



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2M29 / pdb\_00002m29  
BMRB ID : 18877  
Title : NMR structure of Ca<sup>2+</sup> bound CaBP4 N-domain  
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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 : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
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) : 2.49

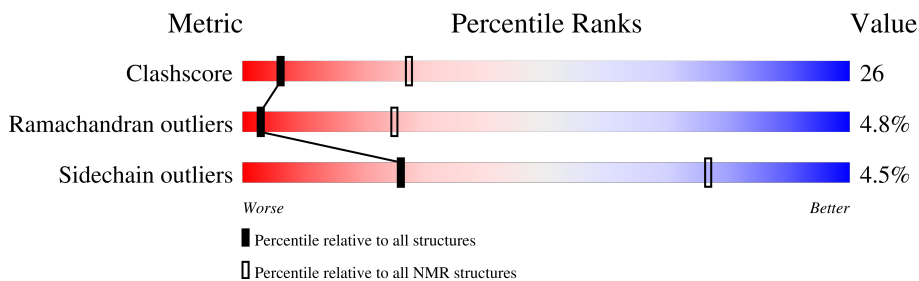
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 69%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	171	

## 2 Ensemble composition and analysis i

This entry contains 15 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:123-A:173, A:179-A:191 (64)	1.02	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 6, 8, 9, 10, 14, 15
2	1, 7, 11, 12
3	5, 13

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

There are 2 unique types of molecules in this entry. The entry contains 1130 atoms, of which 543 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-binding protein 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	72	1129	369	543	90	121	6	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

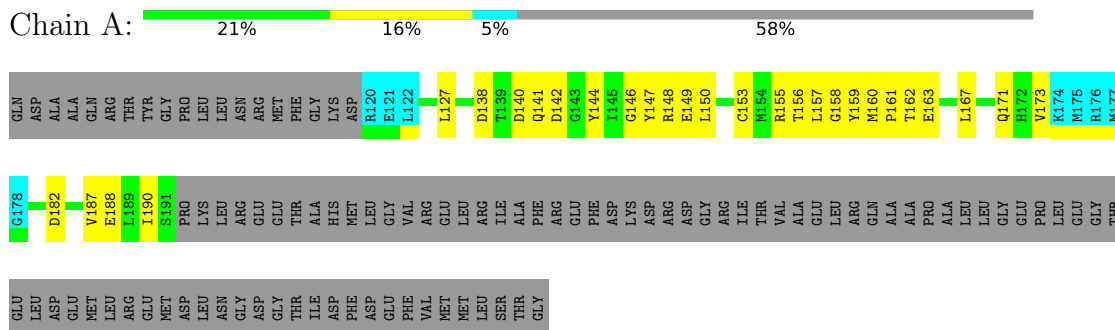
Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	1	1	1

## 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.

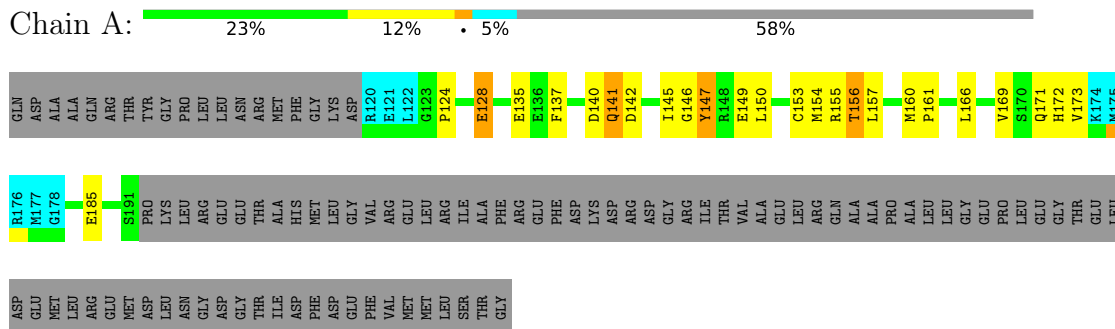
- Molecule 1: Calcium-binding protein 4



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

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

- Molecule 1: Calcium-binding protein 4



## 5 Refinement protocol and experimental data overview

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

Of the 70 calculated structures, 15 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
X-PLOR NIH	structure solution	2.23
X-PLOR NIH	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	1471
Number of shifts mapped to atoms	634
Number of unparsed shifts	0
Number of shifts with mapping errors	837
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	69%

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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

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	518	467	465	25±7
All	All	7785	7005	6996	382

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 26.

5 of 200 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:LEU:C	1:A:127:LEU:HD13	0.76	2.05	13	1
1:A:150:LEU:HD23	1:A:150:LEU:N	0.70	2.01	10	1
1:A:166:LEU:HD23	1:A:166:LEU:N	0.68	2.02	13	1
1:A:150:LEU:C	1:A:150:LEU:HD23	0.68	2.14	8	1
1:A:166:LEU:HD23	1:A:166:LEU:H	0.66	1.49	13	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	63/171 (37%)	55±2 (87±4%)	5±2 (9±3%)	3±1 (5±2%)	3	25
All	All	945/2565 (37%)	818 (87%)	82 (9%)	45 (5%)	3	25

5 of 14 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	162	THR	9
1	A	163	GLU	9
1	A	123	GLY	4
1	A	147	TYR	4
1	A	156	THR	4

### 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	56/145 (39%)	53±1 (95±2%)	3±1 (5±2%)	26	77
All	All	840/2175 (39%)	802 (95%)	38 (5%)	26	77

5 of 15 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	127	LEU	9
1	A	157	LEU	7
1	A	147	TYR	5
1	A	181	VAL	3
1	A	160	MET	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 69% for the well-defined parts and 65% 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 i

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

Total number of shifts	1471
Number of shifts mapped to atoms	634
Number of unparsed shifts	0
Number of shifts with mapping errors	837
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 837) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	GLN	H	8.389	0.02	1
1	A	101	GLN	HA	4.319	0.02	1
1	A	101	GLN	HB2	2.126	0.02	2
1	A	101	GLN	HB3	2.015	0.02	2
1	A	101	GLN	C	175.8	0.3	1
1	A	101	GLN	CA	56.25	0.3	1
1	A	101	GLN	CB	29.45	0.3	1
1	A	101	GLN	N	121.5	0.32	1
1	A	102	ASP	H	8.327	0.02	1
1	A	102	ASP	HA	4.57	0.02	1
1	A	102	ASP	HB2	2.69	0.02	2
1	A	102	ASP	HB3	2.7	0.02	2
1	A	102	ASP	C	176.3	0.3	1
1	A	102	ASP	CA	54.75	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	102	ASP	CB	41.11	0.3	1
1	A	102	ASP	N	121.2	0.3	1
1	A	103	ALA	H	8.17	0.02	1
1	A	103	ALA	HA	4.23	0.02	1
1	A	103	ALA	HB1	1.42	0.02	1
1	A	103	ALA	HB2	1.42	0.02	1
1	A	103	ALA	HB3	1.42	0.02	1
1	A	103	ALA	C	178.0	0.3	1
1	A	103	ALA	CA	53.29	0.3	1
1	A	103	ALA	CB	18.84	0.3	1
1	A	103	ALA	N	123.9	0.3	1
1	A	104	ALA	H	8.229	0.02	1
1	A	104	ALA	HA	4.229	0.02	1
1	A	104	ALA	HB1	1.429	0.02	1
1	A	104	ALA	HB2	1.429	0.02	1
1	A	104	ALA	HB3	1.429	0.02	1
1	A	104	ALA	C	178.0	0.3	1
1	A	104	ALA	CA	53.2	0.3	1
1	A	104	ALA	CB	18.65	0.3	1
1	A	104	ALA	N	122.1	0.3	1
1	A	105	GLN	H	8.144	0.02	1
1	A	105	GLN	HA	4.23	0.02	1
1	A	105	GLN	HB2	2.03	0.02	2
1	A	105	GLN	HB3	2.12	0.02	2
1	A	105	GLN	HE21	6.783	0.02	2
1	A	105	GLN	HE22	7.464	0.02	2
1	A	105	GLN	HG2	2.39	0.02	2
1	A	105	GLN	C	176.3	0.3	1
1	A	105	GLN	CA	56.33	0.3	1
1	A	105	GLN	CB	28.91	0.3	1
1	A	105	GLN	CG	34.02	0.3	1
1	A	105	GLN	N	118.6	0.3	1
1	A	105	GLN	NE2	112.3	0.3	1
1	A	106	ARG	H	8.195	0.02	1
1	A	106	ARG	HA	4.299	0.02	1
1	A	106	ARG	HB2	1.742	0.02	2
1	A	106	ARG	HB3	1.72	0.02	2
1	A	106	ARG	HG2	1.539	0.02	2
1	A	106	ARG	HG3	1.599	0.02	2
1	A	106	ARG	C	176.4	0.3	1
1	A	106	ARG	CA	56.31	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	ARG	CB	29.22	0.3	1
1	A	106	ARG	CG	27.45	0.3	1
1	A	106	ARG	N	121.5	0.3	1
1	A	107	THR	H	8.233	0.02	1
1	A	107	THR	HA	4.258	0.02	1
1	A	107	THR	HB	4.05	0.02	1
1	A	107	THR	HG21	1.009	0.02	1
1	A	107	THR	HG22	1.009	0.02	1
1	A	107	THR	HG23	1.009	0.02	1
1	A	107	THR	CA	62.61	0.3	1
1	A	107	THR	CB	69.72	0.3	1
1	A	107	THR	CG2	21.48	0.3	1
1	A	107	THR	N	115.7	0.3	1
1	A	108	TYR	H	8.59	0.02	1
1	A	108	TYR	HA	4.57	0.02	1
1	A	108	TYR	HB2	3.113	0.02	2
1	A	108	TYR	HB3	2.892	0.02	2
1	A	108	TYR	CA	58.8	0.3	1
1	A	108	TYR	CB	38.55	0.3	1
1	A	108	TYR	N	120.2	0.3	1
1	A	109	GLY	H	8.365	0.02	1
1	A	109	GLY	HA2	3.89	0.02	2
1	A	109	GLY	HA3	4.153	0.02	2
1	A	109	GLY	CA	47.55	0.3	1
1	A	109	GLY	N	109.4	0.3	1
1	A	110	PRO	C	178.6	0.3	1
1	A	110	PRO	CA	64.92	0.3	1
1	A	110	PRO	CB	31.6	0.3	1
1	A	111	LEU	H	7.666	0.02	1
1	A	111	LEU	HA	4.158	0.02	1
1	A	111	LEU	HB2	1.747	0.02	2
1	A	111	LEU	CA	57.67	0.3	1
1	A	111	LEU	CB	41.5	0.3	1
1	A	111	LEU	N	118.5	0.3	1
1	A	112	LEU	H	8.11	0.02	1
1	A	112	LEU	HA	4.143	0.02	1
1	A	112	LEU	C	178.5	0.3	1
1	A	112	LEU	CA	57.47	0.3	1
1	A	112	LEU	CB	41.19	0.3	1
1	A	112	LEU	N	118.7	0.3	1
1	A	113	ASN	H	8.226	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	ASN	HA	4.479	0.02	1
1	A	113	ASN	HB2	2.815	0.02	2
1	A	113	ASN	HB3	2.833	0.02	2
1	A	113	ASN	C	177.3	0.3	1
1	A	113	ASN	CA	56.02	0.3	1
1	A	113	ASN	CB	38.6	0.3	1
1	A	113	ASN	N	116.4	0.3	1
1	A	114	ARG	H	7.819	0.02	1
1	A	114	ARG	C	177.7	0.3	1
1	A	114	ARG	CA	57.96	0.3	1
1	A	114	ARG	CB	29.9	0.3	1
1	A	114	ARG	N	118.6	0.3	1
1	A	115	MET	H	7.9	0.02	1
1	A	115	MET	HA	4.184	0.02	1
1	A	115	MET	C	176.4	0.3	1
1	A	115	MET	CA	57.67	0.3	1
1	A	115	MET	CB	32.84	0.3	1
1	A	115	MET	N	117.2	0.3	1
1	A	116	PHE	H	7.789	0.02	1
1	A	116	PHE	HA	4.78	0.02	1
1	A	116	PHE	HB2	2.88	0.02	2
1	A	116	PHE	HB3	3.37	0.02	2
1	A	116	PHE	HD1	7.345	0.02	3
1	A	116	PHE	HE1	7.234	0.02	3
1	A	116	PHE	HZ	7.148	0.02	1
1	A	116	PHE	C	176.0	0.3	1
1	A	116	PHE	CA	57.7	0.3	1
1	A	116	PHE	CB	39.41	0.3	1
1	A	116	PHE	N	115.6	0.3	1
1	A	117	GLY	H	8.093	0.02	1
1	A	117	GLY	HA2	4.007	0.02	2
1	A	117	GLY	HA3	4.114	0.02	2
1	A	117	GLY	C	174.5	0.3	1
1	A	117	GLY	CA	45.74	0.3	1
1	A	117	GLY	N	108.4	0.3	1
1	A	118	LYS	H	8.087	0.02	1
1	A	118	LYS	HA	4.287	0.02	1
1	A	118	LYS	HB2	1.796	0.02	2
1	A	118	LYS	HB3	1.853	0.02	2
1	A	118	LYS	HD2	1.692	0.02	2
1	A	118	LYS	HE2	3.009	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	118	LYS	HG2	1.445	0.02	2
1	A	118	LYS	C	176.2	0.3	1
1	A	118	LYS	CA	56.86	0.3	1
1	A	118	LYS	CB	32.55	0.3	1
1	A	118	LYS	CD	29.08	0.3	1
1	A	118	LYS	CE	42.04	0.3	1
1	A	118	LYS	CG	24.61	0.3	1
1	A	118	LYS	N	120.0	0.3	1
1	A	119	ASP	H	8.344	0.02	1
1	A	119	ASP	HA	4.622	0.02	1
1	A	119	ASP	HB2	2.613	0.02	2
1	A	119	ASP	HB3	2.71	0.02	2
1	A	119	ASP	C	175.8	0.3	1
1	A	119	ASP	CA	54.46	0.3	1
1	A	119	ASP	CB	40.83	0.3	1
1	A	119	ASP	N	119.8	0.3	1
1	A	120	ARG	H	7.894	0.02	1
1	A	196	GLU	H	8.015	0.02	1
1	A	196	GLU	C	177.2	0.3	1
1	A	196	GLU	CA	57.65	0.3	1
1	A	196	GLU	CB	29.9	0.3	1
1	A	196	GLU	N	120.2	0.3	1
1	A	197	GLU	H	8.356	0.02	1
1	A	197	GLU	HA	4.32	0.02	1
1	A	197	GLU	C	177.1	0.3	1
1	A	197	GLU	CA	57.49	0.3	1
1	A	197	GLU	CB	29.77	0.3	1
1	A	197	GLU	N	120.3	0.3	1
1	A	198	THR	H	7.933	0.02	1
1	A	198	THR	HA	4.35	0.02	1
1	A	198	THR	HB	4.25	0.02	1
1	A	198	THR	HG21	1.2	0.02	1
1	A	198	THR	HG22	1.2	0.02	1
1	A	198	THR	HG23	1.2	0.02	1
1	A	198	THR	C	174.6	0.3	1
1	A	198	THR	CA	62.19	0.3	1
1	A	198	THR	CB	69.71	0.3	1
1	A	198	THR	CG2	21.67	0.3	1
1	A	198	THR	N	112.8	0.3	1
1	A	199	ALA	H	8.098	0.02	1
1	A	199	ALA	HA	4.237	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	199	ALA	HB1	1.385	0.02	1
1	A	199	ALA	HB2	1.385	0.02	1
1	A	199	ALA	HB3	1.385	0.02	1
1	A	199	ALA	C	177.5	0.3	1
1	A	199	ALA	CA	53.3	0.3	1
1	A	199	ALA	CB	19.2	0.3	1
1	A	199	ALA	N	124.8	0.3	1
1	A	201	MET	H	8.036	0.02	1
1	A	201	MET	HA	4.418	0.02	1
1	A	201	MET	HB2	2.068	0.02	2
1	A	201	MET	HB3	1.964	0.02	2
1	A	201	MET	C	175.4	0.3	1
1	A	201	MET	CA	55.89	0.3	1
1	A	201	MET	CB	32.78	0.3	1
1	A	201	MET	N	120.3	0.3	1
1	A	202	LEU	H	8.222	0.02	1
1	A	202	LEU	HA	4.45	0.02	1
1	A	202	LEU	C	176.8	0.3	1
1	A	202	LEU	CA	55.45	0.3	1
1	A	202	LEU	CB	42.04	0.3	1
1	A	202	LEU	N	122.7	0.3	1
1	A	203	GLY	H	8.431	0.02	1
1	A	203	GLY	HA2	3.96	0.02	2
1	A	203	GLY	HA3	4.392	0.02	2
1	A	203	GLY	C	174.3	0.3	1
1	A	203	GLY	CA	44.62	0.3	1
1	A	203	GLY	N	110.2	0.3	1
1	A	204	VAL	H	8.367	0.02	1
1	A	204	VAL	HA	3.83	0.02	1
1	A	204	VAL	HB	2.168	0.02	1
1	A	204	VAL	HG11	1.071	0.02	1
1	A	204	VAL	HG12	1.071	0.02	1
1	A	204	VAL	HG13	1.071	0.02	1
1	A	204	VAL	HG21	1.132	0.02	1
1	A	204	VAL	HG22	1.132	0.02	1
1	A	204	VAL	HG23	1.132	0.02	1
1	A	204	VAL	C	177.4	0.3	1
1	A	204	VAL	CA	66.4	0.3	1
1	A	204	VAL	CB	31.35	0.3	1
1	A	204	VAL	CG1	21.27	0.3	1
1	A	204	VAL	CG2	22.4	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	204	VAL	N	119.6	0.3	1
1	A	205	ARG	H	8.515	0.02	1
1	A	205	ARG	HA	4.041	0.02	1
1	A	205	ARG	HB2	1.891	0.02	2
1	A	205	ARG	C	178.6	0.3	1
1	A	205	ARG	CA	59.84	0.3	1
1	A	205	ARG	CB	29.38	0.3	1
1	A	205	ARG	N	120.3	0.3	1
1	A	206	GLU	H	8.146	0.02	1
1	A	206	GLU	HA	4.049	0.02	1
1	A	206	GLU	C	179.4	0.3	1
1	A	206	GLU	CA	60.34	0.3	1
1	A	206	GLU	CB	28.97	0.3	1
1	A	206	GLU	N	118.2	0.3	1
1	A	207	LEU	H	8.477	0.02	1
1	A	207	LEU	HA	4.339	0.02	1
1	A	207	LEU	HB2	2.262	0.02	2
1	A	207	LEU	HB3	1.636	0.02	2
1	A	207	LEU	HD11	0.836	0.02	2
1	A	207	LEU	HD12	0.836	0.02	2
1	A	207	LEU	HD13	0.836	0.02	2
1	A	207	LEU	C	179.4	0.3	1
1	A	207	LEU	CA	58.42	0.3	1
1	A	207	LEU	CB	41.28	0.3	1
1	A	207	LEU	CD1	26.21	0.3	2
1	A	207	LEU	N	120.3	0.3	1
1	A	208	ARG	H	8.652	0.02	1
1	A	208	ARG	HA	4.045	0.02	1
1	A	208	ARG	HB2	1.981	0.02	2
1	A	208	ARG	HB3	2.017	0.02	2
1	A	208	ARG	C	178.7	0.3	1
1	A	208	ARG	CA	59.9	0.3	1
1	A	208	ARG	CB	29.26	0.3	1
1	A	208	ARG	N	120.3	0.3	1
1	A	209	ILE	H	7.64	0.02	1
1	A	209	ILE	HA	3.66	0.02	1
1	A	209	ILE	HB	2.097	0.02	1
1	A	209	ILE	HD11	0.928	0.02	1
1	A	209	ILE	HD12	0.928	0.02	1
1	A	209	ILE	HD13	0.928	0.02	1
1	A	209	ILE	HG12	1.854	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	209	ILE	HG13	1.205	0.02	2
1	A	209	ILE	HG21	1.013	0.02	1
1	A	209	ILE	HG22	1.013	0.02	1
1	A	209	ILE	HG23	1.013	0.02	1
1	A	209	ILE	C	178.4	0.3	1
1	A	209	ILE	CA	65.1	0.3	1
1	A	209	ILE	CB	37.62	0.3	1
1	A	209	ILE	CD1	13.46	0.3	1
1	A	209	ILE	CG1	29.05	0.3	1
1	A	209	ILE	CG2	17.49	0.3	1
1	A	209	ILE	N	119.9	0.3	1
1	A	210	ALA	H	7.986	0.02	1
1	A	210	ALA	HA	4.042	0.02	1
1	A	210	ALA	HB1	1.66	0.02	1
1	A	210	ALA	HB2	1.66	0.02	1
1	A	210	ALA	HB3	1.66	0.02	1
1	A	210	ALA	C	178.6	0.3	1
1	A	210	ALA	CA	55.19	0.3	1
1	A	210	ALA	CB	17.98	0.3	1
1	A	210	ALA	N	121.6	0.3	1
1	A	211	PHE	H	8.699	0.02	1
1	A	211	PHE	HA	3.334	0.02	1
1	A	211	PHE	HB2	2.983	0.02	2
1	A	211	PHE	HB3	3.089	0.02	2
1	A	211	PHE	HD1	6.475	0.02	3
1	A	211	PHE	HE1	7.015	0.02	3
1	A	211	PHE	HZ	7.238	0.02	1
1	A	211	PHE	C	177.6	0.3	1
1	A	211	PHE	CA	62.07	0.3	1
1	A	211	PHE	CB	39.56	0.3	1
1	A	211	PHE	N	117.8	0.3	1
1	A	212	ARG	H	7.915	0.02	1
1	A	212	ARG	HA	3.933	0.02	1
1	A	212	ARG	HB2	1.991	0.02	2
1	A	212	ARG	C	177.5	0.3	1
1	A	212	ARG	CA	58.85	0.3	1
1	A	212	ARG	CB	29.85	0.3	1
1	A	212	ARG	N	116.5	0.3	1
1	A	213	GLU	H	7.549	0.02	1
1	A	213	GLU	HA	3.976	0.02	1
1	A	213	GLU	C	177.7	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	213	GLU	CA	58.23	0.3	1
1	A	213	GLU	CB	28.7	0.3	1
1	A	213	GLU	N	117.4	0.3	1
1	A	214	PHE	H	7.183	0.02	1
1	A	214	PHE	HA	4.307	0.02	1
1	A	214	PHE	C	177.0	0.3	1
1	A	214	PHE	CA	59.11	0.3	1
1	A	214	PHE	CB	40.67	0.3	1
1	A	214	PHE	N	114.2	0.3	1
1	A	215	ASP	H	7.914	0.02	1
1	A	215	ASP	HA	4.553	0.02	1
1	A	215	ASP	HB2	2.423	0.02	2
1	A	215	ASP	HB3	1.547	0.02	2
1	A	215	ASP	C	177.2	0.3	1
1	A	215	ASP	CA	52.79	0.3	1
1	A	215	ASP	CB	39.08	0.3	1
1	A	215	ASP	N	118.4	0.3	1
1	A	216	LYS	H	7.631	0.02	1
1	A	216	LYS	HA	3.977	0.02	1
1	A	216	LYS	C	177.9	0.3	1
1	A	216	LYS	CA	58.75	0.3	1
1	A	216	LYS	CB	32.29	0.3	1
1	A	216	LYS	N	124.8	0.3	1
1	A	217	ASP	H	7.981	0.02	1
1	A	217	ASP	HA	4.593	0.02	1
1	A	217	ASP	HB2	3.057	0.02	2
1	A	217	ASP	HB3	2.587	0.02	2
1	A	217	ASP	C	176.1	0.3	1
1	A	217	ASP	CA	53.07	0.3	1
1	A	217	ASP	CB	39.08	0.3	1
1	A	217	ASP	N	114.3	0.3	1
1	A	218	ARG	H	7.755	0.02	1
1	A	218	ARG	HA	4.013	0.02	1
1	A	218	ARG	C	176.0	0.3	1
1	A	218	ARG	CA	56.96	0.3	1
1	A	218	ARG	CB	26.43	0.3	1
1	A	218	ARG	N	114.3	0.3	1
1	A	219	ASP	H	8.486	0.02	1
1	A	219	ASP	HA	4.655	0.02	1
1	A	219	ASP	HB2	3.04	0.02	2
1	A	219	ASP	HB3	2.449	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	219	ASP	C	178.0	0.3	1
1	A	219	ASP	CA	53.59	0.3	1
1	A	219	ASP	CB	40.71	0.3	1
1	A	219	ASP	N	119.5	0.3	1
1	A	220	GLY	H	10.55	0.02	1
1	A	220	GLY	HA2	3.704	0.02	2
1	A	220	GLY	HA3	4.333	0.02	2
1	A	220	GLY	C	173.3	0.3	1
1	A	220	GLY	CA	45.53	0.3	1
1	A	220	GLY	N	112.8	0.3	1
1	A	221	ARG	H	8.08	0.02	1
1	A	221	ARG	HA	5.103	0.02	1
1	A	221	ARG	HB2	1.839	0.02	2
1	A	221	ARG	HB3	1.512	0.02	2
1	A	221	ARG	C	174.8	0.3	1
1	A	221	ARG	CA	53.88	0.3	1
1	A	221	ARG	CB	32.69	0.3	1
1	A	221	ARG	N	118.5	0.3	1
1	A	222	ILE	H	9.809	0.02	1
1	A	222	ILE	HA	4.821	0.02	1
1	A	222	ILE	HB	1.804	0.02	1
1	A	222	ILE	HD11	0.207	0.02	1
1	A	222	ILE	HD12	0.207	0.02	1
1	A	222	ILE	HD13	0.207	0.02	1
1	A	222	ILE	HG12	1.8	0.02	2
1	A	222	ILE	HG13	1.138	0.02	2
1	A	222	ILE	HG21	0.839	0.02	1
1	A	222	ILE	HG22	0.839	0.02	1
1	A	222	ILE	HG23	0.839	0.02	1
1	A	222	ILE	C	176.5	0.3	1
1	A	222	ILE	CA	60.79	0.3	1
1	A	222	ILE	CB	38.47	0.3	1
1	A	222	ILE	CD1	14.95	0.3	1
1	A	222	ILE	CG2	17.93	0.3	1
1	A	222	ILE	N	126.4	0.3	1
1	A	223	THR	H	8.722	0.02	1
1	A	223	THR	HA	4.726	0.02	1
1	A	223	THR	HB	4.79	0.02	1
1	A	223	THR	HG21	1.29	0.02	1
1	A	223	THR	HG22	1.29	0.02	1
1	A	223	THR	HG23	1.29	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	223	THR	C	176.1	0.3	1
1	A	223	THR	CA	59.85	0.3	1
1	A	223	THR	CB	71.91	0.3	1
1	A	223	THR	CG2	22.26	0.3	1
1	A	223	THR	N	117.9	0.3	1
1	A	224	VAL	H	9.124	0.02	1
1	A	224	VAL	HA	3.75	0.02	1
1	A	224	VAL	HB	2.168	0.02	1
1	A	224	VAL	HG11	1.049	0.02	1
1	A	224	VAL	HG12	1.049	0.02	1
1	A	224	VAL	HG13	1.049	0.02	1
1	A	224	VAL	HG21	1.126	0.02	1
1	A	224	VAL	HG22	1.126	0.02	1
1	A	224	VAL	HG23	1.126	0.02	1
1	A	224	VAL	C	177.0	0.3	1
1	A	224	VAL	CA	66.61	0.3	1
1	A	224	VAL	CB	30.96	0.3	1
1	A	224	VAL	CG1	20.84	0.3	1
1	A	224	VAL	CG2	23.21	0.3	1
1	A	224	VAL	N	120.4	0.3	1
1	A	225	ALA	H	7.888	0.02	1
1	A	225	ALA	HA	4.13	0.02	1
1	A	225	ALA	HB1	1.45	0.02	1
1	A	225	ALA	HB2	1.45	0.02	1
1	A	225	ALA	HB3	1.45	0.02	1
1	A	225	ALA	C	181.0	0.3	1
1	A	225	ALA	CA	55.2	0.3	1
1	A	225	ALA	CB	18.01	0.3	1
1	A	225	ALA	N	121.4	0.3	1
1	A	226	GLU	H	7.661	0.02	1
1	A	226	GLU	HA	4.122	0.02	1
1	A	226	GLU	C	180.1	0.3	1
1	A	226	GLU	CA	59.14	0.3	1
1	A	226	GLU	CB	29.24	0.3	1
1	A	226	GLU	N	118.8	0.3	1
1	A	227	LEU	H	8.601	0.02	1
1	A	227	LEU	HA	4.068	0.02	1
1	A	227	LEU	HB2	1.747	0.02	2
1	A	227	LEU	HD11	0.782	0.02	1
1	A	227	LEU	HD12	0.782	0.02	1
1	A	227	LEU	HD13	0.782	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	227	LEU	HD21	0.699	0.02	1
1	A	227	LEU	HD22	0.699	0.02	1
1	A	227	LEU	HD23	0.699	0.02	1
1	A	227	LEU	HG	1.64	0.02	1
1	A	227	LEU	C	178.1	0.3	1
1	A	227	LEU	CA	58.52	0.3	1
1	A	227	LEU	CB	41.64	0.3	1
1	A	227	LEU	CD1	24.27	0.3	1
1	A	227	LEU	CD2	24.87	0.3	1
1	A	227	LEU	CG	26.76	0.3	1
1	A	227	LEU	N	122.4	0.3	1
1	A	228	ARG	H	8.456	0.02	1
1	A	228	ARG	C	178.7	0.3	1
1	A	228	ARG	CA	59.57	0.3	1
1	A	228	ARG	CB	29.98	0.3	1
1	A	228	ARG	N	116.9	0.3	1
1	A	229	GLN	H	7.649	0.02	1
1	A	229	GLN	HA	4.19	0.02	1
1	A	229	GLN	HB2	2.2	0.02	2
1	A	229	GLN	HG2	2.56	0.02	2
1	A	229	GLN	C	177.3	0.3	1
1	A	229	GLN	CA	57.83	0.3	1
1	A	229	GLN	CB	28.8	0.3	1
1	A	229	GLN	CG	34.07	0.3	1
1	A	229	GLN	N	115.2	0.3	1
1	A	230	ALA	H	7.765	0.02	1
1	A	230	ALA	HA	4.341	0.02	1
1	A	230	ALA	HB1	1.266	0.02	1
1	A	230	ALA	HB2	1.266	0.02	1
1	A	230	ALA	HB3	1.266	0.02	1
1	A	230	ALA	C	178.1	0.3	1
1	A	230	ALA	CA	53.2	0.3	1
1	A	230	ALA	CB	19.96	0.3	1
1	A	230	ALA	N	119.5	0.3	1
1	A	231	ALA	H	8.072	0.02	1
1	A	231	ALA	HA	4.162	0.02	1
1	A	231	ALA	HB1	1.637	0.02	1
1	A	231	ALA	HB2	1.637	0.02	1
1	A	231	ALA	HB3	1.637	0.02	1
1	A	231	ALA	C	175.3	0.3	1
1	A	231	ALA	CA	57.16	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	231	ALA	CB	16.42	0.3	1
1	A	231	ALA	N	119.1	0.3	1
1	A	232	PRO	HA	4.163	0.02	1
1	A	232	PRO	C	178.7	0.3	1
1	A	232	PRO	CA	66.35	0.3	1
1	A	232	PRO	CB	30.36	0.3	1
1	A	233	ALA	H	7.355	0.02	1
1	A	233	ALA	HA	4.22	0.02	1
1	A	233	ALA	HB1	1.48	0.02	1
1	A	233	ALA	HB2	1.48	0.02	1
1	A	233	ALA	HB3	1.48	0.02	1
1	A	233	ALA	C	178.9	0.3	1
1	A	233	ALA	CA	53.99	0.3	1
1	A	233	ALA	CB	18.67	0.3	1
1	A	233	ALA	N	118.0	0.3	1
1	A	234	LEU	H	7.87	0.02	1
1	A	234	LEU	HA	4.283	0.02	1
1	A	234	LEU	HB2	1.578	0.02	2
1	A	234	LEU	HB3	1.446	0.02	2
1	A	234	LEU	HD11	0.537	0.02	1
1	A	234	LEU	HD12	0.537	0.02	1
1	A	234	LEU	HD13	0.537	0.02	1
1	A	234	LEU	HD21	0.753	0.02	1
1	A	234	LEU	HD22	0.753	0.02	1
1	A	234	LEU	HD23	0.753	0.02	1
1	A	234	LEU	HG	1.61	0.02	1
1	A	234	LEU	C	177.6	0.3	1
1	A	234	LEU	CA	56.4	0.3	1
1	A	234	LEU	CB	42.72	0.3	1
1	A	234	LEU	CD1	25.38	0.3	1
1	A	234	LEU	CD2	23.37	0.3	1
1	A	234	LEU	CG	27.05	0.3	1
1	A	234	LEU	N	116.9	0.3	1
1	A	235	LEU	H	8.518	0.02	1
1	A	235	LEU	HA	4.43	0.02	1
1	A	235	LEU	HB2	1.678	0.02	2
1	A	235	LEU	HB3	1.926	0.02	2
1	A	235	LEU	HD11	0.896	0.02	2
1	A	235	LEU	HD12	0.896	0.02	2
1	A	235	LEU	HD13	0.896	0.02	2
1	A	235	LEU	HD21	0.896	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	235	LEU	HD22	0.896	0.02	2
1	A	235	LEU	HD23	0.896	0.02	2
1	A	235	LEU	C	178.0	0.3	1
1	A	235	LEU	CA	55.12	0.3	1
1	A	235	LEU	CB	42.29	0.3	1
1	A	235	LEU	CD2	23.61	0.3	2
1	A	235	LEU	N	115.8	0.3	1
1	A	236	GLY	H	7.728	0.02	1
1	A	236	GLY	HA2	3.802	0.02	2
1	A	236	GLY	HA3	4.128	0.02	2
1	A	236	GLY	C	173.1	0.3	1
1	A	236	GLY	CA	45.84	0.3	1
1	A	236	GLY	N	106.8	0.3	1
1	A	237	GLU	H	7.317	0.02	1
1	A	237	GLU	HA	4.83	0.02	1
1	A	237	GLU	HB2	2.12	0.02	2
1	A	237	GLU	HB3	1.812	0.02	2
1	A	237	GLU	C	172.6	0.3	1
1	A	237	GLU	CA	53.35	0.3	1
1	A	237	GLU	CB	31.02	0.3	1
1	A	237	GLU	N	117.7	0.3	1
1	A	238	PRO	HA	4.42	0.02	1
1	A	238	PRO	HB2	1.95	0.02	2
1	A	238	PRO	HB3	2.252	0.02	2
1	A	238	PRO	C	176.1	0.3	1
1	A	238	PRO	CA	62.69	0.3	1
1	A	238	PRO	CB	31.38	0.3	1
1	A	239	LEU	H	8.072	0.02	1
1	A	239	LEU	HA	4.523	0.02	1
1	A	239	LEU	HB2	1.463	0.02	2
1	A	239	LEU	HD11	0.835	0.02	2
1	A	239	LEU	HD12	0.835	0.02	2
1	A	239	LEU	HD13	0.835	0.02	2
1	A	239	LEU	C	176.1	0.3	1
1	A	239	LEU	CA	54.53	0.3	1
1	A	239	LEU	CB	43.49	0.3	1
1	A	239	LEU	CD1	25.84	0.3	2
1	A	239	LEU	N	122.3	0.3	1
1	A	240	GLU	H	8.75	0.02	1
1	A	240	GLU	HA	4.513	0.02	1
1	A	240	GLU	HB2	2.178	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	240	GLU	HB3	1.942	0.02	2
1	A	240	GLU	C	177.3	0.3	1
1	A	240	GLU	CA	55.69	0.3	1
1	A	240	GLU	CB	31.59	0.3	1
1	A	240	GLU	N	121.7	0.3	1
1	A	241	GLY	H	8.825	0.02	1
1	A	241	GLY	HA2	3.857	0.02	2
1	A	241	GLY	C	176.1	0.3	1
1	A	241	GLY	CA	47.01	0.3	1
1	A	241	GLY	N	109.8	0.3	1
1	A	242	THR	HA	4.273	0.02	1
1	A	242	THR	HB	4.34	0.02	1
1	A	242	THR	HG21	1.313	0.02	1
1	A	242	THR	HG22	1.313	0.02	1
1	A	242	THR	HG23	1.313	0.02	1
1	A	242	THR	C	176.3	0.3	1
1	A	242	THR	CA	64.45	0.3	1
1	A	242	THR	CB	68.66	0.3	1
1	A	242	THR	CG2	22.09	0.3	1
1	A	243	GLU	H	8.179	0.02	1
1	A	243	GLU	HA	4.168	0.02	1
1	A	243	GLU	HB2	2.076	0.02	2
1	A	243	GLU	HB3	2.179	0.02	2
1	A	243	GLU	C	178.9	0.3	1
1	A	243	GLU	CA	59.52	0.3	1
1	A	243	GLU	CB	29.25	0.3	1
1	A	243	GLU	N	121.7	0.3	1
1	A	244	LEU	H	7.624	0.02	1
1	A	244	LEU	HA	3.994	0.02	1
1	A	244	LEU	HB2	1.633	0.02	2
1	A	244	LEU	HB3	1.595	0.02	2
1	A	244	LEU	HD11	0.91	0.02	2
1	A	244	LEU	HD12	0.91	0.02	2
1	A	244	LEU	HD13	0.91	0.02	2
1	A	244	LEU	HD21	0.867	0.02	2
1	A	244	LEU	HD22	0.867	0.02	2
1	A	244	LEU	HD23	0.867	0.02	2
1	A	244	LEU	HG	1.63	0.02	1
1	A	244	LEU	C	177.8	0.3	1
1	A	244	LEU	CA	57.66	0.3	1
1	A	244	LEU	CB	40.55	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	244	LEU	CD1	24.96	0.3	2
1	A	244	LEU	CG	27.45	0.3	1
1	A	244	LEU	N	120.1	0.3	1
1	A	245	ASP	H	7.793	0.02	1
1	A	245	ASP	HA	4.282	0.02	1
1	A	245	ASP	HB2	2.655	0.02	2
1	A	245	ASP	HB3	2.771	0.02	2
1	A	245	ASP	C	179.1	0.3	1
1	A	245	ASP	CA	57.66	0.3	1
1	A	245	ASP	CB	40.45	0.3	1
1	A	245	ASP	N	118.5	0.3	1
1	A	246	GLU	H	8.016	0.02	1
1	A	246	GLU	HA	4.039	0.02	1
1	A	246	GLU	C	178.3	0.3	1
1	A	246	GLU	CA	59.06	0.3	1
1	A	246	GLU	CB	29.15	0.3	1
1	A	246	GLU	N	119.0	0.3	1
1	A	247	MET	H	7.841	0.02	1
1	A	247	MET	HA	3.976	0.02	1
1	A	247	MET	C	177.8	0.3	1
1	A	247	MET	CA	59.28	0.3	1
1	A	247	MET	CB	32.15	0.3	1
1	A	247	MET	N	120.3	0.3	1
1	A	248	LEU	H	7.961	0.02	1
1	A	248	LEU	HA	3.809	0.02	1
1	A	248	LEU	HB2	1.562	0.02	2
1	A	248	LEU	HB3	1.922	0.02	2
1	A	248	LEU	HD11	0.824	0.02	2
1	A	248	LEU	HD12	0.824	0.02	2
1	A	248	LEU	HD13	0.824	0.02	2
1	A	248	LEU	HD21	0.824	0.02	2
1	A	248	LEU	HD22	0.824	0.02	2
1	A	248	LEU	HD23	0.824	0.02	2
1	A	248	LEU	HG	1.638	0.02	1
1	A	248	LEU	C	178.2	0.3	1
1	A	248	LEU	CA	58.92	0.3	1
1	A	248	LEU	CB	40.48	0.3	1
1	A	248	LEU	CD2	24.69	0.3	2
1	A	248	LEU	CG	27.45	0.3	1
1	A	248	LEU	N	118.9	0.3	1
1	A	249	ARG	H	7.872	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	249	ARG	HA	3.995	0.02	1
1	A	249	ARG	HB2	1.94	0.02	2
1	A	249	ARG	C	178.8	0.3	1
1	A	249	ARG	CA	59.28	0.3	1
1	A	249	ARG	CB	29.65	0.3	1
1	A	249	ARG	N	116.6	0.3	1
1	A	250	GLU	H	7.85	0.02	1
1	A	250	GLU	HA	4.065	0.02	1
1	A	250	GLU	C	177.6	0.3	1
1	A	250	GLU	CA	58.77	0.3	1
1	A	250	GLU	CB	29.68	0.3	1
1	A	250	GLU	N	116.9	0.3	1
1	A	251	MET	H	7.596	0.02	1
1	A	251	MET	HA	4.379	0.02	1
1	A	251	MET	HB2	2.008	0.02	2
1	A	251	MET	C	176.2	0.3	1
1	A	251	MET	CA	56.94	0.3	1
1	A	251	MET	CB	34.5	0.3	1
1	A	251	MET	N	114.1	0.3	1
1	A	252	ASP	H	7.955	0.02	1
1	A	252	ASP	HA	4.615	0.02	1
1	A	252	ASP	HB2	2.938	0.02	2
1	A	252	ASP	HB3	2.297	0.02	2
1	A	252	ASP	C	177.0	0.3	1
1	A	252	ASP	CA	52.84	0.3	1
1	A	252	ASP	CB	39.05	0.3	1
1	A	252	ASP	N	117.1	0.3	1
1	A	253	LEU	H	7.693	0.02	1
1	A	253	LEU	HA	4.07	0.02	1
1	A	253	LEU	HB2	1.601	0.02	2
1	A	253	LEU	HB3	1.863	0.02	2
1	A	253	LEU	HD11	1.049	0.02	1
1	A	253	LEU	HD12	1.049	0.02	1
1	A	253	LEU	HD13	1.049	0.02	1
1	A	253	LEU	HD21	0.928	0.02	1
1	A	253	LEU	HD22	0.928	0.02	1
1	A	253	LEU	HD23	0.928	0.02	1
1	A	253	LEU	HG	1.815	0.02	1
1	A	253	LEU	C	178.9	0.3	1
1	A	253	LEU	CA	57.62	0.3	1
1	A	253	LEU	CB	41.36	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	253	LEU	CD1	25.71	0.3	1
1	A	253	LEU	CD2	22.34	0.3	1
1	A	253	LEU	CG	27.0	0.3	1
1	A	253	LEU	N	126.1	0.3	1
1	A	254	ASN	H	8.365	0.02	1
1	A	254	ASN	HA	4.791	0.02	1
1	A	254	ASN	HB2	2.982	0.02	2
1	A	254	ASN	HB3	3.344	0.02	2
1	A	254	ASN	C	176.9	0.3	1
1	A	254	ASN	CA	51.94	0.3	1
1	A	254	ASN	CB	37.31	0.3	1
1	A	254	ASN	N	112.8	0.3	1
1	A	255	GLY	H	7.668	0.02	1
1	A	255	GLY	HA2	3.9	0.02	2
1	A	255	GLY	C	175.0	0.3	1
1	A	255	GLY	CA	47.56	0.3	1
1	A	255	GLY	N	109.5	0.3	1
1	A	256	ASP	H	8.165	0.02	1
1	A	256	ASP	HA	4.549	0.02	1
1	A	256	ASP	HB2	2.472	0.02	2
1	A	256	ASP	HB3	3.158	0.02	2
1	A	256	ASP	C	177.6	0.3	1
1	A	256	ASP	CA	53.77	0.3	1
1	A	256	ASP	CB	40.27	0.3	1
1	A	256	ASP	N	119.9	0.3	1
1	A	257	GLY	H	10.62	0.02	1
1	A	257	GLY	HA2	3.48	0.02	2
1	A	257	GLY	HA3	4.3	0.02	2
1	A	257	GLY	C	173.3	0.3	1
1	A	257	GLY	CA	45.64	0.3	1
1	A	257	GLY	N	113.8	0.3	1
1	A	258	THR	H	7.948	0.02	1
1	A	258	THR	HA	4.968	0.02	1
1	A	258	THR	HB	3.795	0.02	1
1	A	258	THR	HG21	1.079	0.02	1
1	A	258	THR	HG22	1.079	0.02	1
1	A	258	THR	HG23	1.079	0.02	1
1	A	258	THR	C	173.3	0.3	1
1	A	258	THR	CA	59.33	0.3	1
1	A	258	THR	CB	73.06	0.3	1
1	A	258	THR	CG2	22.65	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	258	THR	N	108.4	0.3	1
1	A	259	ILE	H	9.241	0.02	1
1	A	259	ILE	HA	5.167	0.02	1
1	A	259	ILE	HB	2.015	0.02	1
1	A	259	ILE	HD11	0.838	0.02	1
1	A	259	ILE	HD12	0.838	0.02	1
1	A	259	ILE	HD13	0.838	0.02	1
1	A	259	ILE	HG12	1.471	0.02	2
1	A	259	ILE	HG13	0.973	0.02	2
1	A	259	ILE	HG21	1.289	0.02	1
1	A	259	ILE	HG22	1.289	0.02	1
1	A	259	ILE	HG23	1.289	0.02	1
1	A	259	ILE	C	176.0	0.3	1
1	A	259	ILE	CA	59.52	0.3	1
1	A	259	ILE	CB	39.04	0.3	1
1	A	259	ILE	CD1	14.17	0.3	1
1	A	259	ILE	CG2	18.42	0.3	1
1	A	259	ILE	N	125.1	0.3	1
1	A	260	ASP	H	9.043	0.02	1
1	A	260	ASP	HA	5.45	0.02	1
1	A	260	ASP	HB2	2.637	0.02	2
1	A	260	ASP	HB3	3.325	0.02	2
1	A	260	ASP	C	176.0	0.3	1
1	A	260	ASP	CA	52.46	0.3	1
1	A	260	ASP	CB	41.84	0.3	1
1	A	260	ASP	N	128.1	0.3	1
1	A	261	PHE	H	8.695	0.02	1
1	A	261	PHE	HA	3.61	0.02	1
1	A	261	PHE	HB2	2.193	0.02	2
1	A	261	PHE	HB3	2.58	0.02	2
1	A	261	PHE	HD1	6.607	0.02	3
1	A	261	PHE	HE1	7.085	0.02	3
1	A	261	PHE	HZ	7.241	0.02	1
1	A	261	PHE	C	176.2	0.3	1
1	A	261	PHE	CA	61.87	0.3	1
1	A	261	PHE	CB	38.51	0.3	1
1	A	261	PHE	N	118.6	0.3	1
1	A	262	ASP	H	7.873	0.02	1
1	A	262	ASP	HA	4.162	0.02	1
1	A	262	ASP	HB2	2.595	0.02	2
1	A	262	ASP	HB3	2.788	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	262	ASP	C	179.6	0.3	1
1	A	262	ASP	CA	57.74	0.3	1
1	A	262	ASP	CB	40.02	0.3	1
1	A	262	ASP	N	117.7	0.3	1
1	A	263	GLU	H	8.558	0.02	1
1	A	263	GLU	HA	3.902	0.02	1
1	A	263	GLU	C	178.6	0.3	1
1	A	263	GLU	CA	59.25	0.3	1
1	A	263	GLU	CB	29.06	0.3	1
1	A	263	GLU	N	121.2	0.3	1
1	A	264	PHE	H	8.489	0.02	1
1	A	264	PHE	HA	4.021	0.02	1
1	A	264	PHE	HD1	7.044	0.02	3
1	A	264	PHE	HE1	7.259	0.02	3
1	A	264	PHE	HZ	7.225	0.02	1
1	A	264	PHE	C	176.4	0.3	1
1	A	264	PHE	CA	61.74	0.3	1
1	A	264	PHE	CB	40.35	0.3	1
1	A	264	PHE	N	122.1	0.3	1
1	A	265	VAL	H	8.271	0.02	1
1	A	265	VAL	HA	3.31	0.02	1
1	A	265	VAL	HB	1.833	0.02	1
1	A	265	VAL	HG11	0.709	0.02	1
1	A	265	VAL	HG12	0.709	0.02	1
1	A	265	VAL	HG13	0.709	0.02	1
1	A	265	VAL	HG21	0.43	0.02	1
1	A	265	VAL	HG22	0.43	0.02	1
1	A	265	VAL	HG23	0.43	0.02	1
1	A	265	VAL	C	179.2	0.3	1
1	A	265	VAL	CA	66.14	0.3	1
1	A	265	VAL	CB	31.18	0.3	1
1	A	265	VAL	CG1	21.54	0.3	1
1	A	265	VAL	CG2	23.39	0.3	1
1	A	265	VAL	N	116.0	0.3	1
1	A	266	MET	H	7.937	0.02	1
1	A	266	MET	HA	4.07	0.02	1
1	A	266	MET	C	178.6	0.3	1
1	A	266	MET	CA	59.5	0.3	1
1	A	266	MET	CB	29.21	0.3	1
1	A	266	MET	N	119.4	0.3	1
1	A	267	MET	H	7.767	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	267	MET	HA	4.41	0.02	1
1	A	267	MET	C	177.5	0.3	1
1	A	267	MET	CA	57.09	0.3	1
1	A	267	MET	CB	31.51	0.3	1
1	A	267	MET	N	116.9	0.3	1
1	A	268	LEU	H	7.425	0.02	1
1	A	268	LEU	HA	4.24	0.02	1
1	A	268	LEU	HB2	1.41	0.02	2
1	A	268	LEU	HD11	0.203	0.02	1
1	A	268	LEU	HD12	0.203	0.02	1
1	A	268	LEU	HD13	0.203	0.02	1
1	A	268	LEU	HD21	0.55	0.02	1
1	A	268	LEU	HD22	0.55	0.02	1
1	A	268	LEU	HD23	0.55	0.02	1
1	A	268	LEU	HG	1.32	0.02	1
1	A	268	LEU	C	177.4	0.3	1
1	A	268	LEU	CA	55.72	0.3	1
1	A	268	LEU	CB	41.55	0.3	1
1	A	268	LEU	CD1	25.31	0.3	1
1	A	268	LEU	CD2	23.59	0.3	1
1	A	268	LEU	CG	27.86	0.3	1
1	A	268	LEU	N	117.6	0.3	1
1	A	269	SER	H	7.773	0.02	1
1	A	269	SER	HA	4.523	0.02	1
1	A	269	SER	C	177.4	0.3	1
1	A	269	SER	CA	59.08	0.3	1
1	A	269	SER	CB	63.87	0.3	1
1	A	269	SER	N	113.8	0.3	1
1	A	270	THR	H	7.896	0.02	1
1	A	270	THR	HA	4.41	0.02	1
1	A	270	THR	HB	4.33	0.02	1
1	A	270	THR	HG21	1.239	0.02	1
1	A	270	THR	HG22	1.239	0.02	1
1	A	270	THR	HG23	1.239	0.02	1
1	A	270	THR	C	174.2	0.3	1
1	A	270	THR	CA	62.12	0.3	1
1	A	270	THR	CB	69.99	0.3	1
1	A	270	THR	CG2	21.52	0.3	1
1	A	270	THR	N	114.7	0.3	1
1	A	271	GLY	H	7.945	0.02	1
1	A	271	GLY	HA2	3.793	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	271	GLY	C	178.9	0.3	1
1	A	271	GLY	CA	46.43	0.3	1
1	A	271	GLY	N	117.0	0.3	1

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	162	$-0.26 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	145	$0.46 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	150	$-0.31 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	156	$0.87 \pm 0.25$	Should be applied

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 69%, i.e. 590 atoms were assigned a chemical shift out of a possible 850. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	298/322 (93%)	119/132 (90%)	119/128 (93%)	60/62 (97%)
Sidechain	273/444 (61%)	178/286 (62%)	93/149 (62%)	2/9 (22%)
Aromatic	19/84 (23%)	19/41 (46%)	0/42 (0%)	0/1 (0%)
Overall	590/850 (69%)	316/459 (69%)	212/319 (66%)	62/72 (86%)

### 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.

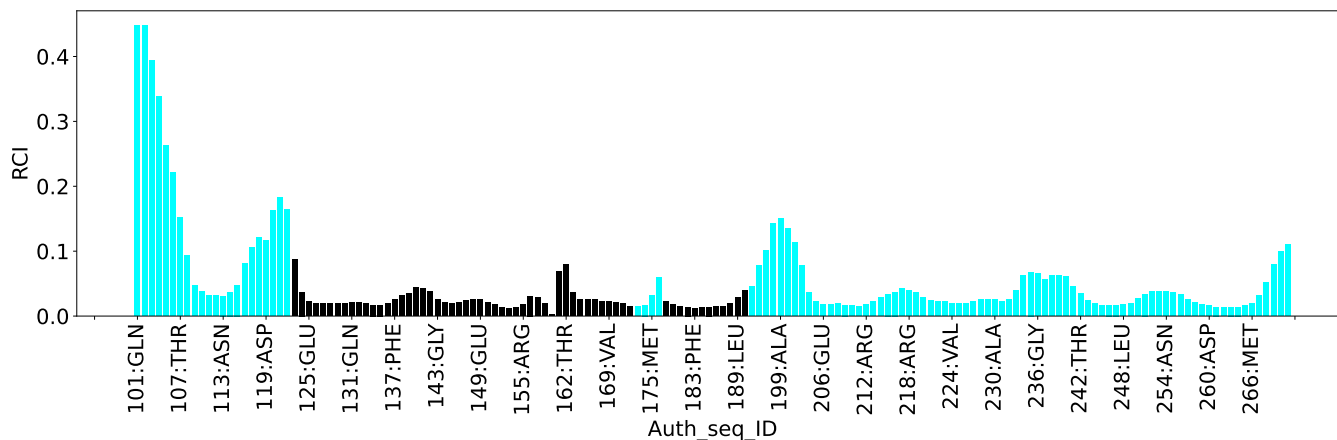
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	159	TYR	C	120.70	165.86 – 185.23	-28.3

### 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	749
Intra-residue ( $ i-j =0$ )	277
Sequential ( $ i-j =1$ )	162
Medium range ( $ i-j >1$ and $ i-j <5$ )	114
Long range ( $ i-j \geq 5$ )	142
Inter-chain	0
Hydrogen bond restraints	54
Disulfide bond restraints	0
Total dihedral-angle restraints	83
Number of unmapped restraints	0
Number of restraints per residue	4.8
Number of long range restraints per residue <sup>1</sup>	0.8

<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)	12.7	0.2
0.2-0.5 (Medium)	12.0	0.5
>0.5 (Large)	10.8	3.99

### 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)	2.5	4.43
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis i

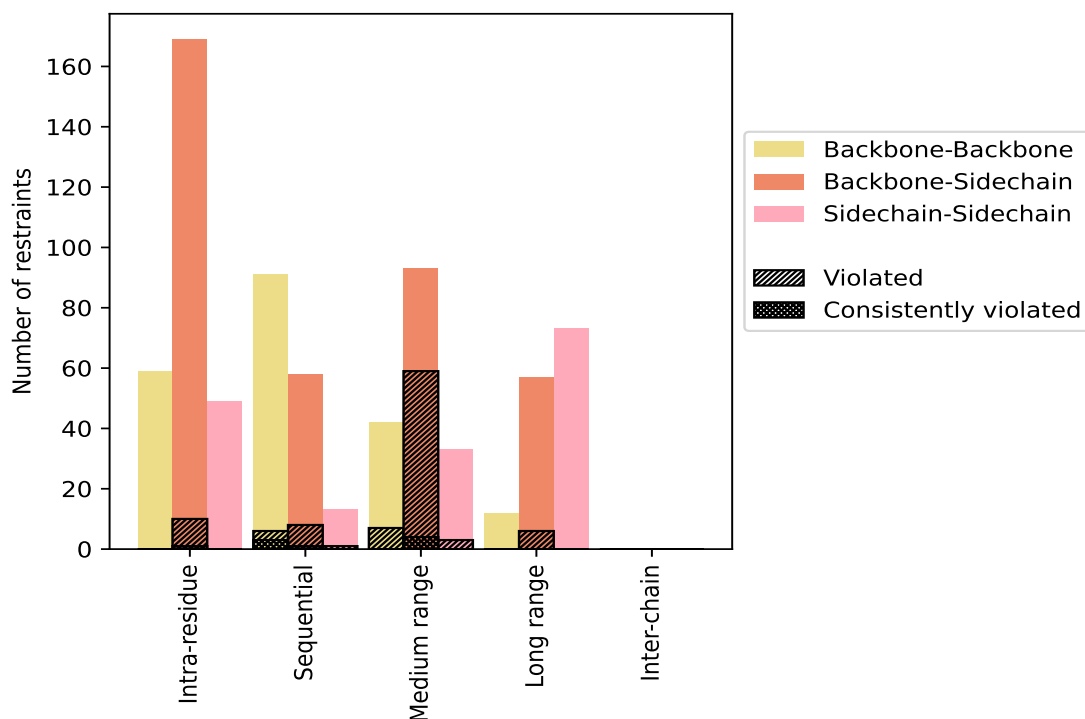
### 9.1 Summary of distance violations i

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>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>277</b>	<b>37.0</b>	<b>10</b>	<b>3.6</b>	<b>1.3</b>	<b>1</b>	<b>0.4</b>	<b>0.1</b>
Backbone-Backbone	59	7.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	169	22.6	10	5.9	1.3	1	0.6	0.1
Sidechain-Sidechain	49	6.5	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>162</b>	<b>21.6</b>	<b>15</b>	<b>9.3</b>	<b>2.0</b>	<b>4</b>	<b>2.5</b>	<b>0.5</b>
Backbone-Backbone	91	12.1	6	6.6	0.8	3	3.3	0.4
Backbone-Sidechain	58	7.7	8	13.8	1.1	1	1.7	0.1
Sidechain-Sidechain	13	1.7	1	7.7	0.1	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>114</b>	<b>15.2</b>	<b>18</b>	<b>15.8</b>	<b>2.4</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	42	5.6	7	16.7	0.9	0	0.0	0.0
Backbone-Sidechain	39	5.2	8	20.5	1.1	0	0.0	0.0
Sidechain-Sidechain	33	4.4	3	9.1	0.4	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>142</b>	<b>19.0</b>	<b>6</b>	<b>4.2</b>	<b>0.8</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	12	1.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	57	7.6	6	10.5	0.8	0	0.0	0.0
Sidechain-Sidechain	73	9.7	0	0.0	0.0	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>54</b>	<b>7.2</b>	<b>51</b>	<b>94.4</b>	<b>6.8</b>	<b>4</b>	<b>7.4</b>	<b>0.5</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>749</b>	<b>100.0</b>	<b>100</b>	<b>13.4</b>	<b>13.4</b>	<b>9</b>	<b>1.2</b>	<b>1.2</b>
Backbone-Backbone	204	27.2	13	6.4	1.7	3	1.5	0.4
Backbone-Sidechain	377	50.3	83	22.0	11.1	6	1.6	0.8
Sidechain-Sidechain	168	22.4	4	2.4	0.5	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	4	7	28	2	0	41	0.43	2.1	0.44	0.26
2	5	10	22	1	0	38	0.39	3.14	0.64	0.2
3	2	6	27	2	0	37	0.62	3.43	0.82	0.32
4	2	5	27	2	0	36	0.47	2.97	0.62	0.28
5	4	7	26	0	0	37	0.55	3.0	0.65	0.32
6	2	7	24	0	0	33	0.46	1.47	0.41	0.28
7	3	6	23	0	0	32	0.49	2.31	0.53	0.29
8	4	7	24	0	0	35	0.51	2.18	0.51	0.28
9	2	7	27	1	0	37	0.49	2.0	0.45	0.28
10	3	6	28	0	0	37	0.65	3.38	0.78	0.4

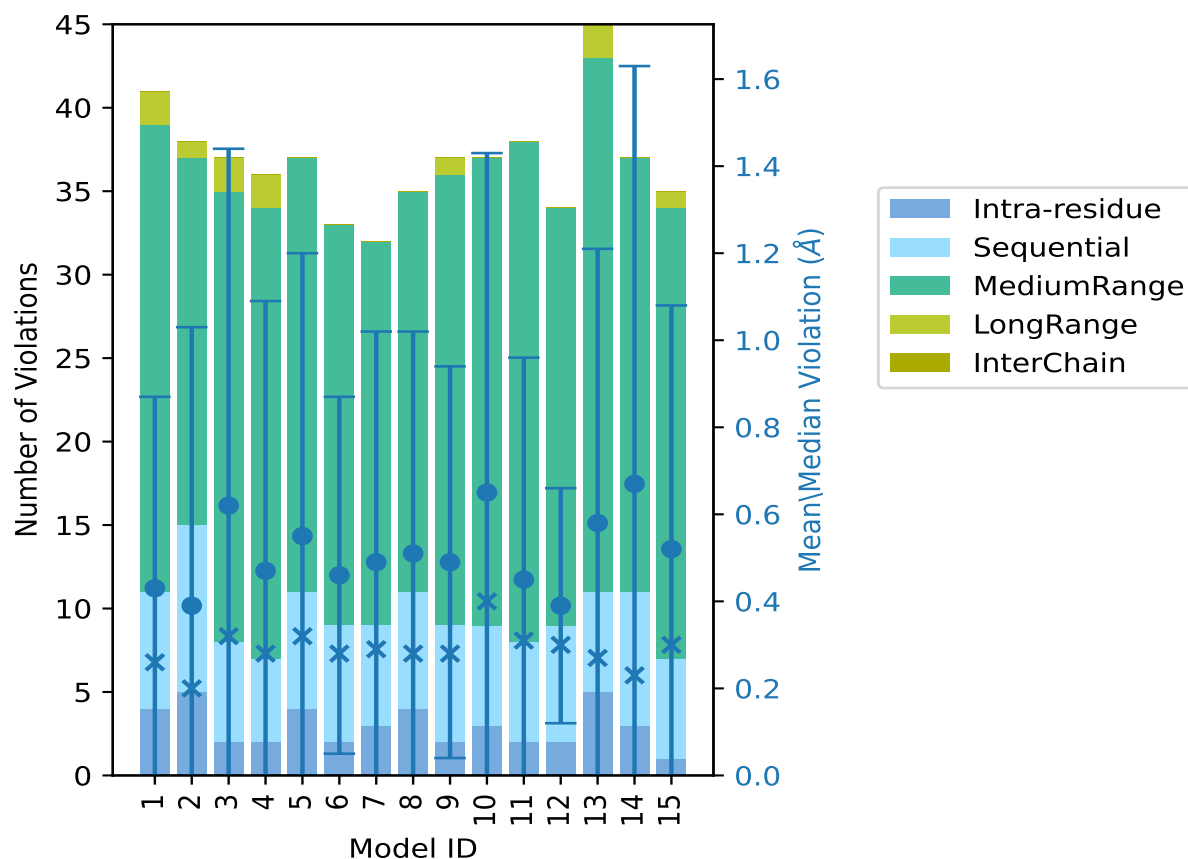
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	2	6	30	0	0	38	0.45	2.5	0.51	0.31
12	2	7	25	0	0	34	0.39	1.08	0.27	0.3
13	5	6	32	2	0	45	0.58	2.54	0.63	0.27
14	3	8	26	0	0	37	0.67	3.99	0.96	0.23
15	1	6	27	1	0	35	0.52	2.4	0.56	0.3

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

### 9.2.1 Bar graph : Distance Violation statistics for each model



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

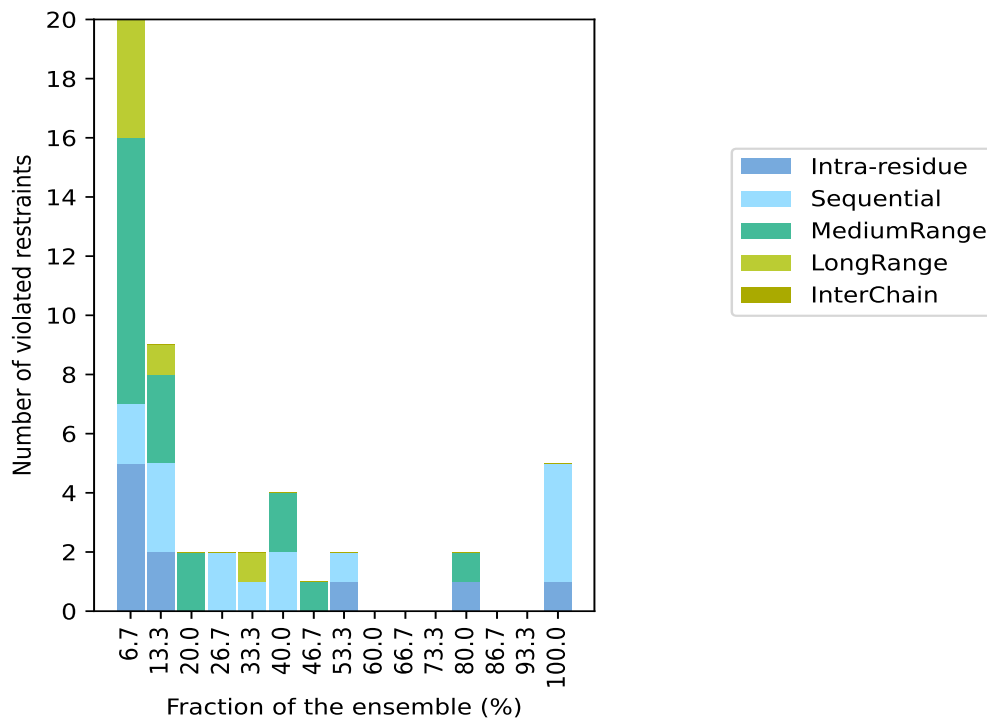
### 9.3 Distance violation statistics for the ensemble

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, 646(IR:267, SQ:147, MR:96, LR:136, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
5	2	9	4	0	20	1	6.7
2	3	3	1	0	9	2	13.3
0	0	2	0	0	2	3	20.0
0	2	0	0	0	2	4	26.7
0	1	0	1	0	2	5	33.3
0	2	2	0	0	4	6	40.0
0	0	1	0	0	1	7	46.7
1	1	0	0	0	2	8	53.3
0	0	0	0	0	0	9	60.0
0	0	0	0	0	0	10	66.7
0	0	0	0	0	0	11	73.3
1	0	1	0	0	2	12	80.0
0	0	0	0	0	0	13	86.7
0	0	0	0	0	0	14	93.3
1	4	0	0	0	5	15	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

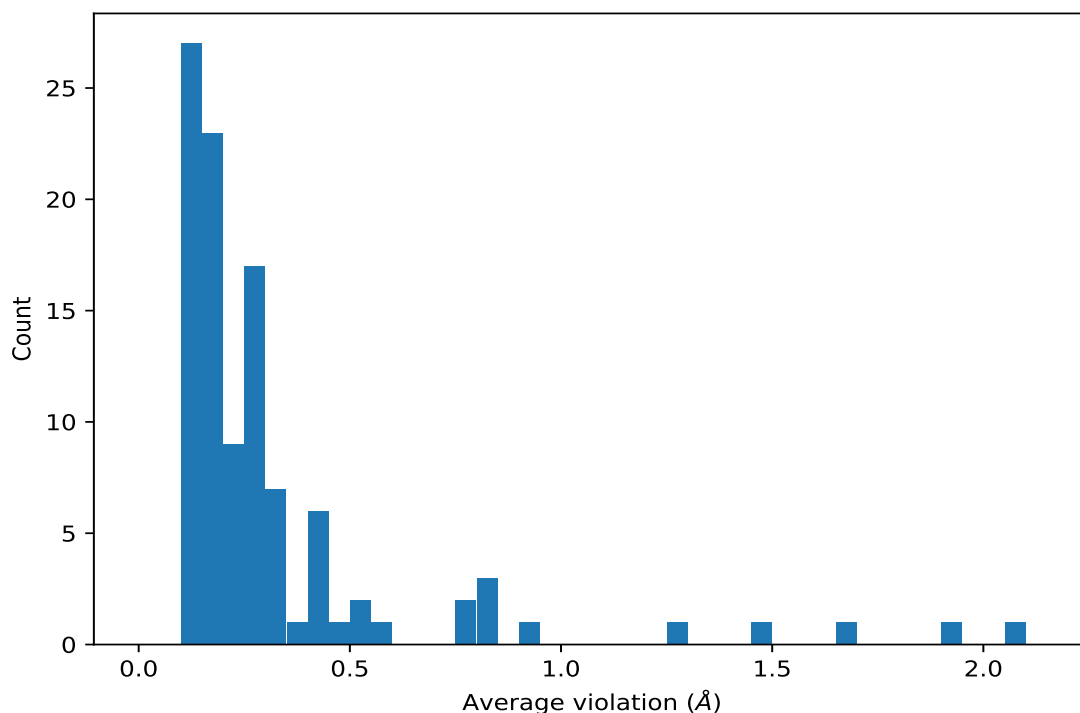
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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.

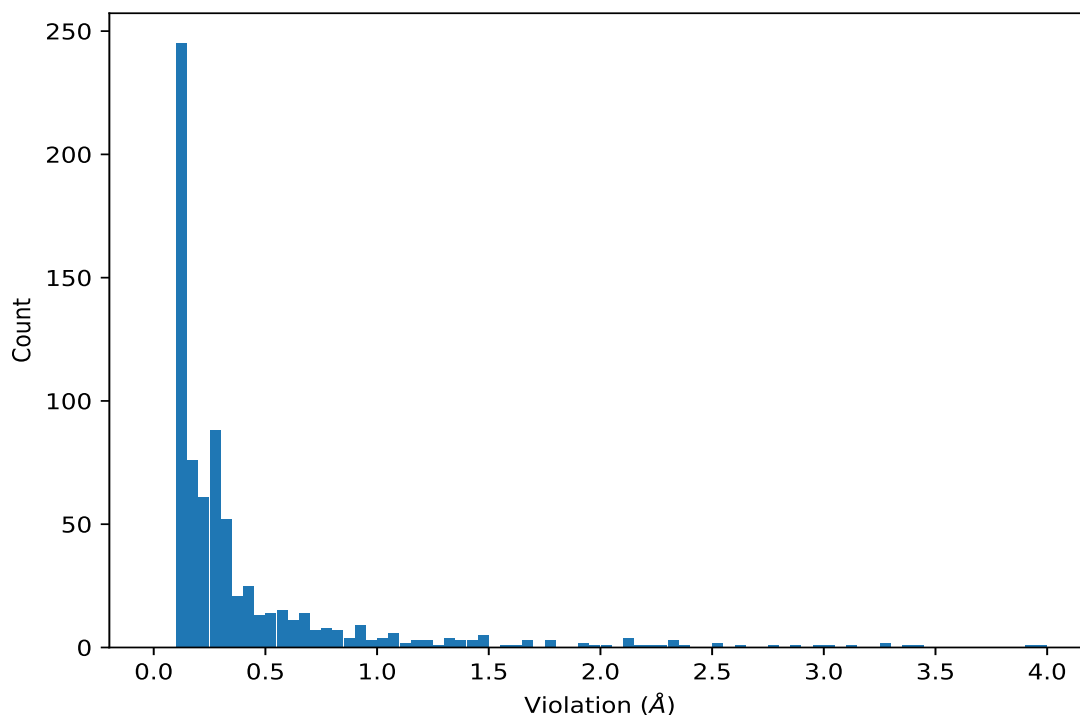
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,20)	1:147:A:TYR:O	1:151:A:GLY:H	15	1.65	1.27	0.97
(1,19)	1:147:A:TYR:O	1:151:A:GLY:N	15	1.49	1.27	0.78
(1,22)	1:148:A:ARG:O	1:152:A:ASP:H	15	0.81	0.32	0.85
(1,21)	1:148:A:ARG:O	1:152:A:ASP:N	15	0.76	0.33	0.82
(2,364)	1:156:A:THR:HA	1:157:A:LEU:H	15	0.35	0.03	0.34
(2,384)	1:179:A:GLY:H	1:180:A:PHE:H	15	0.34	0.03	0.34
(2,471)	1:185:A:GLU:H	1:186:A:PHE:HD1	15	0.26	0.05	0.25
(2,471)	1:185:A:GLU:H	1:186:A:PHE:HD2	15	0.26	0.05	0.25
(2,505)	1:139:A:THR:HA	1:140:A:ASP:H	15	0.2	0.02	0.2
(2,248)	1:169:A:VAL:HA	1:169:A:VAL:HB	15	0.11	0.01	0.11
(1,52)	1:185:A:GLU:O	1:189:A:LEU:H	14	0.54	0.28	0.45

<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)
(1,20)	1:147:A:TYR:O	1:151:A:GLY:H	14	3.99
(1,19)	1:147:A:TYR:O	1:151:A:GLY:N	14	3.91
(1,20)	1:147:A:TYR:O	1:151:A:GLY:H	3	3.43
(1,20)	1:147:A:TYR:O	1:151:A:GLY:H	10	3.38
(1,19)	1:147:A:TYR:O	1:151:A:GLY:N	10	3.3
(1,19)	1:147:A:TYR:O	1:151:A:GLY:N	3	3.28
(1,20)	1:147:A:TYR:O	1:151:A:GLY:H	2	3.14
(1,46)	1:170:A:SER:O	1:174:A:LYS:H	5	3.0
(1,20)	1:147:A:TYR:O	1:151:A:GLY:H	4	2.97
(1,19)	1:147:A:TYR:O	1:151:A:GLY:N	2	2.88

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

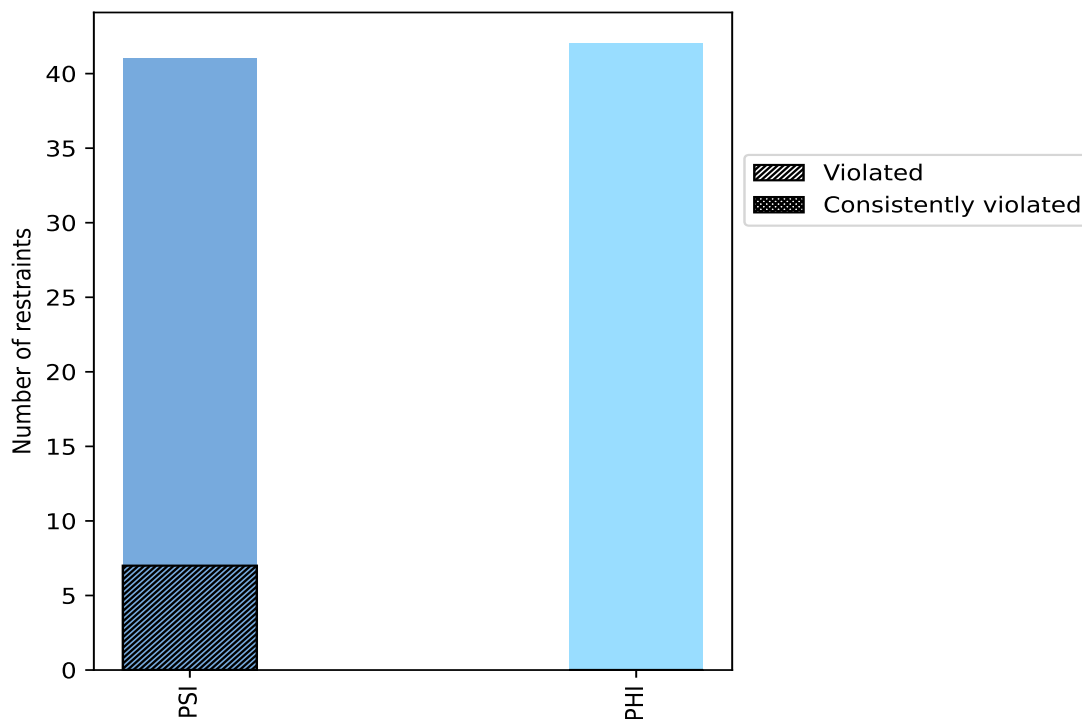
### 10.1 Summary of dihedral-angle violations [i](#)

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	41	49.4	7	17.1	8.4	0	0.0	0.0
PHI	42	50.6	0	0.0	0.0	0	0.0	0.0
Total	83	100.0	7	8.4	8.4	0	0.0	0.0

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

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



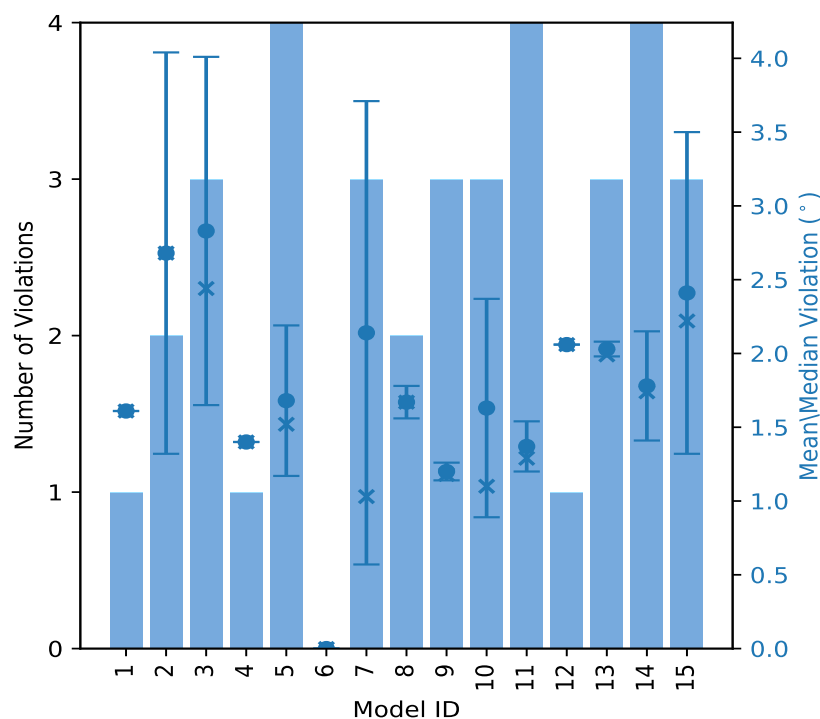
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [\(i\)](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	0	1	1.61	1.61	0.0	1.61
2	2	0	2	2.68	4.04	1.36	2.68
3	3	0	3	2.83	4.43	1.18	2.44
4	1	0	1	1.4	1.4	0.0	1.4
5	4	0	4	1.68	2.49	0.51	1.52
6	0	0	0	0.0	0.0	0.0	0.0
7	3	0	3	2.14	4.36	1.57	1.03
8	2	0	2	1.67	1.78	0.11	1.67
9	3	0	3	1.2	1.29	0.06	1.18
10	3	0	3	1.63	2.68	0.74	1.1
11	4	0	4	1.37	1.66	0.17	1.29
12	1	0	1	2.06	2.06	0.0	2.06
13	3	0	3	2.03	2.1	0.05	1.99
14	4	0	4	1.78	2.25	0.37	1.74
15	3	0	3	2.41	3.82	1.09	2.22

### 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

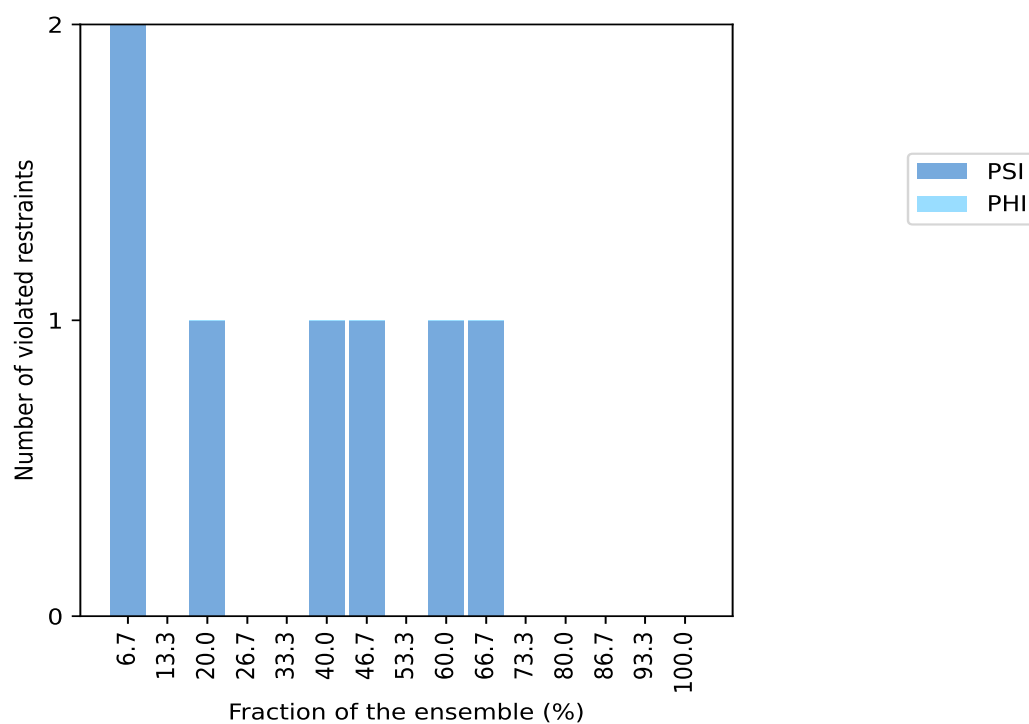
### 10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
2	0	2	1	6.7
0	0	0	2	13.3
1	0	1	3	20.0
0	0	0	4	26.7
0	0	0	5	33.3
1	0	1	6	40.0
1	0	1	7	46.7
0	0	0	8	53.3
1	0	1	9	60.0
1	0	1	10	66.7
0	0	0	11	73.3
0	0	0	12	80.0
0	0	0	13	86.7
0	0	0	14	93.3
0	0	0	15	100.0

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

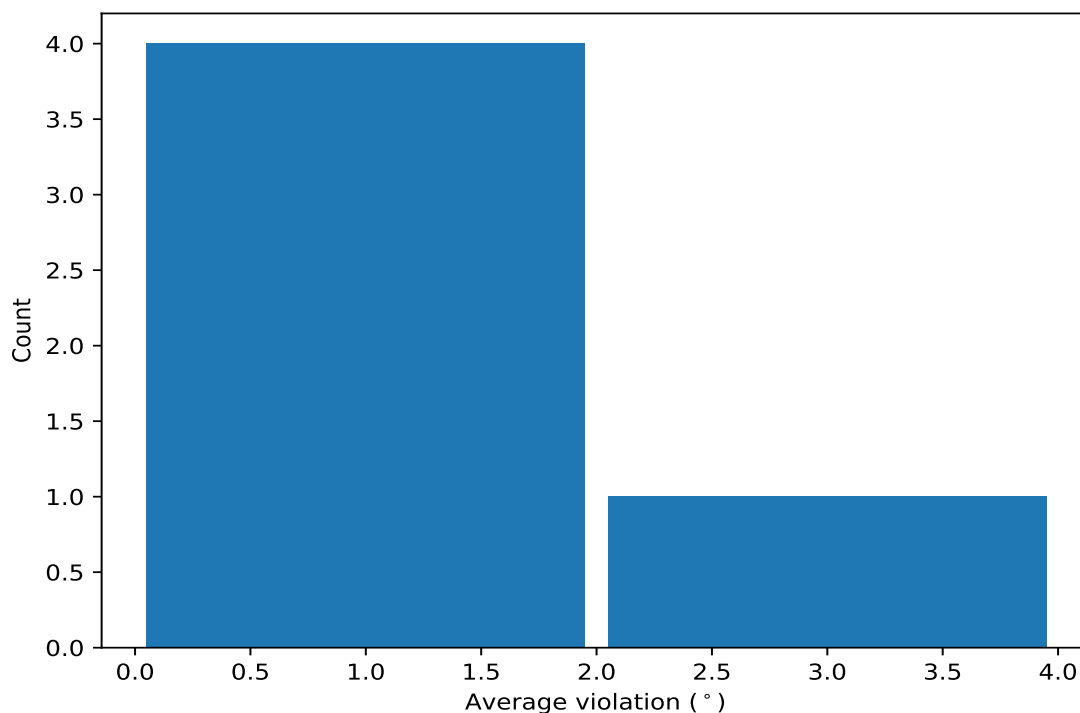
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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.

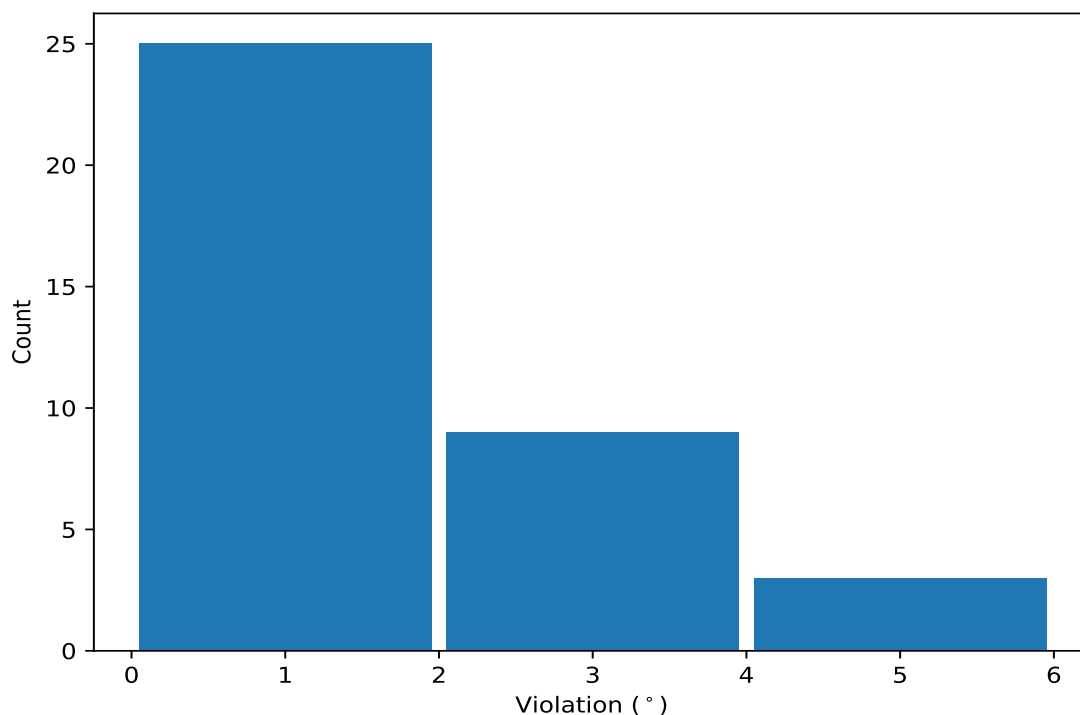
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,65)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:LEU:N	10	1.48	0.34	1.39
(1,66)	1:164:A:MET:N	1:164:A:MET:CA	1:164:A:MET:C	1:165:A:GLU:N	9	2.67	1.37	2.03
(1,72)	1:172:A:HIS:N	1:172:A:HIS:CA	1:172:A:HIS:C	1:173:A:VAL:N	7	1.87	0.57	2.1
(1,83)	1:190:A:ILE:N	1:190:A:ILE:CA	1:190:A:ILE:C	1:191:A:SER:N	6	1.6	0.5	1.35
(1,75)	1:182:A:ASP:N	1:182:A:ASP:CA	1:182:A:ASP:C	1:183:A:PHE:N	3	1.73	0.35	1.56

<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 (°)
(1,66)	1:164:A:MET:N	1:164:A:MET:CA	1:164:A:MET:C	1:165:A:GLU:N	3	4.43
(1,66)	1:164:A:MET:N	1:164:A:MET:CA	1:164:A:MET:C	1:165:A:GLU:N	7	4.36
(1,66)	1:164:A:MET:N	1:164:A:MET:CA	1:164:A:MET:C	1:165:A:GLU:N	2	4.04
(1,66)	1:164:A:MET:N	1:164:A:MET:CA	1:164:A:MET:C	1:165:A:GLU:N	15	3.82
(1,83)	1:190:A:ILE:N	1:190:A:ILE:CA	1:190:A:ILE:C	1:191:A:SER:N	10	2.68
(1,72)	1:172:A:HIS:N	1:172:A:HIS:CA	1:172:A:HIS:C	1:173:A:VAL:N	5	2.49
(1,72)	1:172:A:HIS:N	1:172:A:HIS:CA	1:172:A:HIS:C	1:173:A:VAL:N	3	2.44
(1,72)	1:172:A:HIS:N	1:172:A:HIS:CA	1:172:A:HIS:C	1:173:A:VAL:N	14	2.25
(1,75)	1:182:A:ASP:N	1:182:A:ASP:CA	1:182:A:ASP:C	1:183:A:PHE:N	15	2.22
(1,72)	1:172:A:HIS:N	1:172:A:HIS:CA	1:172:A:HIS:C	1:173:A:VAL:N	13	2.1