



# wwPDB NMR Structure Validation Summary Report ⓘ

Dec 24, 2024 – 01:16 PM EST

PDB ID : 2KHS  
BMRB ID : 15357  
Title : Solution structure of SNase121:SNase(111-143) complex  
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Deposited on : 2009-04-10

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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 : 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

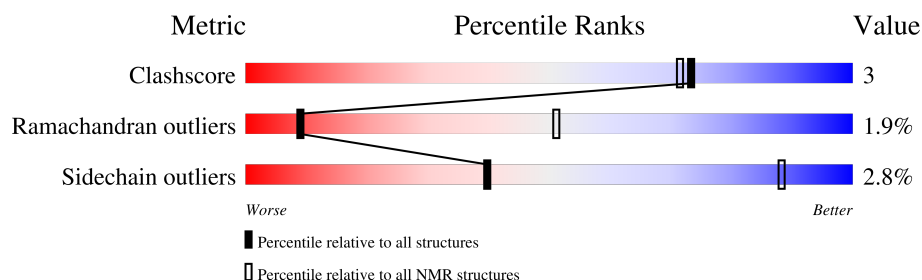
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 62%.

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	121	
2	B	35	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:8-A:41, A:55-A:82, A:87-A:112, B:134-B:156 (111)	0.90	17

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2530 atoms, of which 1286 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thermonuclease.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1955	611	999	165	176	4	

- Molecule 2 is a protein called Nuclease.

Mol	Chain	Residues	Atoms					Trace
2	B	35	Total	C	H	N	O	0
			575	180	287	51	57	

There are 2 discrepancies between the modelled and reference sequences:

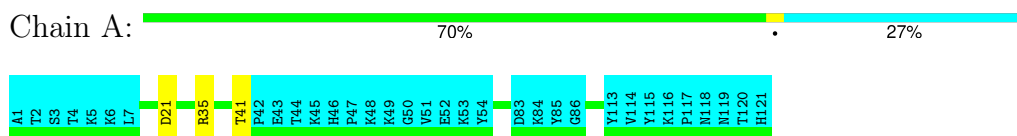
Chain	Residue	Modelled	Actual	Comment	Reference
B	122	GLY	-	expression tag	UNP Q1WCB7
B	123	SER	-	expression tag	UNP Q1WCB7

## 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: Thermonuclease



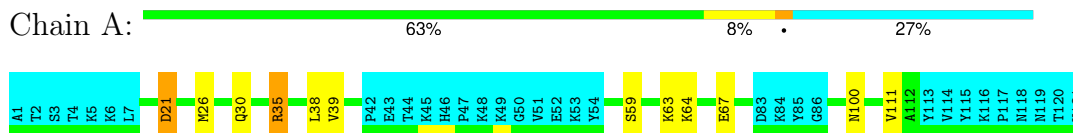
- Molecule 2: Nuclease



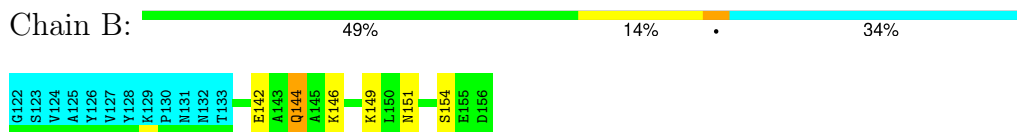
### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 17. Colouring as in section 4.1 above.

- Molecule 1: Thermonuclease



- Molecule 2: Nuclease



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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	1.2
CNS	refinement	1.2

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	1627
Number of shifts mapped to atoms	1264
Number of unparsed shifts	0
Number of shifts with mapping errors	363
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	62%

## 6 Model quality [i](#)

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

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.4±0.5
All	All	0	8

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	35	ARG	Sidechain	3
1	A	81	ARG	Sidechain	2
1	A	87	ARG	Sidechain	2
1	A	105	ARG	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	A	683	719	718	3±2
2	B	196	197	196	2±1
All	All	17580	18320	18280	112

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 3.

5 of 62 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ASP:OD2	1:A:35:ARG:HD2	0.60	1.97	4	1
1:A:21:ASP:OD1	1:A:35:ARG:HD2	0.59	1.97	5	3
1:A:22:THR:HA	1:A:34:PHE:O	0.55	2.00	9	2
2:B:142:GLU:O	2:B:146:LYS:HG3	0.55	2.01	13	14
1:A:101:GLU:O	1:A:105:ARG:HG2	0.55	2.00	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	A	88/121 (73%)	83±2 (95±2%)	4±2 (4±2%)	1±1 (1±1%)	13	60
2	B	22/35 (63%)	20±1 (93±3%)	1±1 (3±3%)	1±0 (5±0%)	3	27
All	All	2200/3120 (71%)	2074 (94%)	84 (4%)	42 (2%)	9	51

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	151	ASN	20
1	A	21	ASP	12
1	A	41	THR	7
1	A	79	GLY	3

### 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	71/101 (70%)	69±1 (97±2%)	2±1 (3±2%)	37	86
2	B	21/31 (68%)	21±0 (98±2%)	0±0 (2±2%)	52	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1840/2640 (70%)	1788 (97%)	52 (3%)	40 88

5 of 28 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	22	THR	6
1	A	87	ARG	4
1	A	35	ARG	4
1	A	65	MET	3
1	A	78	LYS	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 62% for the well-defined parts and 58% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_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	1627
Number of shifts mapped to atoms	1264
Number of unparsed shifts	0
Number of shifts with mapping errors	363
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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 363) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	124	VAL	H	8.28	0.02	1
1	A	124	VAL	HA	4.15	0.02	1
1	A	124	VAL	HB	2.03	0.02	1
1	A	124	VAL	HG21	0.89	0.02	2
1	A	124	VAL	HG22	0.89	0.02	2
1	A	124	VAL	HG23	0.89	0.02	2
1	A	124	VAL	CA	62.1	0.2	1
1	A	124	VAL	CB	32.8	0.2	1
1	A	124	VAL	CG1	20.4	0.2	2
1	A	124	VAL	N	122.1	0.2	1
1	A	125	ALA	H	8.36	0.02	1
1	A	125	ALA	HA	4.3	0.02	1
1	A	125	ALA	HB1	1.31	0.02	1
1	A	125	ALA	HB2	1.31	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	ALA	HB3	1.31	0.02	1
1	A	125	ALA	C	177.0	0.2	1
1	A	125	ALA	CA	52.2	0.2	1
1	A	125	ALA	CB	19.2	0.2	1
1	A	125	ALA	N	128.2	0.2	1
1	A	126	TYR	H	8.16	0.02	1
1	A	126	TYR	HA	4.48	0.02	1
1	A	126	TYR	HB2	2.92	0.02	2
1	A	126	TYR	HD1	6.99	0.02	1
1	A	126	TYR	HE1	6.75	0.02	1
1	A	126	TYR	C	175.1	0.2	1
1	A	126	TYR	CA	58.1	0.2	1
1	A	126	TYR	CB	39.0	0.2	1
1	A	126	TYR	N	120.7	0.2	1
1	A	127	VAL	H	7.83	0.02	1
1	A	127	VAL	HA	4.0	0.02	1
1	A	127	VAL	HB	1.87	0.02	1
1	A	127	VAL	HG21	0.84	0.02	2
1	A	127	VAL	HG22	0.84	0.02	2
1	A	127	VAL	HG23	0.84	0.02	2
1	A	127	VAL	C	174.8	0.2	1
1	A	127	VAL	CA	61.8	0.2	1
1	A	127	VAL	CB	33.3	0.2	1
1	A	127	VAL	CG1	20.7	0.2	2
1	A	127	VAL	N	124.1	0.2	1
1	A	128	TYR	H	8.31	0.02	1
1	A	128	TYR	HA	4.49	0.02	1
1	A	128	TYR	HB2	2.87	0.02	2
1	A	128	TYR	HB3	2.95	0.02	2
1	A	128	TYR	HD2	7.15	0.02	1
1	A	128	TYR	HE2	6.82	0.02	1
1	A	128	TYR	C	174.9	0.2	1
1	A	128	TYR	CA	58.1	0.2	1
1	A	128	TYR	CB	39.2	0.2	1
1	A	128	TYR	N	125.4	0.2	1
1	A	129	LYS	H	8.21	0.02	1
1	A	129	LYS	HA	4.48	0.02	1
1	A	129	LYS	HB2	1.71	0.02	2
1	A	129	LYS	HB3	1.6	0.02	2
1	A	129	LYS	HD2	1.5	0.02	2
1	A	129	LYS	HE3	2.99	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	LYS	HG2	1.37	0.02	2
1	A	129	LYS	HG3	1.45	0.02	2
1	A	129	LYS	C	173.5	0.2	1
1	A	129	LYS	CA	53.5	0.2	1
1	A	129	LYS	CB	33.1	0.2	1
1	A	129	LYS	CD	29.0	0.2	1
1	A	129	LYS	CE	42.0	0.2	1
1	A	129	LYS	CG	24.5	0.2	1
1	A	129	LYS	N	126.2	0.2	1
1	A	130	PRO	HA	4.23	0.02	1
1	A	130	PRO	HB2	2.19	0.02	2
1	A	130	PRO	HB3	1.97	0.02	2
1	A	130	PRO	HD2	3.58	0.02	2
1	A	130	PRO	HD3	3.45	0.02	2
1	A	130	PRO	HG2	1.62	0.02	2
1	A	130	PRO	C	175.2	0.2	1
1	A	130	PRO	CA	62.3	0.2	1
1	A	130	PRO	CB	32.2	0.2	1
1	A	131	ASN	H	8.47	0.02	1
1	A	131	ASN	HA	4.91	0.02	1
1	A	131	ASN	HB2	2.8	0.02	2
1	A	131	ASN	C	175.1	0.2	1
1	A	131	ASN	CA	51.6	0.2	1
1	A	131	ASN	CB	38.6	0.2	1
1	A	131	ASN	N	120.9	0.2	1
1	A	132	ASN	H	7.71	0.02	1
1	A	132	ASN	HA	4.99	0.02	1
1	A	132	ASN	HB2	2.42	0.02	2
1	A	132	ASN	HB3	3.45	0.02	2
1	A	132	ASN	C	177.5	0.2	1
1	A	132	ASN	CA	51.4	0.2	1
1	A	132	ASN	CB	39.5	0.2	1
1	A	132	ASN	N	117.8	0.2	1
1	A	133	THR	H	10.32	0.02	1
1	A	133	THR	HA	3.81	0.02	1
1	A	133	THR	HB	3.75	0.02	1
1	A	133	THR	HG21	0.68	0.02	1
1	A	133	THR	HG22	0.68	0.02	1
1	A	133	THR	HG23	0.68	0.02	1
1	A	133	THR	C	176.3	0.2	1
1	A	133	THR	CA	69.4	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	THR	CB	67.4	0.2	1
1	A	133	THR	CG2	21.1	0.2	1
1	A	133	THR	N	122.9	0.2	1
1	A	134	HIS	H	6.93	0.02	1
1	A	134	HIS	HA	5.41	0.02	1
1	A	134	HIS	HB2	2.31	0.02	2
1	A	134	HIS	HB3	3.23	0.02	2
1	A	134	HIS	C	174.8	0.2	1
1	A	134	HIS	CA	53.9	0.2	1
1	A	134	HIS	CB	29.6	0.2	1
1	A	134	HIS	N	113.4	0.2	1
1	A	135	GLU	H	7.5	0.02	1
1	A	135	GLU	HA	3.74	0.02	1
1	A	135	GLU	HB2	2.21	0.02	2
1	A	135	GLU	HB3	1.99	0.02	2
1	A	135	GLU	HG2	2.21	0.02	2
1	A	135	GLU	C	177.2	0.2	1
1	A	135	GLU	CA	61.7	0.2	1
1	A	135	GLU	CB	30.2	0.2	1
1	A	135	GLU	CG	35.8	0.2	1
1	A	135	GLU	N	120.7	0.2	1
1	A	136	GLN	H	8.87	0.02	1
1	A	136	GLN	HA	4.03	0.02	1
1	A	136	GLN	HB2	1.96	0.02	2
1	A	136	GLN	HB3	2.14	0.02	2
1	A	136	GLN	HG2	2.51	0.02	2
1	A	136	GLN	HG3	2.45	0.02	2
1	A	136	GLN	C	178.3	0.2	1
1	A	136	GLN	CA	59.7	0.2	1
1	A	136	GLN	CB	27.4	0.2	1
1	A	136	GLN	CG	33.9	0.2	1
1	A	136	GLN	N	117.2	0.2	1
1	A	137	LEU	H	7.97	0.02	1
1	A	137	LEU	HA	4.11	0.02	1
1	A	137	LEU	HB2	1.79	0.02	2
1	A	137	LEU	HB3	1.84	0.02	2
1	A	137	LEU	HD11	0.72	0.02	1
1	A	137	LEU	HD12	0.72	0.02	1
1	A	137	LEU	HD13	0.72	0.02	1
1	A	137	LEU	HD21	0.87	0.02	1
1	A	137	LEU	HD22	0.87	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	LEU	HD23	0.87	0.02	1
1	A	137	LEU	HG	1.51	0.02	1
1	A	137	LEU	C	179.0	0.2	1
1	A	137	LEU	CA	58.6	0.2	1
1	A	137	LEU	CB	42.0	0.2	1
1	A	137	LEU	CD1	24.3	0.2	2
1	A	137	LEU	CG	26.8	0.2	1
1	A	137	LEU	N	122.5	0.2	1
1	A	138	LEU	H	8.17	0.02	1
1	A	138	LEU	HA	4.0	0.02	1
1	A	138	LEU	HB2	1.51	0.02	2
1	A	138	LEU	HB3	1.97	0.02	2
1	A	138	LEU	HD11	0.75	0.02	1
1	A	138	LEU	HD12	0.75	0.02	1
1	A	138	LEU	HD13	0.75	0.02	1
1	A	138	LEU	HD21	0.92	0.02	1
1	A	138	LEU	HD22	0.92	0.02	1
1	A	138	LEU	HD23	0.92	0.02	1
1	A	138	LEU	C	179.1	0.2	1
1	A	138	LEU	CA	58.8	0.2	1
1	A	138	LEU	CB	41.1	0.2	1
1	A	138	LEU	CD1	23.6	0.2	2
1	A	138	LEU	CG	26.3	0.2	1
1	A	138	LEU	N	119.5	0.2	1
1	A	139	ARG	H	8.96	0.02	1
1	A	139	ARG	HA	4.05	0.02	1
1	A	139	ARG	HB2	1.95	0.02	2
1	A	139	ARG	HB3	2.05	0.02	2
1	A	139	ARG	HD2	3.25	0.02	2
1	A	139	ARG	HD3	3.14	0.02	2
1	A	139	ARG	HG2	1.72	0.02	2
1	A	139	ARG	HG3	1.75	0.02	2
1	A	139	ARG	C	179.7	0.2	1
1	A	139	ARG	CA	60.1	0.2	1
1	A	139	ARG	CB	29.4	0.2	1
1	A	139	ARG	CD	43.0	0.2	1
1	A	139	ARG	N	119.3	0.2	1
1	A	140	LYS	H	8.13	0.02	1
1	A	140	LYS	HA	4.18	0.02	1
1	A	140	LYS	HB2	1.71	0.02	2
1	A	140	LYS	HB3	2.06	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	140	LYS	HD2	1.64	0.02	2
1	A	140	LYS	HE2	2.97	0.02	2
1	A	140	LYS	HG2	0.88	0.02	2
1	A	140	LYS	HG3	1.45	0.02	2
1	A	140	LYS	C	179.8	0.2	1
1	A	140	LYS	CA	60.0	0.2	1
1	A	140	LYS	CB	31.9	0.2	1
1	A	140	LYS	CD	29.1	0.2	1
1	A	140	LYS	CE	41.9	0.2	1
1	A	140	LYS	CG	25.1	0.2	1
1	A	140	LYS	N	122.1	0.2	1
1	A	141	SER	H	7.83	0.02	1
1	A	141	SER	HA	4.34	0.02	1
1	A	141	SER	HB2	3.65	0.02	2
1	A	141	SER	HB3	4.1	0.02	2
1	A	141	SER	C	175.4	0.2	1
1	A	141	SER	CA	64.0	0.2	1
1	A	141	SER	CB	62.6	0.2	1
1	A	141	SER	N	118.5	0.2	1
1	A	142	GLU	H	8.61	0.02	1
1	A	142	GLU	HA	3.9	0.02	1
1	A	142	GLU	HB2	2.23	0.02	2
1	A	142	GLU	HB3	1.94	0.02	2
1	A	142	GLU	HG3	2.89	0.02	2
1	A	142	GLU	C	177.4	0.2	1
1	A	142	GLU	CA	59.2	0.2	1
1	A	142	GLU	CB	31.0	0.2	1
1	A	142	GLU	CG	38.6	0.2	1
1	A	142	GLU	N	125.2	0.2	1
1	A	143	ALA	H	8.02	0.02	1
1	A	143	ALA	HA	3.84	0.02	1
1	A	143	ALA	HB1	1.5	0.02	1
1	A	143	ALA	HB2	1.5	0.02	1
1	A	143	ALA	HB3	1.5	0.02	1
1	A	143	ALA	C	181.0	0.2	1
1	A	143	ALA	CA	54.8	0.2	1
1	A	143	ALA	CB	17.5	0.2	1
1	A	143	ALA	N	119.5	0.2	1
1	A	144	GLN	H	7.52	0.02	1
1	A	144	GLN	HA	4.0	0.02	1
1	A	144	GLN	HB2	1.96	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	144	GLN	HB3	2.21	0.02	2
1	A	144	GLN	HG3	2.41	0.02	2
1	A	144	GLN	C	177.2	0.2	1
1	A	144	GLN	CA	58.6	0.2	1
1	A	144	GLN	CB	28.0	0.2	1
1	A	144	GLN	CG	33.7	0.2	1
1	A	144	GLN	N	118.7	0.2	1
1	A	145	ALA	H	7.97	0.02	1
1	A	145	ALA	HA	3.94	0.02	1
1	A	145	ALA	HB1	1.76	0.02	1
1	A	145	ALA	HB2	1.76	0.02	1
1	A	145	ALA	HB3	1.76	0.02	1
1	A	145	ALA	C	179.5	0.2	1
1	A	145	ALA	CA	55.8	0.2	1
1	A	145	ALA	CB	18.4	0.2	1
1	A	145	ALA	N	123.3	0.2	1
1	A	146	LYS	H	8.19	0.02	1
1	A	146	LYS	HA	3.43	0.02	1
1	A	146	LYS	HB2	1.26	0.02	2
1	A	146	LYS	HD2	1.02	0.02	2
1	A	146	LYS	HD3	0.82	0.02	2
1	A	146	LYS	HE2	2.22	0.02	2
1	A	146	LYS	HG2	0.18	0.02	2
1	A	146	LYS	HG3	0.47	0.02	2
1	A	146	LYS	C	180.9	0.2	1
1	A	146	LYS	CA	59.5	0.2	1
1	A	146	LYS	CB	32.2	0.2	1
1	A	146	LYS	CD	29.1	0.2	1
1	A	146	LYS	CG	24.3	0.2	1
1	A	146	LYS	N	117.2	0.2	1
1	A	147	LYS	H	7.84	0.02	1
1	A	147	LYS	HA	3.95	0.02	1
1	A	147	LYS	HB2	2.0	0.02	2
1	A	147	LYS	HB3	1.95	0.02	2
1	A	147	LYS	HD2	1.68	0.02	2
1	A	147	LYS	HE2	2.97	0.02	2
1	A	147	LYS	HG2	1.51	0.02	2
1	A	147	LYS	HG3	1.45	0.02	2
1	A	147	LYS	C	178.8	0.2	1
1	A	147	LYS	CA	59.5	0.2	1
1	A	147	LYS	CB	32.2	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	LYS	CD	29.1	0.2	1
1	A	147	LYS	CE	41.6	0.2	1
1	A	147	LYS	CG	24.7	0.2	1
1	A	147	LYS	N	122.5	0.2	1
1	A	148	GLU	H	7.68	0.02	1
1	A	148	GLU	HA	4.03	0.02	1
1	A	148	GLU	HB2	2.06	0.02	2
1	A	148	GLU	HB3	2.14	0.02	2
1	A	148	GLU	HG2	2.28	0.02	2
1	A	148	GLU	HG3	2.53	0.02	2
1	A	148	GLU	C	174.5	0.2	1
1	A	148	GLU	CA	56.6	0.2	1
1	A	148	GLU	CB	30.0	0.2	1
1	A	148	GLU	CG	37.0	0.2	1
1	A	148	GLU	N	116.4	0.2	1
1	A	149	LYS	H	7.86	0.02	1
1	A	149	LYS	HA	3.57	0.02	1
1	A	149	LYS	HB2	1.8	0.02	2
1	A	149	LYS	HB3	2.08	0.02	2
1	A	149	LYS	HD2	1.75	0.02	1
1	A	149	LYS	HE2	3.07	0.02	2
1	A	149	LYS	HG3	1.42	0.02	2
1	A	149	LYS	C	175.0	0.2	1
1	A	149	LYS	CA	56.7	0.2	1
1	A	149	LYS	CB	29.1	0.2	1
1	A	149	LYS	CE	42.1	0.2	1
1	A	149	LYS	CG	24.9	0.2	1
1	A	149	LYS	N	116.8	0.2	1
1	A	150	LEU	H	7.67	0.02	1
1	A	150	LEU	HA	4.2	0.02	1
1	A	150	LEU	HB2	1.39	0.02	2
1	A	150	LEU	HB3	1.55	0.02	2
1	A	150	LEU	HD11	1.0	0.02	2
1	A	150	LEU	HD12	1.0	0.02	2
1	A	150	LEU	HD13	1.0	0.02	2
1	A	150	LEU	HD21	0.84	0.02	2
1	A	150	LEU	HD22	0.84	0.02	2
1	A	150	LEU	HD23	0.84	0.02	2
1	A	150	LEU	HG	1.66	0.02	1
1	A	150	LEU	C	178.5	0.2	1
1	A	150	LEU	CA	55.0	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	150	LEU	CB	44.0	0.2	1
1	A	150	LEU	CD1	22.9	0.2	2
1	A	150	LEU	CG	25.2	0.2	1
1	A	150	LEU	N	117.2	0.2	1
1	A	151	ASN	H	9.13	0.02	1
1	A	151	ASN	HA	3.8	0.02	1
1	A	151	ASN	HB2	2.79	0.02	2
1	A	151	ASN	C	176.3	0.2	1
1	A	151	ASN	CA	56.7	0.2	1
1	A	151	ASN	CB	38.7	0.2	1
1	A	151	ASN	N	119.3	0.2	1
1	A	152	ILE	H	8.42	0.02	1
1	A	152	ILE	HA	3.38	0.02	1
1	A	152	ILE	HB	1.05	0.02	1
1	A	152	ILE	HG13	0.57	0.02	2
1	A	152	ILE	HG21	0.12	0.02	1
1	A	152	ILE	HG22	0.12	0.02	1
1	A	152	ILE	HG23	0.12	0.02	1
1	A	152	ILE	C	176.7	0.2	1
1	A	152	ILE	CA	65.6	0.2	1
1	A	152	ILE	CB	37.2	0.2	1
1	A	152	ILE	CD1	13.6	0.2	1
1	A	152	ILE	CG1	26.0	0.2	1
1	A	152	ILE	CG2	15.3	0.2	1
1	A	152	ILE	N	124.6	0.2	1
1	A	153	TRP	H	7.9	0.02	1
1	A	153	TRP	HA	4.95	0.02	1
1	A	153	TRP	HB2	2.85	0.02	2
1	A	153	TRP	HB3	3.73	0.02	2
1	A	153	TRP	HD1	7.02	0.02	1
1	A	153	TRP	HE3	7.74	0.02	1
1	A	153	TRP	HH2	7.16	0.02	1
1	A	153	TRP	HZ2	7.57	0.02	1
1	A	153	TRP	HZ3	7.11	0.02	1
1	A	153	TRP	C	176.2	0.2	1
1	A	153	TRP	CA	54.7	0.2	1
1	A	153	TRP	CB	30.2	0.2	1
1	A	153	TRP	N	120.1	0.2	1
1	A	154	SER	H	8.11	0.02	1
1	A	154	SER	HA	4.24	0.02	1
1	A	154	SER	HB2	4.18	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	154	SER	HB3	4.06	0.02	2
1	A	154	SER	C	175.3	0.2	1
1	A	154	SER	CA	60.1	0.2	1
1	A	154	SER	CB	64.3	0.2	1
1	A	154	SER	N	116.2	0.2	1
1	A	155	GLU	H	8.07	0.02	1
1	A	155	GLU	HA	4.49	0.02	1
1	A	155	GLU	HB2	1.95	0.02	2
1	A	155	GLU	HB3	2.25	0.02	2
1	A	155	GLU	HG2	2.41	0.02	2
1	A	155	GLU	HG3	2.32	0.02	2
1	A	155	GLU	CA	56.1	0.2	1
1	A	155	GLU	CB	30.5	0.2	1
1	A	155	GLU	N	121.5	0.2	1
1	A	156	ASP	H	8.01	0.02	1
1	A	156	ASP	HA	4.44	0.02	1
1	A	156	ASP	HB2	2.63	0.02	2
1	A	156	ASP	HB3	2.75	0.02	2
1	A	156	ASP	CA	56.1	0.2	1
1	A	156	ASP	CB	42.3	0.2	1
1	A	156	ASP	N	126.8	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
$^{13}\text{C}_\alpha$	149	$-0.06 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	140	$0.02 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	139	$0.12 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	141	$-0.05 \pm 0.39$	None needed ( $< 0.5$ ppm)

### 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 62%, i.e. 966 atoms were assigned a chemical shift out of a possible 1556. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	421/556 (76%)	169/226 (75%)	170/222 (77%)	82/108 (76%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Sidechain	529/915 (58%)	361/592 (61%)	168/285 (59%)	0/38 (0%)
Aromatic	16/85 (19%)	14/41 (34%)	2/39 (5%)	0/5 (0%)
Overall	966/1556 (62%)	544/859 (63%)	340/546 (62%)	82/151 (54%)

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

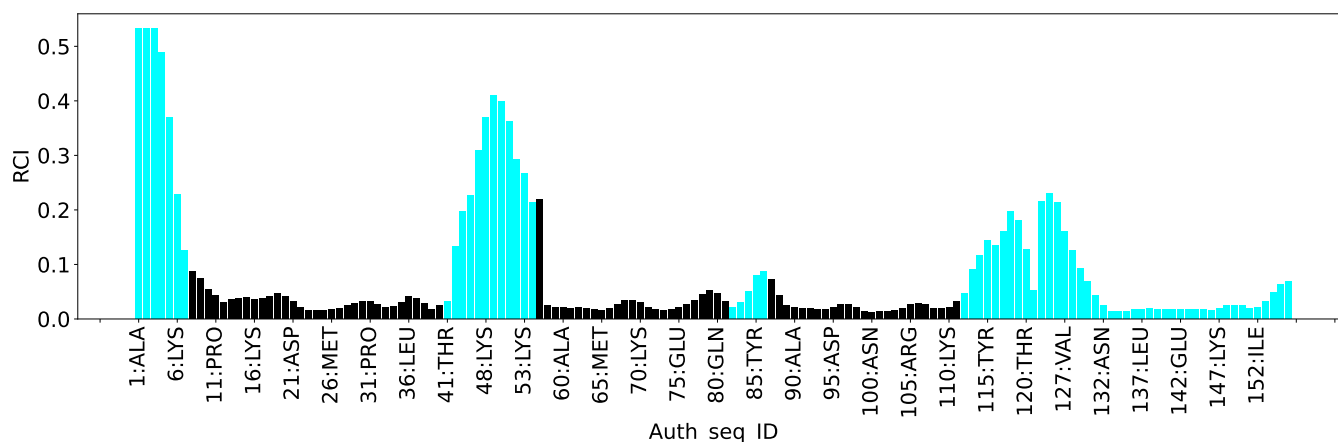
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	120	THR	HG21	4.33	0.08 – 2.19	15.1
1	A	120	THR	HG22	4.33	0.08 – 2.19	15.1
1	A	120	THR	HG23	4.33	0.08 – 2.19	15.1
1	A	44	THR	HG21	3.88	0.08 – 2.19	13.0
1	A	44	THR	HG22	3.88	0.08 – 2.19	13.0
1	A	44	THR	HG23	3.88	0.08 – 2.19	13.0

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis [i](#)

### 8.1 Conformationally restricting restraints [i](#)

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

Description	Value
Total distance restraints	2749
Intra-residue ( $ i-j =0$ )	1197
Sequential ( $ i-j =1$ )	649
Medium range ( $ i-j >1$ and $ i-j <5$ )	260
Long range ( $ i-j \geq 5$ )	459
Inter-chain	72
Hydrogen bond restraints	112
Disulfide bond restraints	0
Total dihedral-angle restraints	185
Number of unmapped restraints	0
Number of restraints per residue	18.8
Number of long range restraints per residue <sup>1</sup>	3.2

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

### 8.2 Residual restraint violations [i](#)

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

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

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.5	0.18
0.2-0.5 (Medium)	0.1	0.27
>0.5 (Large)	None	None

### 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)	7.5	4.99
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

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

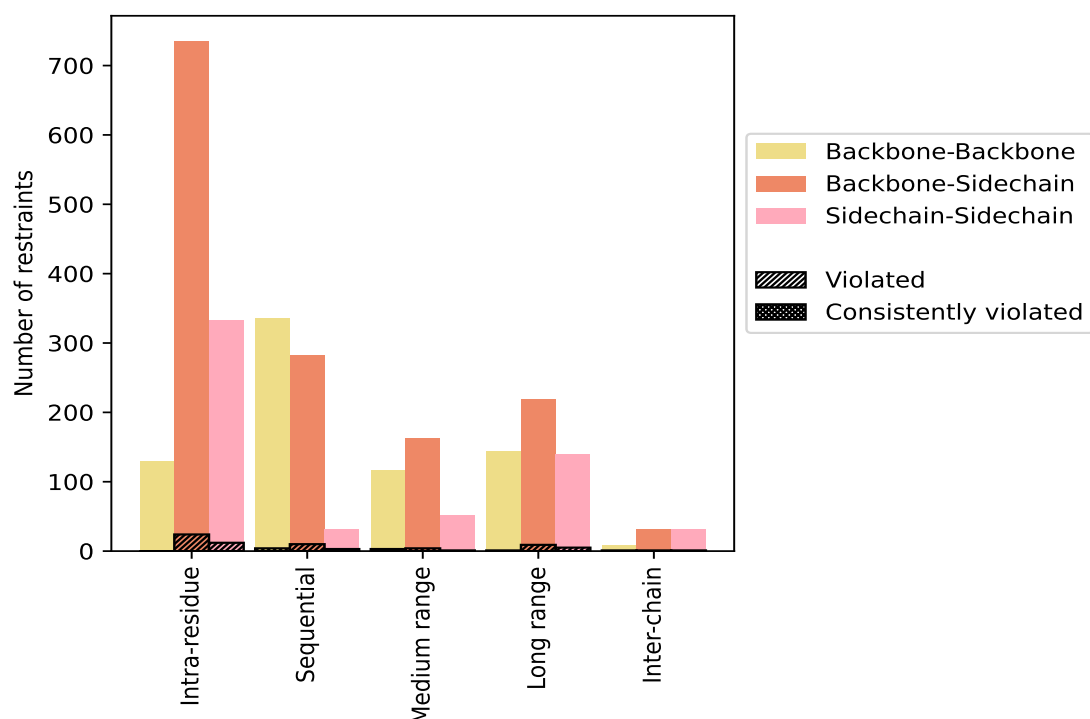
### 9.1 Summary of distance violations [i](#)

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>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">1197</a>	<a href="#">43.5</a>	<a href="#">36</a>	<a href="#">3.0</a>	<a href="#">1.3</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	130	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	735	26.7	24	3.3	0.9	0	0.0	0.0
Sidechain-Sidechain	332	12.1	12	3.6	0.4	0	0.0	0.0
<a href="#">Sequential ( i-j =1)</a>	<a href="#">649</a>	<a href="#">23.6</a>	<a href="#">17</a>	<a href="#">2.6</a>	<a href="#">0.6</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	336	12.2	4	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	282	10.3	10	3.5	0.4	0	0.0	0.0
Sidechain-Sidechain	31	1.1	3	9.7	0.1	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">260</a>	<a href="#">9.5</a>	<a href="#">6</a>	<a href="#">2.3</a>	<a href="#">0.2</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	116	4.2	3	2.6	0.1	0	0.0	0.0
Backbone-Sidechain	93	3.4	2	2.2	0.1	0	0.0	0.0
Sidechain-Sidechain	51	1.9	1	2.0	0.0	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">459</a>	<a href="#">16.7</a>	<a href="#">15</a>	<a href="#">3.3</a>	<a href="#">0.5</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	144	5.2	1	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	175	6.4	9	5.1	0.3	0	0.0	0.0
Sidechain-Sidechain	140	5.1	5	3.6	0.2	0	0.0	0.0
<a href="#">Inter-chain</a>	<a href="#">72</a>	<a href="#">2.6</a>	<a href="#">3</a>	<a href="#">4.2</a>	<a href="#">0.1</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	8	0.3	1	12.5	0.0	0	0.0	0.0
Backbone-Sidechain	32	1.2	1	3.1	0.0	0	0.0	0.0
Sidechain-Sidechain	32	1.2	1	3.1	0.0	0	0.0	0.0
<a href="#">Hydrogen bond</a>	<a href="#">112</a>	<a href="#">4.1</a>	<a href="#">2</a>	<a href="#">1.8</a>	<a href="#">0.1</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">2749</a>	<a href="#">100.0</a>	<a href="#">79</a>	<a href="#">2.9</a>	<a href="#">2.9</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	734	26.7	9	1.2	0.3	0	0.0	0.0
Backbone-Sidechain	1429	52.0	48	3.4	1.7	0	0.0	0.0
Sidechain-Sidechain	586	21.3	22	3.8	0.8	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	2	1	1	0	0	4	0.15	0.18	0.03	0.14
2	2	1	0	0	0	3	0.11	0.12	0.0	0.11
3	4	2	0	0	0	6	0.14	0.17	0.03	0.14
4	1	0	0	0	1	2	0.14	0.16	0.02	0.14
5	5	0	0	0	0	5	0.12	0.16	0.02	0.11
6	1	0	0	2	0	3	0.13	0.18	0.04	0.11
7	1	1	2	0	0	4	0.12	0.14	0.01	0.12
8	9	4	0	2	0	15	0.12	0.16	0.02	0.11
9	1	2	0	2	0	5	0.12	0.13	0.01	0.13
10	2	2	0	2	0	6	0.13	0.16	0.02	0.13

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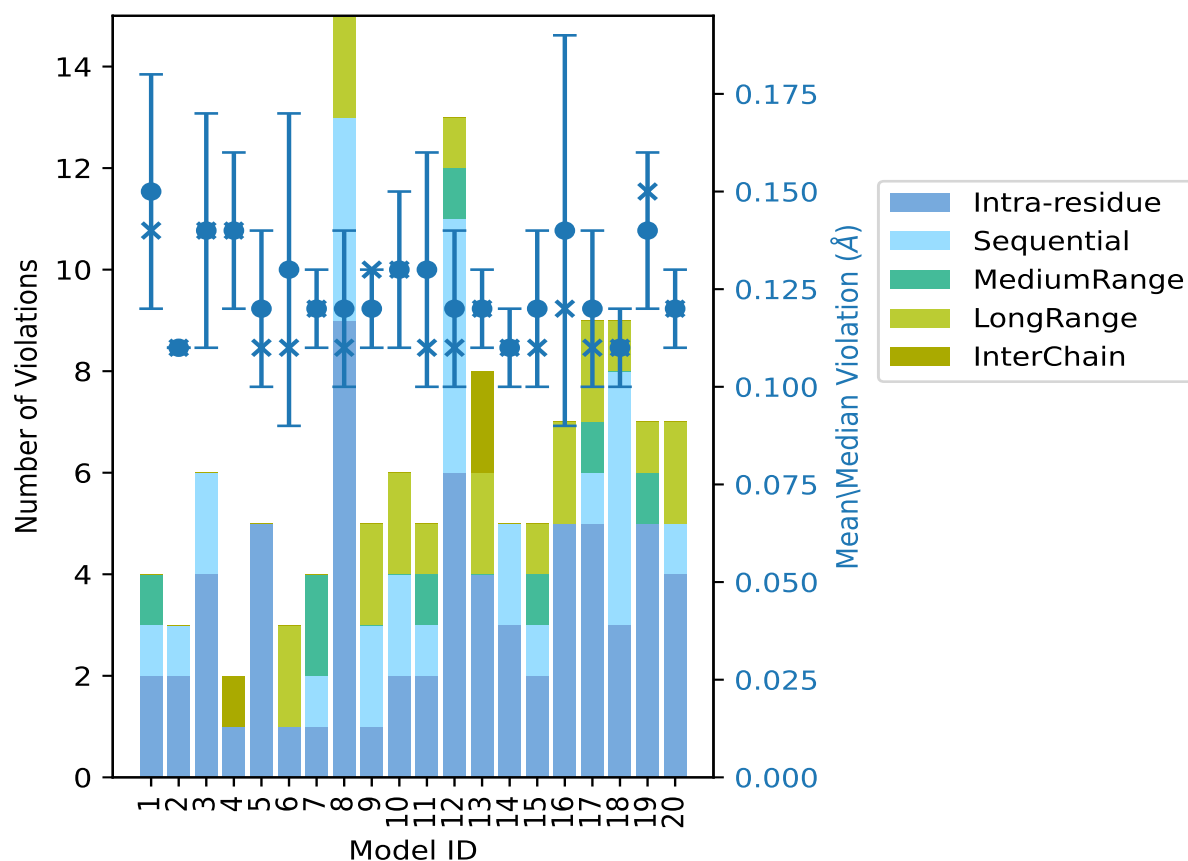
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	2	1	1	1	0	5	0.13	0.18	0.03	0.11
12	6	5	1	1	0	13	0.12	0.15	0.02	0.11
13	4	0	0	2	2	8	0.12	0.14	0.01	0.12
14	3	2	0	0	0	5	0.11	0.14	0.01	0.11
15	2	1	1	1	0	5	0.12	0.15	0.02	0.11
16	5	0	0	2	0	7	0.14	0.27	0.05	0.12
17	5	1	1	2	0	9	0.12	0.17	0.02	0.11
18	3	5	0	1	0	9	0.11	0.13	0.01	0.11
19	5	0	1	1	0	7	0.14	0.15	0.02	0.15
20	4	1	0	2	0	7	0.12	0.14	0.01	0.12

<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 ⓘ

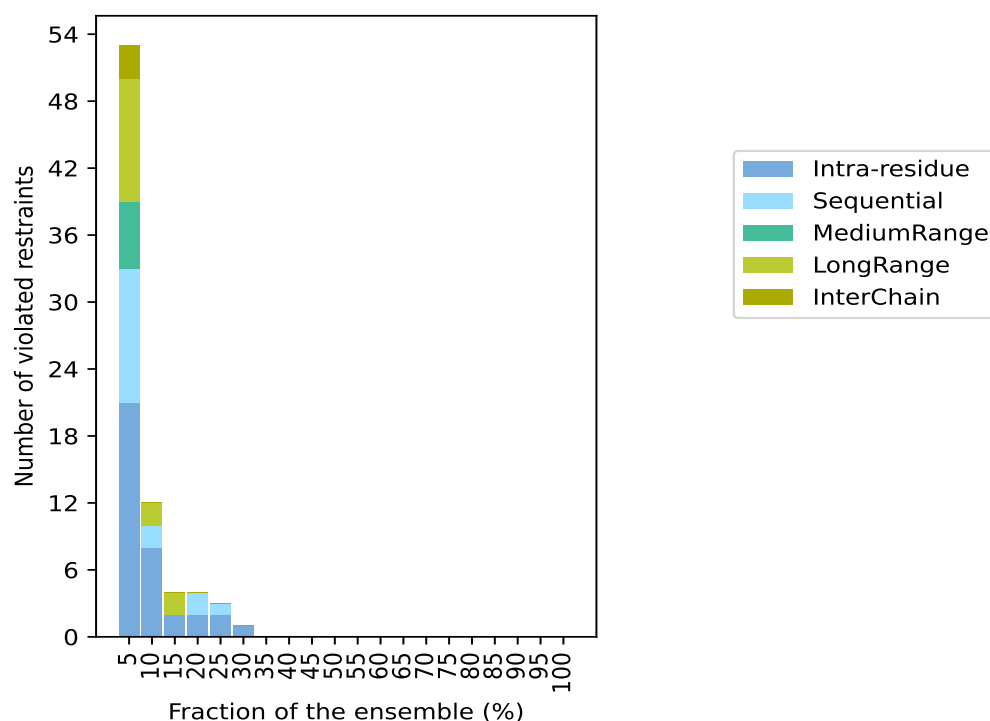
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2560(IR:1161, SQ:632, MR:254, LR:444, IC:69) restraints are 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>	%
21	12	6	11	3	53	1	5.0
8	2	0	2	0	12	2	10.0
2	0	0	2	0	4	3	15.0
2	2	0	0	0	4	4	20.0
2	1	0	0	0	3	5	25.0
1	0	0	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

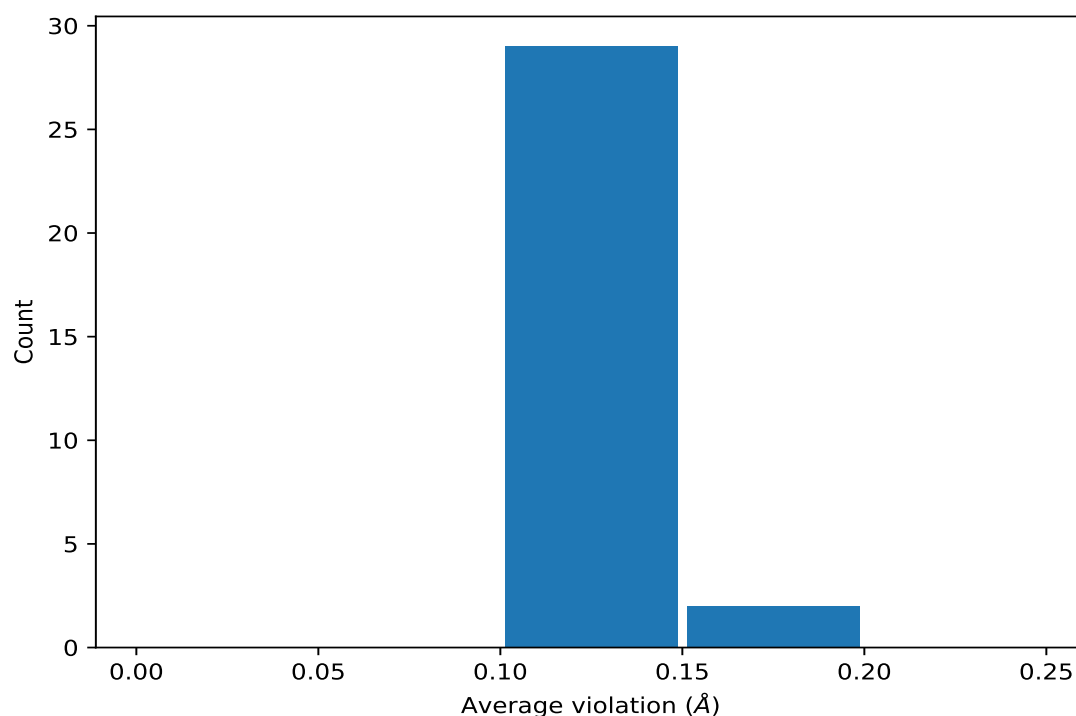
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

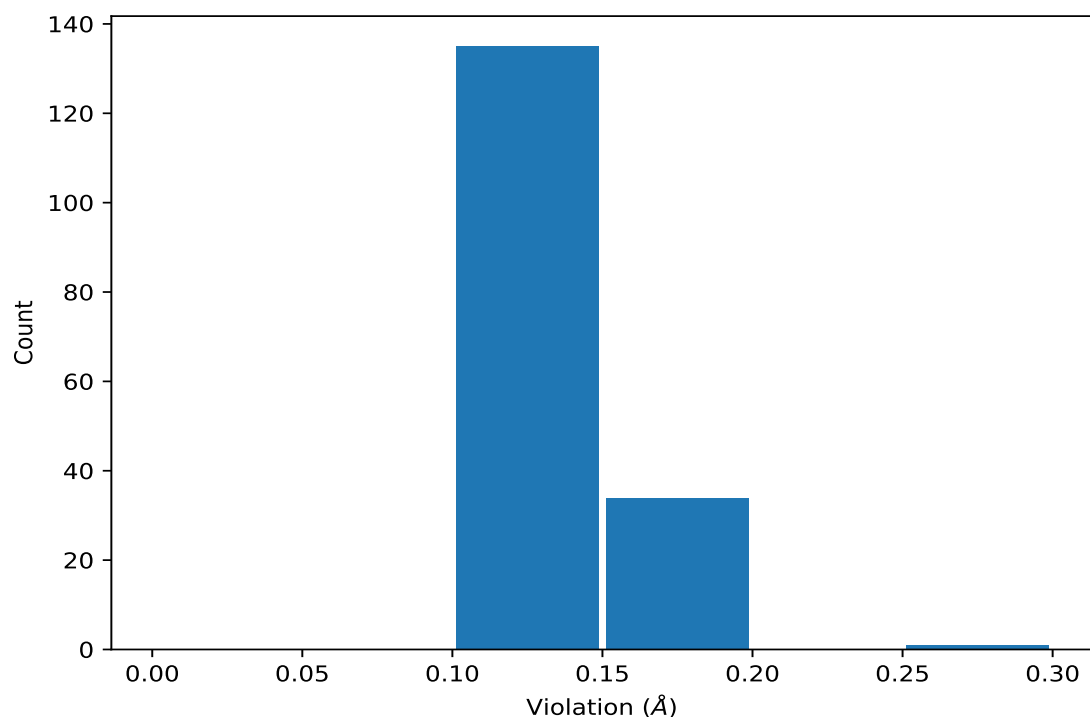
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1449)	1:63:A:LYS:HE3	1:63:A:LYS:HB3	6	0.16	0.01	0.16
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD11	5	0.15	0.02	0.15
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD12	5	0.15	0.02	0.15
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD13	5	0.15	0.02	0.15
(1,2048)	2:133:B:THR:H	2:133:B:THR:HG21	5	0.13	0.02	0.13
(1,2048)	2:133:B:THR:H	2:133:B:THR:HG22	5	0.13	0.02	0.13
(1,2048)	2:133:B:THR:H	2:133:B:THR:HG23	5	0.13	0.02	0.13
(1,43)	1:10:A:GLU:H	1:9:A:LYS:HG2	5	0.12	0.01	0.12
(1,859)	1:99:A:VAL:H	1:98:A:MET:HG3	4	0.14	0.02	0.15
(1,103)	1:16:A:LYS:H	1:16:A:LYS:HG3	4	0.14	0.01	0.14
(1,1630)	1:78:A:LYS:HB2	1:78:A:LYS:HD3	4	0.11	0.0	0.11
(1,1114)	1:10:A:GLU:HB2	1:11:A:PRO:HG3	4	0.11	0.0	0.11
(1,768)	1:92:A:ILE:H	1:36:A:LEU:HB2	3	0.14	0.01	0.14
(1,1226)	1:21:A:ASP:HB3	1:35:A:ARG:HD3	3	0.12	0.02	0.11

<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)
(1,1801)	1:97:A:LYS:HG3	1:97:A:LYS:HB2	16	0.27
(1,1449)	1:63:A:LYS:HE3	1:63:A:LYS:HB3	1	0.18
(1,1425)	1:53:A:LYS:HB3	1:53:A:LYS:HE2	11	0.18
(1,580)	1:75:A:GLU:H	1:91:A:TYR:HB3	6	0.18
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD11	3	0.17
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD12	3	0.17
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD13	3	0.17
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD11	17	0.17
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD12	17	0.17
(1,2407)	2:138:B:LEU:HA	2:138:B:LEU:HD13	17	0.17
(1,2017)	2:129:B:LYS:H	2:128:B:TYR:HD1	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2017)	2:129:B:LYS:H	2:128:B:TYR:HD2	3	0.17
(1,2408)	2:138:B:LEU:HA	2:138:B:LEU:HD21	8	0.16
(1,2408)	2:138:B:LEU:HA	2:138:B:LEU:HD22	8	0.16
(1,2408)	2:138:B:LEU:HA	2:138:B:LEU:HD23	8	0.16
(1,2048)	2:133:B:THR:H	2:133:B:THR:HG21	3	0.16
(1,2048)	2:133:B:THR:H	2:133:B:THR:HG22	3	0.16
(1,2048)	2:133:B:THR:H	2:133:B:THR:HG23	3	0.16
(1,2039)	2:132:B:ASN:H	2:134:B:HIS:H	1	0.16

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

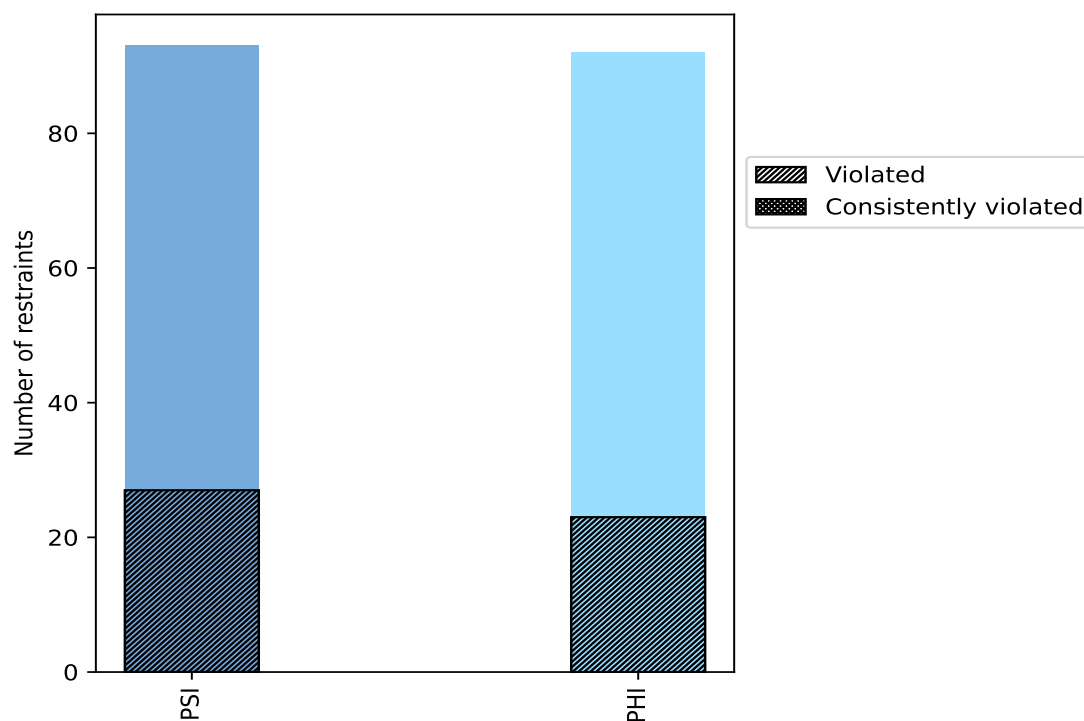
### 10.1 Summary of dihedral-angle violations [i](#)

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	93	50.3	27	29.0	14.6	0	0.0	0.0
PHI	92	49.7	23	25.0	12.4	0	0.0	0.0
Total	185	100.0	50	27.0	27.0	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

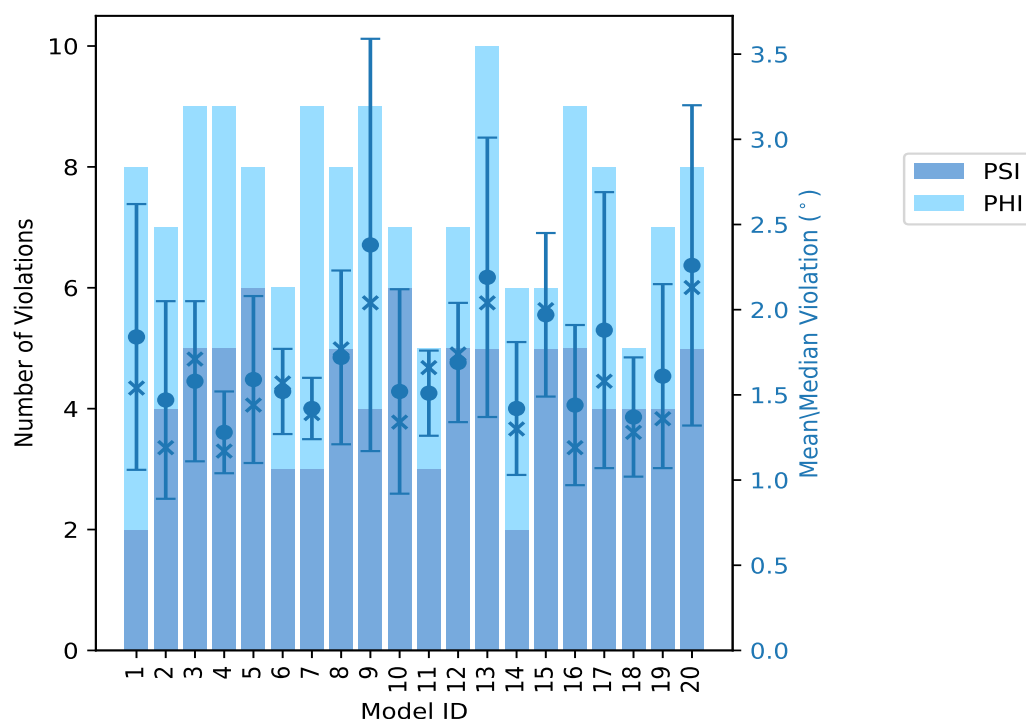
## 10.2 Dihedral-angle violation statistics for each model

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	6	8	1.84	3.64	0.78	1.54
2	4	3	7	1.47	2.81	0.58	1.19
3	5	4	9	1.58	2.21	0.47	1.71
4	5	4	9	1.28	1.78	0.24	1.17
5	6	2	8	1.59	2.74	0.49	1.44
6	3	3	6	1.52	1.83	0.25	1.57
7	3	6	9	1.42	1.81	0.18	1.39
8	5	3	8	1.72	2.52	0.51	1.77
9	4	5	9	2.38	4.99	1.21	2.04
10	6	1	7	1.52	2.9	0.6	1.34
11	3	2	5	1.51	1.77	0.25	1.66
12	5	2	7	1.69	2.17	0.35	1.74
13	5	5	10	2.19	3.53	0.82	2.04
14	2	4	6	1.42	2.2	0.39	1.3
15	5	1	6	1.97	2.53	0.48	2.0
16	5	4	9	1.44	2.33	0.47	1.19
17	4	4	8	1.88	3.67	0.81	1.58
18	4	1	5	1.37	1.98	0.35	1.28
19	4	3	7	1.61	2.51	0.54	1.36
20	5	3	8	2.26	3.61	0.94	2.13



### 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>	%
9	9	18	1	5.0
8	4	12	2	10.0
3	3	6	3	15.0
1	2	3	4	20.0
2	3	5	5	25.0
0	0	0	6	30.0
1	1	2	7	35.0
0	0	0	8	40.0
1	0	1	9	45.0
1	1	2	10	50.0
1	0	1	11	55.0

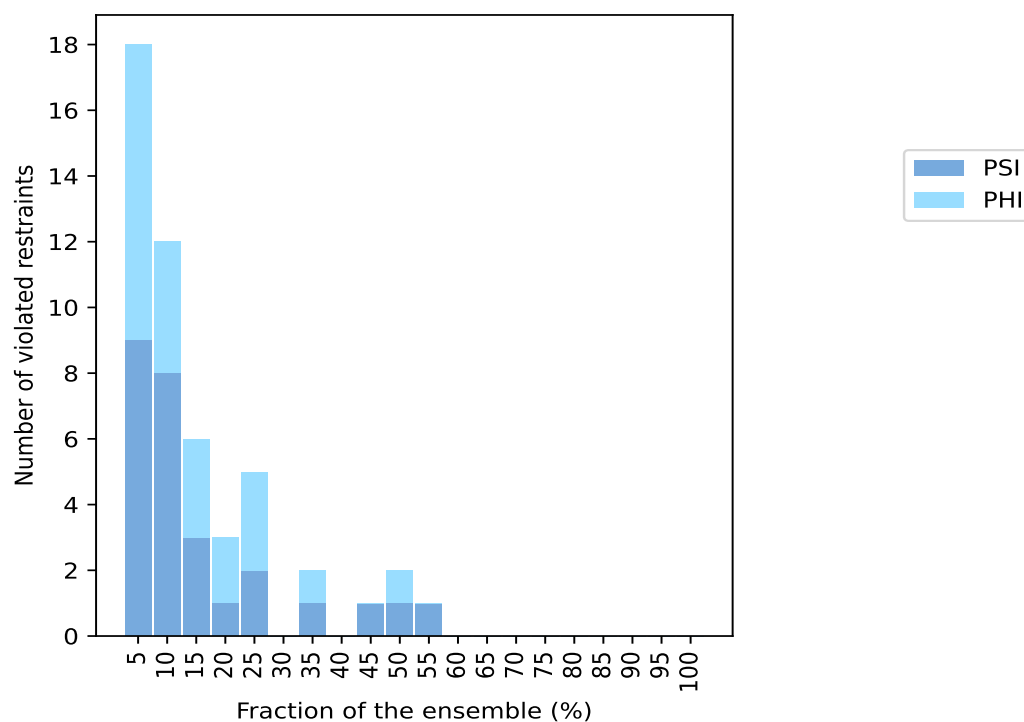
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

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

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

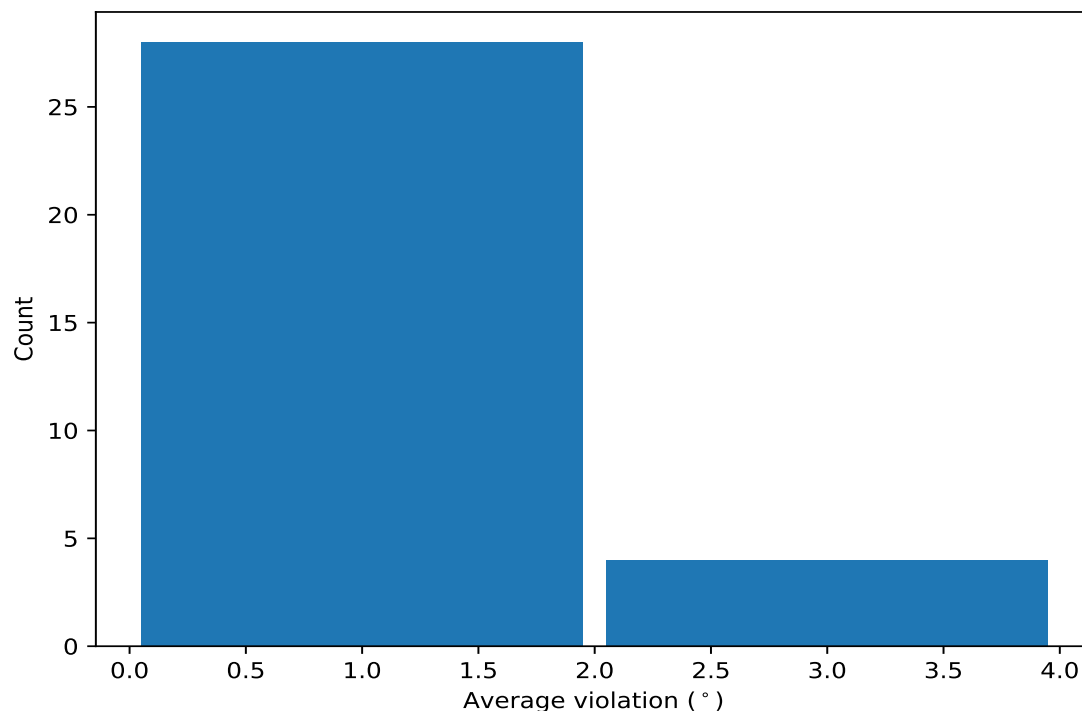


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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

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

in the ensemble



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

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

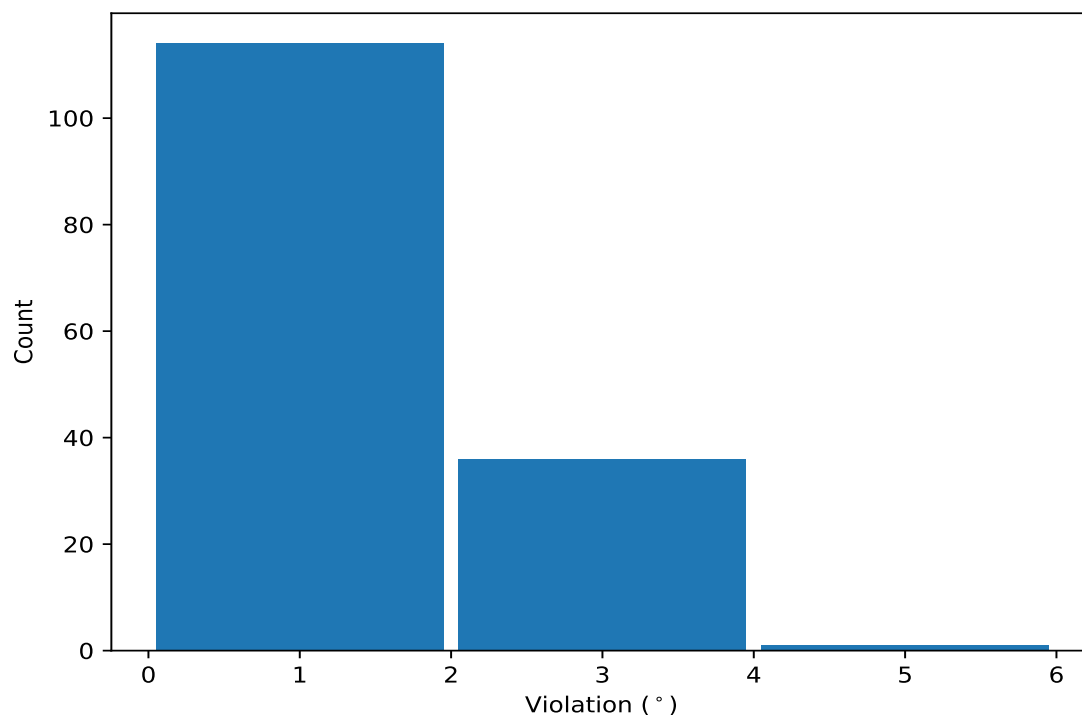
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,134)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:ASP:N	11	1.83	0.52	1.65
(1,74)	1:111:A:VAL:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	10	1.97	1.0	1.44
(1,100)	1:40:A:ASP:N	1:40:A:ASP:CA	1:40:A:ASP:C	1:41:A:THR:N	10	1.77	0.48	1.85
(1,126)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LYS:N	9	1.83	0.45	1.73
(1,151)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:TYR:N	7	2.01	1.0	1.74
(1,58)	1:94:A:ALA:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	7	1.84	0.4	1.95
(1,106)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:TYR:N	5	2.34	0.82	2.81
(1,59)	1:95:A:ASP:C	1:96:A:GLY:N	1:96:A:GLY:CA	1:96:A:GLY:C	5	1.48	0.18	1.46
(1,3)	1:9:A:LYS:C	1:10:A:GLU:N	1:10:A:GLU:CA	1:10:A:GLU:C	5	1.4	0.31	1.34
(1,178)	2:144:B:GLN:N	2:144:B:GLN:CA	2:144:B:GLN:C	2:145:B:ALA:N	5	1.35	0.31	1.36

<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 (°)
(1,75)	1:112:A:ALA:C	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	9	4.99
(1,151)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:TYR:N	9	3.92
(1,74)	1:111:A:VAL:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	17	3.67
(1,74)	1:111:A:VAL:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1	3.64
(1,25)	1:40:A:ASP:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	20	3.61
(1,152)	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	1:114:A:VAL:N	13	3.53
(1,102)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:HIS:N	13	3.48
(1,106)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:TYR:N	20	3.28
(1,74)	1:111:A:VAL:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	20	3.11
(1,106)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:TYR:N	10	2.9