



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 27, 2026 – 08:23 AM UTC

PDB ID : 2N3G / pdb_00002n3g
BMRB ID : 25138
Title : Solution structure of DRB4 dsRBD1 (viz. DRB4(1-72))
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 ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

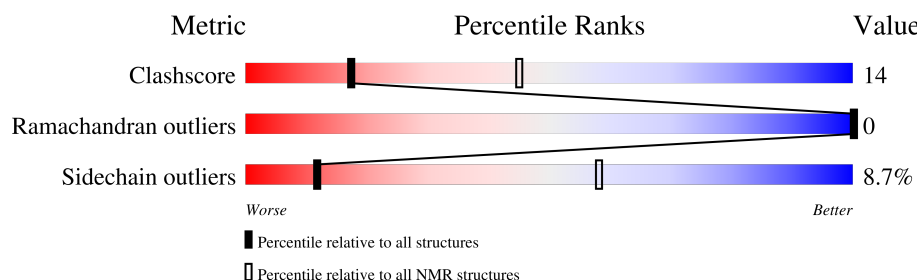
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	153	

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:4-A:27, A:35-A:70 (60)	0.26	4

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 3 clusters and 7 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1112 atoms, of which 546 are hydrogens and 0 are deuteriums.

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

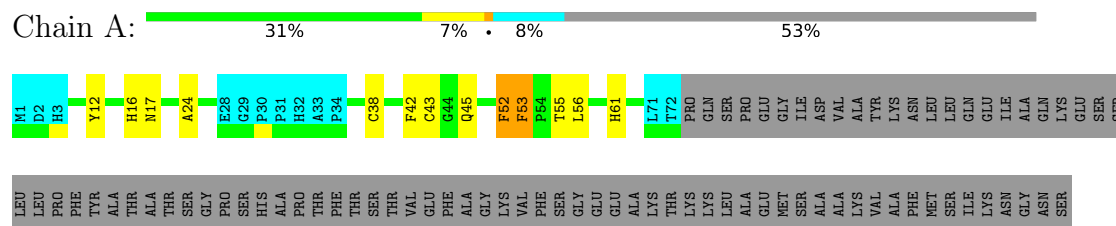
Mol	Chain	Residues	Atoms						Trace
1	A	72	Total	C	H	N	O	S	0
			1112	360	546	100	103	3	

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.

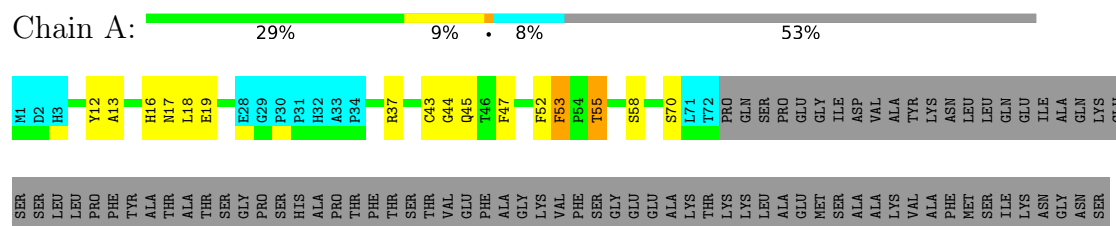
- Molecule 1: Double-stranded RNA-binding protein 4



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

The representative model is number 4. Colouring as in section 4.1 above.

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



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	770
Number of unparsed shifts	0
Number of shifts with mapping errors	888
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.62±0.01	0±0/488 (0.0± 0.0%)	1.07±0.01	0±1/661 (0.1± 0.1%)
All	All	0.62	0/9760 (0.0%)	1.07	10/13220 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	36	PHE	CA-CB-CG	-5.33	108.47	113.80	10	7
1	A	52	PHE	CA-CB-CG	-5.12	108.69	113.80	1	2
1	A	53	PHE	CA-CB-CG	-5.02	108.78	113.80	16	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	476	464	464	13±3
All	All	9520	9280	9280	256

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 14.

5 of 91 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:CD1	1:A:52:PHE:N	0.70	2.59	6	17
1:A:5:TYR:CE1	1:A:61:HIS:ND1	0.67	2.63	11	4
1:A:5:TYR:CE2	1:A:61:HIS:ND1	0.66	2.64	13	1
1:A:12:TYR:CE2	1:A:16:HIS:CE1	0.63	2.86	18	2
1:A:5:TYR:N	1:A:5:TYR:CD1	0.63	2.67	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	60/153 (39%)	58±1 (96±1%)	2±1 (4±1%)	0±0 (0±0%)	100	100
All	All	1200/3060 (39%)	1150 (96%)	50 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	49/124 (40%)	45±1 (91±2%)	4±1 (9±2%)	12	58
All	All	980/2480 (40%)	895 (91%)	85 (9%)	12	58

5 of 11 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	52	PHE	20
1	A	53	PHE	19
1	A	56	LEU	17
1	A	55	THR	15

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Mol	Chain	Res	Type	Models (Total)
1	A	61	HIS	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 83% for the well-defined parts and 80% 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	770
Number of unparsed shifts	0
Number of shifts with mapping errors	888
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 888) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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	HD2	3.7	0.02	2
1	A	73	PRO	HD3	3.63	0.02	2
1	A	73	PRO	HG2	1.9	0.02	2
1	A	73	PRO	HG3	1.83	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	CD	50.7	0.3	1
1	A	73	PRO	CG	27.3	0.3	1
1	A	74	GLN	H	8.41	0.02	1
1	A	74	GLN	HA	4.28	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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
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	HD2	3.57	0.02	1
1	A	76	PRO	HD3	3.57	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	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

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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	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	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
1	A	79	ILE	HG23	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	CD1	12.9	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	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	81	VAL	HA	3.71	0.02	1
1	A	81	VAL	HB	1.58	0.02	1
1	A	81	VAL	HG11	0.21	0.02	1
1	A	81	VAL	HG12	0.21	0.02	1
1	A	81	VAL	HG13	0.21	0.02	1
1	A	81	VAL	HG21	0.58	0.02	1
1	A	81	VAL	HG22	0.58	0.02	1
1	A	81	VAL	HG23	0.58	0.02	1
1	A	81	VAL	C	175.5	0.3	1
1	A	81	VAL	CA	61.8	0.3	1
1	A	81	VAL	CB	32.1	0.3	1
1	A	81	VAL	CG1	20.9	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	VAL	CG2	20.3	0.3	1
1	A	81	VAL	N	120.0	0.3	1
1	A	82	ALA	H	8.04	0.02	1
1	A	82	ALA	HA	4.27	0.02	1
1	A	82	ALA	HB1	1.1	0.02	1
1	A	82	ALA	HB2	1.1	0.02	1
1	A	82	ALA	HB3	1.1	0.02	1
1	A	82	ALA	C	177.8	0.3	1
1	A	82	ALA	CA	50.9	0.3	1
1	A	82	ALA	CB	17.2	0.3	1
1	A	82	ALA	N	128.6	0.3	1
1	A	83	TYR	H	7.33	0.02	1
1	A	83	TYR	HA	3.48	0.02	1
1	A	83	TYR	HB2	2.63	0.02	1
1	A	83	TYR	HB3	2.63	0.02	1
1	A	83	TYR	HD1	6.62	0.02	1
1	A	83	TYR	HD2	6.62	0.02	1
1	A	83	TYR	HE1	6.62	0.02	1
1	A	83	TYR	HE2	6.62	0.02	1
1	A	83	TYR	C	176.9	0.3	1
1	A	83	TYR	CA	63.5	0.3	1
1	A	83	TYR	CB	38.2	0.3	1
1	A	83	TYR	N	119.5	0.3	1
1	A	84	LYS	H	7.95	0.02	1
1	A	84	LYS	HA	3.82	0.02	1
1	A	84	LYS	HB2	1.69	0.02	1
1	A	84	LYS	HB3	1.69	0.02	1
1	A	84	LYS	HD2	1.51	0.02	1
1	A	84	LYS	HD3	1.51	0.02	1
1	A	84	LYS	HG2	1.21	0.02	1
1	A	84	LYS	HG3	1.21	0.02	1
1	A	84	LYS	C	179.6	0.3	1
1	A	84	LYS	CA	60.4	0.3	1
1	A	84	LYS	CB	31.8	0.3	1
1	A	84	LYS	N	117.5	0.3	1
1	A	85	ASN	H	7.41	0.02	1
1	A	85	ASN	HA	4.23	0.02	1
1	A	85	ASN	HB2	2.69	0.02	1
1	A	85	ASN	HB3	2.69	0.02	1
1	A	85	ASN	HD21	7.34	0.02	1
1	A	85	ASN	HD22	6.78	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	ASN	C	177.3	0.3	1
1	A	85	ASN	CA	55.9	0.3	1
1	A	85	ASN	CB	37.3	0.3	1
1	A	85	ASN	N	120.5	0.3	1
1	A	85	ASN	ND2	112.2	0.3	1
1	A	86	LEU	H	7.94	0.02	1
1	A	86	LEU	HA	3.85	0.02	1
1	A	86	LEU	HD11	0.01	0.02	1
1	A	86	LEU	HD12	0.01	0.02	1
1	A	86	LEU	HD13	0.01	0.02	1
1	A	86	LEU	HD21	0.54	0.02	1
1	A	86	LEU	HD22	0.54	0.02	1
1	A	86	LEU	HD23	0.54	0.02	1
1	A	86	LEU	C	179.6	0.3	1
1	A	86	LEU	CA	57.7	0.3	1
1	A	86	LEU	CB	41.1	0.3	1
1	A	86	LEU	N	121.6	0.3	1
1	A	87	LEU	H	8.02	0.02	1
1	A	87	LEU	HA	3.93	0.02	1
1	A	87	LEU	HB2	1.44	0.02	1
1	A	87	LEU	HB3	1.44	0.02	1
1	A	87	LEU	HD11	0.45	0.02	1
1	A	87	LEU	HD12	0.45	0.02	1
1	A	87	LEU	HD13	0.45	0.02	1
1	A	87	LEU	HD21	0.53	0.02	1
1	A	87	LEU	HD22	0.53	0.02	1
1	A	87	LEU	HD23	0.53	0.02	1
1	A	87	LEU	HG	1.44	0.02	1
1	A	87	LEU	C	178.1	0.3	1
1	A	87	LEU	CA	57.5	0.3	1
1	A	87	LEU	CB	41.4	0.3	1
1	A	87	LEU	CD1	23.8	0.3	1
1	A	87	LEU	CD2	24.1	0.3	1
1	A	87	LEU	N	119.1	0.3	1
1	A	88	GLN	H	7.49	0.02	1
1	A	88	GLN	HA	3.69	0.02	1
1	A	88	GLN	HB2	2.24	0.02	1
1	A	88	GLN	HB3	2.24	0.02	1
1	A	88	GLN	HE21	7.53	0.02	1
1	A	88	GLN	HE22	6.86	0.02	1
1	A	88	GLN	HG2	2.24	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	GLN	HG3	2.24	0.02	1
1	A	88	GLN	C	177.3	0.3	1
1	A	88	GLN	CA	59.7	0.3	1
1	A	88	GLN	CB	27.8	0.3	1
1	A	88	GLN	CG	33.8	0.3	1
1	A	88	GLN	N	118.5	0.3	1
1	A	88	GLN	NE2	113.3	0.3	1
1	A	89	GLU	H	7.87	0.02	1
1	A	89	GLU	HA	4.0	0.02	1
1	A	89	GLU	HB2	2.12	0.02	1
1	A	89	GLU	HB3	2.12	0.02	1
1	A	89	GLU	HG2	2.33	0.02	1
1	A	89	GLU	HG3	2.33	0.02	1
1	A	89	GLU	C	179.2	0.3	1
1	A	89	GLU	CA	59.1	0.3	1
1	A	89	GLU	CB	29.2	0.3	1
1	A	89	GLU	CG	36.3	0.3	1
1	A	89	GLU	N	119.5	0.3	1
1	A	90	ILE	H	7.72	0.02	1
1	A	90	ILE	HA	3.72	0.02	1
1	A	90	ILE	HB	1.97	0.02	1
1	A	90	ILE	HD11	0.87	0.02	1
1	A	90	ILE	HD12	0.87	0.02	1
1	A	90	ILE	HD13	0.87	0.02	1
1	A	90	ILE	HG12	1.87	0.02	1
1	A	90	ILE	HG13	1.87	0.02	1
1	A	90	ILE	HG21	0.97	0.02	1
1	A	90	ILE	HG22	0.97	0.02	1
1	A	90	ILE	HG23	0.97	0.02	1
1	A	90	ILE	C	177.7	0.3	1
1	A	90	ILE	CA	65.1	0.3	1
1	A	90	ILE	CB	38.1	0.3	1
1	A	90	ILE	CD1	13.7	0.3	1
1	A	90	ILE	CG1	32.3	0.3	1
1	A	90	ILE	CG2	17.4	0.3	1
1	A	90	ILE	N	120.8	0.3	1
1	A	91	ALA	H	8.05	0.02	1
1	A	91	ALA	HA	4.07	0.02	1
1	A	91	ALA	HB1	1.45	0.02	1
1	A	91	ALA	HB2	1.45	0.02	1
1	A	91	ALA	HB3	1.45	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	ALA	C	179.7	0.3	1
1	A	91	ALA	CA	55.0	0.3	1
1	A	91	ALA	CB	18.4	0.3	1
1	A	91	ALA	N	122.7	0.3	1
1	A	92	GLN	H	8.14	0.02	1
1	A	92	GLN	HA	4.12	0.02	1
1	A	92	GLN	HB2	2.16	0.02	1
1	A	92	GLN	HB3	2.16	0.02	1
1	A	92	GLN	HE21	7.43	0.02	1
1	A	92	GLN	HE22	6.79	0.02	1
1	A	92	GLN	HG2	2.34	0.02	2
1	A	92	GLN	HG3	2.48	0.02	2
1	A	92	GLN	C	178.8	0.3	1
1	A	92	GLN	CA	58.3	0.3	1
1	A	92	GLN	CB	28.3	0.3	1
1	A	92	GLN	CG	34.4	0.3	1
1	A	92	GLN	N	116.5	0.3	1
1	A	92	GLN	NE2	112.6	0.3	1
1	A	93	LYS	H	7.97	0.02	1
1	A	93	LYS	HA	4.07	0.02	1
1	A	93	LYS	HB2	1.93	0.02	1
1	A	93	LYS	HB3	1.93	0.02	1
1	A	93	LYS	HD2	1.56	0.02	1
1	A	93	LYS	HD3	1.56	0.02	1
1	A	93	LYS	HG2	1.47	0.02	1
1	A	93	LYS	HG3	1.47	0.02	1
1	A	93	LYS	C	178.1	0.3	1
1	A	93	LYS	CA	58.7	0.3	1
1	A	93	LYS	CB	32.3	0.3	1
1	A	93	LYS	CD	28.8	0.3	1
1	A	93	LYS	CG	25.1	0.3	1
1	A	93	LYS	N	120.8	0.3	1
1	A	94	GLU	H	7.93	0.02	1
1	A	94	GLU	HA	4.34	0.02	1
1	A	94	GLU	HB2	2.25	0.02	1
1	A	94	GLU	HB3	2.25	0.02	1
1	A	94	GLU	HG2	2.25	0.02	1
1	A	94	GLU	HG3	2.25	0.02	1
1	A	94	GLU	C	176.0	0.3	1
1	A	94	GLU	CA	55.9	0.3	1
1	A	94	GLU	CB	29.7	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	GLU	CG	36.0	0.3	1
1	A	94	GLU	N	116.8	0.3	1
1	A	95	SER	H	7.9	0.02	1
1	A	95	SER	HA	4.25	0.02	1
1	A	95	SER	HB2	3.84	0.02	1
1	A	95	SER	HB3	3.84	0.02	1
1	A	95	SER	C	173.9	0.3	1
1	A	95	SER	CA	58.4	0.3	1
1	A	95	SER	CB	62.6	0.3	1
1	A	95	SER	N	115.0	0.3	1
1	A	96	SER	H	8.37	0.02	1
1	A	96	SER	HA	4.52	0.02	1
1	A	96	SER	HB2	3.76	0.02	1
1	A	96	SER	HB3	3.76	0.02	1
1	A	96	SER	C	173.7	0.3	1
1	A	96	SER	CA	57.1	0.3	1
1	A	96	SER	CB	64.4	0.3	1
1	A	96	SER	N	116.3	0.3	1
1	A	97	LEU	H	7.83	0.02	1
1	A	97	LEU	HA	4.21	0.02	1
1	A	97	LEU	HB2	1.51	0.02	1
1	A	97	LEU	HB3	1.51	0.02	1
1	A	97	LEU	HD11	0.81	0.02	1
1	A	97	LEU	HD12	0.81	0.02	1
1	A	97	LEU	HD13	0.81	0.02	1
1	A	97	LEU	HD21	0.81	0.02	1
1	A	97	LEU	HD22	0.81	0.02	1
1	A	97	LEU	HD23	0.81	0.02	1
1	A	97	LEU	HG	1.51	0.02	1
1	A	97	LEU	C	177.0	0.3	1
1	A	97	LEU	CA	54.9	0.3	1
1	A	97	LEU	CB	42.2	0.3	1
1	A	97	LEU	CD1	24.8	0.3	1
1	A	97	LEU	CD2	23.2	0.3	1
1	A	97	LEU	CG	26.9	0.3	1
1	A	97	LEU	N	122.5	0.3	1
1	A	98	LEU	H	8.14	0.02	1
1	A	98	LEU	HA	4.25	0.02	1
1	A	98	LEU	HB2	1.63	0.02	2
1	A	98	LEU	HB3	1.51	0.02	2
1	A	98	LEU	HD11	0.9	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	LEU	HD12	0.9	0.02	1
1	A	98	LEU	HD13	0.9	0.02	1
1	A	98	LEU	HD21	0.93	0.02	1
1	A	98	LEU	HD22	0.93	0.02	1
1	A	98	LEU	HD23	0.93	0.02	1
1	A	98	LEU	HG	1.45	0.02	1
1	A	98	LEU	C	175.3	0.3	1
1	A	98	LEU	CA	53.5	0.3	1
1	A	98	LEU	CB	39.9	0.3	1
1	A	98	LEU	N	123.1	0.3	1
1	A	99	PRO	HA	4.57	0.02	1
1	A	99	PRO	HB2	2.04	0.02	1
1	A	99	PRO	HB3	2.04	0.02	1
1	A	99	PRO	HD2	3.59	0.02	2
1	A	99	PRO	HD3	3.56	0.02	2
1	A	99	PRO	HG2	1.8	0.02	1
1	A	99	PRO	HG3	1.8	0.02	1
1	A	99	PRO	C	174.8	0.3	1
1	A	99	PRO	CA	63.0	0.3	1
1	A	99	PRO	CB	32.1	0.3	1
1	A	99	PRO	CG	27.6	0.3	1
1	A	100	PHE	H	7.9	0.02	1
1	A	100	PHE	HA	4.89	0.02	1
1	A	100	PHE	HB2	2.9	0.02	2
1	A	100	PHE	HB3	3.04	0.02	2
1	A	100	PHE	C	174.1	0.3	1
1	A	100	PHE	CA	56.4	0.3	1
1	A	100	PHE	CB	41.4	0.3	1
1	A	100	PHE	N	123.5	0.3	1
1	A	101	TYR	H	8.38	0.02	1
1	A	101	TYR	HA	4.96	0.02	1
1	A	101	TYR	HB2	2.55	0.02	1
1	A	101	TYR	HB3	2.55	0.02	1
1	A	101	TYR	HD1	6.82	0.02	3
1	A	101	TYR	HD2	6.81	0.02	3
1	A	101	TYR	HE1	6.82	0.02	1
1	A	101	TYR	HE2	6.82	0.02	1
1	A	101	TYR	C	174.2	0.3	1
1	A	101	TYR	CA	57.5	0.3	1
1	A	101	TYR	CB	40.5	0.3	1
1	A	101	TYR	N	128.7	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	102	ALA	H	8.58	0.02	1
1	A	102	ALA	HA	4.53	0.02	1
1	A	102	ALA	HB1	1.25	0.02	1
1	A	102	ALA	HB2	1.25	0.02	1
1	A	102	ALA	HB3	1.25	0.02	1
1	A	102	ALA	C	176.4	0.3	1
1	A	102	ALA	CA	51.4	0.3	1
1	A	102	ALA	CB	20.9	0.3	1
1	A	102	ALA	N	126.5	0.3	1
1	A	103	THR	H	8.68	0.02	1
1	A	103	THR	HA	5.0	0.02	1
1	A	103	THR	HB	3.77	0.02	1
1	A	103	THR	HG21	1.18	0.02	1
1	A	103	THR	HG22	1.18	0.02	1
1	A	103	THR	HG23	1.18	0.02	1
1	A	103	THR	C	172.5	0.3	1
1	A	103	THR	CA	62.7	0.3	1
1	A	103	THR	CB	70.3	0.3	1
1	A	103	THR	CG2	22.9	0.3	1
1	A	103	THR	N	120.7	0.3	1
1	A	104	ALA	H	9.1	0.02	1
1	A	104	ALA	HA	4.77	0.02	1
1	A	104	ALA	HB1	1.33	0.02	1
1	A	104	ALA	HB2	1.33	0.02	1
1	A	104	ALA	HB3	1.33	0.02	1
1	A	104	ALA	C	176.3	0.3	1
1	A	104	ALA	CA	50.2	0.3	1
1	A	104	ALA	CB	21.7	0.3	1
1	A	104	ALA	N	132.9	0.3	1
1	A	105	THR	H	8.34	0.02	1
1	A	105	THR	HA	4.72	0.02	1
1	A	105	THR	HB	3.83	0.02	1
1	A	105	THR	HG21	0.85	0.02	1
1	A	105	THR	HG22	0.85	0.02	1
1	A	105	THR	HG23	0.85	0.02	1
1	A	105	THR	C	173.7	0.3	1
1	A	105	THR	CA	60.8	0.3	1
1	A	105	THR	CB	70.0	0.3	1
1	A	105	THR	CG2	21.4	0.3	1
1	A	105	THR	N	116.0	0.3	1
1	A	106	SER	H	8.51	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	SER	HA	4.53	0.02	1
1	A	106	SER	HB2	3.66	0.02	2
1	A	106	SER	HB3	3.52	0.02	2
1	A	106	SER	C	173.7	0.3	1
1	A	106	SER	CA	56.5	0.3	1
1	A	106	SER	CB	64.8	0.3	1
1	A	106	SER	N	121.2	0.3	1
1	A	107	GLY	H	8.12	0.02	1
1	A	107	GLY	HA2	4.25	0.02	2
1	A	107	GLY	HA3	3.71	0.02	2
1	A	107	GLY	C	171.3	0.3	1
1	A	107	GLY	CA	44.3	0.3	1
1	A	107	GLY	N	108.3	0.3	1
1	A	108	PRO	HA	4.34	0.02	1
1	A	108	PRO	HB2	2.2	0.02	1
1	A	108	PRO	HB3	2.2	0.02	1
1	A	108	PRO	HG2	1.82	0.02	1
1	A	108	PRO	HG3	1.82	0.02	1
1	A	108	PRO	C	178.4	0.3	1
1	A	108	PRO	CA	61.9	0.3	1
1	A	108	PRO	CB	31.8	0.3	1
1	A	109	SER	H	8.66	0.02	1
1	A	109	SER	HA	4.07	0.02	1
1	A	109	SER	C	178.8	0.3	1
1	A	109	SER	CA	61.3	0.3	1
1	A	109	SER	CB	62.5	0.3	1
1	A	109	SER	N	117.0	0.3	1
1	A	110	HIS	H	8.08	0.02	1
1	A	110	HIS	HA	4.5	0.02	1
1	A	110	HIS	HB2	3.21	0.02	2
1	A	110	HIS	HB3	2.86	0.02	2
1	A	110	HIS	C	175.1	0.3	1
1	A	110	HIS	CA	56.0	0.3	1
1	A	110	HIS	CB	30.2	0.3	1
1	A	110	HIS	N	120.4	0.3	1
1	A	111	ALA	H	6.99	0.02	1
1	A	111	ALA	HA	4.46	0.02	1
1	A	111	ALA	HB1	0.88	0.02	1
1	A	111	ALA	HB2	0.88	0.02	1
1	A	111	ALA	HB3	0.88	0.02	1
1	A	111	ALA	C	175.1	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	ALA	CA	50.6	0.3	1
1	A	111	ALA	CB	18.0	0.3	1
1	A	111	ALA	N	125.0	0.3	1
1	A	112	PRO	HA	4.37	0.02	1
1	A	112	PRO	HB2	1.8	0.02	1
1	A	112	PRO	HB3	1.8	0.02	1
1	A	112	PRO	HD2	3.36	0.02	2
1	A	112	PRO	HD3	3.33	0.02	2
1	A	112	PRO	HG2	1.31	0.02	1
1	A	112	PRO	HG3	1.31	0.02	1
1	A	112	PRO	C	176.7	0.3	1
1	A	112	PRO	CA	63.1	0.3	1
1	A	112	PRO	CB	32.2	0.3	1
1	A	112	PRO	CD	48.5	0.3	1
1	A	112	PRO	CG	26.8	0.3	1
1	A	113	THR	H	8.13	0.02	1
1	A	113	THR	HA	4.34	0.02	1
1	A	113	THR	HB	3.97	0.02	1
1	A	113	THR	HG21	0.94	0.02	1
1	A	113	THR	HG22	0.94	0.02	1
1	A	113	THR	HG23	0.94	0.02	1
1	A	113	THR	C	172.5	0.3	1
1	A	113	THR	CA	60.0	0.3	1
1	A	113	THR	CB	71.0	0.3	1
1	A	113	THR	CG2	21.8	0.3	1
1	A	113	THR	N	113.3	0.3	1
1	A	114	PHE	H	8.84	0.02	1
1	A	114	PHE	HA	5.23	0.02	1
1	A	114	PHE	HB2	2.46	0.02	2
1	A	114	PHE	HB3	2.31	0.02	2
1	A	114	PHE	HD1	6.7	0.02	1
1	A	114	PHE	HD2	6.7	0.02	1
1	A	114	PHE	HE1	6.7	0.02	1
1	A	114	PHE	HE2	6.7	0.02	1
1	A	114	PHE	C	174.5	0.3	1
1	A	114	PHE	CA	56.7	0.3	1
1	A	114	PHE	CB	42.7	0.3	1
1	A	114	PHE	N	120.2	0.3	1
1	A	115	THR	H	8.5	0.02	1
1	A	115	THR	HA	4.52	0.02	1
1	A	115	THR	HB	3.82	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	115	THR	HG21	0.99	0.02	1
1	A	115	THR	HG22	0.99	0.02	1
1	A	115	THR	HG23	0.99	0.02	1
1	A	115	THR	C	173.7	0.3	1
1	A	115	THR	CA	61.9	0.3	1
1	A	115	THR	CB	71.3	0.3	1
1	A	115	THR	CG2	21.3	0.3	1
1	A	115	THR	N	115.5	0.3	1
1	A	116	SER	H	9.98	0.02	1
1	A	116	SER	HA	5.74	0.02	1
1	A	116	SER	HB2	3.76	0.02	2
1	A	116	SER	HB3	3.35	0.02	2
1	A	116	SER	C	173.2	0.3	1
1	A	116	SER	CA	58.0	0.3	1
1	A	116	SER	CB	65.3	0.3	1
1	A	116	SER	N	126.7	0.3	1
1	A	117	THR	H	9.05	0.02	1
1	A	117	THR	HA	5.32	0.02	1
1	A	117	THR	HB	3.97	0.02	1
1	A	117	THR	HG21	1.0	0.02	1
1	A	117	THR	HG22	1.0	0.02	1
1	A	117	THR	HG23	1.0	0.02	1
1	A	117	THR	C	173.5	0.3	1
1	A	117	THR	CA	59.1	0.3	1
1	A	117	THR	CB	71.9	0.3	1
1	A	117	THR	CG2	21.2	0.3	1
1	A	117	THR	N	115.4	0.3	1
1	A	118	VAL	H	9.03	0.02	1
1	A	118	VAL	HA	4.82	0.02	1
1	A	118	VAL	HB	1.42	0.02	1
1	A	118	VAL	HG11	0.65	0.02	1
1	A	118	VAL	HG12	0.65	0.02	1
1	A	118	VAL	HG13	0.65	0.02	1
1	A	118	VAL	HG21	-0.06	0.02	1
1	A	118	VAL	HG22	-0.06	0.02	1
1	A	118	VAL	HG23	-0.06	0.02	1
1	A	118	VAL	C	172.0	0.3	1
1	A	118	VAL	CA	57.9	0.3	1
1	A	118	VAL	CB	35.2	0.3	1
1	A	118	VAL	CG1	21.0	0.3	1
1	A	118	VAL	CG2	22.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	118	VAL	N	120.0	0.3	1
1	A	119	GLU	H	8.52	0.02	1
1	A	119	GLU	HA	5.32	0.02	1
1	A	119	GLU	HB2	2.05	0.02	1
1	A	119	GLU	HB3	2.05	0.02	1
1	A	119	GLU	HG2	1.91	0.02	1
1	A	119	GLU	HG3	1.91	0.02	1
1	A	119	GLU	C	176.2	0.3	1
1	A	119	GLU	CA	54.0	0.3	1
1	A	119	GLU	CB	31.1	0.3	1
1	A	119	GLU	CG	35.9	0.3	1
1	A	119	GLU	N	129.4	0.3	1
1	A	120	PHE	H	9.08	0.02	1
1	A	120	PHE	HA	4.7	0.02	1
1	A	120	PHE	HB2	2.92	0.02	2
1	A	120	PHE	HB3	2.72	0.02	2
1	A	120	PHE	HD1	6.98	0.02	1
1	A	120	PHE	HD2	6.98	0.02	1
1	A	120	PHE	HE1	6.98	0.02	1
1	A	120	PHE	HE2	6.98	0.02	1
1	A	120	PHE	C	173.1	0.3	1
1	A	120	PHE	CA	57.0	0.3	1
1	A	120	PHE	CB	41.7	0.3	1
1	A	120	PHE	N	127.7	0.3	1
1	A	121	ALA	H	8.66	0.02	1
1	A	121	ALA	HA	3.64	0.02	1
1	A	121	ALA	HB1	0.89	0.02	1
1	A	121	ALA	HB2	0.89	0.02	1
1	A	121	ALA	HB3	0.89	0.02	1
1	A	121	ALA	C	176.9	0.3	1
1	A	121	ALA	CA	52.4	0.3	1
1	A	121	ALA	CB	16.5	0.3	1
1	A	121	ALA	N	129.7	0.3	1
1	A	122	GLY	H	8.58	0.02	1
1	A	122	GLY	HA2	3.93	0.02	2
1	A	122	GLY	HA3	3.47	0.02	2
1	A	122	GLY	C	173.6	0.3	1
1	A	122	GLY	CA	45.2	0.3	1
1	A	122	GLY	N	105.0	0.3	1
1	A	123	LYS	H	7.82	0.02	1
1	A	123	LYS	HA	4.32	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	123	LYS	HD2	1.47	0.02	1
1	A	123	LYS	HD3	1.47	0.02	1
1	A	123	LYS	HG2	1.14	0.02	1
1	A	123	LYS	HG3	1.14	0.02	1
1	A	123	LYS	C	173.5	0.3	1
1	A	123	LYS	CA	54.3	0.3	1
1	A	123	LYS	CB	35.5	0.3	1
1	A	123	LYS	CD	28.8	0.3	1
1	A	123	LYS	CE	41.4	0.3	1
1	A	123	LYS	CG	24.7	0.3	1
1	A	123	LYS	N	122.9	0.3	1
1	A	124	VAL	H	7.69	0.02	1
1	A	124	VAL	HA	4.66	0.02	1
1	A	124	VAL	HB	1.63	0.02	1
1	A	124	VAL	HG11	0.86	0.02	1
1	A	124	VAL	HG12	0.86	0.02	1
1	A	124	VAL	HG13	0.86	0.02	1
1	A	124	VAL	HG21	0.69	0.02	1
1	A	124	VAL	HG22	0.69	0.02	1
1	A	124	VAL	HG23	0.69	0.02	1
1	A	124	VAL	C	175.1	0.3	1
1	A	124	VAL	CA	61.0	0.3	1
1	A	124	VAL	CB	33.0	0.3	1
1	A	124	VAL	CG1	20.8	0.3	1
1	A	124	VAL	CG2	20.8	0.3	1
1	A	124	VAL	N	120.4	0.3	1
1	A	125	PHE	H	9.08	0.02	1
1	A	125	PHE	HA	4.7	0.02	1
1	A	125	PHE	HB2	2.77	0.02	1
1	A	125	PHE	HB3	2.77	0.02	1
1	A	125	PHE	HD2	7.14	0.02	1
1	A	125	PHE	HE2	7.14	0.02	1
1	A	125	PHE	C	174.6	0.3	1
1	A	125	PHE	CA	56.3	0.3	1
1	A	125	PHE	CB	41.2	0.3	1
1	A	125	PHE	N	127.1	0.3	1
1	A	126	SER	H	8.8	0.02	1
1	A	126	SER	HA	5.11	0.02	1
1	A	126	SER	HB2	3.71	0.02	1
1	A	126	SER	HB3	3.71	0.02	1
1	A	126	SER	C	174.6	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	126	SER	CA	57.5	0.3	1
1	A	126	SER	CB	64.7	0.3	1
1	A	126	SER	N	117.9	0.3	1
1	A	127	GLY	H	8.52	0.02	1
1	A	127	GLY	HA2	4.25	0.02	1
1	A	127	GLY	HA3	4.25	0.02	1
1	A	127	GLY	C	172.8	0.3	1
1	A	127	GLY	CA	43.3	0.3	1
1	A	127	GLY	N	111.4	0.3	1
1	A	128	GLU	H	8.37	0.02	1
1	A	128	GLU	HA	4.36	0.02	1
1	A	128	GLU	HB2	2.15	0.02	1
1	A	128	GLU	HB3	2.15	0.02	1
1	A	128	GLU	HG2	2.15	0.02	1
1	A	128	GLU	HG3	2.15	0.02	1
1	A	128	GLU	C	176.5	0.3	1
1	A	128	GLU	CA	54.3	0.3	1
1	A	128	GLU	CB	31.5	0.3	1
1	A	128	GLU	CG	36.2	0.3	1
1	A	128	GLU	N	116.4	0.3	1
1	A	129	GLU	H	8.31	0.02	1
1	A	129	GLU	HA	4.5	0.02	1
1	A	129	GLU	HB2	2.09	0.02	2
1	A	129	GLU	HB3	2.06	0.02	2
1	A	129	GLU	HG2	1.78	0.02	2
1	A	129	GLU	HG3	1.75	0.02	2
1	A	129	GLU	C	176.8	0.3	1
1	A	129	GLU	CA	56.9	0.3	1
1	A	129	GLU	CB	30.2	0.3	1
1	A	129	GLU	CG	36.5	0.3	1
1	A	129	GLU	N	121.7	0.3	1
1	A	130	ALA	H	9.57	0.02	1
1	A	130	ALA	HA	4.87	0.02	1
1	A	130	ALA	HB1	1.39	0.02	1
1	A	130	ALA	HB2	1.39	0.02	1
1	A	130	ALA	HB3	1.39	0.02	1
1	A	130	ALA	C	177.4	0.3	1
1	A	130	ALA	CA	50.3	0.3	1
1	A	130	ALA	CB	23.6	0.3	1
1	A	130	ALA	N	127.4	0.3	1
1	A	131	LYS	H	8.68	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	LYS	HA	4.35	0.02	1
1	A	131	LYS	HB2	1.97	0.02	2
1	A	131	LYS	HB3	1.77	0.02	2
1	A	131	LYS	HD2	1.63	0.02	1
1	A	131	LYS	HD3	1.63	0.02	1
1	A	131	LYS	HG2	1.51	0.02	2
1	A	131	LYS	HG3	1.47	0.02	2
1	A	131	LYS	C	176.4	0.3	1
1	A	131	LYS	CA	57.5	0.3	1
1	A	131	LYS	CB	33.5	0.3	1
1	A	131	LYS	N	116.2	0.3	1
1	A	132	THR	H	7.1	0.02	1
1	A	132	THR	HA	4.31	0.02	1
1	A	132	THR	HB	4.26	0.02	1
1	A	132	THR	HG21	1.07	0.02	1
1	A	132	THR	HG22	1.07	0.02	1
1	A	132	THR	HG23	1.07	0.02	1
1	A	132	THR	C	173.3	0.3	1
1	A	132	THR	CA	58.4	0.3	1
1	A	132	THR	CB	72.2	0.3	1
1	A	132	THR	CG2	21.7	0.3	1
1	A	132	THR	N	105.1	0.3	1
1	A	133	LYS	H	7.97	0.02	1
1	A	133	LYS	HA	3.17	0.02	1
1	A	133	LYS	HB2	1.27	0.02	1
1	A	133	LYS	HB3	1.27	0.02	1
1	A	133	LYS	HE2	2.75	0.02	1
1	A	133	LYS	HE3	2.75	0.02	1
1	A	133	LYS	HG2	1.06	0.02	2
1	A	133	LYS	HG3	0.95	0.02	2
1	A	133	LYS	C	177.1	0.3	1
1	A	133	LYS	CA	59.6	0.3	1
1	A	133	LYS	CB	31.7	0.3	1
1	A	133	LYS	CD	30.5	0.3	1
1	A	133	LYS	CE	37.3	0.3	1
1	A	133	LYS	CG	24.2	0.3	1
1	A	133	LYS	N	124.1	0.3	1
1	A	134	LYS	H	7.94	0.02	1
1	A	134	LYS	HA	3.72	0.02	1
1	A	134	LYS	HB2	1.51	0.02	1
1	A	134	LYS	HB3	1.51	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	134	LYS	HD2	1.58	0.02	1
1	A	134	LYS	HD3	1.58	0.02	1
1	A	134	LYS	HE2	2.79	0.02	1
1	A	134	LYS	HE3	2.79	0.02	1
1	A	134	LYS	HG2	1.28	0.02	1
1	A	134	LYS	HG3	1.28	0.02	1
1	A	134	LYS	C	179.7	0.3	1
1	A	134	LYS	CA	59.3	0.3	1
1	A	134	LYS	CB	31.8	0.3	1
1	A	134	LYS	CD	28.6	0.3	1
1	A	134	LYS	CE	40.7	0.3	1
1	A	134	LYS	CG	24.9	0.3	1
1	A	134	LYS	N	118.3	0.3	1
1	A	135	LEU	H	7.59	0.02	1
1	A	135	LEU	HA	3.99	0.02	1
1	A	135	LEU	HB2	1.42	0.02	1
1	A	135	LEU	HB3	1.42	0.02	1
1	A	135	LEU	HD11	0.81	0.02	1
1	A	135	LEU	HD12	0.81	0.02	1
1	A	135	LEU	HD13	0.81	0.02	1
1	A	135	LEU	HD21	0.9	0.02	1
1	A	135	LEU	HD22	0.9	0.02	1
1	A	135	LEU	HD23	0.9	0.02	1
1	A	135	LEU	HG	1.49	0.02	1
1	A	135	LEU	C	179.8	0.3	1
1	A	135	LEU	CA	57.1	0.3	1
1	A	135	LEU	CB	41.8	0.3	1
1	A	135	LEU	CD1	21.9	0.3	1
1	A	135	LEU	CD2	21.9	0.3	1
1	A	135	LEU	CG	25.6	0.3	1
1	A	135	LEU	N	119.3	0.3	1
1	A	136	ALA	H	8.12	0.02	1
1	A	136	ALA	HA	3.98	0.02	1
1	A	136	ALA	HB1	1.51	0.02	1
1	A	136	ALA	HB2	1.51	0.02	1
1	A	136	ALA	HB3	1.51	0.02	1
1	A	136	ALA	C	181.3	0.3	1
1	A	136	ALA	CA	55.6	0.3	1
1	A	136	ALA	CB	18.5	0.3	1
1	A	136	ALA	N	127.3	0.3	1
1	A	137	GLU	H	8.37	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	GLU	HA	3.81	0.02	1
1	A	137	GLU	HB2	1.25	0.02	1
1	A	137	GLU	HB3	1.25	0.02	1
1	A	137	GLU	HG2	2.27	0.02	1
1	A	137	GLU	HG3	2.27	0.02	1
1	A	137	GLU	C	178.4	0.3	1
1	A	137	GLU	CA	59.7	0.3	1
1	A	137	GLU	CB	29.5	0.3	1
1	A	137	GLU	CG	36.1	0.3	1
1	A	137	GLU	N	122.2	0.3	1
1	A	138	MET	H	7.77	0.02	1
1	A	138	MET	HA	3.97	0.02	1
1	A	138	MET	HB2	2.12	0.02	1
1	A	138	MET	HB3	2.12	0.02	1
1	A	138	MET	HG2	2.67	0.02	1
1	A	138	MET	HG3	2.67	0.02	1
1	A	138	MET	C	177.5	0.3	1
1	A	138	MET	CA	58.2	0.3	1
1	A	138	MET	CB	31.3	0.3	1
1	A	138	MET	CG	32.2	0.3	1
1	A	138	MET	N	118.4	0.3	1
1	A	139	SER	H	7.62	0.02	1
1	A	139	SER	HA	4.14	0.02	1
1	A	139	SER	HB2	3.84	0.02	1
1	A	139	SER	HB3	3.84	0.02	1
1	A	139	SER	C	176.5	0.3	1
1	A	139	SER	CA	60.6	0.3	1
1	A	139	SER	CB	62.1	0.3	1
1	A	139	SER	N	113.1	0.3	1
1	A	140	ALA	H	7.59	0.02	1
1	A	140	ALA	HA	3.69	0.02	1
1	A	140	ALA	HB1	1.32	0.02	1
1	A	140	ALA	HB2	1.32	0.02	1
1	A	140	ALA	HB3	1.32	0.02	1
1	A	140	ALA	C	177.8	0.3	1
1	A	140	ALA	CA	55.4	0.3	1
1	A	140	ALA	CB	17.2	0.3	1
1	A	140	ALA	N	121.8	0.3	1
1	A	141	ALA	H	8.24	0.02	1
1	A	141	ALA	HA	3.85	0.02	1
1	A	141	ALA	HB1	1.47	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	141	ALA	HB2	1.47	0.02	1
1	A	141	ALA	HB3	1.47	0.02	1
1	A	141	ALA	C	178.5	0.3	1
1	A	141	ALA	CA	54.8	0.3	1
1	A	141	ALA	CB	18.1	0.3	1
1	A	141	ALA	N	118.8	0.3	1
1	A	142	LYS	H	7.96	0.02	1
1	A	142	LYS	HA	3.83	0.02	1
1	A	142	LYS	HE2	3.0	0.02	1
1	A	142	LYS	HE3	3.0	0.02	1
1	A	142	LYS	C	177.5	0.3	1
1	A	142	LYS	CA	59.9	0.3	1
1	A	142	LYS	CB	32.0	0.3	1
1	A	142	LYS	N	120.3	0.3	1
1	A	143	VAL	H	7.77	0.02	1
1	A	143	VAL	HA	3.34	0.02	1
1	A	143	VAL	HB	1.95	0.02	1
1	A	143	VAL	HG11	0.99	0.02	1
1	A	143	VAL	HG12	0.99	0.02	1
1	A	143	VAL	HG13	0.99	0.02	1
1	A	143	VAL	HG21	1.09	0.02	1
1	A	143	VAL	HG22	1.09	0.02	1
1	A	143	VAL	HG23	1.09	0.02	1
1	A	143	VAL	C	179.4	0.3	1
1	A	143	VAL	CA	66.5	0.3	1
1	A	143	VAL	CB	31.3	0.3	1
1	A	143	VAL	CG1	21.2	0.3	1
1	A	143	VAL	CG2	22.3	0.3	1
1	A	143	VAL	N	119.9	0.3	1
1	A	144	ALA	H	7.82	0.02	1
1	A	144	ALA	HA	2.28	0.02	1
1	A	144	ALA	HB1	0.77	0.02	1
1	A	144	ALA	HB2	0.77	0.02	1
1	A	144	ALA	HB3	0.77	0.02	1
1	A	144	ALA	C	178.3	0.3	1
1	A	144	ALA	CA	54.3	0.3	1
1	A	144	ALA	CB	19.3	0.3	1
1	A	144	ALA	N	123.3	0.3	1
1	A	145	PHE	H	8.73	0.02	1
1	A	145	PHE	HA	3.58	0.02	1
1	A	145	PHE	HB2	2.97	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	145	PHE	HB3	2.97	0.02	1
1	A	145	PHE	HD1	7.24	0.02	1
1	A	145	PHE	HD2	7.24	0.02	1
1	A	145	PHE	HE1	7.24	0.02	1
1	A	145	PHE	HE2	7.24	0.02	1
1	A	145	PHE	C	177.0	0.3	1
1	A	145	PHE	CA	62.0	0.3	1
1	A	145	PHE	CB	39.5	0.3	1
1	A	145	PHE	N	119.2	0.3	1
1	A	146	MET	H	8.53	0.02	1
1	A	146	MET	HA	3.92	0.02	1
1	A	146	MET	HB2	2.66	0.02	1
1	A	146	MET	HB3	2.66	0.02	1
1	A	146	MET	HG2	2.66	0.02	1
1	A	146	MET	HG3	2.66	0.02	1
1	A	146	MET	C	178.1	0.3	1
1	A	146	MET	CA	57.1	0.3	1
1	A	146	MET	CB	30.7	0.3	1
1	A	146	MET	CG	32.8	0.3	1
1	A	146	MET	N	116.2	0.3	1
1	A	147	SER	H	7.51	0.02	1
1	A	147	SER	HA	4.14	0.02	1
1	A	147	SER	HB2	3.84	0.02	1
1	A	147	SER	HB3	3.84	0.02	1
1	A	147	SER	C	176.2	0.3	1
1	A	147	SER	CA	60.9	0.3	1
1	A	147	SER	CB	63.3	0.3	1
1	A	147	SER	N	115.3	0.3	1
1	A	148	ILE	H	7.59	0.02	1
1	A	148	ILE	HA	3.8	0.02	1
1	A	148	ILE	HB	1.61	0.02	1
1	A	148	ILE	HD11	0.64	0.02	1
1	A	148	ILE	HD12	0.64	0.02	1
1	A	148	ILE	HD13	0.64	0.02	1
1	A	148	ILE	HG12	1.4	0.02	2
1	A	148	ILE	HG13	1.09	0.02	2
1	A	148	ILE	HG21	0.74	0.02	1
1	A	148	ILE	HG22	0.74	0.02	1
1	A	148	ILE	HG23	0.74	0.02	1
1	A	148	ILE	C	177.1	0.3	1
1	A	148	ILE	CA	62.9	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	148	ILE	CB	37.6	0.3	1
1	A	148	ILE	CD1	13.4	0.3	1
1	A	148	ILE	CG1	31.4	0.3	1
1	A	148	ILE	CG2	17.2	0.3	1
1	A	148	ILE	N	121.4	0.3	1
1	A	149	LYS	H	7.93	0.02	1
1	A	149	LYS	HA	3.93	0.02	1
1	A	149	LYS	HB2	1.5	0.02	1
1	A	149	LYS	HB3	1.5	0.02	1
1	A	149	LYS	HD2	1.41	0.02	1
1	A	149	LYS	HD3	1.41	0.02	1
1	A	149	LYS	HE2	2.84	0.02	2
1	A	149	LYS	HE3	2.77	0.02	2
1	A	149	LYS	HG2	1.01	0.02	1
1	A	149	LYS	HG3	1.01	0.02	1
1	A	149	LYS	C	176.9	0.3	1
1	A	149	LYS	CA	56.7	0.3	1
1	A	149	LYS	CB	31.6	0.3	1
1	A	149	LYS	CD	29.8	0.3	1
1	A	149	LYS	CG	23.3	0.3	1
1	A	149	LYS	N	122.1	0.3	1
1	A	150	ASN	H	7.93	0.02	1
1	A	150	ASN	HA	4.54	0.02	1
1	A	150	ASN	HB2	2.72	0.02	1
1	A	150	ASN	HB3	2.72	0.02	1
1	A	150	ASN	HD21	7.48	0.02	1
1	A	150	ASN	HD22	6.8	0.02	1
1	A	150	ASN	C	175.8	0.3	1
1	A	150	ASN	CA	53.5	0.3	1
1	A	150	ASN	CB	38.6	0.3	1
1	A	150	ASN	N	118.0	0.3	1
1	A	150	ASN	ND2	113.6	0.3	1
1	A	151	GLY	H	7.98	0.02	1
1	A	151	GLY	HA2	3.84	0.02	1
1	A	151	GLY	HA3	3.84	0.02	1
1	A	151	GLY	C	173.9	0.3	1
1	A	151	GLY	CA	45.6	0.3	1
1	A	151	GLY	N	109.4	0.3	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

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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 ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	150	-0.01 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	141	0.11 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	150	0.25 ± 0.17	None needed (< 0.5 ppm)
^{15}N	139	-0.64 ± 0.30	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 83%, i.e. 679 atoms were assigned a chemical shift out of a possible 819. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	294/298 (99%)	117/120 (98%)	120/120 (100%)	57/58 (98%)
Sidechain	355/430 (83%)	244/280 (87%)	106/130 (82%)	5/20 (25%)
Aromatic	30/91 (33%)	30/45 (67%)	0/44 (0%)	0/2 (0%)
Overall	679/819 (83%)	391/445 (88%)	226/294 (77%)	62/80 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

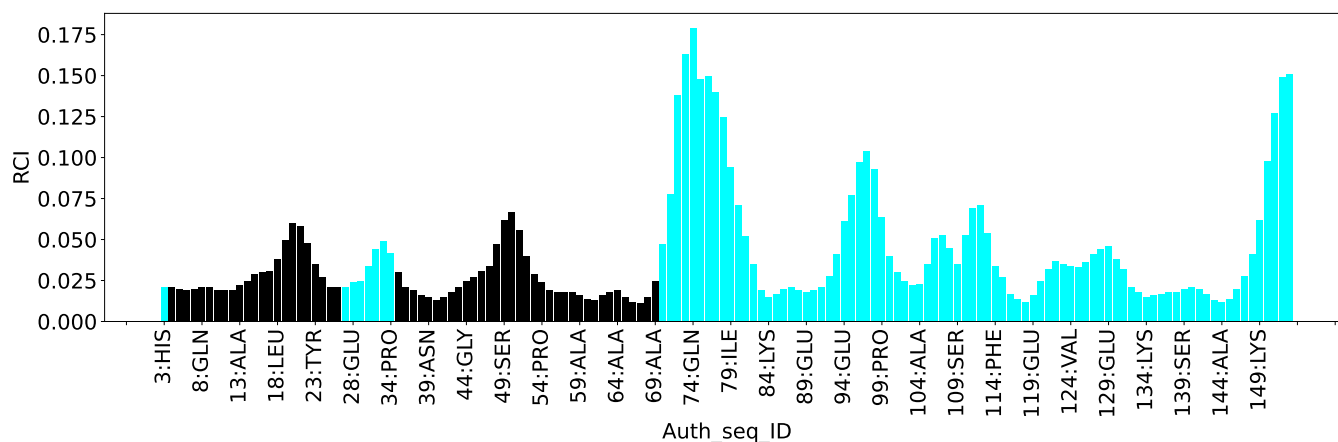
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

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

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1286
Intra-residue ($ i-j =0$)	404
Sequential ($ i-j =1$)	369
Medium range ($ i-j >1$ and $ i-j <5$)	151
Long range ($ i-j \geq 5$)	298
Inter-chain	0
Hydrogen bond restraints	64
Disulfide bond restraints	0
Total dihedral-angle restraints	122
Number of unmapped restraints	0
Number of restraints per residue	9.2
Number of long range restraints per residue ¹	2.1

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	20.2	0.2
0.2-0.5 (Medium)	7.5	0.49
>0.5 (Large)	35.2	3.33

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)	11.6	7.24
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

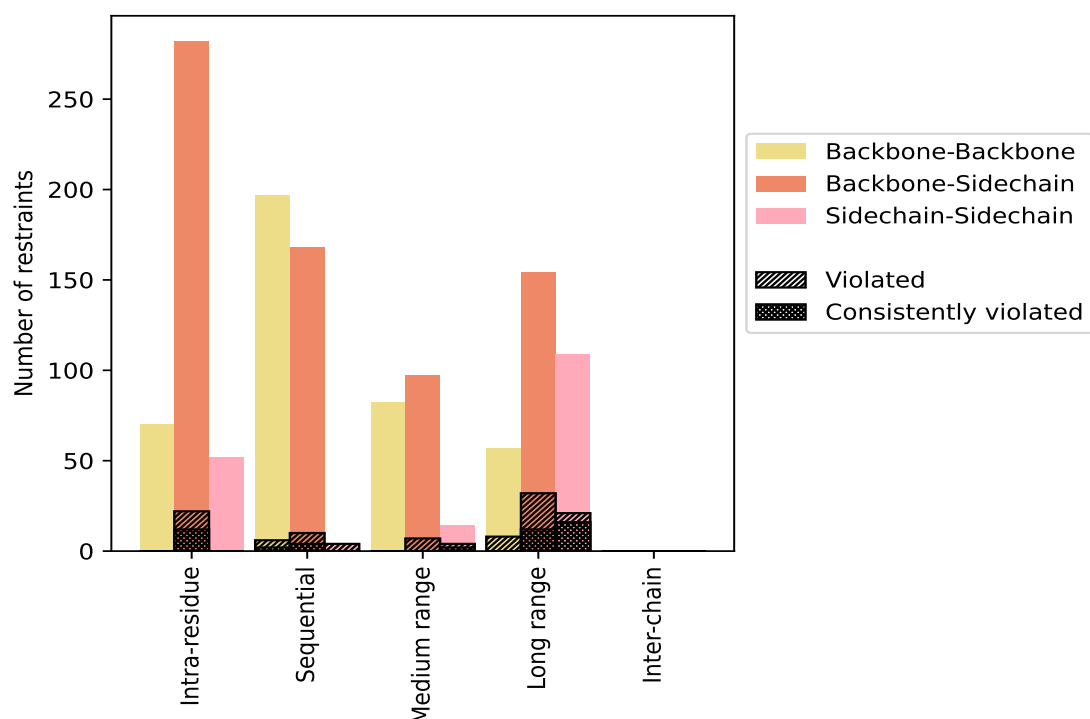
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	404	31.4	22	5.4	1.7	12	3.0	0.9
Backbone-Backbone	70	5.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	282	21.9	22	7.8	1.7	12	4.3	0.9
Sidechain-Sidechain	52	4.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	369	28.7	20	5.4	1.6	6	1.6	0.5
Backbone-Backbone	197	15.3	6	3.0	0.5	2	1.0	0.2
Backbone-Sidechain	168	13.1	10	6.0	0.8	4	2.4	0.3
Sidechain-Sidechain	4	0.3	4	100.0	0.3	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	151	11.7	7	4.6	0.5	2	1.3	0.2
Backbone-Backbone	82	6.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	55	4.3	3	5.5	0.2	0	0.0	0.0
Sidechain-Sidechain	14	1.1	4	28.6	0.3	2	14.3	0.2
Long range (i-j ≥5)	298	23.2	56	18.8	4.4	28	9.4	2.2
Backbone-Backbone	57	4.4	8	14.0	0.6	0	0.0	0.0
Backbone-Sidechain	132	10.3	27	20.5	2.1	12	9.1	0.9
Sidechain-Sidechain	109	8.5	21	19.3	1.6	16	14.7	1.2
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	64	5.0	9	14.1	0.7	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1286	100.0	114	8.9	8.9	48	3.7	3.7
Backbone-Backbone	406	31.6	14	3.4	1.1	2	0.5	0.2
Backbone-Sidechain	701	54.5	71	10.1	5.5	28	4.0	2.2
Sidechain-Sidechain	179	13.9	29	16.2	2.3	18	10.1	1.4

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



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

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	13	10	3	40	0	66	1.18	2.82	0.94	1.26
2	12	7	6	38	0	63	1.05	2.91	0.94	0.79
3	13	7	3	40	0	63	1.07	2.72	0.92	0.77
4	15	9	6	36	0	66	1.02	2.93	0.94	0.66
5	13	7	4	39	0	63	1.06	2.79	0.92	0.78
6	13	9	2	33	0	57	1.2	2.82	0.94	1.26
7	13	7	5	37	0	62	1.08	3.02	0.96	0.86
8	14	10	5	36	0	65	1.03	2.75	0.92	0.76
9	15	12	3	41	0	71	1.14	2.93	0.98	0.95
10	12	6	3	38	0	59	1.13	2.78	0.91	1.24

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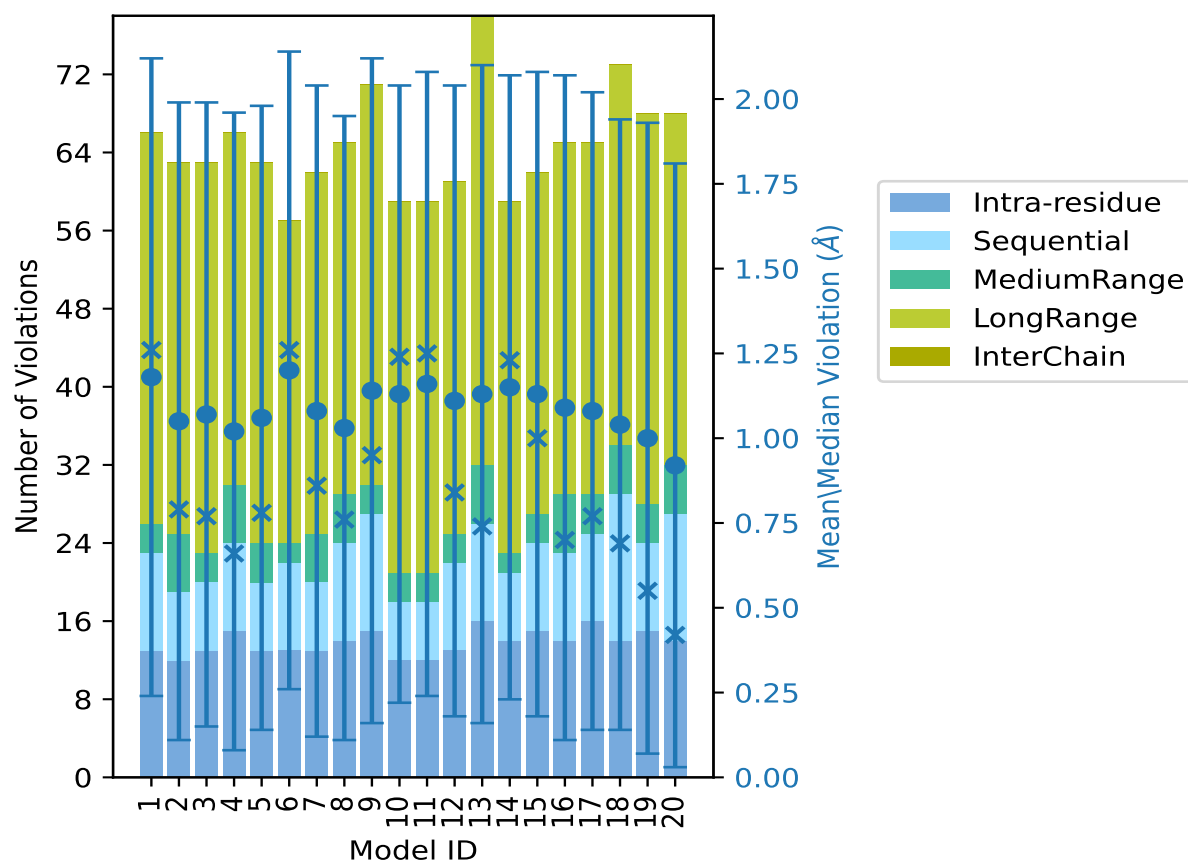
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	12	6	3	38	0	59	1.16	2.68	0.92	1.25
12	13	9	3	36	0	61	1.11	2.89	0.93	0.84
13	16	10	6	46	0	78	1.13	3.33	0.97	0.74
14	14	7	2	36	0	59	1.15	2.75	0.92	1.23
15	15	9	3	35	0	62	1.13	2.84	0.95	1.0
16	14	9	6	36	0	65	1.09	2.91	0.98	0.7
17	16	9	4	36	0	65	1.08	2.76	0.94	0.77
18	14	15	5	39	0	73	1.04	2.79	0.9	0.69
19	15	9	4	40	0	68	1.0	2.83	0.93	0.55
20	14	13	5	36	0	68	0.92	2.96	0.89	0.42

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

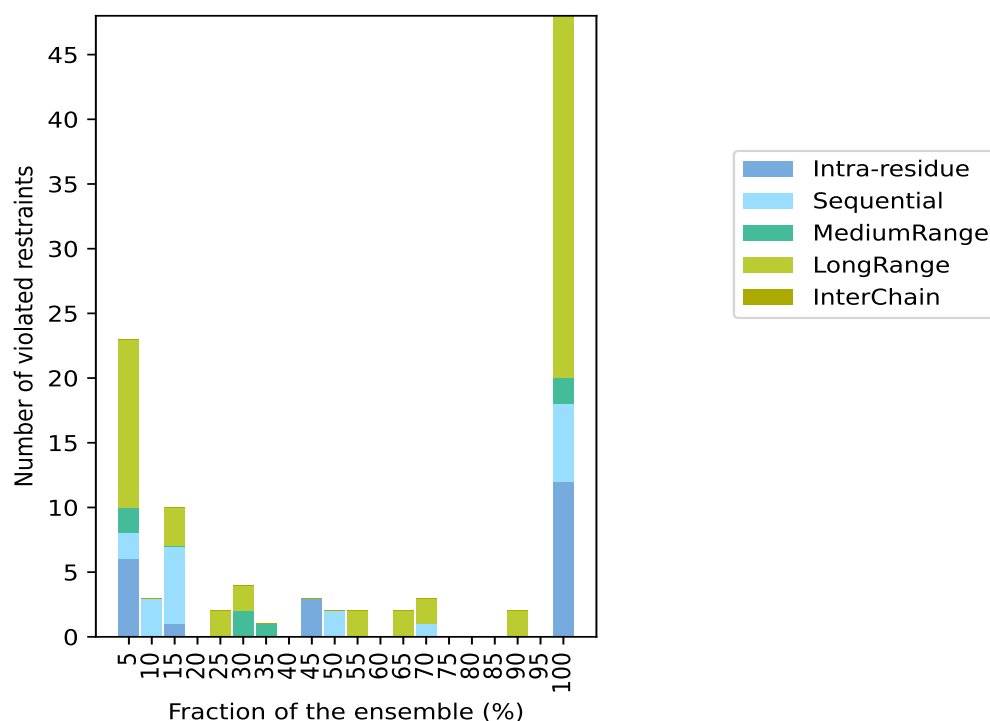
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1117(IR:382, SQ:349, MR:144, LR:242, IC:0) restraints are 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	%
6	2	2	13	0	23	1	5.0
0	3	0	0	0	3	2	10.0
1	6	0	3	0	10	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	2	0	2	5	25.0
0	0	2	2	0	4	6	30.0
0	0	1	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
3	0	0	0	0	3	9	45.0
0	2	0	0	0	2	10	50.0
0	0	0	2	0	2	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	2	0	2	13	65.0
0	1	0	2	0	3	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	2	0	2	18	90.0
0	0	0	0	0	0	19	95.0
12	6	2	28	0	48	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

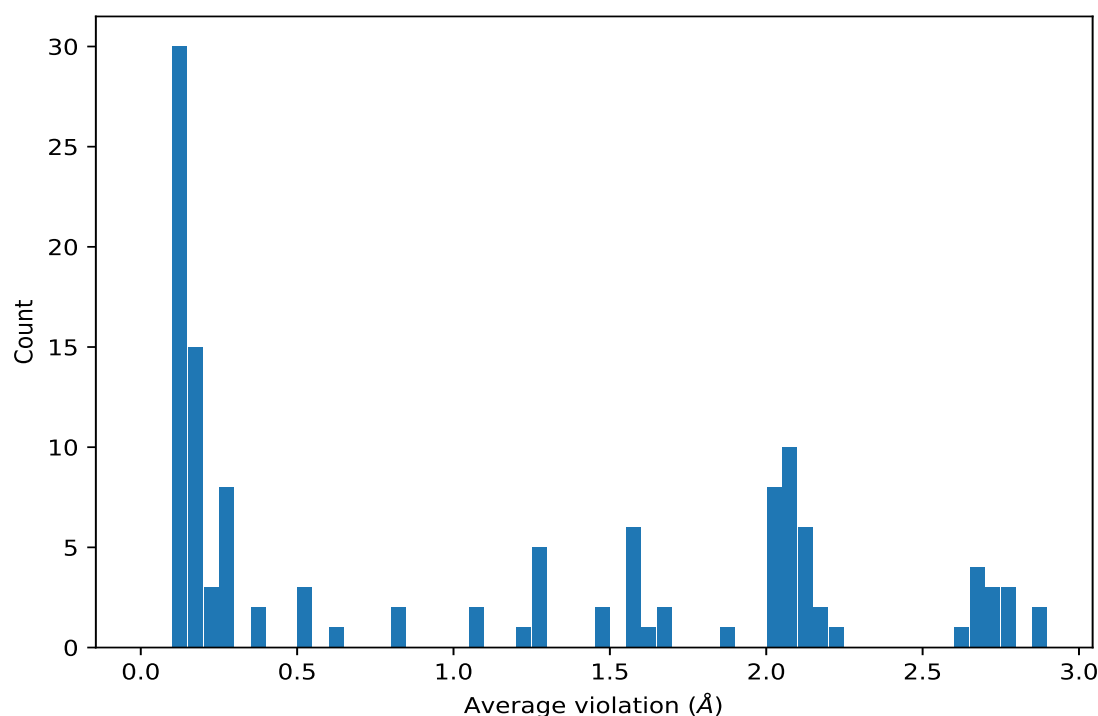
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD11	20	2.79	0.1	2.78
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD12	20	2.79	0.1	2.78
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD13	20	2.79	0.1	2.78
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD11	20	2.72	0.12	2.7
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD12	20	2.72	0.12	2.7
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD13	20	2.72	0.12	2.7
(1,964)	1:27:A:ARG:HB2	1:36:A:PHE:HE2	20	2.66	0.1	2.68
(1,964)	1:27:A:ARG:HB3	1:36:A:PHE:HE2	20	2.66	0.1	2.68
(1,1017)	1:36:A:PHE:HE2	1:27:A:ARG:HB2	20	2.66	0.1	2.68
(1,1017)	1:36:A:PHE:HE2	1:27:A:ARG:HB3	20	2.66	0.1	2.68
(1,1032)	1:36:A:PHE:HE2	1:56:A:LEU:HG	20	2.6	0.14	2.54
(1,1016)	1:36:A:PHE:HE2	1:27:A:ARG:HA	20	2.22	0.07	2.23
(1,965)	1:27:A:ARG:HB2	1:36:A:PHE:HE2	20	2.16	0.1	2.18
(1,965)	1:27:A:ARG:HB3	1:36:A:PHE:HE2	20	2.16	0.1	2.18
(1,1001)	1:34:A:PRO:HG2	1:36:A:PHE:HE1	20	2.11	0.6	2.33
(1,1001)	1:34:A:PRO:HG3	1:36:A:PHE:HE1	20	2.11	0.6	2.33

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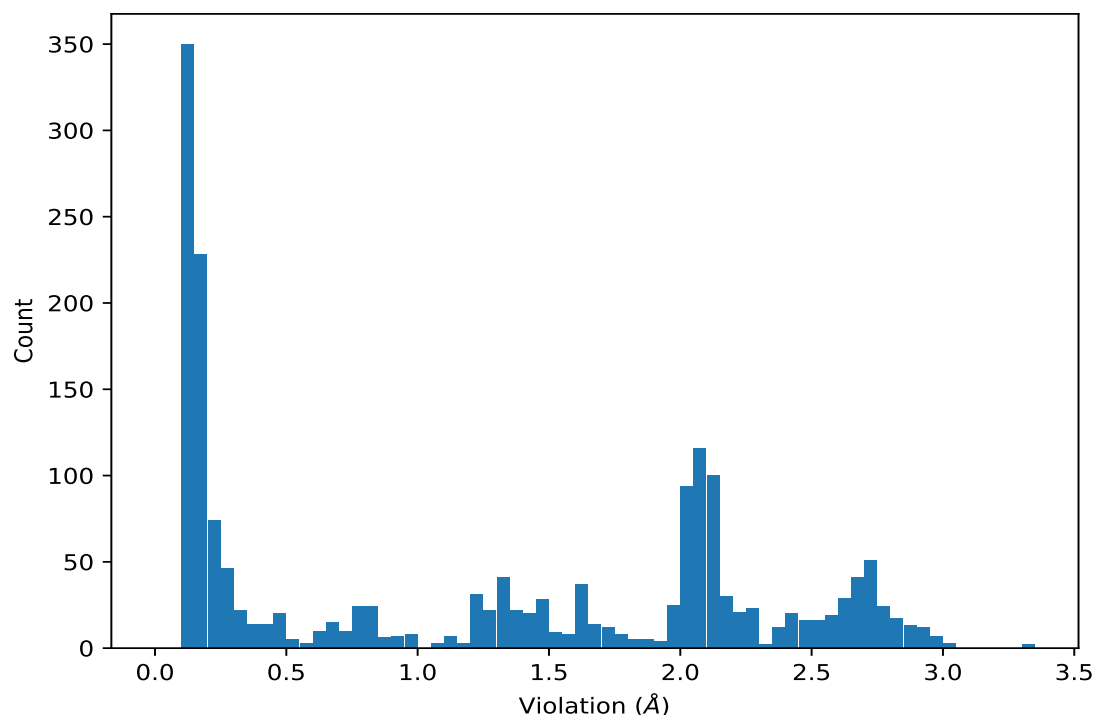
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1021)	1:36:A:PHE:HE1	1:34:A:PRO:HG2	20	2.11	0.6	2.33
(1,1021)	1:36:A:PHE:HE1	1:34:A:PRO:HG3	20	2.11	0.6	2.33
(1,1022)	1:36:A:PHE:HD1	1:55:A:THR:HA	20	2.1	0.03	2.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1157)	1:65:A:LYS:HA	1:5:A:TYR:HE2	13	3.33
(1,753)	1:5:A:TYR:HE2	1:65:A:LYS:HA	13	3.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD11	7	3.02
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD12	7	3.02
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD13	7	3.02
(1,1032)	1:36:A:PHE:HE2	1:56:A:LEU:HG	20	2.96
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD11	7	2.95
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD12	7	2.95
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD13	7	2.95
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD11	20	2.95
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD12	20	2.95
(1,1028)	1:36:A:PHE:HD2	1:56:A:LEU:HD13	20	2.95
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD11	4	2.93
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD12	4	2.93
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD13	4	2.93
(1,833)	1:13:A:ALA:HA	1:12:A:TYR:HD2	9	2.93
(1,826)	1:12:A:TYR:HD2	1:13:A:ALA:HA	9	2.93
(1,1031)	1:36:A:PHE:HE2	1:56:A:LEU:HD11	2	2.91

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

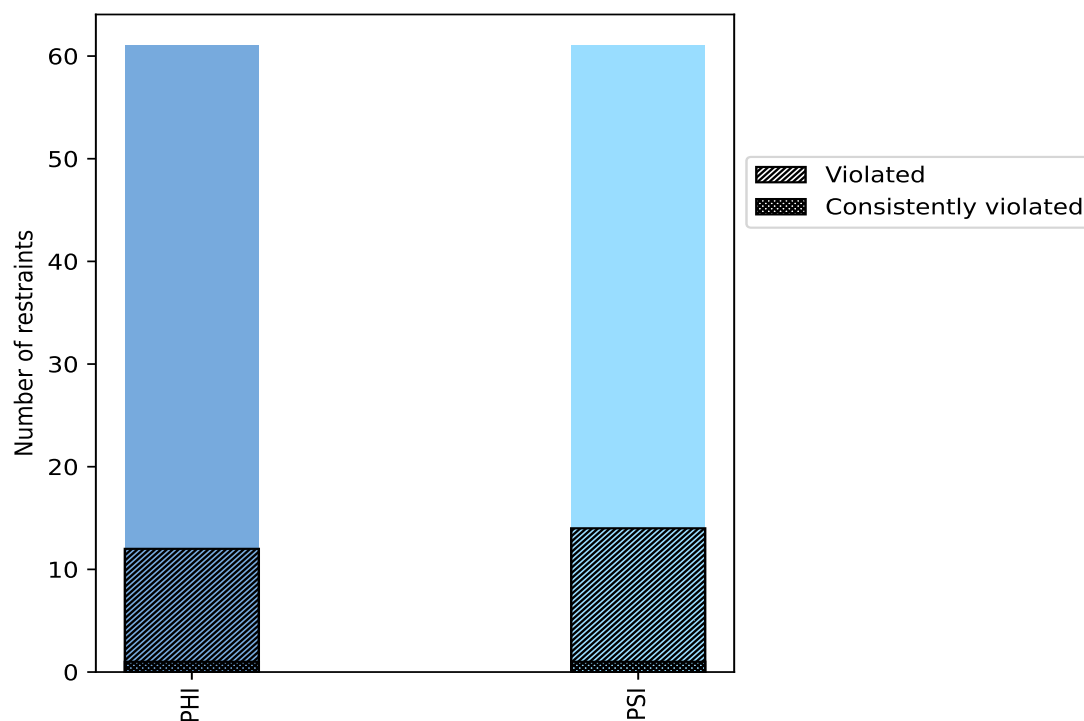
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	61	50.0	12	19.7	9.8	1	1.6	0.8
PSI	61	50.0	14	23.0	11.5	1	1.6	0.8
Total	122	100.0	26	21.3	21.3	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 [i](#)



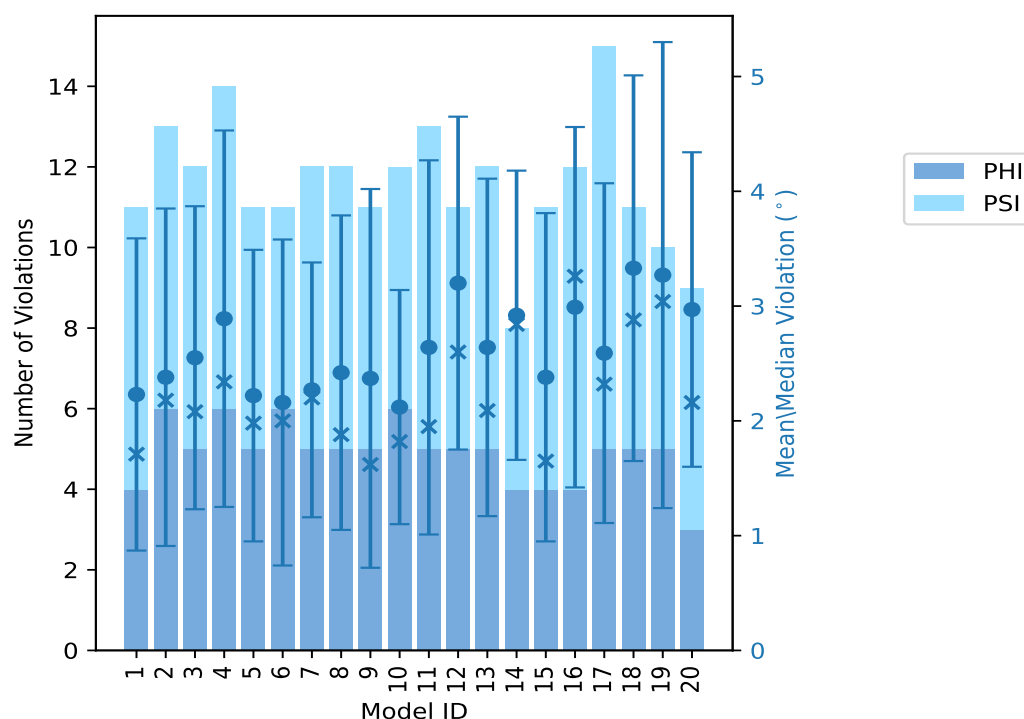
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	4	7	11	2.23	6.09	1.36	1.71
2	6	7	13	2.38	5.88	1.47	2.18
3	5	7	12	2.55	5.65	1.32	2.08
4	6	8	14	2.89	6.73	1.64	2.34
5	5	6	11	2.22	5.6	1.27	1.98
6	6	5	11	2.16	6.36	1.42	2.0
7	5	7	12	2.27	5.3	1.11	2.2
8	5	7	12	2.42	5.47	1.37	1.88
9	5	6	11	2.37	7.04	1.65	1.62
10	6	6	12	2.12	5.08	1.02	1.82
11	5	8	13	2.64	5.38	1.63	1.95
12	5	6	11	3.2	5.54	1.45	2.6
13	5	7	12	2.64	6.03	1.47	2.09
14	4	4	8	2.92	5.6	1.26	2.84
15	4	7	11	2.38	5.28	1.43	1.65
16	4	8	12	2.99	6.1	1.57	3.26
17	5	10	15	2.59	6.28	1.48	2.32
18	5	6	11	3.33	6.75	1.68	2.88
19	5	5	10	3.27	7.24	2.03	3.04
20	3	6	9	2.97	5.65	1.37	2.16

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



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

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

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

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

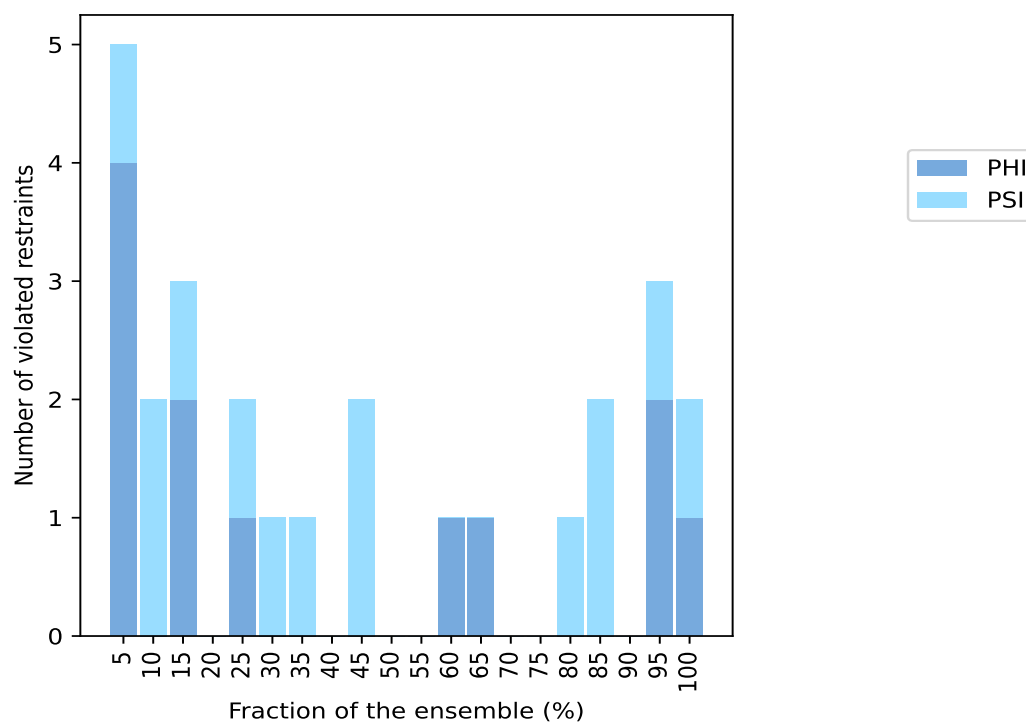
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
1	0	1	12	60.0
1	0	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	1	1	16	80.0
0	2	2	17	85.0
0	0	0	18	90.0
2	1	3	19	95.0
1	1	2	20	100.0

¹ Number of models with violations

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

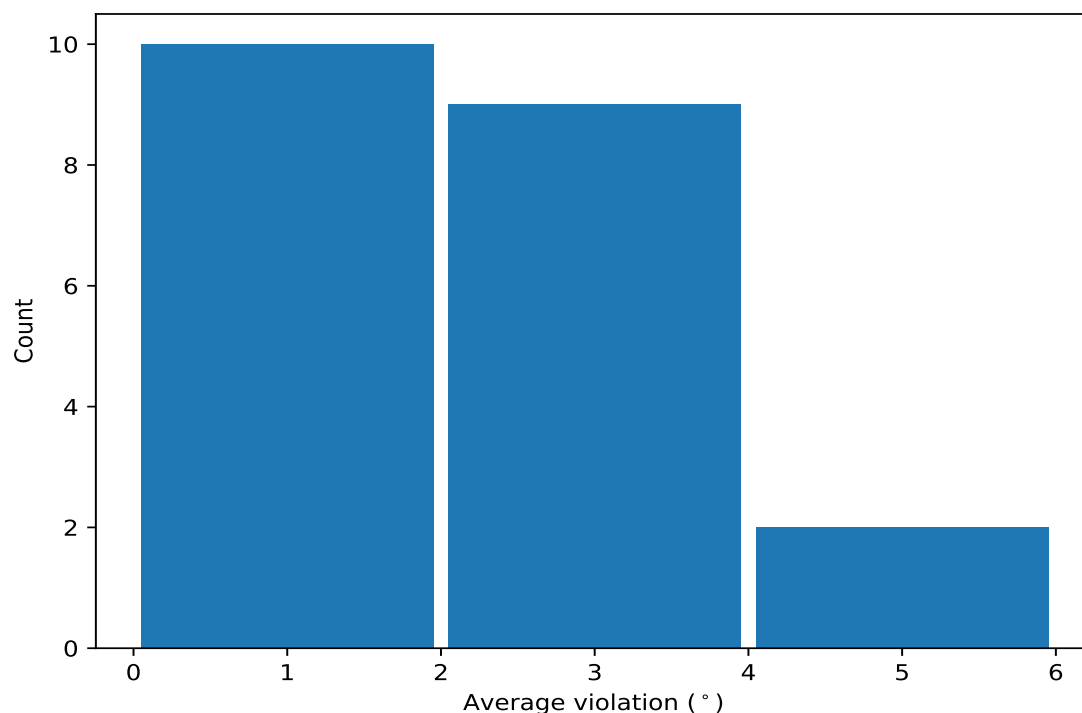


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the 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.

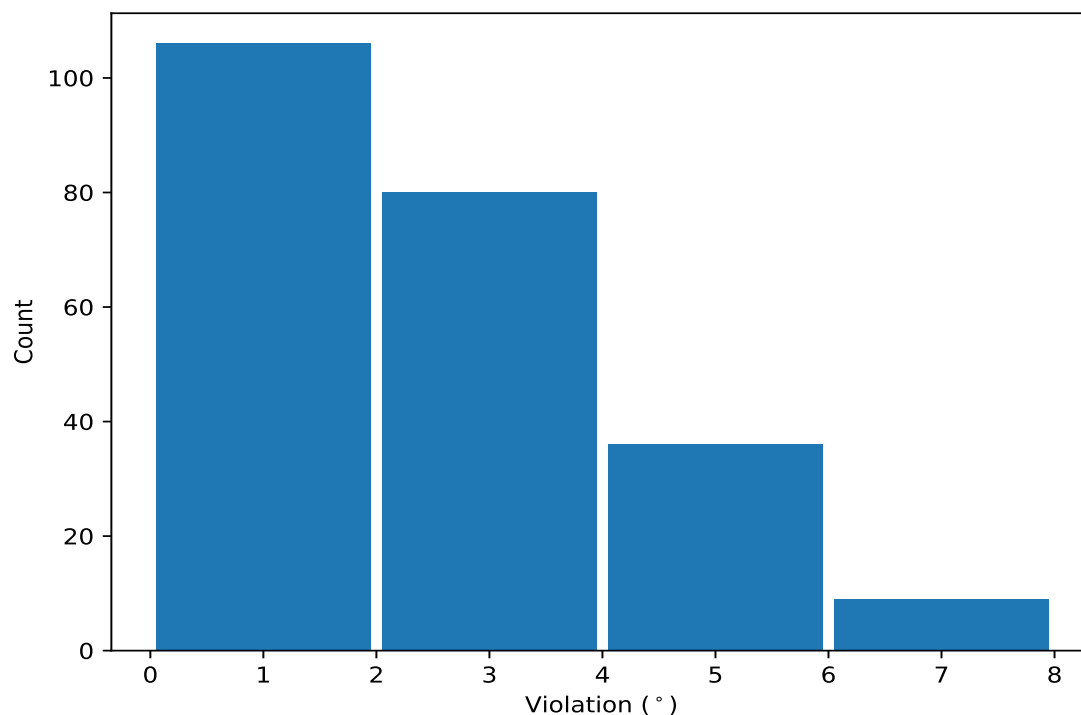
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,90)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ARG:N	20	5.43	1.03	5.5
(1,29)	1:35:A:ARG:C	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	20	2.22	1.01	1.96
(1,108)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LYS:N	19	3.99	1.38	4.31
(1,48)	1:56:A:LEU:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	19	3.08	1.2	2.88
(1,28)	1:32:A:HIS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	19	2.51	1.7	1.79
(1,89)	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	1:34:A:PRO:N	17	2.56	0.72	2.51
(1,101)	1:47:A:PHE:N	1:47:A:PHE:CA	1:47:A:PHE:C	1:48:A:GLN:N	17	1.69	0.61	1.43
(1,91)	1:37:A:ARG:N	1:37:A:ARG:CA	1:37:A:ARG:C	1:38:A:CYS:N	16	2.45	0.85	2.42
(1,25)	1:29:A:GLY:C	1:30:A:PRO:N	1:30:A:PRO:CA	1:30:A:PRO:C	13	2.28	0.64	2.25
(1,4)	1:7:A:GLY:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	12	1.5	0.43	1.32

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,90)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ARG:N	19	7.24
(1,90)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ARG:N	9	7.04
(1,28)	1:32:A:HIS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	18	6.75
(1,108)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LYS:N	4	6.73
(1,90)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ARG:N	6	6.36
(1,108)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LYS:N	17	6.28
(1,28)	1:32:A:HIS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	16	6.1
(1,90)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ARG:N	1	6.09
(1,90)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ARG:N	13	6.03
(1,20)	1:24:A:ALA:C	1:25:A:ASN:N	1:25:A:ASN:CA	1:25:A:ASN:C	19	5.97