W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB NMR Structure Validation Summary Report (i)

Jun 4, 2023 – 07:42 PM EDT

PDB ID	:	2LTS
BMRB ID	:	17703
Title	:	Solution structure of RDE-4(150-235)
Authors	:	Deshmukh, M.; Chiliveri, S.
Deposited on	:	2012-05-31

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

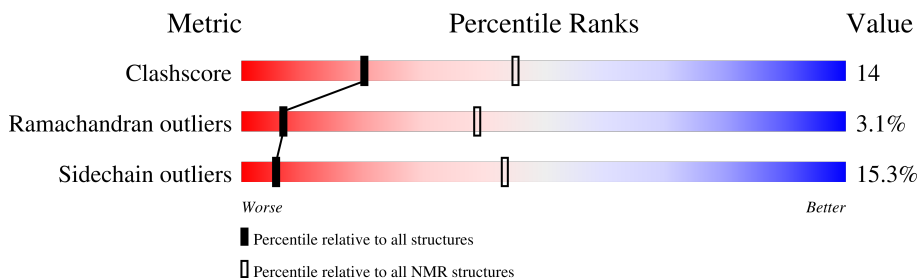|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment is 41%.

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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		3.1%
Sidechain outliers		15.3%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	246	20% 7% • 7% 65%

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 3 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:154-A:158, A:169-A:233 (70)	0.38	3

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 1 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1376 atoms, of which 690 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1376	429	690	121	132	4	0

There are 3 discrepancies between the modelled and reference sequences:

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

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.
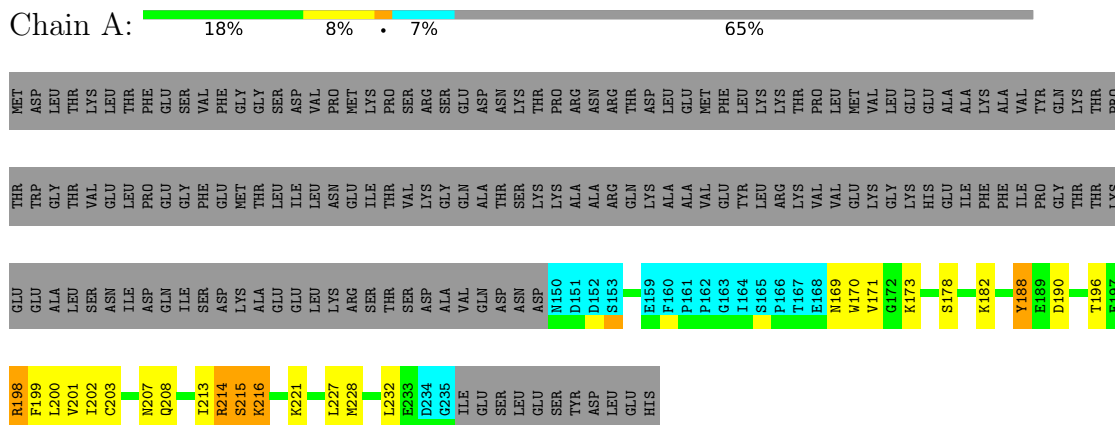
• Molecule 1: Protein RDE-4

Chain A:

20% 7% · 7% 65%
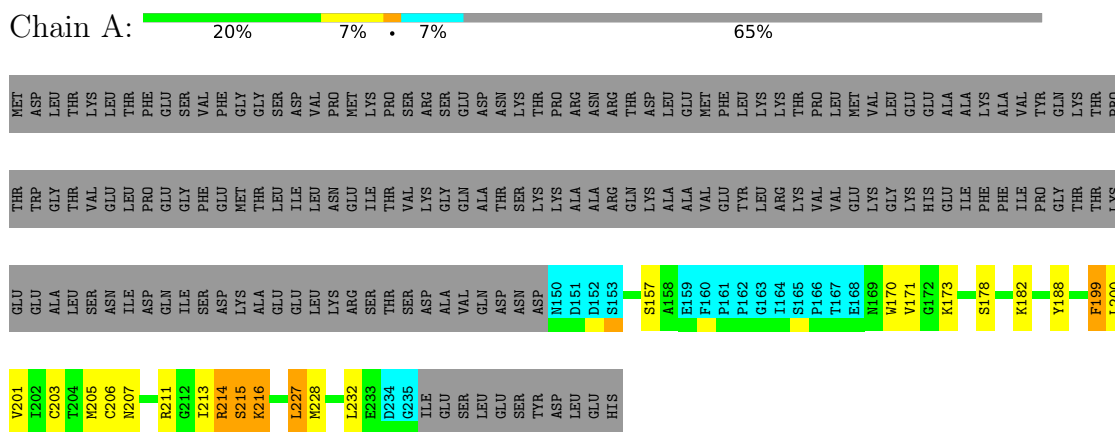
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

• Molecule 1: Protein RDE-4

Chain A:

18% 8% · 7% 65%

5 Refinement protocol and experimental data overview ⓘ

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

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

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

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1441
Number of shifts mapped to atoms	487
Number of unparsed shifts	0
Number of shifts with mapping errors	954
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

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	569	596	596	16±4
All	All	5690	5960	5960	159

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 61 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:203:CYS:SG	1:A:224:ALA:HB1	0.75	2.21	7	5
1:A:213:ILE:HD12	1:A:213:ILE:N	0.63	2.07	3	1
1:A:158:ALA:HB1	1:A:214:ARG:HH12	0.62	1.54	6	1
1:A:226:TRP:CZ3	1:A:229:TRP:CD1	0.62	2.88	6	1
1:A:229:TRP:CD1	1:A:230:LYS:N	0.61	2.69	6	2

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	70/246 (28%)	62±1 (89±2%)	6±1 (8±2%)	2±0 (3±1%)	7	39
All	All	700/2460 (28%)	623 (89%)	55 (8%)	22 (3%)	7	39

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	215	SER	10
1	A	216	LYS	10
1	A	206	CYS	2

6.3.2 Protein sidechains ⓘ

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	62/218 (28%)	52±3 (85±4%)	10±3 (15±4%)	6	43
All	All	620/2180 (28%)	525 (85%)	95 (15%)	6	43

5 of 32 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	171	VAL	10
1	A	227	LEU	9
1	A	214	ARG	7
1	A	199	PHE	7
1	A	157	SER	6

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

WORLDWIDE
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PROTEIN DATA BANK

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 41% for the well-defined parts and 41% 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	1441
Number of shifts mapped to atoms	487
Number of unparsed shifts	0
Number of shifts with mapping errors	954
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 954) occurrences are reported below.

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

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

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

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

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	ASN	CA	52.704	0.300	.
1	A	27	ASN	CB	37.943	0.300	.
1	A	27	ASN	H	8.227	0.020	.
1	A	27	ASN	N	119.643	0.300	.
1	A	28	LYS	C	176.464	0.300	.
1	A	28	LYS	CA	55.658	0.300	.
1	A	28	LYS	CB	31.588	0.300	.
1	A	28	LYS	H	8.174	0.020	.
1	A	28	LYS	N	121.919	0.300	.
1	A	29	THR	C	172.592	0.300	.
1	A	29	THR	CA	59.5	0.300	.
1	A	29	THR	CB	68.774	0.300	.
1	A	29	THR	H	8.12	0.020	.
1	A	29	THR	N	118.711	0.300	.
1	A	30	PRO	C	176.725	0.300	.
1	A	30	PRO	CA	62.61	0.300	.
1	A	30	PRO	CB	30.945	0.300	.
1	A	31	ARG	C	176.007	0.300	.
1	A	31	ARG	CA	55.5	0.300	.
1	A	31	ARG	CB	29.457	0.300	.
1	A	31	ARG	H	8.372	0.020	.
1	A	31	ARG	N	122.183	0.300	.
1	A	32	ASN	C	175.23	0.300	.
1	A	32	ASN	CA	52.81	0.300	.
1	A	32	ASN	CB	37.958	0.300	.
1	A	32	ASN	H	8.4	0.020	.
1	A	32	ASN	N	120.309	0.300	.
1	A	33	ARG	C	176.562	0.300	.
1	A	33	ARG	CA	55.747	0.300	.
1	A	33	ARG	CB	29.386	0.300	.
1	A	33	ARG	H	8.311	0.020	.
1	A	33	ARG	N	122.389	0.300	.
1	A	34	THR	C	174.473	0.300	.
1	A	34	THR	CA	61.98	0.300	.
1	A	34	THR	CB	69.026	0.300	.
1	A	34	THR	H	8.249	0.020	.
1	A	34	THR	N	115.57	0.300	.
1	A	35	ASP	C	177.955	0.300	.
1	A	35	ASP	CA	55.197	0.300	.
1	A	35	ASP	CB	40.012	0.300	.
1	A	35	ASP	H	8.338	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	ASP	N	123.219	0.300	.
1	A	36	LEU	C	177.044	0.300	.
1	A	36	LEU	CA	57.559	0.300	.
1	A	36	LEU	CB	40.367	0.300	.
1	A	36	LEU	CD1	22.206	0.300	.
1	A	36	LEU	CD2	24.896	0.300	.
1	A	36	LEU	H	8.356	0.020	.
1	A	36	LEU	HD11	0.79	0.020	.
1	A	36	LEU	HD12	0.79	0.020	.
1	A	36	LEU	HD13	0.79	0.020	.
1	A	36	LEU	HD21	0.83	0.020	.
1	A	36	LEU	HD22	0.83	0.020	.
1	A	36	LEU	HD23	0.83	0.020	.
1	A	36	LEU	N	125.589	0.300	.
1	A	37	GLU	C	179.333	0.300	.
1	A	37	GLU	CA	58.985	0.300	.
1	A	37	GLU	CB	28.253	0.300	.
1	A	37	GLU	H	8.01	0.020	.
1	A	37	GLU	N	118.091	0.300	.
1	A	38	MET	C	178.737	0.300	.
1	A	38	MET	CA	57.046	0.300	.
1	A	38	MET	CB	31.243	0.300	.
1	A	38	MET	H	7.829	0.020	.
1	A	38	MET	N	116.022	0.300	.
1	A	39	PHE	C	175.855	0.300	.
1	A	39	PHE	CA	61.378	0.300	.
1	A	39	PHE	CB	38.772	0.300	.
1	A	39	PHE	H	8.026	0.020	.
1	A	39	PHE	HD1	7.225	0.020	.
1	A	39	PHE	HE1	7.273	0.020	.
1	A	39	PHE	HZ	6.897	0.020	.
1	A	39	PHE	N	123.397	0.300	.
1	A	40	LEU	C	177.461	0.300	.
1	A	40	LEU	CA	55.451	0.300	.
1	A	40	LEU	CB	40.367	0.300	.
1	A	40	LEU	CD1	25.48	0.300	.
1	A	40	LEU	CD2	22.102	0.300	.
1	A	40	LEU	H	7.995	0.020	.
1	A	40	LEU	HD11	0.813	0.020	.
1	A	40	LEU	HD12	0.813	0.020	.
1	A	40	LEU	HD13	0.813	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	40	LEU	HD21	0.855	0.020	.
1	A	40	LEU	HD22	0.855	0.020	.
1	A	40	LEU	HD23	0.855	0.020	.
1	A	40	LEU	N	113.942	0.300	.
1	A	41	LYS	C	176.539	0.300	.
1	A	41	LYS	CA	55.381	0.300	.
1	A	41	LYS	CB	31.866	0.300	.
1	A	41	LYS	H	6.996	0.020	.
1	A	41	LYS	N	117.082	0.300	.
1	A	42	LYS	C	174.994	0.300	.
1	A	42	LYS	CA	55.245	0.300	.
1	A	42	LYS	CB	33.92	0.300	.
1	A	42	LYS	H	7.691	0.020	.
1	A	42	LYS	N	121.665	0.300	.
1	A	43	THR	C	173.632	0.300	.
1	A	43	THR	CA	58.106	0.300	.
1	A	43	THR	CB	67.64	0.300	.
1	A	43	THR	H	7.06	0.020	.
1	A	43	THR	N	108.411	0.300	.
1	A	44	PRO	C	177.229	0.300	.
1	A	44	PRO	CA	65.454	0.300	.
1	A	44	PRO	CB	31.157	0.300	.
1	A	45	LEU	C	177.815	0.300	.
1	A	45	LEU	CA	57.283	0.300	.
1	A	45	LEU	CB	41.362	0.300	.
1	A	45	LEU	CD1	24.177	0.300	.
1	A	45	LEU	CD2	25.444	0.300	.
1	A	45	LEU	H	8.502	0.020	.
1	A	45	LEU	HD11	0.991	0.020	.
1	A	45	LEU	HD12	0.991	0.020	.
1	A	45	LEU	HD13	0.991	0.020	.
1	A	45	LEU	HD21	0.79	0.020	.
1	A	45	LEU	HD22	0.79	0.020	.
1	A	45	LEU	HD23	0.79	0.020	.
1	A	45	LEU	N	116.774	0.300	.
1	A	46	MET	C	178.368	0.300	.
1	A	46	MET	CA	58.583	0.300	.
1	A	46	MET	CB	33.07	0.300	.
1	A	46	MET	H	7.6	0.020	.
1	A	46	MET	N	119.277	0.300	.
1	A	47	VAL	C	179.12	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	47	VAL	CA	65.771	0.300	.
1	A	47	VAL	CB	30.803	0.300	.
1	A	47	VAL	CG1	21.808	0.300	.
1	A	47	VAL	CG2	23.452	0.300	.
1	A	47	VAL	H	7.846	0.020	.
1	A	47	VAL	HG11	1.205	0.020	.
1	A	47	VAL	HG12	1.205	0.020	.
1	A	47	VAL	HG13	1.205	0.020	.
1	A	47	VAL	HG21	0.818	0.020	.
1	A	47	VAL	HG22	0.818	0.020	.
1	A	47	VAL	HG23	0.818	0.020	.
1	A	47	VAL	N	118.968	0.300	.
1	A	48	LEU	C	177.667	0.300	.
1	A	48	LEU	CA	57.682	0.300	.
1	A	48	LEU	CB	41.258	0.300	.
1	A	48	LEU	CD1	24.574	0.300	.
1	A	48	LEU	CD2	26.597	0.300	.
1	A	48	LEU	H	8.171	0.020	.
1	A	48	LEU	HD11	0.502	0.020	.
1	A	48	LEU	HD12	0.502	0.020	.
1	A	48	LEU	HD13	0.502	0.020	.
1	A	48	LEU	HD21	0.648	0.020	.
1	A	48	LEU	HD22	0.648	0.020	.
1	A	48	LEU	HD23	0.648	0.020	.
1	A	48	LEU	N	120.631	0.300	.
1	A	49	GLU	C	179.957	0.300	.
1	A	49	GLU	CA	59.924	0.300	.
1	A	49	GLU	CB	28.465	0.300	.
1	A	49	GLU	H	8.975	0.020	.
1	A	49	GLU	N	119.032	0.300	.
1	A	50	GLU	C	179.588	0.300	.
1	A	50	GLU	CA	58.698	0.300	.
1	A	50	GLU	CB	28.272	0.300	.
1	A	50	GLU	H	8.681	0.020	.
1	A	50	GLU	N	119.768	0.300	.
1	A	51	ALA	C	178.774	0.300	.
1	A	51	ALA	CA	54.41	0.300	.
1	A	51	ALA	CB	17.773	0.300	.
1	A	51	ALA	H	7.708	0.020	.
1	A	51	ALA	N	122.287	0.300	.
1	A	52	ALA	C	179.561	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	ALA	CA	55.411	0.300	.
1	A	52	ALA	CB	17.556	0.300	.
1	A	52	ALA	H	8.732	0.020	.
1	A	52	ALA	N	120.682	0.300	.
1	A	53	LYS	C	178.227	0.300	.
1	A	53	LYS	CA	58.863	0.300	.
1	A	53	LYS	CB	31.653	0.300	.
1	A	53	LYS	H	7.549	0.020	.
1	A	53	LYS	N	116.775	0.300	.
1	A	54	ALA	C	179.021	0.300	.
1	A	54	ALA	CA	54.228	0.300	.
1	A	54	ALA	CB	18.464	0.300	.
1	A	54	ALA	H	7.924	0.020	.
1	A	54	ALA	N	120.539	0.300	.
1	A	55	VAL	C	177.234	0.300	.
1	A	55	VAL	CA	63.832	0.300	.
1	A	55	VAL	CB	31.519	0.300	.
1	A	55	VAL	CG1	20.106	0.300	.
1	A	55	VAL	CG2	21.919	0.300	.
1	A	55	VAL	H	8.662	0.020	.
1	A	55	VAL	HG11	-0.11	0.020	.
1	A	55	VAL	HG12	-0.11	0.020	.
1	A	55	VAL	HG13	-0.11	0.020	.
1	A	55	VAL	HG21	0.544	0.020	.
1	A	55	VAL	HG22	0.544	0.020	.
1	A	55	VAL	HG23	0.544	0.020	.
1	A	55	VAL	N	116.542	0.300	.
1	A	56	TYR	C	174.818	0.300	.
1	A	56	TYR	CA	56.456	0.300	.
1	A	56	TYR	CB	38.495	0.300	.
1	A	56	TYR	H	6.752	0.020	.
1	A	56	TYR	N	114.496	0.300	.
1	A	57	GLN	C	174.809	0.300	.
1	A	57	GLN	CA	56.712	0.300	.
1	A	57	GLN	CB	24.853	0.300	.
1	A	57	GLN	H	7.643	0.020	.
1	A	57	GLN	N	116.964	0.300	.
1	A	58	LYS	C	174.398	0.300	.
1	A	58	LYS	CA	53.925	0.300	.
1	A	58	LYS	CB	35.62	0.300	.
1	A	58	LYS	H	7.471	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	LYS	N	116.204	0.300	.
1	A	59	THR	C	172.661	0.300	.
1	A	59	THR	CA	58.14	0.300	.
1	A	59	THR	CB	68.774	0.300	.
1	A	59	THR	H	7.893	0.020	.
1	A	59	THR	N	112.295	0.300	.
1	A	60	PRO	C	174.256	0.300	.
1	A	60	PRO	CA	62.089	0.300	.
1	A	60	PRO	CB	30.759	0.300	.
1	A	61	THR	C	172.067	0.300	.
1	A	61	THR	CA	61.655	0.300	.
1	A	61	THR	CB	69.51	0.300	.
1	A	61	THR	H	8.215	0.020	.
1	A	61	THR	N	119.282	0.300	.
1	A	62	TRP	C	177.064	0.300	.
1	A	62	TRP	CA	54.836	0.300	.
1	A	62	TRP	CB	32.149	0.300	.
1	A	62	TRP	H	8.54	0.020	.
1	A	62	TRP	HE1	10.464	0.020	.
1	A	62	TRP	N	125.233	0.300	.
1	A	63	GLY	C	172.583	0.300	.
1	A	63	GLY	CA	44.017	0.300	.
1	A	63	GLY	H	9.522	0.020	.
1	A	63	GLY	N	112.774	0.300	.
1	A	64	THR	C	173.859	0.300	.
1	A	64	THR	CA	62.157	0.300	.
1	A	64	THR	CB	70.12	0.300	.
1	A	64	THR	H	8.624	0.020	.
1	A	64	THR	N	120.888	0.300	.
1	A	65	VAL	C	174.2	0.300	.
1	A	65	VAL	CA	61.249	0.300	.
1	A	65	VAL	CB	34.274	0.300	.
1	A	65	VAL	CG1	20.596	0.300	.
1	A	65	VAL	CG2	21.72	0.300	.
1	A	65	VAL	H	8.734	0.020	.
1	A	65	VAL	HG11	0.802	0.020	.
1	A	65	VAL	HG12	0.802	0.020	.
1	A	65	VAL	HG13	0.802	0.020	.
1	A	65	VAL	HG21	0.915	0.020	.
1	A	65	VAL	HG22	0.915	0.020	.
1	A	65	VAL	HG23	0.915	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	65	VAL	N	128.659	0.300	.
1	A	66	GLU	C	174.582	0.300	.
1	A	66	GLU	CA	55.683	0.300	.
1	A	66	GLU	CB	28.678	0.300	.
1	A	66	GLU	H	8.699	0.020	.
1	A	66	GLU	N	128.468	0.300	.
1	A	67	LEU	C	175.192	0.300	.
1	A	67	LEU	CA	51.683	0.300	.
1	A	67	LEU	CB	40.367	0.300	.
1	A	67	LEU	CD1	25.516	0.300	.
1	A	67	LEU	CD2	21.962	0.300	.
1	A	67	LEU	H	8.055	0.020	.
1	A	67	LEU	HD11	0.606	0.020	.
1	A	67	LEU	HD12	0.606	0.020	.
1	A	67	LEU	HD13	0.606	0.020	.
1	A	67	LEU	HD21	0.695	0.020	.
1	A	67	LEU	HD22	0.695	0.020	.
1	A	67	LEU	HD23	0.695	0.020	.
1	A	67	LEU	N	127.645	0.300	.
1	A	68	PRO	C	177.844	0.300	.
1	A	68	PRO	CA	65.061	0.300	.
1	A	68	PRO	CB	30.166	0.300	.
1	A	69	GLU	C	175.688	0.300	.
1	A	69	GLU	CA	54.974	0.300	.
1	A	69	GLU	CB	28.607	0.300	.
1	A	69	GLU	H	7.877	0.020	.
1	A	69	GLU	N	112.386	0.300	.
1	A	70	GLY	C	170.995	0.300	.
1	A	70	GLY	CA	45.078	0.300	.
1	A	70	GLY	H	7.262	0.020	.
1	A	70	GLY	N	108.767	0.300	.
1	A	71	PHE	C	173.726	0.300	.
1	A	71	PHE	CA	56.864	0.300	.
1	A	71	PHE	CB	43.059	0.300	.
1	A	71	PHE	H	8.757	0.020	.
1	A	71	PHE	N	119.71	0.300	.
1	A	72	GLU	C	175.717	0.300	.
1	A	72	GLU	CA	54.379	0.300	.
1	A	72	GLU	CB	31.937	0.300	.
1	A	72	GLU	H	9.18	0.020	.
1	A	72	GLU	N	122.014	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	73	MET	C	175.471	0.300	.
1	A	73	MET	CA	51.552	0.300	.
1	A	73	MET	CB	31.429	0.300	.
1	A	73	MET	H	9.529	0.020	.
1	A	73	MET	N	128.414	0.300	.
1	A	74	THR	C	171.559	0.300	.
1	A	74	THR	CA	62.105	0.300	.
1	A	74	THR	CB	69.199	0.300	.
1	A	74	THR	H	9.548	0.020	.
1	A	74	THR	N	121.747	0.300	.
1	A	75	LEU	C	173.278	0.300	.
1	A	75	LEU	CA	52.471	0.300	.
1	A	75	LEU	CB	42.846	0.300	.
1	A	75	LEU	CD1	22.695	0.300	.
1	A	75	LEU	CD2	25.298	0.300	.
1	A	75	LEU	H	9.03	0.020	.
1	A	75	LEU	HD11	-0.426	0.020	.
1	A	75	LEU	HD12	-0.426	0.020	.
1	A	75	LEU	HD13	-0.426	0.020	.
1	A	75	LEU	HD21	0.225	0.020	.
1	A	75	LEU	HD22	0.225	0.020	.
1	A	75	LEU	HD23	0.225	0.020	.
1	A	75	LEU	N	132.071	0.300	.
1	A	76	ILE	C	175.391	0.300	.
1	A	76	ILE	CA	59.772	0.300	.
1	A	76	ILE	CB	40.012	0.300	.
1	A	76	ILE	CD1	13.972	0.300	.
1	A	76	ILE	H	8.442	0.020	.
1	A	76	ILE	HD11	0.6	0.020	.
1	A	76	ILE	HD12	0.6	0.020	.
1	A	76	ILE	HD13	0.6	0.020	.
1	A	76	ILE	N	126.389	0.300	.
1	A	77	LEU	C	178.427	0.300	.
1	A	77	LEU	CA	54.801	0.300	.
1	A	77	LEU	CB	40.498	0.300	.
1	A	77	LEU	CD1	22.539	0.300	.
1	A	77	LEU	CD2	21.838	0.300	.
1	A	77	LEU	H	7.965	0.020	.
1	A	77	LEU	HD11	0.472	0.020	.
1	A	77	LEU	HD12	0.472	0.020	.
1	A	77	LEU	HD13	0.472	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	LEU	HD21	0.561	0.020	.
1	A	77	LEU	HD22	0.561	0.020	.
1	A	77	LEU	HD23	0.561	0.020	.
1	A	77	LEU	N	124.234	0.300	.
1	A	79	GLU	C	174.882	0.300	.
1	A	79	GLU	CA	56.621	0.300	.
1	A	79	GLU	CB	27.332	0.300	.
1	A	80	ILE	C	173.264	0.300	.
1	A	80	ILE	CA	60.651	0.300	.
1	A	80	ILE	CB	37.746	0.300	.
1	A	80	ILE	CD1	12.439	0.300	.
1	A	80	ILE	H	7.295	0.020	.
1	A	80	ILE	HD11	0.239	0.020	.
1	A	80	ILE	HD12	0.239	0.020	.
1	A	80	ILE	HD13	0.239	0.020	.
1	A	80	ILE	N	123.564	0.300	.
1	A	81	THR	C	174.473	0.300	.
1	A	81	THR	CA	60.318	0.300	.
1	A	81	THR	CB	70.12	0.300	.
1	A	81	THR	H	7.907	0.020	.
1	A	81	THR	N	123.968	0.300	.
1	A	82	VAL	C	173.164	0.300	.
1	A	82	VAL	CA	58.47	0.300	.
1	A	82	VAL	CB	35.266	0.300	.
1	A	82	VAL	CG1	21.76	0.300	.
1	A	82	VAL	CG2	20.506	0.300	.
1	A	82	VAL	H	8.99	0.020	.
1	A	82	VAL	HG11	0.667	0.020	.
1	A	82	VAL	HG12	0.667	0.020	.
1	A	82	VAL	HG13	0.667	0.020	.
1	A	82	VAL	HG21	0.931	0.020	.
1	A	82	VAL	HG22	0.931	0.020	.
1	A	82	VAL	HG23	0.931	0.020	.
1	A	82	VAL	N	120.397	0.300	.
1	A	83	LYS	C	175.897	0.300	.
1	A	83	LYS	CA	53.974	0.300	.
1	A	83	LYS	CB	35.94	0.300	.
1	A	83	LYS	H	8.278	0.020	.
1	A	83	LYS	N	118.186	0.300	.
1	A	84	GLY	C	171.25	0.300	.
1	A	84	GLY	CA	43.623	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	GLY	H	8.784	0.020	.
1	A	84	GLY	N	106.633	0.300	.
1	A	85	GLN	C	174.2	0.300	.
1	A	85	GLN	CA	53.59	0.300	.
1	A	85	GLN	CB	30.591	0.300	.
1	A	85	GLN	H	8.568	0.020	.
1	A	85	GLN	N	123.301	0.300	.
1	A	86	ALA	C	176.412	0.300	.
1	A	86	ALA	CA	51.077	0.300	.
1	A	86	ALA	CB	21.169	0.300	.
1	A	86	ALA	H	8.518	0.020	.
1	A	86	ALA	N	122.478	0.300	.
1	A	87	THR	C	173.592	0.300	.
1	A	87	THR	CA	63.842	0.300	.
1	A	87	THR	CB	68.543	0.300	.
1	A	87	THR	H	8.681	0.020	.
1	A	87	THR	N	110.462	0.300	.
1	A	88	SER	C	173.845	0.300	.
1	A	88	SER	CA	54.979	0.300	.
1	A	88	SER	CB	65.798	0.300	.
1	A	88	SER	H	7.365	0.020	.
1	A	88	SER	N	112.541	0.300	.
1	A	89	LYS	C	178.227	0.300	.
1	A	89	LYS	CA	59.984	0.300	.
1	A	89	LYS	CB	30.307	0.300	.
1	A	89	LYS	H	8.663	0.020	.
1	A	89	LYS	N	125.762	0.300	.
1	A	90	LYS	C	178.879	0.300	.
1	A	90	LYS	CA	59.166	0.300	.
1	A	90	LYS	CB	30.759	0.300	.
1	A	90	LYS	H	8.345	0.020	.
1	A	90	LYS	N	118.312	0.300	.
1	A	91	ALA	C	179.985	0.300	.
1	A	91	ALA	CA	53.743	0.300	.
1	A	91	ALA	CB	17.627	0.300	.
1	A	91	ALA	H	7.425	0.020	.
1	A	91	ALA	N	120.613	0.300	.
1	A	92	ALA	C	179.049	0.300	.
1	A	92	ALA	CA	54.897	0.300	.
1	A	92	ALA	CB	17.29	0.300	.
1	A	92	ALA	H	8.059	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	92	ALA	N	123.791	0.300	.
1	A	93	ARG	C	178.573	0.300	.
1	A	93	ARG	CA	59.318	0.300	.
1	A	93	ARG	CB	29.457	0.300	.
1	A	93	ARG	H	8.075	0.020	.
1	A	93	ARG	N	117.999	0.300	.
1	A	94	GLN	C	178.363	0.300	.
1	A	94	GLN	CA	58.197	0.300	.
1	A	94	GLN	CB	26.269	0.300	.
1	A	94	GLN	H	7.417	0.020	.
1	A	94	GLN	N	117.299	0.300	.
1	A	95	LYS	C	179.489	0.300	.
1	A	95	LYS	CA	58.533	0.300	.
1	A	95	LYS	CB	31.173	0.300	.
1	A	95	LYS	H	8.034	0.020	.
1	A	95	LYS	N	118.44	0.300	.
1	A	96	ALA	C	178.15	0.300	.
1	A	96	ALA	CA	54.358	0.300	.
1	A	96	ALA	CB	16.737	0.300	.
1	A	96	ALA	H	8.255	0.020	.
1	A	96	ALA	N	122.399	0.300	.
1	A	97	ALA	C	179.092	0.300	.
1	A	97	ALA	CA	54.864	0.300	.
1	A	97	ALA	CB	16.253	0.300	.
1	A	97	ALA	H	8.365	0.020	.
1	A	97	ALA	N	120.184	0.300	.
1	A	98	VAL	C	177.362	0.300	.
1	A	98	VAL	CA	67.209	0.300	.
1	A	98	VAL	CB	30.414	0.300	.
1	A	98	VAL	CG1	20.682	0.300	.
1	A	98	VAL	CG2	24.456	0.300	.
1	A	98	VAL	H	8.321	0.020	.
1	A	98	VAL	HG11	0.892	0.020	.
1	A	98	VAL	HG12	0.892	0.020	.
1	A	98	VAL	HG13	0.892	0.020	.
1	A	98	VAL	HG21	1.092	0.020	.
1	A	98	VAL	HG22	1.092	0.020	.
1	A	98	VAL	HG23	1.092	0.020	.
1	A	98	VAL	N	118.52	0.300	.
1	A	99	GLU	C	179.205	0.300	.
1	A	99	GLU	CA	58.136	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	GLU	CB	27.474	0.300	.
1	A	99	GLU	H	7.794	0.020	.
1	A	99	GLU	N	119.04	0.300	.
1	A	100	TYR	C	177.252	0.300	.
1	A	100	TYR	CA	61.626	0.300	.
1	A	100	TYR	CB	37.943	0.300	.
1	A	100	TYR	H	8.617	0.020	.
1	A	100	TYR	N	122.069	0.300	.
1	A	101	LEU	C	178.51	0.300	.
1	A	101	LEU	CA	56.958	0.300	.
1	A	101	LEU	CB	39.877	0.300	.
1	A	101	LEU	CD1	25.383	0.300	.
1	A	101	LEU	CD2	21.639	0.300	.
1	A	101	LEU	H	8.525	0.020	.
1	A	101	LEU	HD11	0.997	0.020	.
1	A	101	LEU	HD12	0.997	0.020	.
1	A	101	LEU	HD13	0.997	0.020	.
1	A	101	LEU	HD21	0.891	0.020	.
1	A	101	LEU	HD22	0.891	0.020	.
1	A	101	LEU	HD23	0.891	0.020	.
1	A	101	LEU	N	117.726	0.300	.
1	A	102	ARG	C	178.986	0.300	.
1	A	102	ARG	CA	60.106	0.300	.
1	A	102	ARG	CB	28.41	0.300	.
1	A	102	ARG	H	8.45	0.020	.
1	A	102	ARG	N	118.083	0.300	.
1	A	103	LYS	C	178.842	0.300	.
1	A	103	LYS	CA	57.5	0.300	.
1	A	103	LYS	CB	29.811	0.300	.
1	A	103	LYS	H	7.649	0.020	.
1	A	103	LYS	N	120.989	0.300	.
1	A	104	VAL	C	178.206	0.300	.
1	A	104	VAL	CA	65.85	0.300	.
1	A	104	VAL	CB	29.654	0.300	.
1	A	104	VAL	CG1	21.331	0.300	.
1	A	104	VAL	CG2	22.576	0.300	.
1	A	104	VAL	H	7.934	0.020	.
1	A	104	VAL	HG11	0.171	0.020	.
1	A	104	VAL	HG12	0.171	0.020	.
1	A	104	VAL	HG13	0.171	0.020	.
1	A	104	VAL	HG21	0.172	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	VAL	HG22	0.172	0.020	.
1	A	104	VAL	HG23	0.172	0.020	.
1	A	104	VAL	N	119.813	0.300	.
1	A	105	VAL	C	180.16	0.300	.
1	A	105	VAL	CA	65.468	0.300	.
1	A	105	VAL	CB	29.93	0.300	.
1	A	105	VAL	CG2	22.873	0.300	.
1	A	105	VAL	H	7.72	0.020	.
1	A	105	VAL	HG21	0.85	0.020	.
1	A	105	VAL	HG11	0.85	0.020	.
1	A	105	VAL	HG12	0.85	0.020	.
1	A	105	VAL	HG13	0.85	0.020	.
1	A	105	VAL	HG22	0.85	0.020	.
1	A	105	VAL	HG23	0.85	0.020	.
1	A	105	VAL	N	119.945	0.300	.
1	A	106	GLU	C	178.18	0.300	.
1	A	106	GLU	CA	58.701	0.300	.
1	A	106	GLU	CB	28.272	0.300	.
1	A	106	GLU	H	7.996	0.020	.
1	A	106	GLU	N	122.151	0.300	.
1	A	107	LYS	C	176.574	0.300	.
1	A	107	LYS	CA	55.451	0.300	.
1	A	107	LYS	CB	31.243	0.300	.
1	A	107	LYS	H	7.761	0.020	.
1	A	107	LYS	N	116.035	0.300	.
1	A	108	GLY	C	176.015	0.300	.
1	A	108	GLY	CA	45.643	0.300	.
1	A	108	GLY	H	7.919	0.020	.
1	A	108	GLY	N	108.029	0.300	.
1	A	109	LYS	C	176.85	0.300	.
1	A	109	LYS	CA	54.417	0.300	.
1	A	109	LYS	CB	32.14	0.300	.
1	A	109	LYS	H	7.824	0.020	.
1	A	109	LYS	N	118.024	0.300	.
1	A	110	HIS	C	176.057	0.300	.
1	A	110	HIS	CA	60.469	0.300	.
1	A	110	HIS	H	8.559	0.020	.
1	A	110	HIS	N	119.735	0.300	.
1	A	111	GLU	C	178.547	0.300	.
1	A	111	GLU	CA	58.58	0.300	.
1	A	112	ILE	C	174.307	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	112	ILE	CA	61.98	0.300	.
1	A	112	ILE	CB	36.009	0.300	.
1	A	112	ILE	CD1	12.714	0.300	.
1	A	112	ILE	H	7.147	0.020	.
1	A	112	ILE	HD11	0.759	0.020	.
1	A	112	ILE	HD12	0.759	0.020	.
1	A	112	ILE	HD13	0.759	0.020	.
1	A	112	ILE	N	119.91	0.300	.
1	A	113	PHE	C	173.629	0.300	.
1	A	113	PHE	CA	57.076	0.300	.
1	A	113	PHE	CB	38.841	0.300	.
1	A	113	PHE	H	6.86	0.020	.
1	A	113	PHE	HD1	7.176	0.020	.
1	A	113	PHE	HE1	7.237	0.020	.
1	A	113	PHE	HZ	7.379	0.020	.
1	A	113	PHE	N	116.897	0.300	.
1	A	114	PHE	C	174.984	0.300	.
1	A	114	PHE	CA	57.431	0.300	.
1	A	114	PHE	CB	34.487	0.300	.
1	A	114	PHE	H	7.256	0.020	.
1	A	114	PHE	N	112.904	0.300	.
1	A	115	ILE	C	173.788	0.300	.
1	A	115	ILE	CA	57.253	0.300	.
1	A	115	ILE	CB	37.666	0.300	.
1	A	115	ILE	CD1	14.153	0.300	.
1	A	115	ILE	H	7.628	0.020	.
1	A	115	ILE	HD11	0.876	0.020	.
1	A	115	ILE	HD12	0.876	0.020	.
1	A	115	ILE	HD13	0.876	0.020	.
1	A	115	ILE	N	121.347	0.300	.
1	A	116	PRO	C	175.337	0.300	.
1	A	116	PRO	CA	61.915	0.300	.
1	A	116	PRO	CB	30.449	0.300	.
1	A	117	GLY	C	174.696	0.300	.
1	A	117	GLY	CA	43.29	0.300	.
1	A	117	GLY	H	8.069	0.020	.
1	A	117	GLY	N	108.662	0.300	.
1	A	118	THR	C	174.452	0.300	.
1	A	118	THR	CA	63.529	0.300	.
1	A	118	THR	CB	68.128	0.300	.
1	A	118	THR	H	9.063	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	118	THR	N	121.394	0.300	.
1	A	119	THR	C	174.556	0.300	.
1	A	119	THR	CA	58.136	0.300	.
1	A	119	THR	CB	71.961	0.300	.
1	A	119	THR	H	7.305	0.020	.
1	A	119	THR	N	110.277	0.300	.
1	A	120	LYS	C	177.54	0.300	.
1	A	120	LYS	CA	59.53	0.300	.
1	A	120	LYS	CB	31.243	0.300	.
1	A	120	LYS	H	8.951	0.020	.
1	A	120	LYS	N	121.923	0.300	.
1	A	121	GLU	C	179.475	0.300	.
1	A	121	GLU	CA	59.853	0.300	.
1	A	121	GLU	CB	27.305	0.300	.
1	A	121	GLU	H	8.56	0.020	.
1	A	121	GLU	N	117.565	0.300	.
1	A	122	GLU	C	178.17	0.300	.
1	A	122	GLU	CA	58.257	0.300	.
1	A	122	GLU	CB	29.528	0.300	.
1	A	122	GLU	H	7.787	0.020	.
1	A	122	GLU	N	121.874	0.300	.
1	A	123	ALA	C	179.96	0.300	.
1	A	123	ALA	CA	54.44	0.300	.
1	A	123	ALA	CB	16.493	0.300	.
1	A	123	ALA	H	7.714	0.020	.
1	A	123	ALA	N	122.474	0.300	.
1	A	124	LEU	C	179.243	0.300	.
1	A	124	LEU	CA	57.46	0.300	.
1	A	124	LEU	CB	39.739	0.300	.
1	A	124	LEU	CD1	22.624	0.300	.
1	A	124	LEU	CD2	24.675	0.300	.
1	A	124	LEU	H	8.382	0.020	.
1	A	124	LEU	HD11	0.851	0.020	.
1	A	124	LEU	HD12	0.851	0.020	.
1	A	124	LEU	HD13	0.851	0.020	.
1	A	124	LEU	HD21	0.757	0.020	.
1	A	124	LEU	HD22	0.757	0.020	.
1	A	124	LEU	HD23	0.757	0.020	.
1	A	124	LEU	N	117.418	0.300	.
1	A	125	SER	C	177.444	0.300	.
1	A	125	SER	CA	60.59	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	SER	CB	62.326	0.300	.
1	A	125	SER	H	7.769	0.020	.
1	A	125	SER	N	116.137	0.300	.
1	A	126	ASN	C	177.667	0.300	.
1	A	126	ASN	CA	55.776	0.300	.
1	A	126	ASN	CB	35.904	0.300	.
1	A	126	ASN	H	8.092	0.020	.
1	A	126	ASN	N	122.568	0.300	.
1	A	127	ILE	C	178.22	0.300	.
1	A	127	ILE	CA	64.491	0.300	.
1	A	127	ILE	CB	36.285	0.300	.
1	A	127	ILE	CD1	15.053	0.300	.
1	A	127	ILE	H	8.213	0.020	.
1	A	127	ILE	HD11	0.748	0.020	.
1	A	127	ILE	HD12	0.748	0.020	.
1	A	127	ILE	HD13	0.748	0.020	.
1	A	127	ILE	N	122.107	0.300	.
1	A	128	ASP	C	178.978	0.300	.
1	A	128	ASP	CA	57.194	0.300	.
1	A	128	ASP	CB	39.186	0.300	.
1	A	128	ASP	H	8.332	0.020	.
1	A	128	ASP	N	121.49	0.300	.
1	A	129	GLN	C	178.51	0.300	.
1	A	129	GLN	CA	58.53	0.300	.
1	A	129	GLN	H	7.73	0.020	.
1	A	129	GLN	N	117.694	0.300	.
1	A	130	ILE	C	177.183	0.300	.
1	A	130	ILE	CA	62.56	0.300	.
1	A	130	ILE	CB	37.391	0.300	.
1	A	130	ILE	CD1	14.254	0.300	.
1	A	130	ILE	H	7.404	0.020	.
1	A	130	ILE	HD11	0.14	0.020	.
1	A	130	ILE	HD12	0.14	0.020	.
1	A	130	ILE	HD13	0.14	0.020	.
1	A	130	ILE	N	111.546	0.300	.
1	A	131	SER	C	175.05	0.300	.
1	A	131	SER	CA	59.824	0.300	.
1	A	131	SER	CB	62.879	0.300	.
1	A	131	SER	H	7.877	0.020	.
1	A	131	SER	N	118.628	0.300	.
1	A	132	ASP	C	177.044	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	132	ASP	CA	54.661	0.300	.
1	A	132	ASP	CB	40.093	0.300	.
1	A	132	ASP	H	8.275	0.020	.
1	A	132	ASP	N	121.719	0.300	.
1	A	133	LYS	C	176.823	0.300	.
1	A	133	LYS	CA	56.258	0.300	.
1	A	133	LYS	CB	31.299	0.300	.
1	A	133	LYS	H	7.782	0.020	.
1	A	133	LYS	N	120.682	0.300	.
1	A	134	ALA	C	178.04	0.300	.
1	A	134	ALA	CA	52.349	0.300	.
1	A	134	ALA	CB	17.704	0.300	.
1	A	134	ALA	H	7.955	0.020	.
1	A	134	ALA	N	123.659	0.300	.
1	A	135	GLU	C	176.795	0.300	.
1	A	135	GLU	CA	56.44	0.300	.
1	A	135	GLU	CB	28.89	0.300	.
1	A	135	GLU	H	8.074	0.020	.
1	A	135	GLU	N	120.244	0.300	.
1	A	136	GLU	C	176.588	0.300	.
1	A	136	GLU	CA	56.366	0.300	.
1	A	136	GLU	CB	28.894	0.300	.
1	A	136	GLU	H	8.294	0.020	.
1	A	136	GLU	N	121.881	0.300	.
1	A	137	LEU	C	177.305	0.300	.
1	A	137	LEU	CA	54.713	0.300	.
1	A	137	LEU	CB	40.775	0.300	.
1	A	137	LEU	CD1	23.198	0.300	.
1	A	137	LEU	CD2	24.537	0.300	.
1	A	137	LEU	H	8.079	0.020	.
1	A	137	LEU	HD11	0.77	0.020	.
1	A	137	LEU	HD12	0.77	0.020	.
1	A	137	LEU	HD13	0.77	0.020	.
1	A	137	LEU	HD21	0.828	0.020	.
1	A	137	LEU	HD22	0.828	0.020	.
1	A	137	LEU	HD23	0.828	0.020	.
1	A	137	LEU	N	123.233	0.300	.
1	A	138	LYS	C	176.463	0.300	.
1	A	138	LYS	CA	55.773	0.300	.
1	A	138	LYS	CB	31.519	0.300	.
1	A	138	LYS	H	8.086	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	LYS	N	122.904	0.300	.
1	A	139	ARG	C	176.301	0.300	.
1	A	139	ARG	CA	55.532	0.300	.
1	A	139	ARG	CB	29.599	0.300	.
1	A	139	ARG	H	8.237	0.020	.
1	A	139	ARG	N	122.925	0.300	.
1	A	140	SER	C	174.791	0.300	.
1	A	140	SER	CA	57.785	0.300	.
1	A	140	SER	CB	63.285	0.300	.
1	A	140	SER	H	8.404	0.020	.
1	A	140	SER	N	118.057	0.300	.
1	A	141	THR	C	174.638	0.300	.
1	A	141	THR	CA	61.33	0.300	.
1	A	141	THR	CB	69.026	0.300	.
1	A	141	THR	H	8.165	0.020	.
1	A	141	THR	N	116.424	0.300	.
1	A	142	SER	C	174.155	0.300	.
1	A	142	SER	CA	57.963	0.300	.
1	A	142	SER	CB	63.155	0.300	.
1	A	142	SER	H	8.229	0.020	.
1	A	142	SER	N	118.258	0.300	.
1	A	143	ASP	C	175.683	0.300	.
1	A	143	ASP	CA	53.864	0.300	.
1	A	143	ASP	CB	40.367	0.300	.
1	A	143	ASP	H	8.213	0.020	.
1	A	143	ASP	N	123.199	0.300	.
1	A	144	ALA	C	177.532	0.300	.
1	A	144	ALA	CA	51.865	0.300	.
1	A	144	ALA	CB	17.91	0.300	.
1	A	144	ALA	H	8.025	0.020	.
1	A	144	ALA	N	124.487	0.300	.
1	A	145	VAL	C	176.043	0.300	.
1	A	145	VAL	CA	61.733	0.300	.
1	A	145	VAL	CB	31.37	0.300	.
1	A	145	VAL	CG2	20.858	0.300	.
1	A	145	VAL	H	7.986	0.020	.
1	A	145	VAL	HG21	0.812	0.020	.
1	A	145	VAL	HG11	0.812	0.020	.
1	A	145	VAL	HG12	0.812	0.020	.
1	A	145	VAL	HG13	0.812	0.020	.
1	A	145	VAL	HG22	0.812	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	145	VAL	HG23	0.812	0.020	.
1	A	145	VAL	N	120.303	0.300	.
1	A	146	GLN	C	175.32	0.300	.
1	A	146	GLN	CA	54.894	0.300	.
1	A	146	GLN	CB	28.395	0.300	.
1	A	146	GLN	H	8.337	0.020	.
1	A	146	GLN	N	124.575	0.300	.
1	A	147	ASP	C	175.66	0.300	.
1	A	147	ASP	CA	53.747	0.300	.
1	A	147	ASP	CB	40.367	0.300	.
1	A	147	ASP	H	8.288	0.020	.
1	A	147	ASP	N	122.685	0.300	.
1	A	148	ASN	C	174.767	0.300	.
1	A	148	ASN	CA	52.683	0.300	.
1	A	148	ASN	CB	38.241	0.300	.
1	A	148	ASN	H	8.291	0.020	.
1	A	148	ASN	N	119.712	0.300	.
1	A	149	ASP	C	175.828	0.300	.
1	A	149	ASP	CA	53.959	0.300	.
1	A	149	ASP	CB	40.154	0.300	.
1	A	149	ASP	H	8.209	0.020	.
1	A	149	ASP	N	121.997	0.300	.
1	A	236	ILE	C	177.143	0.300	.
1	A	236	ILE	CA	62.14	0.300	.
1	A	236	ILE	CB	37.183	0.300	.
1	A	236	ILE	CD1	13.348	0.300	.
1	A	236	ILE	HD11	0.729	0.020	.
1	A	236	ILE	HD12	0.729	0.020	.
1	A	236	ILE	HD13	0.729	0.020	.
1	A	237	GLU	C	178.081	0.300	.
1	A	237	GLU	CA	57.815	0.300	.
1	A	237	GLU	CB	27.374	0.300	.
1	A	237	GLU	H	9.125	0.020	.
1	A	237	GLU	N	123.401	0.300	.
1	A	238	SER	C	175.62	0.300	.
1	A	238	SER	CA	59.712	0.300	.
1	A	238	SER	CB	62.809	0.300	.
1	A	238	SER	H	7.89	0.020	.
1	A	238	SER	N	117.282	0.300	.
1	A	239	LEU	C	177.915	0.300	.
1	A	239	LEU	CA	55.215	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	239	LEU	CB	40.291	0.300	.
1	A	239	LEU	H	7.556	0.020	.
1	A	239	LEU	N	122.311	0.300	.
1	A	240	GLU	C	177.203	0.300	.
1	A	240	GLU	CA	57.313	0.300	.
1	A	240	GLU	CB	28.48	0.300	.
1	A	240	GLU	H	7.723	0.020	.
1	A	240	GLU	N	119.679	0.300	.
1	A	241	SER	C	174.006	0.300	.
1	A	241	SER	CA	58.76	0.300	.
1	A	241	SER	CB	62.74	0.300	.
1	A	241	SER	H	7.726	0.020	.
1	A	241	SER	N	114.102	0.300	.
1	A	242	TYR	C	174.998	0.300	.
1	A	242	TYR	CA	57.313	0.300	.
1	A	242	TYR	CB	37.736	0.300	.
1	A	242	TYR	H	7.707	0.020	.
1	A	242	TYR	N	121.562	0.300	.
1	A	243	ASP	C	175.993	0.300	.
1	A	243	ASP	CA	53.531	0.300	.
1	A	243	ASP	CB	39.808	0.300	.
1	A	243	ASP	H	8.123	0.020	.
1	A	243	ASP	N	121.714	0.300	.
1	A	244	LEU	C	177.708	0.300	.
1	A	244	LEU	CA	54.92	0.300	.
1	A	244	LEU	CB	40.637	0.300	.
1	A	244	LEU	H	8.194	0.020	.
1	A	244	LEU	N	123.311	0.300	.
1	A	245	GLU	C	176.339	0.300	.
1	A	245	GLU	CA	56.077	0.300	.
1	A	245	GLU	CB	28.82	0.300	.
1	A	245	GLU	H	8.243	0.020	.
1	A	245	GLU	N	119.82	0.300	.
1	A	246	HIS	C	174.445	0.300	.
1	A	246	HIS	CA	55.411	0.300	.
1	A	246	HIS	CB	28.618	0.300	.
1	A	246	HIS	H	8.091	0.020	.
1	A	246	HIS	N	119.252	0.300	.

7.1.2   Chemical shift referencing   ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	242	0.60 ± 0.19	Should be checked
$^{13}C_\beta$	227	1.31 ± 0.14	Should be checked
$^{13}C'$	241	0.13 ± 0.25	None needed (< 0.5 ppm)
^{15}N	225	-0.46 ± 0.22	None needed (< 0.5 ppm)

7.1.3   Completeness of resonance assignments   ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 41%, i.e. 414 atoms were assigned a chemical shift out of a possible 1001. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	267/348 (77%)	65/140 (46%)	137/140 (98%)	65/68 (96%)
Sidechain	144/598 (24%)	59/384 (15%)	85/183 (46%)	0/31 (0%)
Aromatic	3/55 (5%)	2/27 (7%)	0/25 (0%)	1/3 (33%)
Overall	414/1001 (41%)	126/551 (23%)	222/348 (64%)	66/102 (65%)

7.1.4   Statistically unusual chemical shifts   ⓘ

There are no statistically unusual chemical shifts.

7.1.5   Random Coil Index (RCI) plots   ⓘ

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

Random coil index (RCI) for chain A:
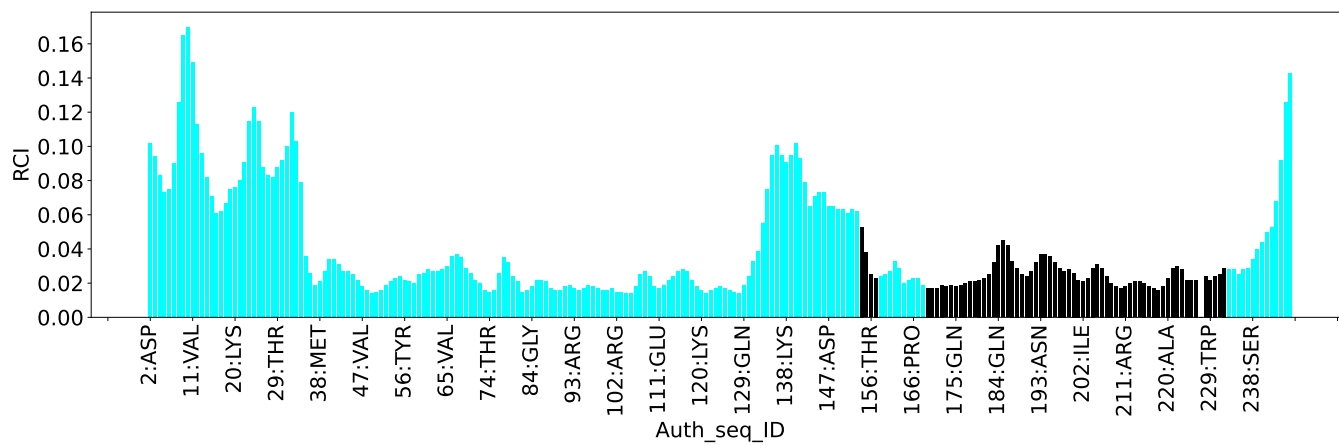
8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

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

Description	Value
Total distance restraints	408
Intra-residue ($|i-j|=0$)	27
Sequential ($|i-j|=1$)	144
Medium range ($|i-j|>1$ and $|i-j|<5$)	80
Long range ($|i-j|\geq 5$)	87
Inter-chain	0
Hydrogen bond restraints	70
Disulfide bond restraints	0
Total dihedral-angle restraints	150
Number of unmapped restraints	2
Number of restraints per residue	2.3
Number of long range restraints per residue[1]	0.5

[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)	4.8	0.19
0.2-0.5 (Medium)	2.9	0.5
>0.5 (Large)	4.5	3.53

8.2.2   Average number of dihedral-angle violations per model ⓘ

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)	12.7	5.0
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.

Restraints type	Count	$\%^1$	Violated[3]			Consistently Violated[4]		
			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
Intra-residue (|i-j|=0)	27	6.6	3	11.1	0.7	2	7.4	0.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	15	3.7	3	20.0	0.7	2	13.3	0.5
Sidechain-Sidechain	12	2.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	144	35.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	127	31.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	4.2	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
Medium range (|i-j|>1 & |i-j|<5)	80	19.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	69	16.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	5	1.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	6	1.5	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	87	21.3	11	12.6	2.7	6	6.9	1.5
Backbone-Backbone	27	6.6	4	14.8	1.0	4	14.8	1.0
Backbone-Sidechain	47	11.5	7	14.9	1.7	2	4.3	0.5
Sidechain-Sidechain	13	3.2	0	0.0	0.0	0	0.0	0.0
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	70	17.2	3	4.3	0.7	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	408	100.0	17	4.2	4.2	8	2.0	2.0
Backbone-Backbone	293	71.8	7	2.4	1.7	4	1.4	1.0
Backbone-Sidechain	84	20.6	10	11.9	2.5	4	4.8	1.0
Sidechain-Sidechain	31	7.6	0	0.0	0.0	0	0.0	0.0

[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 ⓘ
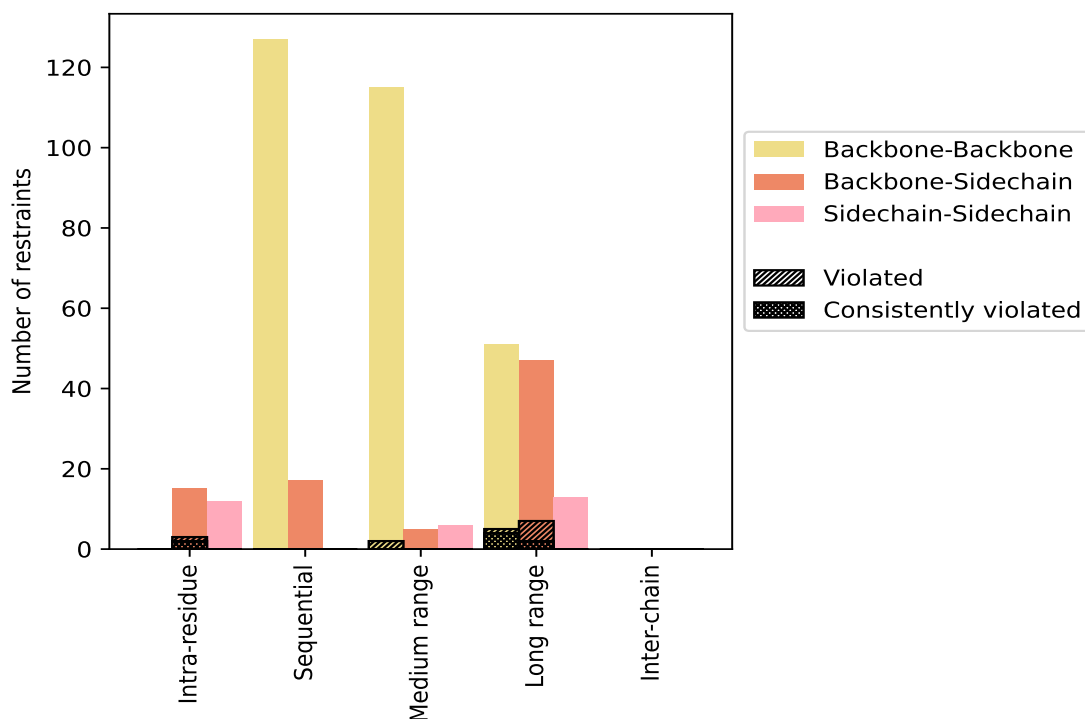
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis
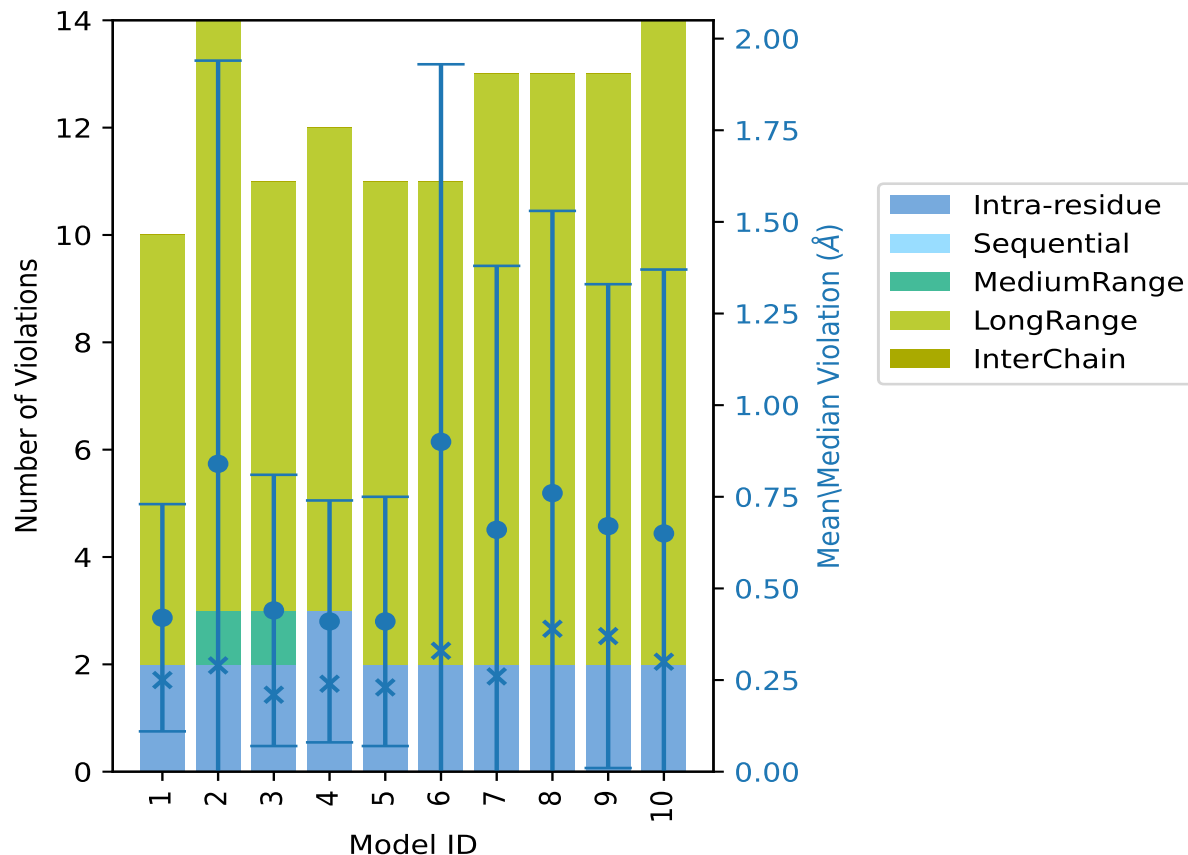
9.2   Distance violation statistics for each model ⓘ

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	2	0	0	8	0	10	0.42	1.02	0.31	0.25
2	2	0	1	11	0	14	0.84	3.53	1.1	0.29
3	2	0	1	8	0	11	0.44	1.11	0.37	0.21
4	3	0	0	9	0	12	0.41	1.08	0.33	0.24
5	2	0	0	9	0	11	0.41	1.11	0.34	0.23
6	2	0	0	9	0	11	0.9	3.08	1.03	0.33
7	2	0	0	11	0	13	0.66	2.48	0.72	0.26
8	2	0	0	11	0	13	0.76	2.61	0.77	0.39
9	2	0	0	11	0	13	0.67	2.27	0.66	0.37
10	2	0	0	12	0	14	0.65	2.5	0.72	0.3

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

[5]Inter-chain restraints, [6]Standard deviation

9.2.1   Bar graph : Distance Violation statistics for each model ⓘ

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

9.3   Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 324(IR:24, SQ:144, MR:80, LR:76, 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]	%
1	0	0	0	0	1	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0
0	0	0	0	0	0	4	40.0

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Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	5	50.0
0	0	0	2	0	2	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	1	0	1	8	80.0
0	0	0	2	0	2	9	90.0
2	0	0	6	0	8	10	100.0

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

9.3.1   Bar graph : Distance violation statistics for the ensemble ⓘ
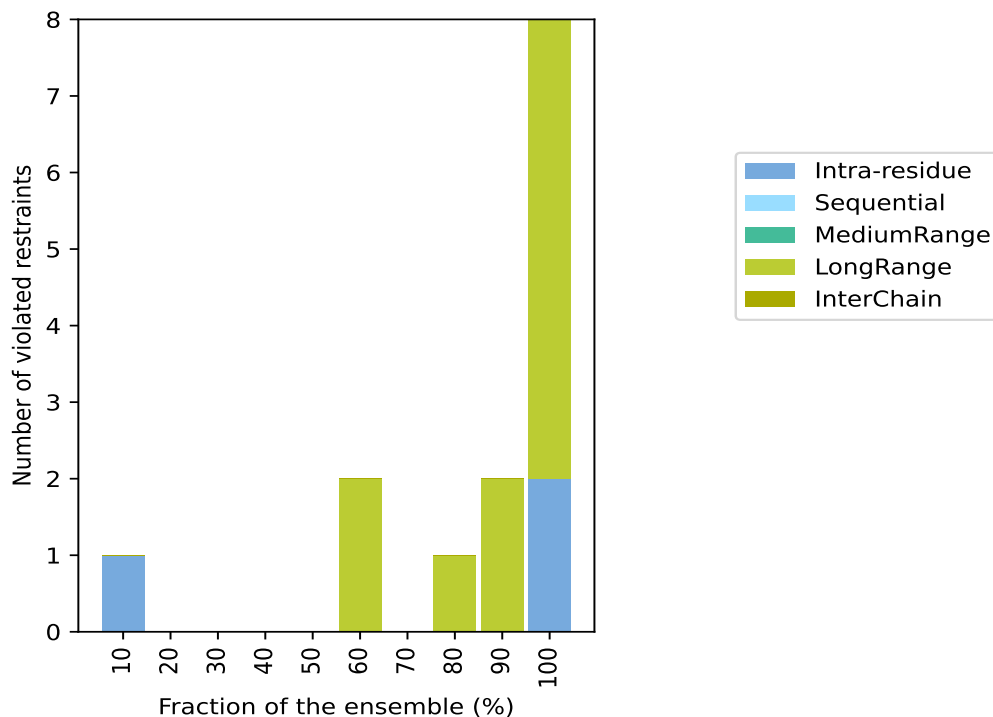
9.4   Most violated distance restraints in the ensemble ⓘ

9.4.1   Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble
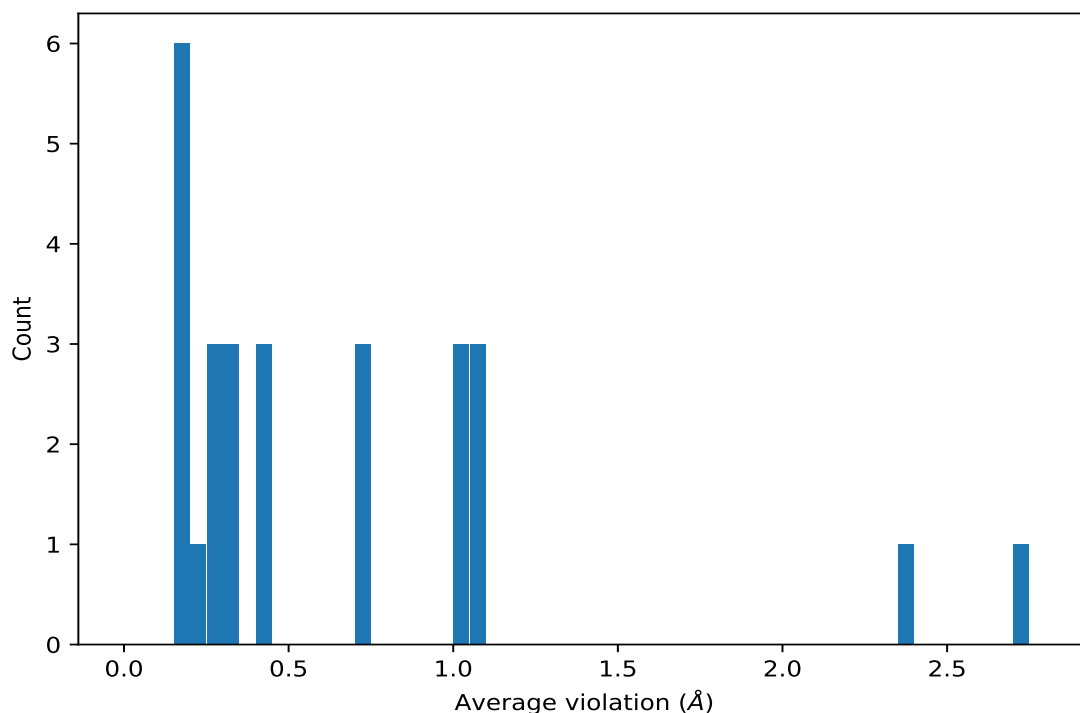
9.4.2 Table: Most violated distance restraints ⓘ

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

| Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,116)	1:A:190:ASP:H	1:A:201:VAL:HG21	10	1.05	0.06	1.06
(1,116)	1:A:190:ASP:H	1:A:201:VAL:HG22	10	1.05	0.06	1.06
(1,116)	1:A:190:ASP:H	1:A:201:VAL:HG23	10	1.05	0.06	1.06
(1,285)	1:A:229:TRP:H	1:A:174:LEU:HD21	10	1.02	0.11	1.08
(1,285)	1:A:229:TRP:H	1:A:174:LEU:HD22	10	1.02	0.11	1.08
(1,285)	1:A:229:TRP:H	1:A:174:LEU:HD23	10	1.02	0.11	1.08
(1,55)	1:A:174:LEU:H	1:A:174:LEU:HD21	10	0.73	0.04	0.74
(1,55)	1:A:174:LEU:H	1:A:174:LEU:HD22	10	0.73	0.04	0.74
(1,55)	1:A:174:LEU:H	1:A:174:LEU:HD23	10	0.73	0.04	0.74
(1,37)	1:A:171:VAL:H	1:A:225:ALA:H	10	0.23	0.03	0.23
(1,34)	1:A:171:VAL:H	1:A:171:VAL:HG21	10	0.18	0.01	0.18
(1,34)	1:A:171:VAL:H	1:A:171:VAL:HG22	10	0.18	0.01	0.18
(1,34)	1:A:171:VAL:H	1:A:171:VAL:HG23	10	0.18	0.01	0.18
(1,38)	1:A:171:VAL:H	1:A:222:ASN:H	10	0.16	0.02	0.16
(1,41)	1:A:171:VAL:H	1:A:226:TRP:H	10	0.15	0.01	0.15
(1,281)	1:A:226:TRP:H	1:A:171:VAL:H	10	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,284)	1:A:229:TRP:H	1:A:174:LEU:HD11	9	0.43	0.15	0.41
(1,284)	1:A:229:TRP:H	1:A:174:LEU:HD12	9	0.43	0.15	0.41
(1,284)	1:A:229:TRP:H	1:A:174:LEU:HD13	9	0.43	0.15	0.41
(1,131)	1:A:193:ASN:H	1:A:200:LEU:HD21	9	0.31	0.05	0.31

[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.
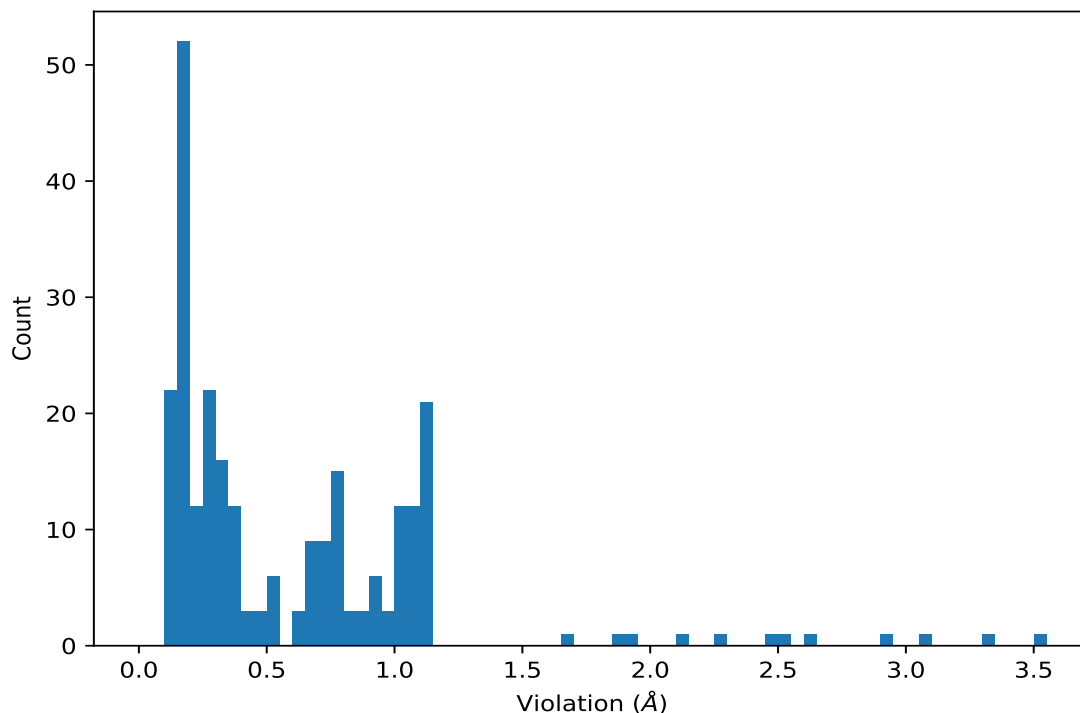
9.5.2 Table : All distance violations (i)

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)
(1,275)	1:A:225:ALA:H	1:A:188:TYR:HE2	2	3.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:A:225:ALA:H	1:A:188:TYR:HD2	2	3.33
(1,276)	1:A:225:ALA:H	1:A:188:TYR:HD2	6	3.08
(1,275)	1:A:225:ALA:H	1:A:188:TYR:HE2	6	2.92
(1,276)	1:A:225:ALA:H	1:A:188:TYR:HD2	8	2.61
(1,276)	1:A:225:ALA:H	1:A:188:TYR:HD2	10	2.5
(1,276)	1:A:225:ALA:H	1:A:188:TYR:HD2	7	2.48
(1,276)	1:A:225:ALA:H	1:A:188:TYR:HD2	9	2.27
(1,275)	1:A:225:ALA:H	1:A:188:TYR:HE2	8	2.13
(1,275)	1:A:225:ALA:H	1:A:188:TYR:HE2	10	1.94

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	76	50.7	19	25.0	12.7	2	2.6	1.3
PHI	74	49.3	13	17.6	8.7	2	2.7	1.3
Total	150	100.0	32	21.3	21.3	4	2.7	2.7

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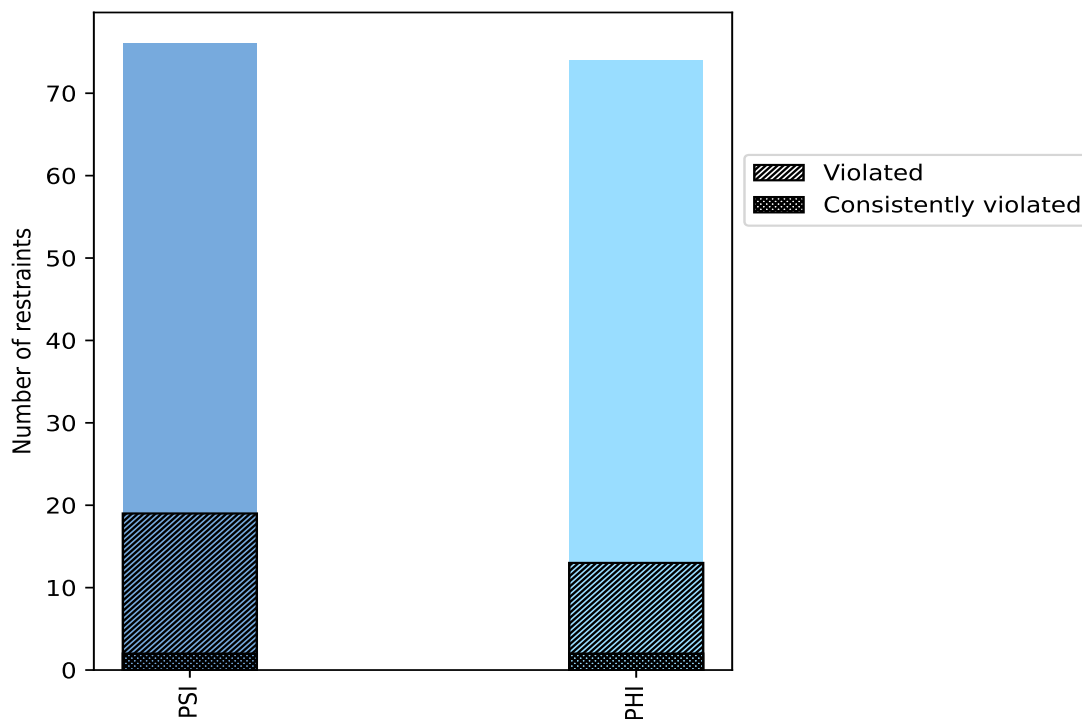
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	8	5	13	2.05	4.5	1.18	1.3
2	6	8	14	2.23	4.3	1.09	2.05
3	8	5	13	2.18	4.4	1.09	1.5
4	5	2	7	2.67	4.2	1.07	2.9
5	10	4	14	1.94	3.8	0.84	1.7
6	10	6	16	2.11	4.7	1.08	1.75
7	9	6	15	2.18	4.7	1.06	1.9
8	7	4	11	2.31	4.1	1.05	1.9
9	7	5	12	2.36	5.0	1.22	1.7
10	6	6	12	2.23	4.3	1.18	1.75

10.2.1 Bar graph : Dihedral violation statistics for each model (i)
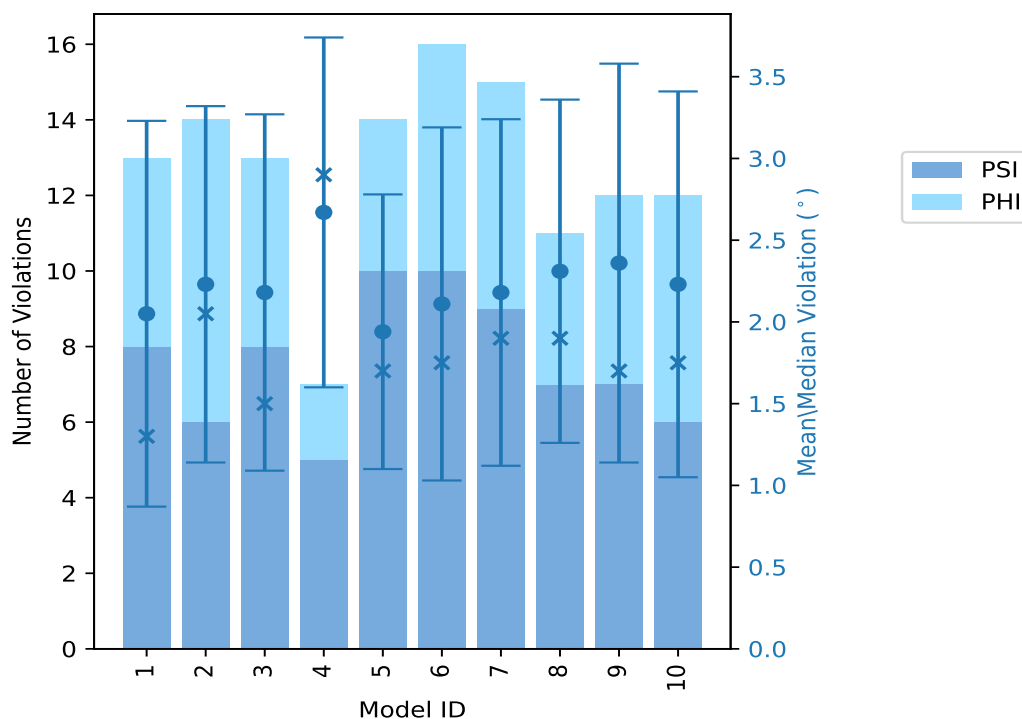
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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.

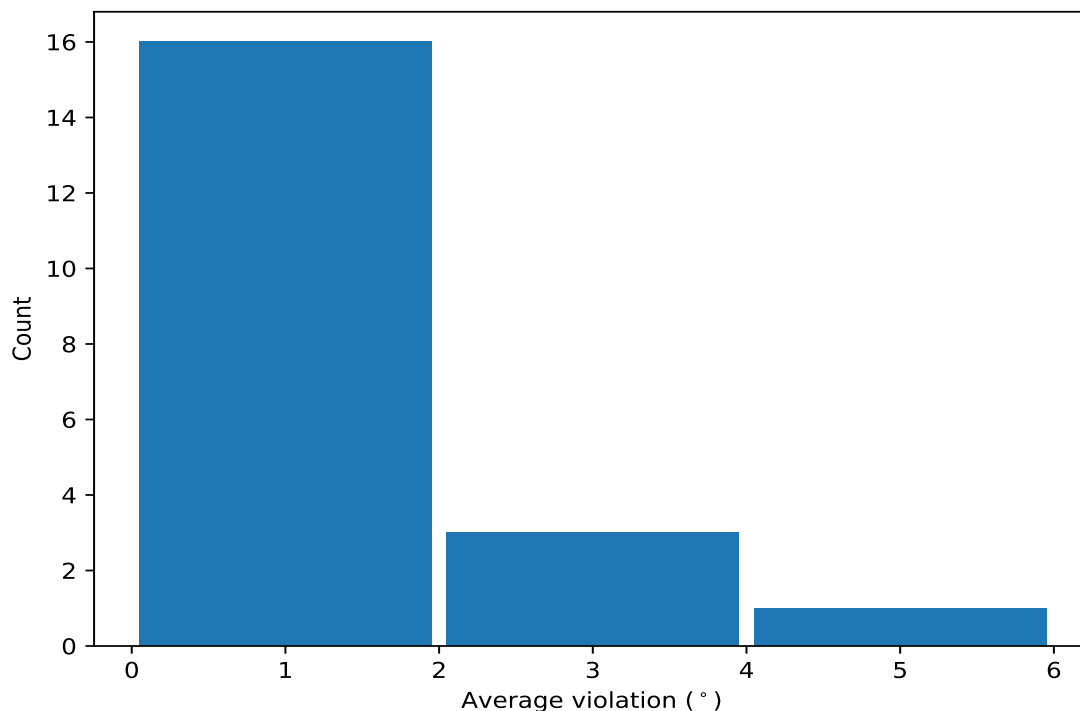| Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
8	4	12	1	10.0
2	1	3	2	20.0
2	2	4	3	30.0
0	2	2	4	40.0
0	1	1	5	50.0
1	1	2	6	60.0
2	0	2	7	70.0
0	0	0	8	80.0
2	0	2	9	90.0
2	2	4	10	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)
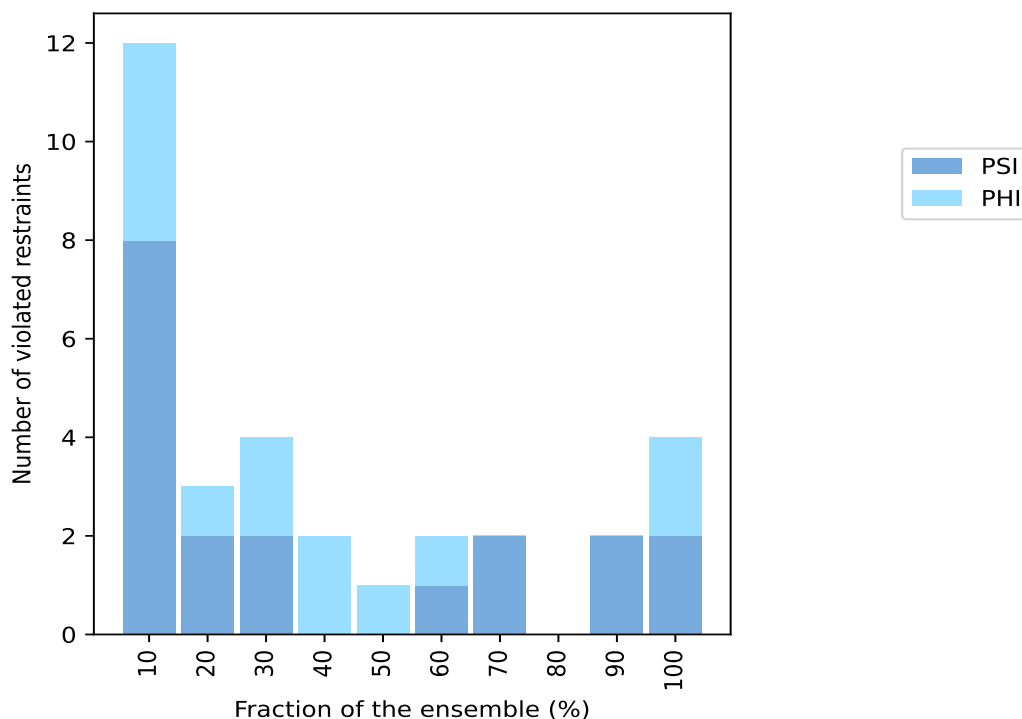
10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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.
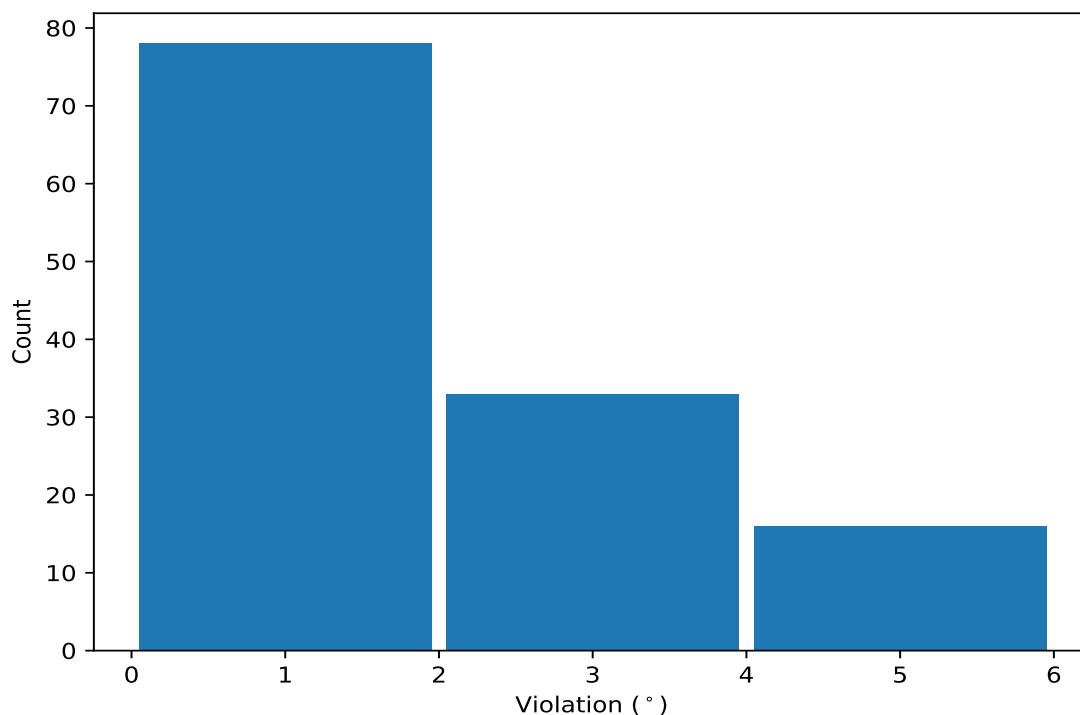
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,134)	1:A:215:SER:N	1:A:215:SER:CA	1:A:215:SER:C	1:A:216:LYS:N	10	4.08	0.55	4.15
(1,18)	1:A:169:ASN:C	1:A:170:TRP:N	1:A:170:TRP:CA	1:A:170:TRP:C	10	3.68	0.64	3.6
(1,79)	1:A:153:SER:N	1:A:153:SER:CA	1:A:153:SER:C	1:A:154:ILE:N	10	3.68	0.44	3.8
(1,60)	1:A:215:SER:C	1:A:216:LYS:N	1:A:216:LYS:CA	1:A:216:LYS:C	10	1.66	0.16	1.65
(1,128)	1:A:209:LYS:N	1:A:209:LYS:CA	1:A:209:LYS:C	1:A:210:THR:N	9	3.14	0.83	3.2
(1,113)	1:A:190:ASP:N	1:A:190:ASP:CA	1:A:190:ASP:C	1:A:191:SER:N	9	1.87	0.49	1.8
(1,140)	1:A:221:LYS:N	1:A:221:LYS:CA	1:A:221:LYS:C	1:A:222:ASN:N	7	1.84	0.43	1.9
(1,135)	1:A:216:LYS:N	1:A:216:LYS:CA	1:A:216:LYS:C	1:A:217:LYS:N	7	1.53	0.27	1.5
(1,73)	1:A:231:ALA:C	1:A:232:LEU:N	1:A:232:LEU:CA	1:A:232:LEU:C	6	1.4	0.31	1.25
(1,143)	1:A:224:ALA:N	1:A:224:ALA:CA	1:A:224:ALA:C	1:A:225:ALA:N	6	1.33	0.33	1.1

[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 (°)
(1,134)	1:A:215:SER:N	1:A:215:SER:CA	1:A:215:SER:C	1:A:216:LYS:N	9	5.0
(1,18)	1:A:169:ASN:C	1:A:170:TRP:N	1:A:170:TRP:CA	1:A:170:TRP:C	7	4.7
(1,134)	1:A:215:SER:N	1:A:215:SER:CA	1:A:215:SER:C	1:A:216:LYS:N	6	4.7
(1,18)	1:A:169:ASN:C	1:A:170:TRP:N	1:A:170:TRP:CA	1:A:170:TRP:C	1	4.5
(1,128)	1:A:209:LYS:N	1:A:209:LYS:CA	1:A:209:LYS:C	1:A:210:THR:N	3	4.4
(1,79)	1:A:153:SER:N	1:A:153:SER:CA	1:A:153:SER:C	1:A:154:ILE:N	9	4.3
(1,18)	1:A:169:ASN:C	1:A:170:TRP:N	1:A:170:TRP:CA	1:A:170:TRP:C	2	4.3
(1,134)	1:A:215:SER:N	1:A:215:SER:CA	1:A:215:SER:C	1:A:216:LYS:N	10	4.3
(1,79)	1:A:153:SER:N	1:A:153:SER:CA	1:A:153:SER:C	1:A:154:ILE:N	3	4.2
(1,134)	1:A:215:SER:N	1:A:215:SER:CA	1:A:215:SER:C	1:A:216:LYS:N	2	4.2