



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2M8T  
BMRB ID : 19268  
Title : Solution NMR structure of the V209M variant of the human prion protein (residues 90-231)  
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Deposited on : 2013-05-28

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

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

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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

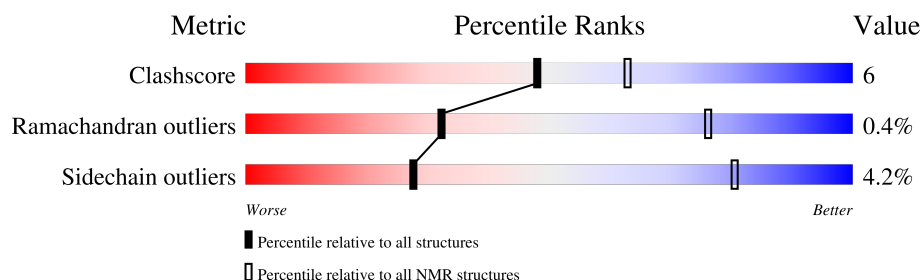
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 79%.

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	146	

## 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: *fewest violations*.

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:128-A:164, A:172-A:225 (91)	0.97	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 2 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1777 atoms, of which 856 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	112	Total	C	H	N	O	S	0
			1777	569	856	161	181	10	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLY	-	expression tag	UNP P04156
A	87	SER	-	expression tag	UNP P04156
A	88	ASP	-	expression tag	UNP P04156
A	89	PRO	-	expression tag	UNP P04156
A	209	MET	VAL	engineered mutation	UNP P04156



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
TALOS	geometry optimization	
CYANA	structure solution	
CNS	geometry optimization	
CYANA	refinement	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1503
Number of shifts mapped to atoms	1174
Number of unparsed shifts	0
Number of shifts with mapping errors	329
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

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	772	721	723	9±3
All	All	15440	14420	14460	171

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 6.

5 of 75 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:THR:HB	1:A:196:GLU:HB3	0.78	1.53	20	1
1:A:204:LYS:HE2	1:A:204:LYS:HA	0.76	1.57	4	1
1:A:130:LEU:HD11	1:A:160:GLN:HG3	0.67	1.65	13	9
1:A:153:ASN:O	1:A:156:ARG:HG2	0.63	1.93	16	1
1:A:163:TYR:HB3	1:A:179:CYS:HB3	0.62	1.71	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	91/146 (62%)	87±1 (95±2%)	4±1 (4±1%)	0±1 (0±1%)	32	76
All	All	1820/2920 (62%)	1736 (95%)	76 (4%)	8 (0%)	32	76

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)
1	A	131	GLY	4
1	A	141	PHE	2
1	A	142	GLY	1
1	A	196	GLU	1

### 6.3.2 Protein sidechains ⓘ

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	86/123 (70%)	82±2 (96±2%)	4±2 (4±2%)	27	80
All	All	1720/2460 (70%)	1648 (96%)	72 (4%)	27	80

5 of 26 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	208	ARG	11
1	A	186	GLN	11
1	A	160	GLN	7
1	A	177	HIS	3
1	A	129	MET	3

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 79% for the well-defined parts and 77% 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	1503
Number of shifts mapped to atoms	1174
Number of unparsed shifts	0
Number of shifts with mapping errors	329
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 329) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	GLY	HA2	3.875	0.020	1
1	A	86	GLY	HA3	3.875	0.020	1
1	A	86	GLY	CA	43.411	0.300	1
1	A	87	SER	H	8.6	0.020	1
1	A	87	SER	HA	4.473	0.020	1
1	A	87	SER	HB2	3.811	0.020	1
1	A	87	SER	HB3	3.811	0.020	1
1	A	87	SER	CA	58.148	0.300	1
1	A	87	SER	CB	63.953	0.300	1
1	A	87	SER	N	115.741	0.300	1
1	A	88	ASP	H	8.438	0.020	1
1	A	88	ASP	HA	4.881	0.020	1
1	A	88	ASP	HB2	2.722	0.020	2
1	A	88	ASP	HB3	2.55	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	ASP	CA	54.716	0.300	1
1	A	88	ASP	CB	41.367	0.300	1
1	A	88	ASP	N	123.605	0.300	1
1	A	89	PRO	HA	4.4	0.020	1
1	A	89	PRO	HB2	2.26	0.020	2
1	A	89	PRO	HB3	1.909	0.020	2
1	A	89	PRO	HG2	1.987	0.020	1
1	A	89	PRO	HG3	1.987	0.020	1
1	A	89	PRO	HD2	3.776	0.020	2
1	A	89	PRO	HD3	3.605	0.020	2
1	A	89	PRO	CA	63.587	0.300	1
1	A	89	PRO	CB	32.113	0.300	1
1	A	89	PRO	CG	27.136	0.300	1
1	A	89	PRO	CD	50.847	0.300	1
1	A	90	GLY	H	8.482	0.020	1
1	A	90	GLY	HA2	3.902	0.020	1
1	A	90	GLY	HA3	3.902	0.020	1
1	A	90	GLY	CA	45.409	0.300	1
1	A	90	GLY	N	108.429	0.300	1
1	A	91	GLN	H	8.084	0.020	1
1	A	91	GLN	HA	4.324	0.020	1
1	A	91	GLN	HB2	2.142	0.020	2
1	A	91	GLN	HB3	1.962	0.020	2
1	A	91	GLN	HG2	2.325	0.020	1
1	A	91	GLN	HG3	2.325	0.020	1
1	A	91	GLN	HE21	7.362	0.020	2
1	A	91	GLN	HE22	6.793	0.020	2
1	A	91	GLN	CA	55.912	0.300	1
1	A	91	GLN	CB	29.28	0.300	1
1	A	91	GLN	CG	33.851	0.300	1
1	A	91	GLN	N	119.598	0.300	1
1	A	91	GLN	NE2	112.348	0.300	1
1	A	92	GLY	H	8.445	0.020	1
1	A	92	GLY	HA2	3.964	0.020	1
1	A	92	GLY	HA3	3.964	0.020	1
1	A	92	GLY	CA	45.43	0.300	1
1	A	92	GLY	N	109.845	0.300	1
1	A	93	GLY	H	8.291	0.020	1
1	A	93	GLY	HA2	3.913	0.020	1
1	A	93	GLY	HA3	3.913	0.020	1
1	A	93	GLY	CA	45.274	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	GLY	N	108.591	0.300	1
1	A	94	GLY	H	8.286	0.020	1
1	A	94	GLY	HA2	3.98	0.020	1
1	A	94	GLY	HA3	3.98	0.020	1
1	A	94	GLY	CA	45.229	0.300	1
1	A	94	GLY	N	108.815	0.300	1
1	A	95	THR	H	8.075	0.020	1
1	A	95	THR	HA	4.255	0.020	1
1	A	95	THR	HB	4.145	0.020	1
1	A	95	THR	HG21	1.135	0.020	1
1	A	95	THR	HG22	1.135	0.020	1
1	A	95	THR	HG23	1.135	0.020	1
1	A	95	THR	CA	62.262	0.300	1
1	A	95	THR	CB	69.627	0.300	1
1	A	95	THR	CG2	21.605	0.300	1
1	A	95	THR	N	113.428	0.300	1
1	A	96	HIS	H	8.522	0.020	1
1	A	96	HIS	HA	4.636	0.020	1
1	A	96	HIS	HB2	3.201	0.020	2
1	A	96	HIS	HB3	3.113	0.020	2
1	A	96	HIS	HD2	7.365	0.020	1
1	A	96	HIS	CA	55.268	0.300	1
1	A	96	HIS	CB	29.219	0.300	1
1	A	96	HIS	CD2	119.831	0.300	1
1	A	96	HIS	N	120.374	0.300	1
1	A	97	SER	H	8.258	0.020	1
1	A	97	SER	HA	4.361	0.020	1
1	A	97	SER	HB2	3.759	0.020	1
1	A	97	SER	HB3	3.759	0.020	1
1	A	97	SER	CA	58.543	0.300	1
1	A	97	SER	CB	63.874	0.300	1
1	A	97	SER	N	116.904	0.300	1
1	A	98	GLN	H	8.429	0.020	1
1	A	98	GLN	HA	4.256	0.020	1
1	A	98	GLN	HB2	1.93	0.020	2
1	A	98	GLN	HB3	1.838	0.020	2
1	A	98	GLN	HG2	2.14	0.020	1
1	A	98	GLN	HG3	2.14	0.020	1
1	A	98	GLN	HE21	7.425	0.020	2
1	A	98	GLN	HE22	6.791	0.020	2
1	A	98	GLN	CA	56.115	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	GLN	CB	29.287	0.300	1
1	A	98	GLN	CG	33.535	0.300	1
1	A	98	GLN	N	121.911	0.300	1
1	A	98	GLN	NE2	112.561	0.300	1
1	A	99	TRP	H	8.065	0.020	1
1	A	99	TRP	HA	4.652	0.020	1
1	A	99	TRP	HB2	3.269	0.020	2
1	A	99	TRP	HB3	3.171	0.020	2
1	A	99	TRP	HD1	7.212	0.020	1
1	A	99	TRP	HE1	10.071	0.020	1
1	A	99	TRP	HE3	7.575	0.020	1
1	A	99	TRP	HZ2	7.413	0.020	1
1	A	99	TRP	HZ3	7.09	0.020	1
1	A	99	TRP	HH2	7.184	0.020	1
1	A	99	TRP	CA	57.131	0.300	1
1	A	99	TRP	CB	29.585	0.300	1
1	A	99	TRP	CD1	126.676	0.300	1
1	A	99	TRP	CE3	120.455	0.300	1
1	A	99	TRP	CZ2	114.19	0.300	1
1	A	99	TRP	CZ3	121.629	0.300	1
1	A	99	TRP	CH2	124.243	0.300	1
1	A	99	TRP	N	121.53	0.300	1
1	A	99	TRP	NE1	129.392	0.300	1
1	A	100	ASN	H	8.065	0.020	1
1	A	100	ASN	HA	4.584	0.020	1
1	A	100	ASN	HB2	2.555	0.020	2
1	A	100	ASN	HB3	2.516	0.020	2
1	A	100	ASN	HD21	7.431	0.020	2
1	A	100	ASN	HD22	6.783	0.020	2
1	A	100	ASN	CA	52.795	0.300	1
1	A	100	ASN	CB	38.908	0.300	1
1	A	100	ASN	N	120.377	0.300	1
1	A	100	ASN	ND2	112.046	0.300	1
1	A	101	LYS	H	7.948	0.020	1
1	A	101	LYS	HA	4.43	0.020	1
1	A	101	LYS	HB2	1.747	0.020	2
1	A	101	LYS	HB3	1.616	0.020	2
1	A	101	LYS	HG2	1.365	0.020	1
1	A	101	LYS	HG3	1.365	0.020	1
1	A	101	LYS	HD2	1.624	0.020	1
1	A	101	LYS	HD3	1.624	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	LYS	HE2	2.941	0.020	1
1	A	101	LYS	HE3	2.941	0.020	1
1	A	101	LYS	CA	54.18	0.300	1
1	A	101	LYS	CB	32.388	0.300	1
1	A	101	LYS	CG	24.909	0.300	1
1	A	101	LYS	CD	28.935	0.300	1
1	A	101	LYS	CE	42.056	0.300	1
1	A	101	LYS	N	122.677	0.300	1
1	A	102	PRO	HA	4.406	0.020	1
1	A	102	PRO	HB2	2.267	0.020	2
1	A	102	PRO	HB3	1.884	0.020	2
1	A	102	PRO	HG2	1.992	0.020	1
1	A	102	PRO	HG3	1.992	0.020	1
1	A	102	PRO	HD2	3.774	0.020	2
1	A	102	PRO	HD3	3.605	0.020	2
1	A	102	PRO	CA	63.094	0.300	1
1	A	102	PRO	CB	32.192	0.300	1
1	A	102	PRO	CG	27.373	0.300	1
1	A	102	PRO	CD	50.759	0.300	1
1	A	103	SER	H	8.382	0.020	1
1	A	103	SER	HA	4.407	0.020	1
1	A	103	SER	HB2	3.82	0.020	1
1	A	103	SER	HB3	3.82	0.020	1
1	A	103	SER	CA	58.08	0.300	1
1	A	103	SER	CB	64.111	0.300	1
1	A	103	SER	N	116.909	0.300	1
1	A	104	LYS	H	8.279	0.020	1
1	A	104	LYS	HA	4.6	0.020	1
1	A	104	LYS	HB2	1.799	0.020	2
1	A	104	LYS	HB3	1.69	0.020	2
1	A	104	LYS	HG2	1.439	0.020	1
1	A	104	LYS	HG3	1.439	0.020	1
1	A	104	LYS	HD2	1.68	0.020	1
1	A	104	LYS	HD3	1.68	0.020	1
1	A	104	LYS	HE2	2.975	0.020	1
1	A	104	LYS	HE3	2.975	0.020	1
1	A	104	LYS	CA	54.184	0.300	1
1	A	104	LYS	CB	32.388	0.300	1
1	A	104	LYS	CG	24.4	0.300	1
1	A	104	LYS	CD	28.935	0.300	1
1	A	104	LYS	CE	42.056	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	LYS	N	124.225	0.300	1
1	A	105	PRO	HA	4.396	0.020	1
1	A	105	PRO	HB2	2.266	0.020	2
1	A	105	PRO	HB3	1.859	0.020	2
1	A	105	PRO	HG2	1.981	0.020	1
1	A	105	PRO	HG3	1.981	0.020	1
1	A	105	PRO	HD2	3.767	0.020	2
1	A	105	PRO	HD3	3.594	0.020	2
1	A	105	PRO	CA	63.018	0.300	1
1	A	105	PRO	CB	32.271	0.300	1
1	A	105	PRO	CG	27.373	0.300	1
1	A	105	PRO	CD	50.759	0.300	1
1	A	106	LYS	H	8.481	0.020	1
1	A	106	LYS	HA	4.321	0.020	1
1	A	106	LYS	HB2	1.84	0.020	2
1	A	106	LYS	HB3	1.747	0.020	2
1	A	106	LYS	HG2	1.464	0.020	2
1	A	106	LYS	HG3	1.428	0.020	2
1	A	106	LYS	HD2	1.679	0.020	1
1	A	106	LYS	HD3	1.679	0.020	1
1	A	106	LYS	HE2	2.995	0.020	1
1	A	106	LYS	HE3	2.995	0.020	1
1	A	106	LYS	CA	56.42	0.300	1
1	A	106	LYS	CB	33.061	0.300	1
1	A	106	LYS	CG	25.081	0.300	1
1	A	106	LYS	CD	29.111	0.300	1
1	A	106	LYS	CE	42.305	0.300	1
1	A	106	LYS	N	121.921	0.300	1
1	A	107	THR	H	8.102	0.020	1
1	A	107	THR	HA	4.304	0.020	1
1	A	107	THR	HB	4.158	0.020	1
1	A	107	THR	HG21	1.159	0.020	1
1	A	107	THR	HG22	1.159	0.020	1
1	A	107	THR	HG23	1.159	0.020	1
1	A	107	THR	CA	61.637	0.300	1
1	A	107	THR	CB	69.799	0.300	1
1	A	107	THR	CG2	21.605	0.300	1
1	A	107	THR	N	115.362	0.300	1
1	A	108	ASN	H	8.495	0.020	1
1	A	108	ASN	HA	4.694	0.020	1
1	A	108	ASN	HB2	2.816	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	ASN	HB3	2.723	0.020	2
1	A	108	ASN	HD21	7.557	0.020	2
1	A	108	ASN	HD22	6.86	0.020	2
1	A	108	ASN	CA	53.168	0.300	1
1	A	108	ASN	CB	38.75	0.300	1
1	A	108	ASN	N	121.166	0.300	1
1	A	108	ASN	ND2	112.704	0.300	1
1	A	109	MET	H	8.302	0.020	1
1	A	109	MET	HA	4.416	0.020	1
1	A	109	MET	HB2	2.037	0.020	2
1	A	109	MET	HB3	1.93	0.020	2
1	A	109	MET	HG2	2.536	0.020	2
1	A	109	MET	HG3	2.48	0.020	2
1	A	109	MET	HE1	1.363	0.020	1
1	A	109	MET	HE2	1.363	0.020	1
1	A	109	MET	HE3	1.363	0.020	1
1	A	109	MET	CA	55.573	0.300	1
1	A	109	MET	CB	31.007	0.300	1
1	A	109	MET	CG	32.388	0.300	1
1	A	109	MET	CE	19.096	0.300	1
1	A	109	MET	N	121.154	0.300	1
1	A	110	LYS	H	8.259	0.020	1
1	A	110	LYS	HA	4.21	0.020	1
1	A	110	LYS	HB2	1.698	0.020	1
1	A	110	LYS	HB3	1.698	0.020	1
1	A	110	LYS	HG2	1.388	0.020	2
1	A	110	LYS	HG3	1.322	0.020	2
1	A	110	LYS	HD2	1.643	0.020	1
1	A	110	LYS	HD3	1.643	0.020	1
1	A	110	LYS	HE2	2.961	0.020	1
1	A	110	LYS	HE3	2.961	0.020	1
1	A	110	LYS	CA	56.488	0.300	1
1	A	110	LYS	CB	33.14	0.300	1
1	A	110	LYS	CG	27.017	0.300	1
1	A	110	LYS	CD	28.935	0.300	1
1	A	110	LYS	CE	42.147	0.300	1
1	A	110	LYS	N	122.304	0.300	1
1	A	111	HIS	H	8.468	0.020	1
1	A	111	HIS	HA	4.619	0.020	1
1	A	111	HIS	HB2	3.216	0.020	2
1	A	111	HIS	HB3	3.107	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	HIS	HD2	7.198	0.020	1
1	A	111	HIS	CA	55.198	0.300	1
1	A	111	HIS	CB	29.111	0.300	1
1	A	111	HIS	CD2	119.62	0.300	1
1	A	111	HIS	N	119.597	0.300	1
1	A	112	MET	H	8.385	0.020	1
1	A	112	MET	HA	4.434	0.020	1
1	A	112	MET	HB2	2.042	0.020	2
1	A	112	MET	HB3	1.936	0.020	2
1	A	112	MET	HG2	2.543	0.020	2
1	A	112	MET	HG3	2.478	0.020	2
1	A	112	MET	HE1	2.061	0.020	1
1	A	112	MET	HE2	2.061	0.020	1
1	A	112	MET	HE3	2.061	0.020	1
1	A	112	MET	CA	55.302	0.300	1
1	A	112	MET	CB	33.078	0.300	1
1	A	112	MET	CG	32.042	0.300	1
1	A	112	MET	CE	16.934	0.300	1
1	A	112	MET	N	122.696	0.300	1
1	A	113	ALA	H	8.39	0.020	1
1	A	113	ALA	HA	4.295	0.020	1
1	A	113	ALA	HB1	1.357	0.020	1
1	A	113	ALA	HB2	1.357	0.020	1
1	A	113	ALA	HB3	1.357	0.020	1
1	A	113	ALA	CA	52.5	0.300	1
1	A	113	ALA	CB	19.0	0.300	1
1	A	113	ALA	N	125.77	0.300	1
1	A	114	GLY	H	8.356	0.020	1
1	A	114	GLY	HA2	3.914	0.020	1
1	A	114	GLY	HA3	3.914	0.020	1
1	A	114	GLY	CA	45.24	0.300	1
1	A	114	GLY	N	108.458	0.300	1
1	A	115	ALA	H	8.107	0.020	1
1	A	115	ALA	HA	4.277	0.020	1
1	A	115	ALA	HB1	1.349	0.020	1
1	A	115	ALA	HB2	1.349	0.020	1
1	A	115	ALA	HB3	1.349	0.020	1
1	A	115	ALA	CA	52.524	0.300	1
1	A	115	ALA	CB	19.393	0.300	1
1	A	115	ALA	N	123.843	0.300	1
1	A	116	ALA	H	8.241	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	ALA	HA	4.264	0.020	1
1	A	116	ALA	HB1	1.355	0.020	1
1	A	116	ALA	HB2	1.355	0.020	1
1	A	116	ALA	HB3	1.355	0.020	1
1	A	116	ALA	CA	52.472	0.300	1
1	A	116	ALA	CB	19.235	0.300	1
1	A	116	ALA	N	123.101	0.300	1
1	A	117	ALA	H	8.155	0.020	1
1	A	117	ALA	HA	4.246	0.020	1
1	A	117	ALA	HB1	1.355	0.020	1
1	A	117	ALA	HB2	1.355	0.020	1
1	A	117	ALA	HB3	1.355	0.020	1
1	A	117	ALA	CA	52.433	0.300	1
1	A	117	ALA	CB	19.235	0.300	1
1	A	117	ALA	N	123.228	0.300	1
1	A	118	ALA	H	8.188	0.020	1
1	A	118	ALA	HA	3.919	0.020	1
1	A	118	ALA	HB1	1.363	0.020	1
1	A	118	ALA	HB2	1.363	0.020	1
1	A	118	ALA	HB3	1.363	0.020	1
1	A	118	ALA	CA	52.539	0.300	1
1	A	118	ALA	CB	19.156	0.300	1
1	A	118	ALA	N	123.218	0.300	1
1	A	119	GLY	H	8.233	0.020	1
1	A	119	GLY	HA2	3.901	0.020	1
1	A	119	GLY	HA3	3.901	0.020	1
1	A	119	GLY	CA	45.24	0.300	1
1	A	119	GLY	N	108.025	0.300	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
$^{13}\text{C}_\alpha$	142	$-0.25 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	125	$0.10 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	133	$0.05 \pm 0.20$	None needed ( $< 0.5$ ppm)

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1011 atoms were assigned a chemical shift out of a possible 1286. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	355/454 (78%)	176/183 (96%)	91/182 (50%)	88/89 (99%)
Sidechain	584/693 (84%)	390/444 (88%)	175/213 (82%)	19/36 (53%)
Aromatic	72/139 (52%)	51/67 (76%)	21/68 (31%)	0/4 (0%)
Overall	1011/1286 (79%)	617/694 (89%)	287/463 (62%)	107/129 (83%)

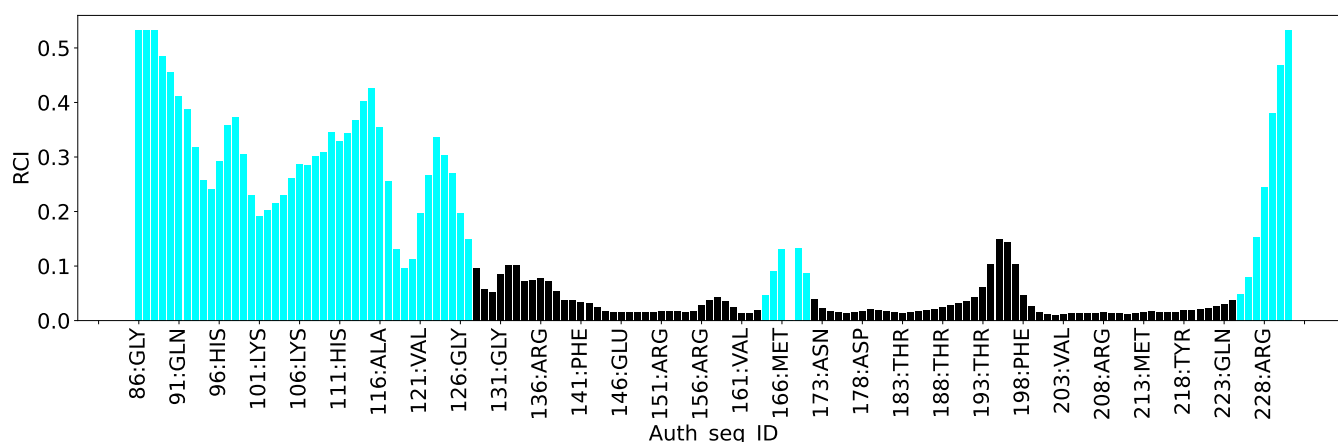
### 7.1.4 Statistically unusual chemical shifts [i](#)

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:



## 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	1318
Intra-residue ( $ i-j =0$ )	462
Sequential ( $ i-j =1$ )	363
Medium range ( $ i-j >1$ and $ i-j <5$ )	216
Long range ( $ i-j \geq 5$ )	277
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	124
Number of unmapped restraints	0
Number of restraints per residue	9.9
Number of long range restraints per residue <sup>1</sup>	1.9

<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)	23.0	0.2
0.2-0.5 (Medium)	34.2	0.5
>0.5 (Large)	45.1	18.31

### 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)	6.2	5.29
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

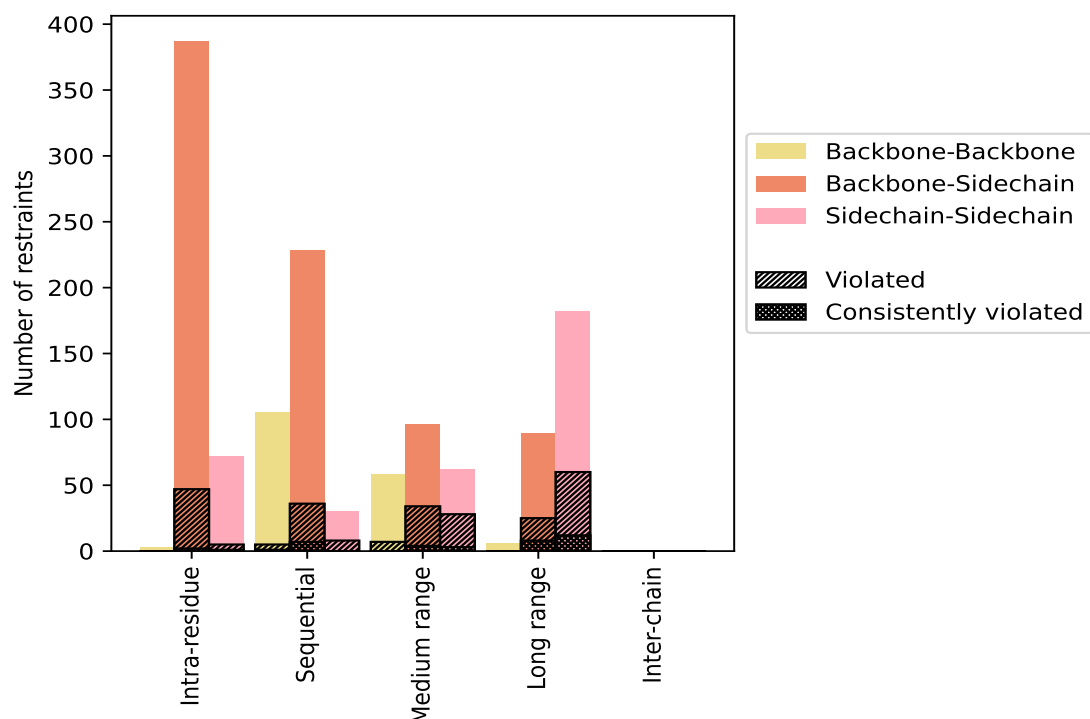
### 9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">462</a>	<a href="#">35.1</a>	<a href="#">52</a>	<a href="#">11.3</a>	<a href="#">3.9</a>	<a href="#">3</a>	<a href="#">0.6</a>	<a href="#">0.2</a>
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	387	29.4	47	12.1	3.6	2	0.5	0.2
Sidechain-Sidechain	72	5.5	5	6.9	0.4	1	1.4	0.1
<a href="#">Sequential ( i-j =1)</a>	<a href="#">363</a>	<a href="#">27.5</a>	<a href="#">49</a>	<a href="#">13.5</a>	<a href="#">3.7</a>	<a href="#">8</a>	<a href="#">2.2</a>	<a href="#">0.6</a>
Backbone-Backbone	105	8.0	5	4.8	0.4	1	1.0	0.1
Backbone-Sidechain	228	17.3	36	15.8	2.7	7	3.1	0.5
Sidechain-Sidechain	30	2.3	8	26.7	0.6	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">216</a>	<a href="#">16.4</a>	<a href="#">69</a>	<a href="#">31.9</a>	<a href="#">5.2</a>	<a href="#">7</a>	<a href="#">3.2</a>	<a href="#">0.5</a>
Backbone-Backbone	58	4.4	7	12.1	0.5	0	0.0	0.0
Backbone-Sidechain	96	7.3	34	35.4	2.6	4	4.2	0.3
Sidechain-Sidechain	62	4.7	28	45.2	2.1	3	4.8	0.2
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">277</a>	<a href="#">21.0</a>	<a href="#">85</a>	<a href="#">30.7</a>	<a href="#">6.4</a>	<a href="#">20</a>	<a href="#">7.2</a>	<a href="#">1.5</a>
Backbone-Backbone	6	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	89	6.8	25	28.1	1.9	8	9.0	0.6
Sidechain-Sidechain	182	13.8	60	33.0	4.6	12	6.6	0.9
<a href="#">Inter-chain</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>
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
<a href="#">Hydrogen 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="#">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="#">1318</a>	<a href="#">100.0</a>	<a href="#">255</a>	<a href="#">19.3</a>	<a href="#">19.3</a>	<a href="#">38</a>	<a href="#">2.9</a>	<a href="#">2.9</a>
Backbone-Backbone	172	13.1	12	7.0	0.9	1	0.6	0.1
Backbone-Sidechain	800	60.7	142	17.8	10.8	21	2.6	1.6
Sidechain-Sidechain	346	26.3	101	29.2	7.7	16	4.6	1.2

<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	16	21	26	38	0	101	1.23	13.68	2.49	0.45
2	13	20	37	38	0	108	1.02	10.01	1.79	0.4
3	17	21	28	48	0	114	0.97	11.91	2.03	0.4
4	14	22	34	36	0	106	1.1	11.83	2.03	0.43
5	13	20	25	36	0	94	1.28	14.92	2.68	0.44
6	16	19	32	31	0	98	1.21	14.54	2.62	0.42
7	13	17	30	34	0	94	1.25	11.38	2.22	0.5
8	15	22	33	38	0	108	1.23	17.74	3.16	0.38
9	15	22	28	39	0	104	1.33	18.31	3.18	0.38
10	17	24	26	46	0	113	1.15	15.31	2.58	0.4

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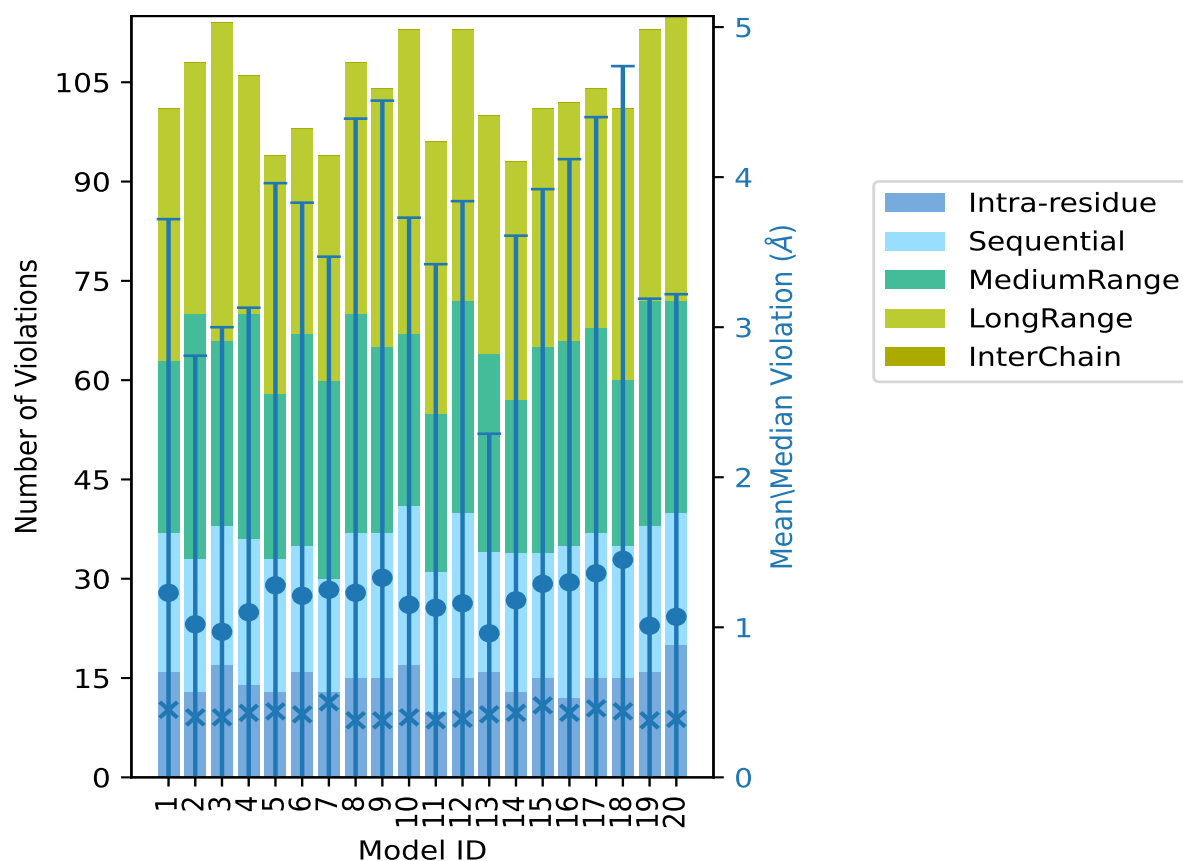
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	10	21	24	41	0	96	1.13	12.96	2.29	0.38
12	15	25	32	41	0	113	1.16	15.86	2.68	0.39
13	16	18	30	36	0	100	0.96	7.2	1.33	0.42
14	13	21	23	36	0	93	1.18	12.56	2.43	0.43
15	15	19	31	36	0	101	1.29	14.74	2.63	0.48
16	12	23	31	36	0	102	1.3	15.81	2.82	0.43
17	15	22	31	36	0	104	1.36	17.24	3.04	0.46
18	15	20	25	41	0	101	1.45	17.75	3.29	0.44
19	16	22	34	41	0	113	1.01	13.26	2.18	0.38
20	20	20	32	43	0	115	1.07	12.95	2.15	0.39

<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

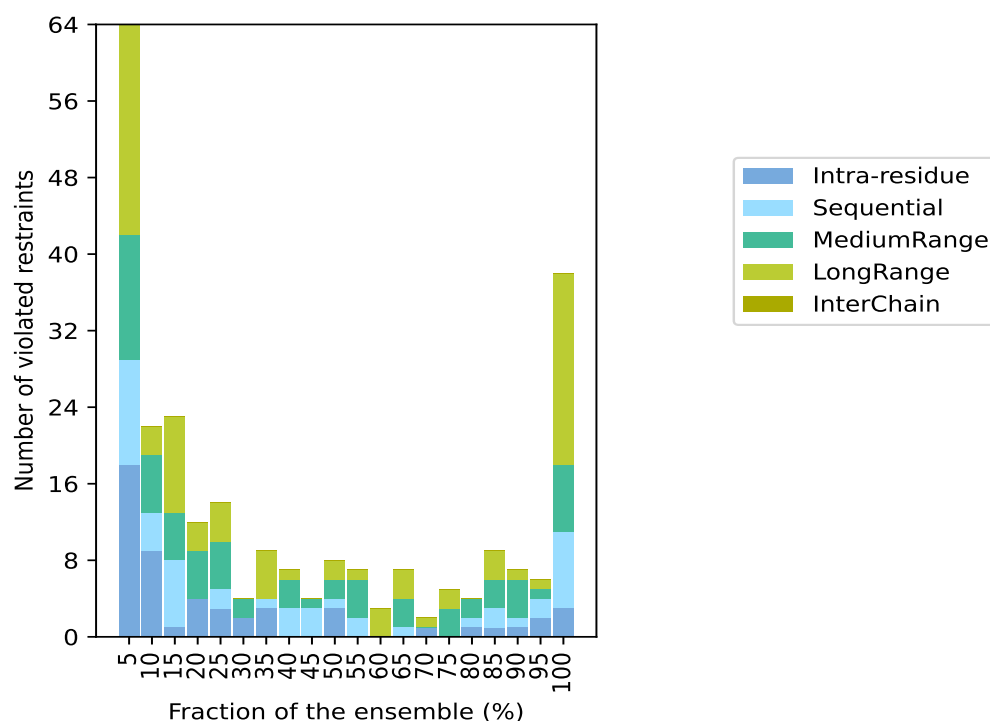
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1063(IR:410, SQ:314, MR:147, LR:192, IC:0) restraints are 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>	%
18	11	13	22	0	64	1	5.0
9	4	6	3	0	22	2	10.0
1	7	5	10	0	23	3	15.0
4	0	5	3	0	12	4	20.0
3	2	5	4	0	14	5	25.0
2	0	2	0	0	4	6	30.0
3	1	0	5	0	9	7	35.0
0	3	3	1	0	7	8	40.0
0	3	1	0	0	4	9	45.0
3	1	2	2	0	8	10	50.0
0	2	4	1	0	7	11	55.0
0	0	0	3	0	3	12	60.0
0	1	3	3	0	7	13	65.0
1	0	0	1	0	2	14	70.0
0	0	3	2	0	5	15	75.0
1	1	2	0	0	4	16	80.0
1	2	3	3	0	9	17	85.0
1	1	4	1	0	7	18	90.0
2	2	1	1	0	6	19	95.0
3	8	7	20	0	38	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

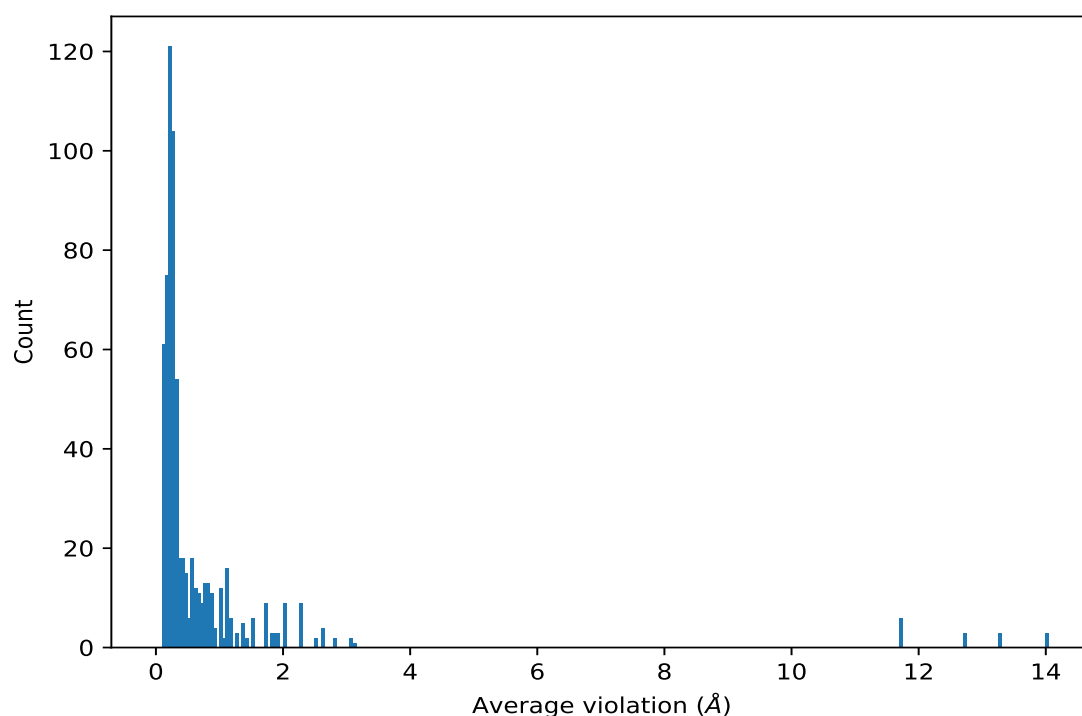
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	20	14.0	2.74	14.11
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	20	14.0	2.74	14.11
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	20	14.0	2.74	14.11
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	20	13.26	2.74	13.06
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	20	13.26	2.74	13.06
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	20	13.26	2.74	13.06
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	20	12.71	2.83	12.98
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	20	12.71	2.83	12.98
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	20	12.71	2.83	12.98
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	20	11.73	2.48	11.97
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	20	3.14	0.96	3.44

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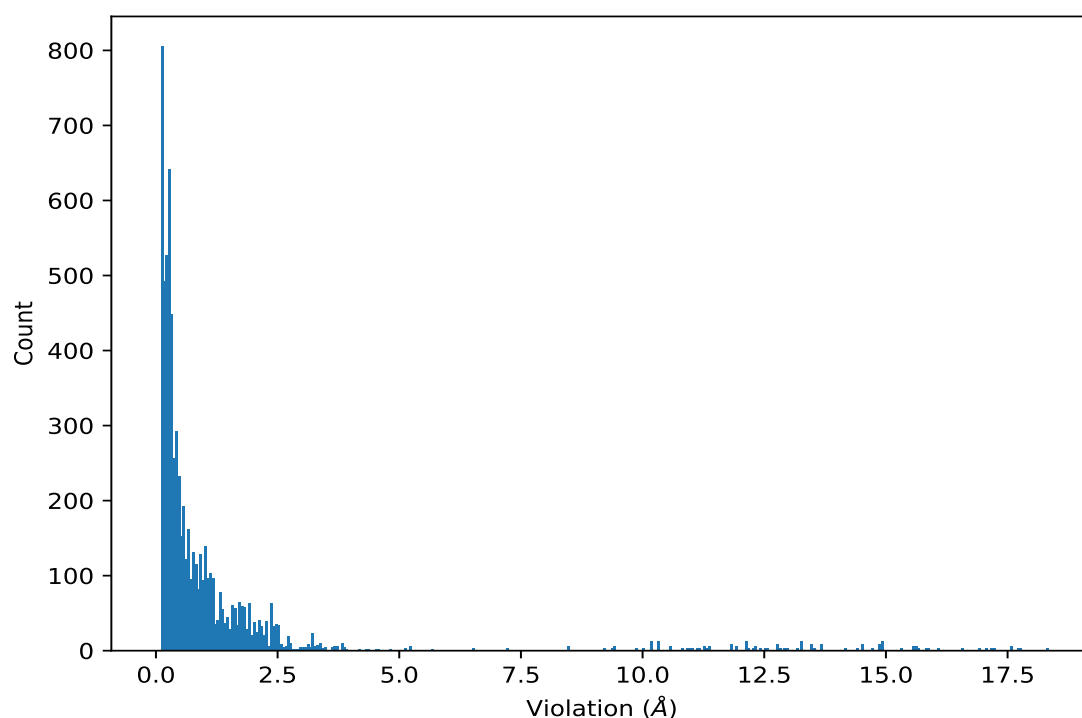
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	20	3.06	0.56	3.13
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	20	3.06	0.56	3.13
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	20	2.61	0.95	2.99
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	20	2.61	0.95	2.99
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	20	2.61	0.95	2.99
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	20	2.61	0.95	2.99
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	20	2.28	0.35	2.38
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	20	2.01	0.34	2.03
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	20	1.94	0.28	1.96

<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)
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	9	18.31
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	9	18.31
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	9	18.31
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	18	17.75
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	18	17.75
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	18	17.75
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	8	17.74
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	8	17.74
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	8	17.74
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	18	17.57
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	18	17.57
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	18	17.57
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	8	17.55
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	8	17.55
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	8	17.55
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	17	17.24
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	17	17.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	17	17.24
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	9	17.18
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	9	17.18
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	9	17.18
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	8	17.08
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	8	17.08
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	8	17.08
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	18	16.93
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	18	16.93
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	18	16.93
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	17	16.57

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

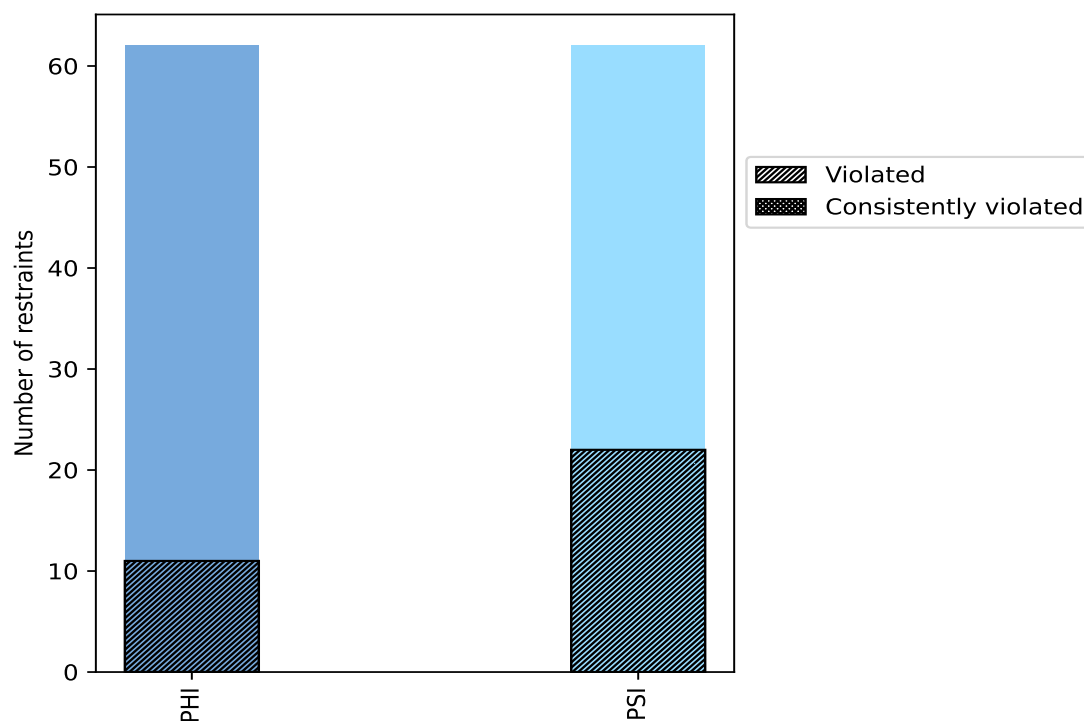
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	62	50.0	11	17.7	8.9	0	0.0	0.0
PSI	62	50.0	22	35.5	17.7	0	0.0	0.0
Total	124	100.0	33	26.6	26.6	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

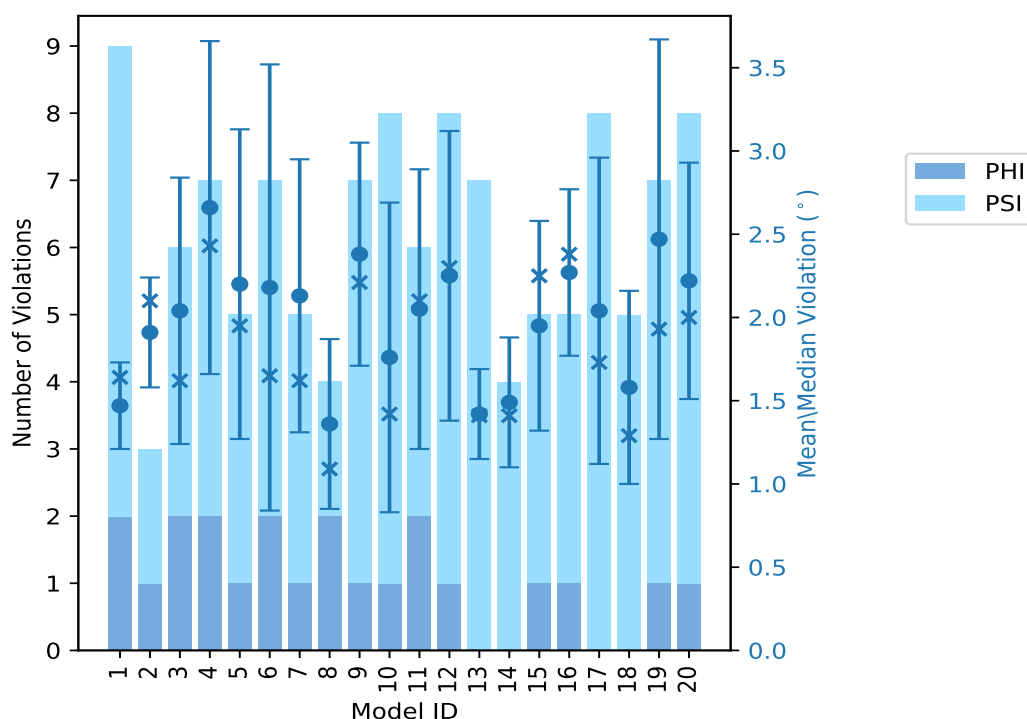
## 10.2 Dihedral-angle violation statistics for each model ⓘ

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 (°)
	PHI	PSI	Total				
1	2	7	9	1.47	1.78	0.26	1.64
2	1	2	3	1.91	2.19	0.33	2.1
3	2	4	6	2.04	3.64	0.8	1.62
4	2	5	7	2.66	4.48	1.0	2.43
5	1	4	5	2.2	3.95	0.93	1.95
6	2	5	7	2.18	5.29	1.34	1.65
7	1	4	5	2.13	3.25	0.82	1.62
8	2	2	4	1.36	2.25	0.51	1.09
9	1	6	7	2.38	3.94	0.67	2.21
10	1	7	8	1.76	4.18	0.93	1.42
11	2	4	6	2.05	3.45	0.84	2.1
12	1	7	8	2.25	3.57	0.87	2.3
13	0	7	7	1.42	1.91	0.27	1.41
14	0	4	4	1.49	2.11	0.39	1.41
15	1	4	5	1.95	2.63	0.63	2.25
16	1	4	5	2.27	2.79	0.5	2.38
17	0	8	8	2.04	3.7	0.92	1.73
18	0	5	5	1.58	2.48	0.58	1.29
19	1	6	7	2.47	4.85	1.2	1.93
20	1	7	8	2.22	3.49	0.71	2.0



### 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	
PHI	PSI	Total	Count <sup>1</sup>	%
7	9	16	1	5.0
3	2	5	2	10.0
0	1	1	3	15.0
0	3	3	4	20.0
0	1	1	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	1	1	8	40.0
1	1	2	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

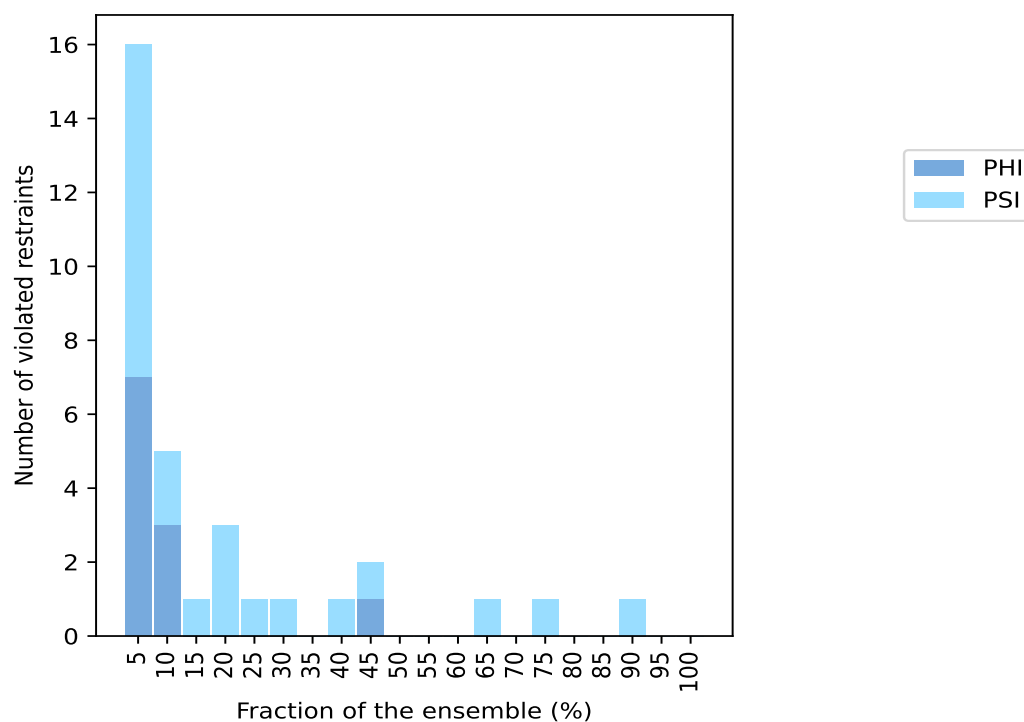
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
0	0	0	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

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

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

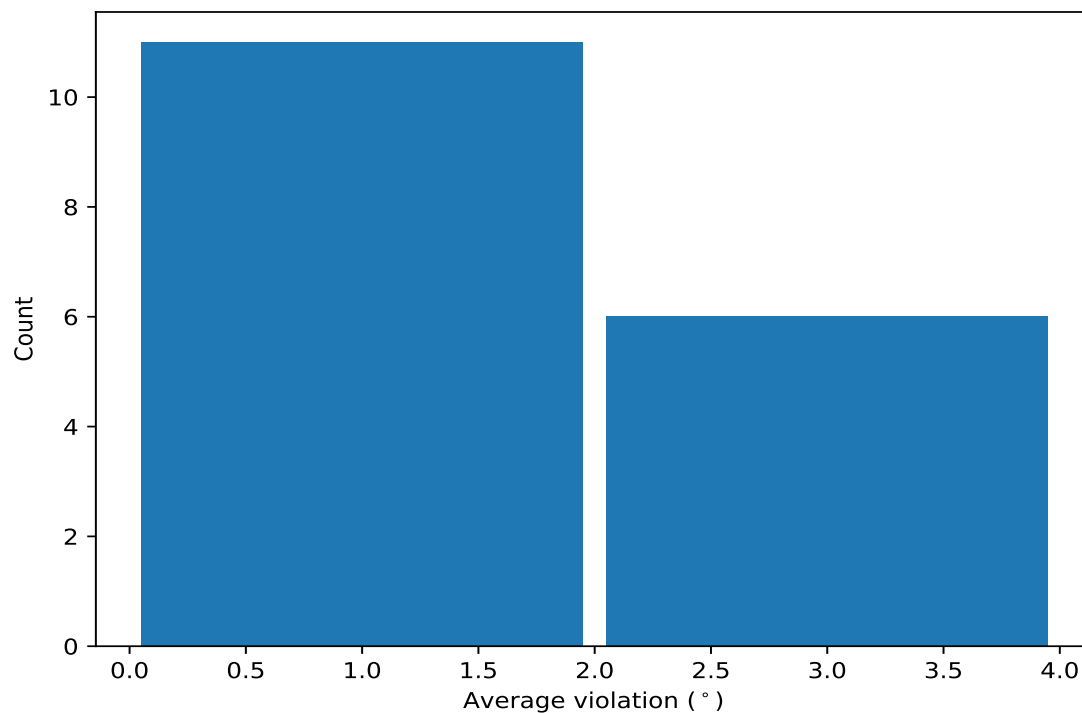


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 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.

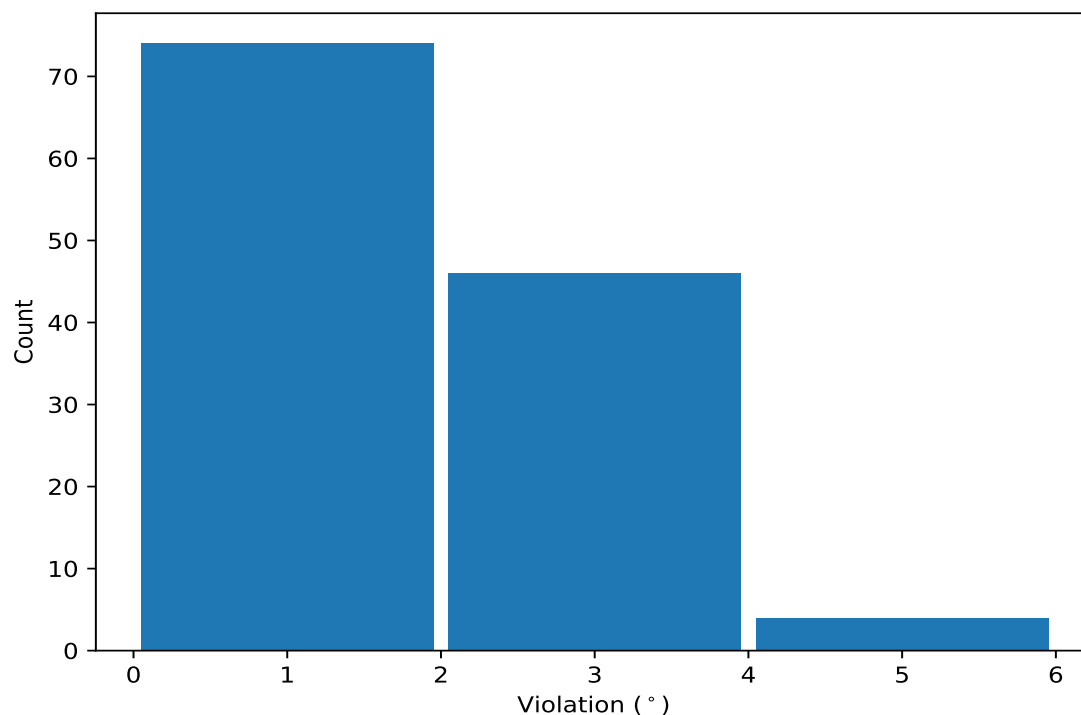
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	18	2.53	1.0	2.16
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	15	2.65	1.12	2.25
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	13	2.06	0.51	1.95
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	9	2.35	1.0	1.9
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	9	1.94	0.72	1.64
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	8	1.67	0.41	1.6
(1,86)	1:206:A:MET:N	1:206:A:MET:CA	1:206:A:MET:C	1:207:A:GLU:N	6	1.44	0.27	1.38
(1,124)	1:225:A:TYR:N	1:225:A:TYR:CA	1:225:A:TYR:C	1:226:A:TYR:N	5	1.78	0.52	1.76
(1,106)	1:216:A:THR:N	1:216:A:THR:CA	1:216:A:THR:C	1:217:A:GLN:N	4	2.45	0.99	2.32
(1,10)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ARG:N	4	1.69	0.46	1.58

<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 (°)
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	6	5.29
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	19	4.85
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	4	4.48
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	10	4.18
(1,106)	1:216:A:THR:N	1:216:A:THR:CA	1:216:A:THR:C	1:217:A:GLN:N	5	3.95
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	9	3.94
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	17	3.7
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	3	3.64
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	12	3.57
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	19	3.53