



# wwPDB NMR Structure Validation Summary Report ⓘ

Dec 24, 2024 – 02:46 PM EST

PDB ID : 2L9B  
BMRB ID : 17161  
Title : Heterodimer between Rna14p monkeytail domain and Rna15p hinge domain of the yeast CF IA complex  
Authors : Moreno-Morcillo, M.; Minvielle-Sebastia, L.; Fribourg, S.; Mackereth, C.D.  
Deposited on : 2011-02-07

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

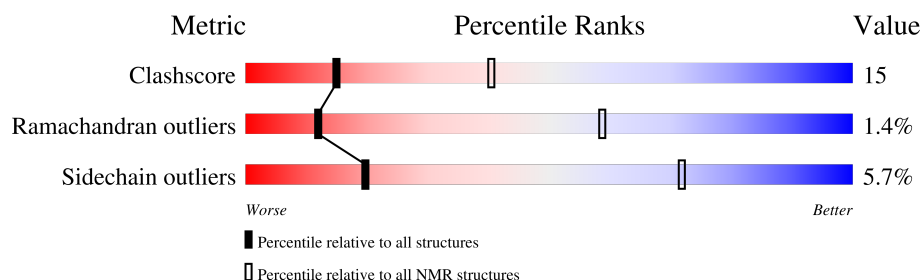
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 96%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	109	
2	B	53	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:141-A:228, B:630-B:647, B:652-B:669 (124)	0.72	8

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 and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 6, 8, 9
2	3, 4, 5
Single-model clusters	7; 10

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2100 atoms, of which 1064 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called mRNA 3'-end-processing protein RNA15.

Mol	Chain	Residues	Atoms						Trace
1	A	91	Total	C	H	N	O	S	0
			1439	458	730	113	133	5	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLY	-	expression tag	UNP P25299
A	125	HIS	-	expression tag	UNP P25299
A	126	MET	-	expression tag	UNP P25299
A	196	ALA	VAL	variant	UNP P25299

- Molecule 2 is a protein called mRNA 3'-end-processing protein RNA14.

Mol	Chain	Residues	Atoms					Trace
2	B	40	Total	C	H	N	O	0
			661	212	334	52	63	

There is a discrepancy between the modelled and reference sequences:

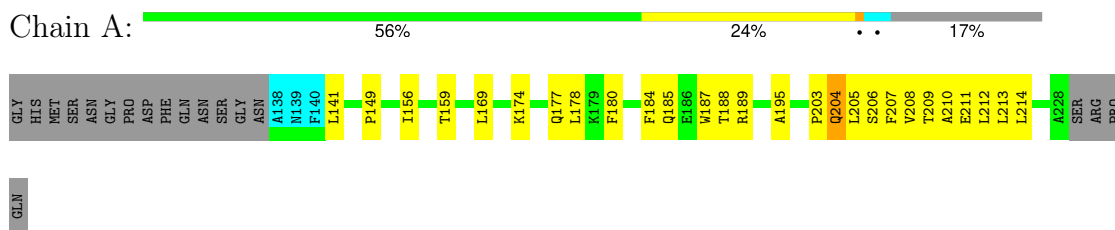
Chain	Residue	Modelled	Actual	Comment	Reference
B	625	MET	-	initiating methionine	UNP P25298

## 4 Residue-property plots

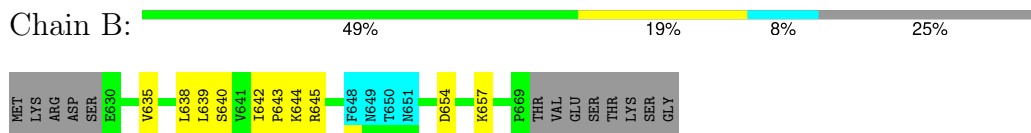
### 4.1 Average score per residue in the NMR ensemble

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: mRNA 3'-end-processing protein RNA15



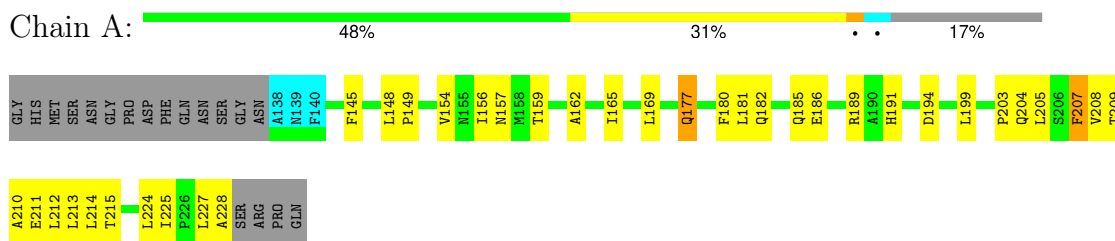
- Molecule 2: mRNA 3'-end-processing protein RNA14



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

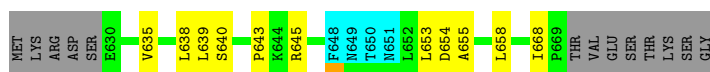
The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: mRNA 3'-end-processing protein RNA15



- Molecule 2: mRNA 3'-end-processing protein RNA14





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 20 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
ARIA	structure solution	1.2
CNS	refinement	1.1
ARIA1.2/CNS1.1	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	2077
Number of shifts mapped to atoms	1767
Number of unparsed shifts	0
Number of shifts with mapping errors	310
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	96%

## 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	0.31±0.03	0±0/698 ( 0.0± 0.0%)	0.43±0.02	0±0/947 ( 0.0± 0.0%)
2	B	0.33±0.04	0±0/297 ( 0.0± 0.0%)	0.49±0.02	0±0/405 ( 0.0± 0.0%)
All	All	0.32	1/9950 ( 0.0%)	0.45	0/13520 ( 0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	207	PHE	CE1-CZ	5.38	1.47	1.37	8	1

There are no bond-angle outliers.

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	685	711	710	26±4
2	B	293	306	306	14±2
All	All	9780	10170	10160	296

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 15.

5 of 144 unique clashes are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:ARG:HH12	2:B:662:LEU:HG	0.72	1.44	9	1
1:A:177:GLN:HB3	1:A:212:LEU:HD22	0.70	1.62	1	9
1:A:204:GLN:O	1:A:208:VAL:HB	0.67	1.88	1	2
1:A:177:GLN:HB2	1:A:216:ASN:HD21	0.66	1.50	4	2
1:A:188:THR:HG21	2:B:662:LEU:HD23	0.66	1.67	2	4

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	87/109 (80%)	82±2 (95±3%)	4±2 (4±2%)	1±0 (1±1%)	19	69
2	B	34/53 (64%)	30±1 (89±3%)	3±1 (8±4%)	1±1 (3±3%)	6	39
All	All	1210/1620 (75%)	1128 (93%)	65 (5%)	17 (1%)	12	59

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	156	ILE	5
2	B	645	ARG	4
2	B	652	LEU	4
2	B	643	PRO	2
1	A	159	THR	1

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	79/96 (82%)	74±2 (93±3%)	5±2 (7±3%)	16	67
2	B	35/51 (69%)	34±1 (97±2%)	1±1 (3±2%)	34	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1140/1470 (78%)	1075 (94%)	65 (6%)	20 72

5 of 30 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	204	GLN	9
1	A	177	GLN	6
1	A	206	SER	6
1	A	207	PHE	6
1	A	208	VAL	3

### 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 [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 96% for the well-defined parts and 96% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: 17161\_chemshifts\_PDB.str

#### 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	2077
Number of shifts mapped to atoms	1767
Number of unparsed shifts	0
Number of shifts with mapping errors	310
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 310) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	625	MET	HA	4.62	0.02	1
1	B	625	MET	HB2	3.06	0.02	1
1	B	625	MET	HB3	3.06	0.02	1
1	B	625	MET	HG2	3.08	0.02	1
1	B	625	MET	HG3	3.08	0.02	1
1	B	625	MET	C	175.23	0.2	1
1	B	625	MET	CA	57.34	0.2	1
1	B	625	MET	CB	39.74	0.2	1
1	B	626	LYS	H	8.2	0.02	1
1	B	626	LYS	HA	4.3	0.02	1
1	B	626	LYS	HB2	1.78	0.02	1
1	B	626	LYS	HB3	1.78	0.02	1
1	B	626	LYS	HD2	1.71	0.02	1
1	B	626	LYS	HD3	1.71	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	626	LYS	HE2	3.0	0.02	1
1	B	626	LYS	HE3	3.0	0.02	1
1	B	626	LYS	HG2	1.39	0.02	1
1	B	626	LYS	HG3	1.39	0.02	1
1	B	626	LYS	C	175.93	0.2	1
1	B	626	LYS	CA	55.91	0.2	1
1	B	626	LYS	CB	33.04	0.2	1
1	B	626	LYS	CD	29.17	0.2	1
1	B	626	LYS	CE	42.12	0.2	1
1	B	626	LYS	CG	24.53	0.2	1
1	B	626	LYS	N	123.67	0.2	1
1	B	627	ARG	H	8.4	0.02	1
1	B	627	ARG	HA	4.34	0.02	1
1	B	627	ARG	HB2	1.89	0.02	2
1	B	627	ARG	HB3	1.78	0.02	2
1	B	627	ARG	HD2	3.2	0.02	1
1	B	627	ARG	HD3	3.2	0.02	1
1	B	627	ARG	HG2	1.67	0.02	1
1	B	627	ARG	HG3	1.67	0.02	1
1	B	627	ARG	C	176.12	0.2	1
1	B	627	ARG	CA	56.0	0.2	1
1	B	627	ARG	CB	30.8	0.2	1
1	B	627	ARG	CD	43.8	0.2	1
1	B	627	ARG	CG	27.17	0.2	1
1	B	627	ARG	N	123.14	0.2	1
1	B	628	ASP	H	8.5	0.02	1
1	B	628	ASP	HA	4.64	0.02	1
1	B	628	ASP	HB2	2.75	0.02	1
1	B	628	ASP	HB3	2.75	0.02	1
1	B	628	ASP	C	176.29	0.2	1
1	B	628	ASP	CA	54.67	0.2	1
1	B	628	ASP	CB	41.12	0.2	1
1	B	628	ASP	N	122.08	0.2	1
1	B	629	SER	H	8.22	0.02	1
1	B	629	SER	HA	4.38	0.02	1
1	B	629	SER	HB2	3.84	0.02	2
1	B	629	SER	HB3	3.91	0.02	2
1	B	629	SER	C	174.61	0.2	1
1	B	629	SER	CA	58.43	0.2	1
1	B	629	SER	CB	63.94	0.2	1
1	B	629	SER	N	114.75	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	630	GLU	H	8.37	0.02	1
1	B	670	THR	H	8.05	0.02	1
1	B	670	THR	HA	4.37	0.02	1
1	B	670	THR	HB	4.25	0.02	1
1	B	670	THR	HG21	1.23	0.02	1
1	B	670	THR	HG22	1.23	0.02	1
1	B	670	THR	HG23	1.23	0.02	1
1	B	670	THR	C	175.17	0.2	1
1	B	670	THR	CA	61.2	0.2	1
1	B	670	THR	CB	70.09	0.2	1
1	B	670	THR	CG2	21.53	0.2	1
1	B	670	THR	N	112.39	0.2	1
1	B	671	VAL	H	8.34	0.02	1
1	B	671	VAL	HA	4.13	0.02	1
1	B	671	VAL	HB	2.12	0.02	1
1	B	671	VAL	HG11	0.96	0.02	2
1	B	671	VAL	HG12	0.96	0.02	2
1	B	671	VAL	HG13	0.96	0.02	2
1	B	671	VAL	HG21	0.96	0.02	2
1	B	671	VAL	HG22	0.96	0.02	2
1	B	671	VAL	HG23	0.96	0.02	2
1	B	671	VAL	C	176.24	0.2	1
1	B	671	VAL	CA	62.37	0.2	1
1	B	671	VAL	CB	32.71	0.2	1
1	B	671	VAL	CG1	21.35	0.2	1
1	B	671	VAL	CG2	20.86	0.2	1
1	B	671	VAL	N	121.96	0.2	1
1	B	672	GLU	H	8.59	0.02	1
1	B	672	GLU	HA	4.32	0.02	1
1	B	672	GLU	HB2	2.09	0.02	2
1	B	672	GLU	HB3	1.98	0.02	2
1	B	672	GLU	HG2	2.29	0.02	1
1	B	672	GLU	HG3	2.29	0.02	1
1	B	672	GLU	C	176.69	0.2	1
1	B	672	GLU	CA	56.72	0.2	1
1	B	672	GLU	CB	29.92	0.2	1
1	B	672	GLU	CG	36.35	0.2	1
1	B	672	GLU	N	124.31	0.2	1
1	B	673	SER	H	8.37	0.02	1
1	B	673	SER	HA	4.5	0.02	1
1	B	673	SER	HB2	3.93	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	673	SER	HB3	3.93	0.02	1
1	B	673	SER	C	174.97	0.2	1
1	B	673	SER	CA	58.58	0.2	1
1	B	673	SER	CB	63.86	0.2	1
1	B	673	SER	N	117.25	0.2	1
1	B	674	THR	H	8.18	0.02	1
1	B	674	THR	HA	4.38	0.02	1
1	B	674	THR	HB	4.27	0.02	1
1	B	674	THR	HG21	1.23	0.02	1
1	B	674	THR	HG22	1.23	0.02	1
1	B	674	THR	HG23	1.23	0.02	1
1	B	674	THR	C	174.58	0.2	1
1	B	674	THR	CA	62.01	0.2	1
1	B	674	THR	CB	69.62	0.2	1
1	B	674	THR	CG2	21.6	0.2	1
1	B	674	THR	N	116.1	0.2	1
1	B	675	LYS	H	8.27	0.02	1
1	B	675	LYS	HA	4.43	0.02	1
1	B	675	LYS	HB2	1.88	0.02	1
1	B	675	LYS	HB3	1.88	0.02	1
1	B	675	LYS	HD2	1.73	0.02	1
1	B	675	LYS	HD3	1.73	0.02	1
1	B	675	LYS	HE2	3.01	0.02	1
1	B	675	LYS	HE3	3.01	0.02	1
1	B	675	LYS	HG2	1.47	0.02	1
1	B	675	LYS	HG3	1.47	0.02	1
1	B	675	LYS	C	176.47	0.2	1
1	B	675	LYS	CA	56.21	0.2	1
1	B	675	LYS	CB	32.91	0.2	1
1	B	675	LYS	CD	28.96	0.2	1
1	B	675	LYS	CE	41.99	0.2	1
1	B	675	LYS	CG	24.61	0.2	1
1	B	675	LYS	N	123.91	0.2	1
1	B	676	SER	H	8.36	0.02	1
1	B	676	SER	HA	4.5	0.02	1
1	B	676	SER	HB2	3.89	0.02	1
1	B	676	SER	HB3	3.89	0.02	1
1	B	676	SER	C	174.02	0.2	1
1	B	676	SER	CA	58.16	0.2	1
1	B	676	SER	CB	64.06	0.2	1
1	B	676	SER	N	117.91	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	677	GLY	H	8.01	0.02	1
1	B	677	GLY	HA2	3.79	0.02	1
1	B	677	GLY	HA3	3.79	0.02	1
1	B	677	GLY	C	179.02	0.2	1
1	B	677	GLY	CA	46.12	0.2	1
1	B	677	GLY	N	117.26	0.2	1
1	A	125	HIS	HA	4.68	0.02	1
1	A	125	HIS	HB2	3.12	0.02	1
1	A	125	HIS	HB3	3.12	0.02	1
1	A	125	HIS	HD2	7.07	0.02	1
1	A	125	HIS	HE1	7.96	0.02	1
1	A	125	HIS	CB	30.74	0.2	1
1	A	125	HIS	CD2	119.44	0.2	1
1	A	125	HIS	CE1	137.6	0.2	1
1	A	127	SER	HA	4.41	0.02	1
1	A	127	SER	HB2	3.84	0.02	1
1	A	127	SER	HB3	3.84	0.02	1
1	A	127	SER	C	174.09	0.2	1
1	A	127	SER	CA	58.26	0.2	1
1	A	127	SER	CB	63.83	0.2	1
1	A	128	ASN	H	8.45	0.02	1
1	A	128	ASN	HA	4.79	0.02	1
1	A	128	ASN	HB2	2.76	0.02	2
1	A	128	ASN	HB3	2.83	0.02	2
1	A	128	ASN	HD21	7.62	0.02	2
1	A	128	ASN	HD22	6.94	0.02	2
1	A	128	ASN	C	175.18	0.2	1
1	A	128	ASN	CA	53.09	0.2	1
1	A	128	ASN	CB	39.08	0.2	1
1	A	128	ASN	CG	177.0	0.2	1
1	A	128	ASN	N	120.6	0.2	1
1	A	128	ASN	ND2	112.67	0.2	1
1	A	129	GLY	H	8.18	0.02	1
1	A	129	GLY	HA2	4.13	0.02	1
1	A	129	GLY	HA3	4.13	0.02	1
1	A	129	GLY	C	171.97	0.2	1
1	A	129	GLY	CA	44.5	0.2	1
1	A	129	GLY	N	109.07	0.2	1
1	A	130	PRO	HA	4.38	0.02	1
1	A	130	PRO	HB2	1.79	0.02	2
1	A	130	PRO	HB3	2.2	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	PRO	HD2	3.62	0.02	1
1	A	130	PRO	HD3	3.62	0.02	1
1	A	130	PRO	HG2	1.98	0.02	1
1	A	130	PRO	HG3	1.98	0.02	1
1	A	130	PRO	C	176.8	0.2	1
1	A	130	PRO	CA	63.4	0.2	1
1	A	130	PRO	CB	31.99	0.2	1
1	A	130	PRO	CD	49.79	0.2	1
1	A	130	PRO	CG	27.16	0.2	1
1	A	131	ASP	H	8.37	0.02	1
1	A	131	ASP	HA	4.56	0.02	1
1	A	131	ASP	HB2	2.57	0.02	2
1	A	131	ASP	HB3	2.66	0.02	2
1	A	131	ASP	C	176.35	0.2	1
1	A	131	ASP	CA	54.15	0.2	1
1	A	131	ASP	CB	40.76	0.2	1
1	A	131	ASP	N	119.64	0.2	1
1	A	132	PHE	H	8.07	0.02	1
1	A	132	PHE	HA	4.55	0.02	1
1	A	132	PHE	HB2	3.15	0.02	2
1	A	132	PHE	HB3	3.05	0.02	2
1	A	132	PHE	HD1	7.25	0.02	1
1	A	132	PHE	HD2	7.25	0.02	1
1	A	132	PHE	C	176.03	0.2	1
1	A	132	PHE	CA	58.17	0.2	1
1	A	132	PHE	CB	39.34	0.2	1
1	A	132	PHE	CD1	131.71	0.2	1
1	A	132	PHE	CD2	131.71	0.2	1
1	A	132	PHE	N	120.51	0.2	1
1	A	133	GLN	H	8.24	0.02	1
1	A	133	GLN	HA	4.25	0.02	1
1	A	133	GLN	HB2	2.07	0.02	1
1	A	133	GLN	HB3	2.07	0.02	1
1	A	133	GLN	HE21	7.5	0.02	2
1	A	133	GLN	HE22	6.83	0.02	2
1	A	133	GLN	HG2	2.28	0.02	1
1	A	133	GLN	HG3	2.28	0.02	1
1	A	133	GLN	C	175.73	0.2	1
1	A	133	GLN	CA	56.05	0.2	1
1	A	133	GLN	CB	28.99	0.2	1
1	A	133	GLN	CD	180.27	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	GLN	CG	33.79	0.2	1
1	A	133	GLN	N	120.83	0.2	1
1	A	133	GLN	NE2	112.36	0.2	1
1	A	134	ASN	H	8.29	0.02	1
1	A	134	ASN	HA	4.72	0.02	1
1	A	134	ASN	HB2	2.76	0.02	2
1	A	134	ASN	HB3	2.88	0.02	2
1	A	134	ASN	HD21	7.69	0.02	2
1	A	134	ASN	HD22	6.93	0.02	2
1	A	134	ASN	C	175.41	0.2	1
1	A	134	ASN	CA	53.29	0.2	1
1	A	134	ASN	CB	38.85	0.2	1
1	A	134	ASN	CG	177.15	0.2	1
1	A	134	ASN	N	119.46	0.2	1
1	A	134	ASN	ND2	113.16	0.2	1
1	A	135	SER	H	8.28	0.02	1
1	A	135	SER	HA	4.42	0.02	1
1	A	135	SER	HB2	3.91	0.02	1
1	A	135	SER	HB3	3.91	0.02	1
1	A	135	SER	C	175.24	0.2	1
1	A	135	SER	CA	58.84	0.2	1
1	A	135	SER	CB	63.83	0.2	1
1	A	135	SER	N	116.3	0.2	1
1	A	136	GLY	H	8.47	0.02	1
1	A	136	GLY	HA2	3.98	0.02	1
1	A	136	GLY	HA3	3.98	0.02	1
1	A	136	GLY	C	174.28	0.2	1
1	A	136	GLY	CA	45.43	0.2	1
1	A	136	GLY	N	110.62	0.2	1
1	A	137	ASN	H	8.25	0.02	1
1	A	137	ASN	HA	4.73	0.02	1
1	A	137	ASN	HB2	2.83	0.02	1
1	A	137	ASN	HB3	2.83	0.02	1
1	A	137	ASN	HD21	7.62	0.02	2
1	A	137	ASN	HD22	6.94	0.02	2
1	A	137	ASN	C	175.51	0.2	1
1	A	137	ASN	CA	53.3	0.2	1
1	A	137	ASN	CB	38.85	0.2	1
1	A	137	ASN	CG	176.93	0.2	1
1	A	137	ASN	N	119.06	0.2	1
1	A	137	ASN	ND2	112.57	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	ALA	H	8.31	0.02	1
1	A	229	SER	H	8.23	0.02	1
1	A	229	SER	HA	4.39	0.02	1
1	A	229	SER	HB2	3.76	0.02	1
1	A	229	SER	HB3	3.76	0.02	1
1	A	229	SER	C	174.27	0.2	1
1	A	229	SER	CA	58.72	0.2	1
1	A	229	SER	CB	63.74	0.2	1
1	A	229	SER	N	116.28	0.2	1
1	A	230	ARG	H	8.44	0.02	1
1	A	230	ARG	HA	4.74	0.02	1
1	A	230	ARG	HB2	1.89	0.02	2
1	A	230	ARG	HB3	1.76	0.02	2
1	A	230	ARG	HD2	3.24	0.02	1
1	A	230	ARG	HD3	3.24	0.02	1
1	A	230	ARG	HG2	1.68	0.02	1
1	A	230	ARG	HG3	1.68	0.02	1
1	A	230	ARG	C	174.04	0.2	1
1	A	230	ARG	CA	53.59	0.2	1
1	A	230	ARG	CB	30.49	0.2	1
1	A	230	ARG	CD	43.81	0.2	1
1	A	230	ARG	CG	26.71	0.2	1
1	A	230	ARG	N	124.16	0.2	1
1	A	231	PRO	HA	4.46	0.02	1
1	A	231	PRO	HB2	2.32	0.02	2
1	A	231	PRO	HB3	1.99	0.02	2
1	A	231	PRO	HD2	3.67	0.02	2
1	A	231	PRO	HD3	3.82	0.02	2
1	A	231	PRO	HG2	2.08	0.02	2
1	A	231	PRO	HG3	2.01	0.02	2
1	A	231	PRO	C	176.24	0.2	1
1	A	231	PRO	CA	63.39	0.2	1
1	A	231	PRO	CB	31.82	0.2	1
1	A	231	PRO	CD	50.67	0.2	1
1	A	231	PRO	CG	27.22	0.2	1
1	A	232	GLN	H	8.03	0.02	1
1	A	232	GLN	HA	4.16	0.02	1
1	A	232	GLN	HB2	2.14	0.02	1
1	A	232	GLN	HB3	2.14	0.02	1
1	A	232	GLN	HE21	7.54	0.02	2
1	A	232	GLN	HE22	6.83	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	232	GLN	HG2	2.35	0.02	1
1	A	232	GLN	HG3	2.35	0.02	1
1	A	232	GLN	C	180.74	0.2	1
1	A	232	GLN	CA	57.32	0.2	1
1	A	232	GLN	CB	30.27	0.2	1
1	A	232	GLN	CD	181.35	0.2	1
1	A	232	GLN	CG	34.32	0.2	1
1	A	232	GLN	N	125.68	0.2	1
1	A	232	GLN	NE2	112.2	0.2	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
$^{13}\text{C}_\alpha$	159	$-0.31 \pm 0.22$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	155	$0.37 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	156	$-0.27 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	143	$1.14 \pm 0.35$	Should be applied

### 7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 96%, i.e. 1679 atoms were assigned a chemical shift out of a possible 1743. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	597/602 (99%)	239/240 (100%)	245/248 (99%)	113/114 (99%)
Sidechain	1008/1062 (95%)	678/696 (97%)	316/338 (93%)	14/28 (50%)
Aromatic	74/79 (94%)	37/39 (95%)	36/37 (97%)	1/3 (33%)
Overall	1679/1743 (96%)	954/975 (98%)	597/623 (96%)	128/145 (88%)

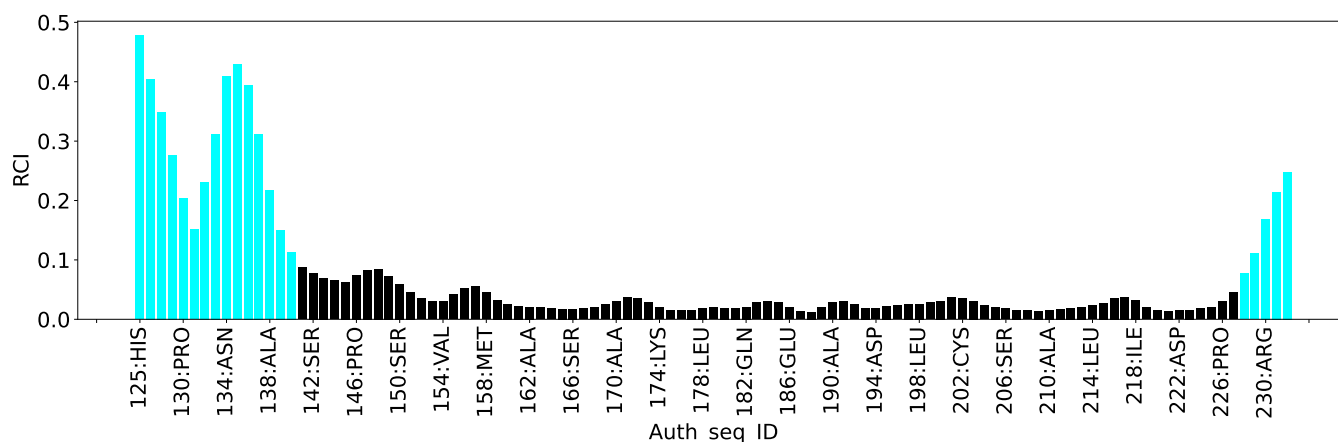
### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

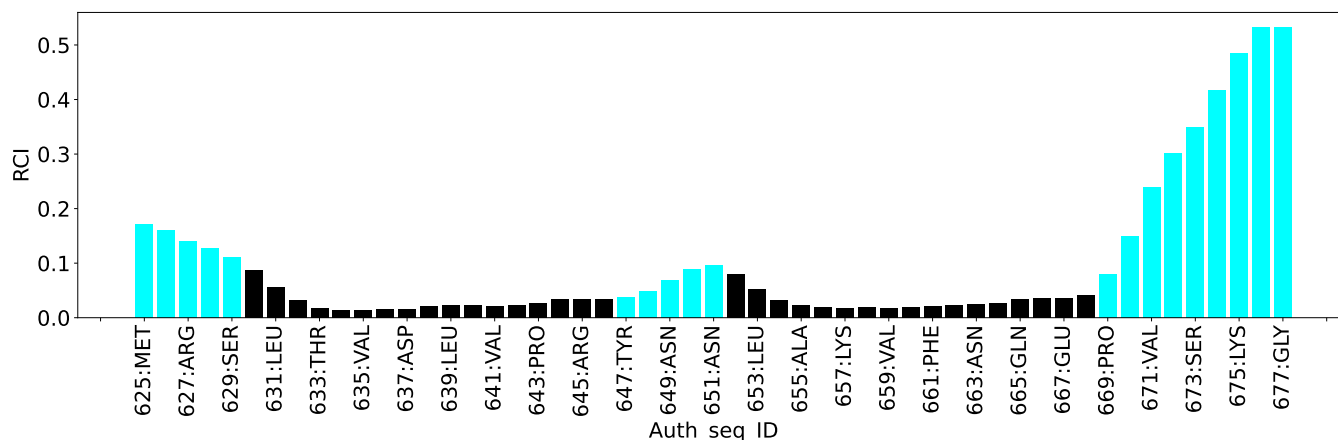
### 7.1.5 Random Coil Index (RCI) plots [i](#)

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 B:



## 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	4260
Intra-residue ( $ i-j =0$ )	1629
Sequential ( $ i-j =1$ )	765
Medium range ( $ i-j >1$ and $ i-j <5$ )	786
Long range ( $ i-j \geq 5$ )	382
Inter-chain	598
Hydrogen bond restraints	100
Disulfide bond restraints	0
Total dihedral-angle restraints	270
Number of unmapped restraints	253
Number of restraints per residue	28.0
Number of long range restraints per residue <sup>1</sup>	2.4

<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)	39.3	0.2
0.2-0.5 (Medium)	50.4	0.5
>0.5 (Large)	47.5	4.04

### 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)	6.7	5.23
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

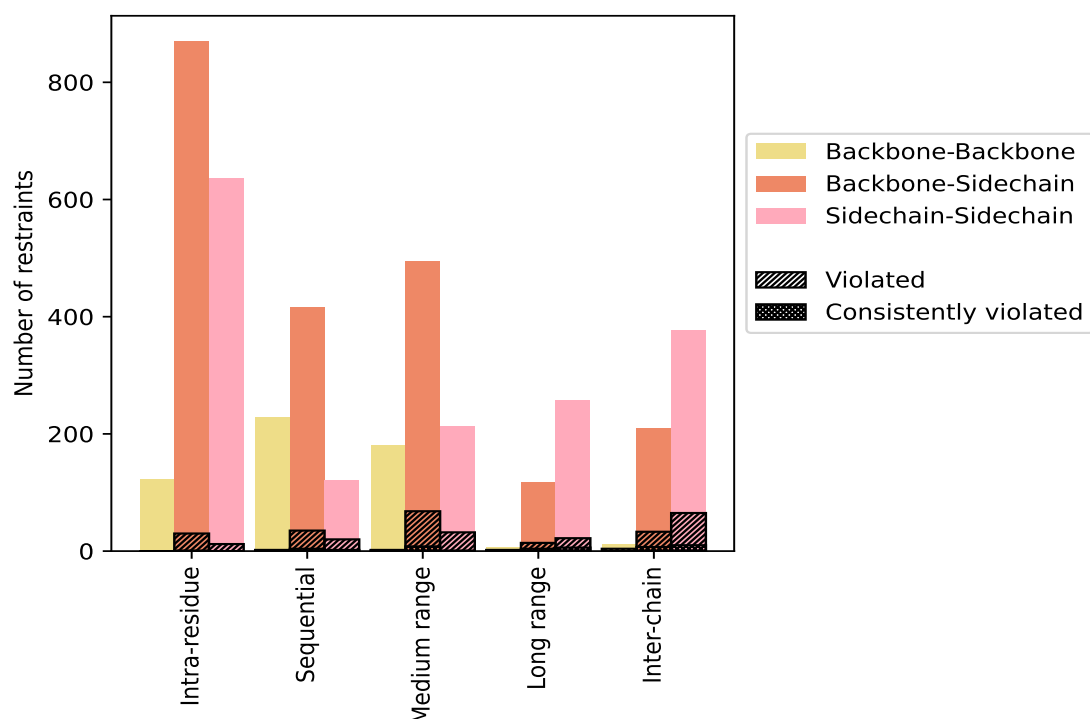
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>1629</b>	<b>38.2</b>	<b>42</b>	<b>2.6</b>	<b>1.0</b>	<b>1</b>	<b>0.1</b>	<b>0.0</b>
Backbone-Backbone	123	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	870	20.4	30	3.4	0.7	1	0.1	0.0
Sidechain-Sidechain	636	14.9	12	1.9	0.3	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>765</b>	<b>18.0</b>	<b>57</b>	<b>7.5</b>	<b>1.3</b>	<b>6</b>	<b>0.8</b>	<b>0.1</b>
Backbone-Backbone	228	5.4	2	0.9	0.0	0	0.0	0.0
Backbone-Sidechain	416	9.8	35	8.4	0.8	4	1.0	0.1
Sidechain-Sidechain	121	2.8	20	16.5	0.5	2	1.7	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>786</b>	<b>18.5</b>	<b>93</b>	<b>11.8</b>	<b>2.2</b>	<b>10</b>	<b>1.3</b>	<b>0.2</b>
Backbone-Backbone	180	4.2	2	1.1	0.0	1	0.6	0.0
Backbone-Sidechain	394	9.2	59	15.0	1.4	8	2.0	0.2
Sidechain-Sidechain	212	5.0	32	15.1	0.8	1	0.5	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>382</b>	<b>9.0</b>	<b>38</b>	<b>9.9</b>	<b>0.9</b>	<b>11</b>	<b>2.9</b>	<b>0.3</b>
Backbone-Backbone	7	0.2	2	28.6	0.0	1	14.3	0.0
Backbone-Sidechain	118	2.8	14	11.9	0.3	4	3.4	0.1
Sidechain-Sidechain	257	6.0	22	8.6	0.5	6	2.3	0.1
<b>Inter-chain</b>	<b>598</b>	<b>14.0</b>	<b>102</b>	<b>17.1</b>	<b>2.4</b>	<b>17</b>	<b>2.8</b>	<b>0.4</b>
Backbone-Backbone	12	0.3	4	33.3	0.1	0	0.0	0.0
Backbone-Sidechain	209	4.9	33	15.8	0.8	7	3.3	0.2
Sidechain-Sidechain	377	8.8	65	17.2	1.5	10	2.7	0.2
<b>Hydrogen bond</b>	<b>100</b>	<b>2.3</b>	<b>9</b>	<b>9.0</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</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>4260</b>	<b>100.0</b>	<b>341</b>	<b>8.0</b>	<b>8.0</b>	<b>45</b>	<b>1.1</b>	<b>1.1</b>
Backbone-Backbone	550	12.9	10	1.8	0.2	2	0.4	0.0
Backbone-Sidechain	2107	49.5	180	8.5	4.2	24	1.1	0.6
Sidechain-Sidechain	1603	37.6	151	9.4	3.5	19	1.2	0.4

<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](#)

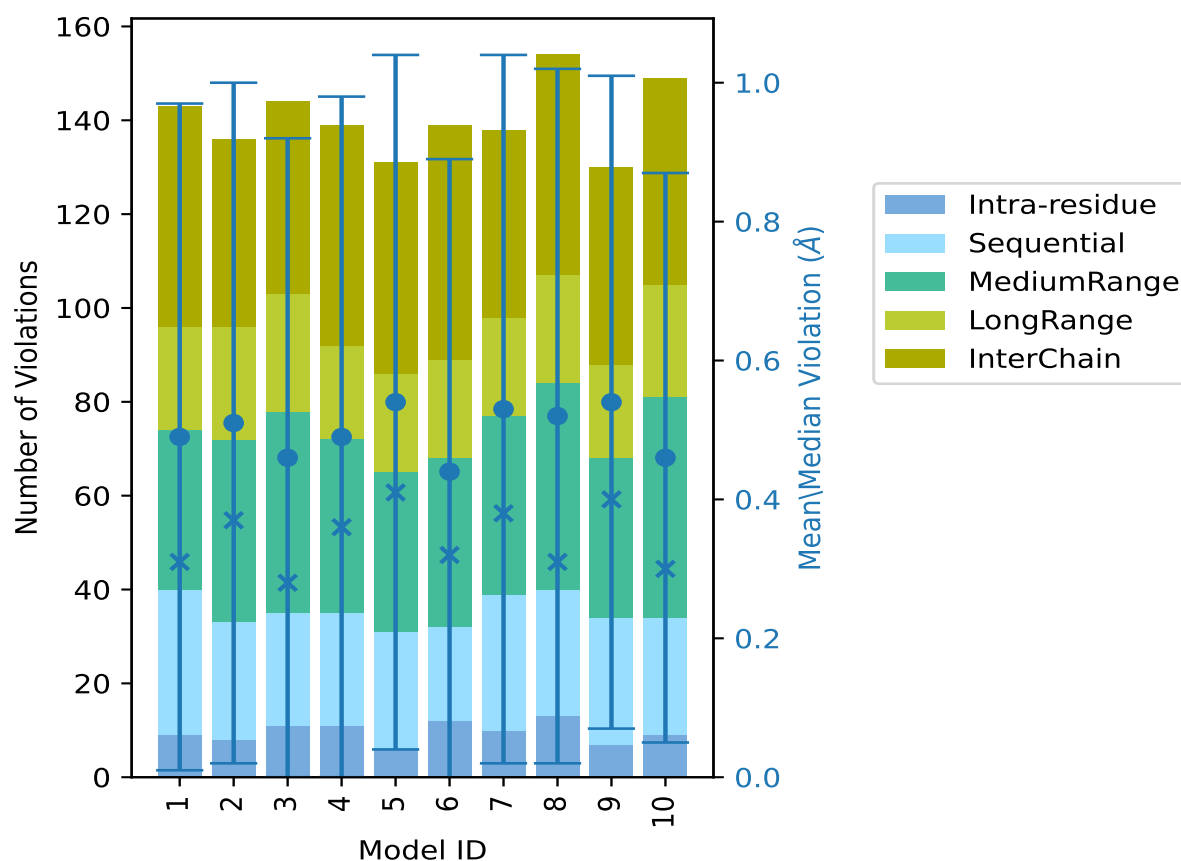
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	9	31	34	22	47	143	0.49	3.21	0.48	0.31
2	8	25	39	24	40	136	0.51	3.33	0.49	0.37
3	11	24	43	25	41	144	0.46	3.1	0.46	0.28
4	11	24	37	20	47	139	0.49	4.02	0.49	0.36
5	6	25	34	21	45	131	0.54	2.69	0.5	0.41
6	12	20	36	21	50	139	0.44	3.46	0.45	0.32
7	10	29	38	21	40	138	0.53	4.04	0.51	0.38
8	13	27	44	23	47	154	0.52	3.18	0.5	0.31
9	7	27	34	20	42	130	0.54	3.08	0.47	0.4
10	9	25	47	24	44	149	0.46	2.08	0.41	0.3



<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, 3828(IR:1587, SQ:708, MR:693, LR:344, IC:496) 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>	%
20	17	32	8	37	114	1	10.0
6	6	13	7	11	43	2	20.0
5	4	10	3	8	30	3	30.0

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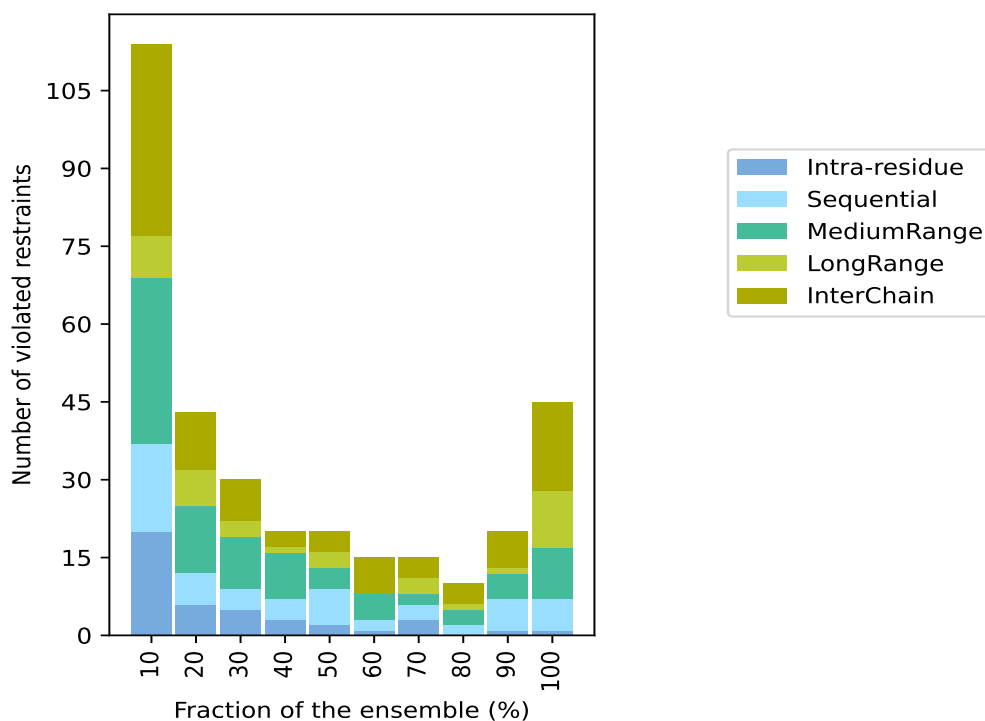
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
3	4	9	1	3	20	4	40.0
2	7	4	3	4	20	5	50.0
1	2	5	0	7	15	6	60.0
3	3	2	3	4	15	7	70.0
0	2	3	1	4	10	8	80.0
1	6	5	1	7	20	9	90.0
1	6	10	11	17	45	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 ⓘ

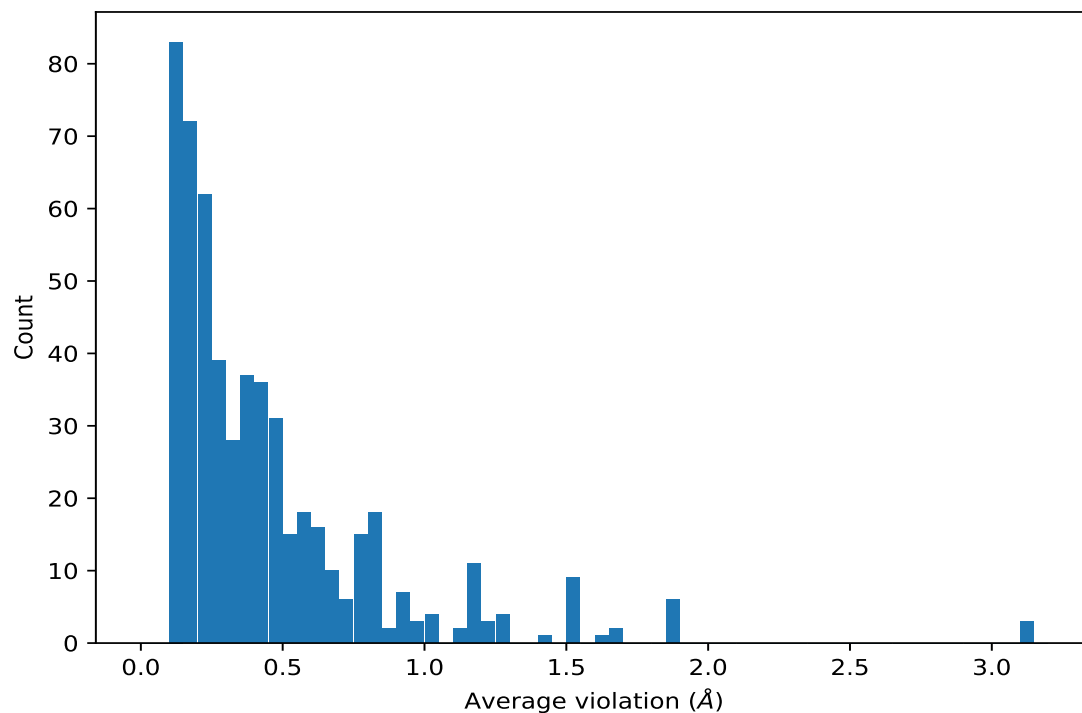


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



#### 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)
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	10	3.13	0.77	3.2
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	10	3.13	0.77	3.2
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	10	3.13	0.77	3.2
(1,3542)	2:644:B:LYS:HB3	1:156:A:ILE:HD11	10	1.88	0.18	1.88
(1,3542)	2:644:B:LYS:HB3	1:156:A:ILE:HD12	10	1.88	0.18	1.88
(1,3542)	2:644:B:LYS:HB3	1:156:A:ILE:HD13	10	1.88	0.18	1.88
(1,3542)	2:644:B:LYS:HB3	1:165:A:ILE:HD11	10	1.88	0.18	1.88
(1,3542)	2:644:B:LYS:HB3	1:165:A:ILE:HD12	10	1.88	0.18	1.88
(1,3542)	2:644:B:LYS:HB3	1:165:A:ILE:HD13	10	1.88	0.18	1.88
(1,557)	2:634:B:GLU:HB3	1:184:A:PHE:HB3	10	1.68	0.38	1.9
(1,557)	2:634:B:GLU:HB2	1:184:A:PHE:HB3	10	1.68	0.38	1.9
(1,3199)	1:192:A:PRO:HB3	2:660:B:ASN:HA	10	1.64	0.26	1.74
(1,3600)	1:204:A:GLN:HA	2:638:B:LEU:HG	10	1.41	0.09	1.44
(1,3058)	1:141:A:LEU:HD11	1:200:A:GLU:HB3	10	1.22	0.66	1.34
(1,3058)	1:141:A:LEU:HD12	1:200:A:GLU:HB3	10	1.22	0.66	1.34

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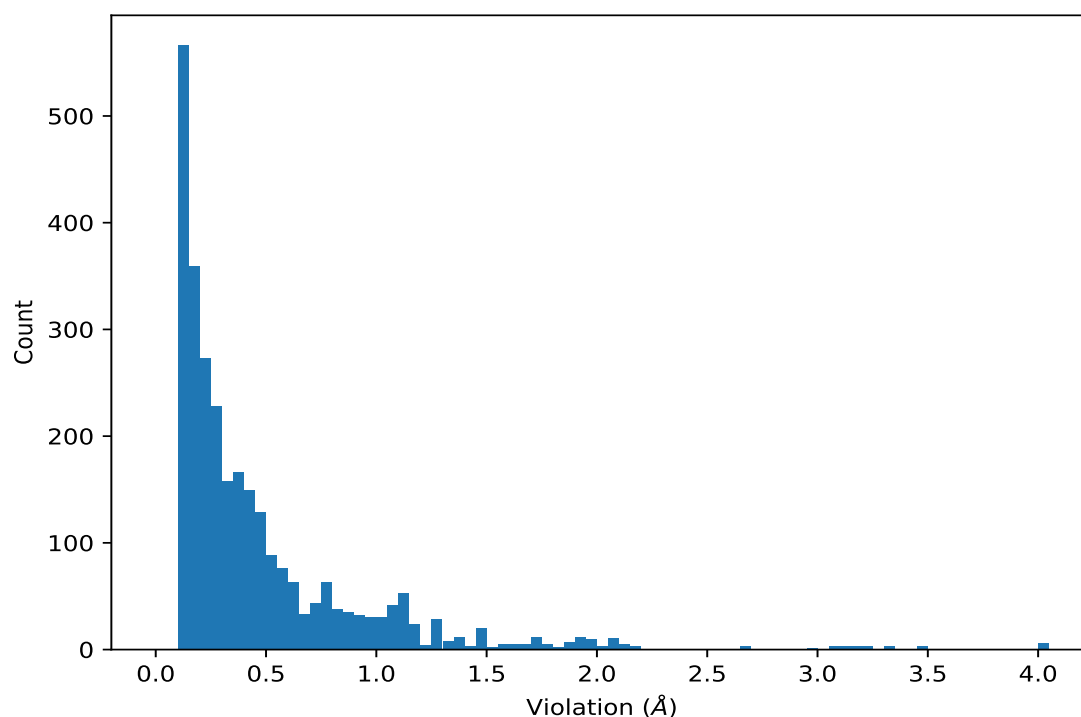
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3058)	1:141:A:LEU:HD13	1:200:A:GLU:HB3	10	1.22	0.66	1.34
(1,3658)	2:635:B:VAL:HG11	1:141:A:LEU:HD21	10	1.16	0.14	1.12
(1,3658)	2:635:B:VAL:HG11	1:141:A:LEU:HD22	10	1.16	0.14	1.12
(1,3658)	2:635:B:VAL:HG11	1:141:A:LEU:HD23	10	1.16	0.14	1.12
(1,3658)	2:635:B:VAL:HG12	1:141:A:LEU:HD21	10	1.16	0.14	1.12
(1,3658)	2:635:B:VAL:HG12	1:141:A:LEU:HD22	10	1.16	0.14	1.12
(1,3658)	2:635:B:VAL:HG12	1:141:A:LEU:HD23	10	1.16	0.14	1.12
(1,3658)	2:635:B:VAL:HG13	1:141:A:LEU:HD21	10	1.16	0.14	1.12
(1,3658)	2:635:B:VAL:HG13	1:141:A:LEU:HD22	10	1.16	0.14	1.12
(1,3658)	2:635:B:VAL:HG13	1:141:A:LEU:HD23	10	1.16	0.14	1.12
(1,3208)	1:147:A:GLU:HG2	1:144:A:LYS:HA	10	1.15	0.39	1.15
(1,3208)	1:193:A:GLU:HG2	1:196:A:ALA:HA	10	1.15	0.39	1.15
(2,54)	2:646:B:GLN:H	1:203:A:PRO:HD3	10	1.0	0.35	1.13
(1,585)	1:140:A:PHE:HZ	1:145:A:PHE:HB3	10	0.98	0.15	0.99

<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

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)
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	7	4.04
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	7	4.04
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	7	4.04
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	4	4.02
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	4	4.02
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	4	4.02
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	6	3.46
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	6	3.46
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	6	3.46
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	2	3.33
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	2	3.33
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	2	3.33
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	1	3.21
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	1	3.21
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	1	3.21
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	8	3.18
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	8	3.18
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	8	3.18
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	3	3.1
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	3	3.1
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	3	3.1
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	9	3.08
(1,3065)	2:652:B:LEU:HD22	2:643:B:PRO:HB3	9	3.08
(1,3065)	2:652:B:LEU:HD23	2:643:B:PRO:HB3	9	3.08
(1,3513)	2:640:B:SER:HB2	1:204:A:GLN:HG3	2	2.95
(1,3065)	2:652:B:LEU:HD21	2:643:B:PRO:HB3	5	2.69

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

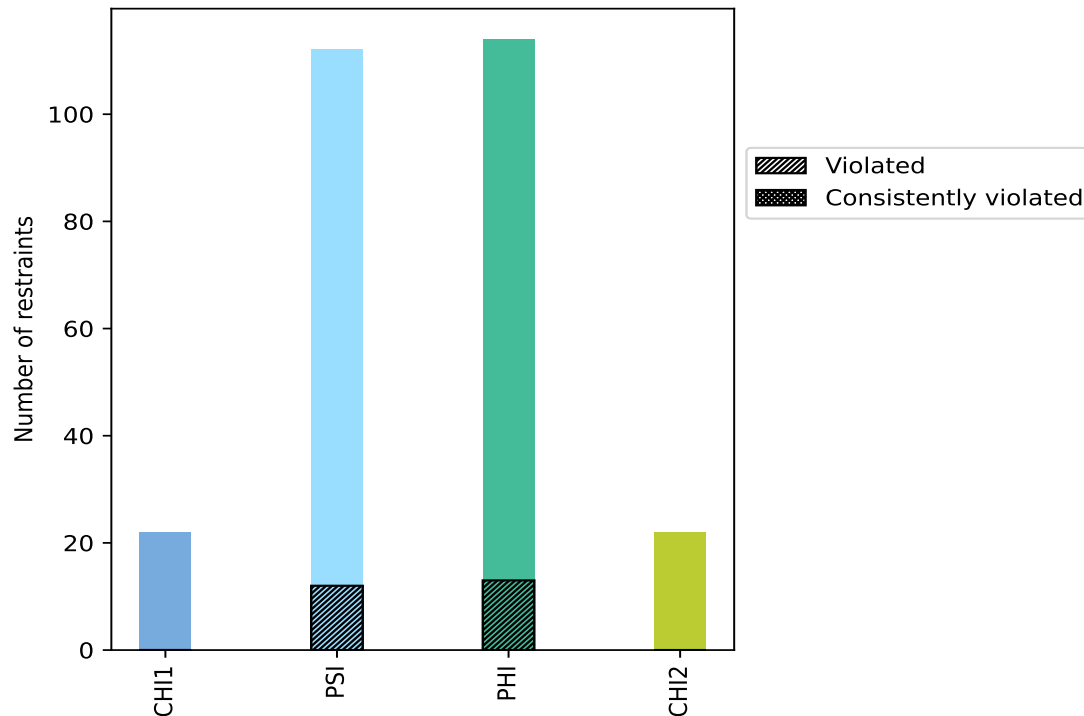
### 10.1 Summary of dihedral-angle violations [i](#)

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>
CHI1	22	8.1	0	0.0	0.0	0	0.0	0.0
PSI	112	41.5	12	10.7	4.4	0	0.0	0.0
PHI	114	42.2	13	11.4	4.8	0	0.0	0.0
CHI2	22	8.1	0	0.0	0.0	0	0.0	0.0
Total	270	100.0	25	9.3	9.3	0	0.0	0.0

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

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



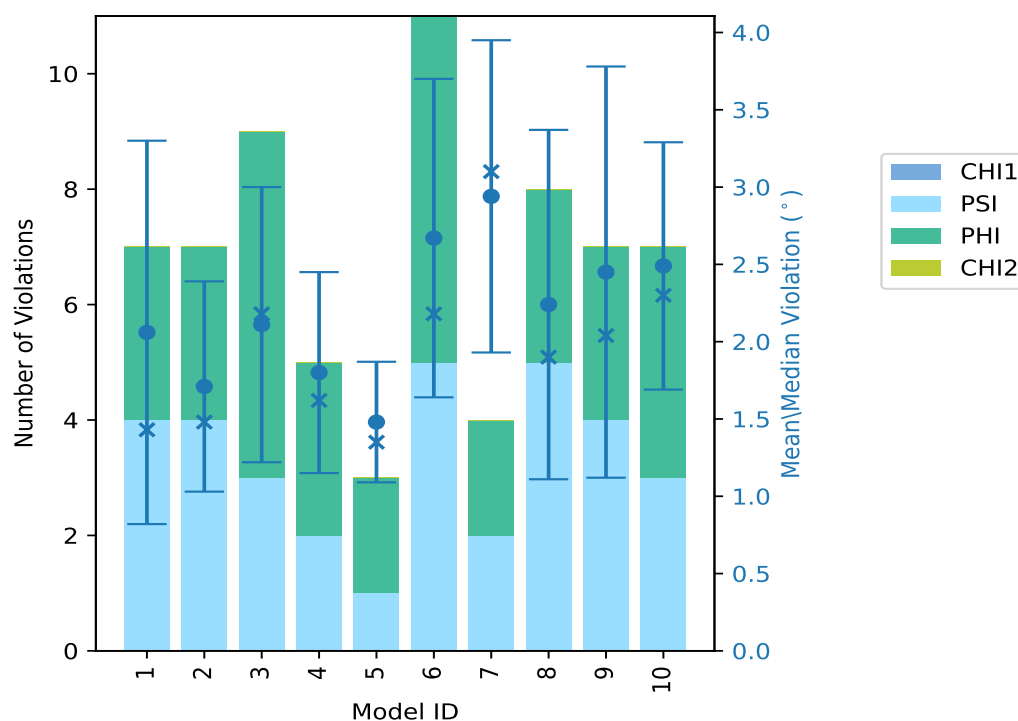
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°)
	CHI1	PSI	PHI	CHI2	Total				
1	0	4	3	0	7	2.06	4.82	1.24	1.43
2	0	4	3	0	7	1.71	3.2	0.68	1.48
3	0	3	6	0	9	2.11	3.25	0.89	2.18
4	0	2	3	0	5	1.8	2.94	0.65	1.62
5	0	1	2	0	3	1.48	2.01	0.39	1.35
6	0	5	6	0	11	2.67	4.46	1.03	2.18
7	0	2	2	0	4	2.94	3.94	1.01	3.1
8	0	5	3	0	8	2.24	5.12	1.13	1.9
9	0	4	3	0	7	2.45	5.23	1.33	2.04
10	0	3	4	0	7	2.49	4.09	0.8	2.3

### 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

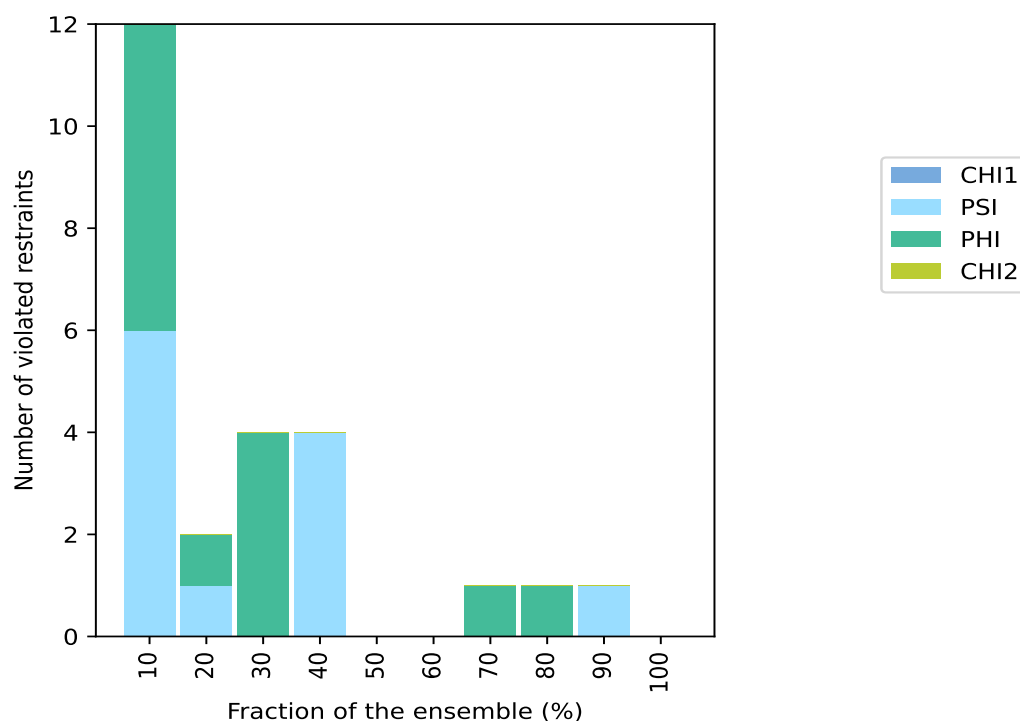
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
CHI1	PSI	PHI	CHI2	Total	Count <sup>1</sup>	%
0	6	6	0	12	1	10.0
0	1	1	0	2	2	20.0
0	0	4	0	4	3	30.0
0	4	0	0	4	4	40.0
0	0	0	0	0	5	50.0
0	0	0	0	0	6	60.0
0	0	1	0	1	7	70.0
0	0	1	0	1	8	80.0
0	1	0	0	1	9	90.0
0	0	0	0	0	10	100.0

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

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

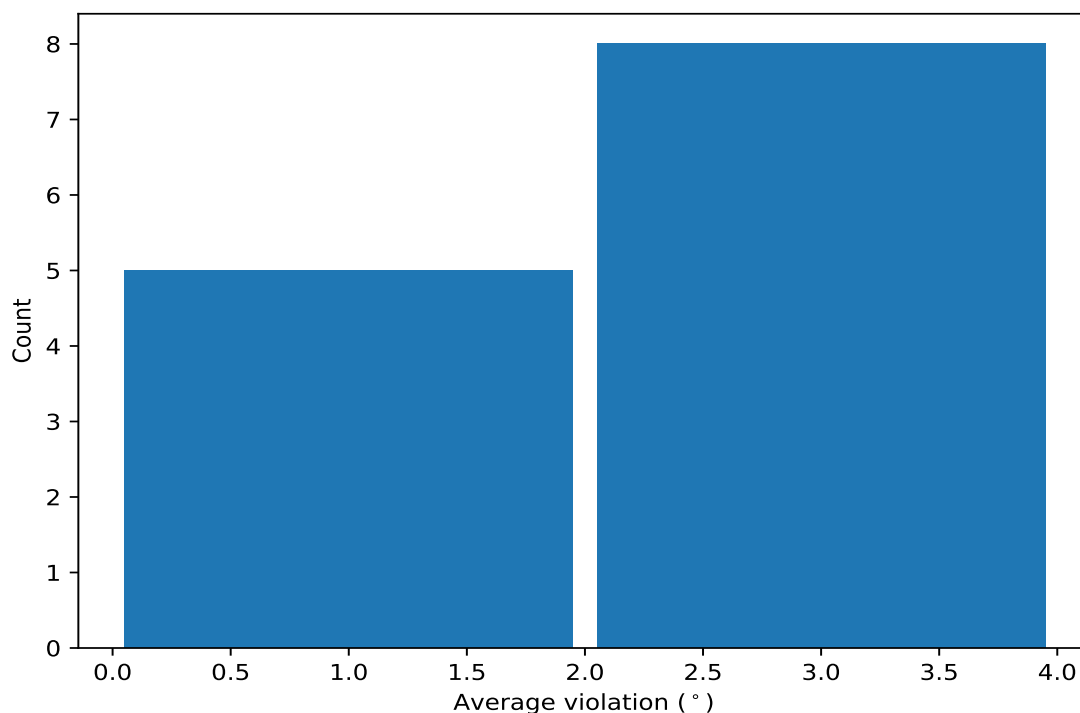




## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

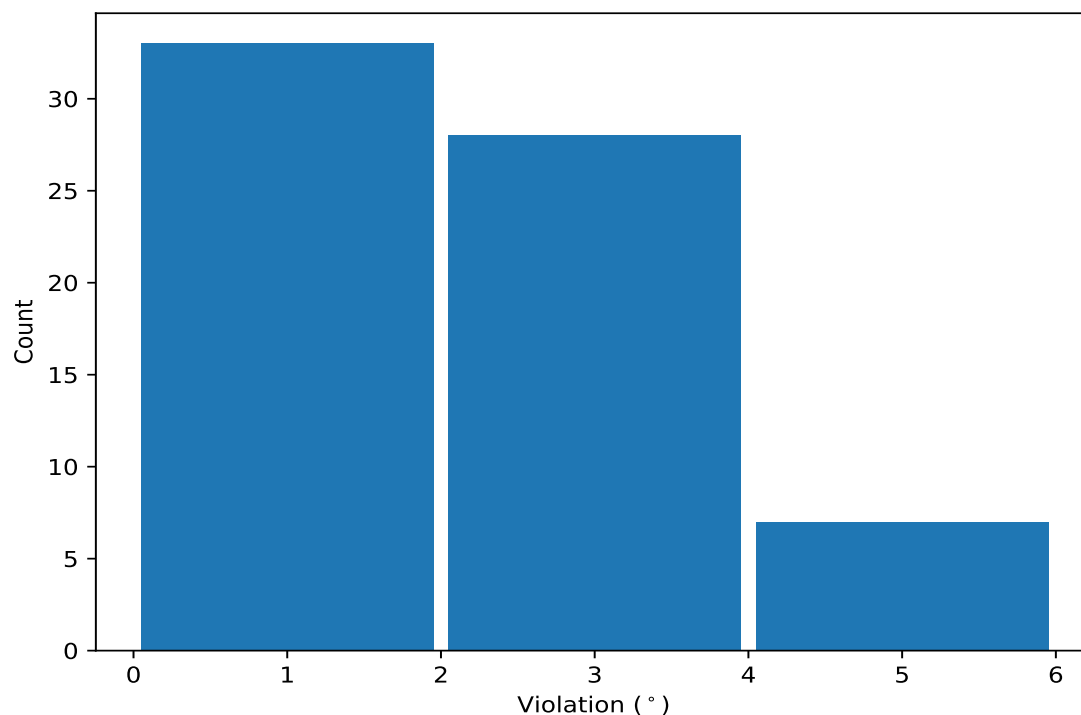
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,45)	1:167:A:SER:N	1:167:A:SER:CA	1:167:A:SER:C	1:168:A:GLU:N	9	2.69	1.27	2.63
(1,216)	2:663:B:ASN:C	2:664:B:ASP:N	2:664:B:ASP:CA	2:664:B:ASP:C	8	1.71	0.37	1.8
(1,150)	1:222:A:ASP:C	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	7	1.72	0.62	1.56
(1,195)	2:653:B:LEU:N	2:653:B:LEU:CA	2:653:B:LEU:C	2:654:B:ASP:N	4	3.57	1.51	3.88
(1,16)	1:147:A:GLU:N	1:147:A:GLU:CA	1:147:A:GLU:C	1:148:A:LEU:N	4	2.45	1.32	2.13
(1,25)	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	1:156:A:ILE:N	4	2.04	1.17	1.62
(1,51)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:LYS:N	4	1.9	0.11	1.92
(1,198)	2:654:B:ASP:C	2:655:B:ALA:N	2:655:B:ALA:CA	2:655:B:ALA:C	3	3.02	0.79	2.75
(1,46)	1:167:A:SER:C	1:168:A:GLU:N	1:168:A:GLU:CA	1:168:A:GLU:C	3	2.92	1.01	3.06
(1,196)	2:653:B:LEU:C	2:654:B:ASP:N	2:654:B:ASP:CA	2:654:B:ASP:C	3	2.55	0.3	2.4

<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 (°)
(1,45)	1:167:A:SER:N	1:167:A:SER:CA	1:167:A:SER:C	1:168:A:GLU:N	9	5.23
(1,195)	2:653:B:LEU:N	2:653:B:LEU:CA	2:653:B:LEU:C	2:654:B:ASP:N	8	5.12
(1,195)	2:653:B:LEU:N	2:653:B:LEU:CA	2:653:B:LEU:C	2:654:B:ASP:N	1	4.82
(1,16)	1:147:A:GLU:N	1:147:A:GLU:CA	1:147:A:GLU:C	1:148:A:LEU:N	6	4.46
(1,6)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:SER:N	6	4.11
(1,198)	2:654:B:ASP:C	2:655:B:ALA:N	2:655:B:ALA:CA	2:655:B:ALA:C	10	4.09
(1,46)	1:167:A:SER:C	1:168:A:GLU:N	1:168:A:GLU:CA	1:168:A:GLU:C	6	4.07
(1,25)	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	1:156:A:ILE:N	7	3.94
(1,45)	1:167:A:SER:N	1:167:A:SER:CA	1:167:A:SER:C	1:168:A:GLU:N	7	3.92
(1,149)	1:222:A:ASP:N	1:222:A:ASP:CA	1:222:A:ASP:C	1:223:A:ASP:N	9	3.32