wwPDB NMR Structure Validation Summary Report

Dec 24, 2024 – 04:58 PM EST

PDB ID	:	2LOX
BMRB ID	:	18229
Title	:	NMR structure of the complex between the PH domain of the Tfb1 subunit from TFIIH and Rad2
Authors	:	Lafrance-Vanasse, J.; Legault, P.; Omichinski, J.
Deposited on	:	2012-01-27

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 (i) 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 (i)) were used in the production of this report:

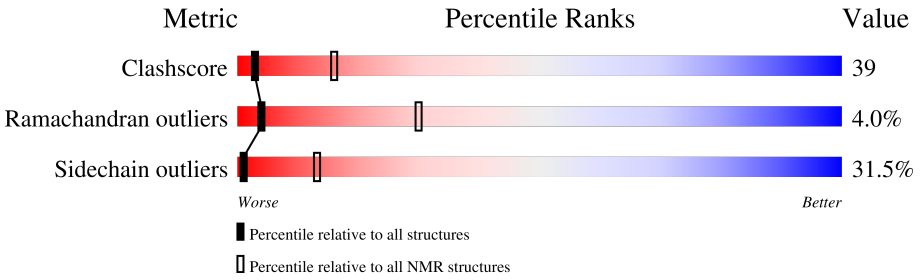
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	119	32% 45% 10% • 9% •
2	B	52	38% 62%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:3-A:51, A:58-A:64, A:86-A:114 (85)	0.23	13
2	A:66-A:84 (19)	1.07	12

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 and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2132 atoms, of which 1072 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA polymerase II transcription factor B subunit 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	115	1820	559	919	161	176	5	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP P32776
A	116	GLY	-	expression tag	UNP P32776
A	117	ASN	-	expression tag	UNP P32776
A	118	SER	-	expression tag	UNP P32776
A	119	SER	-	expression tag	UNP P32776

- Molecule 2 is a protein called DNA repair protein RAD2.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	20	312	100	153	22	37	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	640	GLY	-	expression tag	UNP P07276
B	641	SER	-	expression tag	UNP P07276
B	691	TYR	-	expression tag	UNP P07276

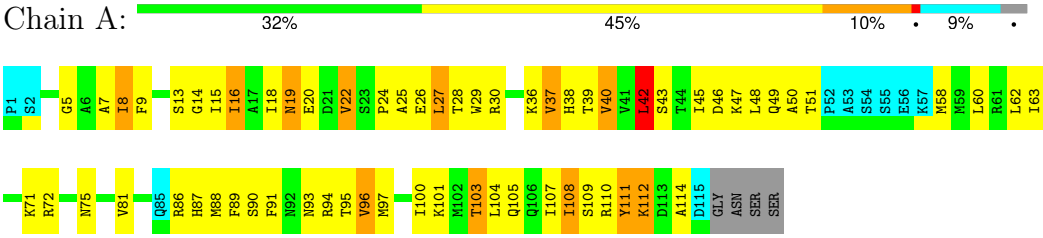
4 Residue-property plots

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.

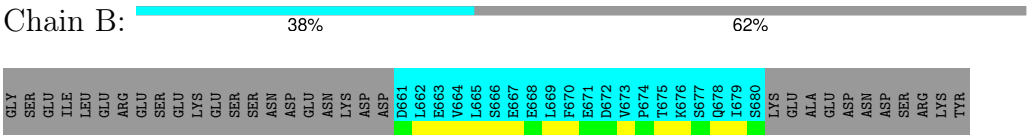
• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A:



• Molecule 2: DNA repair protein RAD2

Chain B:

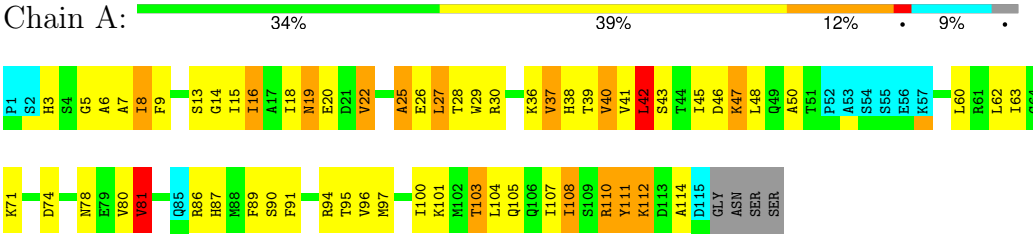


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A:



• Molecule 2: DNA repair protein RAD2

Chain B:


GLY
SER
GLU
ILE
LEU
GLU
ARG
GLU
SER
GLU
LYS
GLU
SER
SER
ASN
ASP
GLU
ASN
LYS
ASP
ASP
D661
L662
E663
V664
L665
S666
E667
E668
L669
F670
E671
D672
V673
P674
T675
K676
S677
Q678
I679
S680
LYS
GLU
ALA
GLU
ASP
ASN
ASP
SER
ARG
LYS
TYR

5 Refinement protocol and experimental data overview

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

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
CNS	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	1958
Number of shifts mapped to atoms	1706
Number of unparsed shifts	0
Number of shifts with mapping errors	252
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality

6.1 Standard geometry

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	820	839	836	65±6
2	B	0	0	0	0±0
All	All	16400	16780	16720	1293

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 39.

5 of 209 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD11	1:A:104:LEU:HD13	0.99	1.34	1	18
1:A:107:ILE:HG22	1:A:111:TYR:CE1	0.85	2.07	7	20
1:A:16:ILE:HD11	1:A:89:PHE:CD2	0.84	2.06	19	9
1:A:16:ILE:HD11	1:A:89:PHE:CD1	0.84	2.06	13	11
1:A:107:ILE:HG22	1:A:111:TYR:HE1	0.83	1.33	7	20

6.3 Torsion angles

6.3.1 Protein backbone

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	104/119 (87%)	85±2 (82±2%)	14±2 (14±2%)	4±1 (4±1%)	4 30
2	B	0	-	-	-	-
All	All	2080/3420 (61%)	1708 (82%)	289 (14%)	83 (4%)	4 30

5 of 13 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	71	LYS	18
1	A	42	LEU	13
1	A	75	ASN	11
1	A	25	ALA	10
1	A	78	ASN	8

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	93/106 (88%)	64±4 (68±4%)	29±4 (32±4%)	1 13
2	B	0	-	-	-
All	All	1860/3120 (60%)	1274 (68%)	586 (32%)	1 13

5 of 62 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	16	ILE	20
1	A	22	VAL	20
1	A	36	LYS	20
1	A	37	VAL	20
1	A	39	THR	20

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 93% 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	1958
Number of shifts mapped to atoms	1706
Number of unparsed shifts	0
Number of shifts with mapping errors	252
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 3 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	LEU	HD11	0.855	0.005	2
1	A	48	LEU	HD12	0.855	0.005	2
1	A	48	LEU	HD13	0.855	0.005	2

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 252) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	117	ASN	H	8.317	.	1
1	A	117	ASN	N	118.871	.	1
1	A	118	SER	H	8.329	.	1
1	A	118	SER	N	116.555	.	1
1	A	116	GLY	H	8.217	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	GLY	N	108.816	.	1
1	A	119	SER	H	8.016	.	1
1	A	119	SER	N	123.353	.	1
1	A	118	SER	C	173.789	.	1
1	A	116	GLY	C	174.366	.	1
1	A	117	ASN	C	175.359	.	1
1	A	118	SER	CB	63.939	0.001	1
1	A	118	SER	CA	58.41	0.013	1
1	A	116	GLY	CA	45.802	.	1
1	A	117	ASN	CA	53.229	0.022	1
1	A	117	ASN	CB	39.193	0.012	1
1	A	119	SER	CB	64.719	0.043	1
1	A	119	SER	CA	60.007	0.019	1
1	A	116	GLY	HA3	4.003	0.001	1
1	A	116	GLY	HA2	4.003	0.001	1
1	A	117	ASN	HA	4.852	0.001	1
1	A	117	ASN	HB3	2.9	0.003	2
1	A	117	ASN	HB2	2.822	0.002	2
1	A	118	SER	HA	4.557	0.003	1
1	A	118	SER	HB3	3.931	0.005	2
1	A	118	SER	HB2	3.931	0.005	2
1	A	119	SER	HA	4.306	0.002	1
1	A	119	SER	HB3	3.875	0.002	2
1	A	119	SER	HB2	3.875	0.002	2
1	A	117	ASN	ND2	113.528	.	1
1	A	117	ASN	HD21	7.663	.	1
1	A	117	ASN	HD22	6.941	.	1
1	B	646	ARG	HE	7.272	.	1
1	B	646	ARG	NE	124.512	.	1
1	B	684	GLU	H	8.313	.	1
1	B	684	GLU	N	120.022	.	1
1	B	681	LYS	H	8.42	.	1
1	B	681	LYS	N	124.077	.	1
1	B	644	LEU	H	8.243	.	1
1	B	644	LEU	N	126.349	.	1
1	B	657	ASN	H	8.454	.	1
1	B	657	ASN	N	119.502	.	1
1	B	686	ASN	H	8.37	.	1
1	B	686	ASN	N	119.403	.	1
1	B	645	GLU	H	8.64	.	1
1	B	645	GLU	N	123.191	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	654	ASN	H	8.496	.	1
1	B	654	ASN	N	120.907	.	1
1	B	690	LYS	H	8.124	.	1
1	B	690	LYS	N	122.478	.	1
1	B	653	SER	H	8.409	.	1
1	B	653	SER	N	117.859	.	1
1	B	652	SER	H	8.371	.	1
1	B	652	SER	N	117.099	.	1
1	B	649	GLU	H	8.43	.	1
1	B	649	GLU	N	122.77	.	1
1	B	648	SER	H	8.326	.	1
1	B	648	SER	N	116.353	.	1
1	B	688	SER	H	8.196	.	1
1	B	688	SER	N	116.057	.	1
1	B	647	GLU	H	8.553	.	1
1	B	647	GLU	N	122.357	.	1
1	B	651	GLU	H	8.459	.	1
1	B	651	GLU	N	122.132	.	1
1	B	683	ALA	H	8.244	.	1
1	B	683	ALA	N	124.346	.	1
1	B	683	ALA	C	177.889	.	1
1	B	645	GLU	C	176.413	.	1
1	B	690	LYS	C	176.363	.	1
1	B	643	ILE	C	176.117	.	1
1	B	656	GLU	C	176.309	.	1
1	B	685	ASP	C	176.312	.	1
1	B	644	LEU	C	176.764	.	1
1	B	652	SER	C	174.62	.	1
1	B	650	LYS	C	176.683	.	1
1	B	646	ARG	C	176.494	.	1
1	B	648	SER	C	174.72	.	1
1	B	660	ASP	C	176.172	.	1
1	B	651	GLU	C	176.624	.	1
1	B	687	ASP	C	176.631	.	1
1	B	647	GLU	C	176.799	.	1
1	B	682	GLU	C	176.442	.	1
1	B	689	ARG	H	8.116	.	1
1	B	689	ARG	N	122.433	.	1
1	B	689	ARG	C	174.692	.	1
1	B	688	SER	C	175.935	.	1
1	B	646	ARG	H	8.307	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	646	ARG	N	121.703	.	1
1	B	682	GLU	H	8.449	.	1
1	B	682	GLU	N	121.869	.	1
1	B	685	ASP	H	8.506	.	1
1	B	685	ASP	N	121.35	.	1
1	B	684	GLU	C	176.09	.	1
1	B	681	LYS	C	176.743	.	1
1	B	684	GLU	CA	56.509	.	1
1	B	684	GLU	CB	30.207	.	1
1	B	681	LYS	CB	33.037	0.0	1
1	B	681	LYS	CA	56.571	0.0	1
1	B	644	LEU	CB	42.369	.	1
1	B	644	LEU	CA	55.212	.	1
1	B	657	ASN	CB	38.994	.	1
1	B	657	ASN	CA	53.394	.	1
1	B	686	ASN	CB	39.218	.	1
1	B	686	ASN	CA	53.954	.	1
1	B	645	GLU	CA	56.974	.	1
1	B	654	ASN	CA	53.414	.	1
1	B	654	ASN	CB	39.171	.	1
1	B	690	LYS	CB	33.021	.	1
1	B	690	LYS	CA	56.203	.	1
1	B	652	SER	CA	58.265	.	1
1	B	652	SER	CB	63.885	.	1
1	B	649	GLU	CA	56.974	.	1
1	B	649	GLU	CB	30.196	.	1
1	B	648	SER	CA	58.679	.	1
1	B	648	SER	CB	63.77	.	1
1	B	688	SER	CA	58.689	.	1
1	B	688	SER	CB	63.591	.	1
1	B	651	GLU	CA	56.722	.	1
1	B	651	GLU	CB	30.229	.	1
1	B	683	ALA	CB	19.346	.	1
1	B	683	ALA	CA	52.68	.	1
1	B	685	ASP	CB	41.143	.	1
1	B	685	ASP	CA	54.347	.	1
1	B	643	ILE	CB	38.518	.	1
1	B	643	ILE	CA	61.194	.	1
1	B	656	GLU	CB	30.3	.	1
1	B	656	GLU	CA	56.864	.	1
1	B	689	ARG	CA	56.228	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	689	ARG	CB	30.57	.	1
1	B	660	ASP	CB	41.226	.	1
1	B	660	ASP	CA	54.605	.	1
1	B	687	ASP	CB	41.166	.	1
1	B	687	ASP	CA	54.842	.	1
1	B	647	GLU	CB	30.123	.	1
1	B	647	GLU	CA	56.974	.	1
1	B	650	LYS	CB	33.225	.	1
1	B	650	LYS	CA	56.443	.	1
1	B	682	GLU	CA	56.858	0.014	1
1	B	682	GLU	CB	30.059	0.013	1
1	B	646	ARG	CB	30.988	.	1
1	B	646	ARG	CA	56.161	.	1
1	B	653	SER	CA	58.293	.	1
1	B	653	SER	CB	63.846	.	1
1	B	653	SER	C	174.407	.	1
1	B	690	LYS	CG	24.521	.	1
1	B	690	LYS	CD	29.046	.	1
1	B	690	LYS	CE	42.471	.	1
1	B	644	LEU	CG	27.089	.	1
1	B	644	LEU	CD2	23.922	.	2
1	B	647	GLU	CG	36.33	.	1
1	B	646	ARG	CG	27.089	.	1
1	B	646	ARG	CD	43.331	.	1
1	B	650	LYS	CE	42.17	.	1
1	B	650	LYS	CD	29.147	.	1
1	B	650	LYS	CG	24.739	.	1
1	B	645	GLU	CG	36.33	.	1
1	B	681	LYS	CE	42.143	0.013	1
1	B	681	LYS	CD	28.975	0.013	1
1	B	681	LYS	CG	24.701	0.0	1
1	B	684	GLU	CG	36.282	.	1
1	B	651	GLU	CG	36.243	.	1
1	B	682	GLU	CG	36.307	0.0	1
1	B	645	GLU	CB	30.123	.	1
1	B	644	LEU	CD1	24.882	.	2
1	B	689	ARG	CD	43.289	.	1
1	B	689	ARG	CG	27.055	.	1
1	B	681	LYS	HA	4.359	0.0	1
1	B	681	LYS	HB3	1.896	0.0	2
1	B	681	LYS	HB2	1.812	0.0	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	681	LYS	HG3	1.479	0.003	2
1	B	681	LYS	HG2	1.48	0.003	2
1	B	681	LYS	HD3	1.728	0.002	1
1	B	681	LYS	HD2	1.728	0.002	1
1	B	681	LYS	HE3	3.038	0.002	2
1	B	681	LYS	HE2	3.038	0.001	2
1	B	682	GLU	HA	4.282	0.002	1
1	B	682	GLU	HB2	2.119	0.004	2
1	B	682	GLU	HB3	1.998	0.002	2
1	B	682	GLU	HG3	2.338	0.001	1
1	B	682	GLU	HG2	2.338	0.001	1
1	B	683	ALA	HA	4.336	.	1
1	B	683	ALA	HB1	1.45	.	1
1	B	683	ALA	HB2	1.45	.	1
1	B	683	ALA	HB3	1.45	.	1
1	B	684	GLU	HB2	2.124	.	2
1	B	684	GLU	HA	4.387	.	1
1	B	684	GLU	HB3	2.004	.	2
1	B	684	GLU	HG2	2.337	.	1
1	B	684	GLU	HG3	2.337	.	1
1	B	685	ASP	HA	4.651	.	1
1	B	685	ASP	HB3	2.762	.	2
1	B	685	ASP	HB2	2.684	.	2
1	B	686	ASN	HA	4.662	.	1
1	B	644	LEU	HA	4.372	.	1
1	B	644	LEU	HB2	1.685	.	1
1	B	644	LEU	HB3	1.685	.	1
1	B	644	LEU	HD11	0.967	.	1
1	B	644	LEU	HD12	0.967	.	1
1	B	644	LEU	HD13	0.967	.	1
1	B	644	LEU	HG	1.685	.	1
1	B	644	LEU	HD21	0.967	.	1
1	B	644	LEU	HD22	0.967	.	1
1	B	644	LEU	HD23	0.967	.	1
1	B	645	GLU	HA	4.314	.	1
1	B	645	GLU	HB3	2.112	.	2
1	B	645	GLU	HB2	2.007	.	2
1	B	645	GLU	HG2	2.338	.	1
1	B	645	GLU	HG3	2.338	.	1
1	B	646	ARG	HA	4.372	.	1
1	B	647	GLU	HA	4.314	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	646	ARG	HB3	1.915	.	2
1	B	646	ARG	HB2	1.825	.	2
1	B	646	ARG	HG2	1.685	.	1
1	B	646	ARG	HG3	1.685	.	1
1	B	646	ARG	HD3	3.254	.	1
1	B	646	ARG	HD2	3.254	.	1
1	B	648	SER	HA	4.444	.	1
1	B	647	GLU	HB3	2.112	.	2
1	B	647	GLU	HB2	2.007	.	2
1	B	647	GLU	HG2	2.338	.	1
1	B	647	GLU	HG3	2.338	.	1
1	B	649	GLU	HA	4.314	.	1
1	B	648	SER	HB2	3.924	.	1
1	B	648	SER	HB3	3.924	.	1
1	B	690	LYS	HA	4.317	.	1
1	B	688	SER	HA	4.406	.	1
1	B	690	LYS	HE3	3.027	.	1
1	B	690	LYS	HE2	3.027	.	1
1	B	690	LYS	HD3	1.702	.	1
1	B	690	LYS	HD2	1.702	.	1
1	B	690	LYS	HG3	1.426	.	1
1	B	690	LYS	HG2	1.426	.	1
1	B	690	LYS	HB3	1.695	.	2
1	B	690	LYS	HB2	1.811	.	2
1	B	689	ARG	HD2	3.192	.	1
1	B	689	ARG	HD3	3.192	.	1
1	B	689	ARG	HG3	1.588	.	1
1	B	689	ARG	HG2	1.588	.	1
1	B	689	ARG	HB2	1.798	.	1
1	B	689	ARG	HB3	1.798	.	1
1	B	689	ARG	HA	4.317	.	1
1	B	688	SER	HB2	3.938	.	1
1	B	688	SER	HB3	3.938	.	1
1	B	654	ASN	ND2	113.243	.	1
1	B	657	ASN	HD22	7.639	.	1
1	B	654	ASN	HD21	6.921	.	1
1	B	657	ASN	ND2	112.704	.	1
1	B	657	ASN	HD21	6.936	.	1
1	B	654	ASN	HD22	7.64	.	1
1	B	686	ASN	ND2	112.412	.	1
1	B	686	ASN	HD22	6.96	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	686	ASN	HD21	7.64	.	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	164	-0.21 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	158	-0.07 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	154	0.05 ± 0.11	None needed (< 0.5 ppm)
^{15}N	153	-0.14 ± 0.24	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 1328 atoms were assigned a chemical shift out of a possible 1441. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	515/519 (99%)	210/210 (100%)	204/208 (98%)	101/101 (100%)
Sidechain	762/847 (90%)	522/549 (95%)	228/262 (87%)	12/36 (33%)
Aromatic	51/75 (68%)	27/37 (73%)	23/31 (74%)	1/7 (14%)
Overall	1328/1441 (92%)	759/796 (95%)	455/501 (91%)	114/144 (79%)

7.1.4 Statistically unusual chemical shifts

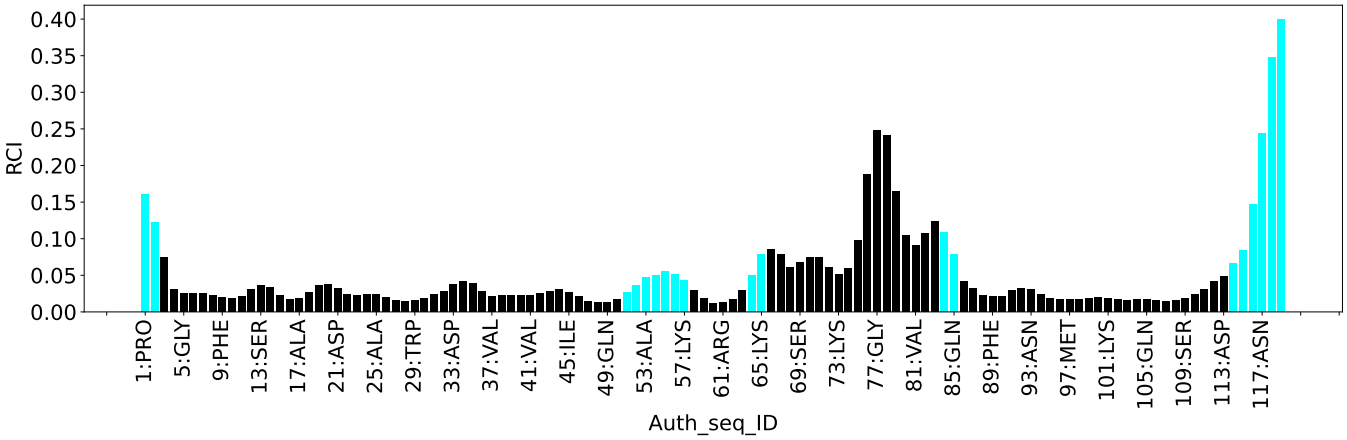
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	646	ARG	NE	124.51	76.53 – 92.65	24.8
1	A	10	GLU	HG3	0.61	1.20 – 3.30	-7.8
1	A	89	PHE	CZ	117.69	121.82 – 136.66	-7.8
1	A	10	GLU	HG2	1.11	1.24 – 3.30	-5.6
1	A	101	LYS	CG	19.14	19.35 – 30.45	-5.2

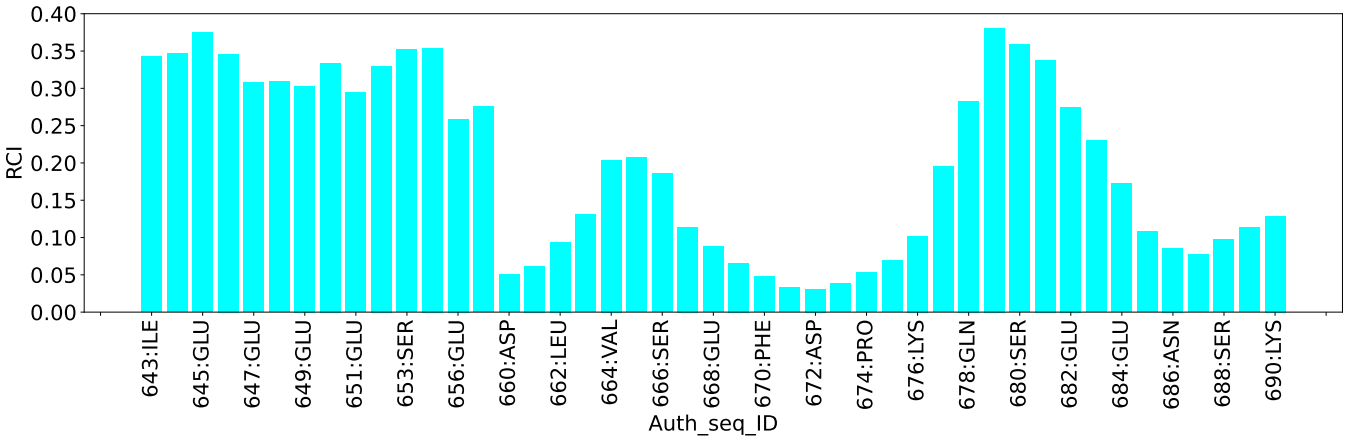
7.1.5 Random Coil Index (RCI) plots

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:



Random coil index (RCI) for chain B:



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	1617
Intra-residue (|i-j|=0)	377
Sequential (|i-j|=1)	409
Medium range (|i-j|>1 and |i-j|<5)	240
Long range (|i-j|≥5)	480
Inter-chain	75
Hydrogen bond restraints	36
Disulfide bond restraints	0
Total dihedral-angle restraints	158
Number of unmapped restraints	0
Number of restraints per residue	10.4
Number of long range restraints per residue[1]	3.0

[1]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)	10.2	0.2
0.2-0.5 (Medium)	1.1	0.49
>0.5 (Large)	0.8	0.86

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)	1.9	1.78
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

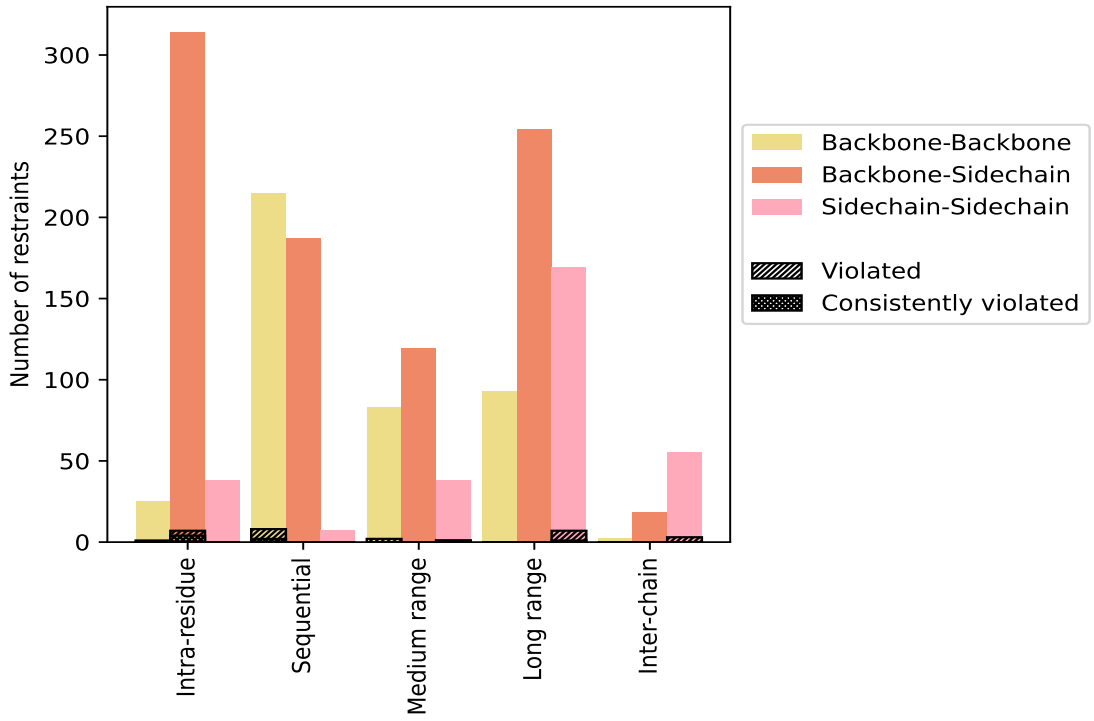
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	377	23.3	8	2.1	0.5	4	1.1	0.2
Backbone-Backbone	25	1.5	1	4.0	0.1	0	0.0	0.0
Backbone-Sidechain	314	19.4	7	2.2	0.4	4	1.3	0.2
Sidechain-Sidechain	38	2.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	409	25.3	8	2.0	0.5	2	0.5	0.1
Backbone-Backbone	215	13.3	8	3.7	0.5	2	0.9	0.1
Backbone-Sidechain	187	11.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	0.4	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	240	14.8	3	1.2	0.2	1	0.4	0.1
Backbone-Backbone	83	5.1	2	2.4	0.1	0	0.0	0.0
Backbone-Sidechain	119	7.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	38	2.4	1	2.6	0.1	1	2.6	0.1
Long range (|i-j|≥5)	480	29.7	7	1.5	0.4	1	0.2	0.1
Backbone-Backbone	93	5.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	218	13.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	169	10.5	7	4.1	0.4	1	0.6	0.1
Inter-chain	75	4.6	3	4.0	0.2	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	1.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	55	3.4	3	5.5	0.2	0	0.0	0.0
Hydrogen bond	36	2.2	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	1617	100.0	29	1.8	1.8	8	0.5	0.5
Backbone-Backbone	418	25.9	11	2.6	0.7	2	0.5	0.1
Backbone-Sidechain	892	55.2	7	0.8	0.4	4	0.4	0.2
Sidechain-Sidechain	307	19.0	11	3.6	0.7	2	0.7	0.1

[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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

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	3	2	2	1	13	0.18	0.67	0.14	0.14
2	6	2	2	4	2	16	0.2	0.54	0.13	0.16
3	5	3	2	2	1	13	0.2	0.86	0.19	0.14
4	7	2	3	2	2	16	0.17	0.66	0.13	0.15
5	5	3	2	2	1	13	0.2	0.86	0.19	0.14
6	6	2	2	1	1	12	0.2	0.72	0.16	0.16
7	6	3	1	1	1	12	0.21	0.86	0.2	0.15
8	5	5	2	2	2	16	0.19	0.86	0.18	0.13
9	6	3	2	1	3	15	0.22	0.86	0.19	0.16
10	4	3	2	2	0	11	0.15	0.21	0.04	0.14

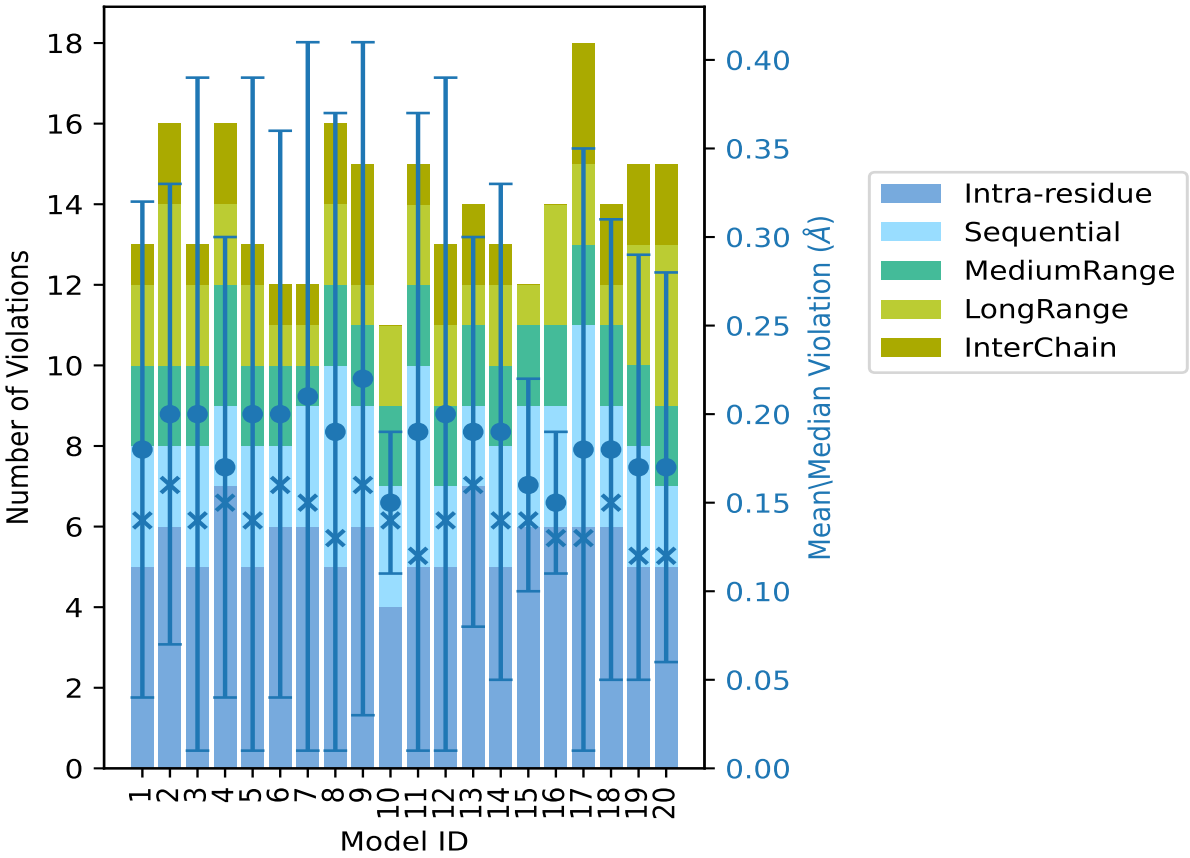
Continued on next page...

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	5	5	2	2	1	15	0.19	0.83	0.18	0.12
12	5	2	2	2	2	13	0.2	0.84	0.19	0.14
13	7	2	2	1	2	14	0.19	0.49	0.11	0.16
14	5	3	2	2	1	13	0.19	0.66	0.14	0.14
15	6	3	2	1	0	12	0.16	0.33	0.06	0.14
16	6	3	2	3	0	14	0.15	0.21	0.04	0.13
17	6	5	2	2	3	18	0.18	0.86	0.17	0.13
18	6	3	2	1	2	14	0.18	0.62	0.13	0.15
19	5	3	2	3	2	15	0.17	0.6	0.12	0.12
20	5	2	2	4	2	15	0.17	0.56	0.11	0.12

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

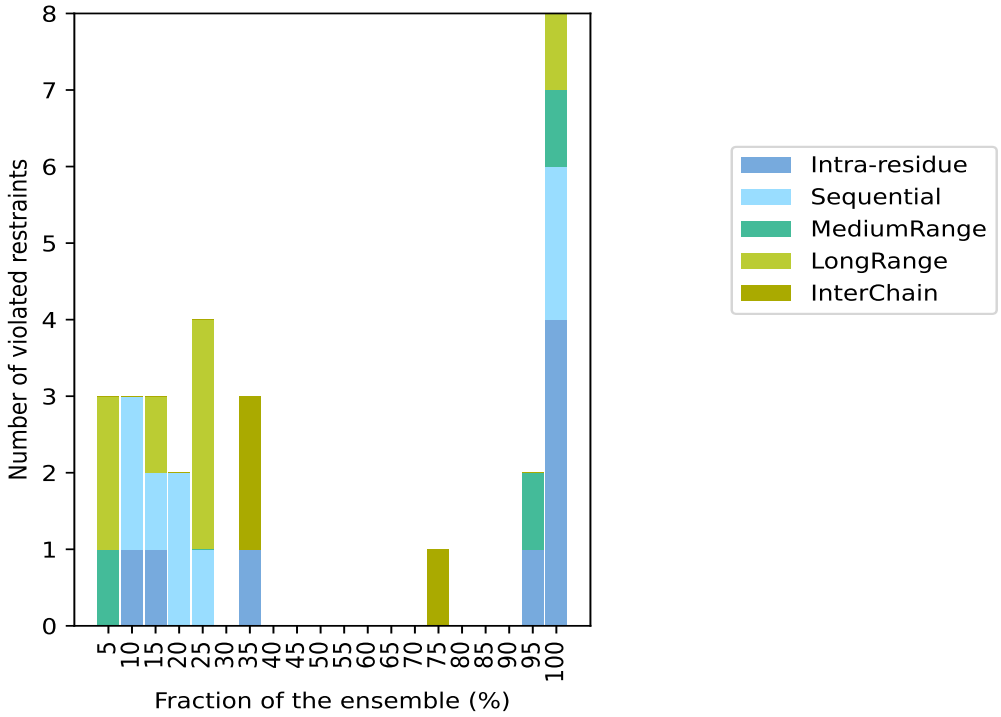
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1552(IR:369, SQ:401, MR:237, LR:473, IC:72) 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]	%
0	0	1	2	0	3	1	5.0
1	2	0	0	0	3	2	10.0
1	1	0	1	0	3	3	15.0
0	2	0	0	0	2	4	20.0
0	1	0	3	0	4	5	25.0
0	0	0	0	0	0	6	30.0
1	0	0	0	2	3	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	1	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
1	0	1	0	0	2	19	95.0
4	2	1	1	0	8	20	100.0

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

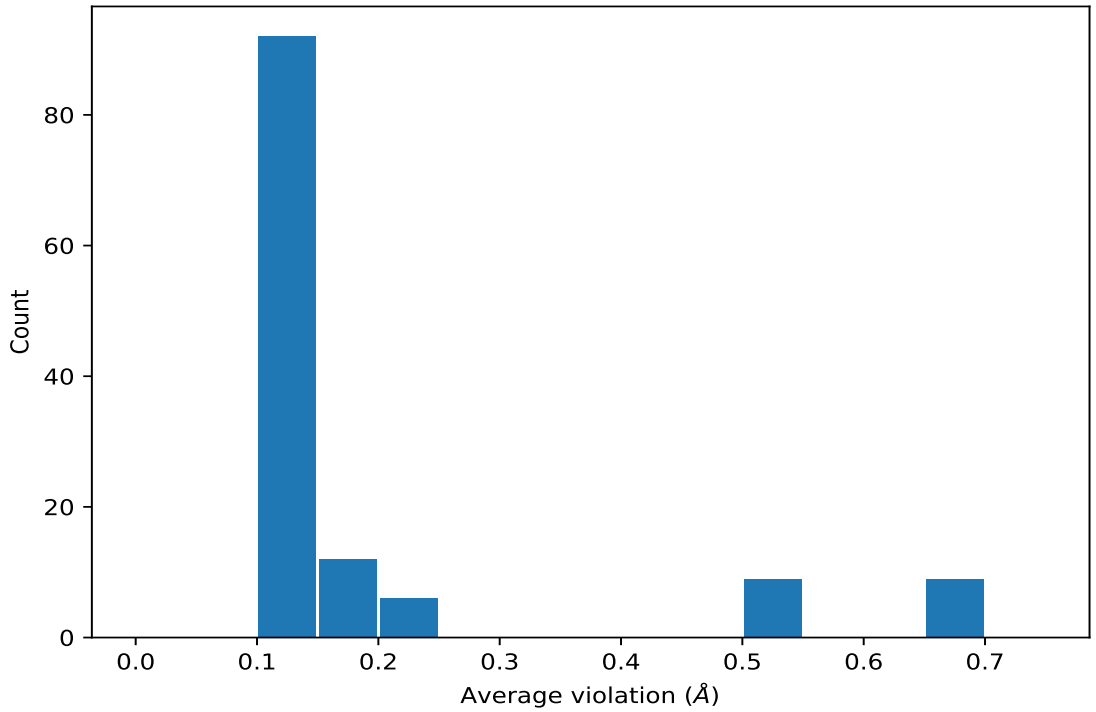
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

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)
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	20	0.22	0.03	0.22
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	20	0.19	0.01	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	20	0.19	0.0	0.19
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	20	0.18	0.0	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	20	0.18	0.01	0.18

Continued on next page...

Continued from previous page...

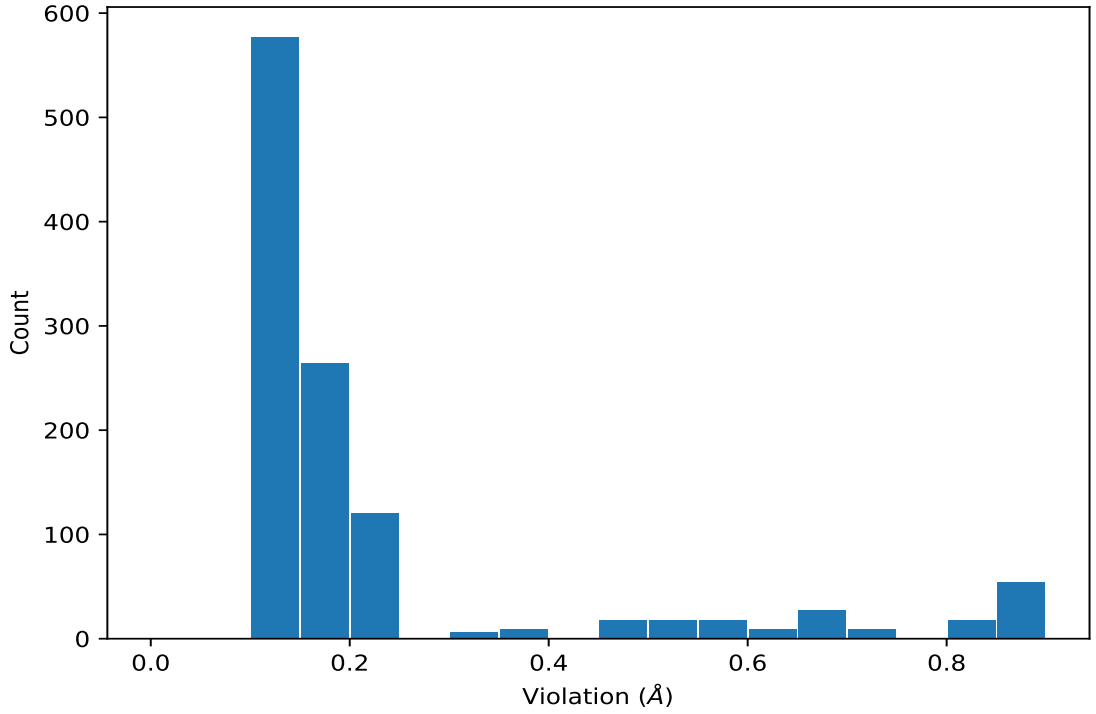
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	20	0.18	0.01	0.18
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	20	0.14	0.0	0.14
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	20	0.12	0.0	0.12
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	20	0.11	0.0	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	19	0.11	0.01	0.11
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	19	0.1	0.0	0.1

[1]Number of violated models, [2]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)
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	9	0.86
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	9	0.86
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	9	0.86
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	9	0.86
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	9	0.86
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	9	0.86
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	9	0.86
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	9	0.86
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	9	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	3	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	3	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	3	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	3	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	3	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	3	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	3	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	3	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	3	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	5	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	5	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	5	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	5	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	5	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	5	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	5	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	5	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	5	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	7	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	7	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	7	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	7	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	7	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	7	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	7	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	7	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	7	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	8	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	8	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	8	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	8	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	8	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	8	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	8	0.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	8	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	8	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	17	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	17	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	17	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	17	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	17	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	17	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	17	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	17	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	17	0.86
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	12	0.84
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	12	0.84
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	12	0.84
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	12	0.84
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	12	0.84
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	12	0.84
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	12	0.84
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	12	0.84
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	12	0.84
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	11	0.83
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	11	0.83
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	11	0.83
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	11	0.83
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	11	0.83
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	11	0.83
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	11	0.83
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	11	0.83
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	11	0.83
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	6	0.72
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	6	0.72
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	6	0.72
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	6	0.72
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	6	0.72
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	6	0.72
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	6	0.72
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	6	0.72
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	6	0.72
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	1	0.67

10 Dihedral-angle violation analysis

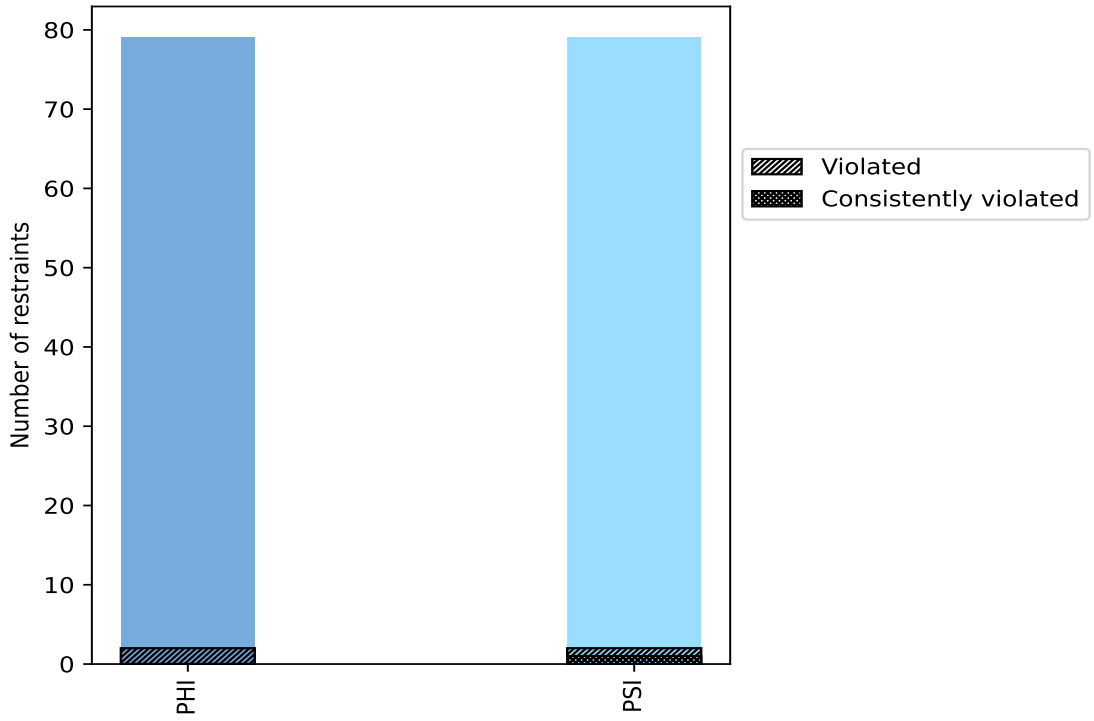
10.1 Summary of dihedral-angle violations

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	79	50.0	2	2.5	1.3	0	0.0	0.0
PSI	79	50.0	2	2.5	1.3	1	1.3	0.6
Total	158	100.0	4	2.5	2.5	1	0.6	0.6

[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



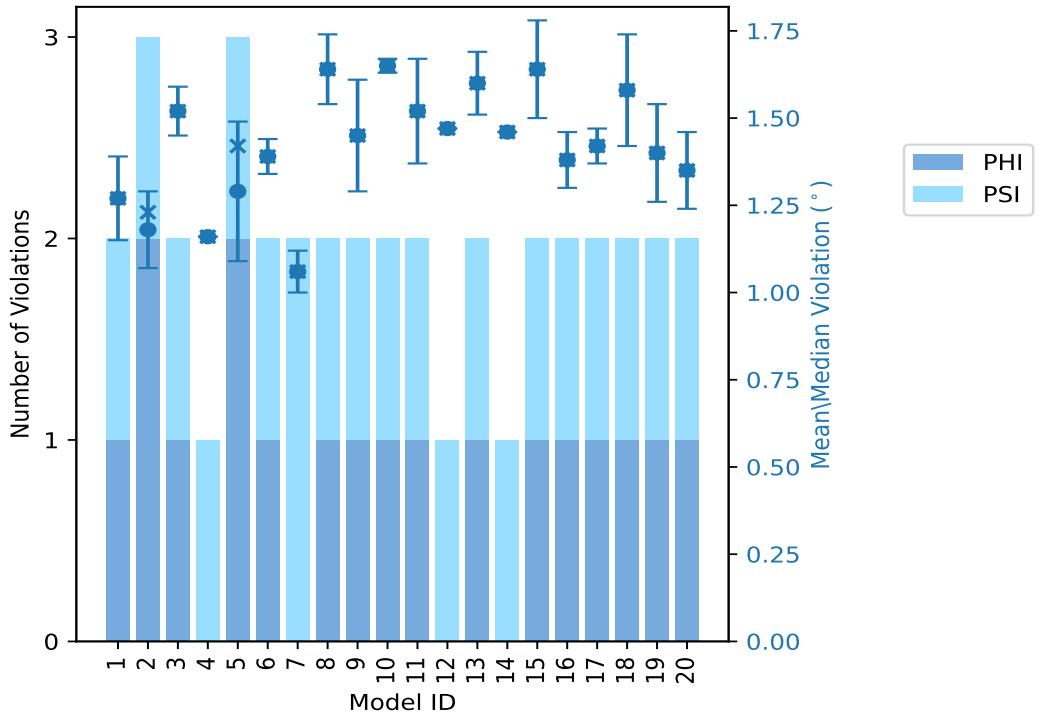
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	1	1	2	1.27	1.39	0.12	1.27
2	2	1	3	1.18	1.28	0.11	1.23
3	1	1	2	1.52	1.59	0.07	1.52
4	0	1	1	1.16	1.16	0.0	1.16
5	2	1	3	1.29	1.45	0.2	1.42
6	1	1	2	1.39	1.44	0.05	1.39
7	0	2	2	1.06	1.12	0.06	1.06
8	1	1	2	1.64	1.74	0.1	1.64
9	1	1	2	1.45	1.61	0.16	1.45
10	1	1	2	1.65	1.67	0.02	1.65
11	1	1	2	1.52	1.68	0.15	1.52
12	0	1	1	1.47	1.47	0.0	1.47
13	1	1	2	1.6	1.69	0.09	1.6
14	0	1	1	1.46	1.46	0.0	1.46
15	1	1	2	1.64	1.78	0.14	1.64
16	1	1	2	1.38	1.47	0.08	1.38
17	1	1	2	1.42	1.47	0.05	1.42
18	1	1	2	1.58	1.74	0.16	1.58
19	1	1	2	1.4	1.54	0.14	1.4
20	1	1	2	1.35	1.46	0.11	1.35

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]	%
0	1	1	1	5.0
1	0	1	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

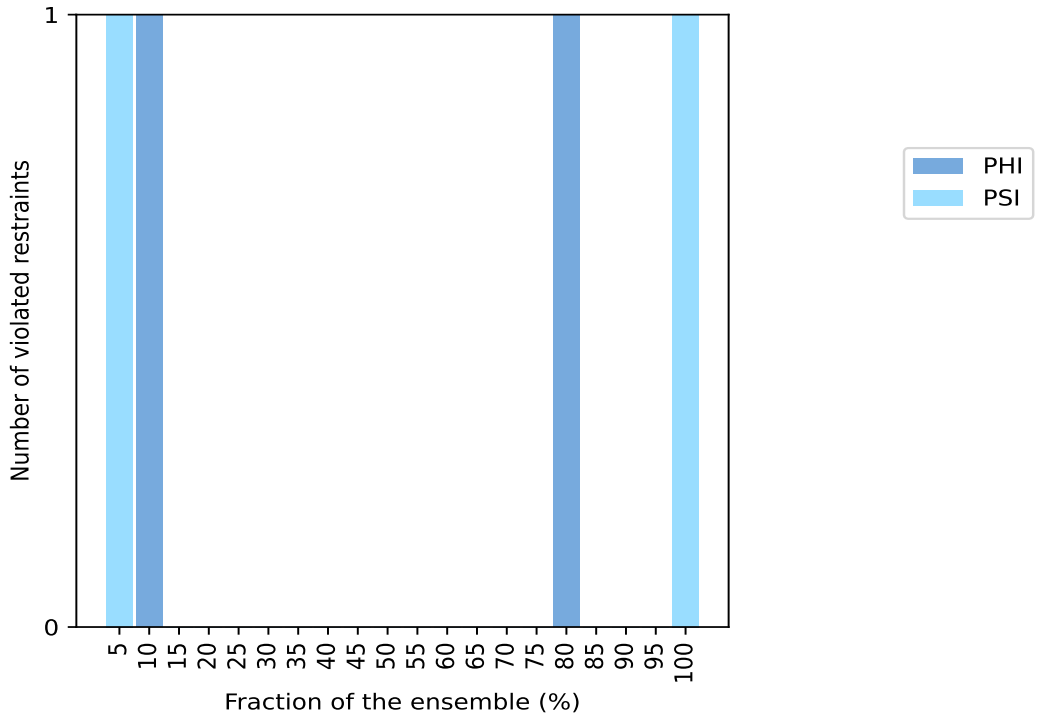
Continued on next page...

Continued from previous page...

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

[1] Number of models with violations

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

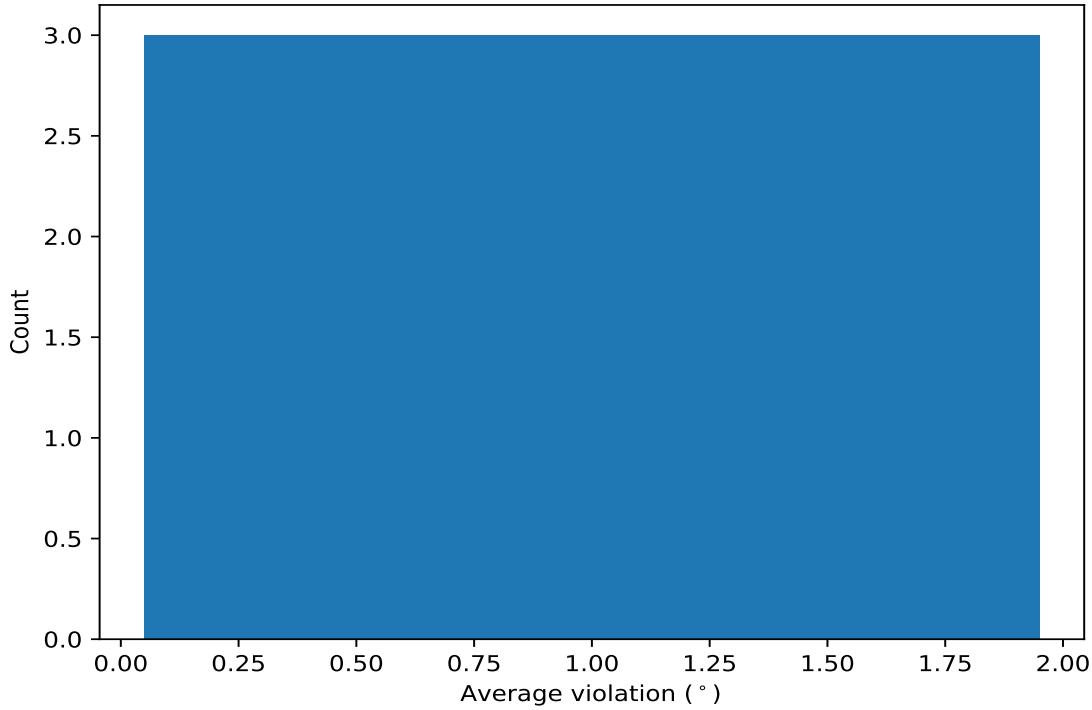


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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.

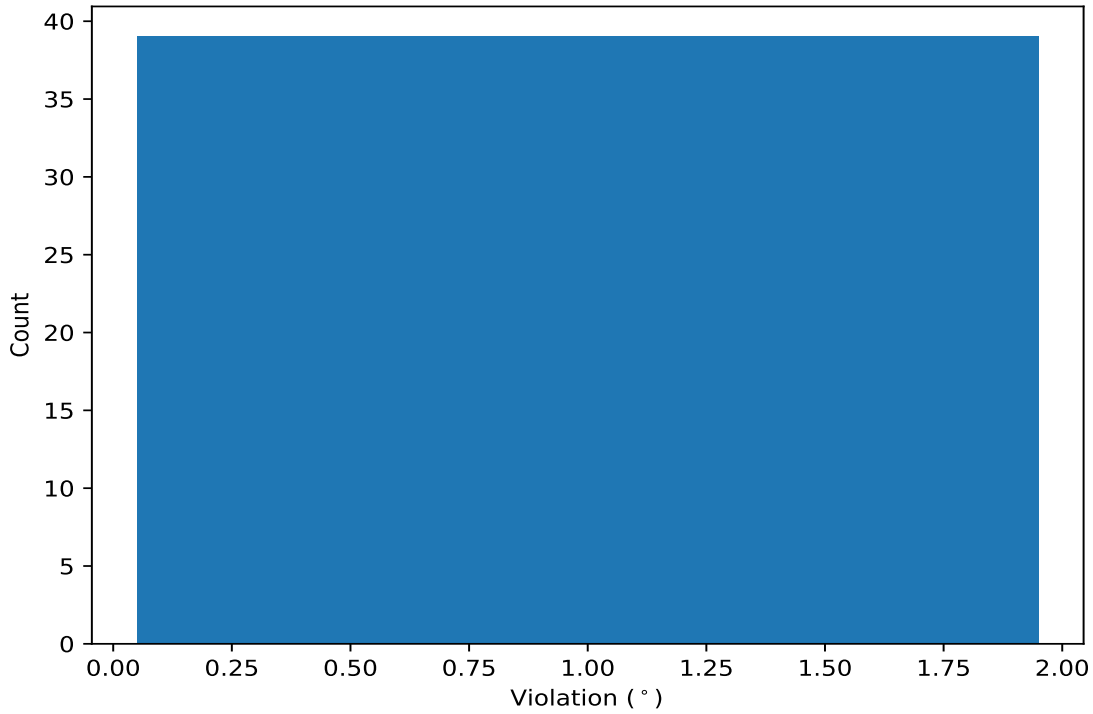
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	20	1.46	0.15	1.46
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	16	1.44	0.19	1.37
(1,33)	1:28:A:THR:C	1:29:A:TRP:N	1:29:A:TRP:CA	1:29:A:TRP:C	2	1.02	0.01	1.02

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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 (°)
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	15	1.78
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	8	1.74
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	18	1.74
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	13	1.69
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	11	1.68
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	10	1.67
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	10	1.63
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	9	1.61
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	3	1.59
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	19	1.54