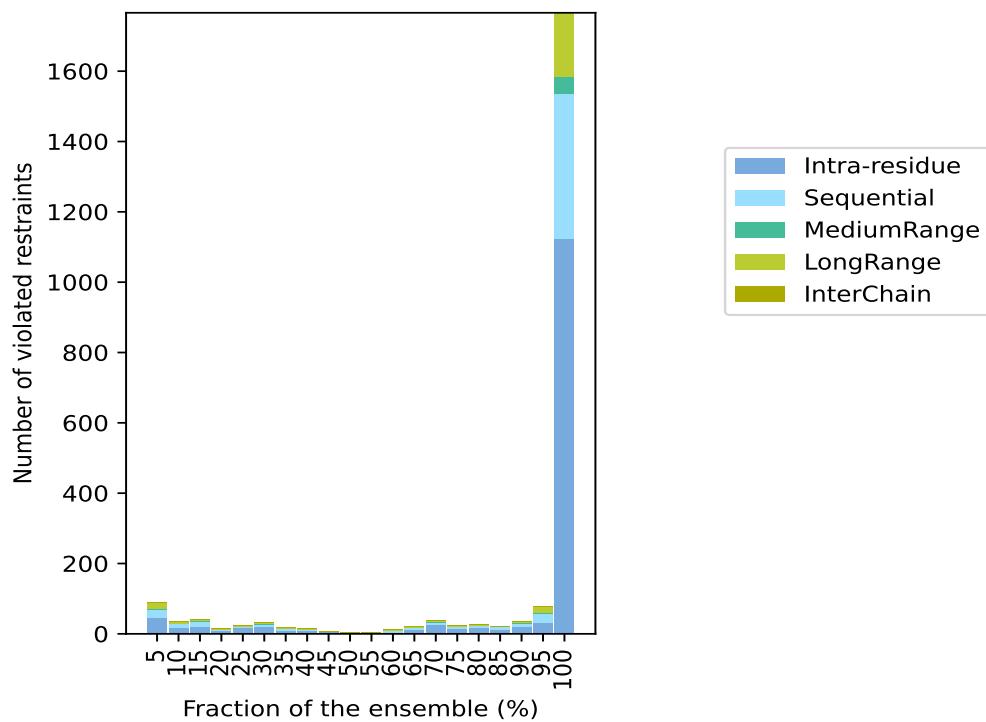
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1922(IR:983, SQ:641, MR:91, LR:207, IC:0) restraints are not violated in the ensemble.

IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Fraction of the ensemble	
						Count <sup>6</sup>	%
45	24	1	19	0	89	1	5.0
19	9	1	6	0	35	2	10.0
19	17	1	5	0	42	3	15.0
10	3	0	3	0	16	4	20.0
17	2	1	3	0	23	5	25.0
20	6	3	3	0	32	6	30.0
9	5	1	2	0	17	7	35.0
9	4	0	1	0	14	8	40.0
5	2	1	0	0	8	9	45.0
1	1	0	1	0	3	10	50.0
3	1	1	0	0	5	11	55.0
3	5	1	2	0	11	12	60.0
12	6	0	2	0	20	13	65.0
25	6	3	5	0	39	14	70.0
15	4	1	4	0	24	15	75.0
18	4	2	2	0	26	16	80.0
13	7	0	2	0	22	17	85.0
19	10	2	3	0	34	18	90.0
33	24	3	18	0	78	19	95.0
1125	410	48	183	0	1766	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

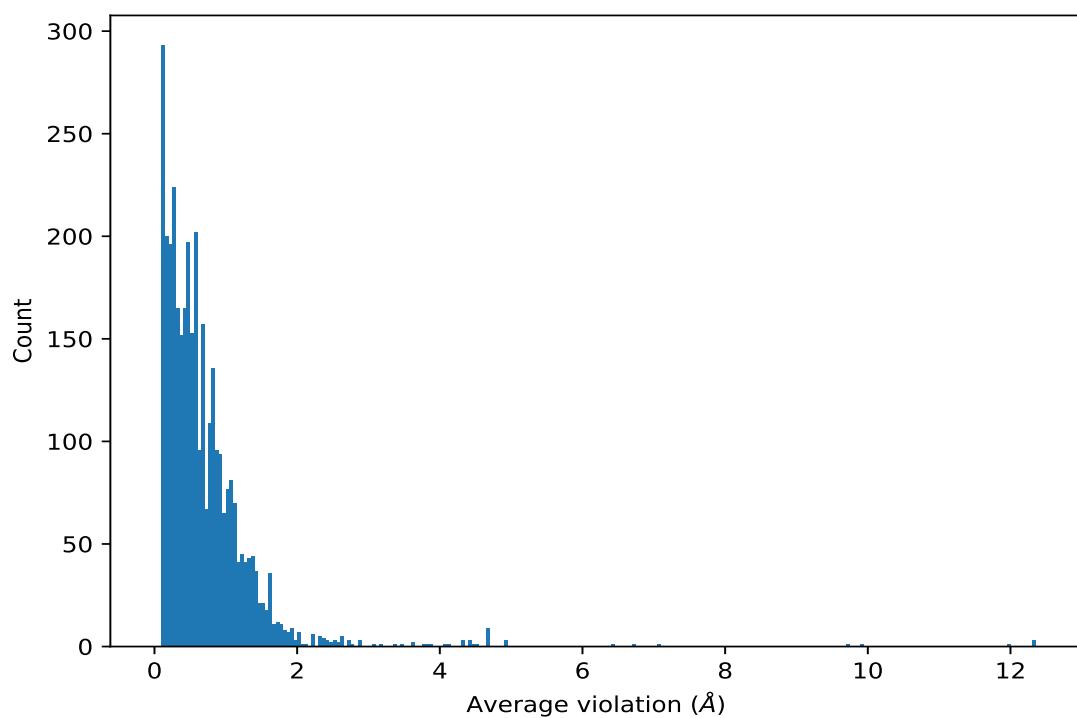
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [\(i\)](#)



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

### 9.4.1 Histogram : Distribution of mean distance violations [\(i\)](#)

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



#### 9.4.2 Table: Most violated distance restraints [\(i\)](#)

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	20	12.33	0.08	12.32
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	20	12.33	0.08	12.32
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	20	12.33	0.08	12.32
(1,3746)	1:A:426:GLN:H	1:A:453:LEU:HA	20	11.98	0.07	11.96
(1,3912)	1:A:451:LYS:H	1:A:347:VAL:HB	20	9.95	0.08	9.98
(1,3929)	1:A:355:TRP:HE1	1:A:420:ILE:HA	20	9.72	0.05	9.73
(1,972)	1:A:396:THR:HB	1:A:375:THR:HA	20	7.06	0.63	6.96
(1,3983)	1:A:428:GLU:H	1:A:352:GLN:HB2	20	6.71	0.24	6.8
(1,3489)	1:A:367:ASP:H	1:A:356:TYR:HA	20	6.44	0.03	6.44
(1,2830)	1:A:450:MET:HE1	1:A:419:GLY:H	20	4.94	0.07	4.92
(1,2830)	1:A:450:MET:HE2	1:A:419:GLY:H	20	4.94	0.07	4.92
(1,2830)	1:A:450:MET:HE3	1:A:419:GLY:H	20	4.94	0.07	4.92
(1,814)	1:A:464:LEU:HD11	1:A:456:MET:HE1	20	4.67	0.04	4.66
(1,814)	1:A:464:LEU:HD11	1:A:456:MET:HE2	20	4.67	0.04	4.66
(1,814)	1:A:464:LEU:HD11	1:A:456:MET:HE3	20	4.67	0.04	4.66
(1,814)	1:A:464:LEU:HD12	1:A:456:MET:HE1	20	4.67	0.04	4.66

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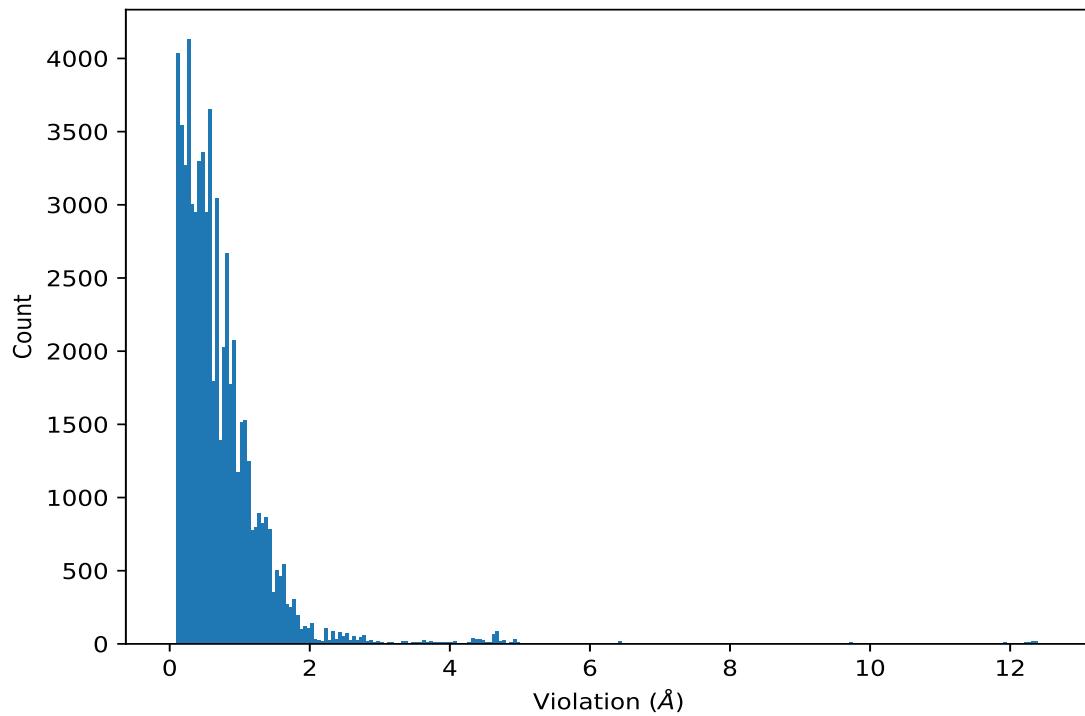
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,814)	1:A:464:LEU:HD12	1:A:456:MET:HE2	20	4.67	0.04	4.66
(1,814)	1:A:464:LEU:HD12	1:A:456:MET:HE3	20	4.67	0.04	4.66
(1,814)	1:A:464:LEU:HD13	1:A:456:MET:HE1	20	4.67	0.04	4.66
(1,814)	1:A:464:LEU:HD13	1:A:456:MET:HE2	20	4.67	0.04	4.66
(1,814)	1:A:464:LEU:HD13	1:A:456:MET:HE3	20	4.67	0.04	4.66
(1,3665)	1:A:371:GLY:H	1:A:419:GLY:HA3	20	4.5	0.16	4.54

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	5	12.55
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	5	12.55
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	5	12.55
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	12	12.46
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	12	12.46
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	12	12.46
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	16	12.4
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	16	12.4
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	16	12.4
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	7	12.38
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	7	12.38
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	7	12.38
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	18	12.38
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	18	12.38
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	18	12.38
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	4	12.37
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	4	12.37
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	4	12.37
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	14	12.36
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	14	12.36
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	14	12.36
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	17	12.36
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	17	12.36
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	17	12.36
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	1	12.35
(1,1537)	1:A:411:MET:HE2	1:A:372:LYS:HA	1	12.35
(1,1537)	1:A:411:MET:HE3	1:A:372:LYS:HA	1	12.35
(1,1537)	1:A:411:MET:HE1	1:A:372:LYS:HA	6	12.34

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

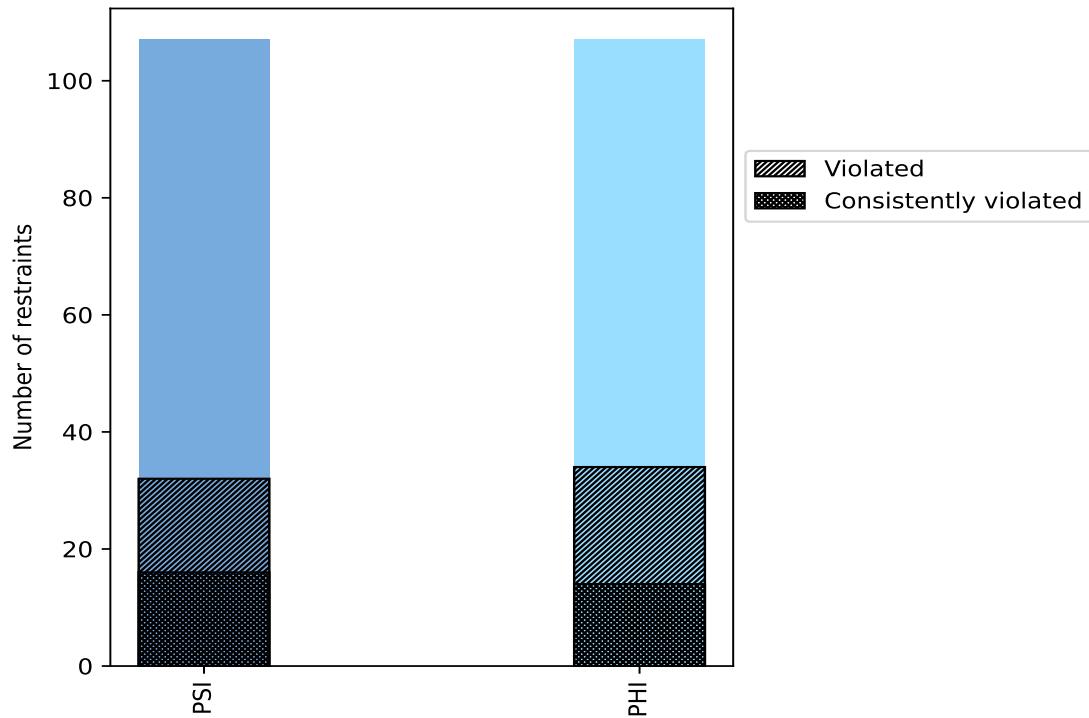
### 10.1 Summary of dihedral-angle violations [\(i\)](#)

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>
PSI	107	50.0	32	29.9	15.0	16	15.0	7.5
PHI	107	50.0	34	31.8	15.9	14	13.1	6.5
Total	214	100.0	66	30.8	30.8	30	14.0	14.0

<sup>1</sup> percentage calculated with respect to total number of dihedral-angle restraints, <sup>2</sup> percentage calculated with respect to number of restraints in a particular dihedral-angle type, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [\(i\)](#)



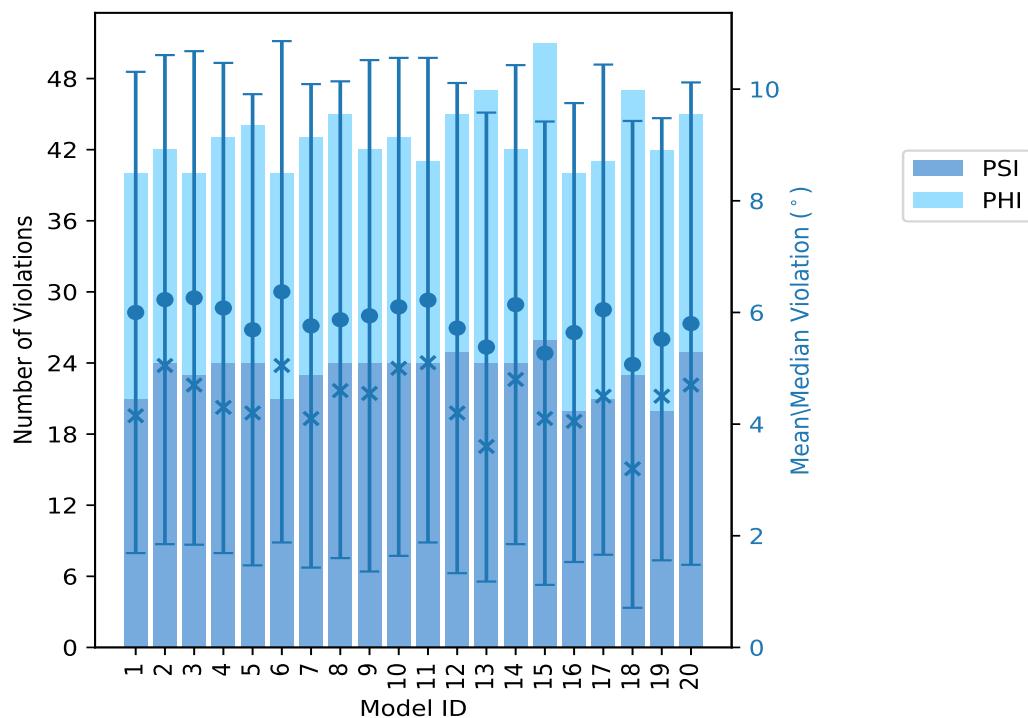
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	21	19	40	6.0	21.4	4.31	4.15
2	24	18	42	6.23	21.3	4.38	5.05
3	23	17	40	6.26	21.4	4.42	4.7
4	24	19	43	6.08	21.6	4.39	4.3
5	24	20	44	5.69	19.5	4.22	4.2
6	21	19	40	6.37	21.9	4.49	5.05
7	23	20	43	5.76	21.0	4.33	4.1
8	24	21	45	5.87	21.1	4.27	4.6
9	24	18	42	5.94	22.2	4.58	4.55
10	24	19	43	6.1	21.8	4.46	5.0
11	24	17	41	6.22	20.6	4.34	5.1
12	25	20	45	5.72	20.4	4.39	4.2
13	24	23	47	5.38	21.1	4.2	3.6
14	24	18	42	6.14	19.4	4.29	4.8
15	26	25	51	5.27	20.3	4.15	4.1
16	20	20	40	5.64	20.9	4.11	4.05
17	21	20	41	6.05	21.1	4.39	4.5
18	23	24	47	5.07	21.2	4.36	3.2
19	20	22	42	5.52	19.9	3.96	4.5
20	25	20	45	5.8	20.8	4.32	4.7

### 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.

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

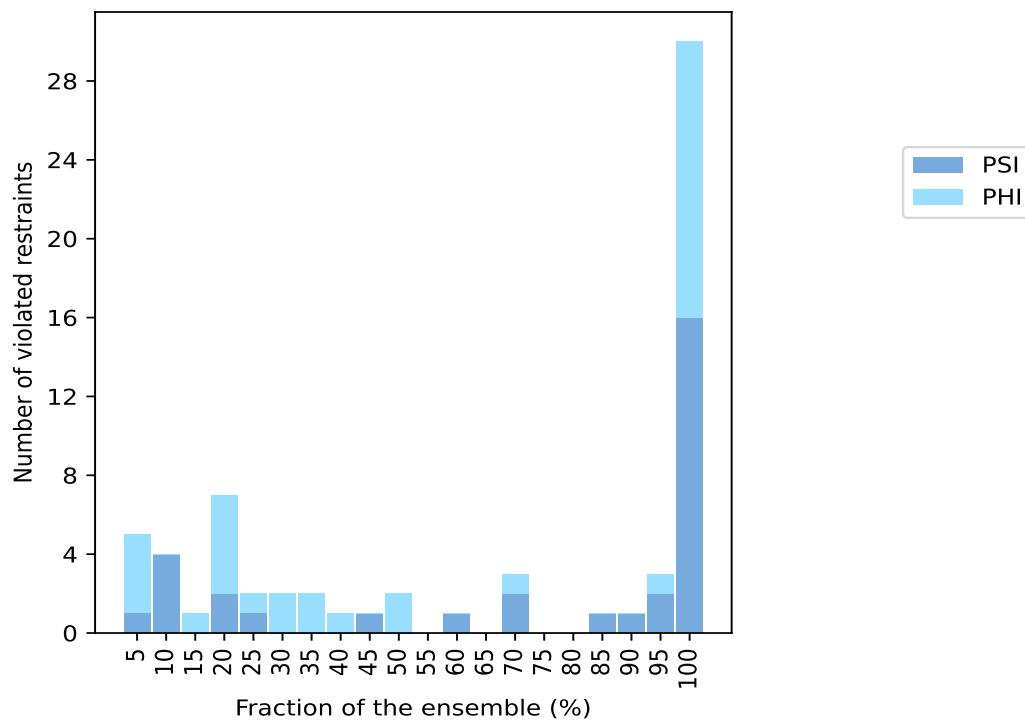
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
1	0	1	12	60.0
0	0	0	13	65.0
2	1	3	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
1	0	1	18	90.0
2	1	3	19	95.0
16	14	30	20	100.0

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

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

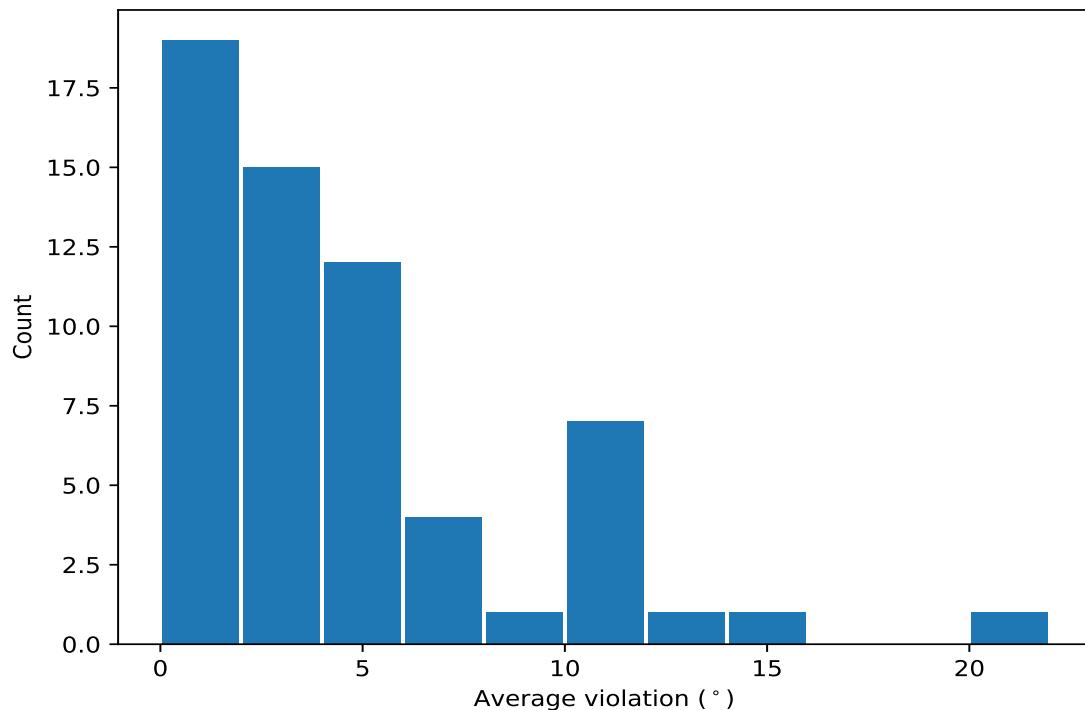


## 10.4 Most violated dihedral-angle restraints in the ensemble [\(i\)](#)

### 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.

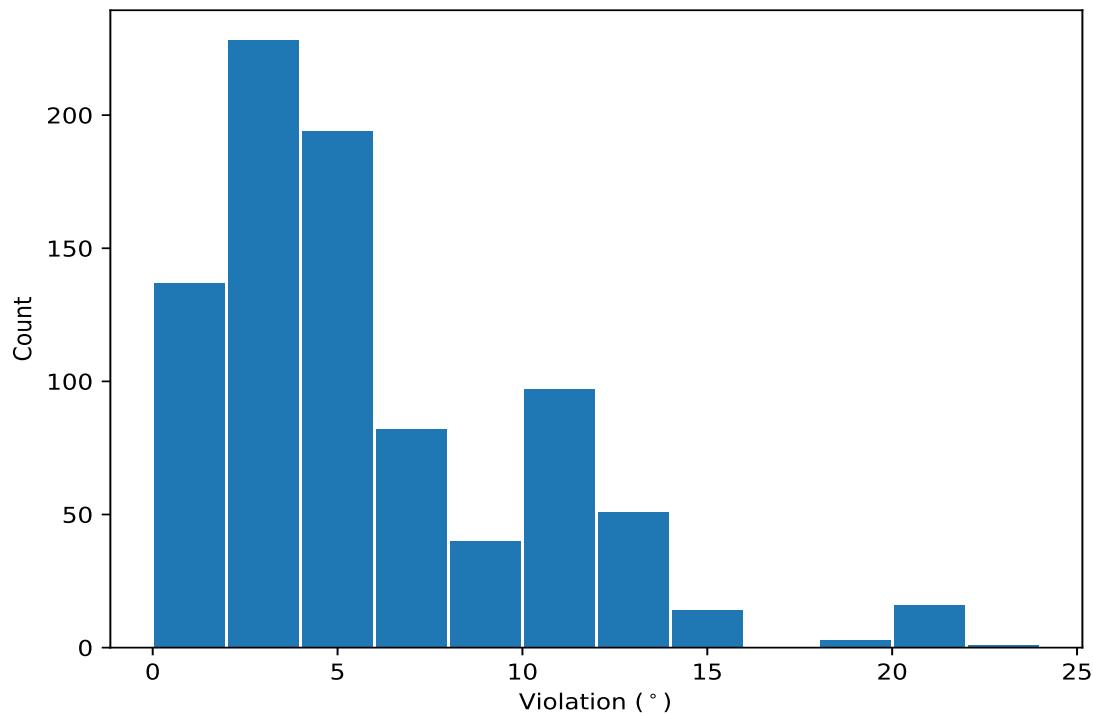
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	20	20.94	0.73	21.1
(1,153)	1:A:431:GLY:C	1:A:432:ASP:N	1:A:432:ASP:CA	1:A:432:ASP:C	20	14.34	0.78	14.35
(1,54)	1:A:370:SER:N	1:A:370:SER:CA	1:A:370:SER:C	1:A:371:GLY:N	20	12.55	0.45	12.5
(1,7)	1:A:344:TYR:C	1:A:345:ILE:N	1:A:345:ILE:CA	1:A:345:ILE:C	20	11.3	0.37	11.2
(1,152)	1:A:431:GLY:N	1:A:431:GLY:CA	1:A:431:GLY:C	1:A:432:ASP:N	20	10.94	3.41	12.3
(1,46)	1:A:365:GLU:N	1:A:365:GLU:CA	1:A:365:GLU:C	1:A:366:THR:N	20	10.62	0.47	10.7
(1,2)	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	1:A:343:THR:N	20	10.51	0.94	10.6
(1,5)	1:A:343:THR:C	1:A:344:TYR:N	1:A:344:TYR:CA	1:A:344:TYR:C	20	10.39	0.43	10.3
(1,134)	1:A:418:VAL:N	1:A:418:VAL:CA	1:A:418:VAL:C	1:A:419:GLY:N	20	10.26	2.0	10.8
(1,154)	1:A:432:ASP:N	1:A:432:ASP:CA	1:A:432:ASP:C	1:A:433:LEU:N	20	8.64	0.64	8.65

<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 (°)
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	9	22.2
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	6	21.9
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	10	21.8
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	4	21.6
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	1	21.4
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	3	21.4
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	2	21.3
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	18	21.2
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	8	21.1
(1,55)	1:A:370:SER:C	1:A:371:GLY:N	1:A:371:GLY:CA	1:A:371:GLY:C	13	21.1