



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LNZ  
BMRB ID : 18186  
Title : Solution structure of the Get5 carboxyl domain from *S. cerevisiae*  
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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

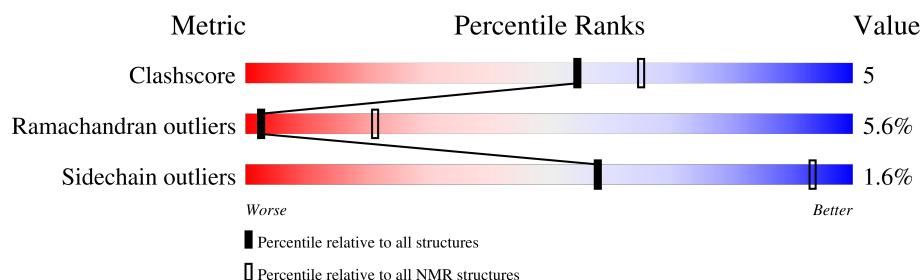
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 45%.

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	64	
1	B	64	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:176-A:211, B:176-B:212 (73)	0.19	1

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, 5, 6, 8, 10
2	2, 3, 4
Single-model clusters	7; 9

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

There is only 1 type of molecule in this entry. The entry contains 1308 atoms, of which 648 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-like protein MDY2.

Mol	Chain	Residues	Atoms						Trace
1	A	40	Total	C	H	N	O	S	0
			654	207	324	58	64	1	
1	B	40	Total	C	H	N	O	S	0
			654	207	324	58	64	1	

There are 6 discrepancies between the modelled and reference sequences:

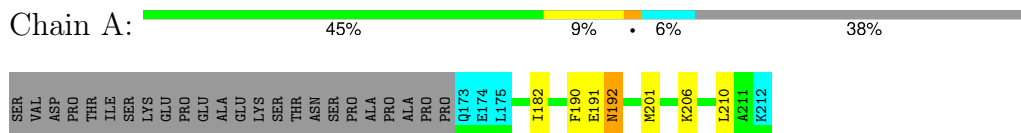
Chain	Residue	Modelled	Actual	Comment	Reference
A	149	SER	-	expression tag	UNP Q12285
A	150	VAL	-	expression tag	UNP Q12285
A	151	ASP	-	expression tag	UNP Q12285
B	149	SER	-	expression tag	UNP Q12285
B	150	VAL	-	expression tag	UNP Q12285
B	151	ASP	-	expression tag	UNP Q12285

## 4 Residue-property plots [i](#)

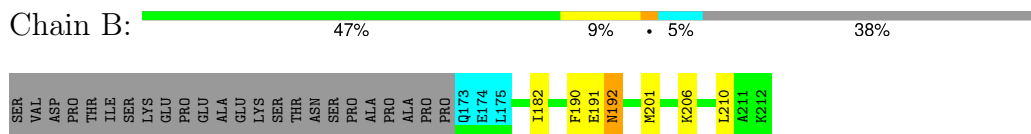
### 4.1 Average score per residue in the NMR ensemble

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: Ubiquitin-like protein MDY2



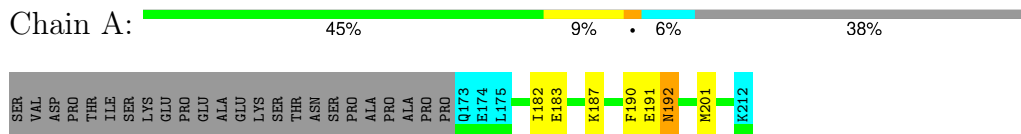
- Molecule 1: Ubiquitin-like protein MDY2



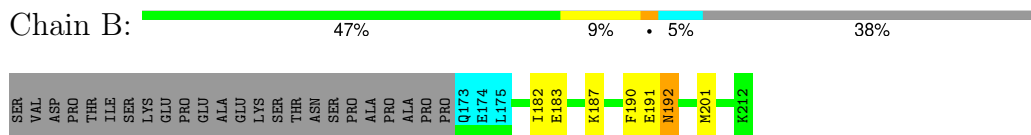
### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 1: Ubiquitin-like protein MDY2



## 5 Refinement protocol and experimental data overview

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

Of the 100 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	2.3
CNS	refinement	1.21

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	762
Number of shifts mapped to atoms	518
Number of unparsed shifts	0
Number of shifts with mapping errors	244
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

## 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	294	286	286	3±1
1	B	304	299	299	3±1
All	All	5980	5850	5850	58

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 5.

5 of 18 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:LYS:O	1:A:210:LEU:HG	0.54	2.03	4	9
1:B:206:LYS:O	1:B:210:LEU:HG	0.53	2.04	4	9
1:B:190:PHE:C	1:B:192:ASN:H	0.52	2.08	7	1
1:A:182:ILE:HG22	1:A:201:MET:SD	0.52	2.45	1	6
1:A:190:PHE:C	1:A:192:ASN:H	0.52	2.08	7	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	36/64 (56%)	32±0 (89±1%)	2±1 (5±2%)	2±0 (6±1%)	2	21
1	B	36/64 (56%)	32±0 (89±1%)	2±1 (5±2%)	2±0 (6±1%)	2	21
All	All	720/1280 (56%)	644 (89%)	36 (5%)	40 (6%)	2	21

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	191	GLU	10
1	B	191	GLU	10
1	A	192	ASN	9
1	B	192	ASN	9
1	A	193	ASP	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	31/56 (55%)	30±1 (98±2%)	0±1 (2±2%)	58	93
1	B	32/56 (57%)	32±1 (98±2%)	0±1 (2±2%)	58	93
All	All	630/1120 (56%)	620 (98%)	10 (2%)	58	93

5 of 6 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	201	MET	2
1	B	201	MET	2
1	A	191	GLU	2
1	B	191	GLU	2
1	A	193	ASP	1



### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no 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 45% for the well-defined parts and 45% 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	762
Number of shifts mapped to atoms	518
Number of unparsed shifts	0
Number of shifts with mapping errors	244
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

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 244) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	150	VAL	HA	4.188	0.001	1
1	A	150	VAL	HB	2.051	0	1
1	A	150	VAL	HG11	0.924	0	2
1	A	150	VAL	HG12	0.924	0	2
1	A	150	VAL	HG13	0.924	0	2
1	A	150	VAL	HG21	0.932	0	2
1	A	150	VAL	HG22	0.932	0	2
1	A	150	VAL	HG23	0.932	0	2
1	A	150	VAL	C	175.422	0	1
1	A	150	VAL	CA	62.042	0.067	1
1	A	150	VAL	CB	32.93	0.074	1
1	A	150	VAL	CG1	21.124	0	2
1	A	150	VAL	CG2	20.404	0.003	2
1	A	151	ASP	H	8.49	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	ASP	HA	4.908	0.001	1
1	A	151	ASP	HB2	2.558	0.007	2
1	A	151	ASP	HB3	2.818	0.002	2
1	A	151	ASP	CA	51.995	0.066	1
1	A	151	ASP	CB	41.174	0.026	1
1	A	151	ASP	N	126.293	0.026	1
1	A	152	PRO	HA	4.5	0.013	1
1	A	152	PRO	HB2	2.019	0	2
1	A	152	PRO	HB3	2.317	0	2
1	A	152	PRO	C	177.321	0	1
1	A	152	PRO	CA	63.537	0.05	1
1	A	152	PRO	CB	32.192	0.086	1
1	A	152	PRO	CG	26.992	0	1
1	A	152	PRO	CD	50.879	0	1
1	A	153	THR	H	8.423	0.002	1
1	A	153	THR	HA	4.259	0.002	1
1	A	153	THR	HB	4.205	0.005	1
1	A	153	THR	HG21	1.227	0.002	1
1	A	153	THR	HG22	1.227	0.002	1
1	A	153	THR	HG23	1.227	0.002	1
1	A	153	THR	C	174.81	0	1
1	A	153	THR	CA	62.769	0.072	1
1	A	153	THR	CB	69.533	0.054	1
1	A	153	THR	CG2	21.769	0.023	1
1	A	153	THR	N	113.744	0.028	1
1	A	154	ILE	H	7.822	0.001	1
1	A	154	ILE	HA	4.214	0.013	1
1	A	154	ILE	HB	1.912	0.007	1
1	A	154	ILE	HG12	1.2	0.002	2
1	A	154	ILE	HG13	1.468	0.002	2
1	A	154	ILE	HG21	0.913	0	1
1	A	154	ILE	HG22	0.913	0	1
1	A	154	ILE	HG23	0.913	0	1
1	A	154	ILE	HD11	0.876	0	1
1	A	154	ILE	HD12	0.876	0	1
1	A	154	ILE	HD13	0.876	0	1
1	A	154	ILE	C	176.15	0	1
1	A	154	ILE	CA	61.08	0.054	1
1	A	154	ILE	CB	38.714	0.052	1
1	A	154	ILE	CG1	27.227	0.033	1
1	A	154	ILE	CG2	17.419	0.017	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	154	ILE	CD1	12.916	0.054	1
1	A	154	ILE	N	122.501	0.018	1
1	A	155	SER	H	8.318	0.002	1
1	A	155	SER	HA	4.458	0.002	1
1	A	155	SER	HB2	3.844	0	1
1	A	155	SER	HB3	3.844	0	1
1	A	155	SER	C	174.203	0	1
1	A	155	SER	CA	58.168	0.08	1
1	A	155	SER	CB	63.742	0.043	1
1	A	155	SER	N	119.956	0.009	1
1	A	156	LYS	H	8.344	0.002	1
1	A	156	LYS	HA	4.384	0.007	1
1	A	156	LYS	HB2	1.735	0	2
1	A	156	LYS	HB3	1.847	0	2
1	A	156	LYS	HG2	1.443	0.004	1
1	A	156	LYS	HG3	1.443	0.004	1
1	A	156	LYS	HD2	1.693	0.003	1
1	A	156	LYS	HD3	1.693	0.003	1
1	A	156	LYS	HE2	2.996	0	1
1	A	156	LYS	HE3	2.996	0	1
1	A	156	LYS	C	176.183	0	1
1	A	156	LYS	CA	55.962	0.049	1
1	A	156	LYS	CB	33.242	0.07	1
1	A	156	LYS	CG	24.526	0.079	1
1	A	156	LYS	CD	28.962	0.082	1
1	A	156	LYS	CE	42.081	0	1
1	A	156	LYS	N	123.765	0.027	1
1	A	157	GLU	H	8.462	0.002	1
1	A	157	GLU	HA	4.555	0.008	1
1	A	157	GLU	HB2	1.878	0	2
1	A	157	GLU	HB3	2.076	0	2
1	A	157	GLU	HG2	2.33	0	1
1	A	157	GLU	HG3	2.33	0	1
1	A	157	GLU	CA	54.6	0.032	1
1	A	157	GLU	CB	29.502	0	1
1	A	157	GLU	N	123.909	0.024	1
1	A	158	PRO	HA	4.39	0.005	1
1	A	158	PRO	HB2	1.925	0	2
1	A	158	PRO	HB3	2.318	0	2
1	A	158	PRO	HG3	2.056	0	1
1	A	158	PRO	HD2	3.707	0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	158	PRO	HD3	3.821	0	2
1	A	158	PRO	C	177.12	0	1
1	A	158	PRO	CA	63.257	0.057	1
1	A	158	PRO	CB	32.063	0.085	1
1	A	158	PRO	CG	27.44	0.001	1
1	A	158	PRO	CD	50.624	0.003	1
1	A	159	GLU	H	8.543	0.001	1
1	A	159	GLU	HA	4.235	0	1
1	A	159	GLU	HB2	1.947	0	2
1	A	159	GLU	HB3	2.051	0	2
1	A	159	GLU	HG2	2.32	0	1
1	A	159	GLU	HG3	2.32	0	1
1	A	159	GLU	C	176.525	0	1
1	A	159	GLU	CA	56.604	0.066	1
1	A	159	GLU	CB	30.199	0.113	1
1	A	159	GLU	CG	36.293	0	1
1	A	159	GLU	N	121.225	0.023	1
1	A	160	ALA	H	8.325	0.002	1
1	A	160	ALA	HA	4.28	0.002	1
1	A	160	ALA	HB1	1.407	0.004	1
1	A	160	ALA	HB2	1.407	0.004	1
1	A	160	ALA	HB3	1.407	0.004	1
1	A	160	ALA	C	177.923	0	1
1	A	160	ALA	CA	52.758	0.105	1
1	A	160	ALA	CB	19.382	0.034	1
1	A	160	ALA	N	125.227	0.019	1
1	A	161	GLU	H	8.388	0.01	1
1	A	161	GLU	HA	4.229	0.012	1
1	A	161	GLU	HB2	2.051	0	2
1	A	161	GLU	HB3	1.96	0	2
1	A	161	GLU	HG2	2.306	0	1
1	A	161	GLU	HG3	2.306	0	1
1	A	161	GLU	C	176.613	0	1
1	A	161	GLU	CA	56.702	0.017	1
1	A	161	GLU	CB	30.11	0.097	1
1	A	161	GLU	CG	36.227	0	1
1	A	161	GLU	N	120.229	0.013	1
1	A	162	LYS	H	8.33	0.006	1
1	A	162	LYS	HA	4.373	0.002	1
1	A	162	LYS	HB2	1.869	0	2
1	A	162	LYS	HB3	1.731	0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	162	LYS	HG2	1.443	0.007	1
1	A	162	LYS	HG3	1.443	0.007	1
1	A	162	LYS	HD2	1.766	0	2
1	A	162	LYS	HD3	1.648	0	2
1	A	162	LYS	HE2	3.012	0.002	2
1	A	162	LYS	HE3	3.01	0	2
1	A	162	LYS	C	176.739	0	1
1	A	162	LYS	CA	56.252	0.086	1
1	A	162	LYS	CB	33.105	0.029	1
1	A	162	LYS	CG	24.754	0.054	1
1	A	162	LYS	CD	29.057	0.007	1
1	A	162	LYS	CE	42.125	0	1
1	A	162	LYS	N	122.474	0.048	1
1	A	163	SER	H	8.413	0.002	1
1	A	163	SER	HA	4.52	0.014	1
1	A	163	SER	HB2	3.892	0.001	2
1	A	163	SER	HB3	3.934	0	2
1	A	163	SER	C	174.994	0	1
1	A	163	SER	CA	58.346	0.064	1
1	A	163	SER	CB	63.753	0.029	1
1	A	163	SER	N	117.125	0.012	1
1	A	164	THR	H	8.246	0.001	1
1	A	164	THR	HA	4.378	0.003	1
1	A	164	THR	HB	4.283	0.001	1
1	A	164	THR	HG21	1.218	0.003	1
1	A	164	THR	HG22	1.218	0.003	1
1	A	164	THR	HG23	1.218	0.003	1
1	A	164	THR	C	174.356	0	1
1	A	164	THR	CA	61.834	0.074	1
1	A	164	THR	CB	69.706	0.026	1
1	A	164	THR	CG2	21.578	0.051	1
1	A	164	THR	N	115.57	0.011	1
1	A	165	ASN	H	8.409	0.002	1
1	A	165	ASN	HA	4.773	0	1
1	A	165	ASN	HB2	2.738	0.006	2
1	A	165	ASN	HB3	2.825	0.011	2
1	A	165	ASN	HD21	6.919	0	1
1	A	165	ASN	HD22	7.597	0	1
1	A	165	ASN	C	174.816	0	1
1	A	165	ASN	CA	53.141	0.055	1
1	A	165	ASN	CB	39.08	0.075	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	165	ASN	N	120.92	0.02	1
1	A	165	ASN	ND2	112.944	0	1
1	A	166	SER	H	8.271	0.002	1
1	A	166	SER	HA	4.762	0.008	1
1	A	166	SER	HB2	3.801	0.004	2
1	A	166	SER	HB3	3.881	0	2
1	A	166	SER	CA	56.442	0.103	1
1	A	166	SER	CB	63.237	0	1
1	A	166	SER	N	117.774	0.045	1
1	A	167	PRO	HA	4.387	0	1
1	A	167	PRO	HB2	1.879	0	2
1	A	167	PRO	HB3	2.263	0	2
1	A	167	PRO	C	176.325	0	1
1	A	167	PRO	CA	62.723	0.079	1
1	A	167	PRO	CB	31.989	0.06	1
1	A	167	PRO	CG	27.271	0	1
1	A	167	PRO	CD	50.403	0	1
1	A	168	ALA	H	8.372	0.002	1
1	A	168	ALA	HA	4.582	0.005	1
1	A	168	ALA	HB1	1.362	0.005	1
1	A	168	ALA	HB2	1.362	0.005	1
1	A	168	ALA	HB3	1.362	0.005	1
1	A	168	ALA	CA	50.374	0.048	1
1	A	168	ALA	CB	18.181	0.028	1
1	A	168	ALA	N	125.934	0.032	1
1	A	169	PRO	HA	4.42	0.016	1
1	A	169	PRO	HB2	1.916	0	2
1	A	169	PRO	HB3	2.275	0	2
1	A	169	PRO	HG3	2.035	0	1
1	A	169	PRO	HD2	3.643	0	2
1	A	169	PRO	HD3	3.819	0	2
1	A	169	PRO	C	176.344	0	1
1	A	169	PRO	CA	62.976	0.049	1
1	A	169	PRO	CB	32.02	0.067	1
1	A	169	PRO	CG	27.693	0	1
1	A	169	PRO	CD	50.668	0.009	1
1	A	170	ALA	H	8.407	0.002	1
1	A	170	ALA	HA	4.584	0.003	1
1	A	170	ALA	HB1	1.362	0.004	1
1	A	170	ALA	HB2	1.362	0.004	1
1	A	170	ALA	HB3	1.362	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	170	ALA	CA	50.424	0.034	1
1	A	170	ALA	CB	18.143	0.01	1
1	A	170	ALA	N	126.15	0.023	1
1	A	171	PRO	HA	4.713	0.003	1
1	A	171	PRO	HB2	1.92	0.001	2
1	A	171	PRO	HB3	2.366	0	2
1	A	171	PRO	HG3	2.046	0.004	1
1	A	171	PRO	HD2	3.826	0.002	2
1	A	171	PRO	HD3	3.647	0.001	2
1	A	171	PRO	CA	61.639	0.047	1
1	A	171	PRO	CB	31.95	0	1
1	A	171	PRO	CG	27.519	0	1
1	A	171	PRO	CD	50.679	0	1
1	A	172	PRO	HA	4.413	0.018	1
1	A	172	PRO	HB2	1.922	0.008	2
1	A	172	PRO	HB3	2.31	0.005	2
1	A	172	PRO	HG2	2.033	0	1
1	A	172	PRO	HG3	2.033	0	1
1	A	172	PRO	HD2	3.707	0.003	2
1	A	172	PRO	HD3	3.824	0.001	2
1	A	172	PRO	C	176.888	0	1
1	A	172	PRO	CA	62.937	0.059	1
1	A	172	PRO	CB	32.074	0.072	1
1	A	172	PRO	CG	27.369	0.002	1
1	A	172	PRO	CD	50.386	0.008	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
$^{13}\text{C}_\alpha$	63	$-0.67 \pm 0.30$	Should be checked
$^{13}\text{C}_\beta$	62	$0.23 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	55	$-0.40 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	55	$-0.14 \pm 0.42$	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 45%, i.e. 464 atoms were assigned a chemical shift out of a possible 1032. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned



stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	178/363 (49%)	72/146 (49%)	71/146 (49%)	35/71 (49%)
Sidechain	252/601 (42%)	170/386 (44%)	76/186 (41%)	6/29 (21%)
Aromatic	34/68 (50%)	17/34 (50%)	15/30 (50%)	2/4 (50%)
Overall	464/1032 (45%)	259/566 (46%)	162/362 (45%)	43/104 (41%)

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

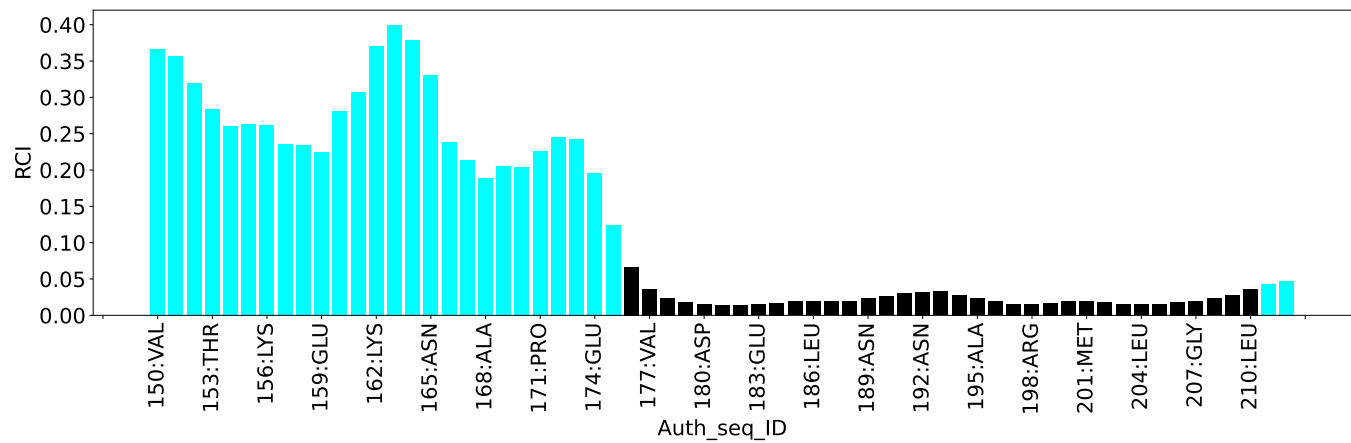
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	205	GLN	HG3	-0.05	0.91 – 3.68	-8.5
1	A	177	VAL	HG11	-0.99	-0.48 – 2.12	-7.0
1	A	177	VAL	HG12	-0.99	-0.48 – 2.12	-7.0
1	A	177	VAL	HG13	-0.99	-0.48 – 2.12	-7.0
1	A	203	ARG	HD2	1.57	1.97 – 4.26	-6.7
1	A	177	VAL	HB	0.16	0.43 – 3.54	-5.9
1	A	205	GLN	HE21	4.66	5.02 – 9.43	-5.8
1	A	177	VAL	HG21	-0.61	-0.58 – 2.19	-5.1
1	A	177	VAL	HG22	-0.61	-0.58 – 2.19	-5.1
1	A	177	VAL	HG23	-0.61	-0.58 – 2.19	-5.1

### 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	2976
Intra-residue ( $ i-j =0$ )	764
Sequential ( $ i-j =1$ )	508
Medium range ( $ i-j >1$ and $ i-j <5$ )	848
Long range ( $ i-j \geq 5$ )	358
Inter-chain	402
Hydrogen bond restraints	96
Disulfide bond restraints	0
Total dihedral-angle restraints	132
Number of unmapped restraints	0
Number of restraints per residue	24.3
Number of long range restraints per residue <sup>1</sup>	2.8

<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)	140.7	0.2
0.2-0.5 (Medium)	254.1	0.5
>0.5 (Large)	333.4	3.49

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	5.9	7.53
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

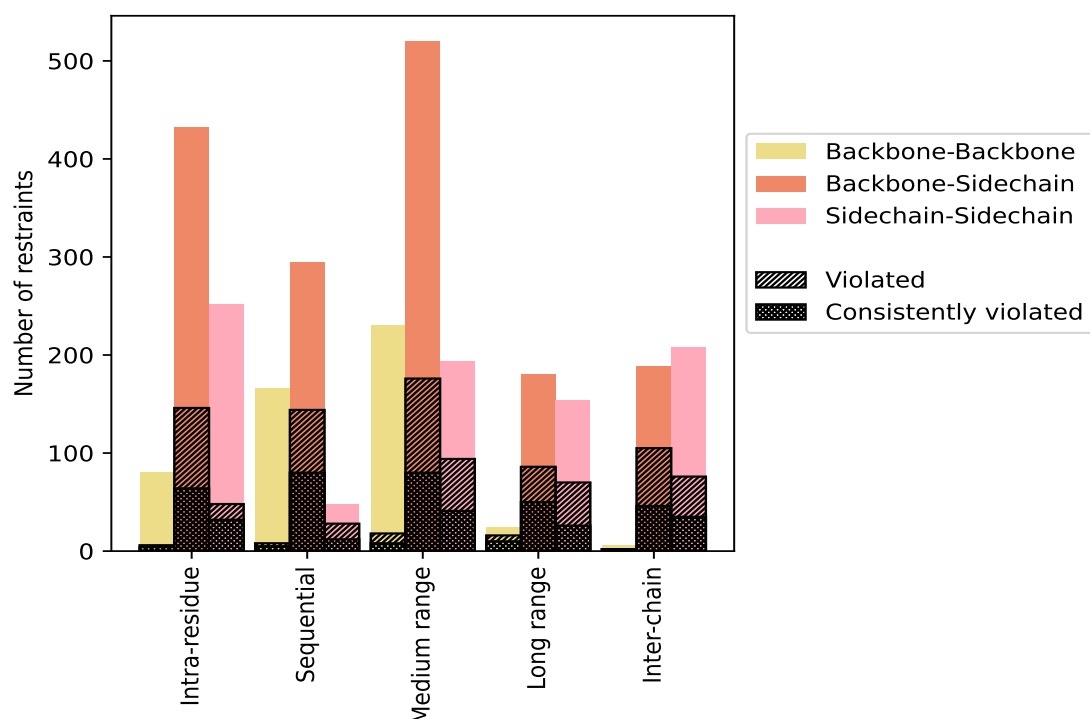
### 9.1 Summary of distance violations ⓘ

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>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>764</b>	<b>25.7</b>	<b>200</b>	<b>26.2</b>	<b>6.7</b>	<b>100</b>	<b>13.1</b>	<b>3.4</b>
Backbone-Backbone	80	2.7	6	7.5	0.2	4	5.0	0.1
Backbone-Sidechain	432	14.5	146	33.8	4.9	64	14.8	2.2
Sidechain-Sidechain	252	8.5	48	19.0	1.6	32	12.7	1.1
<b>Sequential (<math> i-j =1</math>)</b>	<b>508</b>	<b>17.1</b>	<b>180</b>	<b>35.4</b>	<b>6.0</b>	<b>97</b>	<b>19.1</b>	<b>3.3</b>
Backbone-Backbone	166	5.6	8	4.8	0.3	5	3.0	0.2
Backbone-Sidechain	294	9.9	144	49.0	4.8	80	27.2	2.7
Sidechain-Sidechain	48	1.6	28	58.3	0.9	12	25.0	0.4
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>848</b>	<b>28.5</b>	<b>288</b>	<b>34.0</b>	<b>9.7</b>	<b>129</b>	<b>15.2</b>	<b>4.3</b>
Backbone-Backbone	230	7.7	18	7.8	0.6	8	3.5	0.3
Backbone-Sidechain	424	14.2	176	41.5	5.9	80	18.9	2.7
Sidechain-Sidechain	194	6.5	94	48.5	3.2	41	21.1	1.4
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>358</b>	<b>12.0</b>	<b>172</b>	<b>48.0</b>	<b>5.8</b>	<b>86</b>	<b>24.0</b>	<b>2.9</b>
Backbone-Backbone	24	0.8	16	66.7	0.5	10	41.7	0.3
Backbone-Sidechain	180	6.0	86	47.8	2.9	50	27.8	1.7
Sidechain-Sidechain	154	5.2	70	45.5	2.4	26	16.9	0.9
<b>Inter-chain</b>	<b>402</b>	<b>13.5</b>	<b>183</b>	<b>45.5</b>	<b>6.1</b>	<b>83</b>	<b>20.6</b>	<b>2.8</b>
Backbone-Backbone	6	0.2	2	33.3	0.1	2	33.3	0.1
Backbone-Sidechain	188	6.3	105	55.9	3.5	46	24.5	1.5
Sidechain-Sidechain	208	7.0	76	36.5	2.6	35	16.8	1.2
<b>Hydrogen bond</b>	<b>96</b>	<b>3.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</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>2976</b>	<b>100.0</b>	<b>1023</b>	<b>34.4</b>	<b>34.4</b>	<b>495</b>	<b>16.6</b>	<b>16.6</b>
Backbone-Backbone	506	17.0	50	9.9	1.7	29	5.7	1.0
Backbone-Sidechain	1614	54.2	657	40.7	22.1	320	19.8	10.8
Sidechain-Sidechain	856	28.8	316	36.9	10.6	146	17.1	4.9

<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

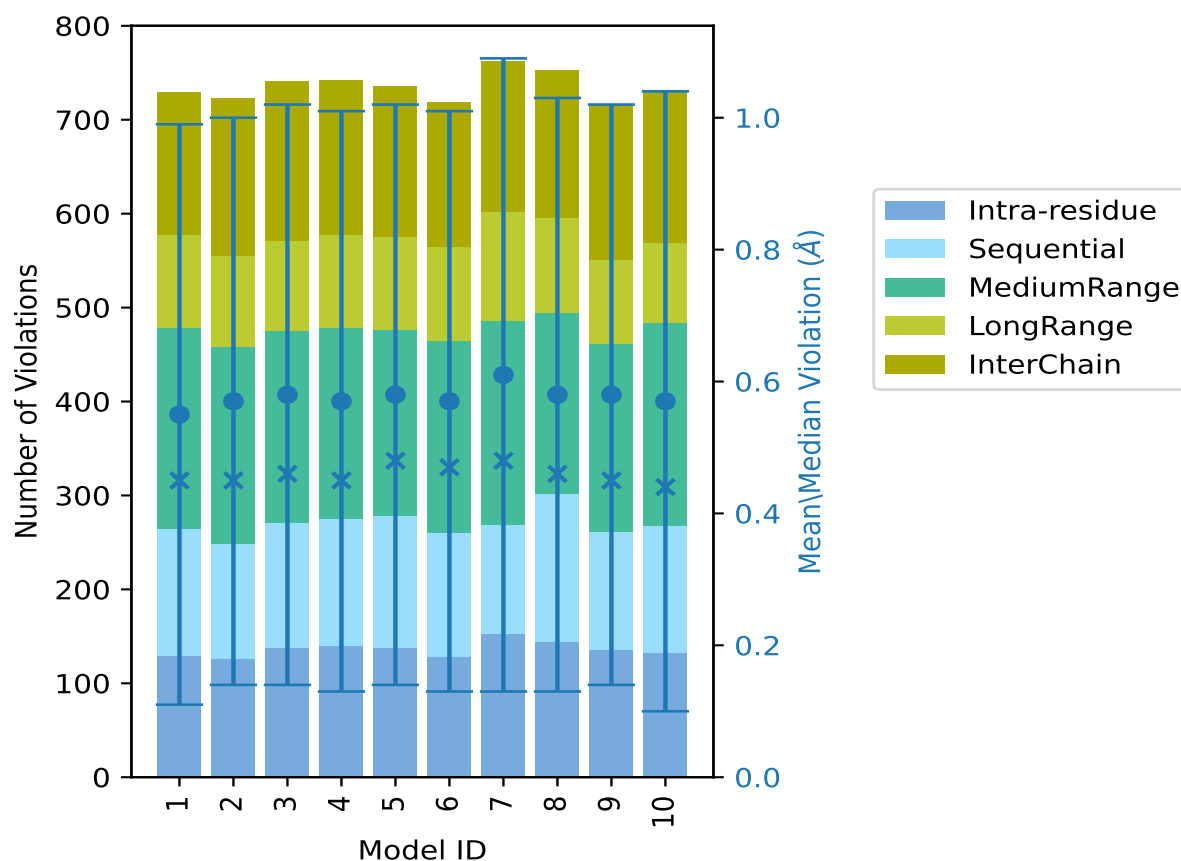
## 9.2 Distance violation statistics for each model [i](#)

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	129	135	215	98	152	729	0.55	3.49	0.44	0.45
2	126	123	210	96	168	723	0.57	2.16	0.43	0.45
3	138	133	205	95	170	741	0.58	2.26	0.44	0.46
4	140	135	204	98	165	742	0.57	2.48	0.44	0.45
5	138	140	198	100	160	736	0.58	2.42	0.44	0.48
6	128	132	204	101	154	719	0.57	3.45	0.44	0.47
7	153	116	217	116	160	762	0.61	3.45	0.48	0.48
8	144	158	192	102	157	753	0.58	3.25	0.45	0.46
9	136	125	200	90	164	715	0.58	2.49	0.44	0.45
10	132	136	216	85	162	731	0.57	2.54	0.47	0.44

<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, 1857(IR:564, SQ:328, MR:560, LR:186, IC:219) 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>	%
22	19	41	20	17	119	1	10.0
22	7	16	10	5	60	2	20.0
6	10	8	10	16	50	3	30.0

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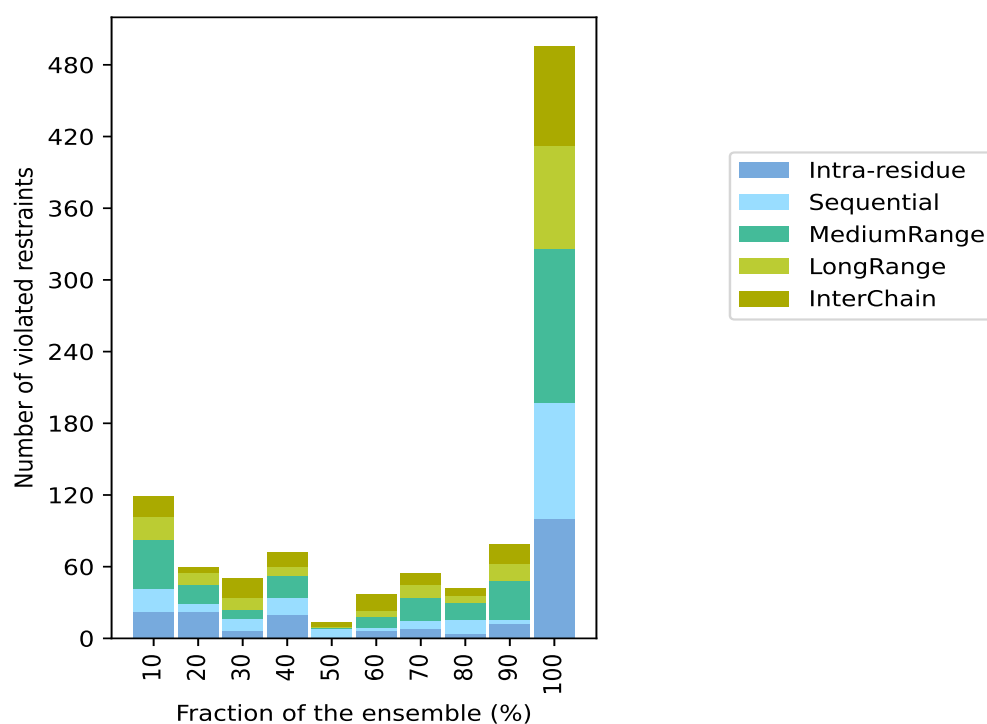
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
20	14	18	8	12	72	4	40.0
0	8	1	1	4	14	5	50.0
6	3	9	5	14	37	6	60.0
8	7	19	11	10	55	7	70.0
4	11	15	6	6	42	8	80.0
12	4	32	15	16	79	9	90.0
100	97	129	86	83	495	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 ⓘ



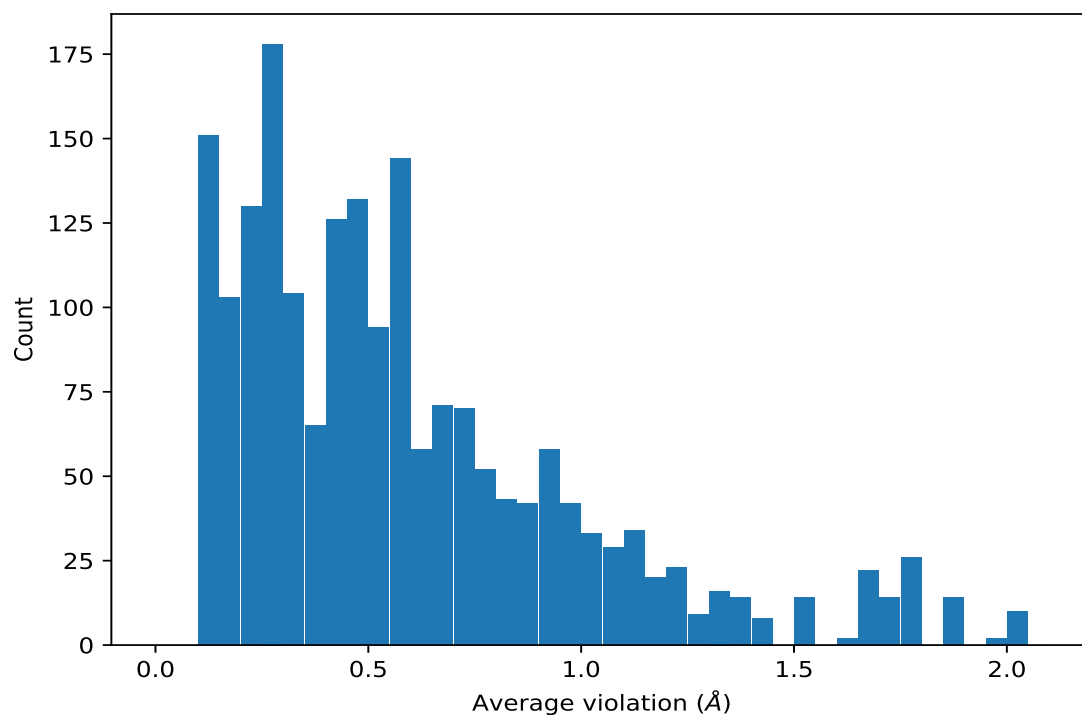
## 9.4 Most violated distance restraints in the ensemble ⓘ

### 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)
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	10	2.02	0.16	2.02
(1,2349)	1:193:A:ASP:H	1:187:A:LYS:HG2	10	2.02	0.16	2.02
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	10	2.02	0.16	2.01
(1,2350)	1:193:B:ASP:H	1:187:B:LYS:HG2	10	2.02	0.16	2.01
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	10	1.98	0.24	2.04
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	10	1.98	0.24	2.02
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD11	10	1.88	0.18	1.96
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD13	10	1.88	0.18	1.96
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD12	10	1.88	0.18	1.96
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD11	10	1.88	0.18	1.96
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD13	10	1.88	0.18	1.96
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD12	10	1.88	0.18	1.96
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	10	1.86	0.47	2.06
(1,2646)	1:188:B:ASN:HD22	1:187:B:LYS:HG3	10	1.86	0.47	2.06
(1,2646)	1:188:B:ASN:HD22	1:178:A:PRO:HG2	10	1.86	0.47	2.06

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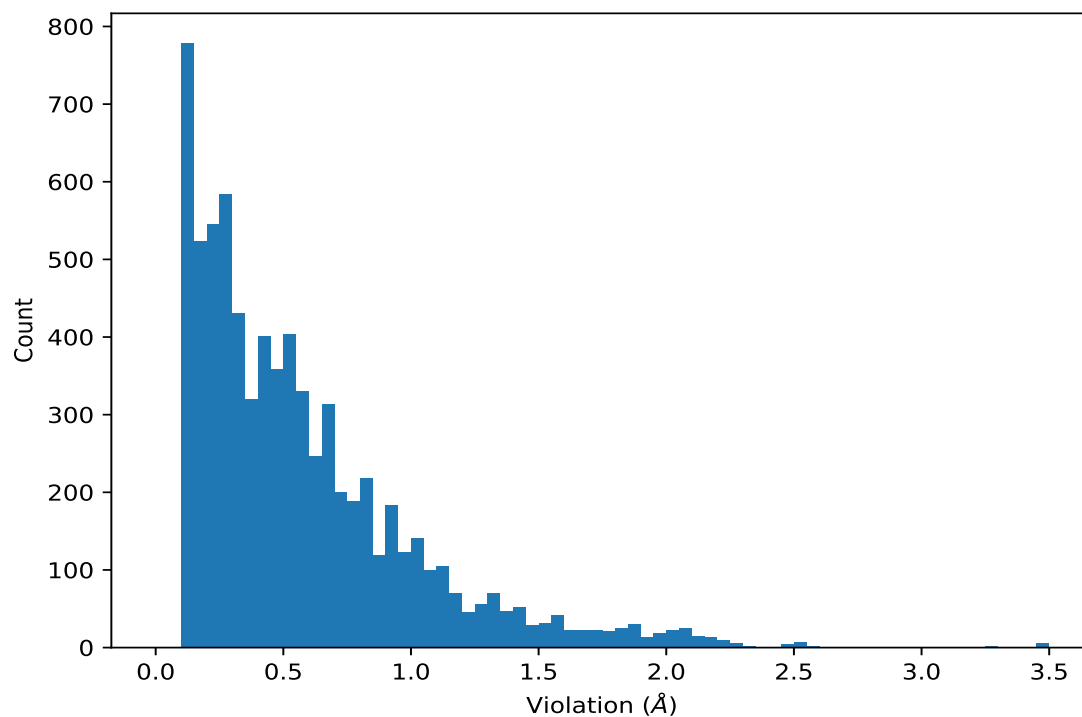
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	10	1.86	0.47	2.06
(1,2645)	1:188:A:ASN:HD22	1:187:A:LYS:HG3	10	1.86	0.47	2.06
(1,2645)	1:188:A:ASN:HD22	1:178:B:PRO:HG2	10	1.86	0.47	2.06
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG13	10	1.79	0.07	1.81
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG12	10	1.79	0.07	1.81
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG11	10	1.79	0.07	1.81
(1,2146)	1:199:B:GLN:HB3	1:200:B:VAL:HG23	10	1.79	0.07	1.81
(1,2146)	1:199:B:GLN:HB3	1:196:B:ALA:HB3	10	1.79	0.07	1.81
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG13	10	1.79	0.07	1.8

<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)
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB3	1	3.49
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB3	1	3.48
(1,2630)	1:173:B:GLN:HE21	1:195:A:ALA:HB1	7	3.45
(1,2629)	1:173:A:GLN:HE21	1:195:B:ALA:HB1	7	3.45
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	6	3.45
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	6	3.45
(1,504)	1:189:B:ASN:HA	1:188:B:ASN:HD22	8	3.25
(1,503)	1:189:A:ASN:HA	1:188:A:ASN:HD22	8	3.25
(1,945)	1:175:A:LEU:HD23	1:199:B:GLN:HB3	7	2.6
(1,946)	1:175:B:LEU:HD23	1:199:A:GLN:HB3	7	2.59

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

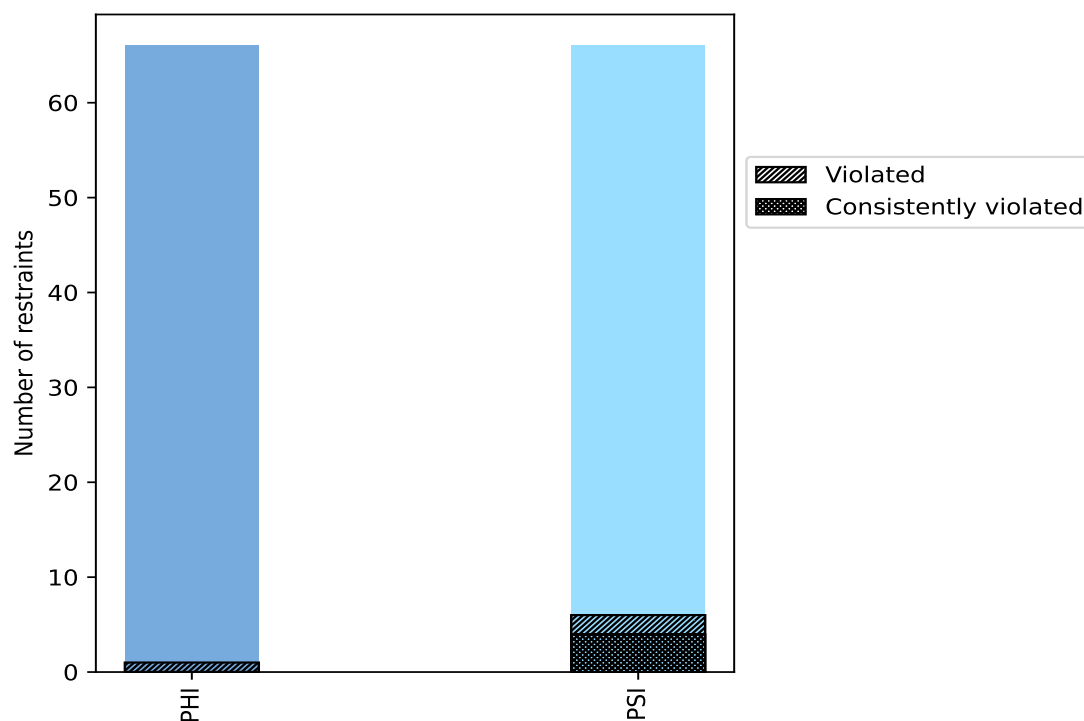
### 10.1 Summary of dihedral-angle violations [i](#)

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	66	50.0	1	1.5	0.8	0	0.0	0.0
PSI	66	50.0	6	9.1	4.5	4	6.1	3.0
Total	132	100.0	7	5.3	5.3	4	3.0	3.0

<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](#)



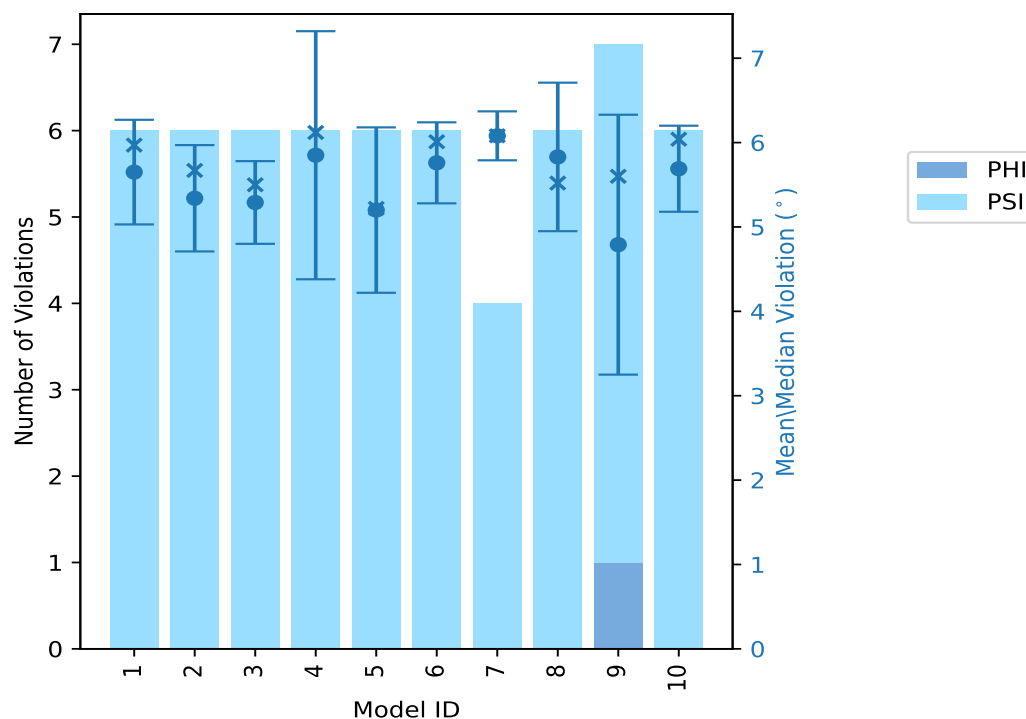
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°)
	PHI	PSI	Total				
1	0	6	6	5.65	6.23	0.62	5.97
2	0	6	6	5.34	6.0	0.63	5.67
3	0	6	6	5.29	5.79	0.49	5.5
4	0	6	6	5.85	7.53	1.47	6.12
5	0	6	6	5.2	6.4	0.98	5.22
6	0	6	6	5.76	6.27	0.48	6.01
7	0	4	4	6.08	6.37	0.29	6.08
8	0	6	6	5.83	7.07	0.88	5.52
9	1	6	7	4.79	5.68	1.54	5.6
10	0	6	6	5.69	6.08	0.51	6.04

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



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

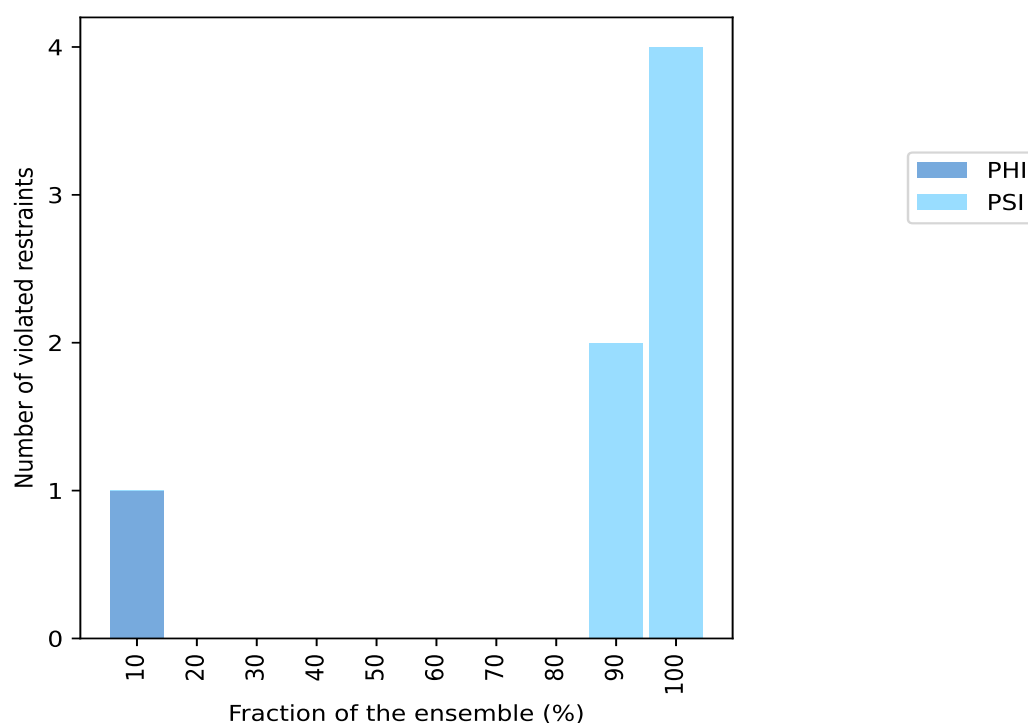
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

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

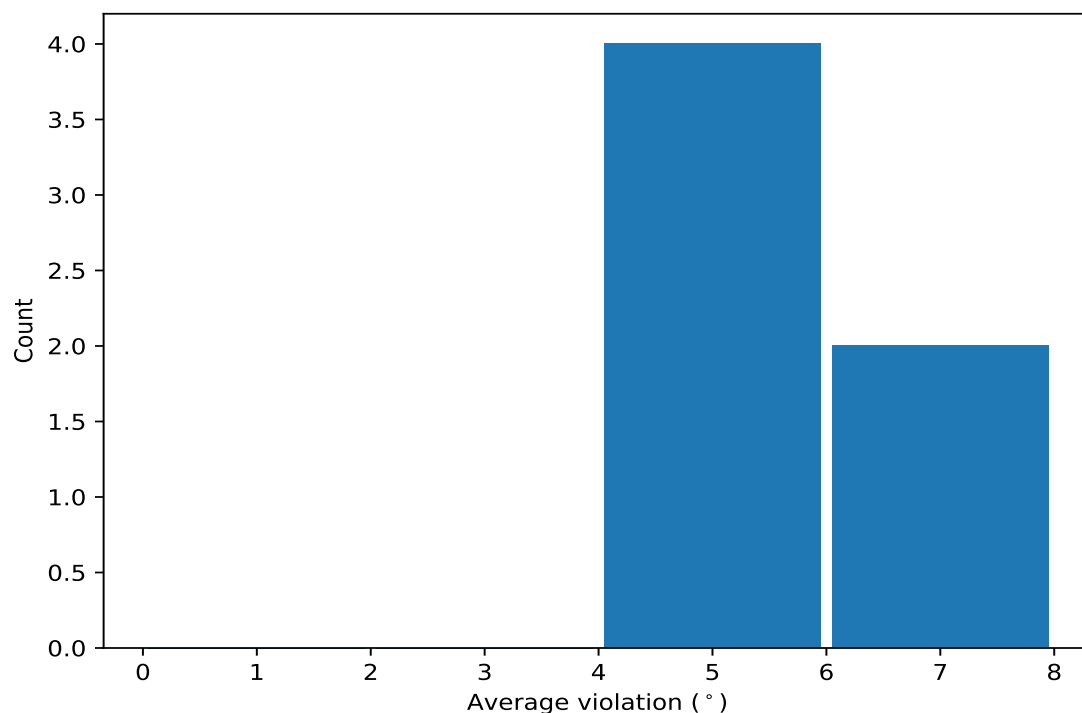
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

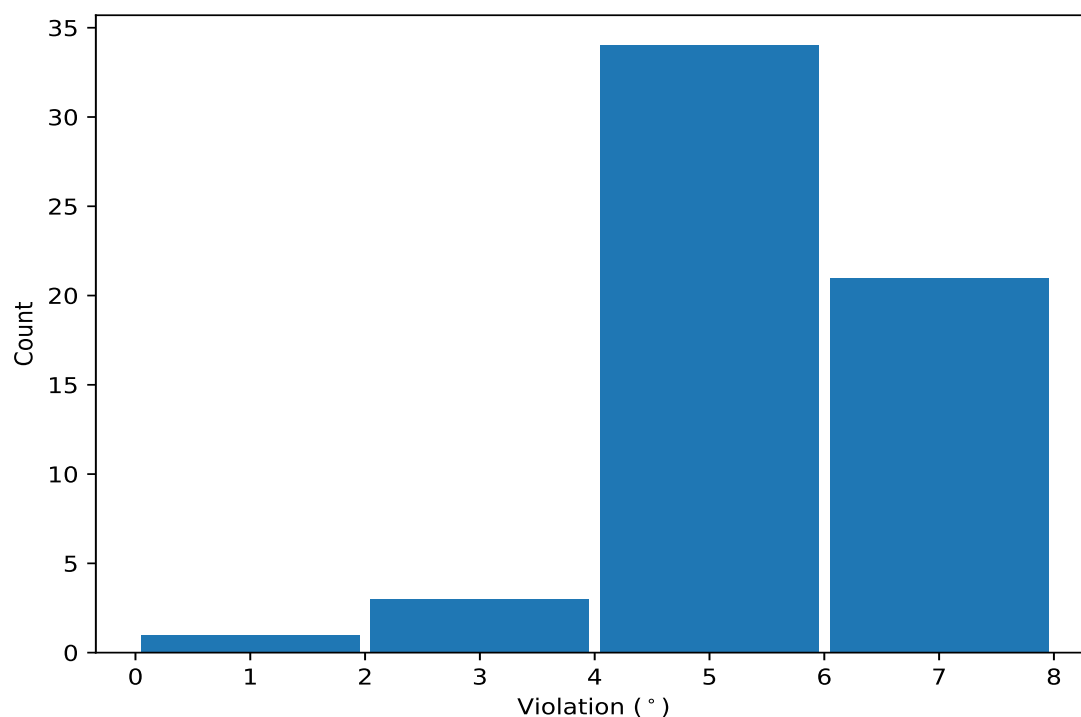
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	10	6.27	0.57	6.22
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	10	6.27	0.56	6.16
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	10	5.81	0.31	5.88
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	10	5.74	0.27	5.8
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	9	4.67	0.41	4.7
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	9	4.61	0.42	4.75

<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 (°)
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	4	7.53
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	4	7.46
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	8	7.07
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	8	6.94
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	5	6.4
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	5	6.37
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	7	6.37
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	7	6.35
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	6	6.27
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	1	6.23