



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:28 PM UTC

PDB ID : 2LFE / pdb_00002lfe
BMRB ID : 17750
Title : Solution NMR structure of N-terminal domain of human E3 ubiquitin-protein ligase HECW2, Northeast structural genomics consortium (NESG) target ht6306A
Authors : Lemak, A.; Yee, A.; Houliston, S.; Garcia, M.; Chitayat, S.; Dhe-Paganon, S.; Montelione, G.T.; Arrowsmith, C.; Northeast Structural Genomics Consortium (NESG); Structural Genomics Consortium (SGC)
Deposited on : 2011-06-29

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

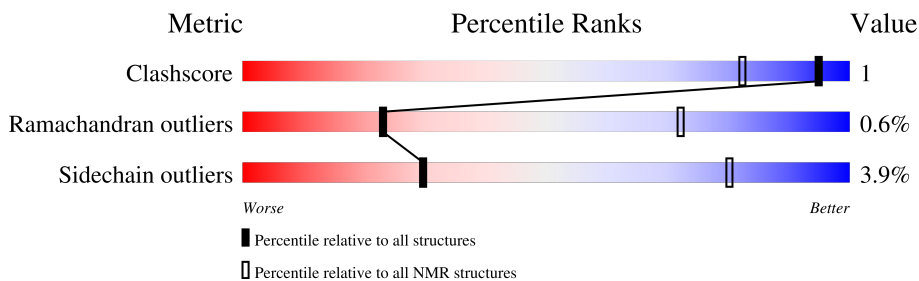
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	138	

2 Ensemble composition and analysis i

This entry contains 16 models. Model 10 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:59-A:144, A:149-A:162 (100)	0.70	10

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1684 atoms, of which 827 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase HECW2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	106	1684	551	827	141	161	4	0

There are 18 discrepancies between the modelled and reference sequences:

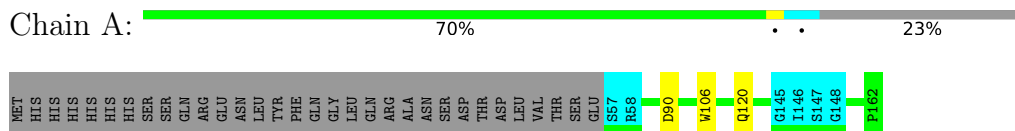
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	expression tag	UNP Q9P2P5
A	26	HIS	-	expression tag	UNP Q9P2P5
A	27	HIS	-	expression tag	UNP Q9P2P5
A	28	HIS	-	expression tag	UNP Q9P2P5
A	29	HIS	-	expression tag	UNP Q9P2P5
A	30	HIS	-	expression tag	UNP Q9P2P5
A	31	HIS	-	expression tag	UNP Q9P2P5
A	32	SER	-	expression tag	UNP Q9P2P5
A	33	SER	-	expression tag	UNP Q9P2P5
A	34	GLN	-	expression tag	UNP Q9P2P5
A	35	ARG	-	expression tag	UNP Q9P2P5
A	36	GLU	-	expression tag	UNP Q9P2P5
A	37	ASN	-	expression tag	UNP Q9P2P5
A	38	LEU	-	expression tag	UNP Q9P2P5
A	39	TYR	-	expression tag	UNP Q9P2P5
A	40	PHE	-	expression tag	UNP Q9P2P5
A	41	GLN	-	expression tag	UNP Q9P2P5
A	42	GLY	-	expression tag	UNP Q9P2P5

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: E3 ubiquitin-protein ligase HECW2



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 16 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	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1434
Number of shifts mapped to atoms	1273
Number of unparsed shifts	0
Number of shifts with mapping errors	161
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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	1.17±0.03	1±1/844 (0.1± 0.1%)	0.82±0.02	0±0/1149 (0.0± 0.0%)
All	All	1.17	9/13504 (0.1%)	0.82	5/18384 (0.0%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	157	ILE	CA-CB	5.78	1.60	1.53	14	1
1	A	82	ILE	CA-CB	5.62	1.60	1.53	14	5
1	A	136	ILE	CA-CB	5.19	1.60	1.53	10	1
1	A	87	ASP	C-N	5.12	1.38	1.33	14	2

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	90	ASP	CA-CB-CG	5.67	118.27	112.60	8	5

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	818	787	785	2±1
All	All	13088	12592	12560	27

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 1.

5 of 17 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:CYS:SG	1:A:141:LYS:HE3	0.53	2.44	1	3
1:A:86:VAL:HG12	1:A:151:ARG:HH12	0.47	1.69	15	1
1:A:109:LYS:HA	1:A:109:LYS:NZ	0.46	2.26	6	1
1:A:144:HIS:HB2	1:A:151:ARG:HD3	0.46	1.87	3	1
1:A:133:GLU:HB2	1:A:136:ILE:HG13	0.46	1.88	7	4

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	99/138 (72%)	88±2 (89±2%)	11±3 (11±3%)	1±1 (1±1%)	23	72
All	All	1584/2208 (72%)	1403 (89%)	171 (11%)	10 (1%)	23	72

All 2 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	105	PHE	8
1	A	97	ILE	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	89/123 (72%)	86±1 (96±1%)	4±1 (4±1%)	30	80
All	All	1424/1968 (72%)	1368 (96%)	56 (4%)	30	80

5 of 16 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	106	TRP	16
1	A	120	GLN	11
1	A	83	LYS	5
1	A	137	LYS	4
1	A	109	LYS	3

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1434
Number of shifts mapped to atoms	1273
Number of unparsed shifts	0
Number of shifts with mapping errors	161
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

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 161) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	43	LEU	H	7.881	0.04	1
1	A	43	LEU	HA	4.206	0.04	1
1	A	43	LEU	HB2	1.527	0.04	2
1	A	43	LEU	HB3	1.469	0.04	2
1	A	43	LEU	HD11	0.799	0.04	2
1	A	43	LEU	HD12	0.799	0.04	2
1	A	43	LEU	HD13	0.799	0.04	2
1	A	43	LEU	HD21	0.741	0.04	2
1	A	43	LEU	HD22	0.741	0.04	2
1	A	43	LEU	HD23	0.741	0.04	2
1	A	43	LEU	HG	1.477	0.04	1
1	A	43	LEU	C	177.422	0.40	1
1	A	43	LEU	CA	55.349	0.40	1
1	A	43	LEU	CB	42.35	0.40	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	43	LEU	CD1	24.83	0.40	2
1	A	43	LEU	CD2	23.468	0.40	2
1	A	43	LEU	CG	26.819	0.40	1
1	A	43	LEU	N	121.393	0.40	1
1	A	44	GLN	H	8.246	0.04	1
1	A	44	GLN	HA	4.182	0.04	1
1	A	44	GLN	HB2	1.965	0.04	2
1	A	44	GLN	HB3	1.86	0.04	2
1	A	44	GLN	HG2	2.223	0.04	2
1	A	44	GLN	HG3	2.223	0.04	2
1	A	44	GLN	C	175.921	0.40	1
1	A	44	GLN	CA	55.977	0.40	1
1	A	44	GLN	CB	29.294	0.40	1
1	A	44	GLN	CG	33.792	0.40	1
1	A	44	GLN	N	120.78	0.40	1
1	A	45	ARG	H	8.18	0.04	1
1	A	45	ARG	HA	4.189	0.04	1
1	A	45	ARG	HB2	1.733	0.04	2
1	A	45	ARG	HB3	1.63	0.04	2
1	A	45	ARG	HD2	3.063	0.04	2
1	A	45	ARG	HD3	3.063	0.04	2
1	A	45	ARG	HG2	1.503	0.04	2
1	A	45	ARG	HG3	1.503	0.04	2
1	A	45	ARG	C	175.962	0.40	1
1	A	45	ARG	CA	55.922	0.40	1
1	A	45	ARG	CB	31.083	0.40	1
1	A	45	ARG	CD	43.244	0.40	1
1	A	45	ARG	CG	26.982	0.40	1
1	A	45	ARG	N	122.04	0.40	1
1	A	46	ALA	H	8.288	0.04	1
1	A	46	ALA	HA	4.19	0.04	1
1	A	46	ALA	HB1	1.282	0.04	1
1	A	46	ALA	HB2	1.282	0.04	1
1	A	46	ALA	HB3	1.282	0.04	1
1	A	46	ALA	C	177.49	0.40	1
1	A	46	ALA	CA	52.592	0.40	1
1	A	46	ALA	CB	19.4	0.40	1
1	A	46	ALA	N	125.104	0.40	1
1	A	47	ASN	H	8.354	0.04	1
1	A	47	ASN	HA	4.593	0.04	1
1	A	47	ASN	HB2	2.748	0.04	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	47	ASN	HB3	2.677	0.04	2
1	A	47	ASN	HD21	6.85	0.04	2
1	A	47	ASN	HD22	7.538	0.04	2
1	A	47	ASN	C	175.279	0.40	1
1	A	47	ASN	CA	53.356	0.40	1
1	A	47	ASN	CB	39.012	0.40	1
1	A	47	ASN	N	117.971	0.40	1
1	A	47	ASN	ND2	113.27	0.40	1
1	A	48	SER	H	8.2	0.04	1
1	A	48	SER	HA	4.36	0.04	1
1	A	48	SER	HB2	3.841	0.04	2
1	A	48	SER	HB3	3.841	0.04	2
1	A	48	SER	C	174.433	0.40	1
1	A	48	SER	CA	58.488	0.40	1
1	A	48	SER	CB	63.947	0.40	1
1	A	48	SER	N	115.74	0.40	1
1	A	49	ASP	H	8.352	0.04	1
1	A	49	ASP	HA	4.556	0.04	1
1	A	49	ASP	HB2	2.654	0.04	2
1	A	49	ASP	HB3	2.571	0.04	2
1	A	49	ASP	C	176.603	0.40	1
1	A	49	ASP	CA	54.694	0.40	1
1	A	49	ASP	CB	40.95	0.40	1
1	A	49	ASP	N	122.414	0.40	1
1	A	50	THR	H	7.934	0.04	1
1	A	50	THR	HA	4.194	0.04	1
1	A	50	THR	HB	4.146	0.04	1
1	A	50	THR	HG21	1.088	0.04	1
1	A	50	THR	HG22	1.088	0.04	1
1	A	50	THR	HG23	1.088	0.04	1
1	A	50	THR	C	174.378	0.40	1
1	A	50	THR	CA	62.064	0.40	1
1	A	50	THR	CB	69.652	0.40	1
1	A	50	THR	CG2	21.466	0.40	1
1	A	50	THR	N	113.34	0.40	1
1	A	51	ASP	H	8.202	0.04	1
1	A	51	ASP	HA	4.507	0.04	1
1	A	51	ASP	HB2	2.606	0.04	2
1	A	51	ASP	HB3	2.517	0.04	2
1	A	51	ASP	C	176.057	0.40	1
1	A	51	ASP	CA	54.53	0.40	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	ASP	CB	41.019	0.40	1
1	A	51	ASP	N	122.584	0.40	1
1	A	52	LEU	H	7.991	0.04	1
1	A	52	LEU	HA	4.216	0.04	1
1	A	52	LEU	HB2	1.529	0.04	2
1	A	52	LEU	HB3	1.468	0.04	2
1	A	52	LEU	HD11	0.798	0.04	2
1	A	52	LEU	HD12	0.798	0.04	2
1	A	52	LEU	HD13	0.798	0.04	2
1	A	52	LEU	HD21	0.741	0.04	2
1	A	52	LEU	HD22	0.741	0.04	2
1	A	52	LEU	HD23	0.741	0.04	2
1	A	52	LEU	HG	1.485	0.04	1
1	A	52	LEU	C	177.381	0.40	1
1	A	52	LEU	CA	55.322	0.40	1
1	A	52	LEU	CB	42.351	0.40	1
1	A	52	LEU	CD1	24.912	0.40	2
1	A	52	LEU	CD2	23.468	0.40	2
1	A	52	LEU	CG	26.873	0.40	1
1	A	52	LEU	N	122.329	0.40	1
1	A	53	VAL	H	8.065	0.04	1
1	A	53	VAL	HA	4.039	0.04	1
1	A	53	VAL	HB	1.985	0.04	1
1	A	53	VAL	HG11	0.828	0.04	2
1	A	53	VAL	HG12	0.828	0.04	2
1	A	53	VAL	HG13	0.828	0.04	2
1	A	53	VAL	HG21	0.842	0.04	2
1	A	53	VAL	HG22	0.842	0.04	2
1	A	53	VAL	HG23	0.842	0.04	2
1	A	53	VAL	C	176.548	0.40	1
1	A	53	VAL	CA	62.637	0.40	1
1	A	53	VAL	CB	32.502	0.40	1
1	A	53	VAL	CG1	21.098	0.40	2
1	A	53	VAL	CG2	20.744	0.40	2
1	A	53	VAL	N	121.478	0.40	1
1	A	54	THR	H	8.158	0.04	1
1	A	54	THR	HA	4.292	0.04	1
1	A	54	THR	HB	4.169	0.04	1
1	A	54	THR	HG21	1.092	0.04	1
1	A	54	THR	HG22	1.092	0.04	1
1	A	54	THR	HG23	1.092	0.04	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	THR	C	174.706	0.40	1
1	A	54	THR	CA	61.681	0.40	1
1	A	54	THR	CB	69.843	0.40	1
1	A	54	THR	CG2	21.466	0.40	1
1	A	54	THR	N	117.715	0.40	1
1	A	55	SER	H	8.244	0.04	1
1	A	55	SER	HA	4.339	0.04	1
1	A	55	SER	HB2	3.807	0.04	2
1	A	55	SER	HB3	3.732	0.04	2
1	A	55	SER	C	174.61	0.40	1
1	A	55	SER	CA	58.652	0.40	1
1	A	55	SER	CB	63.729	0.40	1
1	A	55	SER	N	117.92	0.40	1
1	A	56	GLU	H	8.335	0.04	1
1	A	56	GLU	HA	4.216	0.04	1
1	A	56	GLU	HB2	1.971	0.04	2
1	A	56	GLU	HB3	1.828	0.04	2
1	A	56	GLU	HG2	2.19	0.04	2
1	A	56	GLU	HG3	2.138	0.04	2
1	A	56	GLU	C	176.303	0.40	1
1	A	56	GLU	CA	56.605	0.40	1
1	A	56	GLU	CB	30.264	0.40	1
1	A	56	GLU	CG	36.312	0.40	1
1	A	56	GLU	N	122.567	0.40	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
$^{13}\text{C}_\alpha$	118	0.13 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	110	-0.07 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	106	0.49 ± 0.15	None needed (< 0.5 ppm)
^{15}N	106	0.33 ± 0.35	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 89%, i.e. 1223 atoms were assigned a chemical shift out of a possible 1378. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	470/492 (96%)	194/199 (97%)	187/200 (94%)	89/93 (96%)
Sidechain	645/728 (89%)	439/473 (93%)	197/231 (85%)	9/24 (38%)
Aromatic	108/158 (68%)	54/76 (71%)	51/74 (69%)	3/8 (38%)
Overall	1223/1378 (89%)	687/748 (92%)	435/505 (86%)	101/125 (81%)

7.1.4 Statistically unusual chemical shifts [i](#)

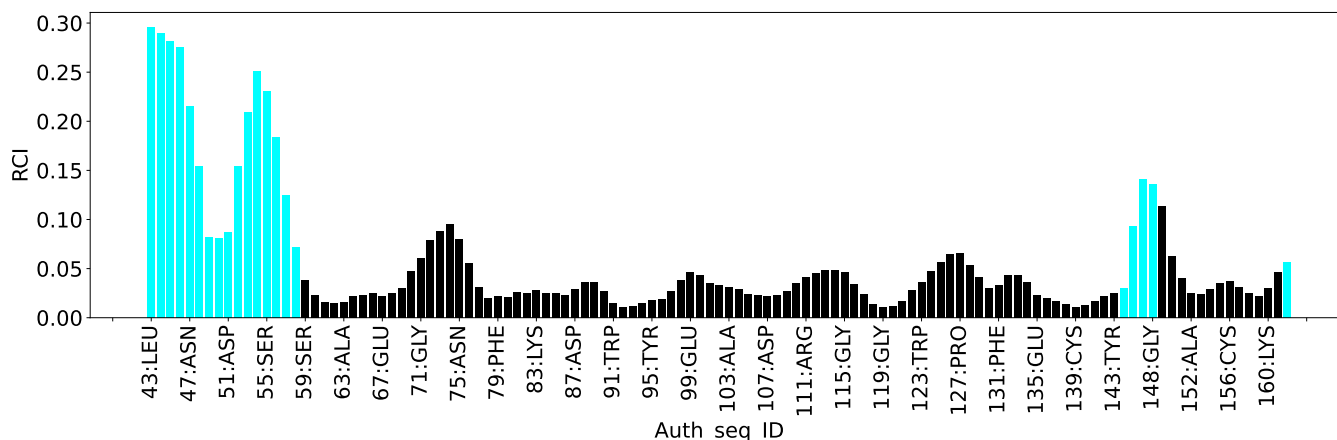
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	123	TRP	CZ3	1000.00	113.48 – 129.28	556.1
1	A	109	LYS	HE3	0.99	1.92 – 3.89	-9.7
1	A	109	LYS	HD2	0.22	0.58 – 2.64	-6.8
1	A	109	LYS	HD3	0.22	0.54 – 2.65	-6.5
1	A	143	TYR	HB3	0.65	0.93 – 4.76	-5.7
1	A	130	TYR	HB3	0.90	0.93 – 4.76	-5.1
1	A	130	TYR	HB2	1.07	1.09 – 4.72	-5.1

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1993
Intra-residue ($ i-j =0$)	469
Sequential ($ i-j =1$)	524
Medium range ($ i-j >1$ and $ i-j <5$)	180
Long range ($ i-j \geq 5$)	764
Inter-chain	0
Hydrogen bond restraints	56
Disulfide bond restraints	0
Total dihedral-angle restraints	175
Number of unmapped restraints	0
Number of restraints per residue	15.7
Number of long range restraints per residue ¹	5.9

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)	12.6	0.2
0.2-0.5 (Medium)	10.8	0.5
>0.5 (Large)	50.2	4.35

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)	8.4	7.34
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

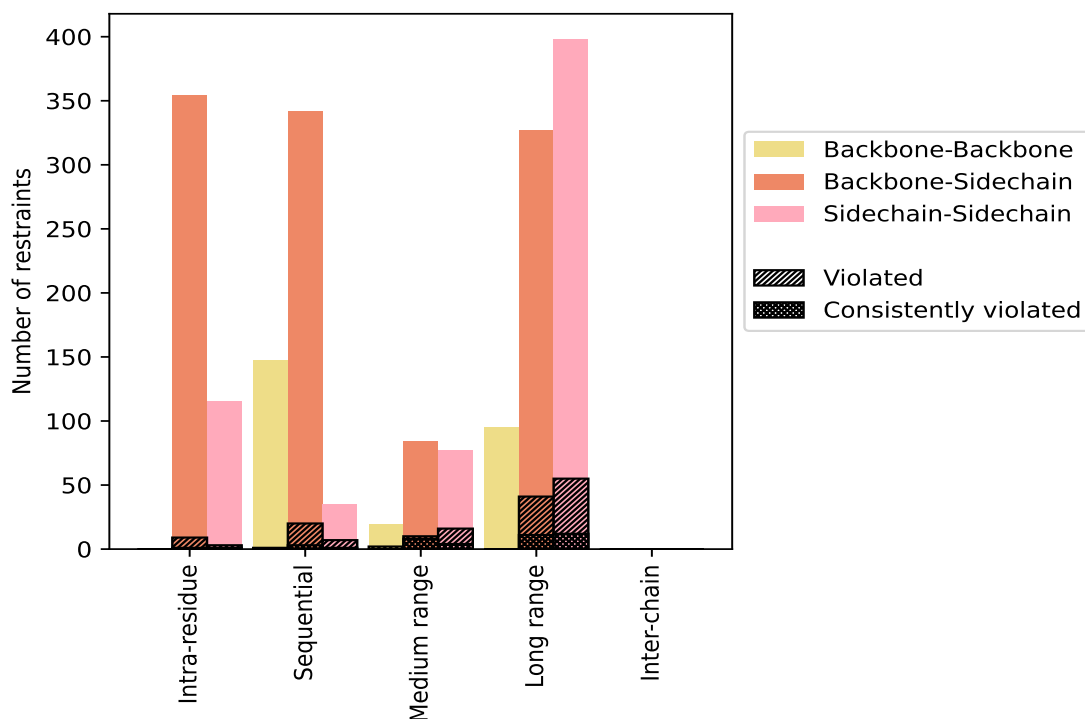
9.1 Summary of distance violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	469	23.5	12	2.6	0.6	2	0.4	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	354	17.8	9	2.5	0.5	1	0.3	0.1
Sidechain-Sidechain	115	5.8	3	2.6	0.2	1	0.9	0.1
Sequential ($i-j =1$)	524	26.3	28	5.3	1.4	4	0.8	0.2
Backbone-Backbone	147	7.4	1	0.7	0.1	0	0.0	0.0
Backbone-Sidechain	342	17.2	20	5.8	1.0	3	0.9	0.2
Sidechain-Sidechain	35	1.8	7	20.0	0.4	1	2.9	0.1
Medium range ($i-j >1$ & $i-j <5$)	180	9.0	28	15.6	1.4	12	6.7	0.6
Backbone-Backbone	19	1.0	2	10.5	0.1	0	0.0	0.0
Backbone-Sidechain	84	4.2	10	11.9	0.5	8	9.5	0.4
Sidechain-Sidechain	77	3.9	16	20.8	0.8	4	5.2	0.2
Long range ($i-j \geq 5$)	764	38.3	89	11.6	4.5	22	2.9	1.1
Backbone-Backbone	95	4.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	271	13.6	34	12.5	1.7	10	3.7	0.5
Sidechain-Sidechain	398	20.0	55	13.8	2.8	12	3.0	0.6
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	56	2.8	7	12.5	0.4	1	1.8	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1993	100.0	164	8.2	8.2	41	2.1	2.1
Backbone-Backbone	261	13.1	3	1.1	0.2	0	0.0	0.0
Backbone-Sidechain	1107	55.5	80	7.2	4.0	23	2.1	1.2
Sidechain-Sidechain	625	31.4	81	13.0	4.1	18	2.9	0.9

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	5	11	17	37	0	70	1.1	3.32	0.87	0.96
2	2	12	14	49	0	77	1.31	4.3	0.97	1.22
3	5	14	16	56	0	91	1.21	4.28	1.01	0.96
4	3	9	16	48	0	76	1.14	4.2	0.92	0.96
5	3	11	16	50	0	80	1.18	4.24	1.01	0.88
6	4	15	15	46	0	80	1.31	4.35	1.03	1.15
7	6	9	15	42	0	72	1.19	4.28	0.97	0.9
8	8	8	19	39	0	74	1.11	3.43	0.89	0.86
9	3	10	21	41	0	75	1.2	4.23	0.92	0.95
10	2	14	16	50	0	82	1.29	4.34	0.99	1.04

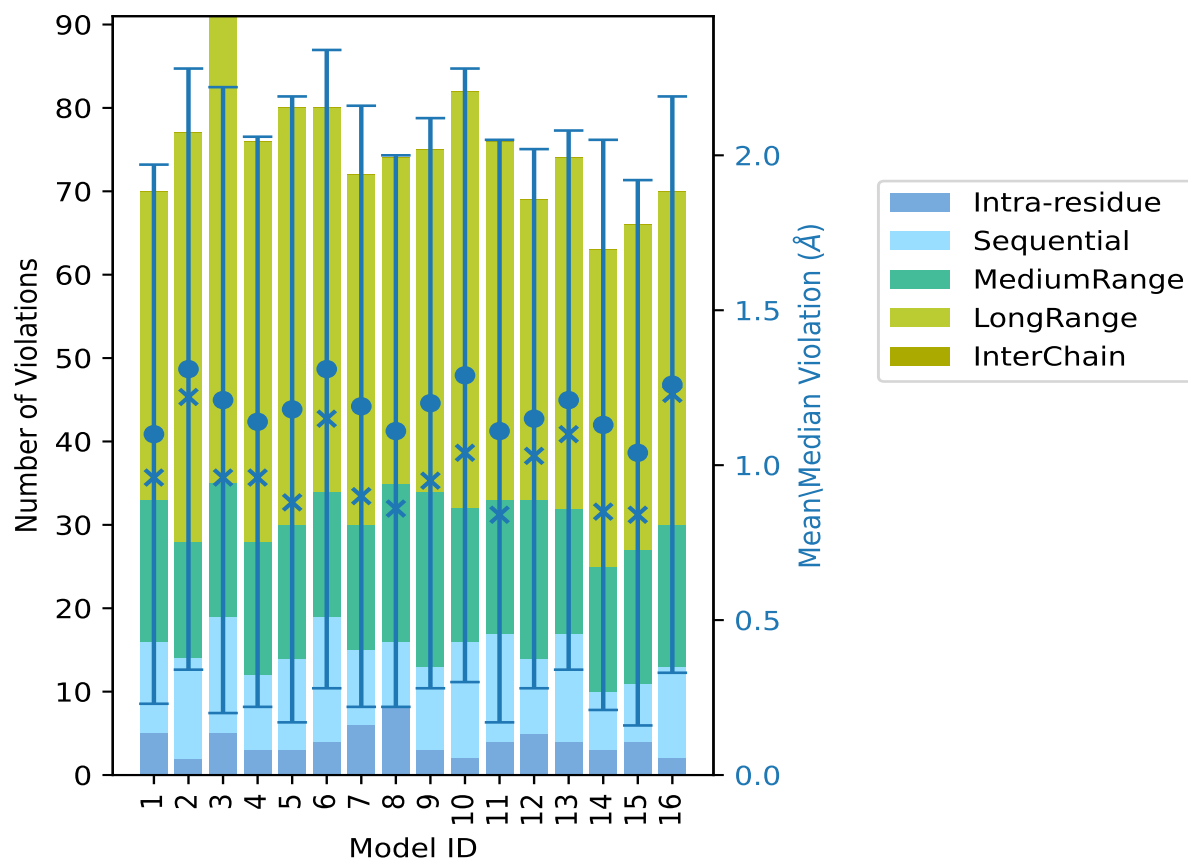
Continued on next page...

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	4	13	16	43	0	76	1.11	3.95	0.94	0.84
12	5	9	19	36	0	69	1.15	3.72	0.87	1.03
13	4	13	15	42	0	74	1.21	3.39	0.87	1.1
14	3	7	15	38	0	63	1.13	3.73	0.92	0.85
15	4	7	16	39	0	66	1.04	3.09	0.88	0.84
16	2	11	17	40	0	70	1.26	3.68	0.93	1.23

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

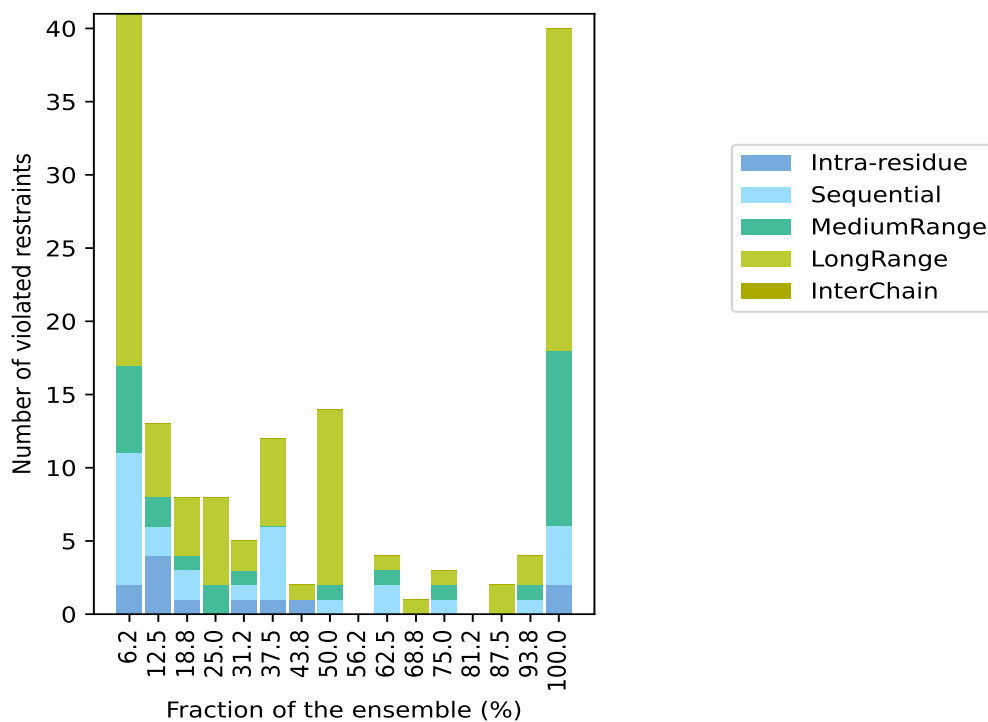
9.3 Distance violation statistics for the ensemble

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, 1780(IR:457, SQ:496, MR:152, LR:675, 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	%
2	9	6	24	0	41	1	6.2
4	2	2	5	0	13	2	12.5
1	2	1	4	0	8	3	18.8
0	0	2	6	0	8	4	25.0
1	1	1	2	0	5	5	31.2
1	5	0	6	0	12	6	37.5
1	0	0	1	0	2	7	43.8
0	1	1	12	0	14	8	50.0
0	0	0	0	0	0	9	56.2
0	2	1	1	0	4	10	62.5
0	0	0	1	0	1	11	68.8
0	1	1	1	0	3	12	75.0
0	0	0	0	0	0	13	81.2
0	0	0	2	0	2	14	87.5
0	1	1	2	0	4	15	93.8
2	4	12	22	0	40	16	100.0

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

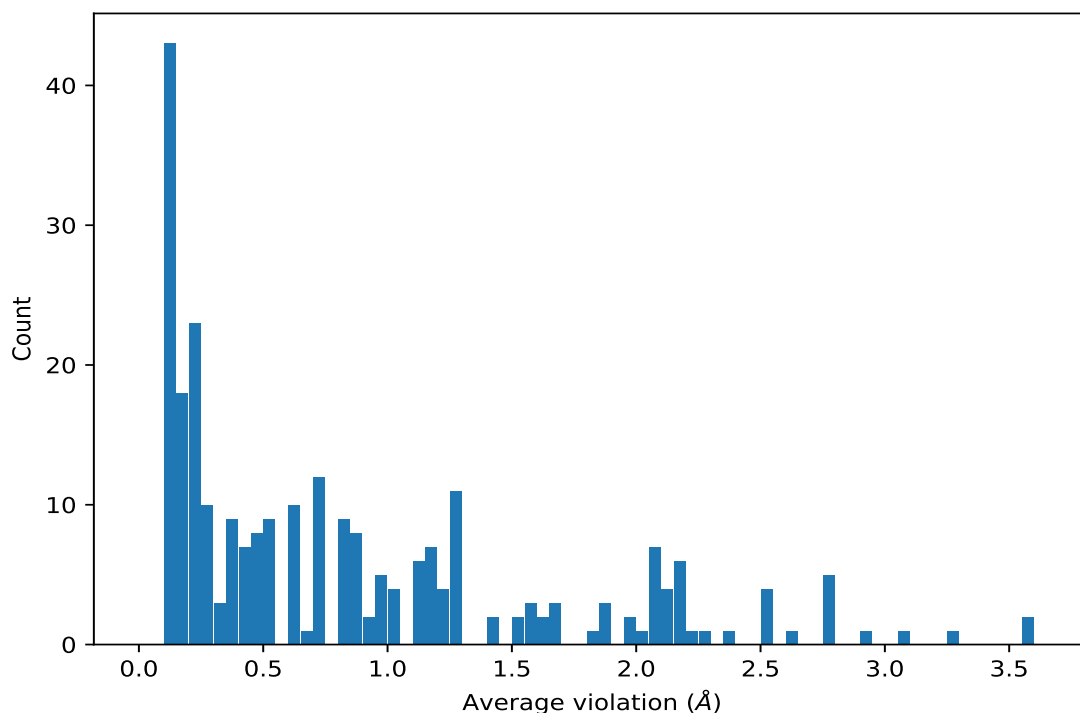
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,891)	1:96:A:HIS:HA	1:131:A:PHE:HE2	16	3.27	0.35	3.28
(1,51)	1:68:A:TYR:HD2	1:70:A:LEU:H	16	2.77	0.17	2.78
(1,835)	1:63:A:ALA:HB1	1:79:A:PHE:HD2	16	2.76	0.17	2.72
(1,835)	1:63:A:ALA:HB2	1:79:A:PHE:HD2	16	2.76	0.17	2.72
(1,835)	1:63:A:ALA:HB3	1:79:A:PHE:HD2	16	2.76	0.17	2.72
(1,73)	1:77:A:ILE:H	1:79:A:PHE:HD2	16	2.36	0.14	2.37
(1,258)	1:142:A:TYR:HD2	1:151:A:ARG:H	16	2.25	0.16	2.26
(1,19)	1:64:A:SER:H	1:79:A:PHE:HD2	16	2.23	0.13	2.23
(1,1652)	1:68:A:TYR:HE2	1:70:A:LEU:HD11	16	2.17	0.25	2.16
(1,1652)	1:68:A:TYR:HE2	1:70:A:LEU:HD12	16	2.17	0.25	2.16
(1,1652)	1:68:A:TYR:HE2	1:70:A:LEU:HD13	16	2.17	0.25	2.16
(1,1652)	1:68:A:TYR:HE2	1:70:A:LEU:HD21	16	2.17	0.25	2.16
(1,1652)	1:68:A:TYR:HE2	1:70:A:LEU:HD22	16	2.17	0.25	2.16
(1,1652)	1:68:A:TYR:HE2	1:70:A:LEU:HD23	16	2.17	0.25	2.16
(1,1086)	1:131:A:PHE:HE2	1:136:A:ILE:HG21	16	2.12	0.17	2.09
(1,1086)	1:131:A:PHE:HE2	1:136:A:ILE:HG22	16	2.12	0.17	2.09

Continued on next page...

Continued from previous page...

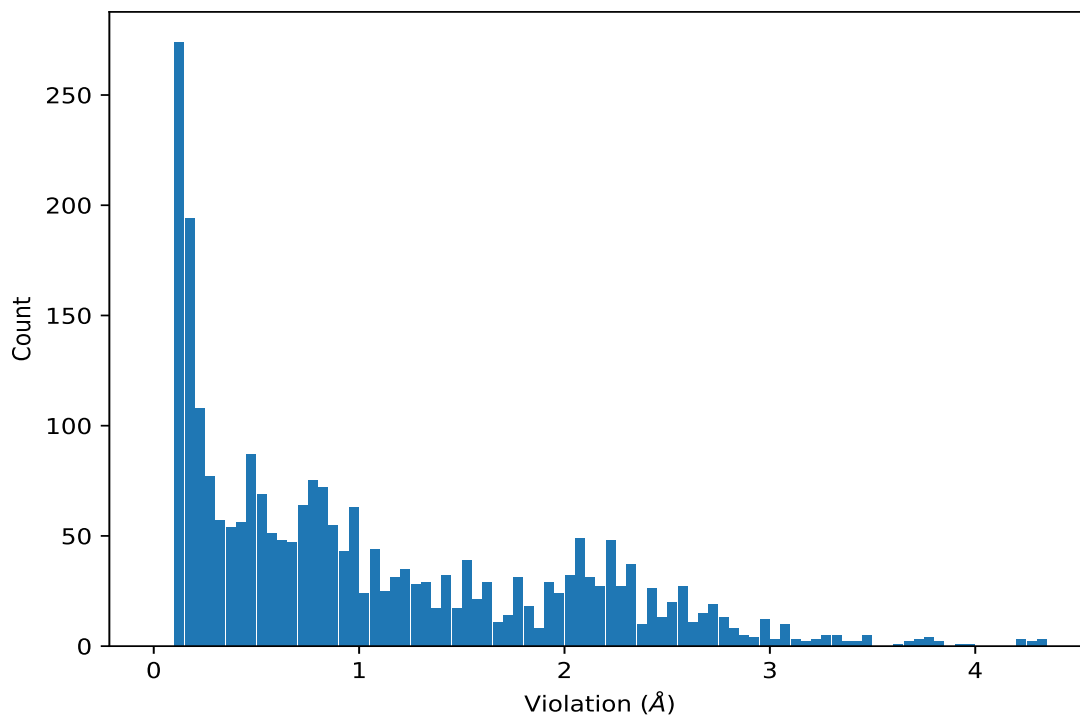
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1086)	1:131:A:PHE:HE2	1:136:A:ILE:HG23	16	2.12	0.17	2.09
(1,790)	1:64:A:SER:HA	1:79:A:PHE:HD2	16	2.1	0.12	2.1
(1,937)	1:68:A:TYR:HD1	1:76:A:LEU:HD21	16	2.08	0.66	2.41

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)
(1,333)	1:109:A:LYS:H	1:140:A:PHE:HE2	6	4.35
(1,333)	1:109:A:LYS:H	1:140:A:PHE:HE2	10	4.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:109:A:LYS:H	1:140:A:PHE:HE2	2	4.3
(1,333)	1:109:A:LYS:H	1:140:A:PHE:HE2	3	4.28
(1,333)	1:109:A:LYS:H	1:140:A:PHE:HE2	7	4.28
(1,333)	1:109:A:LYS:H	1:140:A:PHE:HE2	5	4.24
(1,333)	1:109:A:LYS:H	1:140:A:PHE:HE2	9	4.23
(1,333)	1:109:A:LYS:H	1:140:A:PHE:HE2	4	4.2
(1,891)	1:96:A:HIS:HA	1:131:A:PHE:HE2	11	3.95
(1,1222)	1:108:A:SER:HA	1:140:A:PHE:HE2	6	3.92

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

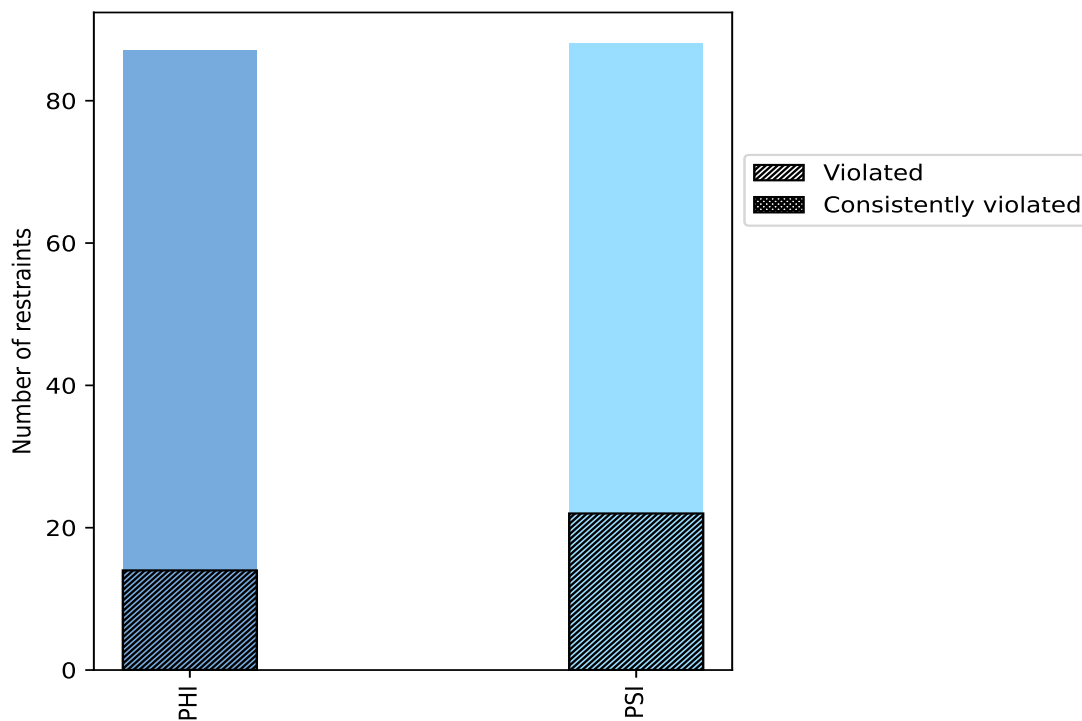
10.1 Summary of dihedral-angle violations [i](#)

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
PHI	87	49.7	14	16.1	8.0	0	0.0	0.0
PSI	88	50.3	22	25.0	12.6	0	0.0	0.0
Total	175	100.0	36	20.6	20.6	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](#)



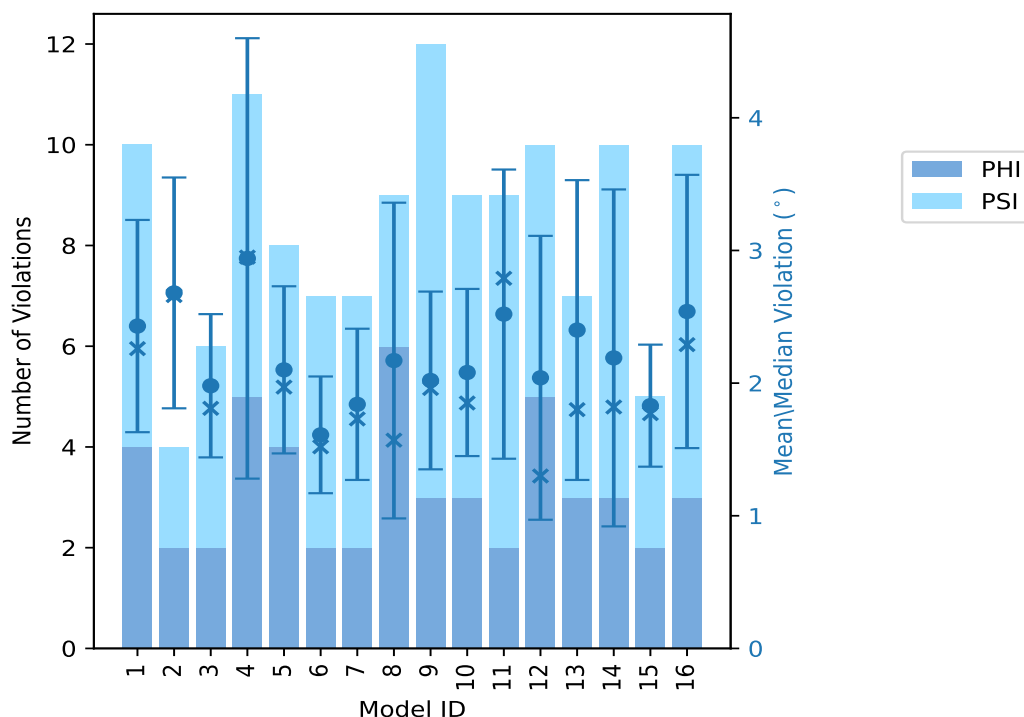
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	4	6	10	2.43	3.87	0.8	2.26
2	2	2	4	2.68	3.73	0.87	2.66
3	2	4	6	1.98	2.74	0.54	1.81
4	5	6	11	2.94	7.34	1.66	2.95
5	4	4	8	2.1	2.99	0.63	1.97
6	2	5	7	1.61	2.21	0.44	1.52
7	2	5	7	1.84	2.84	0.57	1.73
8	6	3	9	2.17	4.23	1.19	1.57
9	3	9	12	2.02	3.2	0.67	1.96
10	3	6	9	2.08	3.01	0.63	1.85
11	2	7	9	2.52	3.99	1.09	2.79
12	5	5	10	2.04	3.82	1.07	1.3
13	3	4	7	2.4	4.47	1.13	1.8
14	3	7	10	2.19	5.3	1.27	1.82
15	2	3	5	1.83	2.58	0.46	1.77
16	3	7	10	2.54	4.88	1.03	2.29

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
6	7	13	1	6.2
2	3	5	2	12.5
1	2	3	3	18.8
2	0	2	4	25.0
0	4	4	5	31.2
0	4	4	6	37.5
1	0	1	7	43.8
0	0	0	8	50.0
1	1	2	9	56.2
0	0	0	10	62.5
0	1	1	11	68.8

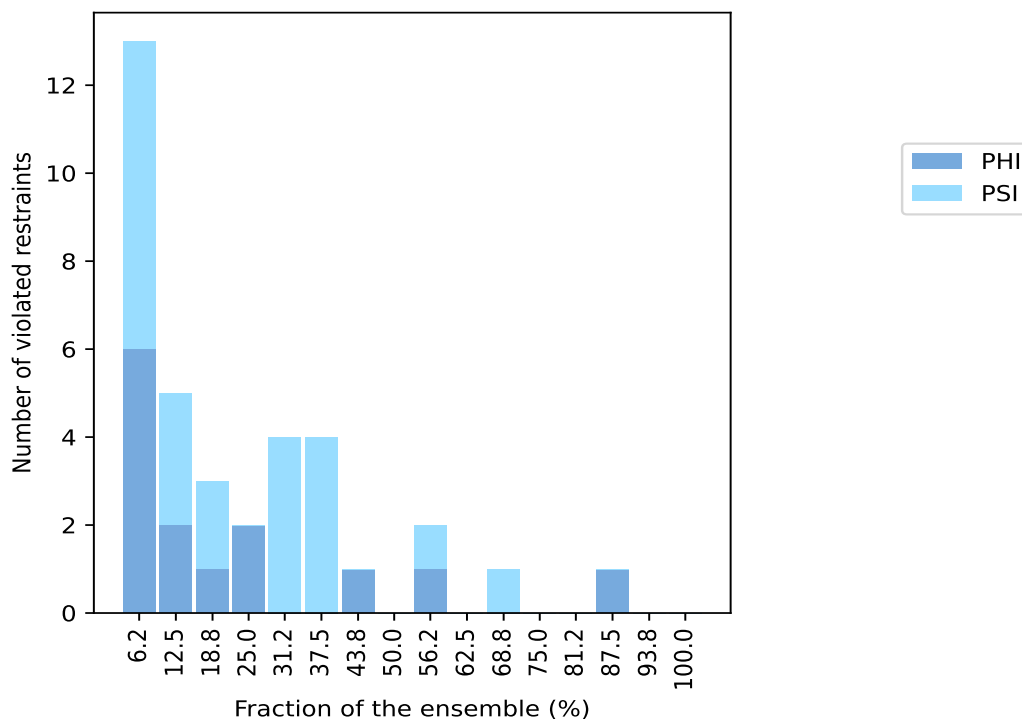
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	75.0
0	0	0	13	81.2
1	0	1	14	87.5
0	0	0	15	93.8
0	0	0	16	100.0

¹ Number of models with violations

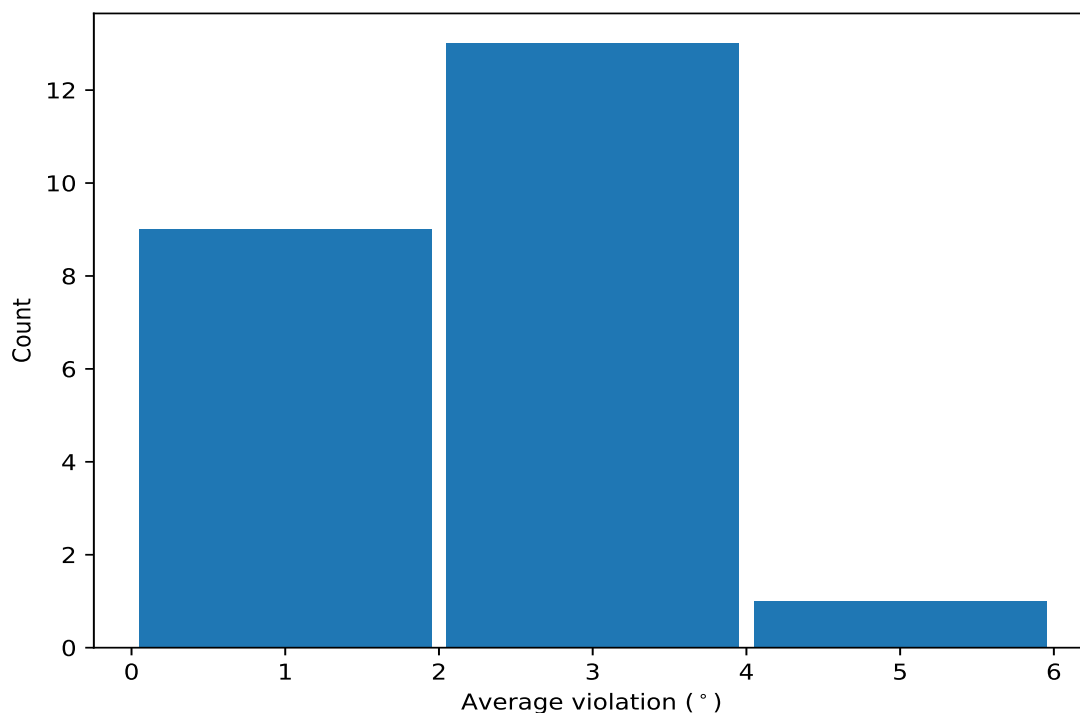
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

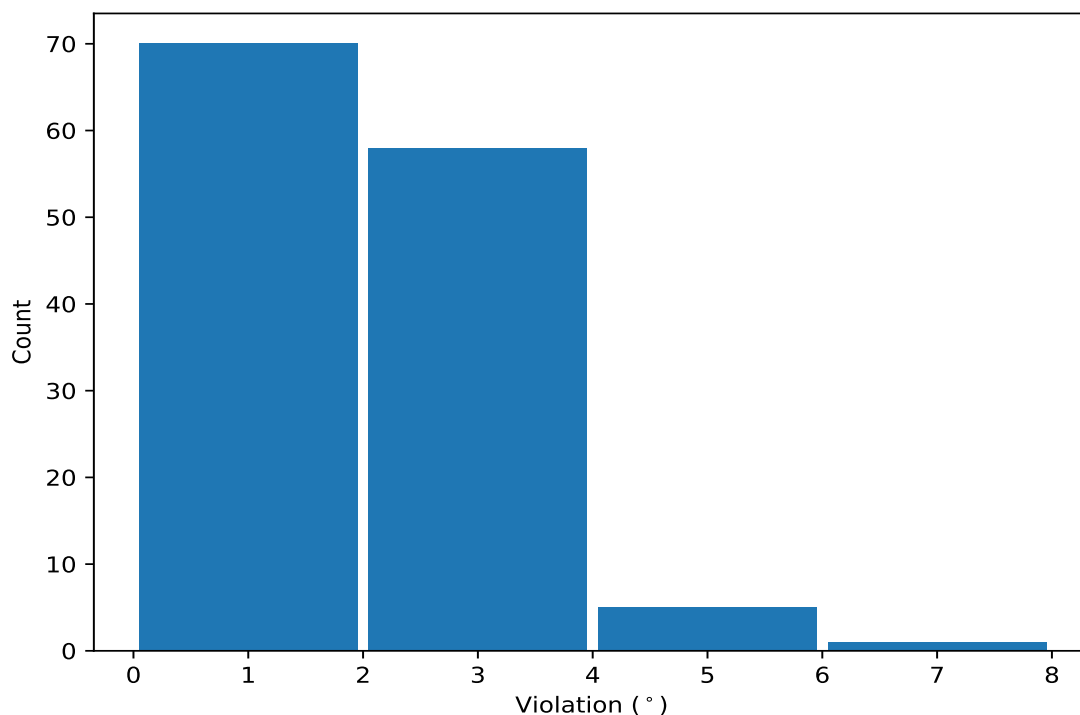
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,162)	1:156:A:CYS:C	1:157:A:ILE:N	1:157:A:ILE:CA	1:157:A:ILE:C	14	2.59	0.9	2.9
(1,123)	1:131:A:PHE:N	1:131:A:PHE:CA	1:131:A:PHE:C	1:132:A:MET:N	11	2.14	0.78	2.15
(1,67)	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	1:100:A:ASN:N	9	2.52	1.23	2.09
(1,114)	1:124:A:ARG:C	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	9	2.11	0.6	2.2
(1,86)	1:109:A:LYS:C	1:110:A:ASN:N	1:110:A:ASN:CA	1:110:A:ASN:C	7	1.99	0.85	1.7
(1,19)	1:68:A:TYR:N	1:68:A:TYR:CA	1:68:A:TYR:C	1:69:A:THR:N	6	2.86	0.82	2.82
(1,87)	1:110:A:ASN:N	1:110:A:ASN:CA	1:110:A:ASN:C	1:111:A:ARG:N	6	2.65	0.88	2.46
(1,65)	1:97:A:ILE:N	1:97:A:ILE:CA	1:97:A:ILE:C	1:98:A:ASP:N	6	2.33	1.21	1.81
(1,133)	1:137:A:LYS:N	1:137:A:LYS:CA	1:137:A:LYS:C	1:138:A:ILE:N	6	1.58	0.42	1.56
(1,149)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:LEU:N	5	2.67	1.1	2.75

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 (°)
(1,3)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:SER:N	4	7.34
(1,81)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:SER:N	14	5.3
(1,67)	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	1:100:A:ASN:N	16	4.88
(1,65)	1:97:A:ILE:N	1:97:A:ILE:CA	1:97:A:ILE:C	1:98:A:ASP:N	13	4.47
(1,149)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:LEU:N	4	4.25
(1,162)	1:156:A:CYS:C	1:157:A:ILE:N	1:157:A:ILE:CA	1:157:A:ILE:C	8	4.23
(1,19)	1:68:A:TYR:N	1:68:A:TYR:CA	1:68:A:TYR:C	1:69:A:THR:N	11	3.99
(1,87)	1:110:A:ASN:N	1:110:A:ASN:CA	1:110:A:ASN:C	1:111:A:ARG:N	1	3.87
(1,67)	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	1:100:A:ASN:N	12	3.82
(1,68)	1:99:A:GLU:C	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	16	3.74