



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2MK0 / pdb\_00002mk0  
BMRB ID : 4958  
Title : Structure of the PSCD4-domain of the cell wall protein pleuralin-1 from the diatom *Cylindrotheca fusiformis*  
Authors : De Sanctis, S.; Wenzler, M.; Kroeger, N.; Malloni, W.M.; Sumper, M.; Deutzmann, R.; Zadavec, P.; Brunner, E.; Kremer, W.; Kalbitzer, S.H.R.  
Deposited on : 2014-01-22

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

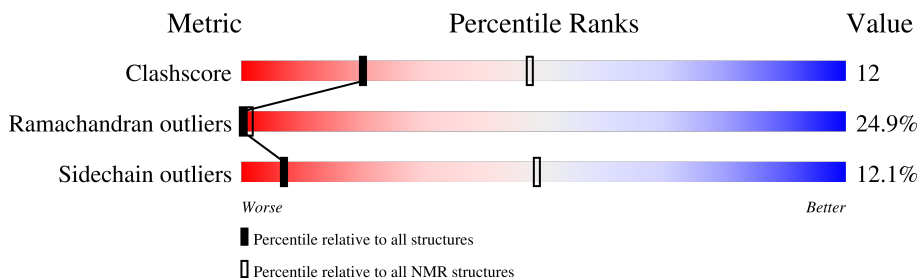
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 88%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	120	 37%      22%      . . 8%      27%

## 2 Ensemble composition and analysis i

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:376-A:453 (78)	0.84	2

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 2 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1204 atoms, of which 570 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HEP200 protein.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	88	1204	388	570	101	133	12	0

There are 16 discrepancies between the modelled and reference sequences:

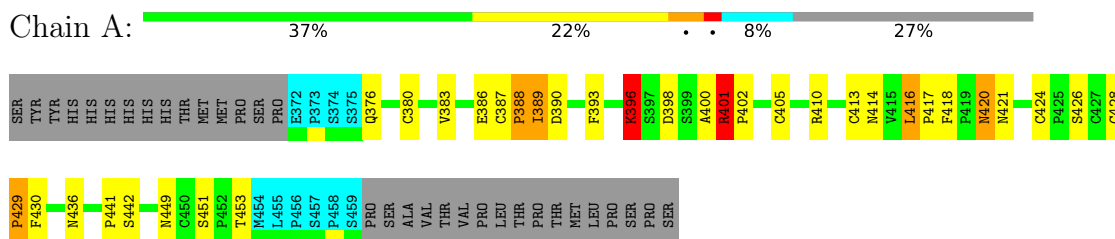
Chain	Residue	Modelled	Actual	Comment	Reference
A	357	SER	-	expression tag	UNP O22015
A	358	TYR	-	expression tag	UNP O22015
A	359	TYR	-	expression tag	UNP O22015
A	360	HIS	-	expression tag	UNP O22015
A	361	HIS	-	expression tag	UNP O22015
A	362	HIS	-	expression tag	UNP O22015
A	363	HIS	-	expression tag	UNP O22015
A	364	HIS	-	expression tag	UNP O22015
A	365	HIS	-	expression tag	UNP O22015
A	470	THR	-	expression tag	UNP O22015
A	471	MET	-	expression tag	UNP O22015
A	472	LEU	-	expression tag	UNP O22015
A	473	PRO	-	expression tag	UNP O22015
A	474	SER	-	expression tag	UNP O22015
A	475	PRO	-	expression tag	UNP O22015
A	476	SER	-	expression tag	UNP O22015

## 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.

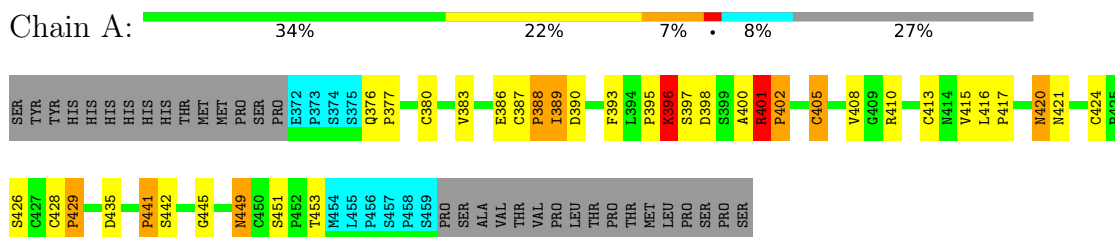
- Molecule 1: HEP200 protein



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

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: HEP200 protein



## 5 Refinement protocol and experimental data overview

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

Of the 2000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.21
CNS	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	1074
Number of shifts mapped to atoms	901
Number of unparsed shifts	0
Number of shifts with mapping errors	173
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

## 6 Model quality [i](#)

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

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	1.37±0.02	3±1/585 ( 0.5± 0.2%)	1.37±0.02	3±1/809 ( 0.3± 0.2%)
All	All	1.37	27/5850 ( 0.5%)	1.37	27/8090 ( 0.3%)

5 of 10 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	416	LEU	C-N	6.69	1.41	1.33	10	8
1	A	415	VAL	N-CA	-5.72	1.40	1.46	7	4
1	A	436	ASN	C-N	5.69	1.41	1.33	8	4
1	A	389	ILE	CA-CB	5.44	1.61	1.54	3	5
1	A	401	ARG	NE-CZ	5.42	1.39	1.33	9	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	420	ASN	CA-CB-CG	8.62	121.22	112.60	7	10
1	A	449	ASN	CA-CB-CG	6.68	119.28	112.60	1	5
1	A	401	ARG	CA-C-N	5.77	126.32	120.38	9	5
1	A	401	ARG	C-N-CA	5.77	126.32	120.38	9	5
1	A	392	CYS	N-CA-C	-5.12	105.35	111.03	9	1

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	564	503	503	13±3
All	All	5640	5030	5030	131

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 12.

5 of 42 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:428:CYS:SG	1:A:429:PRO:HD2	0.63	2.33	5	7
1:A:386:GLU:C	1:A:388:PRO:HD2	0.61	2.20	6	6
1:A:387:CYS:N	1:A:388:PRO:HD2	0.60	2.12	5	8
1:A:387:CYS:SG	1:A:388:PRO:HD3	0.60	2.36	7	2
1:A:396:LYS:HA	1:A:401:ARG:CG	0.59	2.28	1	10

## 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	78/120 (65%)	32±2 (41±2%)	26±2 (34±2%)	19±2 (25±2%)	0	1
All	All	780/1200 (65%)	321 (41%)	265 (34%)	194 (25%)	0	1

5 of 30 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	376	GLN	10
1	A	380	CYS	10
1	A	388	PRO	10
1	A	389	ILE	10
1	A	393	PHE	10

### 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	71/112 (63%)	62±1 (88±2%)	9±1 (12±2%)	<b>7</b> 49
All	All	710/1120 (63%)	624 (88%)	86 (12%)	<b>7</b> 49

5 of 18 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	383	VAL	10
1	A	396	LYS	10
1	A	401	ARG	10
1	A	420	ASN	10
1	A	421	ASN	10

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *shift\_set\_1*

#### 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	1074
Number of shifts mapped to atoms	901
Number of unparsed shifts	0
Number of shifts with mapping errors	173
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- No matching atom found in the structure. First 5 (of 173) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	358	TYR	H	7.64	0.02	1
1	A	358	TYR	HA	4.77	0.05	1
1	A	358	TYR	C	175.42	0.20	1
1	A	358	TYR	CA	57.75	0.20	1
1	A	358	TYR	CB	40.12	0.20	1
1	A	359	TYR	C	176.1	0.20	1
1	A	359	TYR	CA	59.3	0.20	1
1	A	359	TYR	N	115.11	0.33	1
1	A	361	HIS	HA	3.97	0.05	1
1	A	361	HIS	HB2	3.11	0.05	2
1	A	361	HIS	HB3	3.2	0.05	2
1	A	361	HIS	C	176.39	0.20	1
1	A	361	HIS	CA	56.7	0.20	1
1	A	361	HIS	CB	30.07	0.20	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	364	HIS	HA	4.57	0.05	1
1	A	364	HIS	HB2	2.98	0.05	1
1	A	364	HIS	HB3	2.98	0.05	1
1	A	364	HIS	C	173.92	0.20	1
1	A	364	HIS	CA	55.82	0.20	1
1	A	364	HIS	CB	30.6	0.20	1
1	A	365	HIS	H	8.35	0.02	1
1	A	365	HIS	HA	4.65	0.05	1
1	A	365	HIS	HB2	3.08	0.05	1
1	A	365	HIS	HB3	3.08	0.05	1
1	A	365	HIS	C	175.59	0.20	1
1	A	365	HIS	CA	56.17	0.20	1
1	A	365	HIS	CB	30.74	0.20	1
1	A	365	HIS	N	120.44	0.33	1
1	A	366	THR	H	8.12	0.02	1
1	A	366	THR	HA	4.12	0.05	1
1	A	366	THR	HB	4.02	0.05	1
1	A	366	THR	HG21	1.2	0.05	1
1	A	366	THR	HG22	1.2	0.05	1
1	A	366	THR	HG23	1.2	0.05	1
1	A	366	THR	C	172.91	0.20	1
1	A	366	THR	CA	61.36	0.20	1
1	A	366	THR	CB	70.0	0.20	1
1	A	366	THR	CG2	21.2	0.20	1
1	A	366	THR	N	114.95	0.33	1
1	A	367	MET	H	7.91	0.02	1
1	A	367	MET	HA	4.15	0.05	1
1	A	367	MET	C	175.61	0.20	1
1	A	367	MET	CA	58.74	0.20	1
1	A	367	MET	N	120.41	0.33	1
1	A	368	MET	H	8.08	0.02	1
1	A	368	MET	CA	52.83	0.20	1
1	A	368	MET	N	123.73	0.33	1
1	A	369	PRO	HA	4.38	0.05	1
1	A	369	PRO	HB2	1.89	0.05	2
1	A	369	PRO	HB3	2.19	0.05	2
1	A	369	PRO	HD2	3.65	0.05	2
1	A	369	PRO	HD3	3.77	0.05	2
1	A	369	PRO	HG2	1.92	0.05	1
1	A	369	PRO	HG3	1.92	0.05	1
1	A	369	PRO	CA	63.04	0.20	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	369	PRO	CB	32.15	0.20	1
1	A	369	PRO	CD	50.57	0.20	1
1	A	369	PRO	CG	26.98	0.20	1
1	A	370	SER	H	7.98	0.02	1
1	A	370	SER	HA	4.39	0.05	1
1	A	370	SER	CA	55.28	0.20	1
1	A	370	SER	CB	65.53	0.20	1
1	A	370	SER	N	114.78	0.33	1
1	A	371	PRO	HA	4.4	0.05	1
1	A	371	PRO	HB2	1.88	0.05	2
1	A	371	PRO	HB3	2.24	0.05	2
1	A	371	PRO	HD2	3.64	0.05	2
1	A	371	PRO	HD3	3.7	0.05	2
1	A	371	PRO	HG2	1.98	0.05	1
1	A	371	PRO	HG3	1.98	0.05	1
1	A	371	PRO	C	177.97	0.20	1
1	A	371	PRO	CA	62.94	0.20	1
1	A	371	PRO	CB	32.2	0.20	1
1	A	371	PRO	CD	50.69	0.20	1
1	A	371	PRO	CG	26.92	0.20	1
1	A	460	PRO	HA	4.77	0.05	9
1	A	460	PRO	HB2	1.99	0.05	9
1	A	460	PRO	HB3	2.25	0.05	9
1	A	460	PRO	HD2	3.69	0.05	9
1	A	460	PRO	HD3	3.69	0.05	9
1	A	460	PRO	HG2	1.95	0.05	9
1	A	460	PRO	HG3	1.95	0.05	9
1	A	460	PRO	C	176.93	0.20	9
1	A	460	PRO	CA	63.55	0.20	9
1	A	460	PRO	CB	32.2	0.20	9
1	A	460	PRO	CD	50.49	0.20	9
1	A	460	PRO	CG	27.03	0.20	9
1	A	461	SER	H	8.43	0.02	9
1	A	461	SER	HA	4.43	0.05	9
1	A	461	SER	HB2	3.87	0.05	9
1	A	461	SER	HB3	3.87	0.05	9
1	A	461	SER	C	174.26	0.20	9
1	A	461	SER	CA	58.21	0.20	9
1	A	461	SER	CB	63.24	0.20	9
1	A	461	SER	N	115.43	0.33	9
1	A	462	ALA	H	8.27	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	462	ALA	HA	4.16	0.05	1
1	A	462	ALA	HB1	1.38	0.05	1
1	A	462	ALA	HB2	1.38	0.05	1
1	A	462	ALA	HB3	1.38	0.05	1
1	A	462	ALA	C	173.63	0.20	1
1	A	462	ALA	CA	52.38	0.20	1
1	A	462	ALA	CB	19.8	0.20	1
1	A	462	ALA	N	126.03	0.33	1
1	A	463	VAL	H	8.09	0.02	1
1	A	463	VAL	HA	4.1	0.05	1
1	A	463	VAL	HB	2.06	0.05	1
1	A	463	VAL	HG11	0.93	0.05	1
1	A	463	VAL	HG12	0.93	0.05	1
1	A	463	VAL	HG13	0.93	0.05	1
1	A	463	VAL	HG21	0.88	0.05	1
1	A	463	VAL	HG22	0.88	0.05	1
1	A	463	VAL	HG23	0.88	0.05	1
1	A	463	VAL	C	176.35	0.20	1
1	A	463	VAL	CA	62.06	0.20	1
1	A	463	VAL	CB	32.9	0.20	1
1	A	463	VAL	CG1	20.35	0.20	1
1	A	463	VAL	CG2	20.35	0.20	1
1	A	463	VAL	N	119.28	0.33	1
1	A	464	THR	H	8.27	0.02	1
1	A	464	THR	HA	4.33	0.05	1
1	A	464	THR	HB	4.11	0.05	1
1	A	464	THR	HG21	1.18	0.05	1
1	A	464	THR	HG22	1.18	0.05	1
1	A	464	THR	HG23	1.18	0.05	1
1	A	464	THR	C	174.07	0.20	1
1	A	464	THR	CA	61.75	0.20	1
1	A	464	THR	CB	69.65	0.20	1
1	A	464	THR	N	118.96	0.33	1
1	A	465	VAL	H	8.19	0.02	1
1	A	465	VAL	HA	4.43	0.05	1
1	A	465	VAL	HB	2.09	0.05	1
1	A	465	VAL	HG11	0.91	0.05	1
1	A	465	VAL	HG12	0.91	0.05	1
1	A	465	VAL	HG13	0.91	0.05	1
1	A	465	VAL	HG21	0.91	0.05	1
1	A	465	VAL	HG22	0.91	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	465	VAL	HG23	0.91	0.05	1
1	A	465	VAL	CA	59.8	0.20	1
1	A	465	VAL	N	124.42	0.33	1
1	A	466	PRO	HA	4.42	0.05	1
1	A	466	PRO	HB2	2.0	0.05	2
1	A	466	PRO	HB3	2.46	0.05	2
1	A	466	PRO	HD2	3.5	0.05	1
1	A	466	PRO	HD3	3.5	0.05	1
1	A	466	PRO	HG2	1.89	0.05	1
1	A	466	PRO	HG3	1.89	0.05	1
1	A	466	PRO	C	175.45	0.20	1
1	A	466	PRO	CA	62.73	0.20	1
1	A	466	PRO	CB	33.46	0.20	1
1	A	466	PRO	CD	50.34	0.20	1
1	A	466	PRO	CG	25.43	0.20	1
1	A	467	LEU	H	9.35	0.02	1
1	A	467	LEU	HA	4.42	0.05	1
1	A	467	LEU	HB2	1.65	0.05	2
1	A	467	LEU	HB3	1.78	0.05	2
1	A	467	LEU	HD11	1.02	0.05	1
1	A	467	LEU	HD12	1.02	0.05	1
1	A	467	LEU	HD13	1.02	0.05	1
1	A	467	LEU	HD21	0.94	0.05	1
1	A	467	LEU	HD22	0.94	0.05	1
1	A	467	LEU	HD23	0.94	0.05	1
1	A	467	LEU	C	176.95	0.20	1
1	A	467	LEU	CA	55.9	0.20	1
1	A	467	LEU	CB	42.27	0.20	1
1	A	467	LEU	CD1	24.58	0.20	1
1	A	467	LEU	CD2	23.61	0.20	1
1	A	467	LEU	CG	26.92	0.20	1
1	A	467	LEU	N	127.64	0.33	1
1	A	468	THR	H	7.64	0.02	1
1	A	468	THR	HA	4.13	0.05	1
1	A	468	THR	CA	62.75	0.20	1
1	A	468	THR	N	119.28	0.33	1

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	105	$0.42 \pm 0.32$	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	93	$0.28 \pm 0.20$	None needed (< 0.5 ppm)
$^{13}\text{C}'$	91	$-0.03 \pm 0.20$	None needed (< 0.5 ppm)
$^{15}\text{N}$	78	$0.57 \pm 0.74$	None needed (imprecise)

### 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 88%, i.e. 793 atoms were assigned a chemical shift out of a possible 904. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	340/360 (94%)	137/143 (96%)	145/156 (93%)	58/61 (95%)
Sidechain	441/504 (88%)	288/326 (88%)	145/165 (88%)	8/13 (62%)
Aromatic	12/40 (30%)	12/20 (60%)	0/20 (0%)	0/0 (—%)
Overall	793/904 (88%)	437/489 (89%)	290/341 (85%)	66/74 (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	401	ARG	NE	127.48	76.53 – 92.65	26.6
1	A	410	ARG	NE	124.58	76.53 – 92.65	24.8

### 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	1745
Intra-residue ( $ i-j =0$ )	388
Sequential ( $ i-j =1$ )	504
Medium range ( $ i-j >1$ and $ i-j <5$ )	469
Long range ( $ i-j \geq 5$ )	348
Inter-chain	0
Hydrogen bond restraints	36
Disulfide bond restraints	0
Total dihedral-angle restraints	134
Number of unmapped restraints	0
Number of restraints per residue	15.7
Number of long range restraints per residue <sup>1</sup>	3.0

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

### 8.2 Residual restraint violations

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)	37.1	0.2
0.2-0.5 (Medium)	29.9	0.5
>0.5 (Large)	23.5	1.68

### 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)	5.6	4.59
10.0-20.0 (Medium)	None	None
>20.0 (Large)	1.0	121.08

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

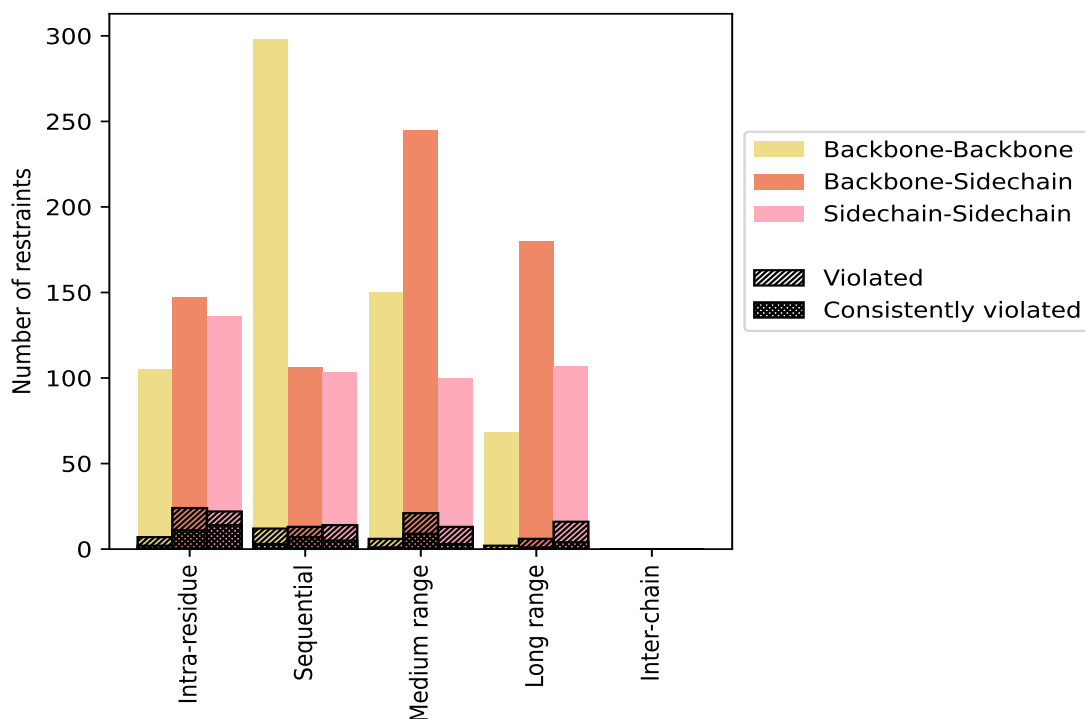
### 9.1 Summary of distance violations [i](#)

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>388</b>	<b>22.2</b>	<b>53</b>	<b>13.7</b>	<b>3.0</b>	<b>27</b>	<b>7.0</b>	<b>1.5</b>
Backbone-Backbone	105	6.0	7	6.7	0.4	2	1.9	0.1
Backbone-Sidechain	147	8.4	24	16.3	1.4	11	7.5	0.6
Sidechain-Sidechain	136	7.8	22	16.2	1.3	14	10.3	0.8
<b>Sequential (<math> i-j =1</math>)</b>	<b>504</b>	<b>28.9</b>	<b>38</b>	<b>7.5</b>	<b>2.2</b>	<b>15</b>	<b>3.0</b>	<b>0.9</b>
Backbone-Backbone	298	17.1	12	4.0	0.7	3	1.0	0.2
Backbone-Sidechain	106	6.1	13	12.3	0.7	7	6.6	0.4
Sidechain-Sidechain	100	5.7	13	13.0	0.7	5	5.0	0.3
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>469</b>	<b>26.9</b>	<b>35</b>	<b>7.5</b>	<b>2.0</b>	<b>12</b>	<b>2.6</b>	<b>0.7</b>
Backbone-Backbone	150	8.6	6	4.0	0.3	1	0.7	0.1
Backbone-Sidechain	219	12.6	16	7.3	0.9	8	3.7	0.5
Sidechain-Sidechain	100	5.7	13	13.0	0.7	3	3.0	0.2
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>348</b>	<b>19.9</b>	<b>24</b>	<b>6.9</b>	<b>1.4</b>	<b>5</b>	<b>1.4</b>	<b>0.3</b>
Backbone-Backbone	68	3.9	2	2.9	0.1	0	0.0	0.0
Backbone-Sidechain	174	10.0	6	3.4	0.3	1	0.6	0.1
Sidechain-Sidechain	106	6.1	16	15.1	0.9	4	3.8	0.2
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>36</b>	<b>2.1</b>	<b>6</b>	<b>16.7</b>	<b>0.3</b>	<b>1</b>	<b>2.8</b>	<b>0.1</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1745</b>	<b>100.0</b>	<b>156</b>	<b>8.9</b>	<b>8.9</b>	<b>60</b>	<b>3.4</b>	<b>3.4</b>
Backbone-Backbone	621	35.6	27	4.3	1.5	6	1.0	0.3
Backbone-Sidechain	678	38.9	64	9.4	3.7	28	4.1	1.6
Sidechain-Sidechain	446	25.6	65	14.6	3.7	26	5.8	1.5

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

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



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

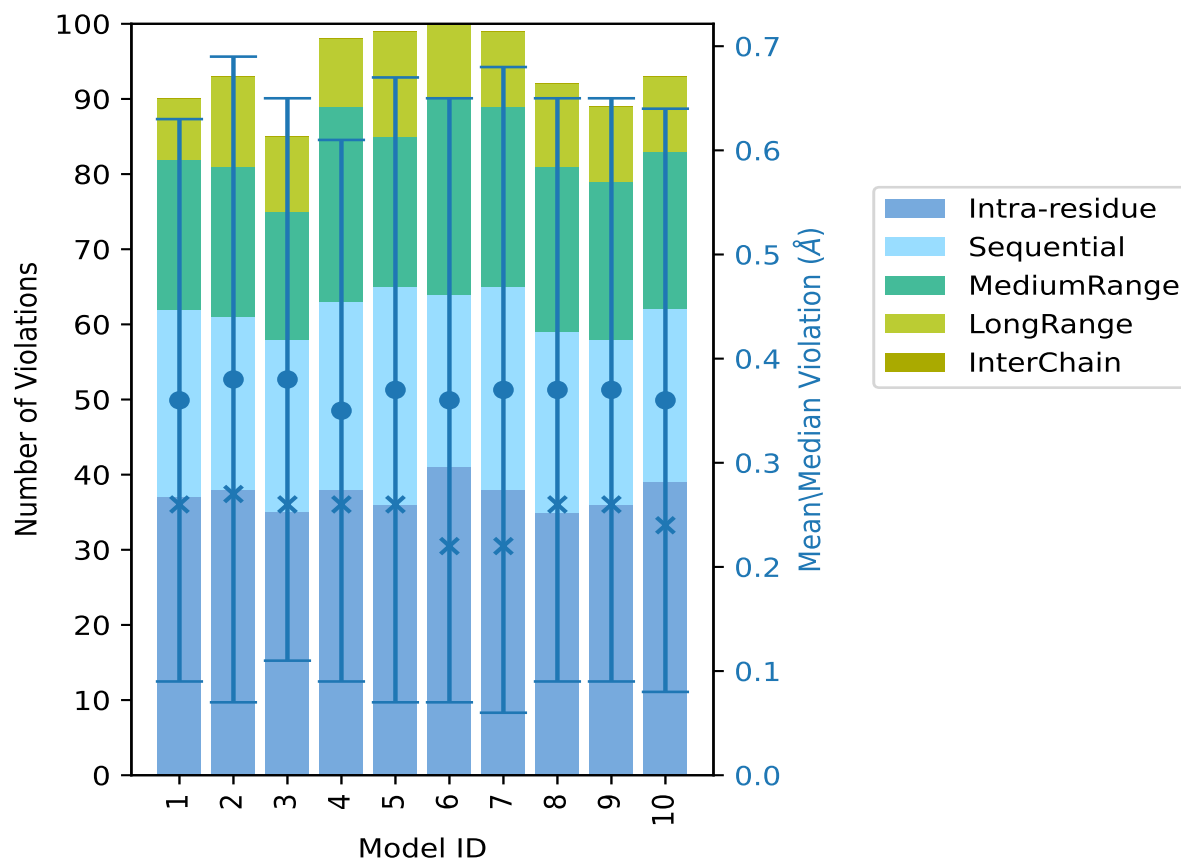
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	37	25	20	8	0	90	0.36	0.99	0.27	0.26
2	38	23	20	12	0	93	0.38	1.56	0.31	0.27
3	35	23	17	10	0	85	0.38	1.29	0.27	0.26
4	38	25	26	9	0	98	0.35	1.14	0.26	0.26
5	36	29	20	14	0	99	0.37	1.64	0.3	0.26
6	41	23	26	10	0	100	0.36	1.68	0.29	0.22
7	38	27	24	10	0	99	0.37	1.58	0.31	0.22
8	35	24	22	11	0	92	0.37	1.22	0.28	0.26
9	36	22	21	10	0	89	0.37	1.47	0.28	0.26
10	39	23	21	10	0	93	0.36	1.54	0.28	0.24

<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, 1559(IR:335, SQ:466, MR:434, LR:324, 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>	%
10	8	11	9	0	38	1	10.0
0	4	4	5	0	13	2	20.0
2	2	2	0	0	6	3	30.0

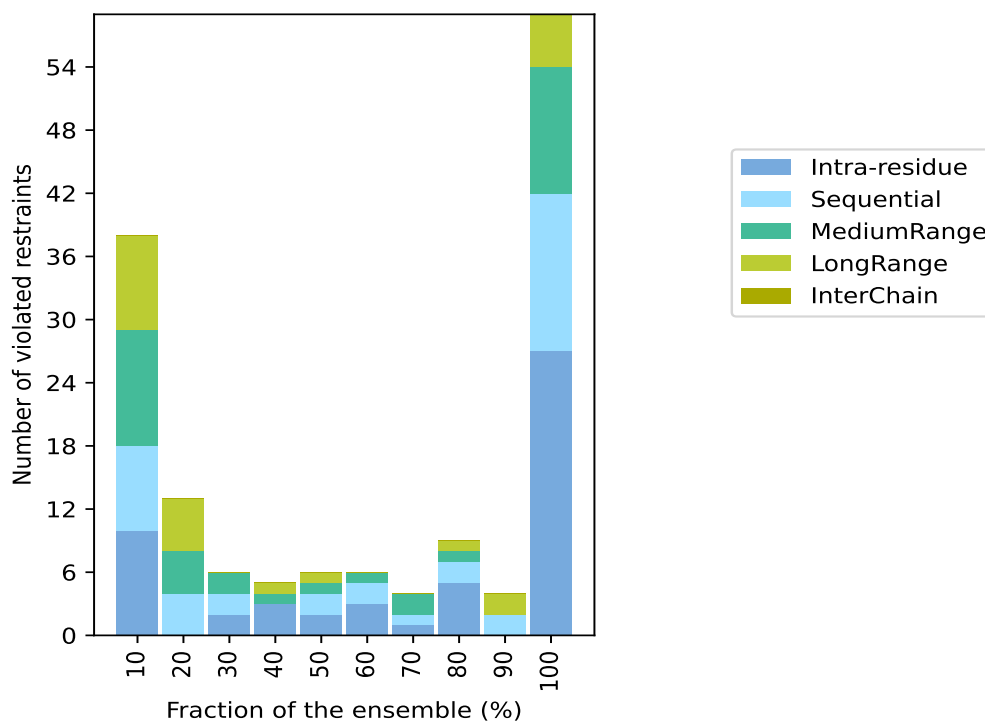
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
3	0	1	1	0	5	4	40.0
2	2	1	1	0	6	5	50.0
3	2	1	0	0	6	6	60.0
1	1	2	0	0	4	7	70.0
5	2	1	1	0	9	8	80.0
0	2	0	2	0	4	9	90.0
27	15	12	5	0	59	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

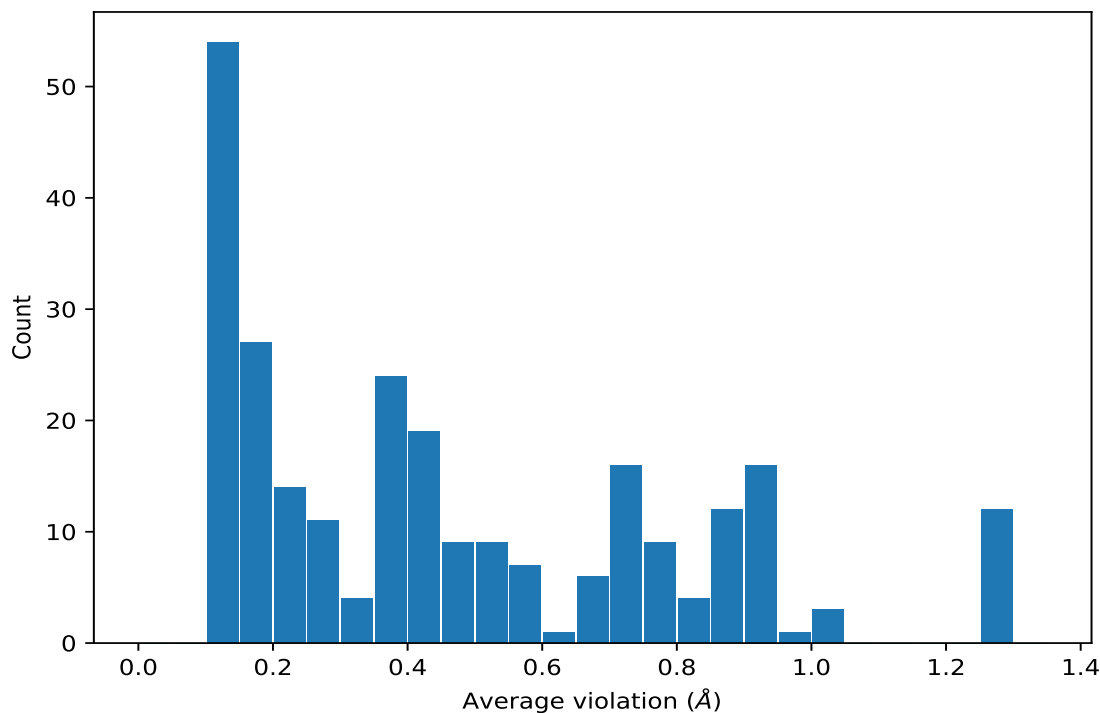


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1012)	1:388:A:PRO:HD2	1:389:A:ILE:HD11	10	1.0	0.04	1.0
(1,1012)	1:388:A:PRO:HD2	1:389:A:ILE:HD12	10	1.0	0.04	1.0
(1,1012)	1:388:A:PRO:HD2	1:389:A:ILE:HD13	10	1.0	0.04	1.0
(1,1694)	1:455:A:LEU:HD11	1:455:A:LEU:HD21	10	0.94	0.01	0.94
(1,1694)	1:455:A:LEU:HD11	1:455:A:LEU:HD22	10	0.94	0.01	0.94
(1,1694)	1:455:A:LEU:HD11	1:455:A:LEU:HD23	10	0.94	0.01	0.94
(1,1694)	1:455:A:LEU:HD12	1:455:A:LEU:HD21	10	0.94	0.01	0.94
(1,1694)	1:455:A:LEU:HD12	1:455:A:LEU:HD22	10	0.94	0.01	0.94
(1,1694)	1:455:A:LEU:HD12	1:455:A:LEU:HD23	10	0.94	0.01	0.94
(1,1694)	1:455:A:LEU:HD13	1:455:A:LEU:HD21	10	0.94	0.01	0.94
(1,1694)	1:455:A:LEU:HD13	1:455:A:LEU:HD22	10	0.94	0.01	0.94
(1,1694)	1:455:A:LEU:HD13	1:455:A:LEU:HD23	10	0.94	0.01	0.94
(1,1508)	1:421:A:ASN:H	1:422:A:ILE:HG21	10	0.93	0.01	0.93
(1,1508)	1:421:A:ASN:H	1:422:A:ILE:HG22	10	0.93	0.01	0.93
(1,1508)	1:421:A:ASN:H	1:422:A:ILE:HG23	10	0.93	0.01	0.93

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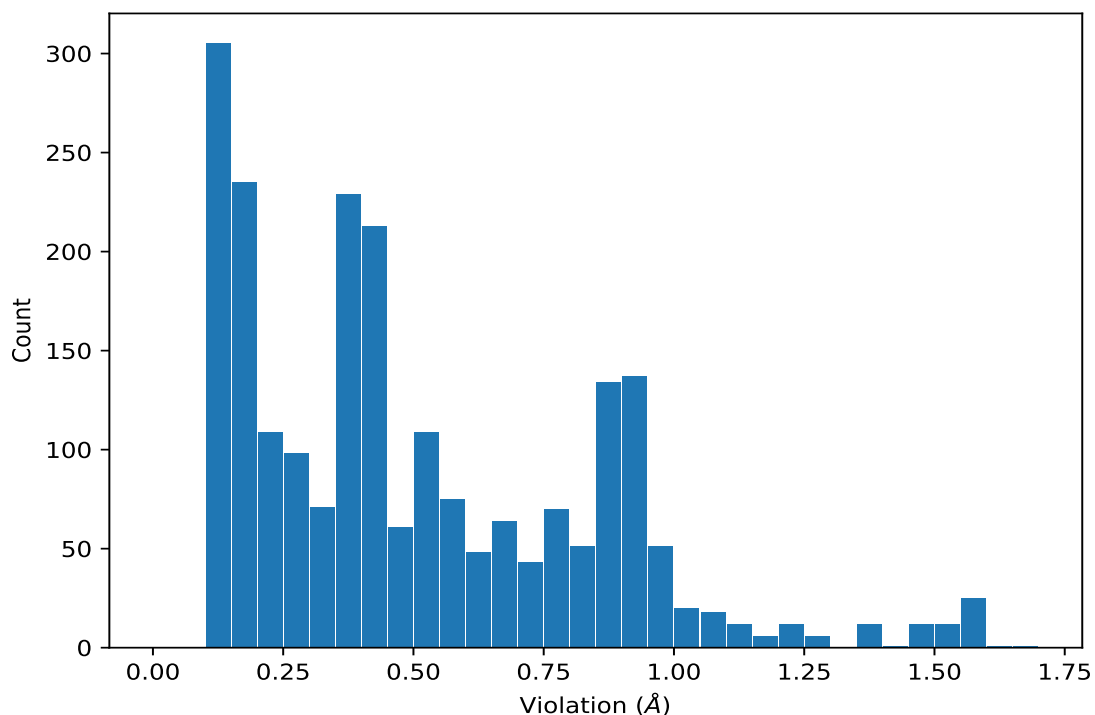
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1250)	1:406:A:THR:H	1:407:A:ALA:HB1	10	0.92	0.01	0.92
(1,1250)	1:406:A:THR:H	1:407:A:ALA:HB2	10	0.92	0.01	0.92
(1,1250)	1:406:A:THR:H	1:407:A:ALA:HB3	10	0.92	0.01	0.92
(1,79)	1:423:A:GLY:HA2	1:424:A:CYS:H	10	0.9	0.16	0.93
(1,1279)	1:407:A:ALA:HB1	1:409:A:GLY:H	10	0.89	0.01	0.89
(1,1279)	1:407:A:ALA:HB2	1:409:A:GLY:H	10	0.89	0.01	0.89
(1,1279)	1:407:A:ALA:HB3	1:409:A:GLY:H	10	0.89	0.01	0.89
(1,1536)	1:422:A:ILE:HG21	1:422:A:ILE:HD11	10	0.86	0.0	0.86
(1,1536)	1:422:A:ILE:HG21	1:422:A:ILE:HD12	10	0.86	0.0	0.86
(1,1536)	1:422:A:ILE:HG21	1:422:A:ILE:HD13	10	0.86	0.0	0.86
(1,1536)	1:422:A:ILE:HG22	1:422:A:ILE:HD11	10	0.86	0.0	0.86
(1,1536)	1:422:A:ILE:HG22	1:422:A:ILE:HD12	10	0.86	0.0	0.86
(1,1536)	1:422:A:ILE:HG22	1:422:A:ILE:HD13	10	0.86	0.0	0.86
(1,1536)	1:422:A:ILE:HG23	1:422:A:ILE:HD11	10	0.86	0.0	0.86
(1,1536)	1:422:A:ILE:HG23	1:422:A:ILE:HD12	10	0.86	0.0	0.86
(1,1536)	1:422:A:ILE:HG23	1:422:A:ILE:HD13	10	0.86	0.0	0.86
(1,975)	1:382:A:GLU:HB3	1:383:A:VAL:HG11	10	0.84	0.01	0.84
(1,975)	1:382:A:GLU:HB3	1:383:A:VAL:HG12	10	0.84	0.01	0.84
(1,975)	1:382:A:GLU:HB3	1:383:A:VAL:HG13	10	0.84	0.01	0.84
(1,1294)	1:408:A:VAL:HG11	1:427:A:CYS:HB2	10	0.78	0.05	0.8
(1,1294)	1:408:A:VAL:HG12	1:427:A:CYS:HB2	10	0.78	0.05	0.8
(1,1294)	1:408:A:VAL:HG13	1:427:A:CYS:HB2	10	0.78	0.05	0.8
(1,1278)	1:407:A:ALA:HB1	1:408:A:VAL:H	10	0.77	0.01	0.77

<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)
(1,920)	1:372:A:GLU:H	1:372:A:GLU:HG3	6	1.68
(1,921)	1:372:A:GLU:H	1:372:A:GLU:HG2	5	1.64
(1,920)	1:372:A:GLU:H	1:372:A:GLU:HG3	7	1.58
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD11	7	1.57
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD12	7	1.57
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD13	7	1.57
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD21	7	1.57
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD22	7	1.57
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD23	7	1.57
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD11	7	1.57
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD12	7	1.57
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD13	7	1.57
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD21	7	1.57
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD22	7	1.57
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD23	7	1.57
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD11	2	1.56
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD12	2	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD13	2	1.56
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD21	2	1.56
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD22	2	1.56
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD23	2	1.56
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD11	2	1.56
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD12	2	1.56
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD13	2	1.56
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD21	2	1.56
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD22	2	1.56
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD23	2	1.56
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD11	10	1.54
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD12	10	1.54
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD13	10	1.54
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD21	10	1.54
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD22	10	1.54
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD23	10	1.54
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD11	10	1.54
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD12	10	1.54
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD13	10	1.54
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD21	10	1.54
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD22	10	1.54
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD23	10	1.54
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD11	9	1.47
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD12	9	1.47
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD13	9	1.47
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD21	9	1.47
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD22	9	1.47
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD23	9	1.47
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD11	9	1.47
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD12	9	1.47
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD13	9	1.47
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD21	9	1.47
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD22	9	1.47
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD23	9	1.47
(1,921)	1:372:A:GLU:H	1:372:A:GLU:HG2	2	1.43
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD11	5	1.36
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD12	5	1.36
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD13	5	1.36
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD21	5	1.36
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD22	5	1.36
(1,1042)	1:393:A:PHE:HD1	1:394:A:LEU:HD23	5	1.36
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD11	5	1.36

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<b>Key</b>	<b>Atom-1</b>	<b>Atom-2</b>	<b>Model ID</b>	<b>Violation (Å)</b>
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD12	5	1.36
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD13	5	1.36
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD21	5	1.36
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD22	5	1.36
(1,1042)	1:393:A:PHE:HD2	1:394:A:LEU:HD23	5	1.36
(1,1696)	1:455:A:LEU:HD11	1:456:A:PRO:HD3	3	1.29

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

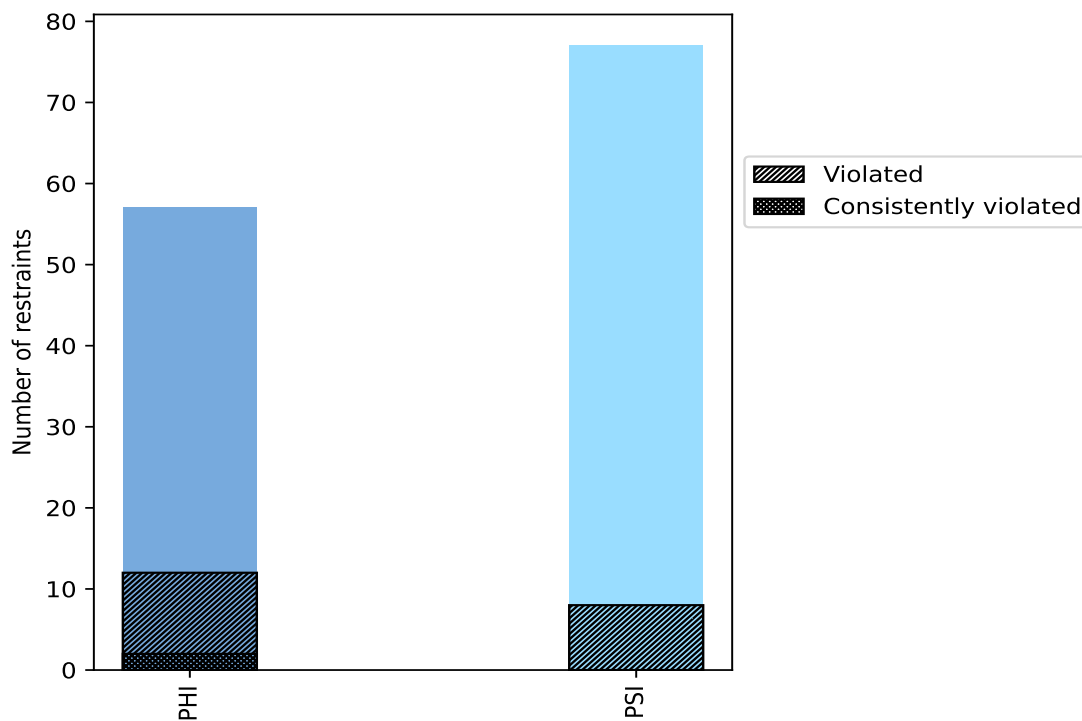
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	57	42.5	12	21.1	9.0	2	3.5	1.5
PSI	77	57.5	8	10.4	6.0	0	0.0	0.0
Total	134	100.0	20	14.9	14.9	2	1.5	1.5

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

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



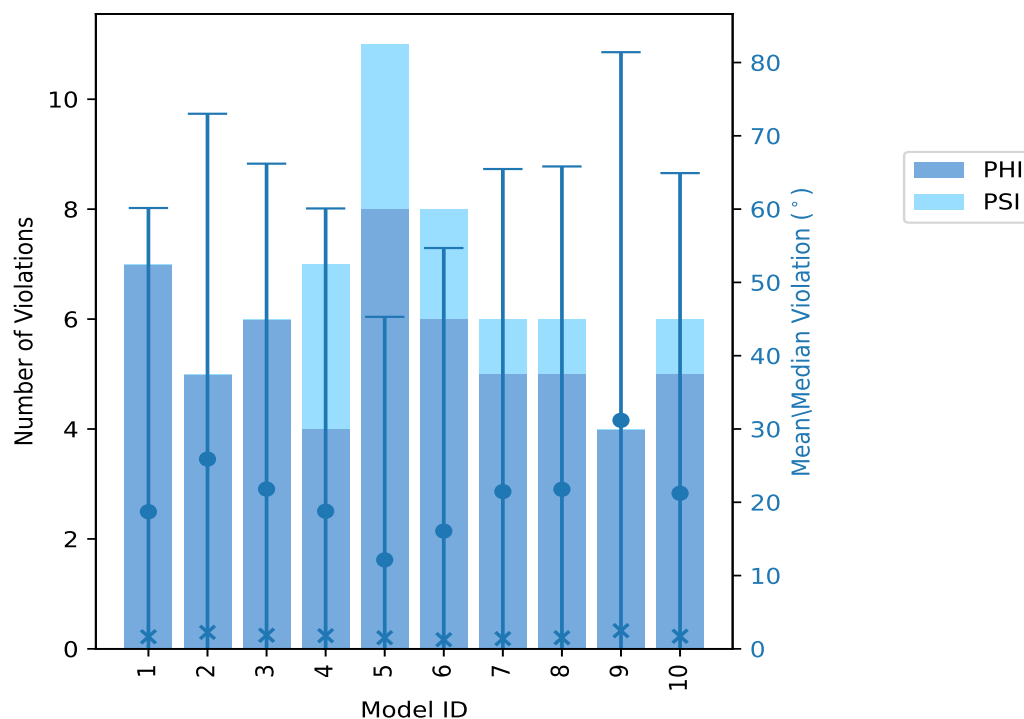
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	7	0	7	18.71	120.2	41.44	1.65
2	5	0	5	25.89	120.1	47.12	2.25
3	6	0	6	21.8	121.08	44.4	1.86
4	4	3	7	18.78	119.97	41.31	1.8
5	8	3	11	12.14	116.99	33.16	1.52
6	6	2	8	16.07	118.23	38.62	1.25
7	5	1	6	21.46	119.84	44.01	1.39
8	5	1	6	21.77	120.23	44.05	1.52
9	4	0	4	31.18	118.17	50.23	2.48
10	5	1	6	21.23	118.88	43.68	1.72

### 10.2.1 Bar graph : Dihedral violation statistics for each model [\(i\)](#)



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

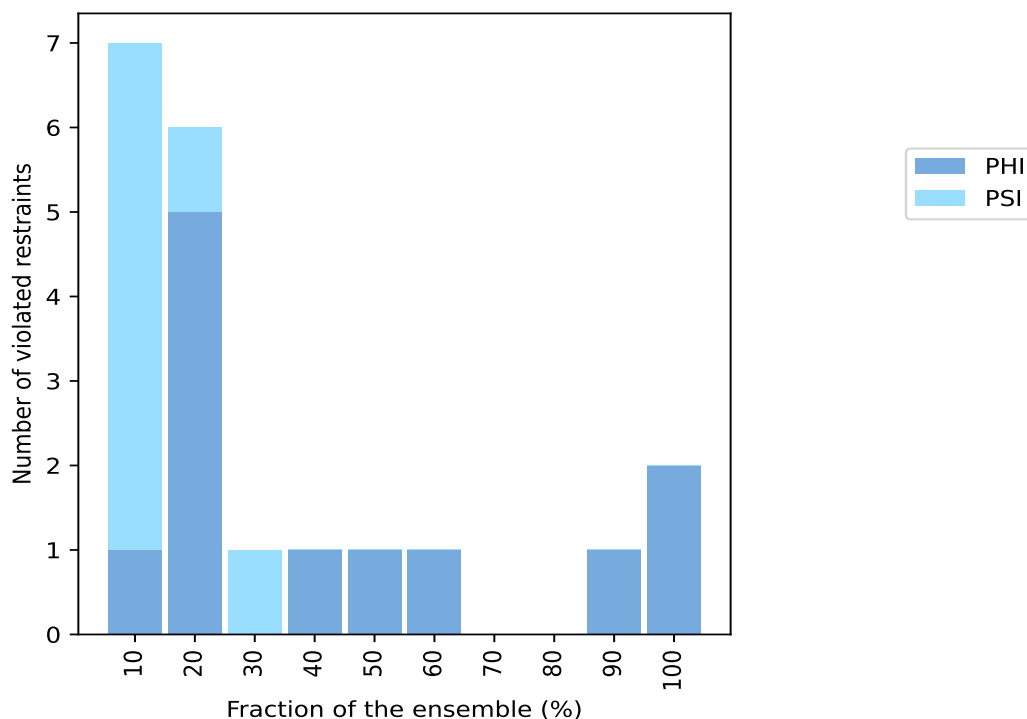
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
1	6	7	1	10.0
5	1	6	2	20.0
0	1	1	3	30.0
1	0	1	4	40.0
1	0	1	5	50.0
1	0	1	6	60.0
0	0	0	7	70.0
0	0	0	8	80.0
1	0	1	9	90.0
2	0	2	10	100.0

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

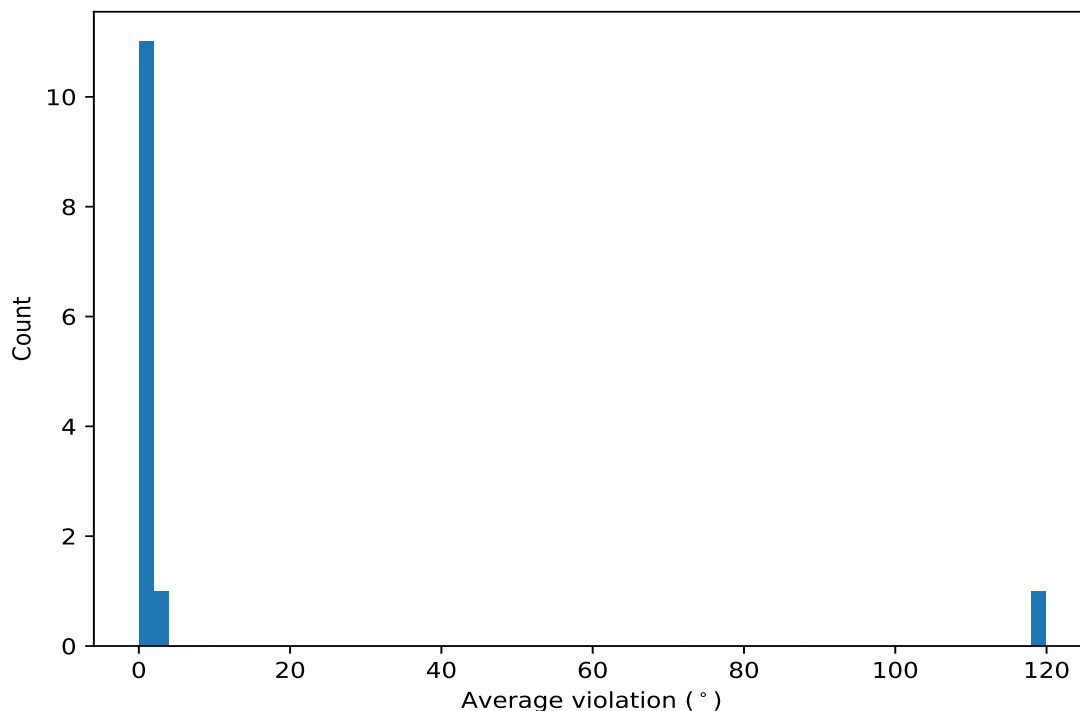
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

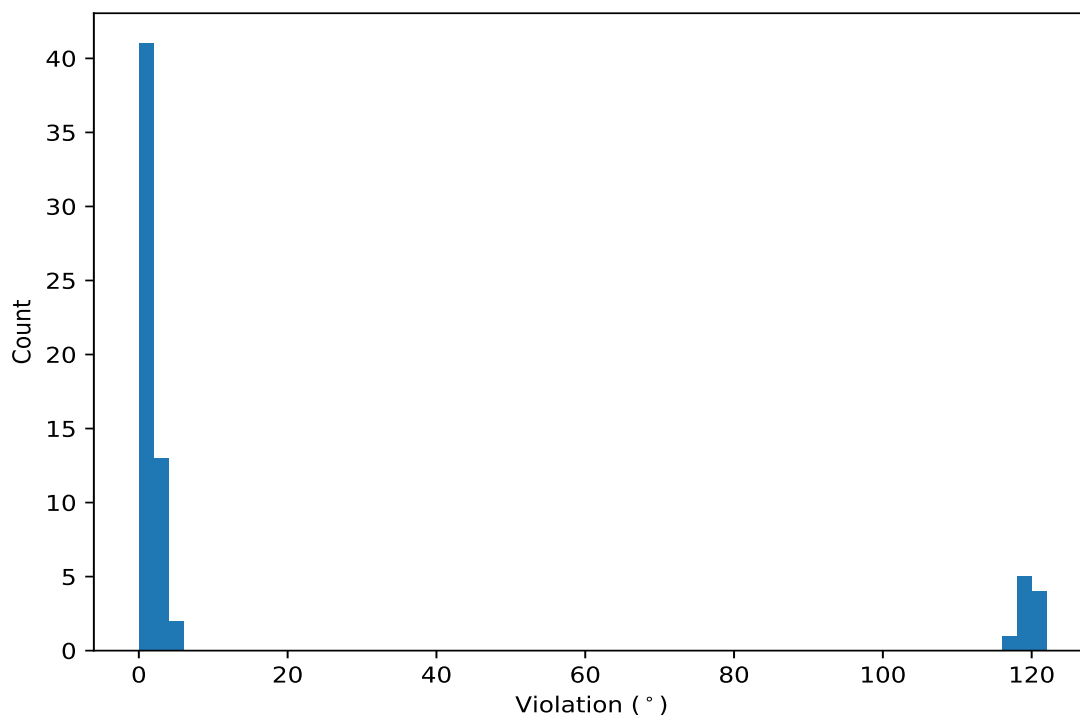
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	10	119.37	1.19	119.9
(1,49)	1:445:A:GLY:C	1:446:A:SER:N	1:446:A:SER:CA	1:446:A:SER:C	10	3.28	0.8	3.15
(1,33)	1:417:A:PRO:C	1:418:A:PHE:N	1:418:A:PHE:CA	1:418:A:PHE:C	9	1.54	0.26	1.5
(1,45)	1:437:A:PRO:C	1:438:A:MET:N	1:438:A:MET:CA	1:438:A:MET:C	6	1.54	0.32	1.46
(1,7)	1:381:A:GLY:C	1:382:A:GLU:N	1:382:A:GLU:CA	1:382:A:GLU:C	5	1.34	0.42	1.07
(1,37)	1:423:A:GLY:C	1:424:A:CYS:N	1:424:A:CYS:CA	1:424:A:CYS:C	4	1.46	0.3	1.51
(1,68)	1:384:A:ILE:N	1:384:A:ILE:CA	1:384:A:ILE:C	1:385:A:GLU:N	3	1.64	0.31	1.8
(1,54)	1:454:A:MET:C	1:455:A:LEU:N	1:455:A:LEU:CA	1:455:A:LEU:C	2	1.88	0.36	1.88
(1,4)	1:377:A:PRO:C	1:378:A:SER:N	1:378:A:SER:CA	1:378:A:SER:C	2	1.58	0.06	1.58
(1,53)	1:453:A:THR:C	1:454:A:MET:N	1:454:A:MET:CA	1:454:A:MET:C	2	1.38	0.27	1.38

<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 (°)
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	3	121.08
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	8	120.23
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	1	120.2
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	2	120.1
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	4	119.97
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	7	119.84
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	10	118.88
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	6	118.23
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	9	118.17
(1,133)	1:404:A:ASP:C	1:405:A:CYS:N	1:405:A:CYS:CA	1:405:A:CYS:C	5	116.99