



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:30 AM UTC

PDB ID : 2LEN / pdb_00002len
BMRB ID : 17260
Title : Solution structure of UCHL1 S18Y variant
Authors : Tse, H.
Deposited on : 2011-06-19

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

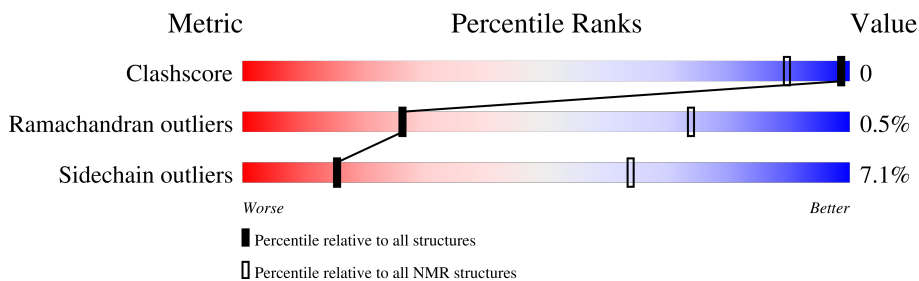
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 ≥ 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	231	88% 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:3-A:151, A:160-A:208, A:214-A:222 (207)	1.11	14

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 4 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3292 atoms, of which 1468 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase isozyme L1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	231	3292	1148	1468	322	342	12	0

There are 9 discrepancies between the modelled and reference sequences:

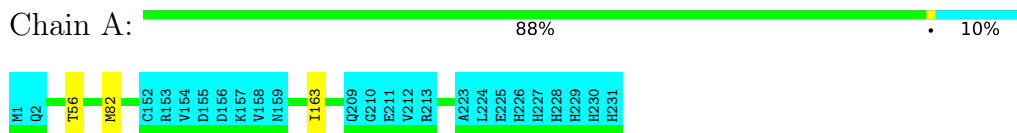
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	TYR	SER	engineered mutation	UNP P09936
A	224	LEU	-	expression tag	UNP P09936
A	225	GLU	-	expression tag	UNP P09936
A	226	HIS	-	expression tag	UNP P09936
A	227	HIS	-	expression tag	UNP P09936
A	228	HIS	-	expression tag	UNP P09936
A	229	HIS	-	expression tag	UNP P09936
A	230	HIS	-	expression tag	UNP P09936
A	231	HIS	-	expression tag	UNP P09936

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.

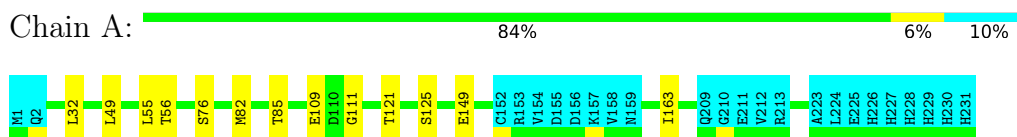
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



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

The representative model is number 14. Colouring as in section 4.1 above.

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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	2
Total number of shifts	4924
Number of shifts mapped to atoms	4404
Number of unparsed shifts	0
Number of shifts with mapping errors	520
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.87±0.01	0±0/1653 (0.0± 0.0%)	1.43±0.02	1±1/2230 (0.0± 0.1%)
All	All	0.87	0/33060 (0.0%)	1.43	17/44600 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

5 of 15 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	91	GLY	CA-C-N	5.42	127.80	120.38	17	1
1	A	91	GLY	C-N-CA	5.42	127.80	120.38	17	1
1	A	86	ILE	CA-C-N	5.38	126.30	122.16	19	1
1	A	86	ILE	C-N-CA	5.38	126.30	122.16	19	1
1	A	192	THR	CA-C-N	5.32	127.72	120.54	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	129	ARG	Sidechain	1

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1620	1315	1602	1±1
All	All	32400	26300	32040	12

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 0.

5 of 8 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:VAL:HG22	1:A:146:VAL:HG11	0.61	1.71	15	4
1:A:165:PHE:CZ	1:A:197:ALA:HB2	0.54	2.38	12	1
1:A:8:ILE:HG21	1:A:50:LEU:HD21	0.48	1.85	5	1
1:A:52:LEU:HD11	1:A:160:PHE:CD1	0.47	2.45	9	1
1:A:67:ILE:HG22	1:A:183:VAL:CG2	0.46	2.39	3	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	207/231 (90%)	193±3 (93±1%)	13±3 (6±1%)	1±1 (1±0%)	26	74
All	All	4140/4620 (90%)	3855 (93%)	264 (6%)	21 (1%)	26	74

5 of 11 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	89	SER	4
1	A	111	GLY	4
1	A	90	CYS	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	72	GLY	2
1	A	83	LYS	2

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	174/196 (89%)	162±3 (93±2%)	12±3 (7±2%)	15	64
All	All	3480/3920 (89%)	3234 (93%)	246 (7%)	15	64

5 of 83 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	82	MET	14
1	A	163	ILE	14
1	A	56	THR	13
1	A	136	ASN	10
1	A	9	ASN	8

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 i

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

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	2462
Number of shifts mapped to atoms	2202
Number of unparsed shifts	0
Number of shifts with mapping errors	260
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 260) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	GLN	HB3	2.066	0.020	2
1	A	2	GLN	HG3	2.309	0.020	2
1	A	3	LEU	HB3	1.353	0.020	2
1	A	5	PRO	HB3	1.86	0.020	2
1	A	6	MET	HB3	1.958	0.020	2
1	A	6	MET	HG3	2.324	0.020	2
1	A	7	GLU	HB3	1.774	0.020	2
1	A	7	GLU	HG3	2.143	0.020	2
1	A	8	ILE	HG13	0.324	0.020	2
1	A	9	ASN	HB3	2.816	0.020	2
1	A	10	PRO	HB3	2.233	0.020	1
1	A	11	GLU	HB3	1.992	0.020	2
1	A	11	GLU	HG3	2.226	0.020	2
1	A	13	LEU	HB3	1.286	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	ASN	HB3	2.788	0.020	2
1	A	15	LYS	HB3	1.85	0.020	2
1	A	15	LYS	HD3	1.685	0.020	2
1	A	15	LYS	HE3	2.995	0.020	2
1	A	15	LYS	HG3	1.521	0.020	2
1	A	17	LEU	HB3	2.086	0.020	2
1	A	18	TYR	HB3	3.247	0.020	2
1	A	19	ARG	HB3	1.937	0.020	2
1	A	19	ARG	HD3	3.26	0.020	2
1	A	19	ARG	HG3	1.883	0.020	2
1	A	20	LEU	HB3	1.934	0.020	2
1	A	21	GLY	HA3	4.037	0.020	2
1	A	24	GLY	HA3	4.12	0.020	2
1	A	25	GLN	HB3	2.101	0.020	1
1	A	25	GLN	HG3	2.292	0.020	2
1	A	26	TRP	HB3	2.645	0.020	2
1	A	27	ARG	HB3	1.83	0.020	2
1	A	27	ARG	HD3	3.158	0.020	2
1	A	27	ARG	HG3	1.59	0.020	1
1	A	28	PHE	HB3	3.002	0.020	2
1	A	30	ASP	HB3	2.551	0.020	2
1	A	32	LEU	HB3	1.665	0.020	2
1	A	33	GLY	HA3	4.093	0.020	2
1	A	34	LEU	HB3	1.523	0.020	2
1	A	35	GLU	HB3	2.224	0.020	1
1	A	35	GLU	HG3	2.334	0.020	2
1	A	36	GLU	HB3	1.998	0.020	2
1	A	36	GLU	HG3	2.265	0.020	2
1	A	37	GLU	HB3	2.038	0.020	2
1	A	37	GLU	HG3	2.294	0.020	2
1	A	38	SER	HB3	3.791	0.020	2
1	A	39	LEU	HB3	1.755	0.020	1
1	A	40	GLY	HA3	4.091	0.020	2
1	A	41	SER	HB3	3.996	0.020	2
1	A	43	PRO	HB3	2.275	0.020	2
1	A	43	PRO	HG3	2.025	0.020	2
1	A	45	PRO	HB3	2.503	0.020	1
1	A	45	PRO	HG3	2.02	0.020	1
1	A	47	CYS	HB3	3.233	0.020	2
1	A	49	LEU	HB3	1.64	0.020	2
1	A	50	LEU	HB3	3.097	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	LEU	HB3	2.305	0.020	2
1	A	53	PHE	HB3	2.948	0.020	2
1	A	55	LEU	HB3	1.564	0.020	2
1	A	58	GLN	HB3	2.433	0.020	2
1	A	58	GLN	HG3	2.707	0.020	2
1	A	59	HIS	HB3	3.536	0.020	2
1	A	60	GLU	HB3	2.118	0.020	2
1	A	60	GLU	HG3	2.414	0.020	2
1	A	61	ASN	HB3	2.918	0.020	2
1	A	62	PHE	HB3	3.252	0.020	2
1	A	64	LYS	HB3	1.926	0.020	2
1	A	64	LYS	HD3	1.703	0.020	2
1	A	64	LYS	HE3	2.968	0.020	2
1	A	64	LYS	HG3	1.415	0.020	2
1	A	65	LYS	HB3	1.883	0.020	2
1	A	65	LYS	HD3	1.672	0.020	2
1	A	65	LYS	HE3	2.961	0.020	2
1	A	65	LYS	HG3	1.338	0.020	2
1	A	67	ILE	HG13	0.83	0.020	2
1	A	68	GLU	HB3	2.117	0.020	2
1	A	68	GLU	HG3	2.405	0.020	2
1	A	69	GLU	HB3	2.131	0.020	2
1	A	70	LEU	HB3	1.765	0.020	2
1	A	71	LYS	HB3	1.913	0.020	2
1	A	71	LYS	HD3	1.738	0.020	2
1	A	71	LYS	HE3	3.004	0.020	2
1	A	71	LYS	HG3	1.495	0.020	2
1	A	72	GLY	HA3	3.898	0.020	2
1	A	73	GLN	HB3	2.036	0.020	2
1	A	73	GLN	HG3	2.284	0.020	2
1	A	74	GLU	HB3	1.824	0.020	2
1	A	74	GLU	HG3	2.003	0.020	2
1	A	76	SER	HB3	4.377	0.020	2
1	A	77	PRO	HB3	2.361	0.020	1
1	A	77	PRO	HD3	3.948	0.020	2
1	A	77	PRO	HG3	2.072	0.020	2
1	A	78	LYS	HB3	1.81	0.020	2
1	A	78	LYS	HD3	1.663	0.020	2
1	A	78	LYS	HE3	2.959	0.020	2
1	A	78	LYS	HG3	1.387	0.020	2
1	A	80	TYR	HB3	2.822	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	PHE	HB3	3.389	0.020	2
1	A	82	MET	HB3	1.818	0.020	1
1	A	82	MET	HG3	2.34	0.020	2
1	A	83	LYS	HB3	1.284	0.020	2
1	A	83	LYS	HE3	3.043	0.020	2
1	A	86	ILE	HG13	1.593	0.020	2
1	A	87	GLY	HA3	4.069	0.020	2
1	A	88	ASN	HB3	2.955	0.020	2
1	A	89	SER	HB3	4.026	0.020	2
1	A	90	CYS	HB3	2.906	0.020	2
1	A	91	GLY	HA3	3.893	0.020	2
1	A	93	ILE	HG13	1.122	0.020	2
1	A	94	GLY	HA3	3.965	0.020	2
1	A	96	ILE	HG13	2.001	0.020	2
1	A	97	HIS	HB3	3.0	0.020	2
1	A	101	ASN	HB3	2.911	0.020	1
1	A	102	ASN	HB3	2.589	0.020	1
1	A	103	GLN	HB3	2.408	0.020	2
1	A	103	GLN	HG3	2.58	0.020	2
1	A	104	ASP	HB3	2.738	0.020	2
1	A	105	LYS	HB3	1.518	0.020	1
1	A	105	LYS	HD3	1.667	0.020	2
1	A	105	LYS	HE3	3.147	0.020	2
1	A	105	LYS	HG3	1.267	0.020	2
1	A	106	LEU	HB3	1.041	0.020	2
1	A	107	GLY	HA3	4.365	0.020	1
1	A	108	PHE	HB3	2.796	0.020	2
1	A	109	GLU	HB3	2.125	0.020	2
1	A	109	GLU	HG3	2.389	0.020	2
1	A	110	ASP	HB3	2.625	0.020	2
1	A	111	GLY	HA3	3.811	0.020	2
1	A	112	SER	HB3	3.867	0.020	2
1	A	114	LEU	HB3	1.602	0.020	2
1	A	115	LYS	HB3	1.612	0.020	2
1	A	115	LYS	HD3	1.299	0.020	2
1	A	115	LYS	HE3	2.771	0.020	2
1	A	115	LYS	HG3	1.129	0.020	2
1	A	116	GLN	HB3	2.142	0.020	2
1	A	116	GLN	HG3	2.463	0.020	2
1	A	117	PHE	HB3	3.29	0.020	1
1	A	118	LEU	HB3	1.74	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	119	SER	HB3	3.946	0.020	2
1	A	120	GLU	HB3	2.086	0.020	2
1	A	120	GLU	HG3	2.208	0.020	2
1	A	122	GLU	HB3	2.46	0.020	1
1	A	122	GLU	HG3	2.233	0.020	2
1	A	123	LYS	HB3	2.066	0.020	2
1	A	123	LYS	HD3	1.675	0.020	2
1	A	123	LYS	HE3	2.964	0.020	2
1	A	123	LYS	HG3	1.366	0.020	2
1	A	124	MET	HB3	2.018	0.020	2
1	A	124	MET	HG3	2.718	0.020	2
1	A	125	SER	HB3	4.148	0.020	2
1	A	126	PRO	HB3	1.948	0.020	2
1	A	127	GLU	HB3	1.954	0.020	2
1	A	127	GLU	HG3	2.464	0.020	2
1	A	128	ASP	HB3	2.856	0.020	2
1	A	129	ARG	HB3	1.915	0.020	2
1	A	129	ARG	HD3	3.037	0.020	2
1	A	129	ARG	HG3	1.724	0.020	2
1	A	131	LYS	HB3	1.984	0.020	2
1	A	131	LYS	HE3	2.962	0.020	2
1	A	132	CYS	HB3	3.089	0.020	1
1	A	133	PHE	HB3	3.507	0.020	1
1	A	134	GLU	HB3	2.221	0.020	2
1	A	134	GLU	HG3	2.643	0.020	2
1	A	135	LYS	HB3	2.055	0.020	2
1	A	135	LYS	HD3	1.686	0.020	2
1	A	135	LYS	HE3	2.982	0.020	2
1	A	135	LYS	HG3	1.574	0.020	2
1	A	136	ASN	HB3	2.901	0.020	2
1	A	137	GLU	HB3	1.98	0.020	2
1	A	137	GLU	HG3	2.34	0.020	2
1	A	139	ILE	HG13	1.555	0.020	2
1	A	140	GLN	HB3	2.002	0.020	2
1	A	140	GLN	HG3	2.289	0.020	2
1	A	143	HIS	HB3	3.476	0.020	2
1	A	148	GLN	HB3	2.194	0.020	2
1	A	148	GLN	HG3	2.54	0.020	2
1	A	149	GLU	HB3	2.136	0.020	2
1	A	149	GLU	HG3	2.577	0.020	2
1	A	150	GLY	HA3	4.31	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	GLN	HB3	1.99	0.020	2
1	A	151	GLN	HG3	2.315	0.020	2
1	A	152	CYS	HB3	2.807	0.020	2
1	A	153	ARG	HB3	1.779	0.020	2
1	A	153	ARG	HD3	3.177	0.020	2
1	A	153	ARG	HG3	1.593	0.020	2
1	A	155	ASP	HB3	2.831	0.020	2
1	A	156	ASP	HB3	2.723	0.020	2
1	A	157	LYS	HB3	1.809	0.020	2
1	A	157	LYS	HD3	1.599	0.020	2
1	A	157	LYS	HE3	2.95	0.020	2
1	A	157	LYS	HG3	1.364	0.020	2
1	A	160	PHE	HB3	2.796	0.020	2
1	A	161	HIS	HB3	2.511	0.020	2
1	A	163	ILE	HG13	1.196	0.020	2
1	A	165	PHE	HB3	2.821	0.020	2
1	A	166	ASN	HB3	2.853	0.020	2
1	A	167	ASN	HB3	2.701	0.020	2
1	A	169	ASP	HB3	3.312	0.020	2
1	A	170	GLY	HA3	4.115	0.020	1
1	A	171	HIS	HB3	2.973	0.020	2
1	A	173	TYR	HB3	2.806	0.020	1
1	A	174	GLU	HB3	2.173	0.020	2
1	A	175	LEU	HB3	1.537	0.020	2
1	A	176	ASP	HB3	2.765	0.020	2
1	A	177	GLY	HA3	3.961	0.020	2
1	A	180	PRO	HB3	2.129	0.020	2
1	A	181	PHE	HB3	3.303	0.020	2
1	A	182	PRO	HB3	1.873	0.020	2
1	A	182	PRO	HG3	1.595	0.020	2
1	A	184	ASN	HB3	3.089	0.020	2
1	A	185	HIS	HB3	3.593	0.020	2
1	A	186	GLY	HA3	4.552	0.020	2
1	A	188	SER	HB3	3.737	0.020	2
1	A	189	SER	HB3	4.06	0.020	2
1	A	190	GLU	HB3	2.151	0.020	2
1	A	190	GLU	HG3	2.415	0.020	2
1	A	191	ASP	HB3	2.717	0.020	2
1	A	193	LEU	HB3	1.734	0.020	2
1	A	194	LEU	HB3	1.766	0.020	1
1	A	195	LYS	HB3	1.752	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	195	LYS	HD3	1.638	0.020	2
1	A	195	LYS	HE3	2.935	0.020	2
1	A	195	LYS	HG3	1.352	0.020	2
1	A	196	ASP	HB3	2.644	0.020	2
1	A	199	LYS	HB3	1.913	0.020	2
1	A	199	LYS	HD3	1.661	0.020	2
1	A	199	LYS	HE3	2.99	0.020	2
1	A	199	LYS	HG3	2.011	0.020	2
1	A	201	CYS	HB3	3.06	0.020	2
1	A	203	GLU	HB3	2.451	0.020	2
1	A	203	GLU	HG3	2.59	0.020	2
1	A	204	PHE	HB3	3.521	0.020	2
1	A	206	GLU	HB3	2.008	0.020	2
1	A	206	GLU	HG3	2.326	0.020	2
1	A	207	ARG	HB3	2.049	0.020	2
1	A	207	ARG	HD3	3.157	0.020	2
1	A	207	ARG	HG3	1.819	0.020	2
1	A	208	GLU	HB3	2.412	0.020	2
1	A	208	GLU	HG3	2.443	0.020	2
1	A	209	GLN	HB3	2.205	0.020	2
1	A	209	GLN	HG3	2.409	0.020	2
1	A	210	GLY	HA3	4.05	0.020	2
1	A	211	GLU	HB3	2.261	0.020	1
1	A	211	GLU	HG3	2.174	0.020	2
1	A	213	ARG	HB3	1.891	0.020	2
1	A	213	ARG	HD3	3.225	0.020	2
1	A	213	ARG	HG3	1.718	0.020	2
1	A	214	PHE	HB3	3.093	0.020	2
1	A	215	SER	HB3	3.919	0.020	2
1	A	219	LEU	HB3	0.768	0.020	2
1	A	220	CYS	HB3	2.797	0.020	2
1	A	221	LYS	HB3	1.05	0.020	1
1	A	221	LYS	HD3	1.188	0.020	2
1	A	221	LYS	HE3	2.662	0.020	2
1	A	221	LYS	HG3	0.568	0.020	2
1	A	224	LEU	HB3	1.501	0.020	2
1	A	225	GLU	HB3	1.837	0.020	2
1	A	225	GLU	HG3	2.14	0.020	2
1	A	226	HIS	HB3	3.041	0.020	2
1	A	229	HIS	HB3	3.099	0.020	2
1	A	230	HIS	HB3	3.118	0.020	2

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
$^{13}\text{C}_\alpha$	229	-0.18 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	208	0.14 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	228	-0.07 ± 0.09	None needed (< 0.5 ppm)
^{15}N	217	0.05 ± 0.18	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 2224 atoms were assigned a chemical shift out of a possible 2803. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1018/1031 (99%)	410/419 (98%)	412/414 (100%)	196/198 (99%)
Sidechain	1204/1561 (77%)	842/1013 (83%)	347/492 (71%)	15/56 (27%)
Aromatic	2/211 (1%)	1/107 (1%)	0/97 (0%)	1/7 (14%)
Overall	2224/2803 (79%)	1253/1539 (81%)	759/1003 (76%)	212/261 (81%)

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.

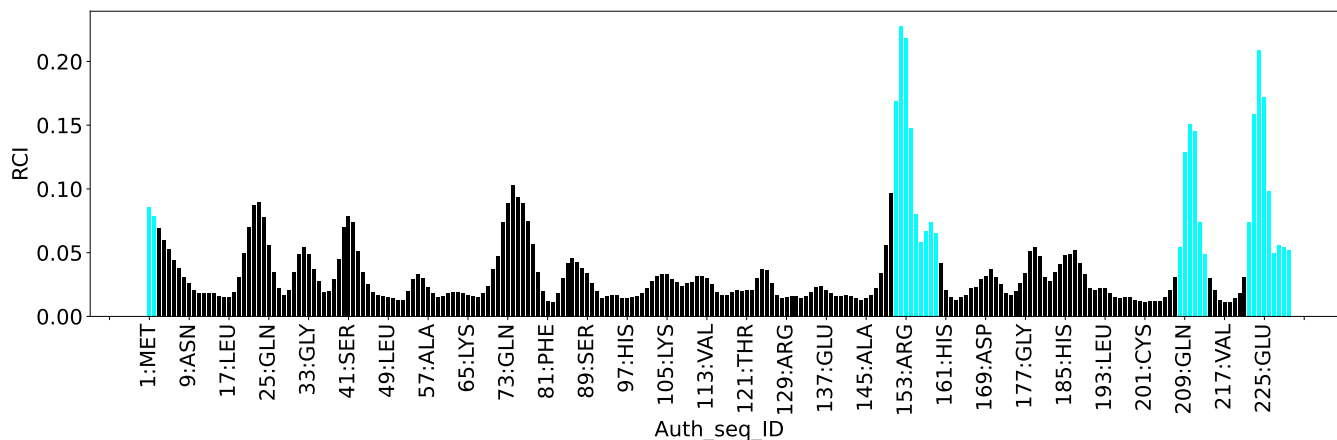
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	221	LYS	HB2	-0.27	0.58 – 2.97	-8.6
1	A	8	ILE	CG1	13.48	19.24 – 36.26	-8.4
1	A	199	LYS	CG	34.11	19.35 – 30.45	8.3
1	A	67	ILE	CG1	14.15	19.24 – 36.26	-8.0
1	A	82	MET	H	11.98	5.39 – 11.10	6.5
1	A	221	LYS	HG2	-0.04	0.13 – 2.61	-5.7

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 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	2462
Number of shifts mapped to atoms	2202
Number of unparsed shifts	0
Number of shifts with mapping errors	260
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 260) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	2	GLN	HB3	2.066	0.020	2
2	A	2	GLN	HG3	2.309	0.020	2
2	A	3	LEU	HB3	1.353	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	5	PRO	HB3	1.86	0.020	2
2	A	6	MET	HB3	1.958	0.020	2
2	A	6	MET	HG3	2.324	0.020	2
2	A	7	GLU	HB3	1.774	0.020	2
2	A	7	GLU	HG3	2.143	0.020	2
2	A	8	ILE	HG13	0.324	0.020	2
2	A	9	ASN	HB3	2.816	0.020	2
2	A	10	PRO	HB3	2.233	0.020	1
2	A	11	GLU	HB3	1.992	0.020	2
2	A	11	GLU	HG3	2.226	0.020	2
2	A	13	LEU	HB3	1.286	0.020	2
2	A	14	ASN	HB3	2.788	0.020	2
2	A	15	LYS	HB3	1.85	0.020	2
2	A	15	LYS	HD3	1.685	0.020	2
2	A	15	LYS	HE3	2.995	0.020	2
2	A	15	LYS	HG3	1.521	0.020	2
2	A	17	LEU	HB3	2.086	0.020	2
2	A	18	TYR	HB3	3.247	0.020	2
2	A	19	ARG	HB3	1.937	0.020	2
2	A	19	ARG	HD3	3.26	0.020	2
2	A	19	ARG	HG3	1.883	0.020	2
2	A	20	LEU	HB3	1.934	0.020	2
2	A	21	GLY	HA3	4.037	0.020	2
2	A	24	GLY	HA3	4.12	0.020	2
2	A	25	GLN	HB3	2.101	0.020	1
2	A	25	GLN	HG3	2.292	0.020	2
2	A	26	TRP	HB3	2.645	0.020	2
2	A	27	ARG	HB3	1.83	0.020	2
2	A	27	ARG	HD3	3.158	0.020	2
2	A	27	ARG	HG3	1.59	0.020	1
2	A	28	PHE	HB3	3.002	0.020	2
2	A	30	ASP	HB3	2.551	0.020	2
2	A	32	LEU	HB3	1.665	0.020	2
2	A	33	GLY	HA3	4.093	0.020	2
2	A	34	LEU	HB3	1.523	0.020	2
2	A	35	GLU	HB3	2.224	0.020	1
2	A	35	GLU	HG3	2.334	0.020	2
2	A	36	GLU	HB3	1.998	0.020	2
2	A	36	GLU	HG3	2.265	0.020	2
2	A	37	GLU	HB3	2.038	0.020	2
2	A	37	GLU	HG3	2.294	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	38	SER	HB3	3.791	0.020	2
2	A	39	LEU	HB3	1.755	0.020	1
2	A	40	GLY	HA3	4.091	0.020	2
2	A	41	SER	HB3	3.996	0.020	2
2	A	43	PRO	HB3	2.275	0.020	2
2	A	43	PRO	HG3	2.025	0.020	2
2	A	45	PRO	HB3	2.503	0.020	1
2	A	45	PRO	HG3	2.02	0.020	1
2	A	47	CYS	HB3	3.233	0.020	2
2	A	49	LEU	HB3	1.64	0.020	2
2	A	50	LEU	HB3	3.097	0.020	2
2	A	52	LEU	HB3	2.305	0.020	2
2	A	53	PHE	HB3	2.948	0.020	2
2	A	55	LEU	HB3	1.564	0.020	2
2	A	58	GLN	HB3	2.433	0.020	2
2	A	58	GLN	HG3	2.707	0.020	2
2	A	59	HIS	HB3	3.536	0.020	2
2	A	60	GLU	HB3	2.118	0.020	2
2	A	60	GLU	HG3	2.414	0.020	2
2	A	61	ASN	HB3	2.918	0.020	2
2	A	62	PHE	HB3	3.252	0.020	2
2	A	64	LYS	HB3	1.926	0.020	2
2	A	64	LYS	HD3	1.703	0.020	2
2	A	64	LYS	HE3	2.968	0.020	2
2	A	64	LYS	HG3	1.415	0.020	2
2	A	65	LYS	HB3	1.883	0.020	2
2	A	65	LYS	HD3	1.672	0.020	2
2	A	65	LYS	HE3	2.961	0.020	2
2	A	65	LYS	HG3	1.338	0.020	2
2	A	67	ILE	HG13	0.83	0.020	2
2	A	68	GLU	HB3	2.117	0.020	2
2	A	68	GLU	HG3	2.405	0.020	2
2	A	69	GLU	HB3	2.131	0.020	2
2	A	70	LEU	HB3	1.765	0.020	2
2	A	71	LYS	HB3	1.913	0.020	2
2	A	71	LYS	HD3	1.738	0.020	2
2	A	71	LYS	HE3	3.004	0.020	2
2	A	71	LYS	HG3	1.495	0.020	2
2	A	72	GLY	HA3	3.898	0.020	2
2	A	73	GLN	HB3	2.036	0.020	2
2	A	73	GLN	HG3	2.284	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	74	GLU	HB3	1.824	0.020	2
2	A	74	GLU	HG3	2.003	0.020	2
2	A	76	SER	HB3	4.377	0.020	2
2	A	77	PRO	HB3	2.361	0.020	1
2	A	77	PRO	HD3	3.948	0.020	2
2	A	77	PRO	HG3	2.072	0.020	2
2	A	78	LYS	HB3	1.81	0.020	2
2	A	78	LYS	HD3	1.663	0.020	2
2	A	78	LYS	HE3	2.959	0.020	2
2	A	78	LYS	HG3	1.387	0.020	2
2	A	80	TYR	HB3	2.822	0.020	2
2	A	81	PHE	HB3	3.389	0.020	2
2	A	82	MET	HB3	1.818	0.020	1
2	A	82	MET	HG3	2.34	0.020	2
2	A	83	LYS	HB3	1.284	0.020	2
2	A	83	LYS	HE3	3.043	0.020	2
2	A	86	ILE	HG13	1.593	0.020	2
2	A	87	GLY	HA3	4.069	0.020	2
2	A	88	ASN	HB3	2.955	0.020	2
2	A	89	SER	HB3	4.026	0.020	2
2	A	90	CYS	HB3	2.906	0.020	2
2	A	91	GLY	HA3	3.893	0.020	2
2	A	93	ILE	HG13	1.122	0.020	2
2	A	94	GLY	HA3	3.965	0.020	2
2	A	96	ILE	HG13	2.001	0.020	2
2	A	97	HIS	HB3	3.0	0.020	2
2	A	101	ASN	HB3	2.911	0.020	1
2	A	102	ASN	HB3	2.589	0.020	1
2	A	103	GLN	HB3	2.408	0.020	2
2	A	103	GLN	HG3	2.58	0.020	2
2	A	104	ASP	HB3	2.738	0.020	2
2	A	105	LYS	HB3	1.518	0.020	1
2	A	105	LYS	HD3	1.667	0.020	2
2	A	105	LYS	HE3	3.147	0.020	2
2	A	105	LYS	HG3	1.267	0.020	2
2	A	106	LEU	HB3	1.041	0.020	2
2	A	107	GLY	HA3	4.365	0.020	1
2	A	108	PHE	HB3	2.796	0.020	2
2	A	109	GLU	HB3	2.125	0.020	2
2	A	109	GLU	HG3	2.389	0.020	2
2	A	110	ASP	HB3	2.625	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	111	GLY	HA3	3.811	0.020	2
2	A	112	SER	HB3	3.867	0.020	2
2	A	114	LEU	HB3	1.602	0.020	2
2	A	115	LYS	HB3	1.612	0.020	2
2	A	115	LYS	HD3	1.299	0.020	2
2	A	115	LYS	HE3	2.771	0.020	2
2	A	115	LYS	HG3	1.129	0.020	2
2	A	116	GLN	HB3	2.142	0.020	2
2	A	116	GLN	HG3	2.463	0.020	2
2	A	117	PHE	HB3	3.29	0.020	1
2	A	118	LEU	HB3	1.74	0.020	2
2	A	119	SER	HB3	3.946	0.020	2
2	A	120	GLU	HB3	2.086	0.020	2
2	A	120	GLU	HG3	2.208	0.020	2
2	A	122	GLU	HB3	2.46	0.020	1
2	A	122	GLU	HG3	2.233	0.020	2
2	A	123	LYS	HB3	2.066	0.020	2
2	A	123	LYS	HD3	1.675	0.020	2
2	A	123	LYS	HE3	2.964	0.020	2
2	A	123	LYS	HG3	1.366	0.020	2
2	A	124	MET	HB3	2.018	0.020	2
2	A	124	MET	HG3	2.718	0.020	2
2	A	125	SER	HB3	4.148	0.020	2
2	A	126	PRO	HB3	1.948	0.020	2
2	A	127	GLU	HB3	1.954	0.020	2
2	A	127	GLU	HG3	2.464	0.020	2
2	A	128	ASP	HB3	2.856	0.020	2
2	A	129	ARG	HB3	1.915	0.020	2
2	A	129	ARG	HD3	3.037	0.020	2
2	A	129	ARG	HG3	1.724	0.020	2
2	A	131	LYS	HB3	1.984	0.020	2
2	A	131	LYS	HE3	2.962	0.020	2
2	A	132	CYS	HB3	3.089	0.020	1
2	A	133	PHE	HB3	3.507	0.020	1
2	A	134	GLU	HB3	2.221	0.020	2
2	A	134	GLU	HG3	2.643	0.020	2
2	A	135	LYS	HB3	2.055	0.020	2
2	A	135	LYS	HD3	1.686	0.020	2
2	A	135	LYS	HE3	2.982	0.020	2
2	A	135	LYS	HG3	1.574	0.020	2
2	A	136	ASN	HB3	2.901	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	137	GLU	HB3	1.98	0.020	2
2	A	137	GLU	HG3	2.34	0.020	2
2	A	139	ILE	HG13	1.555	0.020	2
2	A	140	GLN	HB3	2.002	0.020	2
2	A	140	GLN	HG3	2.289	0.020	2
2	A	143	HIS	HB3	3.476	0.020	2
2	A	148	GLN	HB3	2.194	0.020	2
2	A	148	GLN	HG3	2.54	0.020	2
2	A	149	GLU	HB3	2.136	0.020	2
2	A	149	GLU	HG3	2.577	0.020	2
2	A	150	GLY	HA3	4.31	0.020	2
2	A	151	GLN	HB3	1.99	0.020	2
2	A	151	GLN	HG3	2.315	0.020	2
2	A	152	CYS	HB3	2.807	0.020	2
2	A	153	ARG	HB3	1.779	0.020	2
2	A	153	ARG	HD3	3.177	0.020	2
2	A	153	ARG	HG3	1.593	0.020	2
2	A	155	ASP	HB3	2.831	0.020	2
2	A	156	ASP	HB3	2.723	0.020	2
2	A	157	LYS	HB3	1.809	0.020	2
2	A	157	LYS	HD3	1.599	0.020	2
2	A	157	LYS	HE3	2.95	0.020	2
2	A	157	LYS	HG3	1.364	0.020	2
2	A	160	PHE	HB3	2.796	0.020	2
2	A	161	HIS	HB3	2.511	0.020	2
2	A	163	ILE	HG13	1.196	0.020	2
2	A	165	PHE	HB3	2.821	0.020	2
2	A	166	ASN	HB3	2.853	0.020	2
2	A	167	ASN	HB3	2.701	0.020	2
2	A	169	ASP	HB3	3.312	0.020	2
2	A	170	GLY	HA3	4.115	0.020	1
2	A	171	HIS	HB3	2.973	0.020	2
2	A	173	TYR	HB3	2.806	0.020	1
2	A	174	GLU	HB3	2.173	0.020	2
2	A	175	LEU	HB3	1.537	0.020	2
2	A	176	ASP	HB3	2.765	0.020	2
2	A	177	GLY	HA3	3.961	0.020	2
2	A	180	PRO	HB3	2.129	0.020	2
2	A	181	PHE	HB3	3.303	0.020	2
2	A	182	PRO	HB3	1.873	0.020	2
2	A	182	PRO	HG3	1.595	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	184	ASN	HB3	3.089	0.020	2
2	A	185	HIS	HB3	3.593	0.020	2
2	A	186	GLY	HA3	4.552	0.020	2
2	A	188	SER	HB3	3.737	0.020	2
2	A	189	SER	HB3	4.06	0.020	2
2	A	190	GLU	HB3	2.151	0.020	2
2	A	190	GLU	HG3	2.415	0.020	2
2	A	191	ASP	HB3	2.717	0.020	2
2	A	193	LEU	HB3	1.734	0.020	2
2	A	194	LEU	HB3	1.766	0.020	1
2	A	195	LYS	HB3	1.752	0.020	2
2	A	195	LYS	HD3	1.638	0.020	2
2	A	195	LYS	HE3	2.935	0.020	2
2	A	195	LYS	HG3	1.352	0.020	2
2	A	196	ASP	HB3	2.644	0.020	2
2	A	199	LYS	HB3	1.913	0.020	2
2	A	199	LYS	HD3	1.661	0.020	2
2	A	199	LYS	HE3	2.99	0.020	2
2	A	199	LYS	HG3	2.011	0.020	2
2	A	201	CYS	HB3	3.06	0.020	2
2	A	203	GLU	HB3	2.451	0.020	2
2	A	203	GLU	HG3	2.59	0.020	2
2	A	204	PHE	HB3	3.521	0.020	2
2	A	206	GLU	HB3	2.008	0.020	2
2	A	206	GLU	HG3	2.326	0.020	2
2	A	207	ARG	HB3	2.049	0.020	2
2	A	207	ARG	HD3	3.157	0.020	2
2	A	207	ARG	HG3	1.819	0.020	2
2	A	208	GLU	HB3	2.412	0.020	2
2	A	208	GLU	HG3	2.443	0.020	2
2	A	209	GLN	HB3	2.205	0.020	2
2	A	209	GLN	HG3	2.409	0.020	2
2	A	210	GLY	HA3	4.05	0.020	2
2	A	211	GLU	HB3	2.261	0.020	1
2	A	211	GLU	HG3	2.174	0.020	2
2	A	213	ARG	HB3	1.891	0.020	2
2	A	213	ARG	HD3	3.225	0.020	2
2	A	213	ARG	HG3	1.718	0.020	2
2	A	214	PHE	HB3	3.093	0.020	2
2	A	215	SER	HB3	3.919	0.020	2
2	A	219	LEU	HB3	0.768	0.020	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	220	CYS	HB3	2.797	0.020	2
2	A	221	LYS	HB3	1.05	0.020	1
2	A	221	LYS	HD3	1.188	0.020	2
2	A	221	LYS	HE3	2.662	0.020	2
2	A	221	LYS	HG3	0.568	0.020	2
2	A	224	LEU	HB3	1.501	0.020	2
2	A	225	GLU	HB3	1.837	0.020	2
2	A	225	GLU	HG3	2.14	0.020	2
2	A	226	HIS	HB3	3.041	0.020	2
2	A	229	HIS	HB3	3.099	0.020	2
2	A	230	HIS	HB3	3.118	0.020	2

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	229	-0.18 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	208	0.14 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	228	-0.07 ± 0.09	None needed (< 0.5 ppm)
^{15}N	217	0.05 ± 0.18	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 2224 atoms were assigned a chemical shift out of a possible 2803. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1018/1031 (99%)	410/419 (98%)	412/414 (100%)	196/198 (99%)
Sidechain	1204/1561 (77%)	842/1013 (83%)	347/492 (71%)	15/56 (27%)
Aromatic	2/211 (1%)	1/107 (1%)	0/97 (0%)	1/7 (14%)
Overall	2224/2803 (79%)	1253/1539 (81%)	759/1003 (76%)	212/261 (81%)

7.2.4 Statistically unusual chemical shifts [i](#)

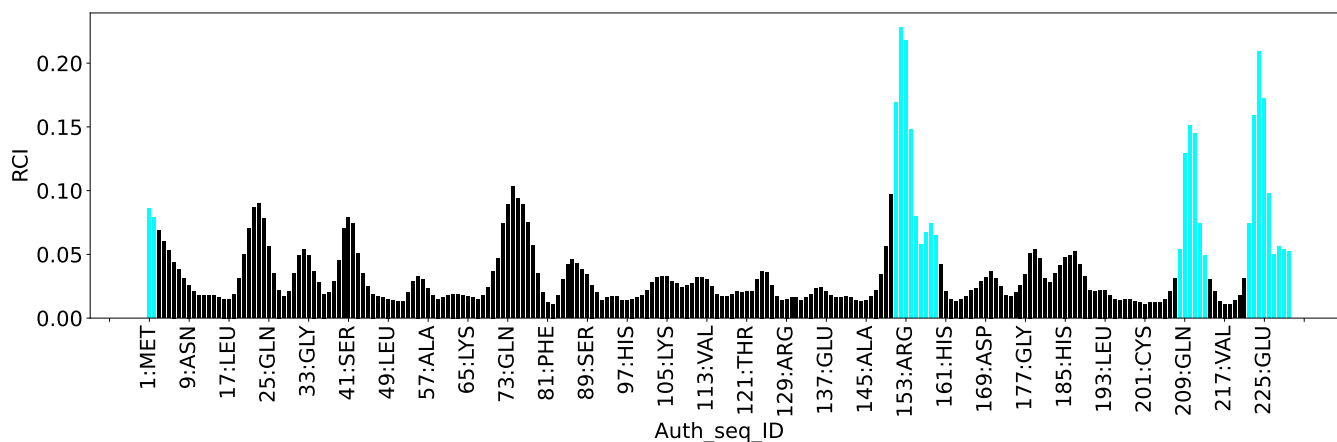
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	221	LYS	HB2	-0.27	0.58 – 2.97	-8.6
2	A	8	ILE	CG1	13.48	19.24 – 36.26	-8.4
2	A	199	LYS	CG	34.11	19.35 – 30.45	8.3
2	A	67	ILE	CG1	14.15	19.24 – 36.26	-8.0
2	A	82	MET	H	11.98	5.39 – 11.10	6.5
2	A	221	LYS	HG2	-0.04	0.13 – 2.61	-5.7

7.2.5 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	2375
Intra-residue ($ i-j =0$)	578
Sequential ($ i-j =1$)	724
Medium range ($ i-j >1$ and $ i-j <5$)	475
Long range ($ i-j \geq 5$)	598
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	733
Number of unmapped restraints	4
Number of restraints per residue	13.5
Number of long range restraints per residue ¹	2.6

¹Long 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)	62.7	0.2
0.2-0.5 (Medium)	78.2	0.5
>0.5 (Large)	32.1	4.28

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)	2.1	9.9
10.0-20.0 (Medium)	0.4	17.55
>20.0 (Large)	0.3	34.04

9 Distance violation analysis [i](#)

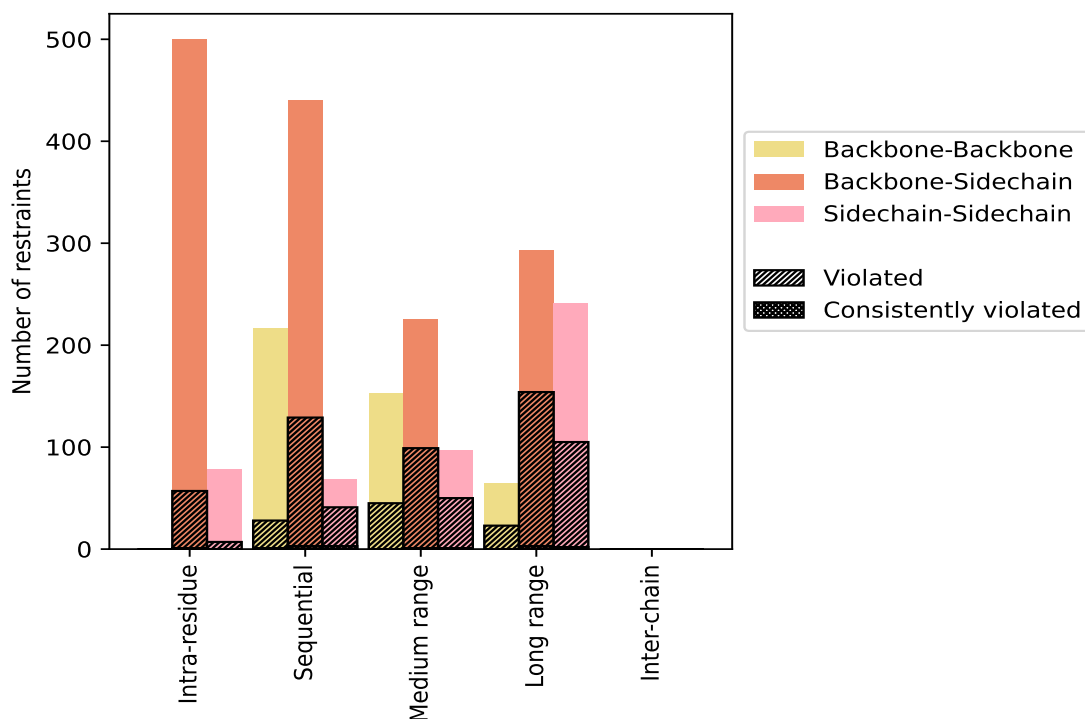
9.1 Summary of distance violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	578	24.3	64	11.1	2.7	1	0.2	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	500	21.1	57	11.4	2.4	1	0.2	0.0
Sidechain-Sidechain	78	3.3	7	9.0	0.3	0	0.0	0.0
Sequential ($i-j =1$)	724	30.5	198	27.3	8.3	7	1.0	0.3
Backbone-Backbone	216	9.1	28	13.0	1.2	1	0.5	0.0
Backbone-Sidechain	440	18.5	129	29.3	5.4	3	0.7	0.1
Sidechain-Sidechain	68	2.9	41	60.3	1.7	3	4.4	0.1
Medium range ($i-j >1$ & $i-j <5$)	475	20.0	194	40.8	8.2	2	0.4	0.1
Backbone-Backbone	153	6.4	45	29.4	1.9	0	0.0	0.0
Backbone-Sidechain	225	9.5	99	44.0	4.2	1	0.4	0.0
Sidechain-Sidechain	97	4.1	50	51.5	2.1	1	1.0	0.0
Long range ($i-j \geq 5$)	598	25.2	282	47.2	11.9	5	0.8	0.2
Backbone-Backbone	64	2.7	23	35.9	1.0	0	0.0	0.0
Backbone-Sidechain	293	12.3	154	52.6	6.5	3	1.0	0.1
Sidechain-Sidechain	241	10.1	105	43.6	4.4	2	0.8	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
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
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2375	100.0	738	31.1	31.1	15	0.6	0.6
Backbone-Backbone	433	18.2	96	22.2	4.0	1	0.2	0.0
Backbone-Sidechain	1458	61.4	439	30.1	18.5	8	0.5	0.3
Sidechain-Sidechain	484	20.4	203	41.9	8.5	6	1.2	0.3

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ 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 ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	13	53	51	76	0	193	0.39	3.89	0.49	0.26
2	13	45	43	58	0	159	0.4	4.1	0.5	0.25
3	8	55	51	54	0	168	0.37	3.96	0.45	0.24
4	12	54	51	62	0	179	0.38	3.34	0.35	0.28
5	13	38	68	73	0	192	0.4	3.57	0.38	0.28
6	11	46	44	68	0	169	0.37	3.6	0.4	0.25
7	9	45	54	78	0	186	0.38	3.77	0.48	0.23
8	8	62	49	68	0	187	0.38	3.3	0.38	0.24
9	13	60	63	69	0	205	0.43	4.17	0.46	0.3
10	11	51	47	61	0	170	0.37	4.08	0.45	0.26

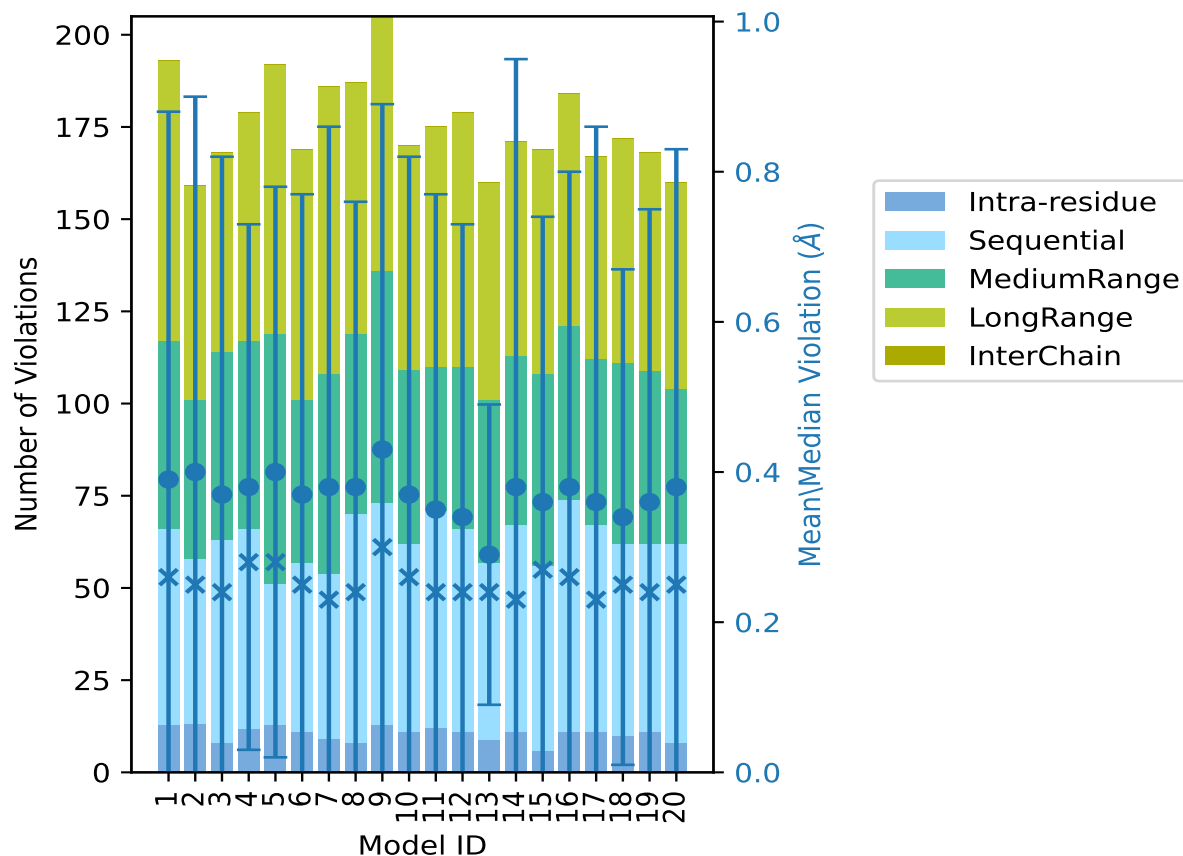
Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	12	59	39	65	0	175	0.35	3.92	0.42	0.24
12	11	55	44	69	0	179	0.34	3.73	0.39	0.24
13	9	48	44	59	0	160	0.29	1.13	0.2	0.24
14	11	56	46	58	0	171	0.38	4.28	0.57	0.23
15	6	50	52	61	0	169	0.36	3.65	0.38	0.27
16	11	63	47	63	0	184	0.38	3.76	0.42	0.26
17	11	56	45	55	0	167	0.36	4.11	0.5	0.23
18	10	52	49	61	0	172	0.34	3.2	0.33	0.25
19	11	51	47	59	0	168	0.36	3.55	0.39	0.24
20	8	54	42	56	0	160	0.38	3.94	0.45	0.25

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

9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



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

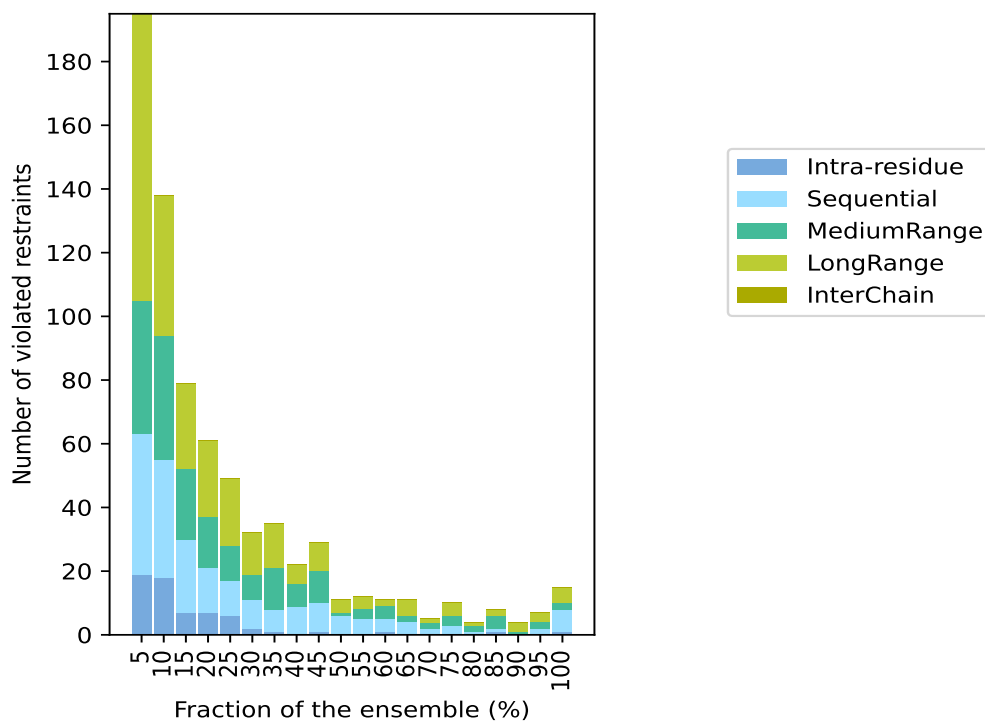
9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1637(IR:514, SQ:526, MR:281, LR:316, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
19	44	42	90	0	195	1	5.0
18	37	39	44	0	138	2	10.0
7	23	22	27	0	79	3	15.0
7	14	16	24	0	61	4	20.0
6	11	11	21	0	49	5	25.0
2	9	8	13	0	32	6	30.0
1	7	13	14	0	35	7	35.0
0	9	7	6	0	22	8	40.0
1	9	10	9	0	29	9	45.0
0	6	1	4	0	11	10	50.0
0	5	3	4	0	12	11	55.0
1	4	4	2	0	11	12	60.0
0	4	2	5	0	11	13	65.0
0	2	2	1	0	5	14	70.0
0	3	3	4	0	10	15	75.0
0	1	2	1	0	4	16	80.0
1	1	4	2	0	8	17	85.0
0	0	1	3	0	4	18	90.0
0	2	2	3	0	7	19	95.0
1	7	2	5	0	15	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

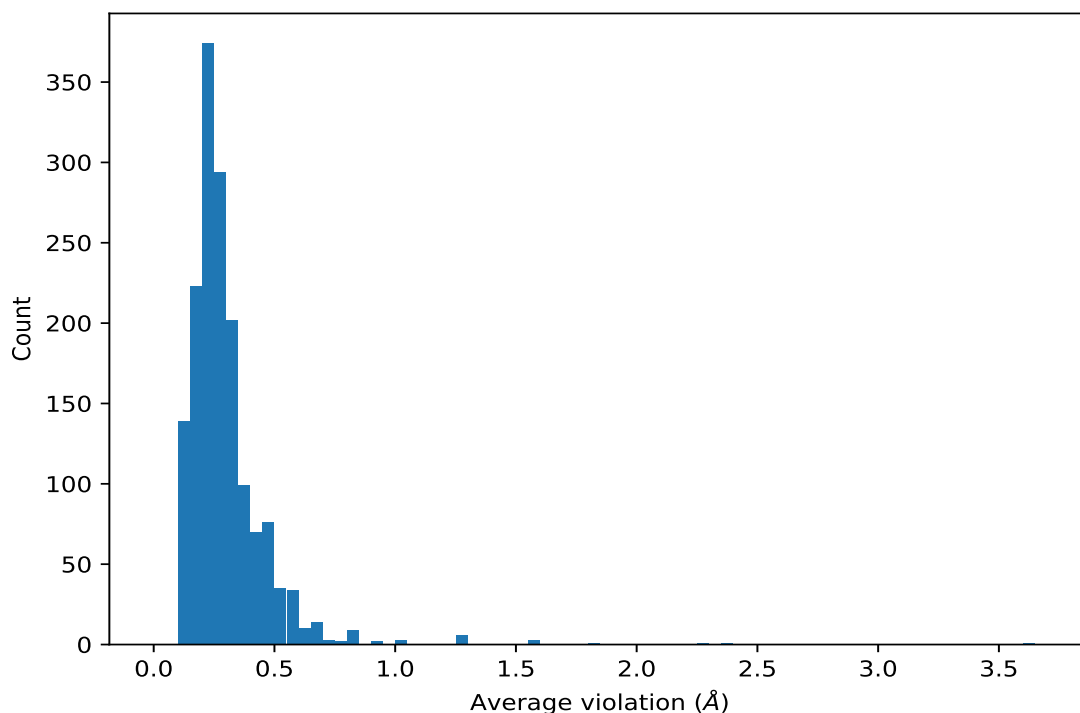
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	20	3.61	0.81	3.76
(1,432)	1:80:A:TYR:HE1	1:124:A:MET:H	20	1.81	0.98	1.54
(1,1328)	1:80:A:TYR:HA	1:80:A:TYR:HE2	20	0.73	0.25	0.78
(1,1912)	1:28:A:PHE:HB2	1:219:A:LEU:H	20	0.64	0.25	0.68
(1,1949)	1:46:A:ALA:HB1	1:220:A:CYS:HB2	20	0.61	0.18	0.64
(1,1949)	1:46:A:ALA:HB2	1:220:A:CYS:HB2	20	0.61	0.18	0.64
(1,1949)	1:46:A:ALA:HB3	1:220:A:CYS:HB2	20	0.61	0.18	0.64
(1,1461)	1:133:A:PHE:HB2	1:135:A:LYS:HG2	20	0.6	0.1	0.62
(1,1232)	1:67:A:ILE:HG21	1:179:A:MET:HE1	20	0.49	0.2	0.56
(1,1232)	1:67:A:ILE:HG21	1:179:A:MET:HE2	20	0.49	0.2	0.56
(1,1232)	1:67:A:ILE:HG21	1:179:A:MET:HE3	20	0.49	0.2	0.56
(1,1232)	1:67:A:ILE:HG22	1:179:A:MET:HE1	20	0.49	0.2	0.56
(1,1232)	1:67:A:ILE:HG22	1:179:A:MET:HE2	20	0.49	0.2	0.56
(1,1232)	1:67:A:ILE:HG22	1:179:A:MET:HE3	20	0.49	0.2	0.56
(1,1232)	1:67:A:ILE:HG23	1:179:A:MET:HE1	20	0.49	0.2	0.56
(1,1232)	1:67:A:ILE:HG23	1:179:A:MET:HE2	20	0.49	0.2	0.56

Continued on next page...

Continued from previous page...

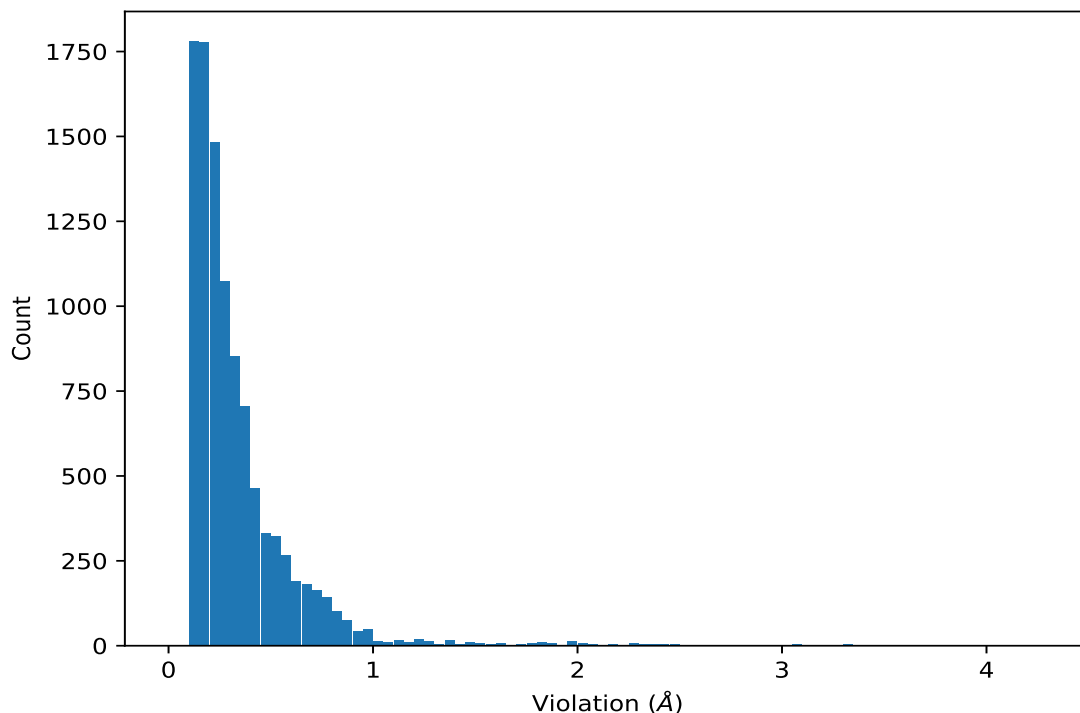
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1232)	1:67:A:ILE:HG23	1:179:A:MET:HE3	20	0.49	0.2	0.56
(1,1779)	1:117:A:PHE:HB2	1:118:A:LEU:HB2	20	0.42	0.11	0.41
(1,439)	1:133:A:PHE:H	1:135:A:LYS:HG2	20	0.34	0.09	0.34
(1,1036)	1:98:A:ALA:H	1:99:A:VAL:HA	20	0.31	0.03	0.3

¹Number of violated models, ²Standard 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)
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	14	4.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	9	4.17
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	17	4.11
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	2	4.1
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	10	4.08
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	3	3.96
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	20	3.94
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	11	3.92
(1,622)	1:80:A:TYR:HE1	1:121:A:THR:H	1	3.89
(1,432)	1:80:A:TYR:HE1	1:124:A:MET:H	1	3.85

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

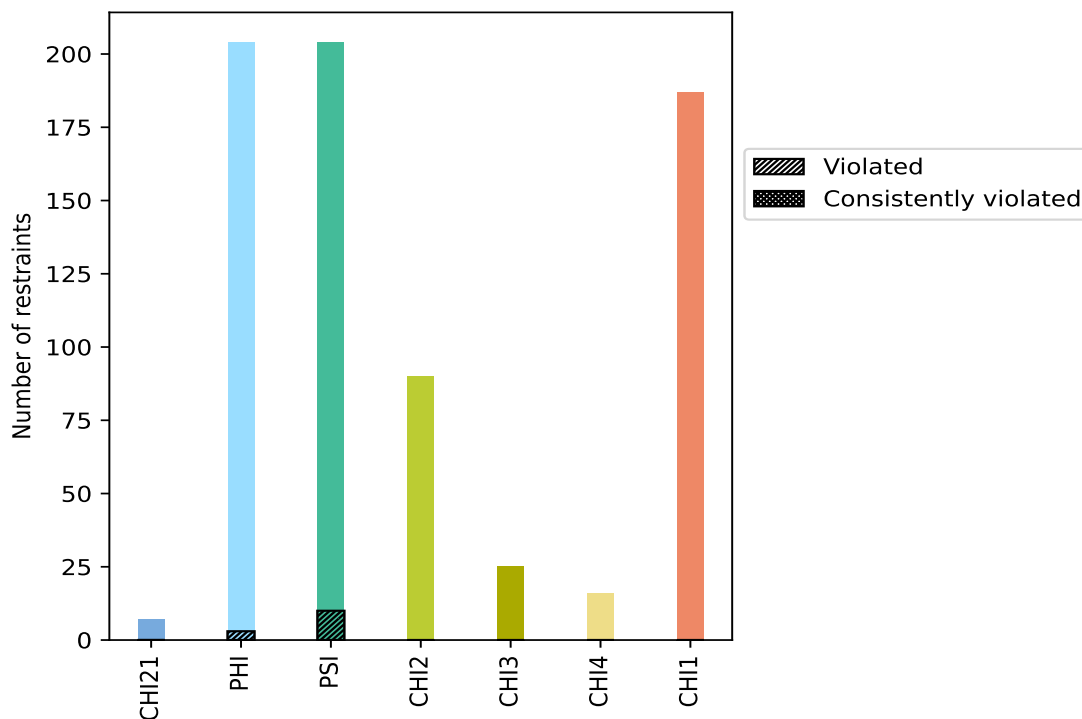
10.1 Summary of dihedral-angle violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
CHI21	7	1.0	0	0.0	0.0	0	0.0	0.0
PHI	204	27.8	3	1.5	0.4	0	0.0	0.0
PSI	204	27.8	10	4.9	1.4	0	0.0	0.0
CHI2	90	12.3	0	0.0	0.0	0	0.0	0.0
CHI3	25	3.4	0	0.0	0.0	0	0.0	0.0
CHI4	16	2.2	0	0.0	0.0	0	0.0	0.0
CHI1	187	25.5	0	0.0	0.0	0	0.0	0.0
Total	733	100.0	13	1.8	1.8	0	0.0	0.0

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

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



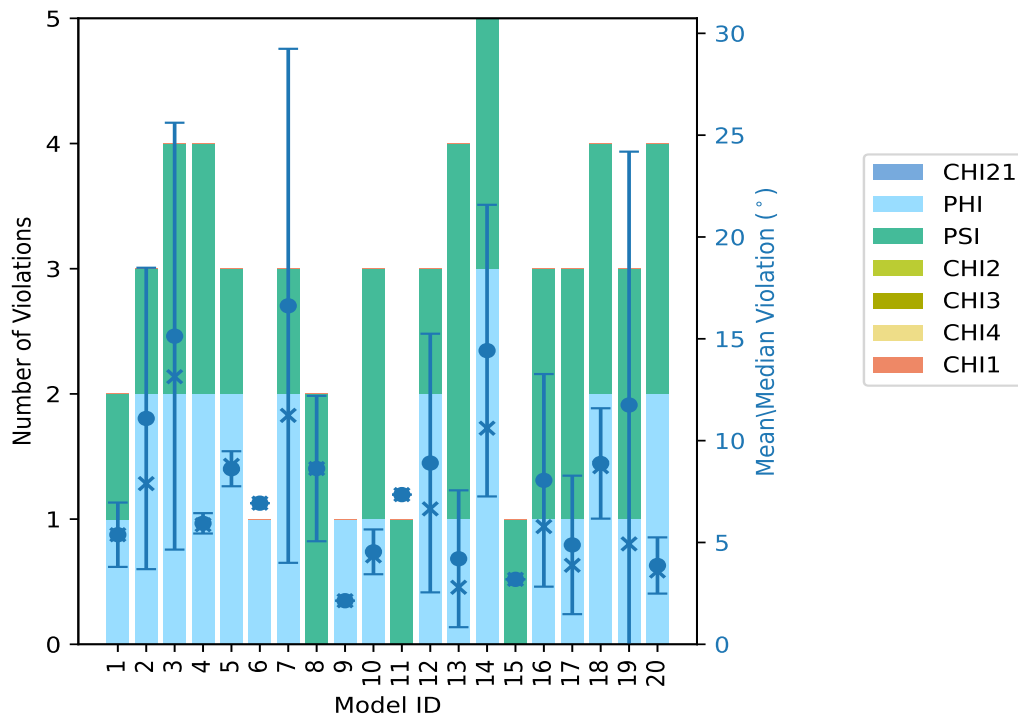
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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							Total	Mean (°)	Max (°)	SD (°)	Median (°)
	CHI21	PHI	PSI	CHI2	CHI3	CHI4	CHI1					
1	0	1	1	0	0	0	0	2	5.38	6.97	1.58	5.38
2	0	2	1	0	0	0	0	3	11.09	21.32	7.4	7.89
3	0	2	2	0	0	0	0	4	15.13	29.22	10.48	13.14
4	0	2	2	0	0	0	0	4	5.94	6.69	0.5	5.87
5	0	2	1	0	0	0	0	3	8.62	9.57	0.86	8.79
6	0	1	0	0	0	0	0	1	6.93	6.93	0.0	6.93
7	0	2	1	0	0	0	0	3	16.62	34.04	12.62	11.24
8	0	0	2	0	0	0	0	2	8.63	12.2	3.57	8.63
9	0	1	0	0	0	0	0	1	2.14	2.14	0.0	2.14
10	0	1	2	0	0	0	0	3	4.54	5.98	1.1	4.34
11	0	0	1	0	0	0	0	1	7.35	7.35	0.0	7.35
12	0	2	1	0	0	0	0	3	8.9	17.55	6.35	6.65
13	0	1	3	0	0	0	0	4	4.2	9.9	3.36	2.8
14	0	3	2	0	0	0	0	5	14.42	27.16	7.16	10.61
15	0	0	1	0	0	0	0	1	3.19	3.19	0.0	3.19
16	0	1	2	0	0	0	0	3	8.05	15.27	5.22	5.78
17	0	1	2	0	0	0	0	3	4.88	9.45	3.4	3.88
18	0	2	2	0	0	0	0	4	8.88	12.69	2.71	8.72
19	0	1	2	0	0	0	0	3	11.75	29.21	12.44	4.93
20	0	2	2	0	0	0	0	4	3.87	5.85	1.38	3.6

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

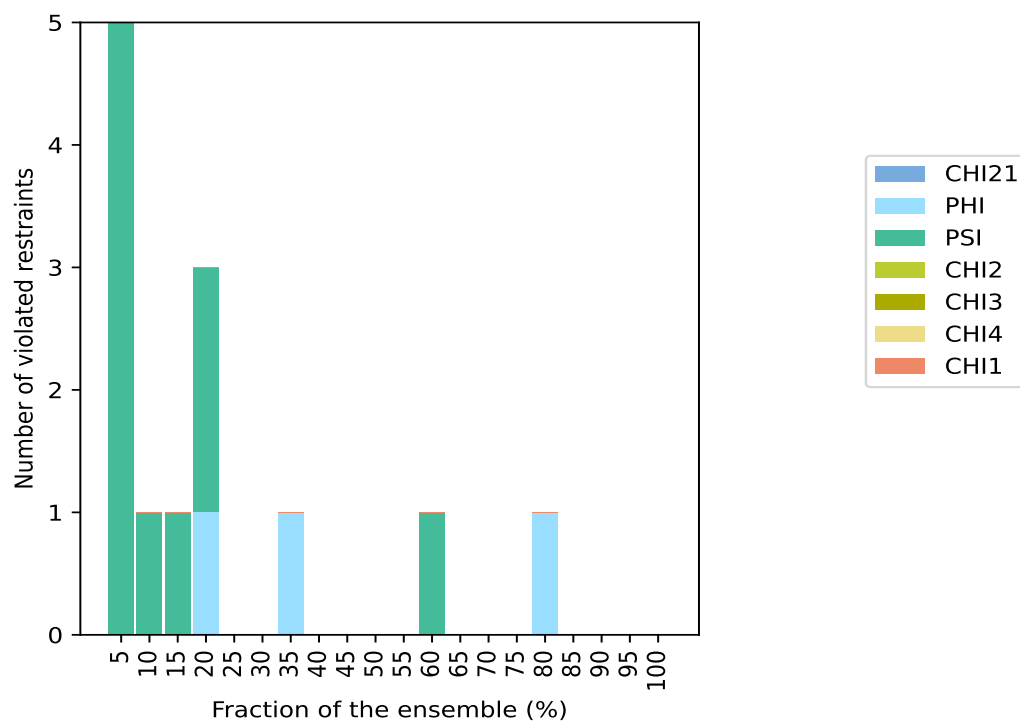
10.3 Dihedral-angle violation statistics for the ensemble i

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	
CHI21	PHI	PSI	CHI2	CHI3	CHI4	CHI1	Total	Count ¹	%
0	0	5	0	0	0	0	5	1	5.0
0	0	1	0	0	0	0	1	2	10.0
0	0	1	0	0	0	0	1	3	15.0
0	1	2	0	0	0	0	3	4	20.0
0	0	0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	0	0	6	30.0
0	1	0	0	0	0	0	1	7	35.0
0	0	0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	0	0	11	55.0
0	0	1	0	0	0	0	1	12	60.0
0	0	0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	0	0	15	75.0
0	1	0	0	0	0	0	1	16	80.0
0	0	0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	0	0	20	100.0

¹ Number of models with violations

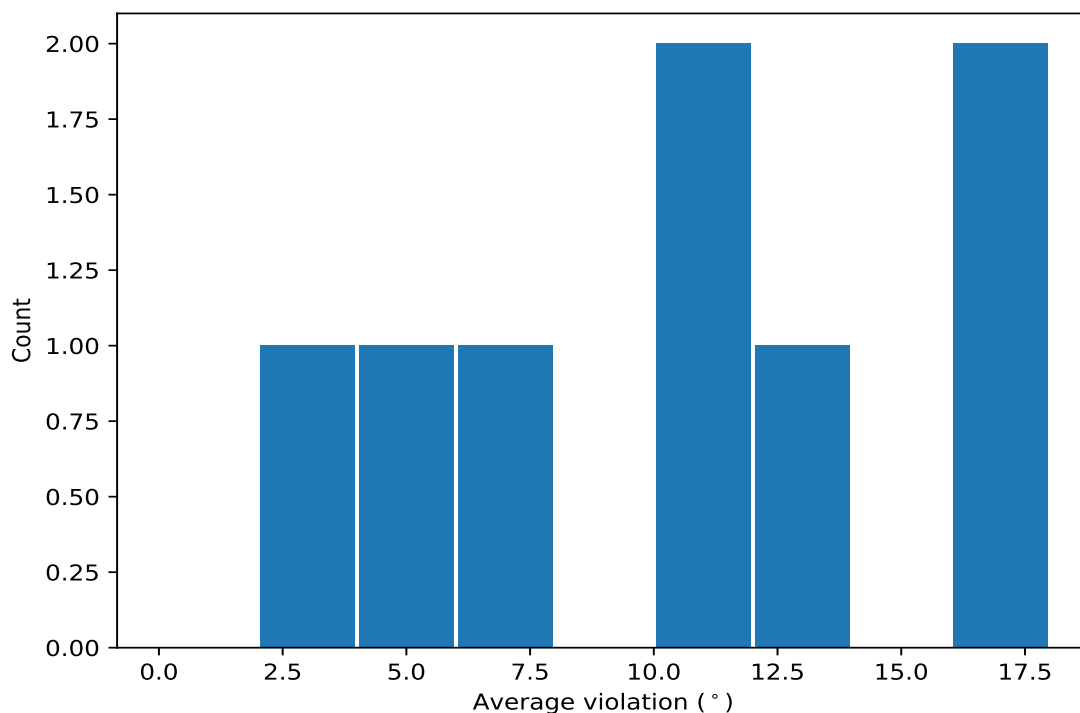
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

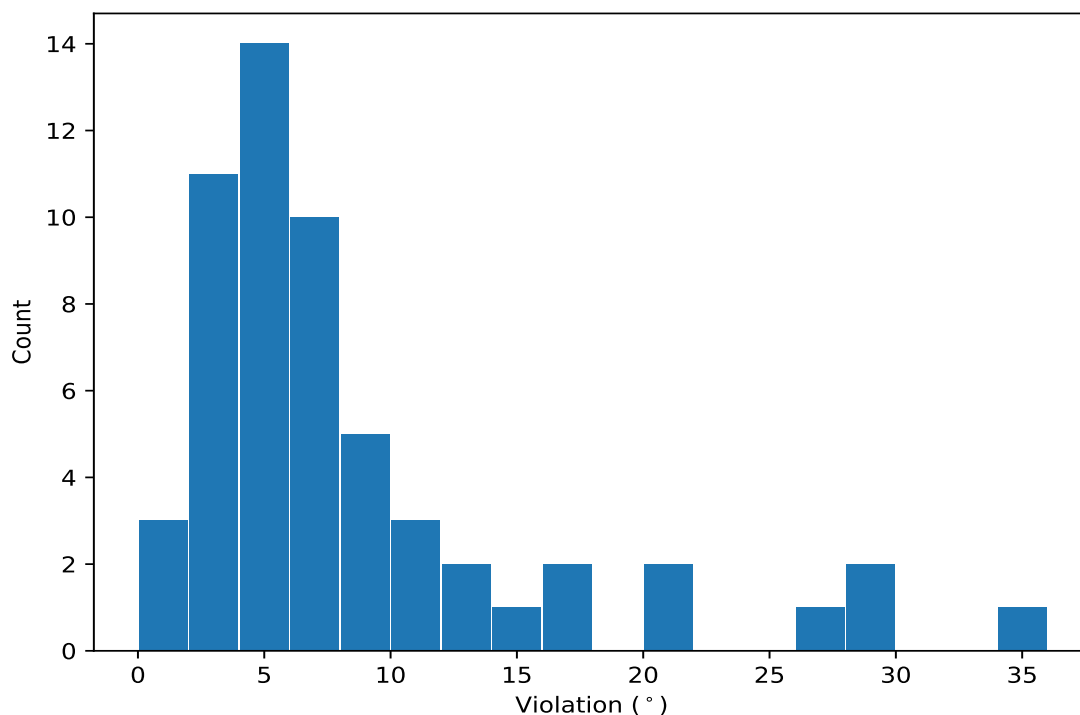
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,53)	1:43:A:PRO:C	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	16	5.59	2.24	5.46
(1,52)	1:42:A:VAL:N	1:42:A:VAL:CA	1:42:A:VAL:C	1:43:A:PRO:N	12	6.82	2.26	6.32
(1,103)	1:75:A:VAL:C	1:76:A:SER:N	1:76:A:SER:CA	1:76:A:SER:C	7	16.38	8.35	15.27
(1,355)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:SER:N	4	17.4	10.42	14.88
(1,381)	1:188:A:SER:N	1:188:A:SER:CA	1:188:A:SER:C	1:189:A:SER:N	4	12.42	10.43	9.59
(1,249)	1:178:A:ARG:C	1:179:A:MET:N	1:179:A:MET:CA	1:179:A:MET:C	4	10.0	7.1	8.13
(1,339)	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	1:84:A:GLN:N	3	2.3	0.75	2.48
(1,395)	1:222:A:ALA:N	1:222:A:ALA:CA	1:222:A:ALA:C	1:223:A:ALA:N	2	11.99	9.24	11.99

¹ Number of violated models, ²Standard 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 (°)
(1,355)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:SER:N	7	34.04
(1,103)	1:75:A:VAL:C	1:76:A:SER:N	1:76:A:SER:CA	1:76:A:SER:C	3	29.22
(1,381)	1:188:A:SER:N	1:188:A:SER:CA	1:188:A:SER:C	1:189:A:SER:N	19	29.21
(1,103)	1:75:A:VAL:C	1:76:A:SER:N	1:76:A:SER:CA	1:76:A:SER:C	14	27.16
(1,249)	1:178:A:ARG:C	1:179:A:MET:N	1:179:A:MET:CA	1:179:A:MET:C	2	21.32
(1,395)	1:222:A:ALA:N	1:222:A:ALA:CA	1:222:A:ALA:C	1:223:A:ALA:N	3	21.23
(1,103)	1:75:A:VAL:C	1:76:A:SER:N	1:76:A:SER:CA	1:76:A:SER:C	12	17.55
(1,355)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:SER:N	14	17.07
(1,103)	1:75:A:VAL:C	1:76:A:SER:N	1:76:A:SER:CA	1:76:A:SER:C	16	15.27
(1,355)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:SER:N	18	12.69