wwPDB NMR Structure Validation Summary Report

Jun 3, 2023 – 07:53 PM EDT

PDB ID	:	2N3H
BMRB ID	:	25138
Title	:	Solution structure of DRB4 dsRBD2 (viz. DRB4(81-151))
Authors	:	Deshmukh, M.; Chiliveri, S.
Deposited on	:	2015-05-29

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (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:

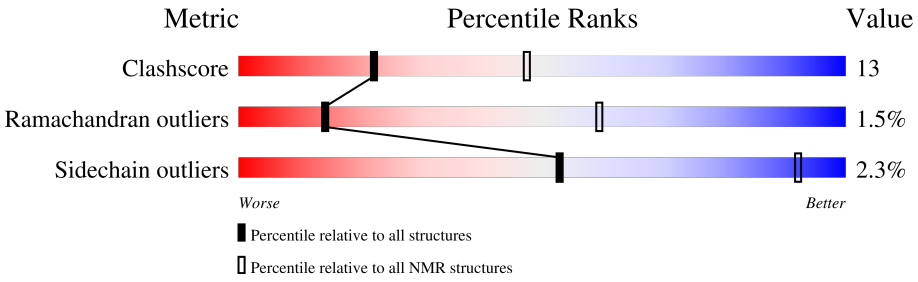
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 86%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	153	38% 7% • 54%

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:82-A:149 (68)	0.47	13

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1069 atoms, of which 538 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Double-stranded RNA-binding protein 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	71	1069	341	538	85	103	2	0

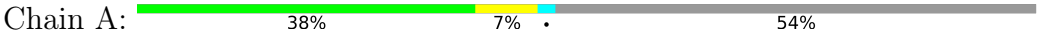
4 Residue-property plots (i)

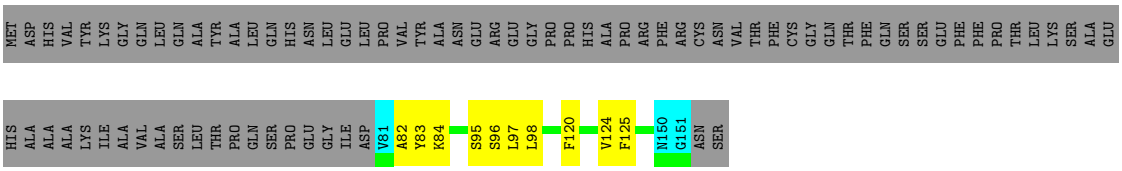
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Double-stranded RNA-binding protein 4

Chain A:



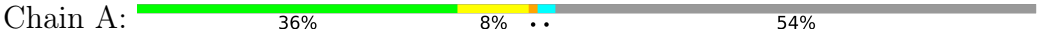


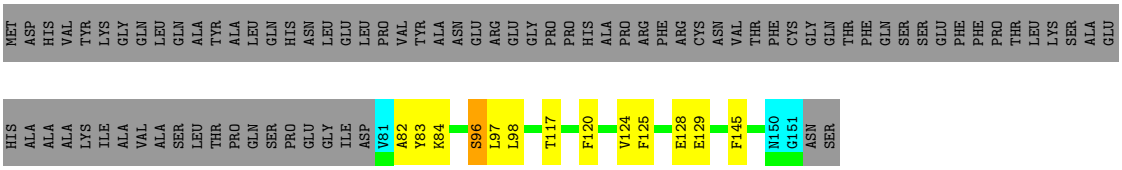
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

• Molecule 1: Double-stranded RNA-binding protein 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, 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
Sparky	structure solution	
Sparky	structure solution	
Sparky	structure solution	
Sparky	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	1658
Number of shifts mapped to atoms	788
Number of unparsed shifts	0
Number of shifts with mapping errors	870
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	512	521	521	13±3
All	All	10240	10420	10420	263

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 13.

5 of 65 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:PHE:CZ	1:A:125:PHE:CE1	0.64	2.86	11	20
1:A:120:PHE:CE1	1:A:125:PHE:CD1	0.58	2.91	15	1
1:A:146:MET:N	1:A:146:MET:SD	0.58	2.76	3	1
1:A:138:MET:N	1:A:138:MET:SD	0.57	2.77	7	1
1:A:120:PHE:CE2	1:A:125:PHE:CD1	0.56	2.94	5	18

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	68/153 (44%)	63±1 (93±2%)	4±2 (6±2%)	1±1 (2±1%)	14 59
All	All	1360/3060 (44%)	1259 (93%)	80 (6%)	21 (2%)	14 59

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	83	TYR	14
1	A	96	SER	5
1	A	95	SER	2

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	54/124 (44%)	53±1 (98±2%)	1±1 (2±2%)	53 92
All	All	1080/2480 (44%)	1055 (98%)	25 (2%)	53 92

5 of 8 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	114	PHE	10
1	A	95	SER	5
1	A	103	THR	3
1	A	132	THR	3
1	A	146	MET	1

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 monosaccharides 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 86% for the well-defined parts and 86% 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	1658
Number of shifts mapped to atoms	788
Number of unparsed shifts	0
Number of shifts with mapping errors	870
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 870) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	HIS	HA	3.68	0.02	1
1	A	3	HIS	HB2	2.58	0.02	2
1	A	3	HIS	HB3	2.2	0.02	2
1	A	3	HIS	C	175.9	0.3	1
1	A	3	HIS	CA	54.1	0.3	1
1	A	3	HIS	CB	28.2	0.3	1
1	A	4	VAL	H	6.86	0.02	1
1	A	4	VAL	HA	4.37	0.02	1
1	A	4	VAL	HB	1.99	0.02	1
1	A	4	VAL	HG11	0.48	0.02	1
1	A	4	VAL	HG12	0.48	0.02	1
1	A	4	VAL	HG13	0.48	0.02	1
1	A	4	VAL	HG21	-0.17	0.02	1
1	A	4	VAL	HG22	-0.17	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	VAL	HG23	-0.17	0.02	1
1	A	4	VAL	C	177.1	0.3	1
1	A	4	VAL	CA	60.4	0.3	1
1	A	4	VAL	CB	32.7	0.3	1
1	A	4	VAL	CG1	20.7	0.3	1
1	A	4	VAL	CG2	16.6	0.3	1
1	A	4	VAL	N	111.8	0.3	1
1	A	5	TYR	H	8.26	0.02	1
1	A	5	TYR	HA	4.19	0.02	1
1	A	5	TYR	HB2	3.09	0.02	2
1	A	5	TYR	HB3	2.75	0.02	2
1	A	5	TYR	HD1	6.94	0.02	3
1	A	5	TYR	HD2	7.01	0.02	3
1	A	5	TYR	C	177.9	0.3	1
1	A	5	TYR	CA	62.3	0.3	1
1	A	5	TYR	CB	39.6	0.3	1
1	A	5	TYR	N	123.6	0.3	1
1	A	6	LYS	H	8.48	0.02	1
1	A	6	LYS	C	180.5	0.3	1
1	A	6	LYS	CA	60.6	0.3	1
1	A	6	LYS	CB	31.6	0.3	1
1	A	6	LYS	N	121.2	0.3	1
1	A	7	GLY	H	8.7	0.02	1
1	A	7	GLY	HA2	3.71	0.02	2
1	A	7	GLY	HA3	3.78	0.02	2
1	A	7	GLY	C	176.5	0.3	1
1	A	7	GLY	CA	46.5	0.3	1
1	A	7	GLY	N	108.8	0.3	1
1	A	8	GLN	H	7.29	0.02	1
1	A	8	GLN	HA	4.03	0.02	1
1	A	8	GLN	HB2	2.08	0.02	2
1	A	8	GLN	HB3	2.19	0.02	2
1	A	8	GLN	HG2	2.48	0.02	1
1	A	8	GLN	HG3	2.48	0.02	1
1	A	8	GLN	HE21	6.94	0.02	1
1	A	8	GLN	HE22	6.45	0.02	1
1	A	8	GLN	C	178.9	0.3	1
1	A	8	GLN	CA	58.8	0.3	1
1	A	8	GLN	CB	28.5	0.3	1
1	A	8	GLN	CG	33.7	0.3	1
1	A	8	GLN	N	122.9	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	GLN	NE2	109.6	0.3	1
1	A	9	LEU	H	7.73	0.02	1
1	A	9	LEU	HA	3.8	0.02	1
1	A	9	LEU	HB2	1.22	0.02	2
1	A	9	LEU	HB3	1.45	0.02	2
1	A	9	LEU	HG	0.99	0.02	1
1	A	9	LEU	HD11	0.18	0.02	1
1	A	9	LEU	HD12	0.18	0.02	1
1	A	9	LEU	HD13	0.18	0.02	1
1	A	9	LEU	HD21	0.37	0.02	1
1	A	9	LEU	HD22	0.37	0.02	1
1	A	9	LEU	HD23	0.37	0.02	1
1	A	9	LEU	C	177.4	0.3	1
1	A	9	LEU	CA	57.1	0.3	1
1	A	9	LEU	CB	41.0	0.3	1
1	A	9	LEU	CG	26.1	0.3	1
1	A	9	LEU	CD1	23.0	0.3	1
1	A	9	LEU	CD2	24.8	0.3	1
1	A	9	LEU	N	121.7	0.3	1
1	A	10	GLN	H	7.75	0.02	1
1	A	10	GLN	HA	3.63	0.02	1
1	A	10	GLN	HB2	2.05	0.02	1
1	A	10	GLN	HB3	2.05	0.02	1
1	A	10	GLN	HG2	1.44	0.02	1
1	A	10	GLN	HG3	1.44	0.02	1
1	A	10	GLN	HE21	7.11	0.02	1
1	A	10	GLN	HE22	6.64	0.02	1
1	A	10	GLN	C	176.9	0.3	1
1	A	10	GLN	CA	59.5	0.3	1
1	A	10	GLN	CB	28.3	0.3	1
1	A	10	GLN	CG	33.4	0.3	1
1	A	10	GLN	N	119.0	0.3	1
1	A	10	GLN	NE2	111.7	0.3	1
1	A	11	ALA	H	8.09	0.02	1
1	A	11	ALA	HA	3.84	0.02	1
1	A	11	ALA	HB1	1.4	0.02	1
1	A	11	ALA	HB2	1.4	0.02	1
1	A	11	ALA	HB3	1.4	0.02	1
1	A	11	ALA	C	180.0	0.3	1
1	A	11	ALA	CA	55.0	0.3	1
1	A	11	ALA	CB	17.6	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ALA	N	120.6	0.3	1
1	A	12	TYR	H	7.75	0.02	1
1	A	12	TYR	HA	4.13	0.02	1
1	A	12	TYR	HB2	3.14	0.02	2
1	A	12	TYR	HB3	3.08	0.02	2
1	A	12	TYR	HD1	7.04	0.02	1
1	A	12	TYR	HD2	7.04	0.02	1
1	A	12	TYR	HE1	7.04	0.02	1
1	A	12	TYR	HE2	7.04	0.02	1
1	A	12	TYR	C	177.7	0.3	1
1	A	12	TYR	CA	61.9	0.3	1
1	A	12	TYR	CB	38.3	0.3	1
1	A	12	TYR	N	120.8	0.3	1
1	A	13	ALA	H	8.26	0.02	1
1	A	13	ALA	HA	4.1	0.02	1
1	A	13	ALA	HB1	1.67	0.02	1
1	A	13	ALA	HB2	1.67	0.02	1
1	A	13	ALA	HB3	1.67	0.02	1
1	A	13	ALA	C	179.5	0.3	1
1	A	13	ALA	CA	55.8	0.3	1
1	A	13	ALA	CB	18.0	0.3	1
1	A	13	ALA	N	122.2	0.3	1
1	A	14	LEU	H	8.25	0.02	1
1	A	14	LEU	HA	4.09	0.02	1
1	A	14	LEU	HB2	1.46	0.02	1
1	A	14	LEU	HB3	1.46	0.02	1
1	A	14	LEU	HG	1.77	0.02	1
1	A	14	LEU	HD11	0.84	0.02	1
1	A	14	LEU	HD12	0.84	0.02	1
1	A	14	LEU	HD13	0.84	0.02	1
1	A	14	LEU	HD21	0.84	0.02	1
1	A	14	LEU	HD22	0.84	0.02	1
1	A	14	LEU	HD23	0.84	0.02	1
1	A	14	LEU	C	180.6	0.3	1
1	A	14	LEU	CA	57.3	0.3	1
1	A	14	LEU	CB	41.5	0.3	1
1	A	14	LEU	CG	26.6	0.3	1
1	A	14	LEU	CD1	22.8	0.3	1
1	A	14	LEU	CD2	25.1	0.3	1
1	A	14	LEU	N	117.6	0.3	1
1	A	15	GLN	H	8.11	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	GLN	HA	3.79	0.02	1
1	A	15	GLN	HB2	1.59	0.02	2
1	A	15	GLN	HB3	1.69	0.02	2
1	A	15	GLN	HG2	1.92	0.02	1
1	A	15	GLN	HG3	1.92	0.02	1
1	A	15	GLN	C	176.7	0.3	1
1	A	15	GLN	CA	58.0	0.3	1
1	A	15	GLN	CB	28.1	0.3	1
1	A	15	GLN	CG	32.9	0.3	1
1	A	15	GLN	N	120.0	0.3	1
1	A	16	HIS	H	7.25	0.02	1
1	A	16	HIS	HA	4.46	0.02	1
1	A	16	HIS	HB2	3.19	0.02	2
1	A	16	HIS	HB3	2.32	0.02	2
1	A	16	HIS	C	173.1	0.3	1
1	A	16	HIS	CA	55.9	0.3	1
1	A	16	HIS	CB	29.5	0.3	1
1	A	16	HIS	N	114.2	0.3	1
1	A	17	ASN	H	7.63	0.02	1
1	A	17	ASN	HA	4.33	0.02	1
1	A	17	ASN	HB2	2.65	0.02	2
1	A	17	ASN	HB3	3.0	0.02	2
1	A	17	ASN	C	173.8	0.3	1
1	A	17	ASN	CA	54.3	0.3	1
1	A	17	ASN	CB	36.6	0.3	1
1	A	17	ASN	N	118.2	0.3	1
1	A	18	LEU	H	8.53	0.02	1
1	A	18	LEU	HA	4.55	0.02	1
1	A	18	LEU	HB2	1.57	0.02	1
1	A	18	LEU	HB3	1.57	0.02	1
1	A	18	LEU	HG	1.47	0.02	1
1	A	18	LEU	HD11	0.84	0.02	1
1	A	18	LEU	HD12	0.84	0.02	1
1	A	18	LEU	HD13	0.84	0.02	1
1	A	18	LEU	HD21	0.75	0.02	1
1	A	18	LEU	HD22	0.75	0.02	1
1	A	18	LEU	HD23	0.75	0.02	1
1	A	18	LEU	C	176.4	0.3	1
1	A	18	LEU	CA	52.8	0.3	1
1	A	18	LEU	CB	44.2	0.3	1
1	A	18	LEU	CG	26.5	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	LEU	CD1	22.0	0.3	1
1	A	18	LEU	CD2	22.2	0.3	1
1	A	18	LEU	N	119.5	0.3	1
1	A	19	GLU	H	8.07	0.02	1
1	A	19	GLU	HA	4.01	0.02	1
1	A	19	GLU	HB2	1.95	0.02	2
1	A	19	GLU	HB3	1.86	0.02	2
1	A	19	GLU	HG2	2.3	0.02	1
1	A	19	GLU	HG3	2.3	0.02	1
1	A	19	GLU	C	176.6	0.3	1
1	A	19	GLU	CA	56.7	0.3	1
1	A	19	GLU	CB	29.3	0.3	1
1	A	19	GLU	CG	36.5	0.3	1
1	A	19	GLU	N	120.6	0.3	1
1	A	20	LEU	H	8.18	0.02	1
1	A	20	LEU	HA	4.37	0.02	1
1	A	20	LEU	HB2	1.67	0.02	1
1	A	20	LEU	HB3	1.67	0.02	1
1	A	20	LEU	HD11	0.92	0.02	1
1	A	20	LEU	HD12	0.92	0.02	1
1	A	20	LEU	HD13	0.92	0.02	1
1	A	20	LEU	HD21	0.92	0.02	1
1	A	20	LEU	HD22	0.92	0.02	1
1	A	20	LEU	HD23	0.92	0.02	1
1	A	20	LEU	C	175.5	0.3	1
1	A	20	LEU	CA	54.0	0.3	1
1	A	20	LEU	CB	39.4	0.3	1
1	A	20	LEU	N	122.5	0.3	1
1	A	21	PRO	HA	4.63	0.02	1
1	A	21	PRO	HB2	1.89	0.02	1
1	A	21	PRO	HB3	1.89	0.02	1
1	A	21	PRO	HG2	1.85	0.02	1
1	A	21	PRO	HG3	1.85	0.02	1
1	A	21	PRO	HD2	3.56	0.02	2
1	A	21	PRO	HD3	3.59	0.02	2
1	A	21	PRO	C	175.0	0.3	1
1	A	21	PRO	CA	62.4	0.3	1
1	A	21	PRO	CB	32.7	0.3	1
1	A	21	PRO	CG	27.2	0.3	1
1	A	21	PRO	CD	49.8	0.3	1
1	A	22	VAL	H	7.97	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	VAL	HA	4.3	0.02	1
1	A	22	VAL	HB	1.74	0.02	1
1	A	22	VAL	HG11	0.84	0.02	1
1	A	22	VAL	HG12	0.84	0.02	1
1	A	22	VAL	HG13	0.84	0.02	1
1	A	22	VAL	HG21	0.92	0.02	1
1	A	22	VAL	HG22	0.92	0.02	1
1	A	22	VAL	HG23	0.92	0.02	1
1	A	22	VAL	C	175.5	0.3	1
1	A	22	VAL	CA	61.3	0.3	1
1	A	22	VAL	CB	34.5	0.3	1
1	A	22	VAL	CG1	20.8	0.3	1
1	A	22	VAL	CG2	20.8	0.3	1
1	A	22	VAL	N	121.0	0.3	1
1	A	23	TYR	H	9.24	0.02	1
1	A	23	TYR	HA	4.82	0.02	1
1	A	23	TYR	HB2	2.77	0.02	1
1	A	23	TYR	HB3	2.77	0.02	1
1	A	23	TYR	HD1	6.88	0.02	1
1	A	23	TYR	HD2	6.88	0.02	1
1	A	23	TYR	HE1	6.88	0.02	1
1	A	23	TYR	HE2	6.88	0.02	1
1	A	23	TYR	C	174.7	0.3	1
1	A	23	TYR	CA	58.1	0.3	1
1	A	23	TYR	CB	40.0	0.3	1
1	A	23	TYR	N	131.0	0.3	1
1	A	24	ALA	H	8.7	0.02	1
1	A	24	ALA	HA	4.73	0.02	1
1	A	24	ALA	HB1	1.35	0.02	1
1	A	24	ALA	HB2	1.35	0.02	1
1	A	24	ALA	HB3	1.35	0.02	1
1	A	24	ALA	C	175.6	0.3	1
1	A	24	ALA	CA	51.2	0.3	1
1	A	24	ALA	CB	21.4	0.3	1
1	A	24	ALA	N	127.2	0.3	1
1	A	25	ASN	H	8.78	0.02	1
1	A	25	ASN	HA	5.68	0.02	1
1	A	25	ASN	HB2	2.62	0.02	2
1	A	25	ASN	HB3	2.44	0.02	2
1	A	25	ASN	HD21	7.66	0.02	1
1	A	25	ASN	HD22	6.81	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	25	ASN	C	173.5	0.3	1
1	A	25	ASN	CA	52.2	0.3	1
1	A	25	ASN	CB	44.6	0.3	1
1	A	25	ASN	N	117.0	0.3	1
1	A	25	ASN	ND2	116.4	0.3	1
1	A	26	GLU	H	8.88	0.02	1
1	A	26	GLU	HA	4.59	0.02	1
1	A	26	GLU	HB2	1.91	0.02	1
1	A	26	GLU	HB3	1.91	0.02	1
1	A	26	GLU	HG2	2.18	0.02	1
1	A	26	GLU	HG3	2.18	0.02	1
1	A	26	GLU	C	173.8	0.3	1
1	A	26	GLU	CA	54.7	0.3	1
1	A	26	GLU	CB	33.5	0.3	1
1	A	26	GLU	CG	36.2	0.3	1
1	A	26	GLU	N	121.3	0.3	1
1	A	27	ARG	H	8.48	0.02	1
1	A	27	ARG	HA	5.28	0.02	1
1	A	27	ARG	HB2	1.51	0.02	1
1	A	27	ARG	HB3	1.51	0.02	1
1	A	27	ARG	HG2	1.15	0.02	2
1	A	27	ARG	HG3	0.99	0.02	2
1	A	27	ARG	HD2	2.96	0.02	2
1	A	27	ARG	HD3	2.91	0.02	2
1	A	27	ARG	C	175.3	0.3	1
1	A	27	ARG	CA	53.9	0.3	1
1	A	27	ARG	CB	33.0	0.3	1
1	A	27	ARG	CG	26.2	0.3	1
1	A	27	ARG	CD	43.4	0.3	1
1	A	27	ARG	N	123.4	0.3	1
1	A	28	GLU	H	8.74	0.02	1
1	A	28	GLU	HA	4.53	0.02	1
1	A	28	GLU	HB2	1.36	0.02	1
1	A	28	GLU	HB3	1.36	0.02	1
1	A	28	GLU	HG2	1.71	0.02	2
1	A	28	GLU	HG3	1.83	0.02	2
1	A	28	GLU	C	174.8	0.3	1
1	A	28	GLU	CA	54.3	0.3	1
1	A	28	GLU	CB	33.1	0.3	1
1	A	28	GLU	CG	35.5	0.3	1
1	A	28	GLU	N	125.4	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	GLY	H	8.14	0.02	1
1	A	29	GLY	HA2	4.26	0.02	2
1	A	29	GLY	HA3	3.61	0.02	2
1	A	29	GLY	C	171.0	0.3	1
1	A	29	GLY	CA	43.6	0.3	1
1	A	29	GLY	N	107.9	0.3	1
1	A	31	PRO	HA	3.97	0.02	1
1	A	31	PRO	HB2	2.25	0.02	2
1	A	31	PRO	HB3	2.08	0.02	2
1	A	31	PRO	HG2	1.95	0.02	2
1	A	31	PRO	HG3	1.88	0.02	2
1	A	31	PRO	HD2	3.72	0.02	2
1	A	31	PRO	HD3	3.68	0.02	2
1	A	31	PRO	C	177.2	0.3	1
1	A	31	PRO	CA	65.1	0.3	1
1	A	31	PRO	CB	31.5	0.3	1
1	A	31	PRO	CG	27.5	0.3	1
1	A	32	HIS	H	7.35	0.02	1
1	A	32	HIS	HA	4.52	0.02	1
1	A	32	HIS	HB2	3.24	0.02	2
1	A	32	HIS	HB3	2.87	0.02	2
1	A	32	HIS	C	175.1	0.3	1
1	A	32	HIS	CA	55.7	0.3	1
1	A	32	HIS	CB	30.0	0.3	1
1	A	32	HIS	N	110.4	0.3	1
1	A	33	ALA	H	7.24	0.02	1
1	A	33	ALA	HA	4.53	0.02	1
1	A	33	ALA	HB1	0.87	0.02	1
1	A	33	ALA	HB2	0.87	0.02	1
1	A	33	ALA	HB3	0.87	0.02	1
1	A	33	ALA	C	175.1	0.3	1
1	A	33	ALA	CA	50.5	0.3	1
1	A	33	ALA	CB	18.3	0.3	1
1	A	33	ALA	N	125.9	0.3	1
1	A	34	PRO	HA	4.31	0.02	1
1	A	34	PRO	HB2	1.71	0.02	1
1	A	34	PRO	HB3	1.71	0.02	1
1	A	34	PRO	HG2	1.2	0.02	1
1	A	34	PRO	HG3	1.2	0.02	1
1	A	34	PRO	HD2	3.38	0.02	2
1	A	34	PRO	HD3	3.29	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	PRO	C	175.7	0.3	1
1	A	34	PRO	CA	62.6	0.3	1
1	A	34	PRO	CB	32.2	0.3	1
1	A	34	PRO	CG	26.6	0.3	1
1	A	34	PRO	CD	49.3	0.3	1
1	A	35	ARG	H	8.14	0.02	1
1	A	35	ARG	HA	4.74	0.02	1
1	A	35	ARG	HB2	1.33	0.02	1
1	A	35	ARG	HB3	1.33	0.02	1
1	A	35	ARG	HG2	1.24	0.02	1
1	A	35	ARG	HG3	1.24	0.02	1
1	A	35	ARG	HD2	2.62	0.02	2
1	A	35	ARG	HD3	2.85	0.02	2
1	A	35	ARG	C	174.6	0.3	1
1	A	35	ARG	CA	54.1	0.3	1
1	A	35	ARG	CB	33.1	0.3	1
1	A	35	ARG	CG	26.7	0.3	1
1	A	35	ARG	CD	43.2	0.3	1
1	A	35	ARG	N	117.1	0.3	1
1	A	36	PHE	H	9.42	0.02	1
1	A	36	PHE	HA	5.7	0.02	1
1	A	36	PHE	HB2	2.7	0.02	1
1	A	36	PHE	HB3	2.7	0.02	1
1	A	36	PHE	HD1	6.91	0.02	1
1	A	36	PHE	HD2	6.91	0.02	1
1	A	36	PHE	HE1	6.91	0.02	1
1	A	36	PHE	HE2	6.91	0.02	1
1	A	36	PHE	C	174.7	0.3	1
1	A	36	PHE	CA	57.2	0.3	1
1	A	36	PHE	CB	43.9	0.3	1
1	A	36	PHE	N	119.0	0.3	1
1	A	37	ARG	H	8.78	0.02	1
1	A	37	ARG	HA	4.97	0.02	1
1	A	37	ARG	HG2	0.92	0.02	2
1	A	37	ARG	HG3	0.96	0.02	2
1	A	37	ARG	HD2	2.93	0.02	2
1	A	37	ARG	HD3	2.88	0.02	2
1	A	37	ARG	C	176.0	0.3	1
1	A	37	ARG	CA	55.1	0.3	1
1	A	37	ARG	CB	34.0	0.3	1
1	A	37	ARG	CG	25.9	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	ARG	CD	43.9	0.3	1
1	A	37	ARG	N	122.9	0.3	1
1	A	38	CYS	H	9.34	0.02	1
1	A	38	CYS	HA	5.59	0.02	1
1	A	38	CYS	HB2	2.95	0.02	2
1	A	38	CYS	HB3	2.59	0.02	2
1	A	38	CYS	C	172.8	0.3	1
1	A	38	CYS	CA	58.2	0.3	1
1	A	38	CYS	CB	31.5	0.3	1
1	A	38	CYS	N	126.0	0.3	1
1	A	39	ASN	H	8.56	0.02	1
1	A	39	ASN	HA	5.32	0.02	1
1	A	39	ASN	HB2	2.47	0.02	1
1	A	39	ASN	HB3	2.47	0.02	1
1	A	39	ASN	HD21	7.3	0.02	1
1	A	39	ASN	HD22	6.69	0.02	1
1	A	39	ASN	C	172.8	0.3	1
1	A	39	ASN	CA	50.9	0.3	1
1	A	39	ASN	CB	42.4	0.3	1
1	A	39	ASN	N	118.7	0.3	1
1	A	39	ASN	ND2	115.7	0.3	1
1	A	40	VAL	H	8.8	0.02	1
1	A	40	VAL	HA	4.91	0.02	1
1	A	40	VAL	HB	1.48	0.02	1
1	A	40	VAL	HG11	0.66	0.02	1
1	A	40	VAL	HG12	0.66	0.02	1
1	A	40	VAL	HG13	0.66	0.02	1
1	A	40	VAL	HG21	-0.09	0.02	1
1	A	40	VAL	HG22	-0.09	0.02	1
1	A	40	VAL	HG23	-0.09	0.02	1
1	A	40	VAL	C	172.6	0.3	1
1	A	40	VAL	CA	58.1	0.3	1
1	A	40	VAL	CB	34.9	0.3	1
1	A	40	VAL	CG1	20.8	0.3	1
1	A	40	VAL	CG2	22.5	0.3	1
1	A	40	VAL	N	119.1	0.3	1
1	A	41	THR	H	8.86	0.02	1
1	A	41	THR	HA	5.36	0.02	1
1	A	41	THR	HB	3.76	0.02	1
1	A	41	THR	HG21	0.89	0.02	1
1	A	41	THR	HG22	0.89	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	THR	HG23	0.89	0.02	1
1	A	41	THR	C	174.2	0.3	1
1	A	41	THR	CA	61.4	0.3	1
1	A	41	THR	CB	69.5	0.3	1
1	A	41	THR	CG2	20.0	0.3	1
1	A	41	THR	N	126.8	0.3	1
1	A	42	PHE	H	9.4	0.02	1
1	A	42	PHE	HA	4.9	0.02	1
1	A	42	PHE	HB2	2.97	0.02	2
1	A	42	PHE	HB3	2.62	0.02	2
1	A	42	PHE	HD1	7.1	0.02	1
1	A	42	PHE	HD2	7.1	0.02	1
1	A	42	PHE	HE1	7.1	0.02	1
1	A	42	PHE	HE2	7.1	0.02	1
1	A	42	PHE	C	173.5	0.3	1
1	A	42	PHE	CA	56.5	0.3	1
1	A	42	PHE	CB	42.1	0.3	1
1	A	42	PHE	N	129.0	0.3	1
1	A	43	CYS	H	9.26	0.02	1
1	A	43	CYS	HA	3.59	0.02	1
1	A	43	CYS	HB2	2.79	0.02	2
1	A	43	CYS	HB3	2.29	0.02	2
1	A	43	CYS	C	174.8	0.3	1
1	A	43	CYS	CA	60.6	0.3	1
1	A	43	CYS	CB	25.2	0.3	1
1	A	43	CYS	N	126.0	0.3	1
1	A	44	GLY	H	8.66	0.02	1
1	A	44	GLY	HA2	3.88	0.02	2
1	A	44	GLY	HA3	3.42	0.02	2
1	A	44	GLY	C	173.1	0.3	1
1	A	44	GLY	CA	45.2	0.3	1
1	A	44	GLY	N	104.8	0.3	1
1	A	45	GLN	H	7.53	0.02	1
1	A	45	GLN	HA	4.36	0.02	1
1	A	45	GLN	HB2	1.41	0.02	1
1	A	45	GLN	HB3	1.41	0.02	1
1	A	45	GLN	HG2	1.75	0.02	2
1	A	45	GLN	HG3	1.85	0.02	2
1	A	45	GLN	C	173.0	0.3	1
1	A	45	GLN	CA	53.7	0.3	1
1	A	45	GLN	CB	32.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	GLN	CG	33.5	0.3	1
1	A	45	GLN	N	120.7	0.3	1
1	A	46	THR	H	8.29	0.02	1
1	A	46	THR	HA	4.77	0.02	1
1	A	46	THR	HB	3.55	0.02	1
1	A	46	THR	HG21	0.85	0.02	1
1	A	46	THR	HG22	0.85	0.02	1
1	A	46	THR	HG23	0.85	0.02	1
1	A	46	THR	C	173.2	0.3	1
1	A	46	THR	CA	61.9	0.3	1
1	A	46	THR	CB	69.7	0.3	1
1	A	46	THR	CG2	21.6	0.3	1
1	A	46	THR	N	119.0	0.3	1
1	A	47	PHE	H	9.38	0.02	1
1	A	47	PHE	HA	4.54	0.02	1
1	A	47	PHE	HB2	2.9	0.02	2
1	A	47	PHE	HB3	2.66	0.02	2
1	A	47	PHE	HD1	7.13	0.02	1
1	A	47	PHE	HD2	7.13	0.02	1
1	A	47	PHE	HE1	7.13	0.02	1
1	A	47	PHE	HE2	7.13	0.02	1
1	A	47	PHE	C	173.9	0.3	1
1	A	47	PHE	CA	56.6	0.3	1
1	A	47	PHE	CB	38.8	0.3	1
1	A	47	PHE	N	128.8	0.3	1
1	A	48	GLN	H	8.92	0.02	1
1	A	48	GLN	HA	4.44	0.02	1
1	A	48	GLN	HB2	2.11	0.02	2
1	A	48	GLN	HB3	1.83	0.02	2
1	A	48	GLN	HE21	7.79	0.02	1
1	A	48	GLN	HE22	7.25	0.02	1
1	A	48	GLN	C	174.9	0.3	1
1	A	48	GLN	CA	54.2	0.3	1
1	A	48	GLN	CB	32.0	0.3	1
1	A	48	GLN	N	124.8	0.3	1
1	A	48	GLN	NE2	116.9	0.3	1
1	A	49	SER	H	7.95	0.02	1
1	A	49	SER	C	175.2	0.3	1
1	A	49	SER	CA	57.5	0.3	1
1	A	49	SER	CB	63.3	0.3	1
1	A	49	SER	N	120.3	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	50	SER	HA	4.41	0.02	1
1	A	50	SER	HB2	3.94	0.02	2
1	A	50	SER	HB3	3.84	0.02	2
1	A	50	SER	C	174.3	0.3	1
1	A	50	SER	CA	59.1	0.3	1
1	A	50	SER	CB	63.7	0.3	1
1	A	51	GLU	H	7.71	0.02	1
1	A	51	GLU	HA	4.3	0.02	1
1	A	51	GLU	HB2	1.65	0.02	1
1	A	51	GLU	HB3	1.65	0.02	1
1	A	51	GLU	HG2	2.02	0.02	1
1	A	51	GLU	HG3	2.02	0.02	1
1	A	51	GLU	C	173.4	0.3	1
1	A	51	GLU	CA	55.4	0.3	1
1	A	51	GLU	CB	32.6	0.3	1
1	A	51	GLU	CG	36.6	0.3	1
1	A	51	GLU	N	123.3	0.3	1
1	A	52	PHE	H	8.1	0.02	1
1	A	52	PHE	HA	5.03	0.02	1
1	A	52	PHE	HB2	2.66	0.02	2
1	A	52	PHE	HB3	2.55	0.02	2
1	A	52	PHE	HD1	6.88	0.02	1
1	A	52	PHE	HD2	6.88	0.02	1
1	A	52	PHE	HE1	6.88	0.02	1
1	A	52	PHE	HE2	6.88	0.02	1
1	A	52	PHE	C	176.4	0.3	1
1	A	52	PHE	CA	56.7	0.3	1
1	A	52	PHE	CB	41.7	0.3	1
1	A	52	PHE	N	117.9	0.3	1
1	A	53	PHE	H	9.7	0.02	1
1	A	53	PHE	HA	4.86	0.02	1
1	A	53	PHE	HB2	3.3	0.02	1
1	A	53	PHE	HB3	3.3	0.02	1
1	A	53	PHE	HD1	7.29	0.02	1
1	A	53	PHE	HD2	7.29	0.02	1
1	A	53	PHE	HE1	7.29	0.02	1
1	A	53	PHE	HE2	7.29	0.02	1
1	A	53	PHE	C	175.2	0.3	1
1	A	53	PHE	CA	56.2	0.3	1
1	A	53	PHE	CB	43.0	0.3	1
1	A	53	PHE	N	119.3	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	PRO	HA	4.89	0.02	1
1	A	54	PRO	HB2	2.41	0.02	1
1	A	54	PRO	HB3	2.41	0.02	1
1	A	54	PRO	HG2	2.21	0.02	1
1	A	54	PRO	HG3	2.21	0.02	1
1	A	54	PRO	HD2	3.68	0.02	1
1	A	54	PRO	HD3	3.68	0.02	1
1	A	54	PRO	C	175.9	0.3	1
1	A	54	PRO	CA	63.9	0.3	1
1	A	54	PRO	CB	32.4	0.3	1
1	A	54	PRO	CG	27.1	0.3	1
1	A	55	THR	H	7.03	0.02	1
1	A	55	THR	HA	4.61	0.02	1
1	A	55	THR	HB	4.28	0.02	1
1	A	55	THR	HG21	1.21	0.02	1
1	A	55	THR	HG22	1.21	0.02	1
1	A	55	THR	HG23	1.21	0.02	1
1	A	55	THR	C	173.0	0.3	1
1	A	55	THR	CA	58.3	0.3	1
1	A	55	THR	CB	72.0	0.3	1
1	A	55	THR	CG2	21.6	0.3	1
1	A	55	THR	N	104.8	0.3	1
1	A	56	LEU	H	8.12	0.02	1
1	A	56	LEU	HA	3.31	0.02	1
1	A	56	LEU	HB2	1.05	0.02	2
1	A	56	LEU	HB3	0.07	0.02	2
1	A	56	LEU	HG	0.87	0.02	1
1	A	56	LEU	HD11	0.53	0.02	1
1	A	56	LEU	HD12	0.53	0.02	1
1	A	56	LEU	HD13	0.53	0.02	1
1	A	56	LEU	HD21	0.47	0.02	1
1	A	56	LEU	HD22	0.47	0.02	1
1	A	56	LEU	HD23	0.47	0.02	1
1	A	56	LEU	C	177.8	0.3	1
1	A	56	LEU	CA	56.9	0.3	1
1	A	56	LEU	CB	40.0	0.3	1
1	A	56	LEU	CG	26.3	0.3	1
1	A	56	LEU	CD1	22.8	0.3	1
1	A	56	LEU	CD2	24.9	0.3	1
1	A	56	LEU	N	126.7	0.3	1
1	A	57	LYS	H	8.05	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	LYS	HA	3.76	0.02	1
1	A	57	LYS	HB2	1.62	0.02	1
1	A	57	LYS	HB3	1.62	0.02	1
1	A	57	LYS	HG2	0.84	0.02	1
1	A	57	LYS	HG3	0.84	0.02	1
1	A	57	LYS	HD2	1.41	0.02	1
1	A	57	LYS	HD3	1.41	0.02	1
1	A	57	LYS	HE2	2.75	0.02	1
1	A	57	LYS	HE3	2.75	0.02	1
1	A	57	LYS	C	178.8	0.3	1
1	A	57	LYS	CA	59.3	0.3	1
1	A	57	LYS	CB	32.1	0.3	1
1	A	57	LYS	CG	24.6	0.3	1
1	A	57	LYS	CD	28.8	0.3	1
1	A	57	LYS	CE	43.9	0.3	1
1	A	57	LYS	N	118.4	0.3	1
1	A	58	SER	H	7.58	0.02	1
1	A	58	SER	HA	3.94	0.02	1
1	A	58	SER	HB2	3.64	0.02	1
1	A	58	SER	HB3	3.64	0.02	1
1	A	58	SER	C	174.9	0.3	1
1	A	58	SER	CA	62.3	0.3	1
1	A	58	SER	N	114.3	0.3	1
1	A	59	ALA	H	7.27	0.02	1
1	A	59	ALA	HA	3.82	0.02	1
1	A	59	ALA	HB1	1.63	0.02	1
1	A	59	ALA	HB2	1.63	0.02	1
1	A	59	ALA	HB3	1.63	0.02	1
1	A	59	ALA	C	180.0	0.3	1
1	A	59	ALA	CA	55.1	0.3	1
1	A	59	ALA	CB	19.2	0.3	1
1	A	59	ALA	N	125.4	0.3	1
1	A	60	GLU	H	8.57	0.02	1
1	A	60	GLU	HA	3.92	0.02	1
1	A	60	GLU	HB2	1.93	0.02	1
1	A	60	GLU	HB3	1.93	0.02	1
1	A	60	GLU	HG2	2.41	0.02	1
1	A	60	GLU	HG3	2.41	0.02	1
1	A	60	GLU	C	179.4	0.3	1
1	A	60	GLU	CA	59.6	0.3	1
1	A	60	GLU	CB	30.1	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	GLU	CG	37.4	0.3	1
1	A	60	GLU	N	120.6	0.3	1
1	A	61	HIS	H	7.93	0.02	1
1	A	61	HIS	HA	4.0	0.02	1
1	A	61	HIS	HB2	3.22	0.02	2
1	A	61	HIS	HB3	2.95	0.02	2
1	A	61	HIS	C	177.1	0.3	1
1	A	61	HIS	CA	61.3	0.3	1
1	A	61	HIS	CB	31.3	0.3	1
1	A	61	HIS	N	118.2	0.3	1
1	A	62	ALA	H	7.9	0.02	1
1	A	62	ALA	HA	3.87	0.02	1
1	A	62	ALA	HB1	1.25	0.02	1
1	A	62	ALA	HB2	1.25	0.02	1
1	A	62	ALA	HB3	1.25	0.02	1
1	A	62	ALA	C	180.5	0.3	1
1	A	62	ALA	CA	54.9	0.3	1
1	A	62	ALA	CB	19.9	0.3	1
1	A	62	ALA	N	122.3	0.3	1
1	A	63	ALA	H	7.56	0.02	1
1	A	63	ALA	HA	3.97	0.02	1
1	A	63	ALA	HB1	1.36	0.02	1
1	A	63	ALA	HB2	1.36	0.02	1
1	A	63	ALA	HB3	1.36	0.02	1
1	A	63	ALA	C	178.4	0.3	1
1	A	63	ALA	CA	55.0	0.3	1
1	A	63	ALA	CB	17.2	0.3	1
1	A	63	ALA	N	121.5	0.3	1
1	A	64	ALA	H	8.42	0.02	1
1	A	64	ALA	HA	3.69	0.02	1
1	A	64	ALA	HB1	1.42	0.02	1
1	A	64	ALA	HB2	1.42	0.02	1
1	A	64	ALA	HB3	1.42	0.02	1
1	A	64	ALA	C	178.2	0.3	1
1	A	64	ALA	CA	55.0	0.3	1
1	A	64	ALA	CB	17.3	0.3	1
1	A	64	ALA	N	120.3	0.3	1
1	A	65	LYS	H	8.31	0.02	1
1	A	65	LYS	HA	3.02	0.02	1
1	A	65	LYS	HB2	1.5	0.02	1
1	A	65	LYS	HB3	1.5	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	65	LYS	HG2	0.72	0.02	1
1	A	65	LYS	HG3	0.72	0.02	1
1	A	65	LYS	HD2	1.09	0.02	1
1	A	65	LYS	HD3	1.09	0.02	1
1	A	65	LYS	HE2	2.74	0.02	1
1	A	65	LYS	HE3	2.74	0.02	1
1	A	65	LYS	C	178.0	0.3	1
1	A	65	LYS	CA	59.9	0.3	1
1	A	65	LYS	CB	32.4	0.3	1
1	A	65	LYS	CG	24.5	0.3	1
1	A	65	LYS	CD	29.8	0.3	1
1	A	65	LYS	CE	42.0	0.3	1
1	A	65	LYS	N	120.2	0.3	1
1	A	66	ILE	H	6.78	0.02	1
1	A	66	ILE	HA	3.48	0.02	1
1	A	66	ILE	HB	1.81	0.02	1
1	A	66	ILE	HG12	1.04	0.02	1
1	A	66	ILE	HG13	1.04	0.02	1
1	A	66	ILE	HG21	0.95	0.02	1
1	A	66	ILE	HG22	0.95	0.02	1
1	A	66	ILE	HG23	0.95	0.02	1
1	A	66	ILE	HD11	0.84	0.02	1
1	A	66	ILE	HD12	0.84	0.02	1
1	A	66	ILE	HD13	0.84	0.02	1
1	A	66	ILE	C	178.3	0.3	1
1	A	66	ILE	CA	64.0	0.3	1
1	A	66	ILE	CB	37.9	0.3	1
1	A	66	ILE	CG1	27.9	0.3	1
1	A	66	ILE	CG2	17.7	0.3	1
1	A	66	ILE	CD1	13.3	0.3	1
1	A	66	ILE	N	119.2	0.3	1
1	A	67	ALA	H	7.0	0.02	1
1	A	67	ALA	HA	2.3	0.02	1
1	A	67	ALA	HB1	0.68	0.02	1
1	A	67	ALA	HB2	0.68	0.02	1
1	A	67	ALA	HB3	0.68	0.02	1
1	A	67	ALA	C	179.5	0.3	1
1	A	67	ALA	CA	54.3	0.3	1
1	A	67	ALA	CB	18.9	0.3	1
1	A	67	ALA	N	123.6	0.3	1
1	A	68	VAL	H	8.65	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	VAL	HA	3.12	0.02	1
1	A	68	VAL	HB	1.9	0.02	1
1	A	68	VAL	HG11	0.83	0.02	1
1	A	68	VAL	HG12	0.83	0.02	1
1	A	68	VAL	HG13	0.83	0.02	1
1	A	68	VAL	HG21	0.91	0.02	1
1	A	68	VAL	HG22	0.91	0.02	1
1	A	68	VAL	HG23	0.91	0.02	1
1	A	68	VAL	C	178.2	0.3	1
1	A	68	VAL	CA	66.1	0.3	1
1	A	68	VAL	CB	31.4	0.3	1
1	A	68	VAL	CG1	21.0	0.3	1
1	A	68	VAL	CG2	24.0	0.3	1
1	A	68	VAL	N	118.9	0.3	1
1	A	69	ALA	H	7.55	0.02	1
1	A	69	ALA	HA	3.94	0.02	1
1	A	69	ALA	HB1	1.33	0.02	1
1	A	69	ALA	HB2	1.33	0.02	1
1	A	69	ALA	HB3	1.33	0.02	1
1	A	69	ALA	C	178.9	0.3	1
1	A	69	ALA	CA	54.2	0.3	1
1	A	69	ALA	CB	17.6	0.3	1
1	A	69	ALA	N	122.7	0.3	1
1	A	70	SER	H	7.24	0.02	1
1	A	70	SER	HA	4.27	0.02	1
1	A	70	SER	HB2	3.83	0.02	1
1	A	70	SER	HB3	3.83	0.02	1
1	A	70	SER	C	174.8	0.3	1
1	A	70	SER	CA	60.0	0.3	1
1	A	70	SER	CB	63.9	0.3	1
1	A	70	SER	N	112.9	0.3	1
1	A	71	LEU	H	7.33	0.02	1
1	A	71	LEU	HA	4.11	0.02	1
1	A	71	LEU	HB2	1.44	0.02	1
1	A	71	LEU	HB3	1.44	0.02	1
1	A	71	LEU	HG	1.01	0.02	1
1	A	71	LEU	HD11	0.18	0.02	1
1	A	71	LEU	HD12	0.18	0.02	1
1	A	71	LEU	HD13	0.18	0.02	1
1	A	71	LEU	HD21	0.47	0.02	1
1	A	71	LEU	HD22	0.47	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	LEU	HD23	0.47	0.02	1
1	A	71	LEU	C	177.1	0.3	1
1	A	71	LEU	CA	55.1	0.3	1
1	A	71	LEU	CB	41.8	0.3	1
1	A	71	LEU	CG	24.6	0.3	1
1	A	71	LEU	CD1	24.8	0.3	1
1	A	71	LEU	CD2	21.5	0.3	1
1	A	71	LEU	N	121.2	0.3	1
1	A	72	THR	H	7.66	0.02	1
1	A	72	THR	HA	4.48	0.02	1
1	A	72	THR	HB	4.06	0.02	1
1	A	72	THR	HG21	1.07	0.02	1
1	A	72	THR	HG22	1.07	0.02	1
1	A	72	THR	HG23	1.07	0.02	1
1	A	72	THR	C	172.4	0.3	1
1	A	72	THR	CA	59.7	0.3	1
1	A	72	THR	CB	69.5	0.3	1
1	A	72	THR	N	115.3	0.3	1
1	A	73	PRO	HA	4.32	0.02	1
1	A	73	PRO	HB2	2.21	0.02	1
1	A	73	PRO	HB3	2.21	0.02	1
1	A	73	PRO	HG2	1.9	0.02	2
1	A	73	PRO	HG3	1.83	0.02	2
1	A	73	PRO	HD2	3.7	0.02	2
1	A	73	PRO	HD3	3.63	0.02	2
1	A	73	PRO	C	176.8	0.3	1
1	A	73	PRO	CA	63.3	0.3	1
1	A	73	PRO	CB	31.7	0.3	1
1	A	73	PRO	CG	27.3	0.3	1
1	A	73	PRO	CD	50.7	0.3	1
1	A	74	GLN	H	8.41	0.02	1
1	A	74	GLN	HA	4.28	0.02	1
1	A	74	GLN	HB2	1.89	0.02	2
1	A	74	GLN	HB3	2.04	0.02	2
1	A	74	GLN	HG2	2.28	0.02	1
1	A	74	GLN	HG3	2.28	0.02	1
1	A	74	GLN	C	175.7	0.3	1
1	A	74	GLN	CA	55.3	0.3	1
1	A	74	GLN	CB	29.4	0.3	1
1	A	74	GLN	CG	33.6	0.3	1
1	A	74	GLN	N	121.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	75	SER	H	8.3	0.02	1
1	A	75	SER	HA	4.78	0.02	1
1	A	75	SER	C	172.9	0.3	1
1	A	75	SER	CA	56.2	0.3	1
1	A	75	SER	CB	63.1	0.3	1
1	A	75	SER	N	119.2	0.3	1
1	A	76	PRO	HA	4.33	0.02	1
1	A	76	PRO	HB2	2.19	0.02	1
1	A	76	PRO	HB3	2.19	0.02	1
1	A	76	PRO	HG2	1.83	0.02	2
1	A	76	PRO	HG3	1.9	0.02	2
1	A	76	PRO	HD2	3.57	0.02	1
1	A	76	PRO	HD3	3.57	0.02	1
1	A	76	PRO	C	176.8	0.3	1
1	A	76	PRO	CA	63.4	0.3	1
1	A	76	PRO	CB	31.7	0.3	1
1	A	76	PRO	CG	27.3	0.3	1
1	A	77	GLU	H	8.38	0.02	1
1	A	77	GLU	HA	4.14	0.02	1
1	A	77	GLU	HB2	1.88	0.02	1
1	A	77	GLU	HB3	1.88	0.02	1
1	A	77	GLU	HG2	2.17	0.02	1
1	A	77	GLU	HG3	2.17	0.02	1
1	A	77	GLU	C	176.8	0.3	1
1	A	77	GLU	CA	56.7	0.3	1
1	A	77	GLU	CB	29.8	0.3	1
1	A	77	GLU	CG	36.2	0.3	1
1	A	77	GLU	N	121.0	0.3	1
1	A	78	GLY	H	8.21	0.02	1
1	A	78	GLY	HA2	3.83	0.02	1
1	A	78	GLY	HA3	3.83	0.02	1
1	A	78	GLY	C	174.0	0.3	1
1	A	78	GLY	CA	45.1	0.3	1
1	A	78	GLY	N	110.3	0.3	1
1	A	79	ILE	H	7.76	0.02	1
1	A	79	ILE	HA	4.03	0.02	1
1	A	79	ILE	HB	1.72	0.02	1
1	A	79	ILE	HG12	1.26	0.02	2
1	A	79	ILE	HG13	1.02	0.02	2
1	A	79	ILE	HG21	0.75	0.02	1
1	A	79	ILE	HG22	0.75	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	ILE	HG23	0.75	0.02	1
1	A	79	ILE	HD11	0.75	0.02	1
1	A	79	ILE	HD12	0.75	0.02	1
1	A	79	ILE	HD13	0.75	0.02	1
1	A	79	ILE	C	175.5	0.3	1
1	A	79	ILE	CA	61.0	0.3	1
1	A	79	ILE	CB	38.4	0.3	1
1	A	79	ILE	CG1	26.9	0.3	1
1	A	79	ILE	CG2	17.3	0.3	1
1	A	79	ILE	CD1	12.9	0.3	1
1	A	79	ILE	N	120.3	0.3	1
1	A	80	ASP	H	8.27	0.02	1
1	A	80	ASP	HA	4.49	0.02	1
1	A	80	ASP	HB2	2.52	0.02	1
1	A	80	ASP	HB3	2.52	0.02	1
1	A	80	ASP	C	175.6	0.3	1
1	A	80	ASP	CA	54.3	0.3	1
1	A	80	ASP	CB	40.7	0.3	1
1	A	80	ASP	N	124.2	0.3	1
1	A	81	VAL	H	7.58	0.02	1
1	A	152	ASN	H	8.18	0.02	1
1	A	152	ASN	HA	4.66	0.02	1
1	A	152	ASN	HB2	2.7	0.02	1
1	A	152	ASN	HB3	2.7	0.02	1
1	A	152	ASN	C	175.2	0.3	1
1	A	152	ASN	CA	53.0	0.3	1
1	A	152	ASN	CB	38.8	0.3	1
1	A	152	ASN	N	119.4	0.3	1
1	A	153	SER	H	8.19	0.02	1
1	A	153	SER	HA	4.3	0.02	1
1	A	153	SER	HB2	3.78	0.02	2
1	A	153	SER	HB3	3.82	0.02	2
1	A	153	SER	C	174.5	0.3	1
1	A	153	SER	CA	58.6	0.3	1
1	A	153	SER	CB	63.4	0.3	1
1	A	153	SER	N	116.8	0.3	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	150	0.12 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	141	0.45 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	150	0.07 ± 0.17	None needed (< 0.5 ppm)
^{15}N	139	-0.60 ± 0.29	Should be applied

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 86%, i.e. 757 atoms were assigned a chemical shift out of a possible 881. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	337/337 (100%)	136/136 (100%)	136/136 (100%)	65/65 (100%)
Sidechain	398/469 (85%)	278/309 (90%)	117/149 (79%)	3/11 (27%)
Aromatic	22/75 (29%)	22/37 (59%)	0/37 (0%)	0/1 (0%)
Overall	757/881 (86%)	436/482 (90%)	253/322 (79%)	68/77 (88%)

7.1.4 Statistically unusual chemical shifts

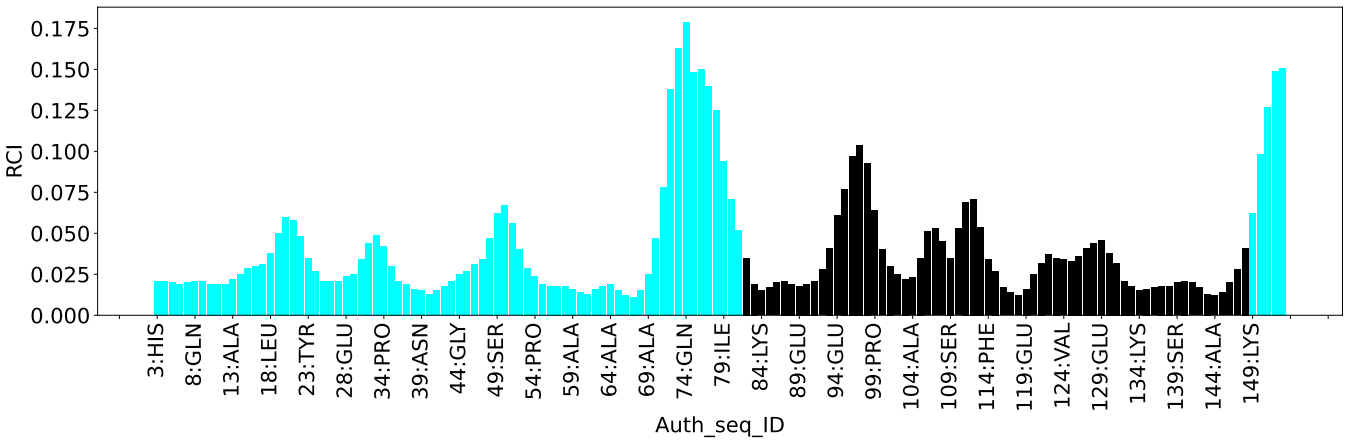
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	133	LYS	CE	37.30	37.57 – 46.21	-5.3

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:


RCI
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
3:HIS
8:GLN
13:ALA
18:LEU
23:TYR
28:GLU
34:PRO
39:ASN
44:GLY
49:SER
54:PRO
59:ALA
64:ALA
69:ALA
74:GLN
79:ILE
84:LYS
89:GLU
94:GLU
99:PRO
104:ALA
109:SER
114:PHE
119:GLU
124:VAL
129:GLU
134:LYS
139:SER
144:ALA
149:LYS
Auth_seq_ID

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	1321
Intra-residue (|i-j|=0)	401
Sequential (|i-j|=1)	322
Medium range (|i-j|>1 and |i-j|<5)	226
Long range (|i-j|≥5)	310
Inter-chain	0
Hydrogen bond restraints	62
Disulfide bond restraints	0
Total dihedral-angle restraints	122
Number of unmapped restraints	0
Number of restraints per residue	9.4
Number of long range restraints per residue[1]	2.1

[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)	9.9	0.2
0.2-0.5 (Medium)	9.3	0.5
>0.5 (Large)	48.1	3.99

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	11.0	6.5
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

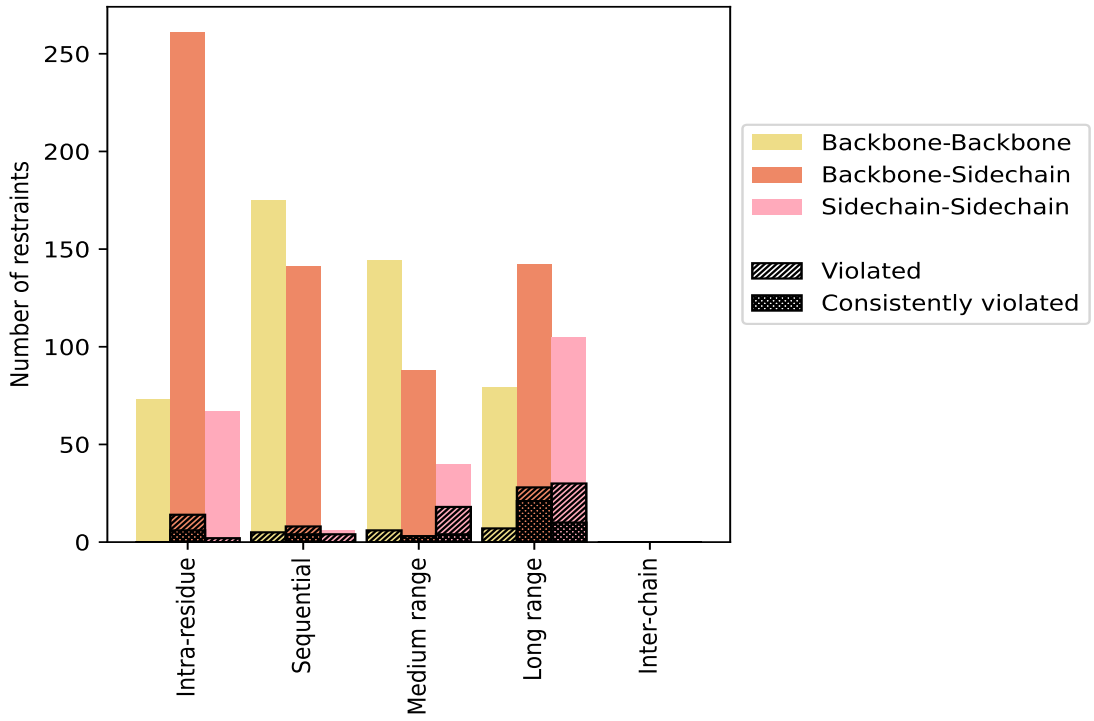
9.1 Summary of distance violations (i)

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)	401	30.4	16	4.0	1.2	6	1.5	0.5
Backbone-Backbone	73	5.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	261	19.8	14	5.4	1.1	6	2.3	0.5
Sidechain-Sidechain	67	5.1	2	3.0	0.2	0	0.0	0.0
Sequential (|i-j|=1)	322	24.4	17	5.3	1.3	4	1.2	0.3
Backbone-Backbone	175	13.2	5	2.9	0.4	0	0.0	0.0
Backbone-Sidechain	141	10.7	8	5.7	0.6	4	2.8	0.3
Sidechain-Sidechain	6	0.5	4	66.7	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	226	17.1	25	11.1	1.9	7	3.1	0.5
Backbone-Backbone	98	7.4	4	4.1	0.3	0	0.0	0.0
Backbone-Sidechain	88	6.7	3	3.4	0.2	3	3.4	0.2
Sidechain-Sidechain	40	3.0	18	45.0	1.4	4	10.0	0.3
Long range (|i-j|≥5)	310	23.5	63	20.3	4.8	31	10.0	2.3
Backbone-Backbone	63	4.8	5	7.9	0.4	0	0.0	0.0
Backbone-Sidechain	142	10.7	28	19.7	2.1	21	14.8	1.6
Sidechain-Sidechain	105	7.9	30	28.6	2.3	10	9.5	0.8
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	62	4.7	4	6.5	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1321	100.0	125	9.5	9.5	48	3.6	3.6
Backbone-Backbone	471	35.7	18	3.8	1.4	0	0.0	0.0
Backbone-Sidechain	632	47.8	53	8.4	4.0	34	5.4	2.6
Sidechain-Sidechain	218	16.5	54	24.8	4.1	14	6.4	1.1

[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	10	10	10	38	0	68	1.59	3.92	1.25	1.34
2	10	6	7	38	0	61	1.76	3.94	1.19	1.85
3	9	7	8	32	0	56	1.7	3.83	1.26	1.8
4	10	9	9	39	0	67	1.64	3.53	1.14	1.71
5	8	7	7	34	0	56	1.77	3.59	1.2	2.33
6	7	7	7	31	0	52	1.87	3.91	1.26	2.15
7	12	9	9	38	0	68	1.65	3.66	1.19	1.62
8	11	9	7	38	0	65	1.7	3.59	1.19	1.79
9	8	8	12	41	0	69	1.58	3.52	1.16	1.52
10	9	9	9	40	0	67	1.62	3.99	1.22	1.41
11	12	9	9	40	0	70	1.51	3.95	1.23	1.32

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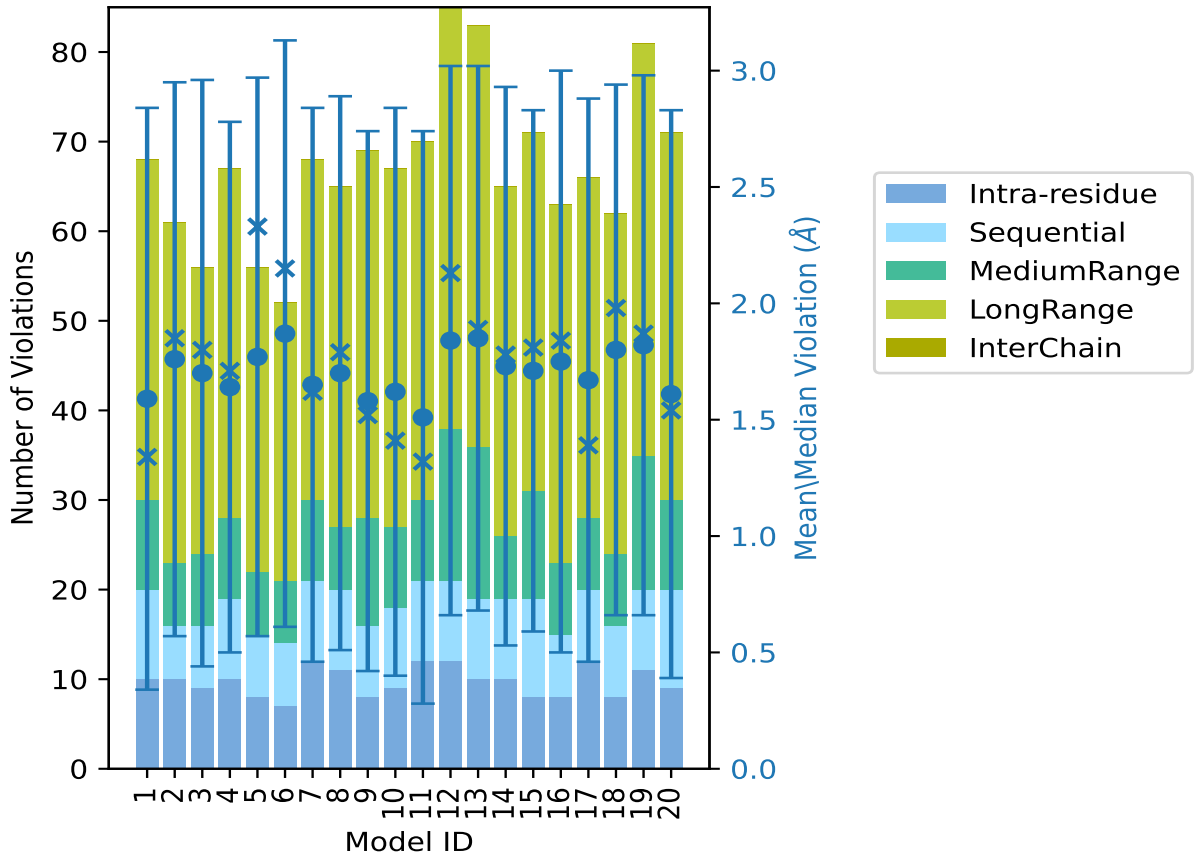
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	12	9	17	47	0	85	1.84	3.63	1.18	2.13
13	10	9	17	47	0	83	1.85	3.7	1.17	1.89
14	10	9	7	39	0	65	1.73	3.61	1.2	1.78
15	8	11	12	40	0	71	1.71	3.6	1.12	1.81
16	8	7	8	40	0	63	1.75	3.94	1.25	1.84
17	12	8	8	38	0	66	1.67	3.9	1.21	1.39
18	8	8	8	38	0	62	1.8	3.78	1.14	1.98
19	11	9	15	46	0	81	1.82	3.68	1.16	1.87
20	9	11	10	41	0	71	1.61	3.88	1.22	1.54

[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

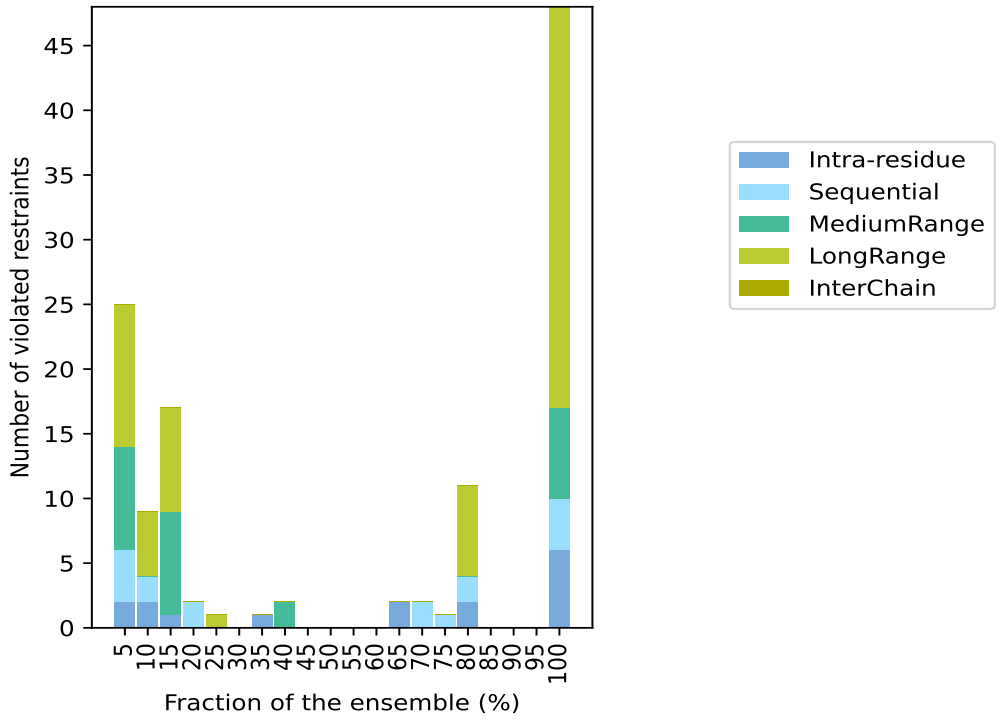
9.3 Distance violation statistics for the ensemble (i)

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, 1138(IR:385, SQ:305, MR:201, LR:247, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
2	4	8	11	0	25	1	5.0
2	2	0	5	0	9	2	10.0
1	0	8	8	0	17	3	15.0
0	2	0	0	0	2	4	20.0
0	0	0	1	0	1	5	25.0
0	0	0	0	0	0	6	30.0
1	0	0	0	0	1	7	35.0
0	0	2	0	0	2	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
2	0	0	0	0	2	13	65.0
0	2	0	0	0	2	14	70.0
0	1	0	0	0	1	15	75.0
2	2	0	7	0	11	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
6	4	7	31	0	48	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

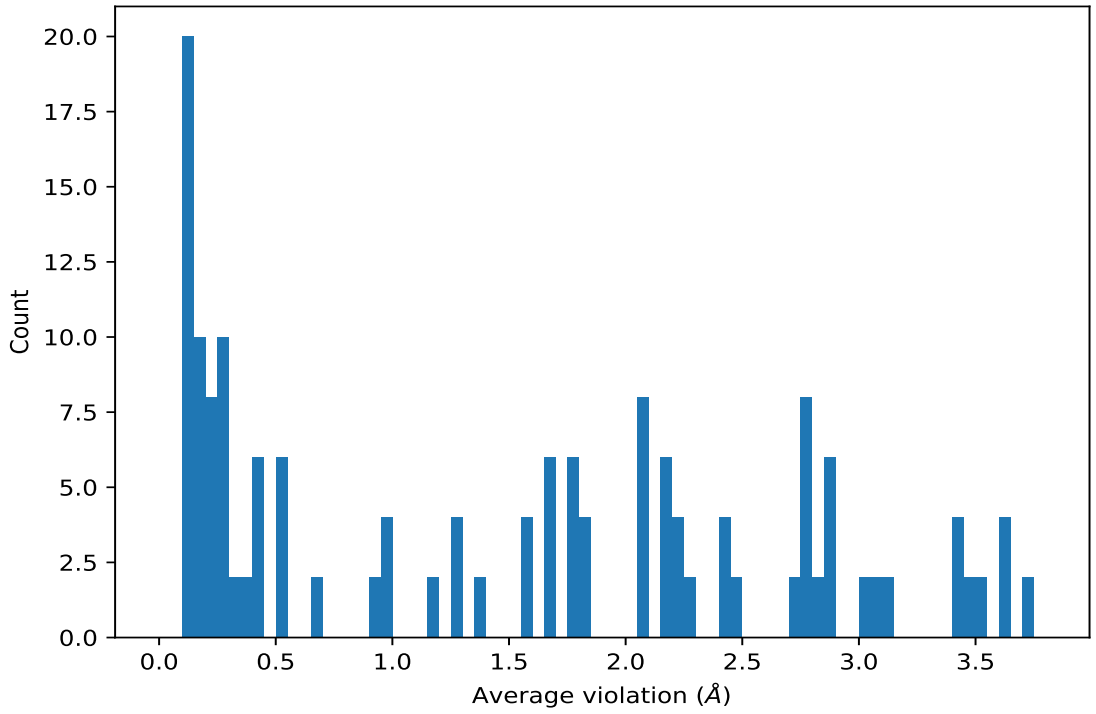
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

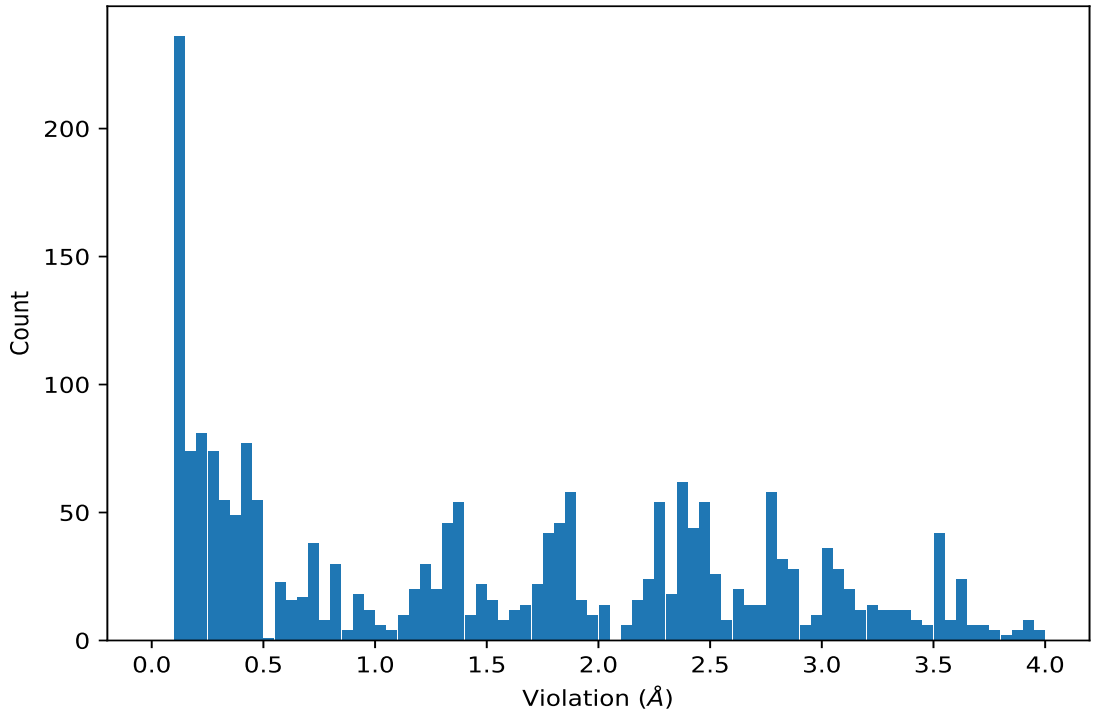
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,931)	1:A:105:THR:HB	1:A:114:PHE:HE2	20	3.74	0.18	3.74
(1,989)	1:A:114:PHE:HE2	1:A:105:THR:HB	20	3.74	0.18	3.74
(1,404)	1:A:114:PHE:HE1	1:A:132:THR:H	20	3.53	0.02	3.52
(1,581)	1:A:132:THR:H	1:A:114:PHE:HE1	20	3.53	0.02	3.52
(1,930)	1:A:105:THR:HB	1:A:114:PHE:HD2	20	3.48	0.19	3.46
(1,986)	1:A:114:PHE:HD2	1:A:105:THR:HB	20	3.48	0.19	3.46
(1,1001)	1:A:114:PHE:HD1	1:A:132:THR:HA	20	3.14	0.12	3.11
(1,1112)	1:A:132:THR:HA	1:A:114:PHE:HD1	20	3.14	0.12	3.11
(1,403)	1:A:114:PHE:HD1	1:A:132:THR:H	20	3.07	0.05	3.06
(1,580)	1:A:132:THR:H	1:A:114:PHE:HD1	20	3.07	0.05	3.06

[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)
(1,989)	1:A:114:PHE:HE2	1:A:105:THR:HB	10	3.99
(1,931)	1:A:105:THR:HB	1:A:114:PHE:HE2	10	3.99
(1,989)	1:A:114:PHE:HE2	1:A:105:THR:HB	11	3.95
(1,931)	1:A:105:THR:HB	1:A:114:PHE:HE2	11	3.95
(1,989)	1:A:114:PHE:HE2	1:A:105:THR:HB	2	3.94
(1,989)	1:A:114:PHE:HE2	1:A:105:THR:HB	16	3.94
(1,931)	1:A:105:THR:HB	1:A:114:PHE:HE2	2	3.94
(1,931)	1:A:105:THR:HB	1:A:114:PHE:HE2	16	3.94
(1,989)	1:A:114:PHE:HE2	1:A:105:THR:HB	1	3.92
(1,931)	1:A:105:THR:HB	1:A:114:PHE:HE2	1	3.92

10 Dihedral-angle violation analysis

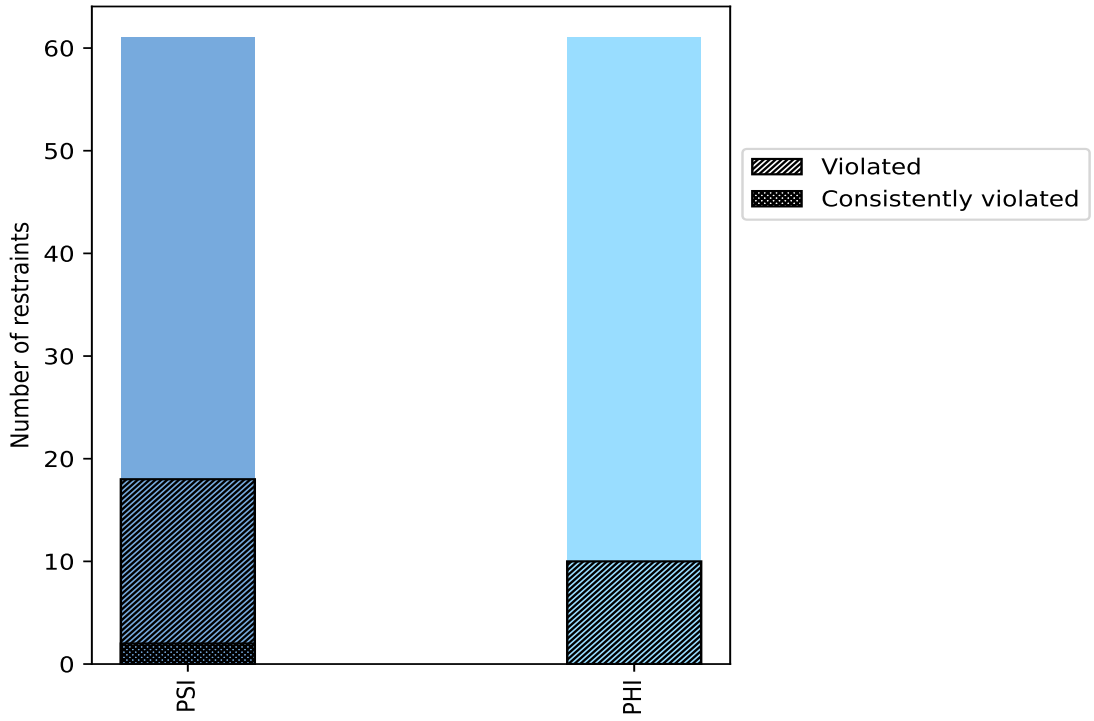
10.1 Summary of dihedral-angle violations

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]
PSI	61	50.0	18	29.5	14.8	2	3.3	1.6
PHI	61	50.0	10	16.4	8.2	0	0.0	0.0
Total	122	100.0	28	23.0	23.0	2	1.6	1.6

[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



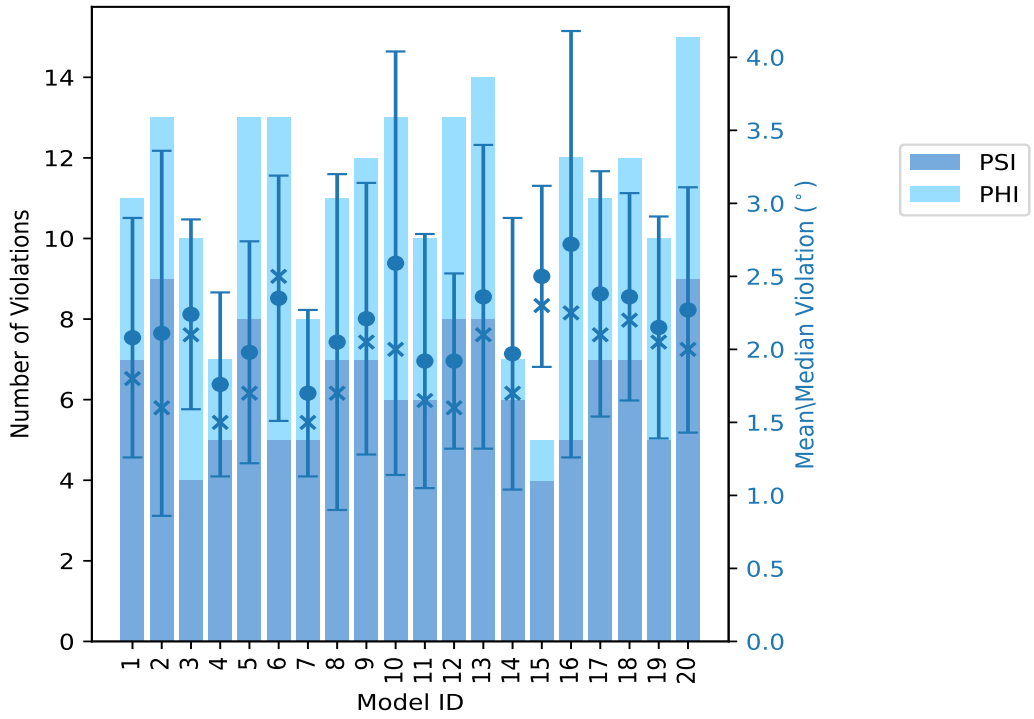
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	7	4	11	2.08	3.8	0.82	1.8
2	9	4	13	2.11	5.4	1.25	1.6
3	4	6	10	2.24	3.5	0.65	2.1
4	5	2	7	1.76	3.1	0.63	1.5
5	8	5	13	1.98	3.8	0.76	1.7
6	5	8	13	2.35	3.8	0.84	2.5
7	5	3	8	1.7	3.0	0.57	1.5
8	7	4	11	2.05	5.5	1.15	1.7
9	7	5	12	2.21	4.4	0.93	2.05
10	6	7	13	2.59	6.3	1.45	2.0
11	6	4	10	1.92	3.9	0.87	1.65
12	8	5	13	1.92	2.9	0.6	1.6
13	8	6	14	2.36	5.3	1.04	2.1
14	6	1	7	1.97	4.1	0.93	1.7
15	4	1	5	2.5	3.6	0.62	2.3
16	5	7	12	2.72	6.5	1.46	2.25
17	7	4	11	2.38	4.0	0.84	2.1
18	7	5	12	2.36	3.3	0.71	2.2
19	5	5	10	2.15	3.3	0.76	2.05
20	9	6	15	2.27	3.9	0.84	2.0

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
4	1	5	1	5.0
3	0	3	2	10.0
1	0	1	3	15.0
2	2	4	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
1	1	2	7	35.0
1	2	3	8	40.0
1	0	1	9	45.0
0	1	1	10	50.0
1	0	1	11	55.0

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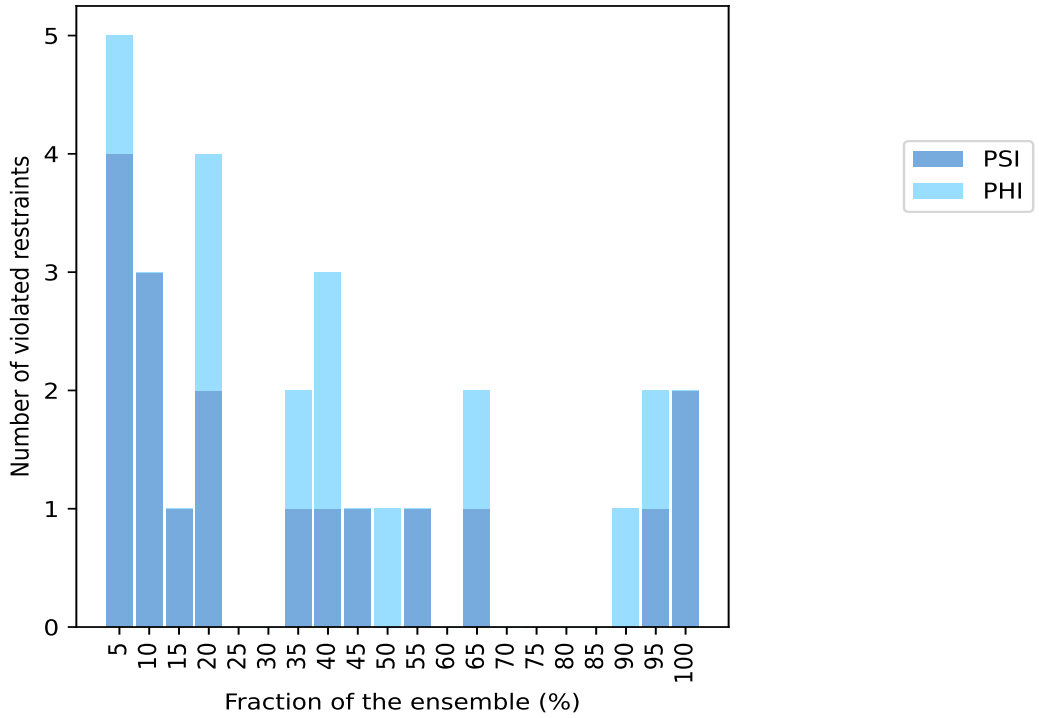
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
1	1	2	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
1	1	2	19	95.0
2	0	2	20	100.0

[1] Number of models with violations

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

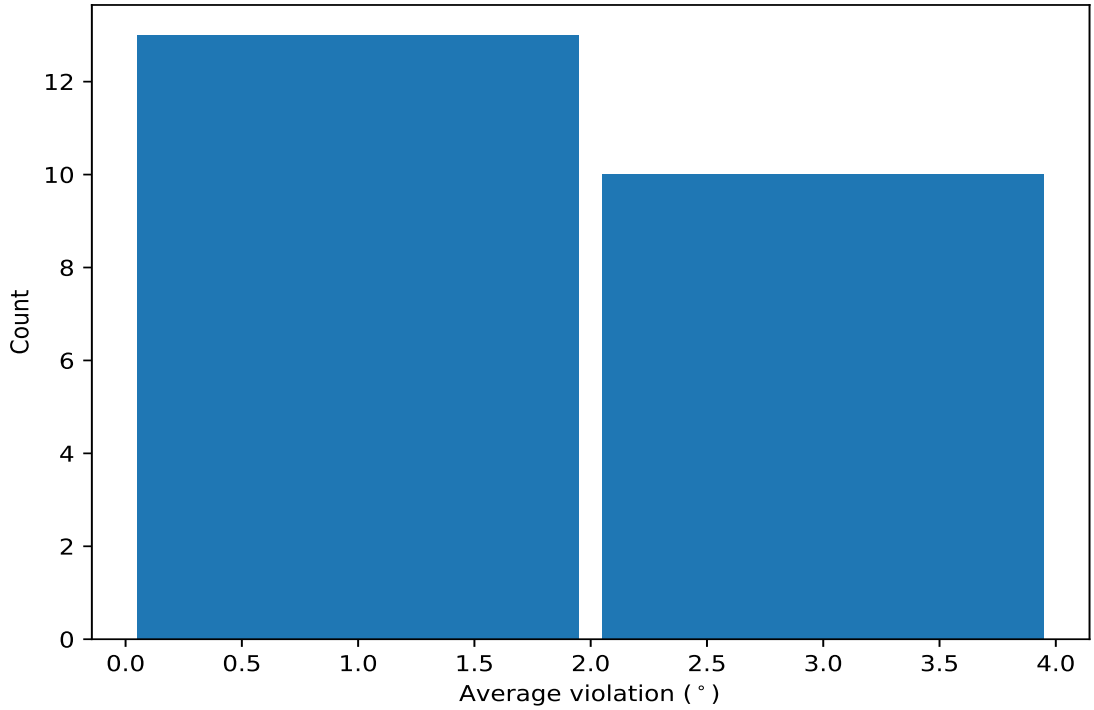


10.4 Most violated dihedral-angle restraints in the ensemble

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 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.

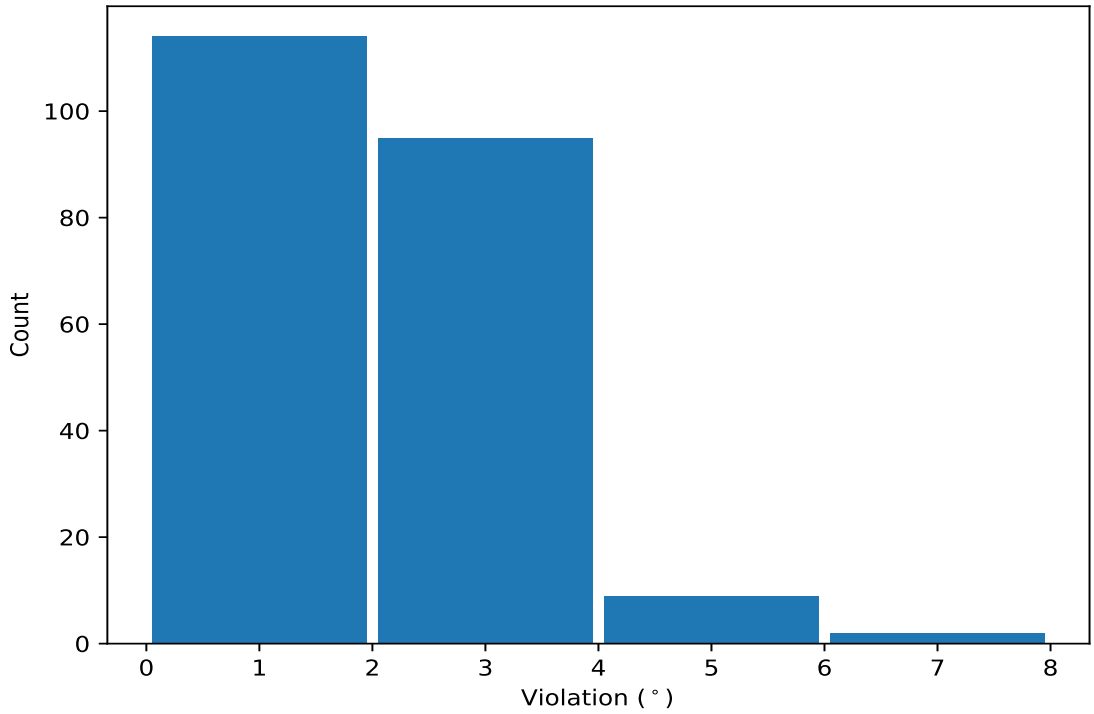
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,104)	1:A:131:LYS:N	1:A:131:LYS:CA	1:A:131:LYS:C	1:A:132:THR:N	20	3.78	1.36	3.6
(1,63)	1:A:83:TYR:N	1:A:83:TYR:CA	1:A:83:TYR:C	1:A:84:LYS:N	20	1.84	0.33	1.8
(1,87)	1:A:111:ALA:N	1:A:111:ALA:CA	1:A:111:ALA:C	1:A:112:PRO:N	19	3.26	0.71	3.4
(1,1)	1:A:81:VAL:C	1:A:82:ALA:N	1:A:82:ALA:CA	1:A:82:ALA:C	19	1.69	0.34	1.7
(1,54)	1:A:141:ALA:C	1:A:142:LYS:N	1:A:142:LYS:CA	1:A:142:LYS:C	18	2.22	0.58	2.3
(1,2)	1:A:82:ALA:C	1:A:83:TYR:N	1:A:83:TYR:CA	1:A:83:TYR:C	13	1.87	0.44	1.8
(1,62)	1:A:82:ALA:N	1:A:82:ALA:CA	1:A:82:ALA:C	1:A:83:TYR:N	13	1.69	0.2	1.7
(1,114)	1:A:141:ALA:N	1:A:141:ALA:CA	1:A:141:ALA:C	1:A:142:LYS:N	11	1.8	0.45	1.7
(1,42)	1:A:129:GLU:C	1:A:130:ALA:N	1:A:130:ALA:CA	1:A:130:ALA:C	10	2.81	1.08	2.5
(1,109)	1:A:136:ALA:N	1:A:136:ALA:CA	1:A:136:ALA:C	1:A:137:GLU:N	9	1.2	0.11	1.2

[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 violationsfor 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 (°)
(1,104)	1:A:131:LYS:N	1:A:131:LYS:CA	1:A:131:LYS:C	1:A:132:THR:N	16	6.5
(1,104)	1:A:131:LYS:N	1:A:131:LYS:CA	1:A:131:LYS:C	1:A:132:THR:N	10	6.3
(1,104)	1:A:131:LYS:N	1:A:131:LYS:CA	1:A:131:LYS:C	1:A:132:THR:N	8	5.5
(1,104)	1:A:131:LYS:N	1:A:131:LYS:CA	1:A:131:LYS:C	1:A:132:THR:N	2	5.4
(1,104)	1:A:131:LYS:N	1:A:131:LYS:CA	1:A:131:LYS:C	1:A:132:THR:N	13	5.3
(1,42)	1:A:129:GLU:C	1:A:130:ALA:N	1:A:130:ALA:CA	1:A:130:ALA:C	10	5.0
(1,87)	1:A:111:ALA:N	1:A:111:ALA:CA	1:A:111:ALA:C	1:A:112:PRO:N	9	4.4
(1,87)	1:A:111:ALA:N	1:A:111:ALA:CA	1:A:111:ALA:C	1:A:112:PRO:N	2	4.1
(1,104)	1:A:131:LYS:N	1:A:131:LYS:CA	1:A:131:LYS:C	1:A:132:THR:N	14	4.1
(1,42)	1:A:129:GLU:C	1:A:130:ALA:N	1:A:130:ALA:CA	1:A:130:ALA:C	16	4.0