wwPDB NMR Structure Validation Summary Report

Dec 24, 2024 – 05:48 PM EST

PDB ID	:	2LTR
BMRB ID	:	17703
Title	:	Solution structure of RDE-4(32-136)
Authors	:	Deshmukh, M.; Chiliveri, S.
Deposited on	:	2012-05-31

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

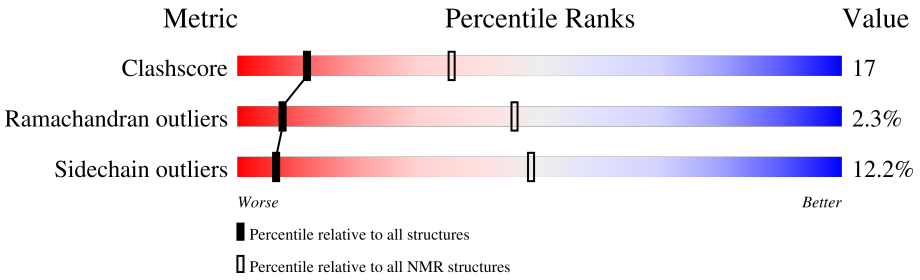
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 45%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=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	246	25% 10% • 7% 57%

2 Ensemble composition and analysis

This entry contains 10 models. Model 7 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:44-A:131 (88)	0.55	7

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 6, 7, 9
2	2, 8
Single-model clusters	4; 5; 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1688 atoms, of which 857 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein RDE-4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	105	1688	530	857	137	161	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	LEU	-	expression tag	UNP G5EBF5
A	245	GLU	-	expression tag	UNP G5EBF5
A	246	HIS	-	expression tag	UNP G5EBF5

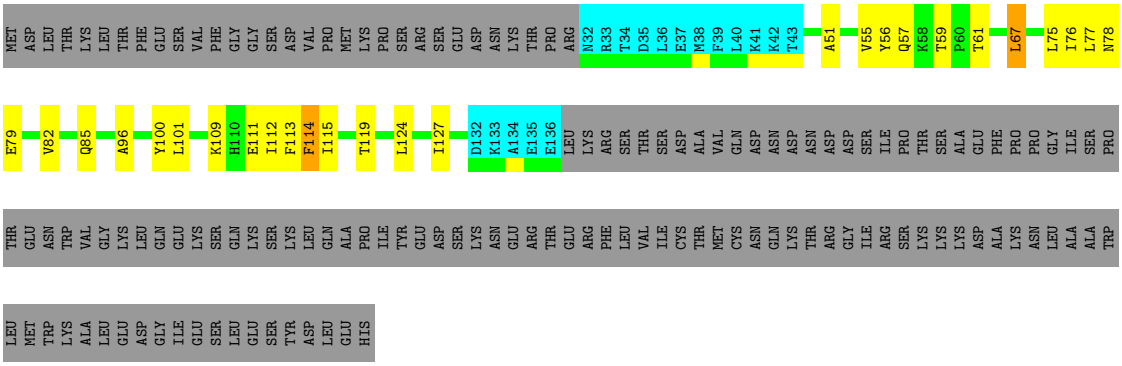
4 Residue-property plots

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: Protein RDE-4

Chain A: 

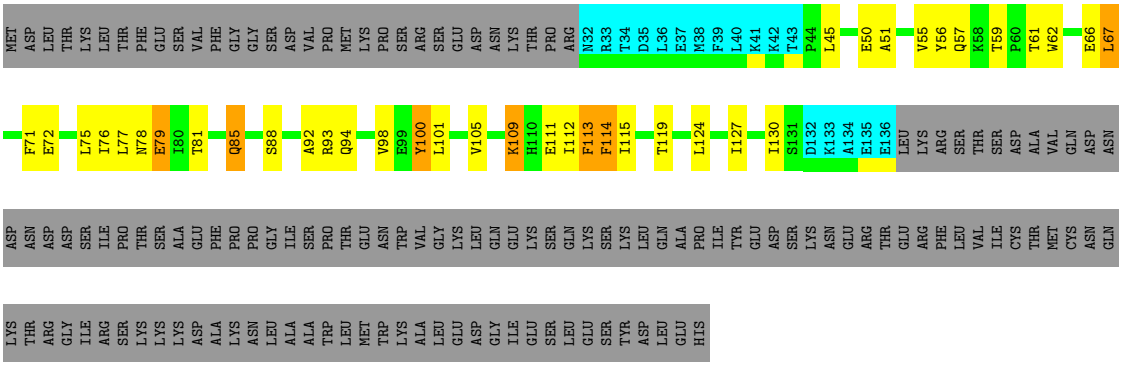


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 7. Colouring as in section 4.1 above.

• Molecule 1: Protein RDE-4

Chain A: 



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1435
Number of shifts mapped to atoms	654
Number of unparsed shifts	0
Number of shifts with mapping errors	781
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

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	688	715	715	24±4
All	All	6880	7150	7150	245

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 17.

5 of 85 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HD12	1:A:76:ILE:N	0.84	1.88	3	7
1:A:67:LEU:HD12	1:A:67:LEU:N	0.82	1.89	8	6
1:A:66:GLU:C	1:A:67:LEU:HD23	0.81	1.96	10	2
1:A:112:ILE:HD12	1:A:113:PHE:H	0.80	1.34	4	9
1:A:112:ILE:HD12	1:A:113:PHE:N	0.74	1.96	10	9

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	88/246 (36%)	80±1 (91±2%)	6±1 (7±2%)	2±0 (2±1%)	7	46
All	All	880/2460 (36%)	799 (91%)	61 (7%)	20 (2%)	7	46

All 3 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	114	PHE	10
1	A	78	ASN	9
1	A	44	PRO	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	74/218 (34%)	65±2 (88±2%)	9±2 (12±2%)	6	48
All	All	740/2180 (34%)	650 (88%)	90 (12%)	6	48

5 of 33 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	59	THR	9
1	A	61	THR	9
1	A	67	LEU	8
1	A	100	TYR	8
1	A	119	THR	6

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 45% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1435
Number of shifts mapped to atoms	654
Number of unparsed shifts	0
Number of shifts with mapping errors	781
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 781) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ASP	C	175.988	0.300	.
1	A	2	ASP	CA	53.203	0.300	.
1	A	2	ASP	CB	40.154	0.300	.
1	A	3	LEU	C	177.901	0.300	.
1	A	3	LEU	CA	55.018	0.300	.
1	A	3	LEU	CB	40.437	0.300	.
1	A	3	LEU	H	8.559	0.020	.
1	A	3	LEU	N	125.503	0.300	.
1	A	4	THR	C	174.724	0.300	.
1	A	4	THR	CA	62.489	0.300	.
1	A	4	THR	CB	68.703	0.300	.
1	A	4	THR	H	8.241	0.020	.
1	A	4	THR	N	114.697	0.300	.
1	A	5	LYS	C	176.227	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LYS	CA	55.621	0.300	.
1	A	5	LYS	CB	31.512	0.300	.
1	A	5	LYS	H	7.896	0.020	.
1	A	5	LYS	N	123.285	0.300	.
1	A	6	LEU	C	177.127	0.300	.
1	A	6	LEU	CA	54.624	0.300	.
1	A	6	LEU	CB	41.051	0.300	.
1	A	6	LEU	H	7.952	0.020	.
1	A	6	LEU	N	123.293	0.300	.
1	A	7	THR	C	174.072	0.300	.
1	A	7	THR	CA	60.977	0.300	.
1	A	7	THR	CB	69.199	0.300	.
1	A	7	THR	H	7.881	0.020	.
1	A	7	THR	N	114.868	0.300	.
1	A	8	PHE	C	175.547	0.300	.
1	A	8	PHE	CA	57.47	0.300	.
1	A	8	PHE	CB	38.737	0.300	.
1	A	8	PHE	H	8.187	0.020	.
1	A	8	PHE	N	122.698	0.300	.
1	A	9	GLU	C	176.236	0.300	.
1	A	9	GLU	CA	56.131	0.300	.
1	A	9	GLU	CB	29.101	0.300	.
1	A	9	GLU	H	8.322	0.020	.
1	A	9	GLU	N	122.332	0.300	.
1	A	10	SER	C	174.398	0.300	.
1	A	10	SER	CA	57.924	0.300	.
1	A	10	SER	CB	63.319	0.300	.
1	A	10	SER	H	8.17	0.020	.
1	A	10	SER	N	117.453	0.300	.
1	A	11	VAL	C	175.859	0.300	.
1	A	11	VAL	CA	61.854	0.300	.
1	A	11	VAL	CB	31.37	0.300	.
1	A	11	VAL	CG1	20.615	0.300	.
1	A	11	VAL	CG2	20.003	0.300	.
1	A	11	VAL	H	7.963	0.020	.
1	A	11	VAL	HG11	0.64	0.020	.
1	A	11	VAL	HG12	0.64	0.020	.
1	A	11	VAL	HG13	0.64	0.020	.
1	A	11	VAL	HG21	0.704	0.020	.
1	A	11	VAL	HG22	0.704	0.020	.
1	A	11	VAL	HG23	0.704	0.020	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	VAL	N	122.156	0.300	.
1	A	12	PHE	C	176.162	0.300	.
1	A	12	PHE	CA	57.253	0.300	.
1	A	12	PHE	CB	38.495	0.300	.
1	A	12	PHE	H	8.235	0.020	.
1	A	12	PHE	HD1	7.194	0.020	.
1	A	12	PHE	HE1	7.249	0.020	.
1	A	12	PHE	HZ	7.161	0.020	.
1	A	12	PHE	N	123.643	0.300	.
1	A	13	GLY	C	174.313	0.300	.
1	A	13	GLY	CA	44.714	0.300	.
1	A	13	GLY	H	8.196	0.020	.
1	A	13	GLY	N	111.925	0.300	.
1	A	14	GLY	C	173.93	0.300	.
1	A	14	GLY	CA	44.55	0.300	.
1	A	14	GLY	H	7.887	0.020	.
1	A	14	GLY	N	109.26	0.300	.
1	A	15	SER	C	173.948	0.300	.
1	A	15	SER	CA	57.726	0.300	.
1	A	15	SER	CB	63.293	0.300	.
1	A	15	SER	H	8.175	0.020	.
1	A	15	SER	N	116.147	0.300	.
1	A	16	ASP	C	175.476	0.300	.
1	A	16	ASP	CA	53.682	0.300	.
1	A	16	ASP	CB	40.154	0.300	.
1	A	16	ASP	H	8.383	0.020	.
1	A	16	ASP	N	123.055	0.300	.
1	A	17	VAL	C	174.157	0.300	.
1	A	17	VAL	CA	59.166	0.300	.
1	A	17	VAL	CB	31.37	0.300	.
1	A	17	VAL	CG1	20.725	0.300	.
1	A	17	VAL	CG2	19.906	0.300	.
1	A	17	VAL	H	7.89	0.020	.
1	A	17	VAL	HG11	0.84	0.020	.
1	A	17	VAL	HG12	0.84	0.020	.
1	A	17	VAL	HG13	0.84	0.020	.
1	A	17	VAL	HG21	0.808	0.020	.
1	A	17	VAL	HG22	0.808	0.020	.
1	A	17	VAL	HG23	0.808	0.020	.
1	A	17	VAL	N	121.964	0.300	.
1	A	18	PRO	C	176.578	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	PRO	CA	62.459	0.300	.
1	A	18	PRO	CB	30.874	0.300	.
1	A	19	MET	C	175.703	0.300	.
1	A	19	MET	CA	54.622	0.300	.
1	A	19	MET	CB	32.007	0.300	.
1	A	19	MET	H	8.294	0.020	.
1	A	19	MET	N	121.632	0.300	.
1	A	20	LYS	C	174.2	0.300	.
1	A	20	LYS	CA	53.501	0.300	.
1	A	20	LYS	CB	31.299	0.300	.
1	A	20	LYS	H	8.255	0.020	.
1	A	20	LYS	N	124.923	0.300	.
1	A	21	PRO	C	176.75	0.300	.
1	A	21	PRO	CA	62.429	0.300	.
1	A	21	PRO	CB	30.874	0.300	.
1	A	22	SER	C	174.469	0.300	.
1	A	22	SER	CA	57.651	0.300	.
1	A	22	SER	CB	63.319	0.300	.
1	A	22	SER	H	8.387	0.020	.
1	A	22	SER	N	117.436	0.300	.
1	A	23	ARG	C	176.327	0.300	.
1	A	23	ARG	CA	55.409	0.300	.
1	A	23	ARG	CB	29.457	0.300	.
1	A	23	ARG	H	8.391	0.020	.
1	A	23	ARG	N	123.817	0.300	.
1	A	24	SER	C	174.666	0.300	.
1	A	24	SER	CA	58.14	0.300	.
1	A	24	SER	CB	63.086	0.300	.
1	A	24	SER	H	8.361	0.020	.
1	A	24	SER	N	118.159	0.300	.
1	A	25	GLU	C	176.063	0.300	.
1	A	25	GLU	CA	56.042	0.300	.
1	A	25	GLU	CB	28.963	0.300	.
1	A	25	GLU	H	8.476	0.020	.
1	A	25	GLU	N	123.248	0.300	.
1	A	26	ASP	C	175.8	0.300	.
1	A	26	ASP	CA	53.886	0.300	.
1	A	26	ASP	CB	40.222	0.300	.
1	A	26	ASP	H	8.165	0.020	.
1	A	26	ASP	N	121.489	0.300	.
1	A	27	ASN	C	174.97	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	ASN	CA	52.704	0.300	.
1	A	27	ASN	CB	37.943	0.300	.
1	A	27	ASN	H	8.227	0.020	.
1	A	27	ASN	N	119.643	0.300	.
1	A	28	LYS	C	176.464	0.300	.
1	A	28	LYS	CA	55.658	0.300	.
1	A	28	LYS	CB	31.588	0.300	.
1	A	28	LYS	H	8.174	0.020	.
1	A	28	LYS	N	121.919	0.300	.
1	A	29	THR	C	172.592	0.300	.
1	A	29	THR	CA	59.5	0.300	.
1	A	29	THR	CB	68.774	0.300	.
1	A	29	THR	H	8.12	0.020	.
1	A	29	THR	N	118.711	0.300	.
1	A	30	PRO	C	176.725	0.300	.
1	A	30	PRO	CA	62.61	0.300	.
1	A	30	PRO	CB	30.945	0.300	.
1	A	31	ARG	C	176.007	0.300	.
1	A	31	ARG	CA	55.5	0.300	.
1	A	31	ARG	CB	29.457	0.300	.
1	A	31	ARG	H	8.372	0.020	.
1	A	31	ARG	N	122.183	0.300	.
1	A	32	ASN	H	8.4	0.020	.
1	A	137	LEU	C	177.305	0.300	.
1	A	137	LEU	CA	54.713	0.300	.
1	A	137	LEU	CB	40.775	0.300	.
1	A	137	LEU	CD1	23.198	0.300	.
1	A	137	LEU	CD2	24.537	0.300	.
1	A	137	LEU	H	8.079	0.020	.
1	A	137	LEU	HD11	0.77	0.020	.
1	A	137	LEU	HD12	0.77	0.020	.
1	A	137	LEU	HD13	0.77	0.020	.
1	A	137	LEU	HD21	0.828	0.020	.
1	A	137	LEU	HD22	0.828	0.020	.
1	A	137	LEU	HD23	0.828	0.020	.
1	A	137	LEU	N	123.233	0.300	.
1	A	138	LYS	C	176.463	0.300	.
1	A	138	LYS	CA	55.773	0.300	.
1	A	138	LYS	CB	31.519	0.300	.
1	A	138	LYS	H	8.086	0.020	.
1	A	138	LYS	N	122.904	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	139	ARG	C	176.301	0.300	.
1	A	139	ARG	CA	55.532	0.300	.
1	A	139	ARG	CB	29.599	0.300	.
1	A	139	ARG	H	8.237	0.020	.
1	A	139	ARG	N	122.925	0.300	.
1	A	140	SER	C	174.791	0.300	.
1	A	140	SER	CA	57.785	0.300	.
1	A	140	SER	CB	63.285	0.300	.
1	A	140	SER	H	8.404	0.020	.
1	A	140	SER	N	118.057	0.300	.
1	A	141	THR	C	174.638	0.300	.
1	A	141	THR	CA	61.33	0.300	.
1	A	141	THR	CB	69.026	0.300	.
1	A	141	THR	H	8.165	0.020	.
1	A	141	THR	N	116.424	0.300	.
1	A	142	SER	C	174.155	0.300	.
1	A	142	SER	CA	57.963	0.300	.
1	A	142	SER	CB	63.155	0.300	.
1	A	142	SER	H	8.229	0.020	.
1	A	142	SER	N	118.258	0.300	.
1	A	143	ASP	C	175.683	0.300	.
1	A	143	ASP	CA	53.864	0.300	.
1	A	143	ASP	CB	40.367	0.300	.
1	A	143	ASP	H	8.213	0.020	.
1	A	143	ASP	N	123.199	0.300	.
1	A	144	ALA	C	177.532	0.300	.
1	A	144	ALA	CA	51.865	0.300	.
1	A	144	ALA	CB	17.91	0.300	.
1	A	144	ALA	H	8.025	0.020	.
1	A	144	ALA	N	124.487	0.300	.
1	A	145	VAL	C	176.043	0.300	.
1	A	145	VAL	CA	61.733	0.300	.
1	A	145	VAL	CB	31.37	0.300	.
1	A	145	VAL	CG2	20.858	0.300	.
1	A	145	VAL	H	7.986	0.020	.
1	A	145	VAL	HG21	0.812	0.020	.
1	A	145	VAL	HG22	0.812	0.020	.
1	A	145	VAL	HG23	0.812	0.020	.
1	A	145	VAL	N	120.303	0.300	.
1	A	146	GLN	C	175.32	0.300	.
1	A	146	GLN	CA	54.894	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	GLN	CB	28.395	0.300	.
1	A	146	GLN	H	8.337	0.020	.
1	A	146	GLN	N	124.575	0.300	.
1	A	147	ASP	C	175.66	0.300	.
1	A	147	ASP	CA	53.747	0.300	.
1	A	147	ASP	CB	40.367	0.300	.
1	A	147	ASP	H	8.288	0.020	.
1	A	147	ASP	N	122.685	0.300	.
1	A	148	ASN	C	174.767	0.300	.
1	A	148	ASN	CA	52.683	0.300	.
1	A	148	ASN	CB	38.241	0.300	.
1	A	148	ASN	H	8.291	0.020	.
1	A	148	ASN	N	119.712	0.300	.
1	A	149	ASP	C	175.828	0.300	.
1	A	149	ASP	CA	53.959	0.300	.
1	A	149	ASP	CB	40.154	0.300	.
1	A	149	ASP	H	8.209	0.020	.
1	A	149	ASP	N	121.997	0.300	.
1	A	150	ASN	C	174.809	0.300	.
1	A	150	ASN	CA	52.719	0.300	.
1	A	150	ASN	CB	38.312	0.300	.
1	A	150	ASN	H	8.176	0.020	.
1	A	150	ASN	N	119.279	0.300	.
1	A	151	ASP	C	175.717	0.300	.
1	A	151	ASP	CA	53.915	0.300	.
1	A	151	ASP	CB	40.222	0.300	.
1	A	151	ASP	H	8.284	0.020	.
1	A	151	ASP	N	121.526	0.300	.
1	A	152	ASP	C	176.256	0.300	.
1	A	152	ASP	CA	53.856	0.300	.
1	A	152	ASP	CB	40.084	0.300	.
1	A	152	ASP	H	8.18	0.020	.
1	A	152	ASP	N	121.423	0.300	.
1	A	153	SER	C	174.1	0.300	.
1	A	153	SER	CA	57.937	0.300	.
1	A	153	SER	CB	62.894	0.300	.
1	A	153	SER	H	8.221	0.020	.
1	A	153	SER	N	115.689	0.300	.
1	A	154	ILE	C	174.145	0.300	.
1	A	154	ILE	CA	58.612	0.300	.
1	A	154	ILE	CB	38.357	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	154	ILE	CD1	13.708	0.300	.
1	A	154	ILE	H	7.64	0.020	.
1	A	154	ILE	HD11	0.599	0.020	.
1	A	154	ILE	HD12	0.599	0.020	.
1	A	154	ILE	HD13	0.599	0.020	.
1	A	154	ILE	N	124.619	0.300	.
1	A	155	PRO	C	174.895	0.300	.
1	A	155	PRO	CA	63.609	0.300	.
1	A	155	PRO	CB	30.874	0.300	.
1	A	156	THR	C	172.992	0.300	.
1	A	156	THR	CA	60.799	0.300	.
1	A	156	THR	CB	72.457	0.300	.
1	A	156	THR	H	8.486	0.020	.
1	A	156	THR	N	123.089	0.300	.
1	A	157	SER	C	171.431	0.300	.
1	A	157	SER	CA	56.249	0.300	.
1	A	157	SER	CB	65.434	0.300	.
1	A	157	SER	H	8.291	0.020	.
1	A	157	SER	N	118.301	0.300	.
1	A	158	ALA	C	176.412	0.300	.
1	A	158	ALA	CA	49.966	0.300	.
1	A	158	ALA	CB	19.54	0.300	.
1	A	158	ALA	H	8.841	0.020	.
1	A	158	ALA	N	127.456	0.300	.
1	A	159	GLU	C	175.306	0.300	.
1	A	159	GLU	CA	54.319	0.300	.
1	A	159	GLU	CB	31.724	0.300	.
1	A	159	GLU	H	7.847	0.020	.
1	A	159	GLU	N	117.099	0.300	.
1	A	160	PHE	C	173.561	0.300	.
1	A	160	PHE	CA	56.652	0.300	.
1	A	160	PHE	CB	37.533	0.300	.
1	A	160	PHE	H	9.23	0.020	.
1	A	160	PHE	N	124.986	0.300	.
1	A	162	PRO	C	177.549	0.300	.
1	A	162	PRO	CA	63.276	0.300	.
1	A	162	PRO	CB	30.378	0.300	.
1	A	163	GLY	C	173.264	0.300	.
1	A	163	GLY	CA	44.351	0.300	.
1	A	163	GLY	H	8.575	0.020	.
1	A	163	GLY	N	111.972	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	164	ILE	C	175.362	0.300	.
1	A	164	ILE	CA	56.682	0.300	.
1	A	164	ILE	CB	33.849	0.300	.
1	A	164	ILE	CD1	8.709	0.300	.
1	A	164	ILE	H	7.575	0.020	.
1	A	164	ILE	HD11	0.523	0.020	.
1	A	164	ILE	HD12	0.523	0.020	.
1	A	164	ILE	HD13	0.523	0.020	.
1	A	164	ILE	N	122.817	0.300	.
1	A	165	SER	C	174.292	0.300	.
1	A	165	SER	CA	54.743	0.300	.
1	A	165	SER	CB	63.248	0.300	.
1	A	165	SER	H	8.644	0.020	.
1	A	165	SER	N	122.181	0.300	.
1	A	166	PRO	C	176.725	0.300	.
1	A	166	PRO	CA	61.703	0.300	.
1	A	166	PRO	CB	31.653	0.300	.
1	A	167	THR	C	175.419	0.300	.
1	A	167	THR	CA	60.439	0.300	.
1	A	167	THR	CB	67.711	0.300	.
1	A	167	THR	H	7.427	0.020	.
1	A	167	THR	N	106.805	0.300	.
1	A	168	GLU	C	173.958	0.300	.
1	A	168	GLU	CA	54.652	0.300	.
1	A	168	GLU	CB	28.465	0.300	.
1	A	168	GLU	H	6.402	0.020	.
1	A	168	GLU	N	124.439	0.300	.
1	A	169	ASN	C	175.674	0.300	.
1	A	169	ASN	CA	49.835	0.300	.
1	A	169	ASN	CB	34.983	0.300	.
1	A	169	ASN	H	8.723	0.020	.
1	A	169	ASN	N	123.071	0.300	.
1	A	170	TRP	C	177.998	0.300	.
1	A	170	TRP	CA	59.5	0.300	.
1	A	170	TRP	CB	28.111	0.300	.
1	A	170	TRP	H	8.769	0.020	.
1	A	170	TRP	HE1	9.743	0.020	.
1	A	170	TRP	N	128.988	0.300	.
1	A	170	TRP	NE1	129.111	0.300	.
1	A	171	VAL	C	179.985	0.300	.
1	A	171	VAL	CA	65.165	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	171	VAL	CB	31.157	0.300	.
1	A	171	VAL	CG1	20.315	0.300	.
1	A	171	VAL	CG2	22.235	0.300	.
1	A	171	VAL	H	7.436	0.020	.
1	A	171	VAL	HG11	0.828	0.020	.
1	A	171	VAL	HG12	0.828	0.020	.
1	A	171	VAL	HG13	0.828	0.020	.
1	A	171	VAL	HG21	0.949	0.020	.
1	A	171	VAL	HG22	0.949	0.020	.
1	A	171	VAL	HG23	0.949	0.020	.
1	A	171	VAL	N	119.871	0.300	.
1	A	172	GLY	C	176.44	0.300	.
1	A	172	GLY	CA	46.744	0.300	.
1	A	172	GLY	H	7.801	0.020	.
1	A	172	GLY	N	110.098	0.300	.
1	A	173	LYS	C	179.865	0.300	.
1	A	173	LYS	CA	58.761	0.300	.
1	A	173	LYS	CB	30.266	0.300	.
1	A	173	LYS	H	7.98	0.020	.
1	A	173	LYS	N	123.784	0.300	.
1	A	174	LEU	C	178.468	0.300	.
1	A	174	LEU	CA	57.253	0.300	.
1	A	174	LEU	CB	40.792	0.300	.
1	A	174	LEU	CD1	23.052	0.300	.
1	A	174	LEU	CD2	25.496	0.300	.
1	A	174	LEU	H	8.631	0.020	.
1	A	174	LEU	HD11	0.959	0.020	.
1	A	174	LEU	HD12	0.959	0.020	.
1	A	174	LEU	HD13	0.959	0.020	.
1	A	174	LEU	HD21	1.046	0.020	.
1	A	174	LEU	HD22	1.046	0.020	.
1	A	174	LEU	HD23	1.046	0.020	.
1	A	174	LEU	N	122.4	0.300	.
1	A	175	GLN	C	179.106	0.300	.
1	A	175	GLN	CA	58.5	0.300	.
1	A	175	GLN	CB	26.624	0.300	.
1	A	175	GLN	H	8.059	0.020	.
1	A	175	GLN	N	121.515	0.300	.
1	A	176	GLU	C	178.351	0.300	.
1	A	176	GLU	CA	58.863	0.300	.
1	A	176	GLU	CB	28.341	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	176	GLU	H	8.336	0.020	.
1	A	176	GLU	N	121.629	0.300	.
1	A	177	LYS	C	178.883	0.300	.
1	A	177	LYS	CA	58.612	0.300	.
1	A	177	LYS	CB	30.966	0.300	.
1	A	177	LYS	H	8.207	0.020	.
1	A	177	LYS	N	121.385	0.300	.
1	A	178	SER	C	175.123	0.300	.
1	A	178	SER	CA	61.53	0.300	.
1	A	178	SER	CB	62.256	0.300	.
1	A	178	SER	H	8.428	0.020	.
1	A	178	SER	N	115.948	0.300	.
1	A	179	GLN	C	179.574	0.300	.
1	A	179	GLN	CA	57.861	0.300	.
1	A	179	GLN	CB	27.474	0.300	.
1	A	179	GLN	H	7.737	0.020	.
1	A	179	GLN	N	121.448	0.300	.
1	A	180	LYS	C	178.454	0.300	.
1	A	180	LYS	CA	58.376	0.300	.
1	A	180	LYS	CB	31.37	0.300	.
1	A	180	LYS	H	8.463	0.020	.
1	A	180	LYS	N	121.226	0.300	.
1	A	181	SER	C	171.945	0.300	.
1	A	181	SER	CA	58.287	0.300	.
1	A	181	SER	CB	63.319	0.300	.
1	A	181	SER	H	7.973	0.020	.
1	A	181	SER	N	112.898	0.300	.
1	A	182	LYS	C	175.291	0.300	.
1	A	182	LYS	CA	56.47	0.300	.
1	A	182	LYS	CB	27.332	0.300	.
1	A	182	LYS	H	7.555	0.020	.
1	A	182	LYS	N	118.016	0.300	.
1	A	183	LEU	C	176.752	0.300	.
1	A	183	LEU	CA	51.986	0.300	.
1	A	183	LEU	CB	43.2	0.300	.
1	A	183	LEU	CD1	25.43	0.300	.
1	A	183	LEU	CD2	21.933	0.300	.
1	A	183	LEU	H	8.274	0.020	.
1	A	183	LEU	HD11	0.648	0.020	.
1	A	183	LEU	HD12	0.648	0.020	.
1	A	183	LEU	HD13	0.648	0.020	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	183	LEU	HD21	0.707	0.020	.
1	A	183	LEU	HD22	0.707	0.020	.
1	A	183	LEU	HD23	0.707	0.020	.
1	A	183	LEU	N	119.293	0.300	.
1	A	184	GLN	C	174.864	0.300	.
1	A	184	GLN	CA	55.591	0.300	.
1	A	184	GLN	CB	27.757	0.300	.
1	A	184	GLN	H	8.014	0.020	.
1	A	184	GLN	N	121.634	0.300	.
1	A	185	ALA	C	175.771	0.300	.
1	A	185	ALA	CA	50.136	0.300	.
1	A	185	ALA	CB	16.362	0.300	.
1	A	185	ALA	H	8.03	0.020	.
1	A	185	ALA	N	126.077	0.300	.
1	A	186	PRO	C	175.411	0.300	.
1	A	186	PRO	CA	61.885	0.300	.
1	A	186	PRO	CB	31.866	0.300	.
1	A	187	ILE	C	174.426	0.300	.
1	A	187	ILE	CA	59.106	0.300	.
1	A	187	ILE	CB	39.946	0.300	.
1	A	187	ILE	CD1	12.988	0.300	.
1	A	187	ILE	H	8.044	0.020	.
1	A	187	ILE	HD11	0.746	0.020	.
1	A	187	ILE	HD12	0.746	0.020	.
1	A	187	ILE	HD13	0.746	0.020	.
1	A	187	ILE	N	121.091	0.300	.
1	A	188	TYR	C	175.759	0.300	.
1	A	188	TYR	CA	56.046	0.300	.
1	A	188	TYR	CB	40.083	0.300	.
1	A	188	TYR	H	8.664	0.020	.
1	A	188	TYR	N	123.672	0.300	.
1	A	189	GLU	C	174.1	0.300	.
1	A	189	GLU	CA	54.531	0.300	.
1	A	189	GLU	CB	32.716	0.300	.
1	A	189	GLU	H	8.914	0.020	.
1	A	189	GLU	N	123.03	0.300	.
1	A	190	ASP	C	174.327	0.300	.
1	A	190	ASP	CA	52.168	0.300	.
1	A	190	ASP	CB	44.688	0.300	.
1	A	190	ASP	H	8.714	0.020	.
1	A	190	ASP	N	121.583	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	191	SER	C	171.874	0.300	.
1	A	191	SER	CA	57.227	0.300	.
1	A	191	SER	CB	64.807	0.300	.
1	A	191	SER	H	8.81	0.020	.
1	A	191	SER	N	114.934	0.300	.
1	A	192	LYS	C	175.263	0.300	.
1	A	192	LYS	CA	54.231	0.300	.
1	A	192	LYS	CB	33.708	0.300	.
1	A	192	LYS	H	8.468	0.020	.
1	A	192	LYS	N	122.639	0.300	.
1	A	193	ASN	C	175.547	0.300	.
1	A	193	ASN	CA	51.902	0.300	.
1	A	193	ASN	CB	38.383	0.300	.
1	A	193	ASN	H	8.516	0.020	.
1	A	193	ASN	N	125.717	0.300	.
1	A	194	GLU	C	177.183	0.300	.
1	A	194	GLU	CA	57.712	0.300	.
1	A	194	GLU	CB	28.395	0.300	.
1	A	194	GLU	H	8.959	0.020	.
1	A	194	GLU	N	125.865	0.300	.
1	A	195	ARG	C	177.773	0.300	.
1	A	195	ARG	CA	57.519	0.300	.
1	A	195	ARG	CB	28.89	0.300	.
1	A	195	ARG	H	8.214	0.020	.
1	A	195	ARG	N	119.005	0.300	.
1	A	196	THR	C	174.68	0.300	.
1	A	196	THR	CA	60.499	0.300	.
1	A	196	THR	CB	68.986	0.300	.
1	A	196	THR	H	7.559	0.020	.
1	A	196	THR	N	108.424	0.300	.
1	A	197	GLU	C	175.05	0.300	.
1	A	197	GLU	CA	56.5	0.300	.
1	A	197	GLU	CB	25.915	0.300	.
1	A	197	GLU	H	7.857	0.020	.
1	A	197	GLU	N	118.543	0.300	.
1	A	198	ARG	C	174.299	0.300	.
1	A	198	ARG	CA	53.804	0.300	.
1	A	198	ARG	CB	31.795	0.300	.
1	A	198	ARG	H	7.277	0.020	.
1	A	198	ARG	N	117.332	0.300	.
1	A	199	PHE	C	173.311	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	199	PHE	CA	57.803	0.300	.
1	A	199	PHE	CB	40.775	0.300	.
1	A	199	PHE	H	8.697	0.020	.
1	A	199	PHE	HD1	7.119	0.020	.
1	A	199	PHE	N	119.812	0.300	.
1	A	200	LEU	C	176.412	0.300	.
1	A	200	LEU	CA	54.016	0.300	.
1	A	200	LEU	CB	41.854	0.300	.
1	A	200	LEU	CD1	24.878	0.300	.
1	A	200	LEU	CD2	26.662	0.300	.
1	A	200	LEU	H	8.694	0.020	.
1	A	200	LEU	HD11	0.687	0.020	.
1	A	200	LEU	HD12	0.687	0.020	.
1	A	200	LEU	HD13	0.687	0.020	.
1	A	200	LEU	HD21	0.685	0.020	.
1	A	200	LEU	HD22	0.685	0.020	.
1	A	200	LEU	HD23	0.685	0.020	.
1	A	200	LEU	N	122.665	0.300	.
1	A	201	VAL	C	173.961	0.300	.
1	A	201	VAL	CA	60.015	0.300	.
1	A	201	VAL	CB	32.624	0.300	.
1	A	201	VAL	CG1	21.816	0.300	.
1	A	201	VAL	CG2	21.816	0.300	.
1	A	201	VAL	H	9.071	0.020	.
1	A	201	VAL	HG11	0.944	0.020	.
1	A	201	VAL	HG12	0.944	0.020	.
1	A	201	VAL	HG13	0.944	0.020	.
1	A	201	VAL	HG21	0.868	0.020	.
1	A	201	VAL	HG22	0.868	0.020	.
1	A	201	VAL	HG23	0.868	0.020	.
1	A	201	VAL	N	124.642	0.300	.
1	A	202	ILE	C	175.646	0.300	.
1	A	202	ILE	CA	58.406	0.300	.
1	A	202	ILE	CB	39.304	0.300	.
1	A	202	ILE	CD1	13.373	0.300	.
1	A	202	ILE	H	8.9	0.020	.
1	A	202	ILE	HD11	0.704	0.020	.
1	A	202	ILE	HD12	0.704	0.020	.
1	A	202	ILE	HD13	0.704	0.020	.
1	A	202	ILE	N	127.312	0.300	.
1	A	203	CYS	C	173.008	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	203	CYS	CA	56.318	0.300	.
1	A	203	CYS	CB	27.899	0.300	.
1	A	203	CYS	H	9.206	0.020	.
1	A	203	CYS	N	131.048	0.300	.
1	A	204	THR	C	174.37	0.300	.
1	A	204	THR	CA	60.772	0.300	.
1	A	204	THR	CB	69.199	0.300	.
1	A	204	THR	H	8.779	0.020	.
1	A	204	THR	N	124.615	0.300	.
1	A	205	MET	C	174.086	0.300	.
1	A	205	MET	CA	55.531	0.300	.
1	A	205	MET	CB	33.495	0.300	.
1	A	205	MET	H	8.644	0.020	.
1	A	205	MET	N	127.382	0.300	.
1	A	206	CYS	C	173.823	0.300	.
1	A	206	CYS	CA	59.863	0.300	.
1	A	206	CYS	CB	24.994	0.300	.
1	A	206	CYS	H	9.237	0.020	.
1	A	206	CYS	N	122.519	0.300	.
1	A	207	ASN	C	173.249	0.300	.
1	A	207	ASN	CA	53.804	0.300	.
1	A	207	ASN	CB	37.108	0.300	.
1	A	207	ASN	H	8.749	0.020	.
1	A	207	ASN	N	113.021	0.300	.
1	A	208	GLN	C	173.285	0.300	.
1	A	208	GLN	CA	53.561	0.300	.
1	A	208	GLN	CB	30.166	0.300	.
1	A	208	GLN	H	7.992	0.020	.
1	A	208	GLN	HE21	7.065	0.020	.
1	A	208	GLN	HE22	7.065	0.020	.
1	A	208	GLN	N	119.926	0.300	.
1	A	209	LYS	C	175.66	0.300	.
1	A	209	LYS	CA	54.379	0.300	.
1	A	209	LYS	CB	36.683	0.300	.
1	A	209	LYS	H	7.771	0.020	.
1	A	209	LYS	N	119.942	0.300	.
1	A	210	THR	C	173.203	0.300	.
1	A	210	THR	CA	59.681	0.300	.
1	A	210	THR	CB	71.466	0.300	.
1	A	210	THR	H	8.779	0.020	.
1	A	210	THR	N	111.409	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	211	ARG	C	173.311	0.300	.
1	A	211	ARG	CA	54.142	0.300	.
1	A	211	ARG	CB	32.787	0.300	.
1	A	211	ARG	H	8.511	0.020	.
1	A	211	ARG	N	120.129	0.300	.
1	A	212	GLY	C	172.399	0.300	.
1	A	212	GLY	CA	42.381	0.300	.
1	A	212	GLY	H	8.958	0.020	.
1	A	212	GLY	N	112.548	0.300	.
1	A	213	ILE	C	176.547	0.300	.
1	A	213	ILE	CA	59.621	0.300	.
1	A	213	ILE	CB	39.393	0.300	.
1	A	213	ILE	CD1	13.942	0.300	.
1	A	213	ILE	H	8.1	0.020	.
1	A	213	ILE	HD11	0.574	0.020	.
1	A	213	ILE	HD12	0.574	0.020	.
1	A	213	ILE	HD13	0.574	0.020	.
1	A	213	ILE	N	123.768	0.300	.
1	A	214	ARG	C	176.1	0.300	.
1	A	214	ARG	CA	51.683	0.300	.
1	A	214	ARG	CB	34.345	0.300	.
1	A	214	ARG	H	8.512	0.020	.
1	A	214	ARG	N	121.124	0.300	.
1	A	215	SER	C	173.395	0.300	.
1	A	215	SER	CA	61.098	0.300	.
1	A	215	SER	CB	62.74	0.300	.
1	A	216	LYS	C	176.547	0.300	.
1	A	216	LYS	CA	53.838	0.300	.
1	A	216	LYS	CB	32.831	0.300	.
1	A	216	LYS	H	7.622	0.020	.
1	A	216	LYS	N	118.28	0.300	.
1	A	217	LYS	C	177.73	0.300	.
1	A	217	LYS	CA	60.136	0.300	.
1	A	217	LYS	CB	29.811	0.300	.
1	A	217	LYS	H	8.35	0.020	.
1	A	217	LYS	N	129.559	0.300	.
1	A	218	LYS	C	178.546	0.300	.
1	A	218	LYS	CA	58.712	0.300	.
1	A	218	LYS	CB	30.69	0.300	.
1	A	218	LYS	H	8.713	0.020	.
1	A	218	LYS	N	117.32	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	219	ASP	C	176.965	0.300	.
1	A	219	ASP	CA	55.743	0.300	.
1	A	219	ASP	CB	39.871	0.300	.
1	A	219	ASP	H	6.517	0.020	.
1	A	219	ASP	N	119.568	0.300	.
1	A	220	ALA	C	178.413	0.300	.
1	A	220	ALA	CA	54.949	0.300	.
1	A	220	ALA	CB	17.566	0.300	.
1	A	220	ALA	H	7.959	0.020	.
1	A	220	ALA	N	123.866	0.300	.
1	A	221	LYS	C	176.712	0.300	.
1	A	221	LYS	CA	58.76	0.300	.
1	A	221	LYS	CB	31.795	0.300	.
1	A	221	LYS	H	8.234	0.020	.
1	A	221	LYS	N	118.925	0.300	.
1	A	222	ASN	C	176.989	0.300	.
1	A	222	ASN	CA	55.451	0.300	.
1	A	222	ASN	CB	38.703	0.300	.
1	A	222	ASN	H	7.734	0.020	.
1	A	222	ASN	N	118.189	0.300	.
1	A	223	LEU	C	177.501	0.300	.
1	A	223	LEU	CA	56.591	0.300	.
1	A	223	LEU	CB	39.877	0.300	.
1	A	223	LEU	CD1	20.1	0.300	.
1	A	223	LEU	CD2	26.721	0.300	.
1	A	223	LEU	H	8.267	0.020	.
1	A	223	LEU	HD11	-0.053	0.020	.
1	A	223	LEU	HD12	-0.053	0.020	.
1	A	223	LEU	HD13	-0.053	0.020	.
1	A	223	LEU	HD21	0.245	0.020	.
1	A	223	LEU	HD22	0.245	0.020	.
1	A	223	LEU	HD23	0.245	0.020	.
1	A	223	LEU	N	120.287	0.300	.
1	A	224	ALA	C	180.501	0.300	.
1	A	224	ALA	CA	55.215	0.300	.
1	A	224	ALA	CB	16.806	0.300	.
1	A	224	ALA	H	8.25	0.020	.
1	A	224	ALA	N	122.439	0.300	.
1	A	225	ALA	C	178.925	0.300	.
1	A	225	ALA	CA	54.319	0.300	.
1	A	225	ALA	CB	17.704	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	225	ALA	H	8.512	0.020	.
1	A	225	ALA	N	120.368	0.300	.
1	A	226	TRP	CA	54.319	0.300	.
1	A	226	TRP	H	8.419	0.020	.
1	A	226	TRP	N	121.963	0.300	.
1	A	227	LEU	CD1	27.151	0.300	.
1	A	227	LEU	CD2	24.146	0.300	.
1	A	227	LEU	HD11	0.662	0.020	.
1	A	227	LEU	HD12	0.662	0.020	.
1	A	227	LEU	HD13	0.662	0.020	.
1	A	227	LEU	HD21	0.666	0.020	.
1	A	227	LEU	HD22	0.666	0.020	.
1	A	227	LEU	HD23	0.666	0.020	.
1	A	228	MET	C	176.553	0.300	.
1	A	228	MET	CA	55.532	0.300	.
1	A	228	MET	CB	28.111	0.300	.
1	A	229	TRP	C	177.791	0.300	.
1	A	229	TRP	CA	60.946	0.300	.
1	A	229	TRP	CB	27.789	0.300	.
1	A	229	TRP	H	8.974	0.020	.
1	A	229	TRP	N	123.396	0.300	.
1	A	230	LYS	C	177.957	0.300	.
1	A	230	LYS	CA	56.751	0.300	.
1	A	230	LYS	CB	29.239	0.300	.
1	A	230	LYS	H	8.507	0.020	.
1	A	230	LYS	N	120.069	0.300	.
1	A	231	ALA	C	180.791	0.300	.
1	A	231	ALA	CA	53.687	0.300	.
1	A	231	ALA	CB	16.599	0.300	.
1	A	231	ALA	H	7.858	0.020	.
1	A	231	ALA	N	122.28	0.300	.
1	A	232	LEU	C	178.87	0.300	.
1	A	232	LEU	CA	56.076	0.300	.
1	A	232	LEU	CB	40.222	0.300	.
1	A	232	LEU	CD1	25.456	0.300	.
1	A	232	LEU	H	8.135	0.020	.
1	A	232	LEU	HD11	0.59	0.020	.
1	A	232	LEU	HD12	0.59	0.020	.
1	A	232	LEU	HD13	0.59	0.020	.
1	A	232	LEU	N	118.143	0.300	.
1	A	233	GLU	C	177.459	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	233	GLU	CA	57.924	0.300	.
1	A	233	GLU	CB	28.894	0.300	.
1	A	233	GLU	H	7.778	0.020	.
1	A	233	GLU	N	120.978	0.300	.
1	A	234	ASP	C	176.63	0.300	.
1	A	234	ASP	CA	54.107	0.300	.
1	A	234	ASP	CB	41.535	0.300	.
1	A	234	ASP	H	8.212	0.020	.
1	A	234	ASP	N	116.859	0.300	.
1	A	235	GLY	C	175.589	0.300	.
1	A	235	GLY	CA	44.284	0.300	.
1	A	235	GLY	H	7.408	0.020	.
1	A	235	GLY	N	110.973	0.300	.
1	A	236	ILE	C	177.143	0.300	.
1	A	236	ILE	CA	62.14	0.300	.
1	A	236	ILE	CB	37.183	0.300	.
1	A	236	ILE	CD1	13.348	0.300	.
1	A	236	ILE	HD11	0.729	0.020	.
1	A	236	ILE	HD12	0.729	0.020	.
1	A	236	ILE	HD13	0.729	0.020	.
1	A	237	GLU	C	178.081	0.300	.
1	A	237	GLU	CA	57.815	0.300	.
1	A	237	GLU	CB	27.374	0.300	.
1	A	237	GLU	H	9.125	0.020	.
1	A	237	GLU	N	123.401	0.300	.
1	A	238	SER	C	175.62	0.300	.
1	A	238	SER	CA	59.712	0.300	.
1	A	238	SER	CB	62.809	0.300	.
1	A	238	SER	H	7.89	0.020	.
1	A	238	SER	N	117.282	0.300	.
1	A	239	LEU	C	177.915	0.300	.
1	A	239	LEU	CA	55.215	0.300	.
1	A	239	LEU	CB	40.291	0.300	.
1	A	239	LEU	H	7.556	0.020	.
1	A	239	LEU	N	122.311	0.300	.
1	A	240	GLU	C	177.203	0.300	.
1	A	240	GLU	CA	57.313	0.300	.
1	A	240	GLU	CB	28.48	0.300	.
1	A	240	GLU	H	7.723	0.020	.
1	A	240	GLU	N	119.679	0.300	.
1	A	241	SER	C	174.006	0.300	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	241	SER	CA	58.76	0.300	.
1	A	241	SER	CB	62.74	0.300	.
1	A	241	SER	H	7.726	0.020	.
1	A	241	SER	N	114.102	0.300	.
1	A	242	TYR	C	174.998	0.300	.
1	A	242	TYR	CA	57.313	0.300	.
1	A	242	TYR	CB	37.736	0.300	.
1	A	242	TYR	H	7.707	0.020	.
1	A	242	TYR	N	121.562	0.300	.
1	A	243	ASP	C	175.993	0.300	.
1	A	243	ASP	CA	53.531	0.300	.
1	A	243	ASP	CB	39.808	0.300	.
1	A	243	ASP	H	8.123	0.020	.
1	A	243	ASP	N	121.714	0.300	.
1	A	244	LEU	C	177.708	0.300	.
1	A	244	LEU	CA	54.92	0.300	.
1	A	244	LEU	CB	40.637	0.300	.
1	A	244	LEU	H	8.194	0.020	.
1	A	244	LEU	N	123.311	0.300	.
1	A	245	GLU	C	176.339	0.300	.
1	A	245	GLU	CA	56.077	0.300	.
1	A	245	GLU	CB	28.82	0.300	.
1	A	245	GLU	H	8.243	0.020	.
1	A	245	GLU	N	119.82	0.300	.
1	A	246	HIS	C	174.445	0.300	.
1	A	246	HIS	CA	55.411	0.300	.
1	A	246	HIS	CB	28.618	0.300	.
1	A	246	HIS	H	8.091	0.020	.
1	A	246	HIS	N	119.252	0.300	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	242	0.27 ± 0.41	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	227	1.28 ± 0.12	Should be checked
$^{13}C'$	241	0.02 ± 0.20	None needed (< 0.5 ppm)
^{15}N	225	0.09 ± 0.42	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 551 atoms were assigned a chemical shift out of a possible 1214. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	336/437 (77%)	81/177 (46%)	174/176 (99%)	81/84 (96%)
Sidechain	211/710 (30%)	99/463 (21%)	112/225 (50%)	0/22 (0%)
Aromatic	4/67 (6%)	4/33 (12%)	0/32 (0%)	0/2 (0%)
Overall	551/1214 (45%)	184/673 (27%)	286/433 (66%)	81/108 (75%)

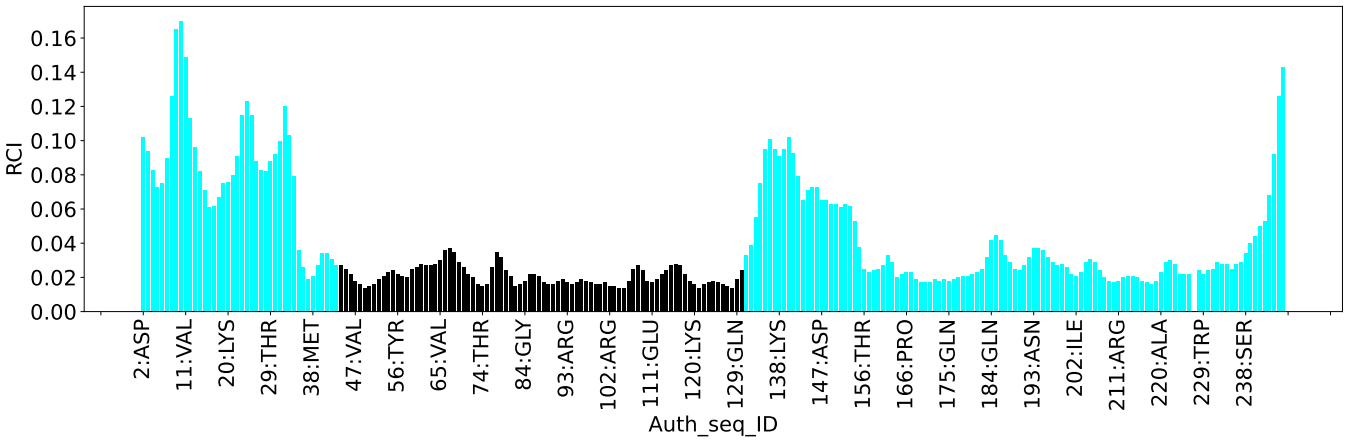
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

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:



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	551
Intra-residue (|i-j|=0)	56
Sequential (|i-j|=1)	170
Medium range (|i-j|>1 and |i-j|<5)	96
Long range (|i-j|≥5)	127
Inter-chain	0
Hydrogen bond restraints	102
Disulfide bond restraints	0
Total dihedral-angle restraints	182
Number of unmapped restraints	7
Number of restraints per residue	3.0
Number of long range restraints per residue[1]	0.6

[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)	3.8	0.16
0.2-0.5 (Medium)	0.4	0.49
>0.5 (Large)	5.6	1.62

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)	16.9	4.96
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

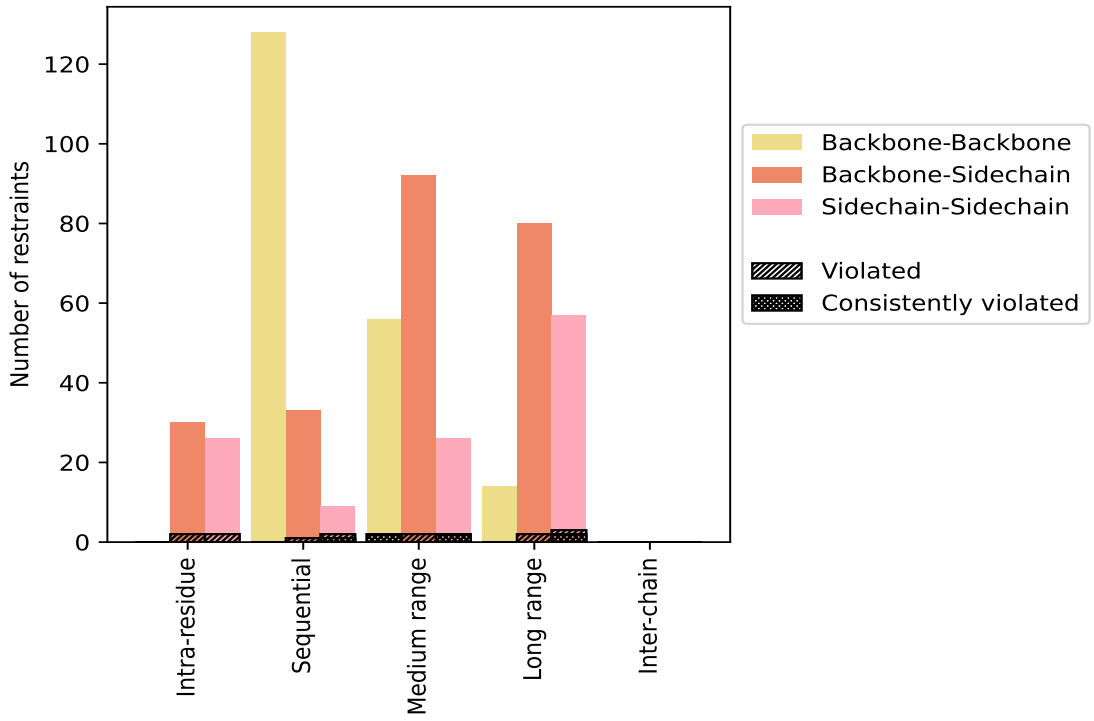
9.1 Summary of distance violations (i)

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)	56	10.2	4	7.1	0.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	30	5.4	2	6.7	0.4	0	0.0	0.0
Sidechain-Sidechain	26	4.7	2	7.7	0.4	0	0.0	0.0
Sequential (|i-j|=1)	170	30.9	3	1.8	0.5	1	0.6	0.2
Backbone-Backbone	128	23.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	33	6.0	1	3.0	0.2	0	0.0	0.0
Sidechain-Sidechain	9	1.6	2	22.2	0.4	1	11.1	0.2
Medium range (|i-j|>1 & |i-j|<5)	96	17.4	4	4.2	0.7	4	4.2	0.7
Backbone-Backbone	56	10.2	2	3.6	0.4	2	3.6	0.4
Backbone-Sidechain	14	2.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	26	4.7	2	7.7	0.4	2	7.7	0.4
Long range (|i-j|≥5)	127	23.0	4	3.1	0.7	2	1.6	0.4
Backbone-Backbone	14	2.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	56	10.2	1	1.8	0.2	0	0.0	0.0
Sidechain-Sidechain	57	10.3	3	5.3	0.5	2	3.5	0.4
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	102	18.5	3	2.9	0.5	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	551	100.0	18	3.3	3.3	7	1.3	1.3
Backbone-Backbone	198	35.9	2	1.0	0.4	2	1.0	0.4
Backbone-Sidechain	235	42.6	7	3.0	1.3	0	0.0	0.0
Sidechain-Sidechain	118	21.4	9	7.6	1.6	5	4.2	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



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

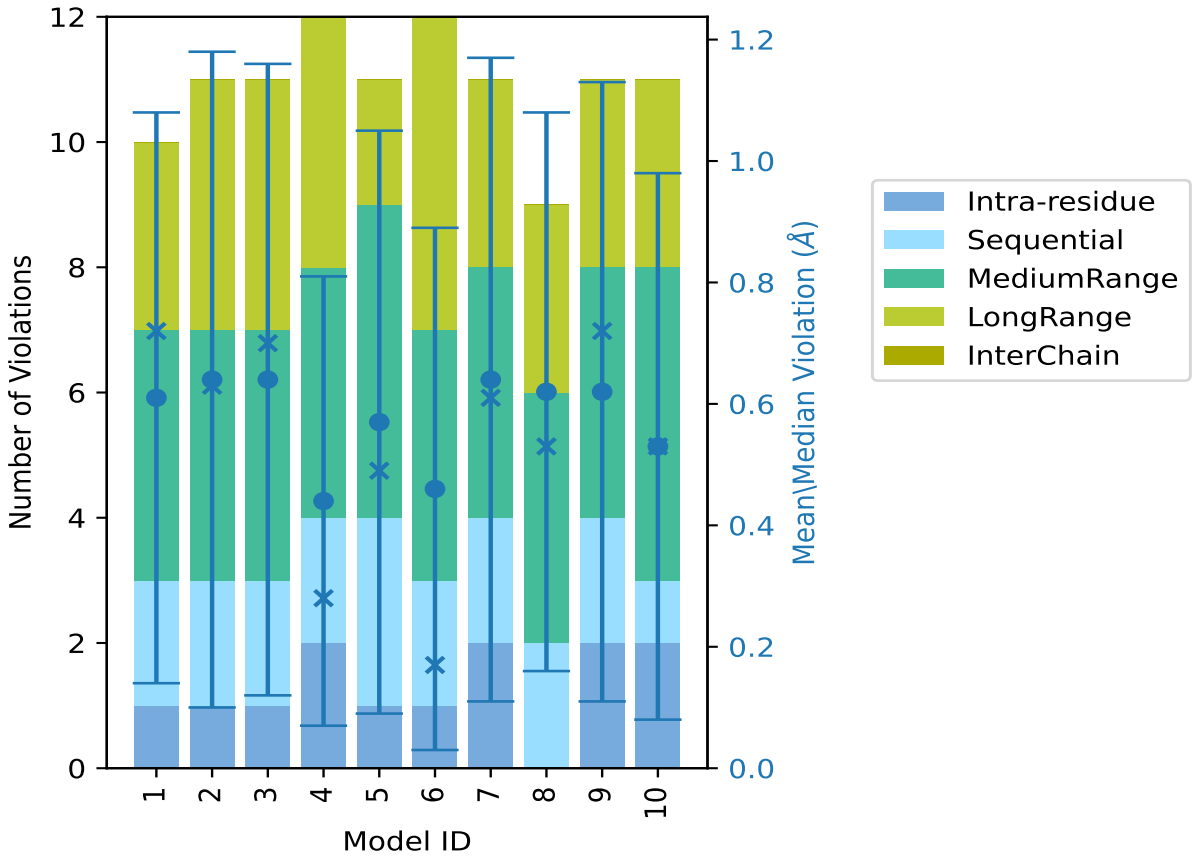
9.2 Distance violation statistics for each model

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	1	2	4	3	0	10	0.61	1.6	0.47	0.72
2	1	2	4	4	0	11	0.64	1.62	0.54	0.63
3	1	2	4	4	0	11	0.64	1.6	0.52	0.7
4	2	2	4	4	0	12	0.44	1.23	0.37	0.28
5	1	3	5	2	0	11	0.57	1.37	0.48	0.49
6	1	2	4	5	0	12	0.46	1.45	0.43	0.17
7	2	2	4	3	0	11	0.64	1.57	0.53	0.61
8	0	2	4	3	0	9	0.62	1.59	0.46	0.53
9	2	2	4	3	0	11	0.62	1.58	0.51	0.72
10	2	1	5	3	0	11	0.53	1.53	0.45	0.53

[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

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, 434(IR:52, SQ:167, MR:92, LR:123, 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]	%
0	1	0	1	0	2	1	10.0
2	0	0	0	0	2	2	20.0
0	0	0	0	0	0	3	30.0

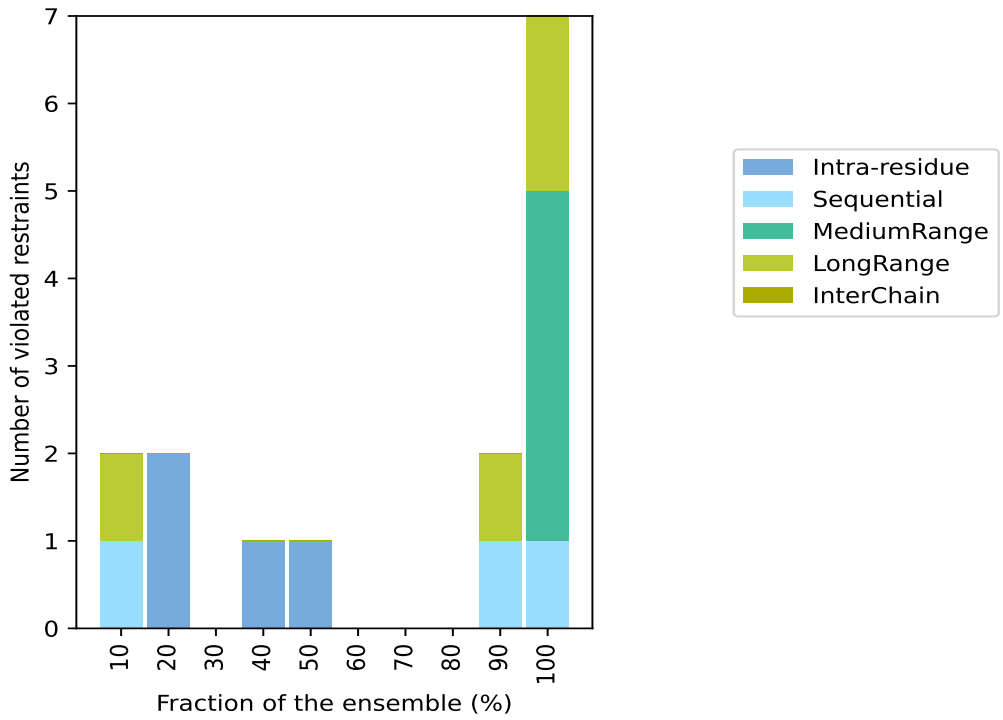
Continued on next page...

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	0	0	0	0	1	4	40.0
1	0	0	0	0	1	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	1	0	1	0	2	9	90.0
0	1	4	2	0	7	10	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

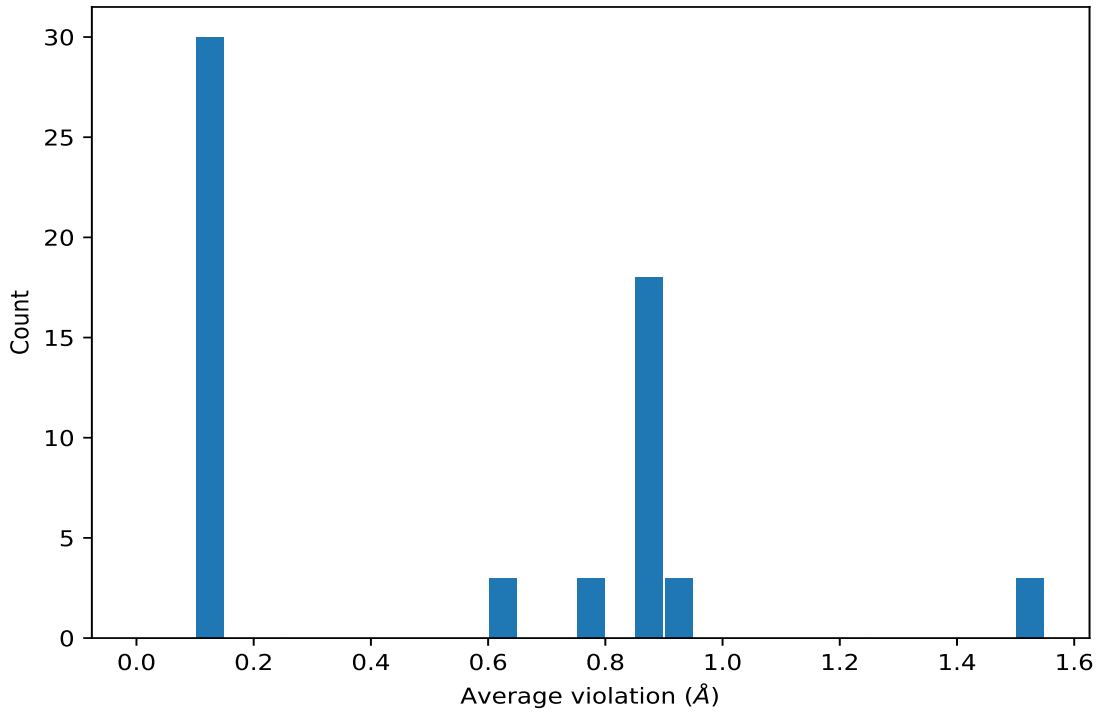


9.4 Most violated distance restraints in the ensemble

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)
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	10	1.5	0.14	1.58
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	10	1.5	0.14	1.58
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	10	1.5	0.14	1.58
(1,399)	1:115:A:ILE:HD11	1:113:A:PHE:HE1	10	0.93	0.25	1.06
(1,399)	1:115:A:ILE:HD12	1:113:A:PHE:HE1	10	0.93	0.25	1.06
(1,399)	1:115:A:ILE:HD13	1:113:A:PHE:HE1	10	0.93	0.25	1.06
(1,328)	1:55:A:VAL:HG21	1:77:A:LEU:HD21	10	0.88	0.22	0.8
(1,328)	1:55:A:VAL:HG21	1:77:A:LEU:HD22	10	0.88	0.22	0.8
(1,328)	1:55:A:VAL:HG21	1:77:A:LEU:HD23	10	0.88	0.22	0.8
(1,328)	1:55:A:VAL:HG22	1:77:A:LEU:HD21	10	0.88	0.22	0.8
(1,328)	1:55:A:VAL:HG22	1:77:A:LEU:HD22	10	0.88	0.22	0.8
(1,328)	1:55:A:VAL:HG22	1:77:A:LEU:HD23	10	0.88	0.22	0.8
(1,328)	1:55:A:VAL:HG23	1:77:A:LEU:HD21	10	0.88	0.22	0.8
(1,328)	1:55:A:VAL:HG23	1:77:A:LEU:HD22	10	0.88	0.22	0.8
(1,328)	1:55:A:VAL:HG23	1:77:A:LEU:HD23	10	0.88	0.22	0.8

Continued on next page...

Continued from previous page...

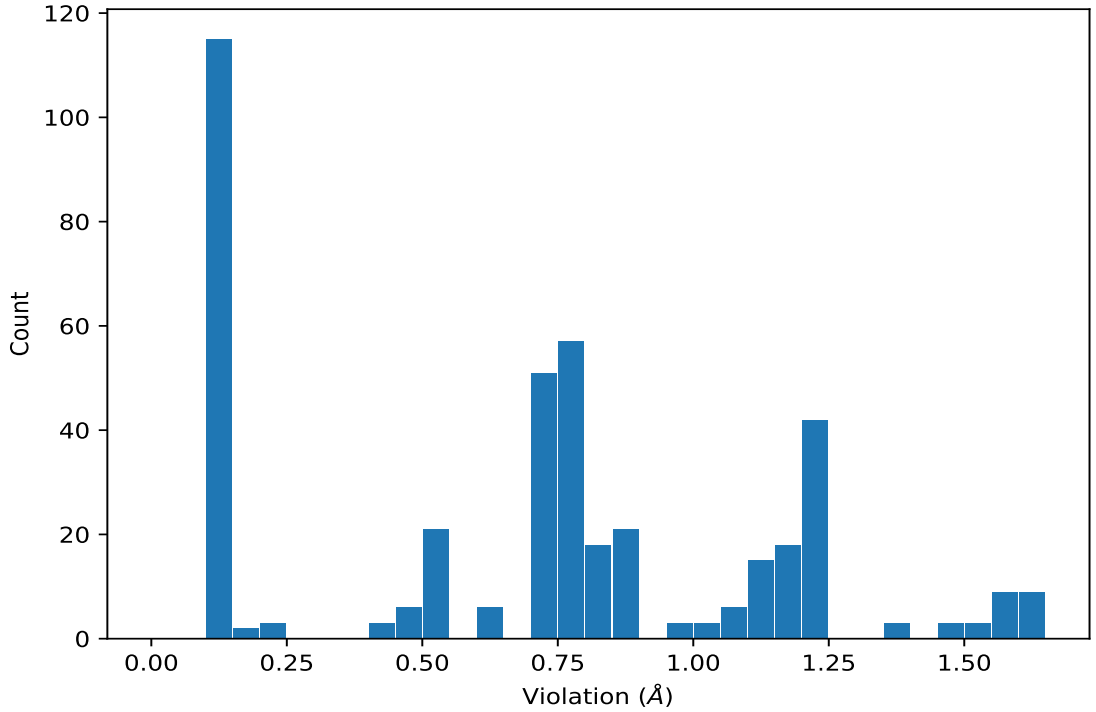
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,357)	1:77:A:LEU:HD21	1:55:A:VAL:HG21	10	0.88	0.22	0.8
(1,357)	1:77:A:LEU:HD21	1:55:A:VAL:HG22	10	0.88	0.22	0.8
(1,357)	1:77:A:LEU:HD21	1:55:A:VAL:HG23	10	0.88	0.22	0.8
(1,357)	1:77:A:LEU:HD22	1:55:A:VAL:HG21	10	0.88	0.22	0.8
(1,357)	1:77:A:LEU:HD22	1:55:A:VAL:HG22	10	0.88	0.22	0.8
(1,357)	1:77:A:LEU:HD22	1:55:A:VAL:HG23	10	0.88	0.22	0.8
(1,357)	1:77:A:LEU:HD23	1:55:A:VAL:HG21	10	0.88	0.22	0.8
(1,357)	1:77:A:LEU:HD23	1:55:A:VAL:HG22	10	0.88	0.22	0.8
(1,357)	1:77:A:LEU:HD23	1:55:A:VAL:HG23	10	0.88	0.22	0.8
(1,391)	1:112:A:ILE:HD11	1:113:A:PHE:HE1	10	0.78	0.2	0.72
(1,391)	1:112:A:ILE:HD12	1:113:A:PHE:HE1	10	0.78	0.2	0.72
(1,391)	1:112:A:ILE:HD13	1:113:A:PHE:HE1	10	0.78	0.2	0.72
(1,112)	1:67:A:LEU:H	1:70:A:GLY:H	10	0.13	0.02	0.13
(1,118)	1:70:A:GLY:H	1:67:A:LEU:H	10	0.13	0.02	0.13
(1,412)	1:130:A:ILE:HD11	1:113:A:PHE:HE1	9	0.64	0.22	0.63
(1,412)	1:130:A:ILE:HD12	1:113:A:PHE:HE1	9	0.64	0.22	0.63
(1,412)	1:130:A:ILE:HD13	1:113:A:PHE:HE1	9	0.64	0.22	0.63
(1,85)	1:56:A:TYR:H	1:55:A:VAL:HG21	9	0.11	0.01	0.11
(1,85)	1:56:A:TYR:H	1:55:A:VAL:HG22	9	0.11	0.01	0.11
(1,85)	1:56:A:TYR:H	1:55:A:VAL:HG23	9	0.11	0.01	0.11
(1,256)	1:124:A:LEU:H	1:124:A:LEU:HD11	5	0.12	0.01	0.12

[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)
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	2	1.62
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	2	1.62
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	2	1.62
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	1	1.6
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	1	1.6
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	1	1.6
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	3	1.6
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	3	1.6
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	3	1.6
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	8	1.59
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	8	1.59
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	8	1.59
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	9	1.58
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	9	1.58
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	9	1.58
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	7	1.57
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	7	1.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	7	1.57
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	10	1.53
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	10	1.53
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	10	1.53
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	6	1.45
(1,398)	1:115:A:ILE:HD12	1:113:A:PHE:HD1	6	1.45
(1,398)	1:115:A:ILE:HD13	1:113:A:PHE:HD1	6	1.45
(1,391)	1:112:A:ILE:HD11	1:113:A:PHE:HE1	5	1.37
(1,391)	1:112:A:ILE:HD12	1:113:A:PHE:HE1	5	1.37
(1,391)	1:112:A:ILE:HD13	1:113:A:PHE:HE1	5	1.37
(1,398)	1:115:A:ILE:HD11	1:113:A:PHE:HD1	5	1.24

10 Dihedral-angle violation analysis

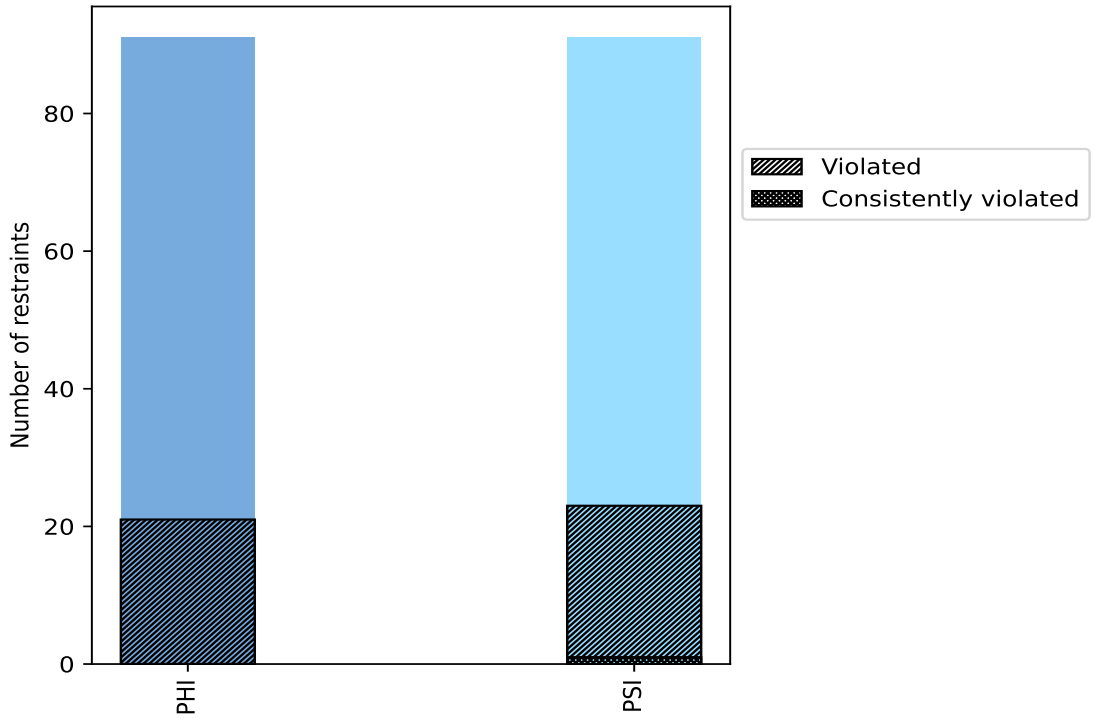
10.1 Summary of dihedral-angle violations

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	91	50.0	21	23.1	11.5	0	0.0	0.0
PSI	91	50.0	23	25.3	12.6	1	1.1	0.5
Total	182	100.0	44	24.2	24.2	1	0.5	0.5

[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



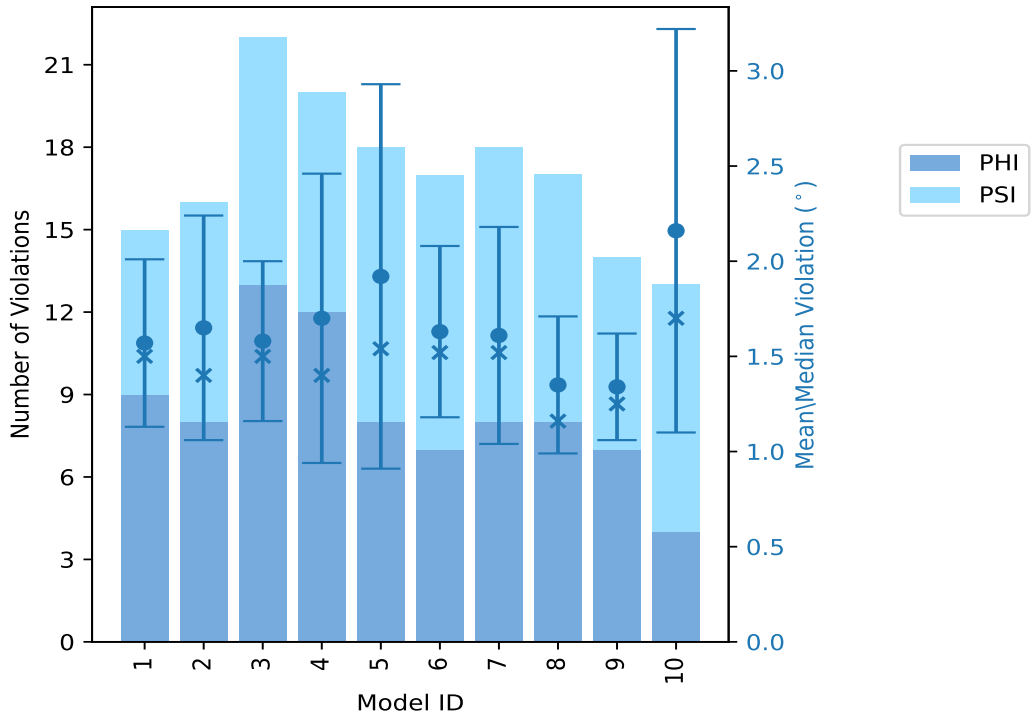
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	9	6	15	1.57	2.56	0.44	1.5
2	8	8	16	1.65	3.28	0.59	1.4
3	13	9	22	1.58	2.52	0.42	1.5
4	12	8	20	1.7	3.83	0.76	1.4
5	8	10	18	1.92	4.87	1.01	1.54
6	7	10	17	1.63	2.51	0.45	1.52
7	8	10	18	1.61	2.93	0.57	1.52
8	8	9	17	1.35	2.1	0.36	1.16
9	7	7	14	1.34	1.9	0.28	1.25
10	4	9	13	2.16	4.96	1.06	1.7

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



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

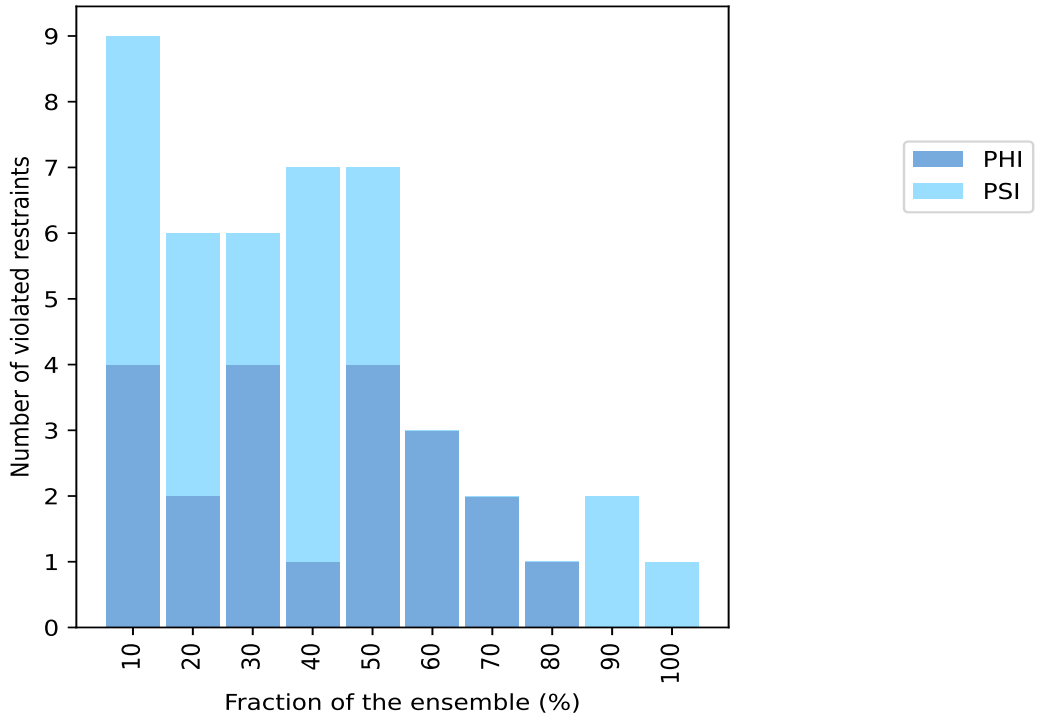
10.3 Dihedral-angle violation statistics for the ensemble

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

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

[1] Number of models with violations

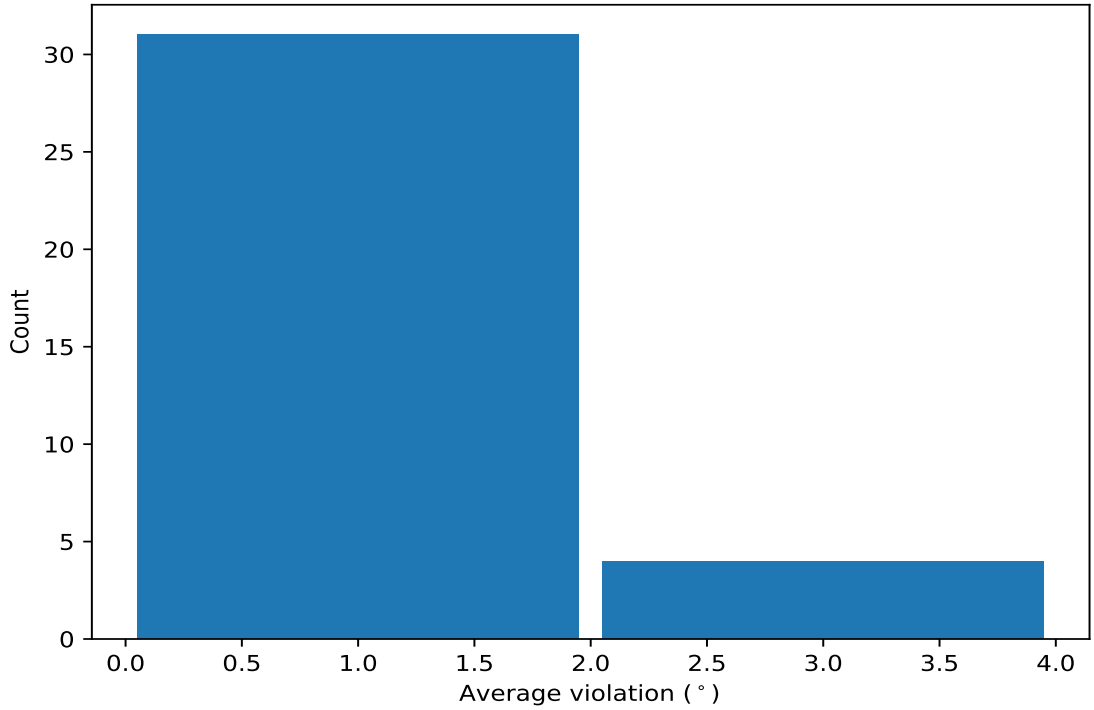
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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 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.

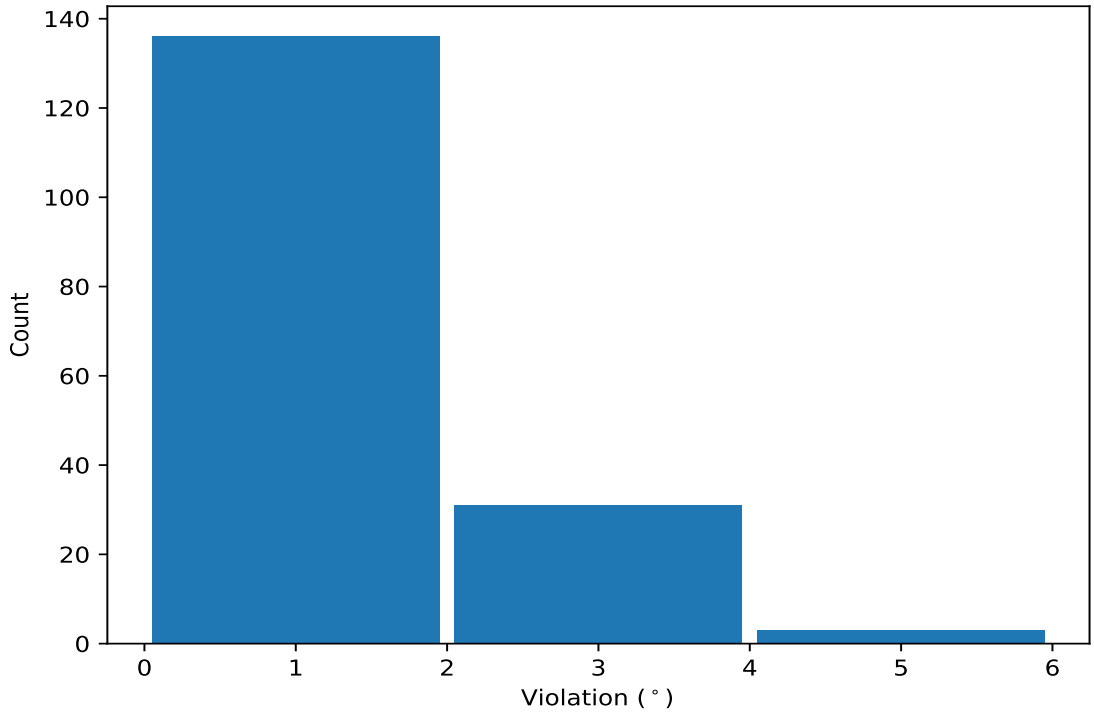
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,163)	1:112:A:ILE:N	1:112:A:ILE:CA	1:112:A:ILE:C	1:113:A:PHE:N	10	2.84	1.08	2.47
(1,101)	1:46:A:MET:N	1:46:A:MET:CA	1:46:A:MET:C	1:47:A:VAL:N	9	1.87	0.53	1.88
(1,103)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:GLU:N	9	1.77	0.28	1.83
(1,73)	1:112:A:ILE:C	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	8	2.37	1.24	1.65
(1,83)	1:124:A:LEU:C	1:125:A:SER:N	1:125:A:SER:CA	1:125:A:SER:C	7	1.66	0.35	1.68
(1,20)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	7	1.38	0.23	1.3
(1,18)	1:53:A:LYS:C	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	6	1.57	0.53	1.48
(1,76)	1:116:A:PRO:C	1:117:A:GLY:N	1:117:A:GLY:CA	1:117:A:GLY:C	6	1.52	0.2	1.56
(1,87)	1:128:A:ASP:C	1:129:A:GLN:N	1:129:A:GLN:CA	1:129:A:GLN:C	6	1.28	0.26	1.16
(1,173)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:SER:N	5	2.35	0.33	2.37

[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

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 (°)
(1,163)	1:112:A:ILE:N	1:112:A:ILE:CA	1:112:A:ILE:C	1:113:A:PHE:N	10	4.96
(1,73)	1:112:A:ILE:C	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	5	4.87
(1,163)	1:112:A:ILE:N	1:112:A:ILE:CA	1:112:A:ILE:C	1:113:A:PHE:N	5	4.02
(1,163)	1:112:A:ILE:N	1:112:A:ILE:CA	1:112:A:ILE:C	1:113:A:PHE:N	4	3.83
(1,120)	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	1:66:A:GLU:N	10	3.58
(1,73)	1:112:A:ILE:C	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	4	3.37
(1,73)	1:112:A:ILE:C	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	10	3.35
(1,163)	1:112:A:ILE:N	1:112:A:ILE:CA	1:112:A:ILE:C	1:113:A:PHE:N	2	3.28
(1,120)	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	1:66:A:GLU:N	7	2.93
(1,173)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:SER:N	7	2.84