



# wwPDB NMR Structure Validation Summary Report ⓘ

Jun 6, 2023 – 06:46 pm BST

PDB ID : 7AFQ  
BMRB ID : 34561  
Title : Ribosome binding factor A (RbfA)  
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Deposited on : 2020-09-19

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<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 : 4.02b-467  
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

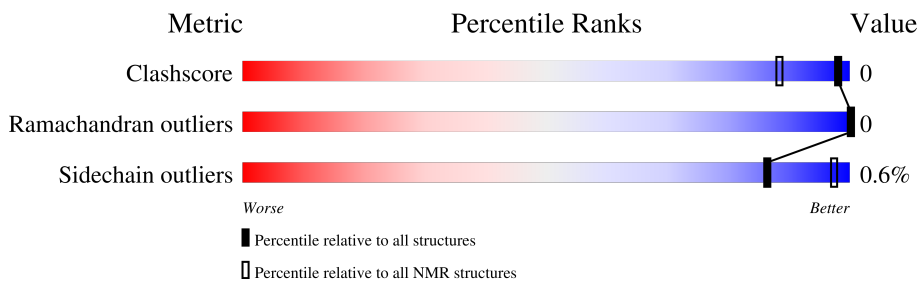
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 80%.

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	V	133	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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	V:9-V:100 (92)	0.53	3

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

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

There is only 1 type of molecule in this entry. The entry contains 1509 atoms, of which 770 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome-binding factor A.

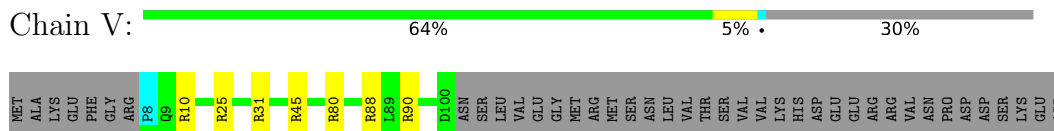
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	V	93	1509	471	770	127	136	5	0

## 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.

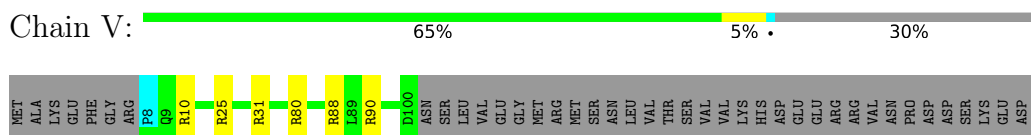
- Molecule 1: Ribosome-binding factor A



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

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: Ribosome-binding factor A



## 5 Refinement protocol and experimental data overview

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

Of the 60 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
X-PLOR NIH	structure calculation	
GROMACS	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	1472
Number of shifts mapped to atoms	1060
Number of unparsed shifts	0
Number of shifts with mapping errors	412
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

## 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	V	0.73±0.01	0±0/740 ( 0.0± 0.0%)	1.07±0.04	6±1/991 ( 0.6± 0.1%)
All	All	0.73	0/14800 ( 0.0%)	1.07	113/19820 ( 0.6%)

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	V	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

5 of 13 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	V	10	ARG	NE-CZ-NH2	10.56	125.58	120.30	4	13
1	V	90	ARG	NE-CZ-NH2	9.13	124.86	120.30	13	16
1	V	88	ARG	NE-CZ-NH2	8.98	124.79	120.30	6	15
1	V	80	ARG	NE-CZ-NH2	8.59	124.59	120.30	1	20
1	V	45	ARG	NE-CZ-NH2	8.54	124.57	120.30	6	15

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	V	80	ARG	Sidechain	1
1	V	49	TYR	Sidechain	1

## 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	V	732	763	763	0±1
All	All	14640	15260	15260	8

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 0.

5 of 8 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:V:27:ILE:HD11	1:V:79:ILE:HD11	0.79	1.55	18	1
1:V:27:ILE:CD1	1:V:79:ILE:HD11	0.64	2.22	18	1
1:V:23:LEU:O	1:V:27:ILE:CG1	0.57	2.53	6	1
1:V:35:MET:HB3	1:V:57:LEU:HB2	0.46	1.87	14	1
1:V:91:ILE:O	1:V:91:ILE:HG23	0.44	2.12	12	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	V	91/133 (68%)	88±1 (97±1%)	3±1 (3±1%)	0±0 (0±0%)	100	100
All	All	1820/2660 (68%)	1768 (97%)	52 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	V	78/116 (67%)	78±0 (99±1%)	0±0 (1±1%)	86	97
All	All	1560/2320 (67%)	1551 (99%)	9 (1%)	86	97

5 of 6 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	V	58	ASN	4
1	V	46	ASP	1
1	V	16	GLN	1
1	V	99	TYR	1
1	V	91	ILE	1

### 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](#)

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 [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 80% for the well-defined parts and 80% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts\_1*

#### 7.1.1 Bookkeeping i

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1472
Number of shifts mapped to atoms	1060
Number of unparsed shifts	0
Number of shifts with mapping errors	412
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. First 5 (of 412) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	6	GLY	HA2	3.94	0.02	1
1	V	6	GLY	HA3	3.79	0.02	1
1	V	6	GLY	CA	44.9	0.3	1
1	V	101	ASN	H	7.92	0.02	1
1	V	101	ASN	HA	4.45	0.02	1
1	V	101	ASN	HB2	2.74	0.02	1
1	V	101	ASN	HB3	2.64	0.02	1
1	V	101	ASN	C	176.0	0.3	1
1	V	101	ASN	CA	52.8	0.3	1
1	V	101	ASN	CB	38.7	0.3	1
1	V	101	ASN	N	122.9	0.3	1
1	V	102	SER	H	8.23	0.02	1
1	V	102	SER	HA	4.04	0.02	1
1	V	102	SER	HB2	3.69	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	102	SER	HB3	3.69	0.02	1
1	V	102	SER	C	174.1	0.3	1
1	V	102	SER	CA	60.2	0.3	1
1	V	102	SER	CB	63.3	0.3	1
1	V	102	SER	N	115.8	0.3	1
1	V	103	LEU	H	7.91	0.02	1
1	V	103	LEU	HA	4.17	0.02	1
1	V	103	LEU	HB2	1.5	0.02	1
1	V	103	LEU	HB3	1.43	0.02	1
1	V	103	LEU	HG	1.48	0.02	1
1	V	103	LEU	HD11	0.72	0.02	1
1	V	103	LEU	HD12	0.72	0.02	1
1	V	103	LEU	HD13	0.72	0.02	1
1	V	103	LEU	HD21	0.67	0.02	1
1	V	103	LEU	HD22	0.67	0.02	1
1	V	103	LEU	HD23	0.67	0.02	1
1	V	103	LEU	C	177.7	0.3	1
1	V	103	LEU	CA	55.7	0.3	1
1	V	103	LEU	CB	41.9	0.3	1
1	V	103	LEU	CG	26.9	0.3	1
1	V	103	LEU	CD1	24.8	0.3	1
1	V	103	LEU	CD2	23.5	0.3	1
1	V	103	LEU	N	122.9	0.3	1
1	V	104	VAL	H	7.73	0.02	1
1	V	104	VAL	HA	3.88	0.02	1
1	V	104	VAL	HB	1.94	0.02	1
1	V	104	VAL	HG11	0.81	0.02	1
1	V	104	VAL	HG12	0.81	0.02	1
1	V	104	VAL	HG13	0.81	0.02	1
1	V	104	VAL	C	176.7	0.3	1
1	V	104	VAL	CA	63.0	0.3	1
1	V	104	VAL	CB	32.5	0.3	1
1	V	104	VAL	CG1	21.0	0.3	1
1	V	104	VAL	CG2	21.0	0.3	1
1	V	104	VAL	N	120.0	0.3	1
1	V	105	GLU	H	8.36	0.02	1
1	V	105	GLU	HA	4.01	0.02	1
1	V	105	GLU	HB2	1.89	0.02	1
1	V	105	GLU	HB3	1.82	0.02	1
1	V	105	GLU	HG2	2.12	0.02	1
1	V	105	GLU	HG3	2.12	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	105	GLU	C	177.4	0.3	1
1	V	105	GLU	CA	57.4	0.3	1
1	V	105	GLU	CB	29.6	0.3	1
1	V	105	GLU	CG	36.2	0.3	1
1	V	105	GLU	N	123.5	0.3	1
1	V	106	GLY	H	8.22	0.02	1
1	V	106	GLY	HA2	3.83	0.02	1
1	V	106	GLY	HA3	3.75	0.02	1
1	V	106	GLY	C	174.5	0.3	1
1	V	106	GLY	CA	45.5	0.3	1
1	V	106	GLY	N	108.7	0.3	1
1	V	107	MET	H	7.91	0.02	1
1	V	107	MET	HA	4.29	0.02	1
1	V	107	MET	HB2	1.93	0.02	1
1	V	107	MET	HB3	1.93	0.02	1
1	V	107	MET	HG2	2.45	0.02	1
1	V	107	MET	HG3	2.38	0.02	1
1	V	107	MET	C	176.3	0.3	1
1	V	107	MET	CA	55.7	0.3	1
1	V	107	MET	CB	32.8	0.3	1
1	V	107	MET	CG	32.0	0.3	1
1	V	107	MET	N	119.5	0.3	1
1	V	111	ASN	HA	4.57	0.02	1
1	V	111	ASN	C	174.9	0.3	1
1	V	111	ASN	CA	53.4	0.3	1
1	V	111	ASN	CB	38.6	0.3	1
1	V	112	LEU	H	7.94	0.02	1
1	V	112	LEU	HA	4.2	0.02	1
1	V	112	LEU	HB2	1.51	0.02	1
1	V	112	LEU	HB3	1.43	0.02	1
1	V	112	LEU	HG	1.47	0.02	1
1	V	112	LEU	HD11	0.78	0.02	1
1	V	112	LEU	HD12	0.78	0.02	1
1	V	112	LEU	HD13	0.78	0.02	1
1	V	112	LEU	C	177.2	0.3	1
1	V	112	LEU	CA	55.3	0.3	1
1	V	112	LEU	CB	42.2	0.3	1
1	V	112	LEU	CG	26.9	0.3	1
1	V	112	LEU	CD1	24.7	0.3	1
1	V	112	LEU	CD2	24.7	0.3	1
1	V	112	LEU	N	121.5	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	113	VAL	H	7.98	0.02	1
1	V	113	VAL	HA	4.03	0.02	1
1	V	113	VAL	HB	1.94	0.02	1
1	V	113	VAL	HG11	0.81	0.02	1
1	V	113	VAL	HG12	0.81	0.02	1
1	V	113	VAL	HG13	0.81	0.02	1
1	V	113	VAL	HG21	0.75	0.02	1
1	V	113	VAL	HG22	0.75	0.02	1
1	V	113	VAL	HG23	0.75	0.02	1
1	V	113	VAL	C	176.2	0.3	1
1	V	113	VAL	CA	62.4	0.3	1
1	V	113	VAL	CB	32.5	0.3	1
1	V	113	VAL	CG1	20.7	0.3	1
1	V	113	VAL	CG2	21.1	0.3	1
1	V	113	VAL	N	120.9	0.3	1
1	V	114	THR	H	8.08	0.02	1
1	V	114	THR	HA	4.25	0.02	1
1	V	114	THR	HB	4.08	0.02	1
1	V	114	THR	HG21	1.05	0.02	1
1	V	114	THR	HG22	1.05	0.02	1
1	V	114	THR	HG23	1.05	0.02	1
1	V	114	THR	CA	61.6	0.3	1
1	V	114	THR	CB	69.7	0.3	1
1	V	114	THR	CG2	21.4	0.3	1
1	V	114	THR	N	117.6	0.3	1
1	V	115	SER	HA	4.36	0.02	1
1	V	115	SER	HB2	3.7	0.02	1
1	V	115	SER	HB3	3.7	0.02	1
1	V	115	SER	C	174.1	0.3	1
1	V	115	SER	CA	58.1	0.3	1
1	V	115	SER	CB	63.7	0.3	1
1	V	116	VAL	H	8.02	0.02	1
1	V	116	VAL	HA	4.0	0.02	1
1	V	116	VAL	HB	1.93	0.02	1
1	V	116	VAL	HG11	0.8	0.02	1
1	V	116	VAL	HG12	0.8	0.02	1
1	V	116	VAL	HG13	0.8	0.02	1
1	V	116	VAL	C	175.9	0.3	1
1	V	116	VAL	CA	62.3	0.3	1
1	V	116	VAL	CB	32.6	0.3	1
1	V	116	VAL	CG1	20.6	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	116	VAL	CG2	20.6	0.3	1
1	V	116	VAL	N	122.0	0.3	1
1	V	117	VAL	H	8.08	0.02	1
1	V	117	VAL	HA	3.89	0.02	1
1	V	117	VAL	HB	1.88	0.02	1
1	V	117	VAL	HG11	0.77	0.02	1
1	V	117	VAL	HG12	0.77	0.02	1
1	V	117	VAL	HG13	0.77	0.02	1
1	V	117	VAL	C	175.7	0.3	1
1	V	117	VAL	CA	62.2	0.3	1
1	V	117	VAL	CB	32.6	0.3	1
1	V	117	VAL	CG1	20.7	0.3	1
1	V	117	VAL	CG2	20.7	0.3	1
1	V	117	VAL	N	124.7	0.3	1
1	V	118	LYS	H	8.29	0.02	1
1	V	118	LYS	HA	4.18	0.02	1
1	V	118	LYS	HB2	1.63	0.02	1
1	V	118	LYS	HB3	1.56	0.02	1
1	V	118	LYS	HG2	1.27	0.02	1
1	V	118	LYS	HG3	1.21	0.02	1
1	V	118	LYS	HD2	1.52	0.02	1
1	V	118	LYS	HD3	1.52	0.02	1
1	V	118	LYS	HE2	2.84	0.02	1
1	V	118	LYS	HE3	2.83	0.02	1
1	V	118	LYS	C	176.0	0.3	1
1	V	118	LYS	CA	55.8	0.3	1
1	V	118	LYS	CB	33.0	0.3	1
1	V	118	LYS	CG	24.6	0.3	1
1	V	118	LYS	CD	29.0	0.3	1
1	V	118	LYS	CE	42.1	0.3	1
1	V	118	LYS	N	126.0	0.3	1
1	V	120	ASP	HA	4.41	0.02	1
1	V	120	ASP	C	176.2	0.3	1
1	V	120	ASP	CA	54.4	0.3	1
1	V	120	ASP	CB	40.9	0.3	1
1	V	121	GLU	H	8.29	0.02	1
1	V	121	GLU	HA	4.07	0.02	1
1	V	121	GLU	HB2	1.84	0.02	1
1	V	121	GLU	HB3	1.84	0.02	1
1	V	121	GLU	HG2	2.12	0.02	1
1	V	121	GLU	HG3	2.12	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	121	GLU	C	176.6	0.3	1
1	V	121	GLU	CA	56.7	0.3	1
1	V	121	GLU	CB	30.0	0.3	1
1	V	121	GLU	CG	36.2	0.3	1
1	V	121	GLU	N	121.2	0.3	1
1	V	122	GLU	H	8.26	0.02	1
1	V	122	GLU	HA	4.07	0.02	1
1	V	122	GLU	HB2	1.84	0.02	1
1	V	122	GLU	HB3	1.84	0.02	1
1	V	122	GLU	HG2	2.12	0.02	1
1	V	122	GLU	HG3	2.12	0.02	1
1	V	122	GLU	C	176.4	0.3	1
1	V	122	GLU	CA	56.7	0.3	1
1	V	122	GLU	CB	29.9	0.3	1
1	V	122	GLU	CG	36.2	0.3	1
1	V	122	GLU	N	121.5	0.3	1
1	V	123	ARG	H	8.13	0.02	1
1	V	123	ARG	HA	4.16	0.02	1
1	V	123	ARG	HB2	1.68	0.02	1
1	V	123	ARG	HB3	1.61	0.02	1
1	V	123	ARG	HG2	1.45	0.02	1
1	V	123	ARG	HG3	1.45	0.02	1
1	V	123	ARG	HD2	3.04	0.02	1
1	V	123	ARG	HD3	3.04	0.02	1
1	V	123	ARG	C	175.9	0.3	1
1	V	123	ARG	CA	55.9	0.3	1
1	V	123	ARG	CB	30.5	0.3	1
1	V	123	ARG	CG	26.9	0.3	1
1	V	123	ARG	CD	43.2	0.3	1
1	V	123	ARG	N	122.1	0.3	1
1	V	124	ARG	H	8.21	0.02	1
1	V	124	ARG	HA	4.21	0.02	1
1	V	124	ARG	HB2	1.68	0.02	1
1	V	124	ARG	HB3	1.61	0.02	1
1	V	124	ARG	HG2	1.45	0.02	1
1	V	124	ARG	HG3	1.45	0.02	1
1	V	124	ARG	HD2	3.04	0.02	1
1	V	124	ARG	HD3	3.04	0.02	1
1	V	124	ARG	C	176.1	0.3	1
1	V	124	ARG	CA	55.9	0.3	1
1	V	124	ARG	CB	30.6	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	124	ARG	CG	26.9	0.3	1
1	V	124	ARG	CD	43.0	0.3	1
1	V	124	ARG	N	122.8	0.3	1
1	V	125	VAL	H	8.12	0.02	1
1	V	125	VAL	HA	3.93	0.02	1
1	V	125	VAL	HB	1.86	0.02	1
1	V	125	VAL	HG11	0.76	0.02	1
1	V	125	VAL	HG12	0.76	0.02	1
1	V	125	VAL	HG13	0.76	0.02	1
1	V	125	VAL	HG21	0.76	0.02	1
1	V	125	VAL	HG22	0.76	0.02	1
1	V	125	VAL	HG23	0.76	0.02	1
1	V	125	VAL	C	175.4	0.3	1
1	V	125	VAL	CA	62.1	0.3	1
1	V	125	VAL	CB	32.7	0.3	1
1	V	125	VAL	CG1	20.6	0.3	1
1	V	125	VAL	CG2	21.0	0.3	1
1	V	125	VAL	N	121.6	0.3	1
1	V	126	ASN	H	8.54	0.02	1
1	V	126	ASN	HA	4.86	0.02	1
1	V	126	ASN	HB2	2.78	0.02	1
1	V	126	ASN	HB3	2.56	0.02	1
1	V	126	ASN	HD21	7.56	0.02	1
1	V	126	ASN	HD22	7.56	0.02	1
1	V	126	ASN	CA	50.9	0.3	1
1	V	126	ASN	CB	38.8	0.3	1
1	V	126	ASN	N	123.9	0.3	1
1	V	126	ASN	ND2	113.3	0.3	1
1	V	127	PRO	HA	4.24	0.02	1
1	V	127	PRO	HB2	2.15	0.02	1
1	V	127	PRO	HB3	1.84	0.02	1
1	V	127	PRO	HG2	1.88	0.02	1
1	V	127	PRO	HG3	1.88	0.02	1
1	V	127	PRO	HD2	3.68	0.02	1
1	V	127	PRO	HD3	3.68	0.02	1
1	V	127	PRO	C	176.7	0.3	1
1	V	127	PRO	CA	63.7	0.3	1
1	V	127	PRO	CB	32.0	0.3	1
1	V	127	PRO	CG	27.1	0.3	1
1	V	127	PRO	CD	50.7	0.3	1
1	V	128	ASP	H	8.14	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	128	ASP	HA	4.44	0.02	1
1	V	128	ASP	HB2	2.58	0.02	1
1	V	128	ASP	HB3	2.46	0.02	1
1	V	128	ASP	C	176.1	0.3	1
1	V	128	ASP	CA	54.5	0.3	1
1	V	128	ASP	CB	40.7	0.3	1
1	V	128	ASP	N	118.8	0.3	1
1	V	129	ASP	H	7.94	0.02	1
1	V	129	ASP	HA	4.45	0.02	1
1	V	129	ASP	HB2	2.57	0.02	1
1	V	129	ASP	HB3	2.46	0.02	1
1	V	129	ASP	C	176.4	0.3	1
1	V	129	ASP	CA	54.4	0.3	1
1	V	129	ASP	CB	40.8	0.3	1
1	V	129	ASP	N	120.7	0.3	1
1	V	130	SER	H	8.09	0.02	1
1	V	130	SER	HA	4.26	0.02	1
1	V	130	SER	HB2	3.75	0.02	1
1	V	130	SER	HB3	3.75	0.02	1
1	V	130	SER	C	174.7	0.3	1
1	V	130	SER	CA	58.6	0.3	1
1	V	130	SER	CB	63.7	0.3	1
1	V	130	SER	N	115.9	0.3	1
1	V	131	LYS	H	8.16	0.02	1
1	V	131	LYS	HA	4.2	0.02	1
1	V	131	LYS	HB2	1.72	0.02	1
1	V	131	LYS	HB3	1.63	0.02	1
1	V	131	LYS	HG2	1.27	0.02	1
1	V	131	LYS	HG3	1.27	0.02	1
1	V	131	LYS	HD2	1.52	0.02	1
1	V	131	LYS	HD3	1.52	0.02	1
1	V	131	LYS	HE2	2.51	0.02	1
1	V	131	LYS	HE3	2.51	0.02	1
1	V	131	LYS	C	176.6	0.3	1
1	V	131	LYS	CA	56.2	0.3	1
1	V	131	LYS	CB	32.8	0.3	1
1	V	131	LYS	CG	24.6	0.3	1
1	V	131	LYS	CD	29.0	0.3	1
1	V	131	LYS	CE	42.0	0.3	1
1	V	131	LYS	N	123.0	0.3	1
1	V	132	GLU	H	8.28	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	V	132	GLU	HA	4.1	0.02	1
1	V	132	GLU	HB2	1.89	0.02	1
1	V	132	GLU	HB3	1.8	0.02	1
1	V	132	GLU	HG2	2.11	0.02	1
1	V	132	GLU	HG3	2.11	0.02	1
1	V	132	GLU	C	176.4	0.3	1
1	V	132	GLU	CA	56.6	0.3	1
1	V	132	GLU	CB	30.1	0.3	1
1	V	132	GLU	CG	36.2	0.3	1
1	V	132	GLU	N	121.6	0.3	1
1	V	133	ASP	H	8.24	0.02	1
1	V	133	ASP	HA	4.42	0.02	1
1	V	133	ASP	HB2	2.56	0.02	1
1	V	133	ASP	HB3	2.46	0.02	1
1	V	133	ASP	C	176.0	0.3	1
1	V	133	ASP	CA	54.3	0.3	1
1	V	133	ASP	CB	41.0	0.3	1
1	V	133	ASP	N	121.4	0.3	1
1	A	134	ALA	H	8.06	0.02	1
1	A	134	ALA	HA	4.16	0.02	1
1	A	134	ALA	HB1	1.25	0.02	1
1	A	134	ALA	HB2	1.25	0.02	1
1	A	134	ALA	HB3	1.25	0.02	1
1	A	134	ALA	C	177.6	0.3	1
1	A	134	ALA	CA	52.5	0.3	1
1	A	134	ALA	CB	19.1	0.3	1
1	A	134	ALA	N	124.1	0.3	1
1	A	135	LEU	H	8.05	0.02	1
1	A	135	LEU	HA	4.15	0.02	1
1	A	135	LEU	HB2	1.51	0.02	1
1	A	135	LEU	HB3	1.43	0.02	1
1	A	135	LEU	HG	1.48	0.02	1
1	A	135	LEU	HD11	0.79	0.02	1
1	A	135	LEU	HD12	0.79	0.02	1
1	A	135	LEU	HD13	0.79	0.02	1
1	A	135	LEU	HD21	0.73	0.02	1
1	A	135	LEU	HD22	0.73	0.02	1
1	A	135	LEU	HD23	0.73	0.02	1
1	A	135	LEU	C	177.4	0.3	1
1	A	135	LEU	CA	55.2	0.3	1
1	A	135	LEU	CB	42.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	135	LEU	CG	26.9	0.3	1
1	A	135	LEU	CD1	24.9	0.3	1
1	A	135	LEU	CD2	23.4	0.3	1
1	A	135	LEU	N	120.8	0.3	1
1	A	136	GLU	H	8.15	0.02	1
1	A	136	GLU	HA	4.11	0.02	1
1	A	136	GLU	HB2	1.85	0.02	1
1	A	136	GLU	HB3	1.79	0.02	1
1	A	136	GLU	HG2	2.11	0.02	1
1	A	136	GLU	HG3	2.11	0.02	1
1	A	136	GLU	C	176.2	0.3	1
1	A	136	GLU	CA	56.6	0.3	1
1	A	136	GLU	CB	30.0	0.3	1
1	A	136	GLU	CG	36.1	0.3	1
1	A	136	GLU	N	121.6	0.3	1
1	A	137	VAL	H	7.96	0.02	1
1	A	137	VAL	HA	3.88	0.02	1
1	A	137	VAL	HB	1.85	0.02	1
1	A	137	VAL	HG11	0.76	0.02	1
1	A	137	VAL	HG12	0.76	0.02	1
1	A	137	VAL	HG13	0.76	0.02	1
1	A	137	VAL	HG21	0.67	0.02	1
1	A	137	VAL	HG22	0.67	0.02	1
1	A	137	VAL	HG23	0.67	0.02	1
1	A	137	VAL	C	175.7	0.3	1
1	A	137	VAL	CA	62.2	0.3	1
1	A	137	VAL	CB	32.5	0.3	1
1	A	137	VAL	CG1	20.6	0.3	1
1	A	137	VAL	CG2	21.1	0.3	1
1	A	137	VAL	N	121.4	0.3	1
1	A	138	LEU	H	8.05	0.02	1
1	A	138	LEU	HA	4.16	0.02	1
1	A	138	LEU	HB2	1.39	0.02	1
1	A	138	LEU	HB3	1.23	0.02	1
1	A	138	LEU	HG	1.36	0.02	1
1	A	138	LEU	HD11	0.73	0.02	1
1	A	138	LEU	HD12	0.73	0.02	1
1	A	138	LEU	HD13	0.73	0.02	1
1	A	138	LEU	HD21	0.66	0.02	1
1	A	138	LEU	HD22	0.66	0.02	1
1	A	138	LEU	HD23	0.66	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	LEU	C	176.7	0.3	1
1	A	138	LEU	CA	54.9	0.3	1
1	A	138	LEU	CB	42.5	0.3	1
1	A	138	LEU	CG	26.8	0.3	1
1	A	138	LEU	CD1	24.7	0.3	1
1	A	138	LEU	CD2	23.3	0.3	1
1	A	138	LEU	N	125.3	0.3	1
1	A	139	PHE	H	8.05	0.02	1
1	A	139	PHE	HA	4.5	0.02	1
1	A	139	PHE	HB2	3.06	0.02	1
1	A	139	PHE	HB3	2.85	0.02	1
1	A	139	PHE	C	174.6	0.3	1
1	A	139	PHE	CA	57.5	0.3	1
1	A	139	PHE	CB	39.4	0.3	1
1	A	139	PHE	N	120.7	0.3	1
1	A	140	GLN	H	7.69	0.02	1
1	A	140	GLN	HA	4.0	0.02	1
1	A	140	GLN	HB2	1.94	0.02	1
1	A	140	GLN	HB3	1.76	0.02	1
1	A	140	GLN	HG2	2.1	0.02	1
1	A	140	GLN	HG3	2.1	0.02	1
1	A	140	GLN	HE21	7.41	0.02	1
1	A	140	GLN	HE22	6.7	0.02	1
1	A	140	GLN	C	180.1	0.3	1
1	A	140	GLN	CA	57.2	0.3	1
1	A	140	GLN	CB	30.5	0.3	1
1	A	140	GLN	CG	34.1	0.3	1
1	A	140	GLN	N	126.1	0.3	1
1	A	140	GLN	NE2	112.2	0.3	1

### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	126	$-0.01 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	119	$0.14 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	111	$-0.02 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	109	$0.68 \pm 0.31$	Should be applied

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 1049 atoms were assigned a chemical shift out of a possible 1314. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	412/461 (89%)	170/187 (91%)	165/184 (90%)	77/90 (86%)
Sidechain	630/786 (80%)	424/512 (83%)	203/240 (85%)	3/34 (9%)
Aromatic	7/67 (10%)	7/32 (22%)	0/35 (0%)	0/0 (—%)
Overall	1049/1314 (80%)	601/731 (82%)	368/459 (80%)	80/124 (65%)

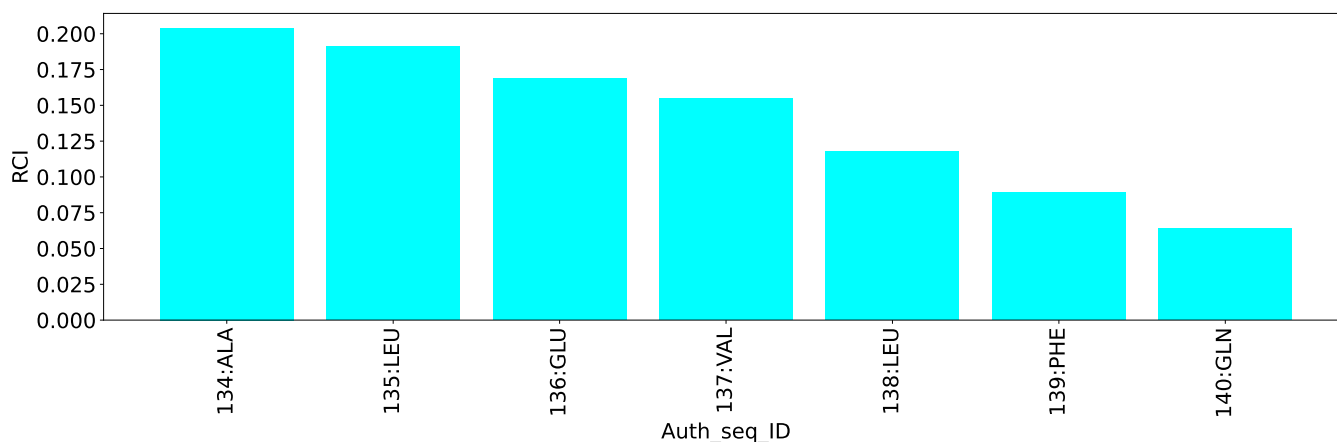
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

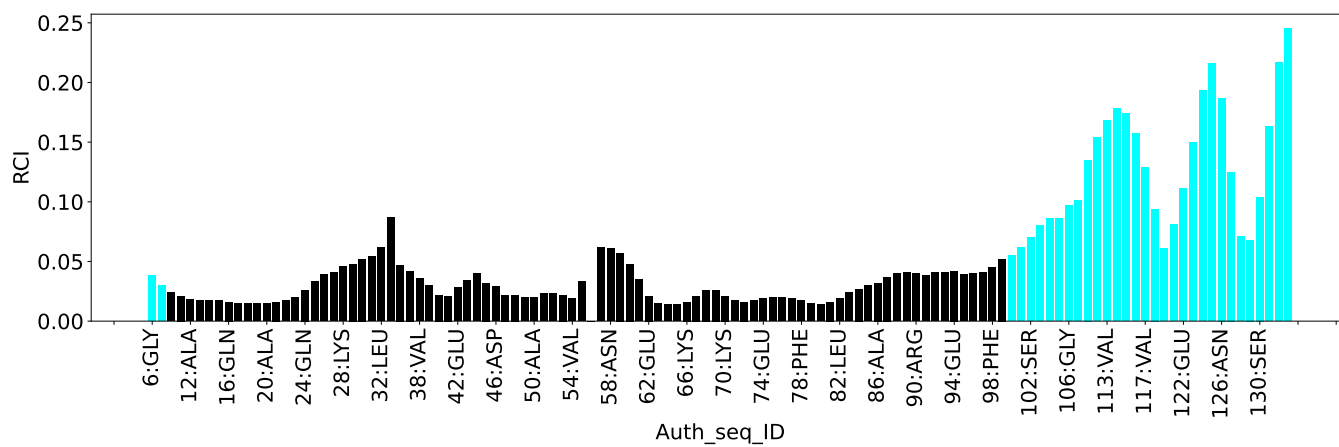
### 7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain V:



## 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	2062
Intra-residue ( $ i-j =0$ )	810
Sequential ( $ i-j =1$ )	575
Medium range ( $ i-j >1$ and $ i-j <5$ )	376
Long range ( $ i-j \geq 5$ )	191
Inter-chain	0
Hydrogen bond restraints	110
Disulfide bond restraints	0
Total dihedral-angle restraints	178
Number of unmapped restraints	159
Number of restraints per residue	16.8
Number of long range restraints per residue <sup>1</sup>	1.7

<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

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)	33.9	0.2
0.2-0.5 (Medium)	43.2	0.5
>0.5 (Large)	19.9	2.36

### 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)	5.0	9.8
10.0-20.0 (Medium)	0.3	18.8
>20.0 (Large)	0.1	54.2



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

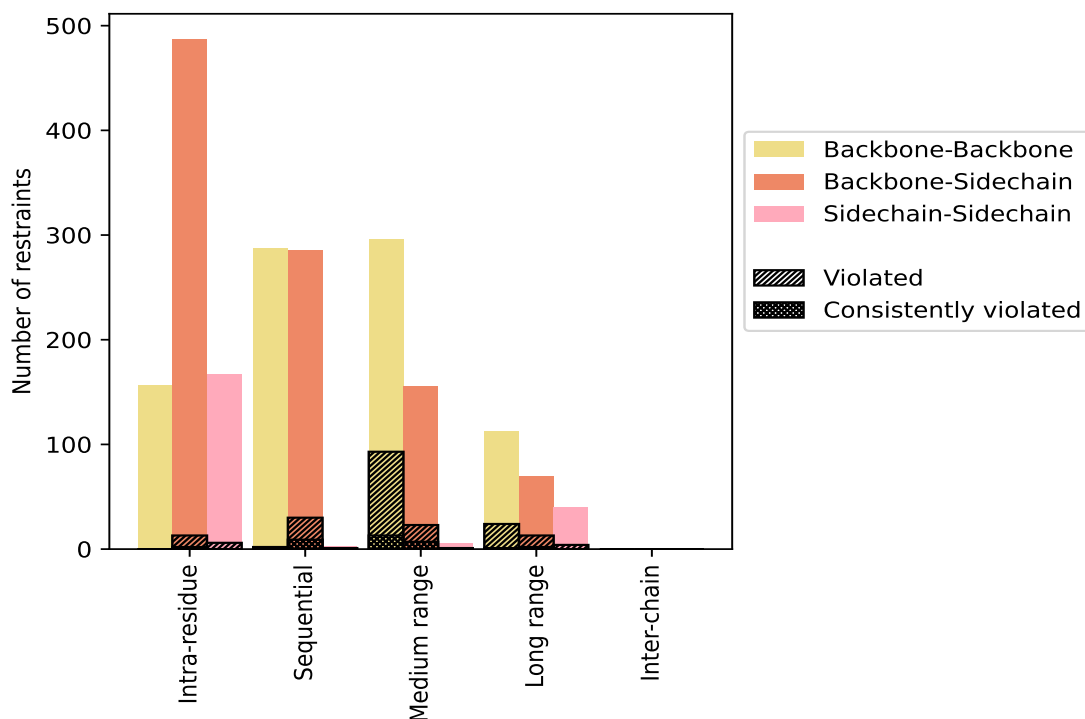
### 9.1 Summary of distance violations [i](#)

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.

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>810</b>	<b>39.3</b>	<b>19</b>	<b>2.3</b>	<b>0.9</b>	<b>2</b>	<b>0.2</b>	<b>0.1</b>
Backbone-Backbone	156	7.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	487	23.6	13	2.7	0.6	2	0.4	0.1
Sidechain-Sidechain	167	8.1	6	3.6	0.3	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>575</b>	<b>27.9</b>	<b>33</b>	<b>5.7</b>	<b>1.6</b>	<b>9</b>	<b>1.6</b>	<b>0.4</b>
Backbone-Backbone	287	13.9	2	0.7	0.1	0	0.0	0.0
Backbone-Sidechain	285	13.8	30	10.5	1.5	9	3.2	0.4
Sidechain-Sidechain	3	0.1	1	33.3	0.0	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>376</b>	<b>18.2</b>	<b>77</b>	<b>20.5</b>	<b>3.7</b>	<b>17</b>	<b>4.5</b>	<b>0.8</b>
Backbone-Backbone	216	10.5	53	24.5	2.6	10	4.6	0.5
Backbone-Sidechain	155	7.5	23	14.8	1.1	7	4.5	0.3
Sidechain-Sidechain	5	0.2	1	20.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>191</b>	<b>9.3</b>	<b>37</b>	<b>19.4</b>	<b>1.8</b>	<b>3</b>	<b>1.6</b>	<b>0.1</b>
Backbone-Backbone	82	4.0	20	24.4	1.0	1	1.2	0.0
Backbone-Sidechain	69	3.3	13	18.8	0.6	2	2.9	0.1
Sidechain-Sidechain	40	1.9	4	10.0	0.2	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>110</b>	<b>5.3</b>	<b>44</b>	<b>40.0</b>	<b>2.1</b>	<b>3</b>	<b>2.7</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>2062</b>	<b>100.0</b>	<b>210</b>	<b>10.2</b>	<b>10.2</b>	<b>34</b>	<b>1.6</b>	<b>1.6</b>
Backbone-Backbone	851	41.3	119	14.0	5.8	14	1.6	0.7
Backbone-Sidechain	996	48.3	79	7.9	3.8	20	2.0	1.0
Sidechain-Sidechain	215	10.4	12	5.6	0.6	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 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	10	14	64	18	0	106	0.36	1.38	0.27	0.25
2	10	14	58	18	0	100	0.36	1.58	0.27	0.27
3	9	16	69	18	0	112	0.34	1.55	0.27	0.26
4	6	16	65	12	0	99	0.37	1.39	0.29	0.26
5	10	18	54	17	0	99	0.36	1.51	0.28	0.26
6	10	15	56	16	0	97	0.39	1.4	0.32	0.27
7	9	12	54	15	0	90	0.36	1.54	0.29	0.26
8	11	14	49	15	0	89	0.37	1.64	0.3	0.26
9	8	12	53	17	0	90	0.37	1.42	0.3	0.25
10	8	18	56	11	0	93	0.37	1.38	0.28	0.27
11	10	20	55	20	0	105	0.39	2.36	0.38	0.24

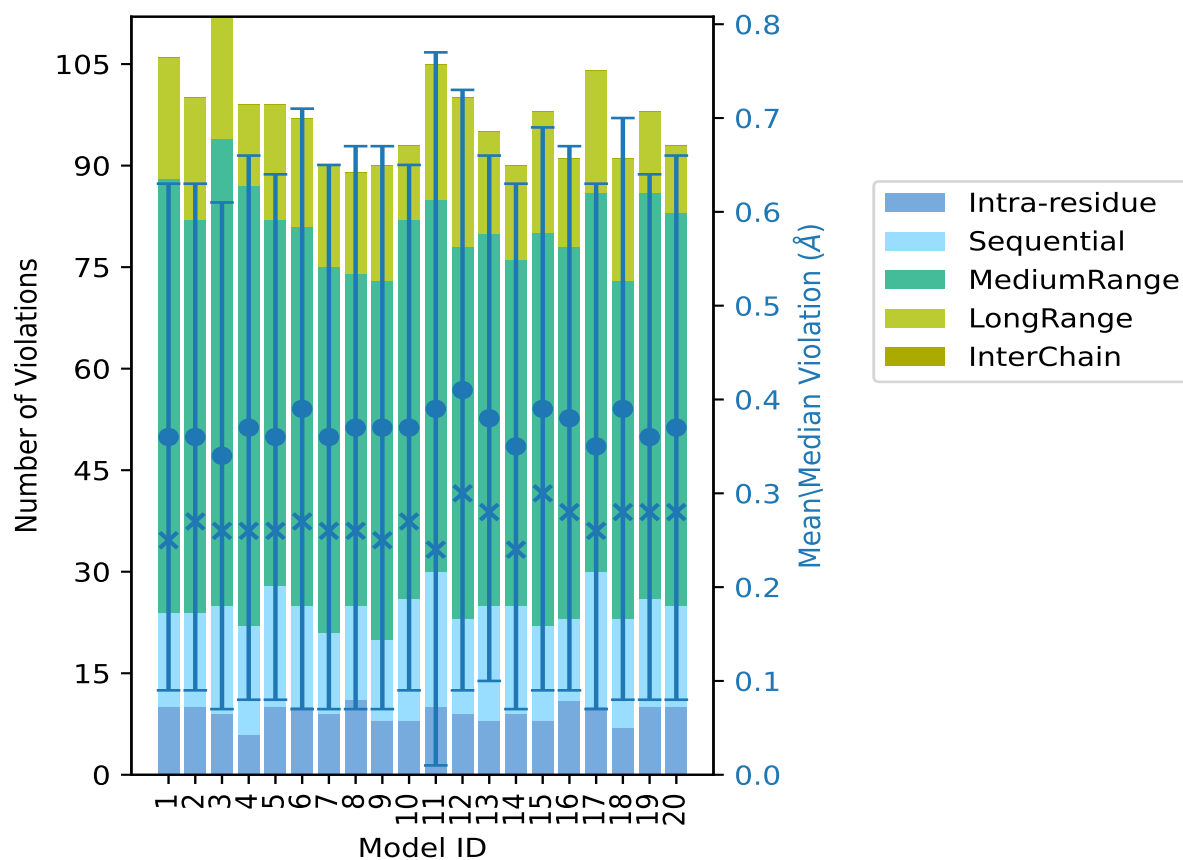
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
12	9	14	55	22	0	100	0.41	1.67	0.32	0.3
13	8	17	55	15	0	95	0.38	1.34	0.28	0.28
14	9	16	51	14	0	90	0.35	1.31	0.28	0.24
15	8	14	58	18	0	98	0.39	1.34	0.3	0.3
16	11	12	55	13	0	91	0.38	1.54	0.29	0.28
17	10	20	56	18	0	104	0.35	1.52	0.28	0.26
18	7	16	50	18	0	91	0.39	1.45	0.31	0.28
19	10	16	60	12	0	98	0.36	1.55	0.28	0.28
20	10	15	58	10	0	93	0.37	1.53	0.29	0.28

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

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



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

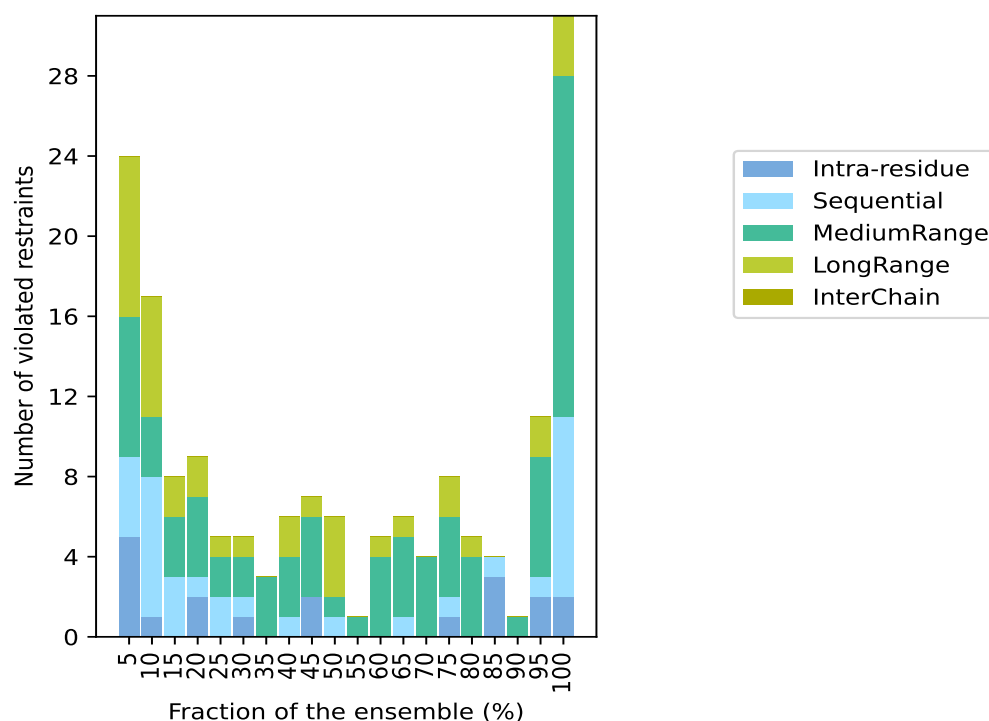
### 9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1786(IR:791, SQ:542, MR:299, LR:154, 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>	%
5	4	7	8	0	24	1	5.0
1	7	3	6	0	17	2	10.0
0	3	3	2	0	8	3	15.0
2	1	4	2	0	9	4	20.0
0	2	2	1	0	5	5	25.0
1	1	2	1	0	5	6	30.0
0	0	3	0	0	3	7	35.0
0	1	3	2	0	6	8	40.0
2	0	4	1	0	7	9	45.0
0	1	1	4	0	6	10	50.0
0	0	1	0	0	1	11	55.0
0	0	4	1	0	5	12	60.0
0	1	4	1	0	6	13	65.0
0	0	4	0	0	4	14	70.0
1	1	4	2	0	8	15	75.0
0	0	4	1	0	5	16	80.0
3	1	0	0	0	4	17	85.0
0	0	1	0	0	1	18	90.0
2	1	6	2	0	11	19	95.0
2	9	17	3	0	31	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

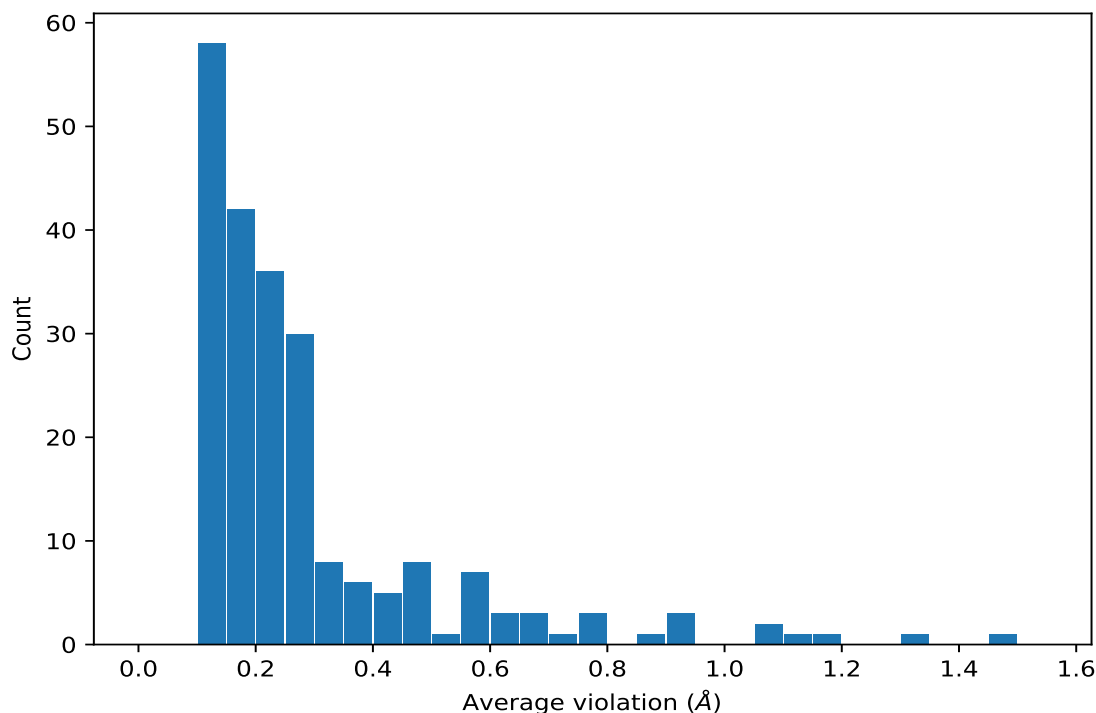
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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.

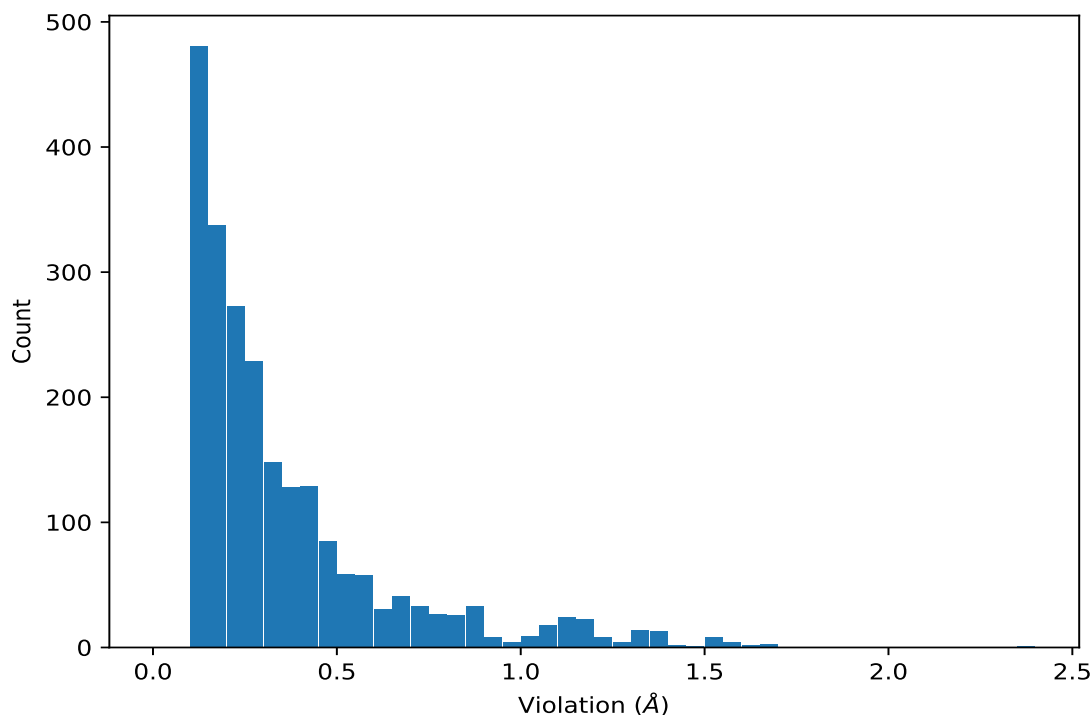
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	20	1.46	0.11	1.52
(3,298)	1:V:47:LEU:H	1:V:48:ALA:HB1	20	1.3	0.05	1.31
(3,473)	1:V:70:LYS:H	1:V:71:ALA:HB1	20	1.16	0.03	1.15
(3,513)	1:V:74:GLU:H	1:V:75:ALA:HB1	20	1.1	0.03	1.09
(3,5)	1:V:11:VAL:H	1:V:12:ALA:HB1	20	1.09	0.05	1.09
(3,530)	1:V:76:SER:H	1:V:75:ALA:HB1	20	0.86	0.03	0.87
(1,639)	1:V:100:ASP:H	1:V:55:THR:CG2	20	0.77	0.05	0.76
(4,47)	1:V:57:LEU:O	1:V:60:LYS:H	20	0.77	0.14	0.78
(1,176)	1:V:27:ILE:H	1:V:25:ARG:CA	20	0.76	0.2	0.68
(5,24)	1:V:57:LEU:C	1:V:60:LYS:H	20	0.69	0.13	0.68

<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)
(1,587)	1:V:92:VAL:H	1:V:89:LEU:CG	11	2.36
(2,36)	1:V:15:MET:HE1	1:V:91:ILE:HD11	12	1.67
(2,36)	1:V:15:MET:HE1	1:V:91:ILE:HD12	12	1.67
(2,36)	1:V:15:MET:HE1	1:V:91:ILE:HD13	12	1.67
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	8	1.64
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	11	1.63
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	2	1.58
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	3	1.55
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	12	1.55
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	19	1.55
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	7	1.54

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<b>Key</b>	<b>Atom-1</b>	<b>Atom-2</b>	<b>Model ID</b>	<b>Violation (Å)</b>
(3,442)	1:V:67:ALA:H	1:V:71:ALA:HB1	16	1.54



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

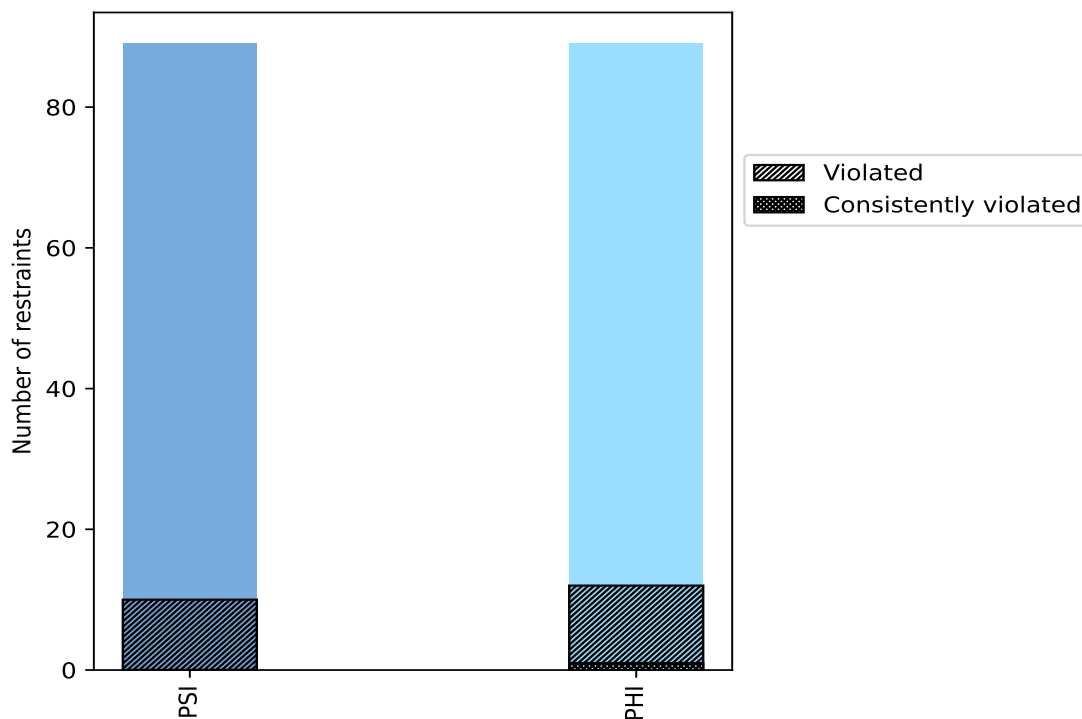
### 10.1 Summary of dihedral-angle violations [i](#)

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	89	50.0	10	11.2	5.6	0	0.0	0.0
PHI	89	50.0	12	13.5	6.7	1	1.1	0.6
Total	178	100.0	22	12.4	12.4	1	0.6	0.6

<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](#)



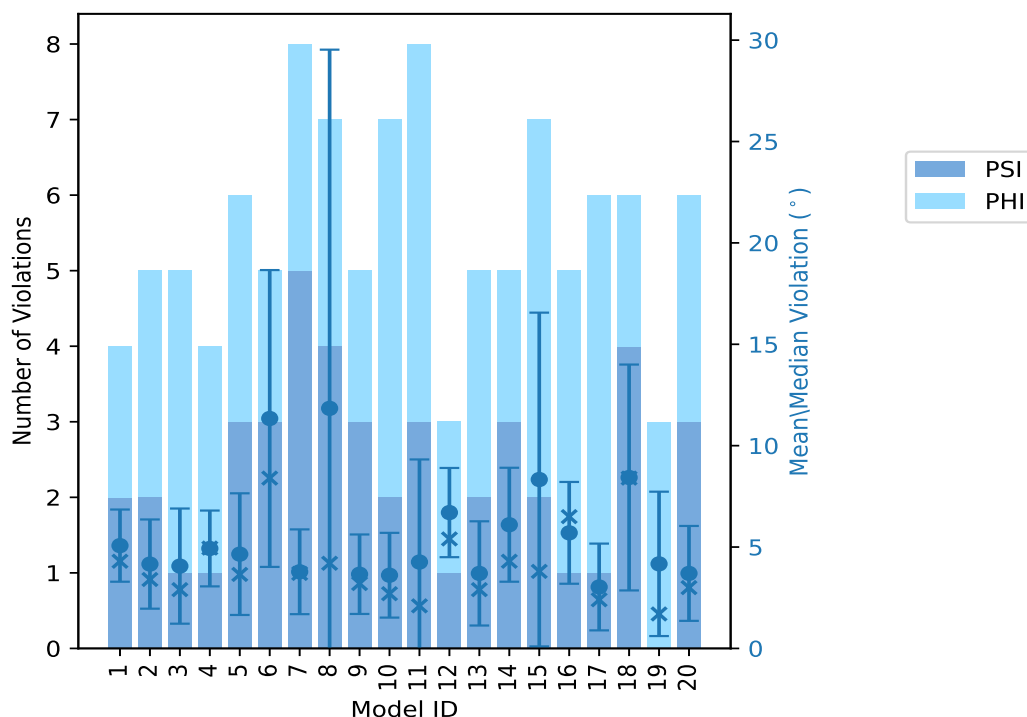
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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	2	2	4	5.07	8.1	1.78	4.3
2	2	3	5	4.16	8.4	2.2	3.4
3	1	4	5	4.06	9.7	2.84	2.9
4	1	3	4	4.93	7.5	1.87	4.95
5	3	3	6	4.65	10.1	3.0	3.65
6	3	2	5	11.34	21.9	7.32	8.4
7	5	3	8	3.78	8.2	2.09	3.7
8	4	3	7	11.84	54.2	17.69	4.2
9	3	2	5	3.66	7.3	1.96	3.2
10	2	5	7	3.61	6.8	2.09	2.7
11	3	5	8	4.26	17.2	5.06	2.1
12	1	2	3	6.7	9.8	2.2	5.4
13	2	3	5	3.7	8.1	2.57	2.9
14	3	2	5	6.1	9.8	2.81	4.3
15	2	5	7	8.33	26.1	8.23	3.8
16	1	4	5	5.7	9.0	2.51	6.5
17	1	5	6	3.03	7.2	2.14	2.4
18	4	2	6	8.43	18.8	5.57	8.4
19	0	3	3	4.17	9.2	3.56	1.7
20	3	3	6	3.7	8.4	2.34	3.0

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

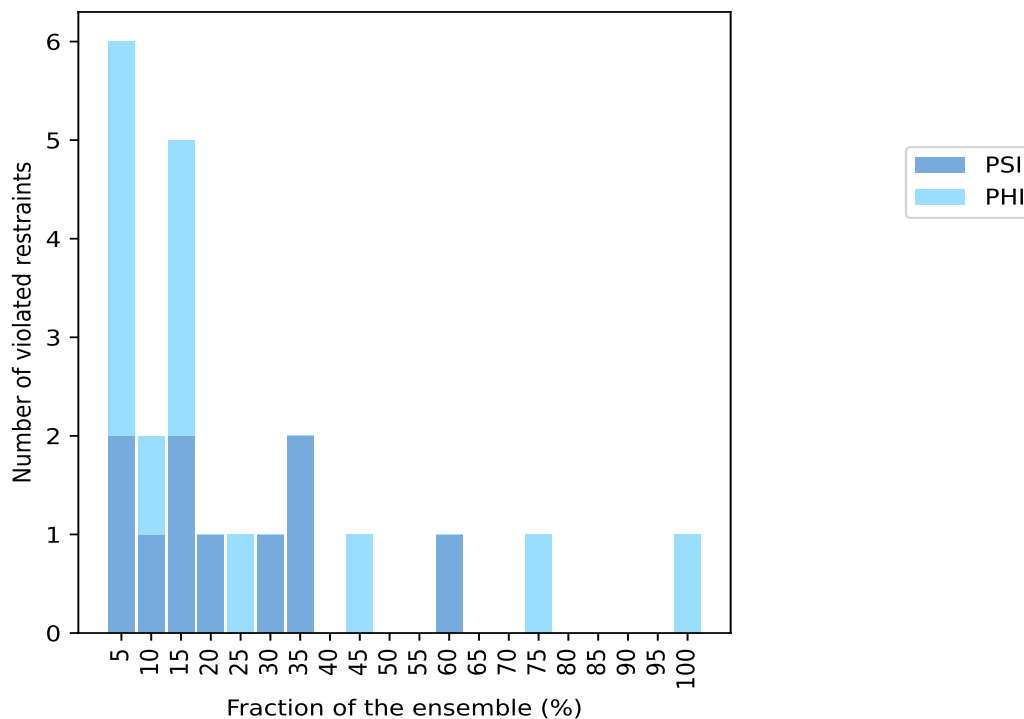
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
1	0	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	1	1	20	100.0

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

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

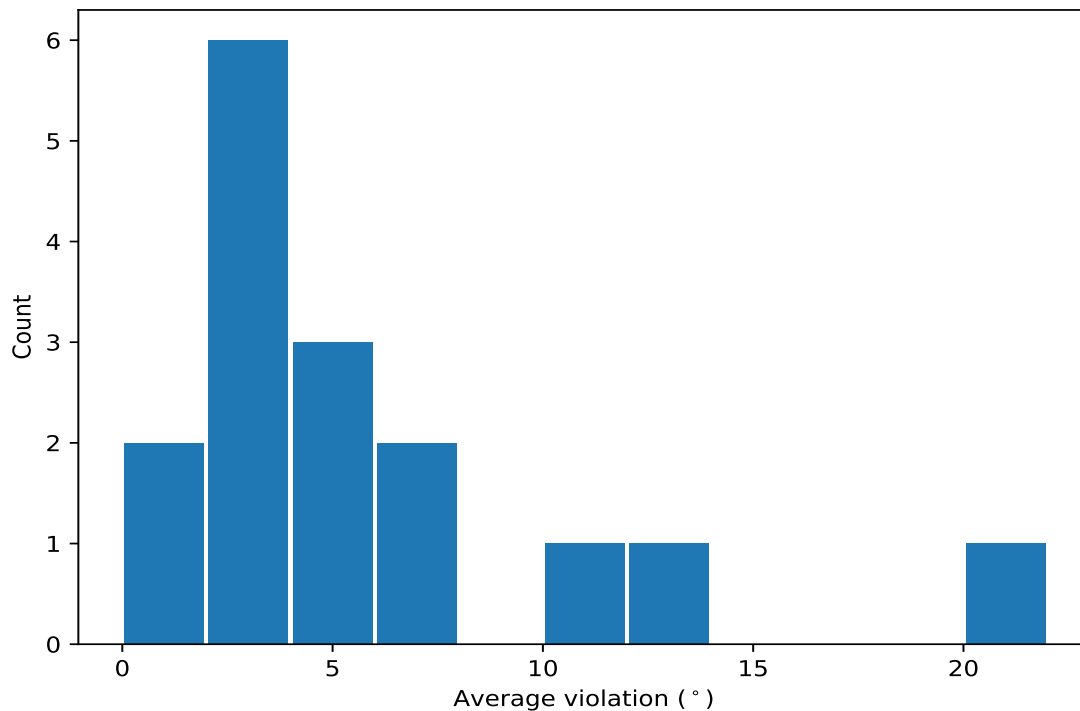


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

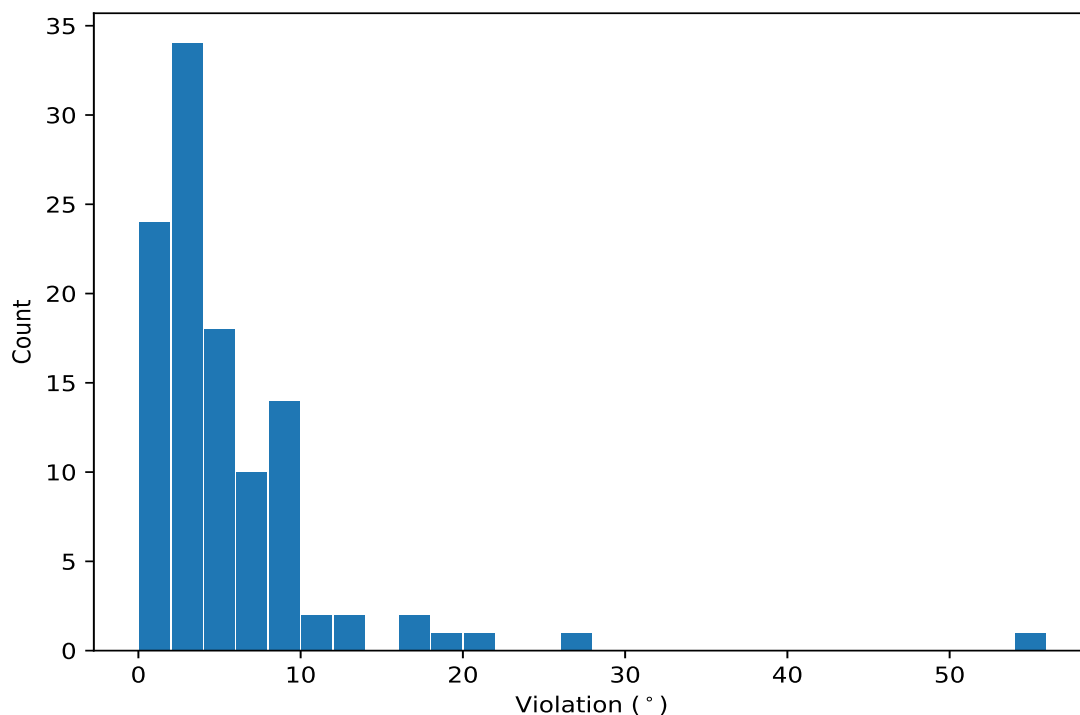
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,93)	1:V:59:ASP:C	1:V:60:LYS:N	1:V:60:LYS:CA	1:V:60:LYS:C	20	7.54	1.86	8.1
(1,85)	1:V:55:THR:C	1:V:56:PHE:N	1:V:56:PHE:CA	1:V:56:PHE:C	15	3.59	1.31	3.3
(1,40)	1:V:28:LYS:N	1:V:28:LYS:CA	1:V:28:LYS:C	1:V:29:ASP:N	12	5.72	4.22	4.7
(1,89)	1:V:57:LEU:C	1:V:58:ASN:N	1:V:58:ASN:CA	1:V:58:ASN:C	9	2.7	0.97	2.9
(1,38)	1:V:27:ILE:N	1:V:27:ILE:CA	1:V:27:ILE:C	1:V:28:LYS:N	7	4.29	2.53	3.2
(1,82)	1:V:54:VAL:N	1:V:54:VAL:CA	1:V:54:VAL:C	1:V:55:THR:N	7	2.43	1.05	2.7
(1,156)	1:V:91:ILE:N	1:V:91:ILE:CA	1:V:91:ILE:C	1:V:92:VAL:N	6	12.73	18.74	3.8
(1,157)	1:V:91:ILE:C	1:V:92:VAL:N	1:V:92:VAL:CA	1:V:92:VAL:C	5	10.98	9.23	6.0
(1,92)	1:V:59:ASP:N	1:V:59:ASP:CA	1:V:59:ASP:C	1:V:60:LYS:N	4	2.2	1.39	1.4
(1,152)	1:V:89:LEU:N	1:V:89:LEU:CA	1:V:89:LEU:C	1:V:90:ARG:N	3	6.47	4.87	3.8

<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 (°)
(1,156)	1:V:91:ILE:N	1:V:91:ILE:CA	1:V:91:ILE:C	1:V:92:VAL:N	8	54.2
(1,157)	1:V:91:ILE:C	1:V:92:VAL:N	1:V:92:VAL:CA	1:V:92:VAL:C	15	26.1
(1,36)	1:V:26:GLU:N	1:V:26:GLU:CA	1:V:26:GLU:C	1:V:27:ILE:N	6	21.9
(1,36)	1:V:26:GLU:N	1:V:26:GLU:CA	1:V:26:GLU:C	1:V:27:ILE:N	18	18.8
(1,40)	1:V:28:LYS:N	1:V:28:LYS:CA	1:V:28:LYS:C	1:V:29:ASP:N	6	17.5
(1,157)	1:V:91:ILE:C	1:V:92:VAL:N	1:V:92:VAL:CA	1:V:92:VAL:C	11	17.2
(1,152)	1:V:89:LEU:N	1:V:89:LEU:CA	1:V:89:LEU:C	1:V:90:ARG:N	8	13.3
(1,33)	1:V:24:GLN:C	1:V:25:ARG:N	1:V:25:ARG:CA	1:V:25:ARG:C	15	13.1
(1,93)	1:V:59:ASP:C	1:V:60:LYS:N	1:V:60:LYS:CA	1:V:60:LYS:C	18	10.3
(1,156)	1:V:91:ILE:N	1:V:91:ILE:CA	1:V:91:ILE:C	1:V:92:VAL:N	5	10.1