wwPDB NMR Structure Validation Summary Report

Jun 6, 2023 – 06:50 pm BST

PDB ID	:	6HJ7
BMRB ID	:	34310
Title	:	The NMR structure of NRADD death domain
Authors	:	Nadezhdin, K.D.; Mineev, K.S.; Goncharuk, S.A.; Arseniev, A.S.
Deposited on	:	2018-09-01

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

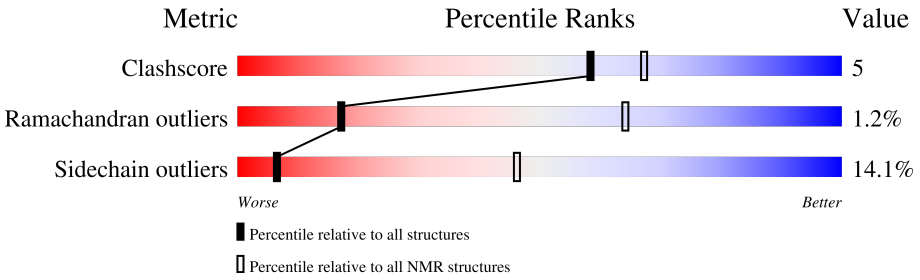
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 87%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	246	29% 5% 8% 59%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:155-A:237 (83)	1.52	14

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1549 atoms, of which 765 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Death domain-containing membrane protein NRADD.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	102	1549	487	765	137	154	6	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8CJ26
A	2	HIS	-	expression tag	UNP Q8CJ26
A	3	HIS	-	expression tag	UNP Q8CJ26
A	4	HIS	-	expression tag	UNP Q8CJ26
A	5	HIS	-	expression tag	UNP Q8CJ26
A	6	HIS	-	expression tag	UNP Q8CJ26
A	7	HIS	-	expression tag	UNP Q8CJ26
A	8	GLY	-	expression tag	UNP Q8CJ26
A	9	SER	-	expression tag	UNP Q8CJ26
A	10	GLY	-	expression tag	UNP Q8CJ26
A	11	SER	-	expression tag	UNP Q8CJ26
A	12	GLY	-	expression tag	UNP Q8CJ26
A	13	LEU	-	expression tag	UNP Q8CJ26
A	14	VAL	-	expression tag	UNP Q8CJ26
A	15	PRO	-	expression tag	UNP Q8CJ26
A	16	ARG	-	expression tag	UNP Q8CJ26
A	17	GLY	-	expression tag	UNP Q8CJ26
A	18	SER	-	expression tag	UNP Q8CJ26
A	19	MET	-	expression tag	UNP Q8CJ26
A	20	LEU	-	expression tag	UNP Q8CJ26
A	21	TYR	-	expression tag	UNP Q8CJ26
A	22	ASN	-	expression tag	UNP Q8CJ26
A	23	VAL	-	expression tag	UNP Q8CJ26
A	24	SER	-	expression tag	UNP Q8CJ26
A	25	LYS	-	expression tag	UNP Q8CJ26
A	26	GLY	-	expression tag	UNP Q8CJ26
A	27	VAL	-	expression tag	UNP Q8CJ26
A	28	VAL	-	expression tag	UNP Q8CJ26
A	29	TYR	-	expression tag	UNP Q8CJ26
A	30	SER	-	expression tag	UNP Q8CJ26
A	31	ASP	-	expression tag	UNP Q8CJ26

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	THR	-	expression tag	UNP Q8CJ26
A	33	ALA	-	expression tag	UNP Q8CJ26
A	34	LEU	-	expression tag	UNP Q8CJ26
A	35	GLN	-	expression tag	UNP Q8CJ26
A	36	GLY	-	expression tag	UNP Q8CJ26
A	37	GLN	-	expression tag	UNP Q8CJ26
A	38	ASP	-	expression tag	UNP Q8CJ26
A	39	GLY	-	expression tag	UNP Q8CJ26
A	40	ASP	-	expression tag	UNP Q8CJ26
A	41	ARG	-	expression tag	UNP Q8CJ26
A	42	GLU	-	expression tag	UNP Q8CJ26
A	43	GLY	-	expression tag	UNP Q8CJ26
A	44	MET	-	expression tag	UNP Q8CJ26
A	45	TRP	-	expression tag	UNP Q8CJ26
A	46	VAL	-	expression tag	UNP Q8CJ26
A	47	GLY	-	expression tag	UNP Q8CJ26
A	48	ALA	-	expression tag	UNP Q8CJ26
A	49	GLY	-	expression tag	UNP Q8CJ26
A	50	GLY	-	expression tag	UNP Q8CJ26
A	51	ALA	-	expression tag	UNP Q8CJ26
A	52	LEU	-	expression tag	UNP Q8CJ26
A	53	ALA	-	expression tag	UNP Q8CJ26
A	54	PRO	-	expression tag	UNP Q8CJ26
A	55	ASN	-	expression tag	UNP Q8CJ26
A	56	THR	-	expression tag	UNP Q8CJ26
A	57	SER	-	expression tag	UNP Q8CJ26
A	58	SER	-	expression tag	UNP Q8CJ26
A	59	LEU	-	expression tag	UNP Q8CJ26
A	60	PHE	-	expression tag	UNP Q8CJ26
A	61	PRO	-	expression tag	UNP Q8CJ26
A	62	PRO	-	expression tag	UNP Q8CJ26
A	63	GLU	-	expression tag	UNP Q8CJ26
A	64	PRO	-	expression tag	UNP Q8CJ26
A	65	PRO	-	expression tag	UNP Q8CJ26
A	66	GLY	-	expression tag	UNP Q8CJ26
A	67	ALA	-	expression tag	UNP Q8CJ26
A	68	SER	-	expression tag	UNP Q8CJ26
A	69	SER	-	expression tag	UNP Q8CJ26
A	70	ASN	-	expression tag	UNP Q8CJ26
A	71	ILE	-	expression tag	UNP Q8CJ26
A	72	ILE	-	expression tag	UNP Q8CJ26
A	73	PRO	-	expression tag	UNP Q8CJ26

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Chain	Residue	Modelled	Actual	Comment	Reference
A	74	VAL	-	expression tag	UNP Q8CJ26
A	75	TYR	-	expression tag	UNP Q8CJ26
A	76	CYS	-	expression tag	UNP Q8CJ26
A	77	ALA	-	expression tag	UNP Q8CJ26
A	78	LEU	-	expression tag	UNP Q8CJ26
A	79	LEU	-	expression tag	UNP Q8CJ26
A	80	ALA	-	expression tag	UNP Q8CJ26
A	81	THR	-	expression tag	UNP Q8CJ26
A	82	VAL	-	expression tag	UNP Q8CJ26
A	83	ILE	-	expression tag	UNP Q8CJ26
A	84	LEU	-	expression tag	UNP Q8CJ26
A	85	GLY	-	expression tag	UNP Q8CJ26
A	86	LEU	-	expression tag	UNP Q8CJ26
A	87	LEU	-	expression tag	UNP Q8CJ26
A	88	ALA	-	expression tag	UNP Q8CJ26
A	89	TYR	-	expression tag	UNP Q8CJ26
A	90	VAL	-	expression tag	UNP Q8CJ26
A	91	ALA	-	expression tag	UNP Q8CJ26
A	92	PHE	-	expression tag	UNP Q8CJ26
A	93	LYS	-	expression tag	UNP Q8CJ26
A	94	CYS	-	expression tag	UNP Q8CJ26
A	95	TRP	-	expression tag	UNP Q8CJ26
A	96	ARG	-	expression tag	UNP Q8CJ26
A	97	SER	-	expression tag	UNP Q8CJ26
A	98	HIS	-	expression tag	UNP Q8CJ26
A	99	LYS	-	expression tag	UNP Q8CJ26
A	100	GLN	-	expression tag	UNP Q8CJ26
A	101	ARG	-	expression tag	UNP Q8CJ26
A	102	GLN	-	expression tag	UNP Q8CJ26
A	103	GLN	-	expression tag	UNP Q8CJ26
A	104	LEU	-	expression tag	UNP Q8CJ26
A	105	ALA	-	expression tag	UNP Q8CJ26
A	106	LYS	-	expression tag	UNP Q8CJ26
A	107	ALA	-	expression tag	UNP Q8CJ26
A	108	ARG	-	expression tag	UNP Q8CJ26
A	109	THR	-	expression tag	UNP Q8CJ26
A	110	VAL	-	expression tag	UNP Q8CJ26
A	111	GLU	-	expression tag	UNP Q8CJ26
A	112	LEU	-	expression tag	UNP Q8CJ26
A	113	GLY	-	expression tag	UNP Q8CJ26
A	114	ASP	-	expression tag	UNP Q8CJ26
A	115	PRO	-	expression tag	UNP Q8CJ26

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Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ASP	-	expression tag	UNP Q8CJ26
A	117	ARG	-	expression tag	UNP Q8CJ26
A	118	ASP	-	expression tag	UNP Q8CJ26
A	119	GLN	-	expression tag	UNP Q8CJ26
A	120	ARG	-	expression tag	UNP Q8CJ26
A	121	ARG	-	expression tag	UNP Q8CJ26
A	122	GLY	-	expression tag	UNP Q8CJ26
A	123	ASP	-	expression tag	UNP Q8CJ26
A	124	SER	-	expression tag	UNP Q8CJ26
A	125	ASN	-	expression tag	UNP Q8CJ26
A	126	VAL	-	expression tag	UNP Q8CJ26
A	127	PHE	-	expression tag	UNP Q8CJ26
A	128	VAL	-	expression tag	UNP Q8CJ26
A	129	ASP	-	expression tag	UNP Q8CJ26
A	130	SER	-	expression tag	UNP Q8CJ26
A	131	PRO	-	expression tag	UNP Q8CJ26
A	132	PRO	-	expression tag	UNP Q8CJ26
A	133	SER	-	expression tag	UNP Q8CJ26
A	134	LEU	-	expression tag	UNP Q8CJ26
A	135	GLU	-	expression tag	UNP Q8CJ26
A	136	PRO	-	expression tag	UNP Q8CJ26
A	137	CYS	-	expression tag	UNP Q8CJ26
A	138	ILE	-	expression tag	UNP Q8CJ26
A	139	PRO	-	expression tag	UNP Q8CJ26
A	140	SER	-	expression tag	UNP Q8CJ26
A	141	GLN	-	expression tag	UNP Q8CJ26
A	142	GLY	-	expression tag	UNP Q8CJ26
A	143	PRO	-	expression tag	UNP Q8CJ26
A	144	HIS	-	expression tag	UNP Q8CJ26

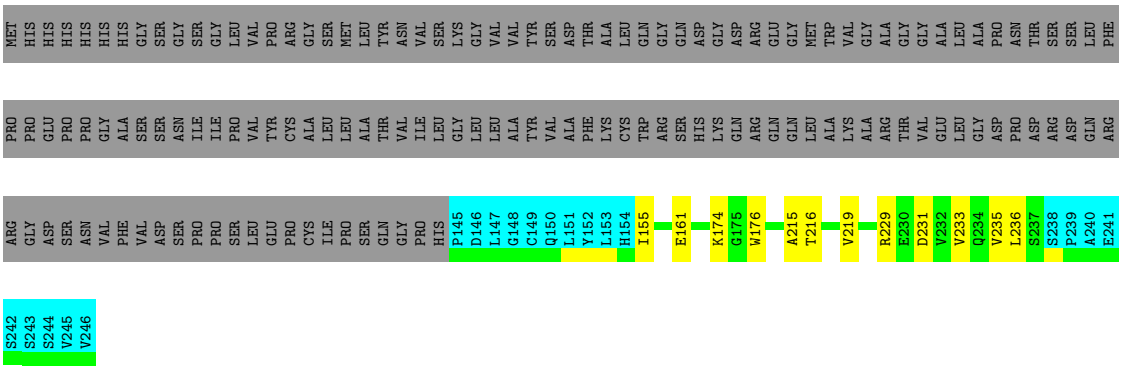
4 Residue-property plots

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: Death domain-containing membrane protein NRADD

Chain A: 29% 5% 8% 59%

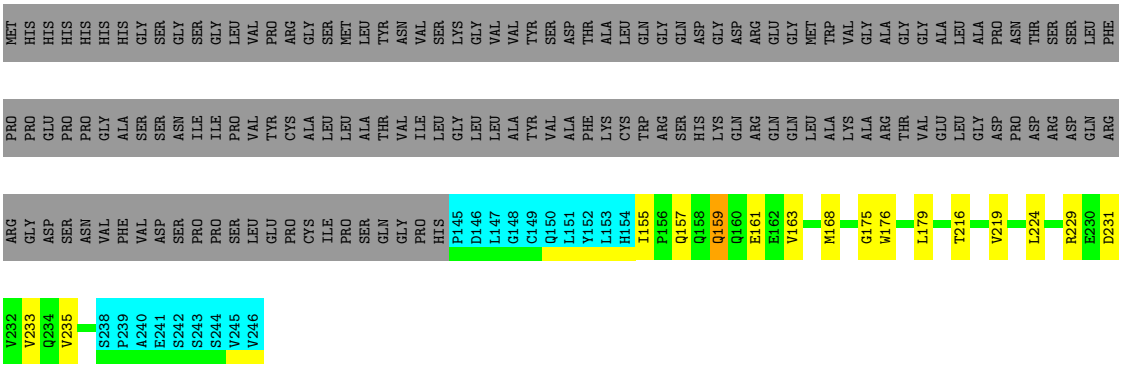


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 14. Colouring as in section 4.1 above.

• Molecule 1: Death domain-containing membrane protein NRADD

Chain A: 27% 6% 8% 59%



5 Refinement protocol and experimental data overview

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

Of the 2000 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure calculation	

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	1903
Number of shifts mapped to atoms	1178
Number of unparsed shifts	0
Number of shifts with mapping errors	725
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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	645	633	633	6±2
All	All	12900	12660	12660	125

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 5.

5 of 58 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:231:ASP:O	1:A:235:VAL:HG23	0.62	1.94	12	8
1:A:233:VAL:O	1:A:236:LEU:HD23	0.61	1.96	12	1
1:A:221:GLU:OE2	1:A:233:VAL:HG22	0.60	1.97	6	2
1:A:179:LEU:HD21	1:A:224:LEU:HD13	0.60	1.73	19	1
1:A:216:THR:O	1:A:219:VAL:HG12	0.60	1.96	13	20

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	83/246 (34%)	75±2 (91±3%)	7±2 (8±2%)	1±1 (1±1%)	17	64
All	All	1660/4920 (34%)	1506 (91%)	134 (8%)	20 (1%)	17	64

5 of 6 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	ALA	9
1	A	175	GLY	4
1	A	197	GLN	3
1	A	196	ASP	2
1	A	174	LYS	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/199 (33%)	56±3 (86±4%)	9±3 (14±4%)	6	46
All	All	1300/3980 (33%)	1117 (86%)	183 (14%)	6	46

5 of 40 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	161	GLU	13
1	A	176	TRP	13
1	A	174	LYS	12
1	A	201	TYR	9
1	A	236	LEU	9

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_ output*

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	1903
Number of shifts mapped to atoms	1178
Number of unparsed shifts	0
Number of shifts with mapping errors	725
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- No matching atom found in the structure. First 5 (of 725) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	GLY	C	173.274	0.3	1
1	A	26	GLY	CA	44.856	0.3	1
1	A	27	VAL	C	175.176	0.3	1
1	A	27	VAL	CA	61.775	0.3	1
1	A	27	VAL	CB	32.412	0.3	1
1	A	27	VAL	H	7.844	0.020	1
1	A	27	VAL	HA	3.933	0.020	1
1	A	27	VAL	HB	1.973	0.020	1
1	A	27	VAL	N	119.502	0.3	1
1	A	28	VAL	C	175.164	0.3	1
1	A	28	VAL	CA	61.53	0.3	1
1	A	28	VAL	CB	32.412	0.3	1
1	A	28	VAL	CG1	20.549	0.3	1
1	A	28	VAL	CG2	19.886	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	28	VAL	H	8.12	0.020	1
1	A	28	VAL	HA	4.106	0.020	1
1	A	28	VAL	HB	1.968	0.020	1
1	A	28	VAL	HG11	0.874	0.020	2
1	A	28	VAL	HG12	0.874	0.020	2
1	A	28	VAL	HG13	0.874	0.020	2
1	A	28	VAL	HG21	0.896	0.020	2
1	A	28	VAL	HG22	0.896	0.020	2
1	A	28	VAL	HG23	0.896	0.020	2
1	A	28	VAL	N	123.796	0.3	1
1	A	29	TYR	C	175.164	0.3	1
1	A	29	TYR	CA	57.453	0.3	1
1	A	29	TYR	CB	38.492	0.3	1
1	A	29	TYR	CD1	133.159	0.3	1
1	A	29	TYR	H	8.343	0.020	1
1	A	29	TYR	HA	4.606	0.020	1
1	A	29	TYR	HB2	3.046	0.020	2
1	A	29	TYR	HB3	2.915	0.020	2
1	A	29	TYR	HD1	7.172	0.020	1
1	A	29	TYR	HD2	7.172	0.020	1
1	A	29	TYR	N	124.726	0.3	1
1	A	30	SER	C	173.581	0.3	1
1	A	30	SER	CA	57.606	0.3	1
1	A	30	SER	CB	63.526	0.3	1
1	A	30	SER	H	8.152	0.020	1
1	A	30	SER	HA	4.454	0.020	1
1	A	30	SER	HB2	3.858	0.020	2
1	A	30	SER	HB3	3.751	0.020	2
1	A	30	SER	N	117.214	0.3	1
1	A	31	ASP	C	176.341	0.3	1
1	A	31	ASP	CA	54.204	0.3	1
1	A	31	ASP	CB	40.566	0.3	1
1	A	31	ASP	H	8.385	0.020	1
1	A	31	ASP	HA	4.642	0.020	1
1	A	31	ASP	HB2	2.714	0.020	1
1	A	31	ASP	HB3	2.714	0.020	1
1	A	31	ASP	N	122.652	0.3	1
1	A	32	THR	C	174.281	0.3	1
1	A	32	THR	CA	61.826	0.3	1
1	A	32	THR	CB	69.042	0.3	1
1	A	32	THR	CG2	21.058	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	THR	H	8.06	0.020	1
1	A	32	THR	HA	4.261	0.020	1
1	A	32	THR	HB	4.26	0.020	1
1	A	32	THR	HG21	1.216	0.020	1
1	A	32	THR	HG22	1.216	0.020	1
1	A	32	THR	HG23	1.216	0.020	1
1	A	32	THR	N	113.882	0.3	1
1	A	33	ALA	C	177.383	0.3	1
1	A	33	ALA	CA	52.457	0.3	1
1	A	33	ALA	CB	18.393	0.3	1
1	A	33	ALA	H	8.192	0.020	1
1	A	33	ALA	HA	4.32	0.020	1
1	A	33	ALA	HB1	1.411	0.020	1
1	A	33	ALA	HB2	1.411	0.020	1
1	A	33	ALA	HB3	1.411	0.020	1
1	A	33	ALA	N	125.741	0.3	1
1	A	34	LEU	C	176.929	0.3	1
1	A	34	LEU	CA	54.694	0.3	1
1	A	34	LEU	CB	41.639	0.3	1
1	A	34	LEU	CG	26.424	0.3	1
1	A	34	LEU	CD1	24.405	0.3	1
1	A	34	LEU	CD2	22.795	0.3	1
1	A	34	LEU	H	8.038	0.020	1
1	A	34	LEU	HA	4.31	0.020	1
1	A	34	LEU	HB2	1.619	0.020	1
1	A	34	LEU	HB3	1.619	0.020	1
1	A	34	LEU	HG	1.6	0.020	1
1	A	34	LEU	HD11	0.921	0.020	2
1	A	34	LEU	HD12	0.921	0.020	2
1	A	34	LEU	HD13	0.921	0.020	2
1	A	34	LEU	HD21	0.857	0.020	2
1	A	34	LEU	HD22	0.857	0.020	2
1	A	34	LEU	HD23	0.857	0.020	2
1	A	34	LEU	N	120.265	0.3	1
1	A	35	GLN	C	176.046	0.3	1
1	A	35	GLN	CA	55.737	0.3	1
1	A	35	GLN	CB	28.907	0.3	1
1	A	35	GLN	CG	33.192	0.3	1
1	A	35	GLN	H	8.187	0.020	1
1	A	35	GLN	HA	4.325	0.020	1
1	A	35	GLN	HB2	2.006	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	GLN	HB3	2.006	0.020	1
1	A	35	GLN	HG2	2.382	0.020	1
1	A	35	GLN	HG3	2.382	0.020	1
1	A	35	GLN	N	120.309	0.3	1
1	A	36	GLY	C	173.79	0.3	1
1	A	36	GLY	CA	44.948	0.3	1
1	A	36	GLY	H	8.42	0.020	1
1	A	36	GLY	HA2	3.968	0.020	1
1	A	36	GLY	HA3	3.968	0.020	1
1	A	36	GLY	N	109.868	0.3	1
1	A	37	GLN	C	175.36	0.3	1
1	A	37	GLN	CA	55.307	0.3	1
1	A	37	GLN	CB	29.083	0.3	1
1	A	37	GLN	CG	33.267	0.3	1
1	A	37	GLN	H	8.28	0.020	1
1	A	37	GLN	HA	4.395	0.020	1
1	A	37	GLN	HB2	1.976	0.020	1
1	A	37	GLN	HB3	1.976	0.020	1
1	A	37	GLN	HG2	2.338	0.020	1
1	A	37	GLN	HG3	2.338	0.020	1
1	A	37	GLN	N	119.596	0.3	1
1	A	38	ASP	C	176.291	0.3	1
1	A	38	ASP	CA	54.184	0.3	1
1	A	38	ASP	CB	40.675	0.3	1
1	A	38	ASP	H	8.455	0.020	1
1	A	38	ASP	HA	4.603	0.020	1
1	A	38	ASP	HB2	2.675	0.020	1
1	A	38	ASP	HB3	2.675	0.020	1
1	A	38	ASP	N	121.071	0.3	1
1	A	39	GLY	C	173.557	0.3	1
1	A	39	GLY	CA	45.101	0.3	1
1	A	39	GLY	H	8.292	0.020	1
1	A	39	GLY	HA2	3.949	0.020	1
1	A	39	GLY	HA3	3.949	0.020	1
1	A	39	GLY	N	108.937	0.3	1
1	A	40	ASP	C	176.125	0.3	1
1	A	40	ASP	CA	53.928	0.3	1
1	A	40	ASP	CB	40.709	0.3	1
1	A	40	ASP	H	8.229	0.020	1
1	A	40	ASP	HA	4.638	0.020	1
1	A	40	ASP	HB2	2.695	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	40	ASP	HB3	2.695	0.020	1
1	A	40	ASP	N	120.486	0.3	1
1	A	41	ARG	C	176.083	0.3	1
1	A	41	ARG	CA	55.921	0.3	1
1	A	41	ARG	CB	30.148	0.3	1
1	A	41	ARG	CG	26.442	0.3	1
1	A	41	ARG	CD	42.8	0.3	1
1	A	41	ARG	H	8.222	0.020	1
1	A	41	ARG	HA	4.31	0.020	1
1	A	41	ARG	HB2	1.797	0.020	1
1	A	41	ARG	HB3	1.797	0.020	1
1	A	41	ARG	HG2	1.619	0.020	1
1	A	41	ARG	HG3	1.619	0.020	1
1	A	41	ARG	N	120.884	0.3	1
1	A	42	GLU	C	176.672	0.3	1
1	A	42	GLU	CA	56.595	0.3	1
1	A	42	GLU	CB	29.408	0.3	1
1	A	42	GLU	CG	35.752	0.3	1
1	A	42	GLU	H	8.399	0.020	1
1	A	42	GLU	HA	4.241	0.020	1
1	A	42	GLU	HB2	1.981	0.020	1
1	A	42	GLU	HB3	1.981	0.020	1
1	A	42	GLU	HG2	2.313	0.020	1
1	A	42	GLU	HG3	2.313	0.020	1
1	A	42	GLU	N	120.815	0.3	1
1	A	43	GLY	C	173.851	0.3	1
1	A	43	GLY	CA	45.04	0.3	1
1	A	43	GLY	H	8.328	0.020	1
1	A	43	GLY	HA2	3.893	0.020	1
1	A	43	GLY	HA3	3.893	0.020	1
1	A	43	GLY	N	109.297	0.3	1
1	A	44	MET	C	175.406	0.3	1
1	A	44	MET	CA	55.399	0.3	1
1	A	44	MET	CB	32.339	0.3	1
1	A	44	MET	CG	31.354	0.3	1
1	A	44	MET	H	8.061	0.020	1
1	A	44	MET	HA	4.393	0.020	1
1	A	44	MET	HB2	1.901	0.020	1
1	A	44	MET	HB3	1.901	0.020	1
1	A	44	MET	HG2	2.402	0.020	1
1	A	44	MET	HG3	2.402	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	44	MET	N	119.372	0.3	1
1	A	45	TRP	C	175.715	0.3	1
1	A	45	TRP	CA	56.687	0.3	1
1	A	45	TRP	CB	29.041	0.3	1
1	A	45	TRP	H	8.19	0.020	1
1	A	45	TRP	HA	4.751	0.020	1
1	A	45	TRP	HB2	3.309	0.020	2
1	A	45	TRP	HB3	3.24	0.020	2
1	A	45	TRP	N	121.636	0.3	1
1	A	46	VAL	C	175.777	0.3	1
1	A	46	VAL	CA	61.976	0.3	1
1	A	46	VAL	CB	32.126	0.3	1
1	A	46	VAL	CG1	20.568	0.3	1
1	A	46	VAL	CG2	20.131	0.3	1
1	A	46	VAL	H	7.887	0.020	1
1	A	46	VAL	HA	4.042	0.020	1
1	A	46	VAL	HB	2.025	0.020	1
1	A	46	VAL	HG11	0.881	0.020	2
1	A	46	VAL	HG12	0.881	0.020	2
1	A	46	VAL	HG13	0.881	0.020	2
1	A	46	VAL	HG21	0.871	0.020	2
1	A	46	VAL	HG22	0.871	0.020	2
1	A	46	VAL	HG23	0.871	0.020	2
1	A	46	VAL	N	121.341	0.3	1
1	A	47	GLY	C	173.422	0.3	1
1	A	47	GLY	CA	44.587	0.3	1
1	A	47	GLY	H	7.881	0.020	1
1	A	47	GLY	HA2	3.813	0.020	1
1	A	47	GLY	HA3	3.813	0.020	1
1	A	47	GLY	N	111.269	0.3	1
1	A	48	ALA	C	177.947	0.3	1
1	A	48	ALA	CA	52.334	0.3	1
1	A	48	ALA	CB	18.679	0.3	1
1	A	48	ALA	H	8.14	0.020	1
1	A	48	ALA	HA	4.315	0.020	1
1	A	48	ALA	HB1	1.416	0.020	1
1	A	48	ALA	HB2	1.416	0.020	1
1	A	48	ALA	HB3	1.416	0.020	1
1	A	48	ALA	N	123.653	0.3	1
1	A	49	GLY	C	174.317	0.3	1
1	A	49	GLY	CA	45.04	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	GLY	H	8.458	0.020	1
1	A	49	GLY	HA2	3.941	0.020	1
1	A	49	GLY	HA3	3.941	0.020	1
1	A	49	GLY	N	108.038	0.3	1
1	A	50	GLY	C	173.376	0.3	1
1	A	50	GLY	CA	44.682	0.3	1
1	A	50	GLY	H	8.155	0.020	1
1	A	50	GLY	HA2	3.91	0.020	1
1	A	50	GLY	HA3	3.91	0.020	1
1	A	50	GLY	N	108.486	0.3	1
1	A	51	ALA	C	177.052	0.3	1
1	A	51	ALA	CA	51.967	0.3	1
1	A	51	ALA	CB	18.849	0.3	1
1	A	51	ALA	H	8.073	0.020	1
1	A	51	ALA	HA	4.32	0.020	1
1	A	51	ALA	HB1	1.377	0.020	1
1	A	51	ALA	HB2	1.377	0.020	1
1	A	51	ALA	HB3	1.377	0.020	1
1	A	51	ALA	N	123.286	0.3	1
1	A	52	LEU	C	176.217	0.3	1
1	A	52	LEU	CA	54.265	0.3	1
1	A	52	LEU	CB	41.925	0.3	1
1	A	52	LEU	CG	26.513	0.3	1
1	A	52	LEU	CD1	24.424	0.3	1
1	A	52	LEU	CD2	22.922	0.3	1
1	A	52	LEU	H	8.123	0.020	1
1	A	52	LEU	HA	4.355	0.020	1
1	A	52	LEU	HB2	1.6	0.020	1
1	A	52	LEU	HB3	1.6	0.020	1
1	A	52	LEU	HG	1.614	0.020	1
1	A	52	LEU	HD11	0.904	0.020	2
1	A	52	LEU	HD12	0.904	0.020	2
1	A	52	LEU	HD13	0.904	0.020	2
1	A	52	LEU	HD21	0.863	0.020	2
1	A	52	LEU	HD22	0.863	0.020	2
1	A	52	LEU	HD23	0.863	0.020	2
1	A	52	LEU	N	120.781	0.3	1
1	A	53	ALA	C	174.979	0.3	1
1	A	53	ALA	CA	49.882	0.3	1
1	A	53	ALA	CB	17.767	0.3	1
1	A	53	ALA	H	8.149	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	ALA	HA	4.558	0.020	1
1	A	53	ALA	HB1	1.351	0.020	1
1	A	53	ALA	HB2	1.351	0.020	1
1	A	53	ALA	HB3	1.351	0.020	1
1	A	53	ALA	N	125.674	0.3	1
1	A	54	PRO	C	176.258	0.3	1
1	A	54	PRO	CA	62.756	0.3	1
1	A	54	PRO	CB	31.482	0.3	1
1	A	54	PRO	HA	4.418	0.020	1
1	A	55	ASN	C	175.212	0.3	1
1	A	55	ASN	CA	52.886	0.3	1
1	A	55	ASN	CB	38.134	0.3	1
1	A	55	ASN	H	8.508	0.020	1
1	A	55	ASN	HA	4.747	0.020	1
1	A	55	ASN	HB2	2.882	0.020	1
1	A	55	ASN	HB3	2.882	0.020	1
1	A	55	ASN	HD21	7.559	0.020	1
1	A	55	ASN	HD22	6.888	0.020	1
1	A	55	ASN	N	118.288	0.3	1
1	A	55	ASN	ND2	111.617	0.3	1
1	A	56	THR	C	174.327	0.3	1
1	A	56	THR	CA	61.683	0.3	1
1	A	56	THR	CB	69.049	0.3	1
1	A	56	THR	CG2	21.099	0.3	1
1	A	56	THR	H	8.126	0.020	1
1	A	56	THR	HA	4.364	0.020	1
1	A	56	THR	HB	4.331	0.020	1
1	A	56	THR	HG21	1.223	0.020	1
1	A	56	THR	HG22	1.223	0.020	1
1	A	56	THR	HG23	1.223	0.020	1
1	A	56	THR	N	113.97	0.3	1
1	A	57	SER	C	174.173	0.3	1
1	A	57	SER	CA	57.943	0.3	1
1	A	57	SER	H	8.323	0.020	1
1	A	57	SER	HA	4.479	0.020	1
1	A	57	SER	HB2	3.915	0.020	1
1	A	57	SER	HB3	3.915	0.020	1
1	A	57	SER	N	117.671	0.3	1
1	A	58	SER	C	173.724	0.3	1
1	A	58	SER	CA	58.066	0.3	1
1	A	58	SER	CB	63.24	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	SER	H	8.225	0.020	1
1	A	58	SER	HA	4.444	0.020	1
1	A	58	SER	HB2	3.813	0.020	1
1	A	58	SER	HB3	3.813	0.020	1
1	A	58	SER	N	117.276	0.3	1
1	A	59	LEU	C	175.826	0.3	1
1	A	59	LEU	CA	55.02	0.3	1
1	A	59	LEU	CB	41.948	0.3	1
1	A	59	LEU	CG	26.351	0.3	1
1	A	59	LEU	CD1	24.274	0.3	1
1	A	59	LEU	CD2	23.018	0.3	1
1	A	59	LEU	H	8.064	0.020	1
1	A	59	LEU	HA	4.2	0.020	1
1	A	59	LEU	HB2	1.457	0.020	1
1	A	59	LEU	HB3	1.457	0.020	1
1	A	59	LEU	HG	1.443	0.020	1
1	A	59	LEU	HD11	0.859	0.020	2
1	A	59	LEU	HD12	0.859	0.020	2
1	A	59	LEU	HD13	0.859	0.020	2
1	A	59	LEU	HD21	0.782	0.020	2
1	A	59	LEU	HD22	0.782	0.020	2
1	A	59	LEU	HD23	0.782	0.020	2
1	A	59	LEU	N	123.16	0.3	1
1	A	60	PHE	C	172.674	0.3	1
1	A	60	PHE	CA	54.664	0.3	1
1	A	60	PHE	CB	38.571	0.3	1
1	A	60	PHE	H	7.97	0.020	1
1	A	60	PHE	HA	4.895	0.020	1
1	A	60	PHE	HB2	3.177	0.020	2
1	A	60	PHE	HB3	2.878	0.020	2
1	A	60	PHE	N	119.243	0.3	1
1	A	63	GLU	C	173.68	0.3	1
1	A	63	GLU	CA	53.775	0.3	1
1	A	63	GLU	CB	29.328	0.3	1
1	A	63	GLU	H	8.355	0.020	1
1	A	63	GLU	HB2	2.022	0.020	2
1	A	63	GLU	HB3	1.889	0.020	2
1	A	63	GLU	HG2	2.298	0.020	1
1	A	63	GLU	HG3	2.298	0.020	1
1	A	63	GLU	N	121.97	0.3	1
1	A	106	LYS	C	176.094	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	LYS	CA	56.012	0.3	1
1	A	107	ALA	C	177.236	0.3	1
1	A	107	ALA	CA	52.15	0.3	1
1	A	107	ALA	CB	18.595	0.3	1
1	A	107	ALA	H	8.136	0.020	1
1	A	107	ALA	HA	4.324	0.020	1
1	A	107	ALA	HB1	1.404	0.020	1
1	A	107	ALA	HB2	1.404	0.020	1
1	A	107	ALA	HB3	1.404	0.020	1
1	A	107	ALA	N	124.476	0.3	1
1	A	108	ARG	C	176.064	0.3	1
1	A	108	ARG	CA	55.829	0.3	1
1	A	108	ARG	CB	30.338	0.3	1
1	A	108	ARG	CG	26.637	0.3	1
1	A	108	ARG	CD	42.771	0.3	1
1	A	108	ARG	H	8.239	0.020	1
1	A	108	ARG	HA	4.387	0.020	1
1	A	108	ARG	HB2	1.912	0.020	2
1	A	108	ARG	HB3	1.809	0.020	2
1	A	108	ARG	HG2	1.625	0.020	1
1	A	108	ARG	HG3	1.625	0.020	1
1	A	108	ARG	HD2	3.202	0.020	1
1	A	108	ARG	HD3	3.202	0.020	1
1	A	108	ARG	N	119.942	0.3	1
1	A	109	THR	C	174.097	0.3	1
1	A	109	THR	CA	61.621	0.3	1
1	A	109	THR	CB	69.28	0.3	1
1	A	109	THR	CG2	21.155	0.3	1
1	A	109	THR	H	8.142	0.020	1
1	A	109	THR	HA	4.36	0.020	1
1	A	109	THR	HB	4.228	0.020	1
1	A	109	THR	HG21	1.217	0.020	1
1	A	109	THR	HG22	1.217	0.020	1
1	A	109	THR	HG23	1.217	0.020	1
1	A	109	THR	N	115.679	0.3	1
1	A	110	VAL	C	175.531	0.3	1
1	A	110	VAL	CA	61.941	0.3	1
1	A	110	VAL	CB	32.054	0.3	1
1	A	110	VAL	CG1	20.672	0.3	1
1	A	110	VAL	CG2	20.041	0.3	1
1	A	110	VAL	H	8.106	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	110	VAL	HA	4.133	0.020	1
1	A	110	VAL	HB	2.093	0.020	1
1	A	110	VAL	HG11	0.934	0.020	2
1	A	110	VAL	HG12	0.934	0.020	2
1	A	110	VAL	HG13	0.934	0.020	2
1	A	110	VAL	HG21	0.96	0.020	2
1	A	110	VAL	HG22	0.96	0.020	2
1	A	110	VAL	HG23	0.96	0.020	2
1	A	110	VAL	N	121.897	0.3	1
1	A	111	GLU	C	175.936	0.3	1
1	A	111	GLU	CA	55.951	0.3	1
1	A	111	GLU	CB	29.622	0.3	1
1	A	111	GLU	CG	35.603	0.3	1
1	A	111	GLU	H	8.459	0.020	1
1	A	111	GLU	HA	4.293	0.020	1
1	A	111	GLU	HB2	1.949	0.020	1
1	A	111	GLU	HB3	1.949	0.020	1
1	A	111	GLU	HG2	2.254	0.020	1
1	A	111	GLU	HG3	2.254	0.020	1
1	A	111	GLU	N	124.476	0.3	1
1	A	112	LEU	C	177.272	0.3	1
1	A	112	LEU	CA	54.887	0.3	1
1	A	112	LEU	CB	41.925	0.3	1
1	A	112	LEU	CG	26.397	0.3	1
1	A	112	LEU	CD1	24.406	0.3	1
1	A	112	LEU	CD2	22.825	0.3	1
1	A	112	LEU	H	8.287	0.020	1
1	A	112	LEU	HA	4.33	0.020	1
1	A	112	LEU	HB2	1.662	0.020	1
1	A	112	LEU	HB3	1.662	0.020	1
1	A	112	LEU	HG	1.602	0.020	1
1	A	112	LEU	HD11	0.929	0.020	2
1	A	112	LEU	HD12	0.929	0.020	2
1	A	112	LEU	HD13	0.929	0.020	2
1	A	112	LEU	HD21	0.87	0.020	2
1	A	112	LEU	HD22	0.87	0.020	2
1	A	112	LEU	HD23	0.87	0.020	2
1	A	112	LEU	N	123.026	0.3	1
1	A	113	GLY	C	172.907	0.3	1
1	A	113	GLY	CA	44.549	0.3	1
1	A	113	GLY	H	8.343	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	GLY	HA2	3.943	0.020	1
1	A	113	GLY	HA3	3.943	0.020	1
1	A	113	GLY	N	109.116	0.3	1
1	A	114	ASP	C	174.55	0.3	1
1	A	114	ASP	CA	51.752	0.3	1
1	A	114	ASP	CB	40.864	0.3	1
1	A	114	ASP	H	8.211	0.020	1
1	A	114	ASP	HA	4.875	0.020	1
1	A	114	ASP	HB2	2.742	0.020	2
1	A	114	ASP	HB3	2.572	0.020	2
1	A	114	ASP	N	121.331	0.3	1
1	A	115	PRO	C	176.728	0.3	1
1	A	115	PRO	CA	63.483	0.3	1
1	A	115	PRO	CB	31.5	0.3	1
1	A	115	PRO	CG	26.672	0.3	1
1	A	115	PRO	CD	50.238	0.3	1
1	A	115	PRO	HA	4.411	0.020	1
1	A	115	PRO	HB2	2.306	0.020	2
1	A	115	PRO	HB3	1.957	0.020	2
1	A	115	PRO	HG2	2.024	0.020	1
1	A	115	PRO	HG3	2.024	0.020	1
1	A	115	PRO	HD2	3.831	0.020	1
1	A	115	PRO	HD3	3.831	0.020	1
1	A	116	ASP	C	176.267	0.3	1
1	A	116	ASP	CA	54.357	0.3	1
1	A	116	ASP	CB	40.494	0.3	1
1	A	116	ASP	H	8.345	0.020	1
1	A	116	ASP	HA	4.63	0.020	1
1	A	116	ASP	HB2	2.744	0.020	2
1	A	116	ASP	HB3	2.639	0.020	2
1	A	116	ASP	N	118.674	0.3	1
1	A	117	ARG	C	176.074	0.3	1
1	A	117	ARG	CA	56.564	0.3	1
1	A	117	ARG	CB	30.189	0.3	1
1	A	117	ARG	CG	26.782	0.3	1
1	A	117	ARG	CD	42.8	0.3	1
1	A	117	ARG	H	7.891	0.020	1
1	A	117	ARG	HA	4.226	0.020	1
1	A	117	ARG	HB2	1.876	0.020	2
1	A	117	ARG	HB3	1.806	0.020	2
1	A	117	ARG	HG2	1.625	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	117	ARG	HG3	1.625	0.020	1
1	A	117	ARG	HD2	3.205	0.020	1
1	A	117	ARG	HD3	3.205	0.020	1
1	A	117	ARG	N	120.334	0.3	1
1	A	118	ASP	C	176.135	0.3	1
1	A	118	ASP	CA	54.419	0.3	1
1	A	118	ASP	CB	40.555	0.3	1
1	A	118	ASP	H	8.331	0.020	1
1	A	118	ASP	HA	4.618	0.020	1
1	A	118	ASP	HB2	2.745	0.020	2
1	A	118	ASP	HB3	2.651	0.020	2
1	A	118	ASP	N	120.127	0.3	1
1	A	119	GLN	C	175.752	0.3	1
1	A	119	GLN	CA	55.737	0.3	1
1	A	119	GLN	CB	28.749	0.3	1
1	A	119	GLN	CG	33.272	0.3	1
1	A	119	GLN	H	8.202	0.020	1
1	A	119	GLN	HA	4.305	0.020	1
1	A	119	GLN	HB2	2.002	0.020	1
1	A	119	GLN	HB3	2.002	0.020	1
1	A	119	GLN	HG2	2.36	0.020	1
1	A	119	GLN	HG3	2.36	0.020	1
1	A	119	GLN	N	120.314	0.3	1
1	A	120	ARG	C	176.059	0.3	1
1	A	120	ARG	CA	55.829	0.3	1
1	A	120	ARG	CB	29.86	0.3	1
1	A	120	ARG	CG	26.405	0.3	1
1	A	120	ARG	CD	42.804	0.3	1
1	A	120	ARG	H	8.269	0.020	1
1	A	120	ARG	HA	4.314	0.020	1
1	A	120	ARG	HB2	1.814	0.020	2
1	A	120	ARG	HB3	1.878	0.020	2
1	A	120	ARG	HG2	1.654	0.020	1
1	A	120	ARG	HG3	1.654	0.020	1
1	A	120	ARG	HD2	3.202	0.020	1
1	A	120	ARG	HD3	3.202	0.020	1
1	A	120	ARG	N	120.978	0.3	1
1	A	121	ARG	C	176.475	0.3	1
1	A	121	ARG	CA	55.921	0.3	1
1	A	121	ARG	CB	30.356	0.3	1
1	A	121	ARG	CG	26.611	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	121	ARG	CD	42.781	0.3	1
1	A	121	ARG	H	8.286	0.020	1
1	A	121	ARG	HA	4.337	0.020	1
1	A	121	ARG	HB2	1.9	0.020	2
1	A	121	ARG	HB3	1.809	0.020	2
1	A	121	ARG	HG2	1.658	0.020	1
1	A	121	ARG	HG3	1.658	0.020	1
1	A	121	ARG	HD2	3.203	0.020	1
1	A	121	ARG	HD3	3.203	0.020	1
1	A	121	ARG	N	121.67	0.3	1
1	A	122	GLY	C	173.447	0.3	1
1	A	122	GLY	CA	44.978	0.3	1
1	A	122	GLY	H	8.401	0.020	1
1	A	122	GLY	HA2	3.973	0.020	1
1	A	122	GLY	HA3	3.973	0.020	1
1	A	122	GLY	N	109.691	0.3	1
1	A	123	ASP	C	176.083	0.3	1
1	A	123	ASP	CA	53.903	0.3	1
1	A	123	ASP	CB	40.709	0.3	1
1	A	123	ASP	H	8.223	0.020	1
1	A	123	ASP	HA	4.635	0.020	1
1	A	123	ASP	HB2	2.688	0.020	1
1	A	123	ASP	HB3	2.688	0.020	1
1	A	123	ASP	N	120.363	0.3	1
1	A	124	SER	C	173.913	0.3	1
1	A	124	SER	CA	58.127	0.3	1
1	A	124	SER	CB	63.24	0.3	1
1	A	124	SER	H	8.255	0.020	1
1	A	124	SER	HA	4.432	0.020	1
1	A	124	SER	HB2	3.878	0.020	1
1	A	124	SER	HB3	3.878	0.020	1
1	A	124	SER	N	115.666	0.3	1
1	A	125	ASN	C	174.403	0.3	1
1	A	125	ASN	CA	52.947	0.3	1
1	A	125	ASN	CB	38.266	0.3	1
1	A	125	ASN	H	8.469	0.020	1
1	A	125	ASN	HA	4.717	0.020	1
1	A	125	ASN	HB2	2.871	0.020	2
1	A	125	ASN	HB3	2.785	0.020	2
1	A	125	ASN	HD21	7.606	0.020	1
1	A	125	ASN	HD22	6.89	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	ASN	N	120.712	0.3	1
1	A	125	ASN	ND2	112.89	0.3	1
1	A	126	VAL	C	175.078	0.3	1
1	A	126	VAL	CA	61.928	0.3	1
1	A	126	VAL	CB	32.19	0.3	1
1	A	126	VAL	CG1	20.558	0.3	1
1	A	126	VAL	CG2	19.74	0.3	1
1	A	126	VAL	H	7.844	0.020	1
1	A	126	VAL	HA	4.072	0.020	1
1	A	126	VAL	HB	1.989	0.020	1
1	A	126	VAL	HG11	0.818	0.020	2
1	A	126	VAL	HG12	0.818	0.020	2
1	A	126	VAL	HG13	0.818	0.020	2
1	A	126	VAL	HG21	0.82	0.020	2
1	A	126	VAL	HG22	0.82	0.020	2
1	A	126	VAL	HG23	0.82	0.020	2
1	A	126	VAL	N	119.156	0.3	1
1	A	127	PHE	C	174.943	0.3	1
1	A	127	PHE	CA	57.116	0.3	1
1	A	127	PHE	CB	39.037	0.3	1
1	A	127	PHE	CD1	130.938	0.3	1
1	A	127	PHE	CE1	129.313	0.3	1
1	A	127	PHE	H	8.274	0.020	1
1	A	127	PHE	HA	4.685	0.020	1
1	A	127	PHE	HB2	3.137	0.020	2
1	A	127	PHE	HB3	3.013	0.020	2
1	A	127	PHE	HD1	7.354	0.020	1
1	A	127	PHE	HD2	7.354	0.020	1
1	A	127	PHE	HE1	7.308	0.020	1
1	A	127	PHE	HE2	7.308	0.020	1
1	A	127	PHE	HZ	7.266	0.020	1
1	A	127	PHE	N	123.772	0.3	1
1	A	128	VAL	C	174.747	0.3	1
1	A	128	VAL	CA	61.499	0.3	1
1	A	128	VAL	CB	32.587	0.3	1
1	A	128	VAL	CG1	20.558	0.3	1
1	A	128	VAL	CG2	19.953	0.3	1
1	A	128	VAL	H	7.961	0.020	1
1	A	128	VAL	HA	4.093	0.020	1
1	A	128	VAL	HB	2.018	0.020	1
1	A	128	VAL	HG11	0.916	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	128	VAL	HG12	0.916	0.020	2
1	A	128	VAL	HG13	0.916	0.020	2
1	A	128	VAL	HG21	0.869	0.020	2
1	A	128	VAL	HG22	0.869	0.020	2
1	A	128	VAL	HG23	0.869	0.020	2
1	A	128	VAL	N	122.089	0.3	1
1	A	129	ASP	C	175.311	0.3	1
1	A	129	ASP	CA	53.714	0.3	1
1	A	129	ASP	CB	40.852	0.3	1
1	A	129	ASP	H	8.279	0.020	1
1	A	129	ASP	HA	4.605	0.020	1
1	A	129	ASP	HB2	2.69	0.020	2
1	A	129	ASP	HB3	2.581	0.020	2
1	A	129	ASP	N	123.882	0.3	1
1	A	130	SER	C	171.448	0.3	1
1	A	130	SER	CA	55.89	0.3	1
1	A	130	SER	CB	62.867	0.3	1
1	A	130	SER	H	8.139	0.020	1
1	A	130	SER	HA	4.43	0.020	1
1	A	130	SER	HB2	3.754	0.020	2
1	A	130	SER	HB3	3.861	0.020	2
1	A	130	SER	N	117.076	0.3	1
1	A	132	PRO	C	176.38	0.3	1
1	A	132	PRO	CA	62.633	0.3	1
1	A	132	PRO	CB	31.499	0.3	1
1	A	132	PRO	HA	4.462	0.020	1
1	A	132	PRO	HB2	2.317	0.020	2
1	A	132	PRO	HB3	1.926	0.020	2
1	A	133	SER	C	174.011	0.3	1
1	A	133	SER	CA	57.514	0.3	1
1	A	133	SER	CB	63.251	0.3	1
1	A	133	SER	H	8.307	0.020	1
1	A	133	SER	HA	4.438	0.020	1
1	A	133	SER	HB2	3.875	0.020	1
1	A	133	SER	HB3	3.875	0.020	1
1	A	133	SER	N	115.617	0.3	1
1	A	134	LEU	C	176.586	0.3	1
1	A	134	LEU	CA	54.438	0.3	1
1	A	134	LEU	CB	41.925	0.3	1
1	A	134	LEU	CG	26.577	0.3	1
1	A	134	LEU	CD1	24.502	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	134	LEU	CD2	22.825	0.3	1
1	A	134	LEU	H	8.311	0.020	1
1	A	134	LEU	HA	4.409	0.020	1
1	A	134	LEU	HB2	1.611	0.020	1
1	A	134	LEU	HB3	1.611	0.020	1
1	A	134	LEU	HG	1.63	0.020	1
1	A	134	LEU	HD11	0.935	0.020	2
1	A	134	LEU	HD12	0.935	0.020	2
1	A	134	LEU	HD13	0.935	0.020	2
1	A	134	LEU	HD21	0.874	0.020	2
1	A	134	LEU	HD22	0.874	0.020	2
1	A	134	LEU	HD23	0.874	0.020	2
1	A	134	LEU	N	124.414	0.3	1
1	A	135	GLU	C	174.072	0.3	1
1	A	135	GLU	CA	53.873	0.3	1
1	A	135	GLU	CB	29.243	0.3	1
1	A	135	GLU	CG	35.422	0.3	1
1	A	135	GLU	H	8.274	0.020	1
1	A	135	GLU	HA	4.584	0.020	1
1	A	135	GLU	HB2	1.888	0.020	1
1	A	135	GLU	HB3	1.888	0.020	1
1	A	135	GLU	HG2	2.283	0.020	1
1	A	135	GLU	HG3	2.283	0.020	1
1	A	135	GLU	N	122.852	0.3	1
1	A	136	PRO	C	176.176	0.3	1
1	A	136	PRO	CA	62.694	0.3	1
1	A	136	PRO	CB	31.554	0.3	1
1	A	136	PRO	HA	4.436	0.020	1
1	A	137	CYS	C	173.888	0.3	1
1	A	137	CYS	CA	57.698	0.3	1
1	A	137	CYS	CB	27.345	0.3	1
1	A	137	CYS	H	8.433	0.020	1
1	A	137	CYS	HA	4.518	0.020	1
1	A	137	CYS	HB2	2.903	0.020	1
1	A	137	CYS	HB3	2.903	0.020	1
1	A	137	CYS	N	119.686	0.3	1
1	A	138	ILE	C	174.158	0.3	1
1	A	138	ILE	CA	58.189	0.3	1
1	A	138	ILE	CB	38.063	0.3	1
1	A	138	ILE	CG1	26.4	0.3	1
1	A	138	ILE	CG2	16.63	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	ILE	CD1	12.125	0.3	1
1	A	138	ILE	H	8.275	0.020	1
1	A	138	ILE	HA	4.5	0.020	1
1	A	138	ILE	HB	1.881	0.020	1
1	A	138	ILE	HG12	1.187	0.020	2
1	A	138	ILE	HG13	1.508	0.020	2
1	A	138	ILE	HG21	0.961	0.020	1
1	A	138	ILE	HG22	0.961	0.020	1
1	A	138	ILE	HG23	0.961	0.020	1
1	A	138	ILE	HD11	0.867	0.020	1
1	A	138	ILE	HD12	0.867	0.020	1
1	A	138	ILE	HD13	0.867	0.020	1
1	A	138	ILE	N	125.089	0.3	1
1	A	139	PRO	C	176.575	0.3	1
1	A	139	PRO	CA	62.97	0.3	1
1	A	139	PRO	CB	31.554	0.3	1
1	A	139	PRO	HA	4.464	0.020	1
1	A	139	PRO	HB2	2.308	0.020	2
1	A	139	PRO	HB3	1.96	0.020	2
1	A	140	SER	C	174.281	0.3	1
1	A	140	SER	CA	58.066	0.3	1
1	A	140	SER	CB	63.277	0.3	1
1	A	140	SER	H	8.376	0.020	1
1	A	140	SER	HA	4.428	0.020	1
1	A	140	SER	HB2	3.893	0.020	1
1	A	140	SER	HB3	3.893	0.020	1
1	A	140	SER	N	115.891	0.3	1
1	A	141	GLN	C	175.556	0.3	1
1	A	141	GLN	CA	55.282	0.3	1
1	A	141	GLN	CB	29.289	0.3	1
1	A	141	GLN	CG	33.34	0.3	1
1	A	141	GLN	H	8.409	0.020	1
1	A	141	GLN	HA	4.447	0.020	1
1	A	141	GLN	HB2	2.008	0.020	1
1	A	141	GLN	HB3	2.008	0.020	1
1	A	141	GLN	HG2	2.407	0.020	1
1	A	141	GLN	HG3	2.407	0.020	1
1	A	141	GLN	HE21	7.772	0.020	1
1	A	141	GLN	HE22	6.789	0.020	1
1	A	141	GLN	N	121.97	0.3	1
1	A	141	GLN	NE2	112.24	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	142	GLY	C	171.092	0.3	1
1	A	142	GLY	CA	43.969	0.3	1
1	A	142	GLY	H	8.237	0.020	1
1	A	142	GLY	HA2	4.125	0.020	2
1	A	142	GLY	HA3	4.07	0.020	2
1	A	142	GLY	N	109.906	0.3	1
1	A	144	HIS	C	172.601	0.3	1
1	A	144	HIS	CA	53.254	0.3	1
1	A	144	HIS	CB	28.71	0.3	1
1	A	144	HIS	H	8.489	0.020	1
1	A	144	HIS	HA	4.96	0.020	1
1	A	144	HIS	HB2	3.204	0.020	2
1	A	144	HIS	HB3	3.144	0.020	2
1	A	144	HIS	N	119.666	0.3	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	174	0.16 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	151	0.82 ± 0.12	Should be checked
$^{13}C'$	170	0.17 ± 0.13	None needed (< 0.5 ppm)
^{15}N	161	0.36 ± 0.20	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 87%, i.e. 975 atoms were assigned a chemical shift out of a possible 1126. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	405/415 (98%)	166/169 (98%)	161/166 (97%)	78/80 (98%)
Sidechain	540/662 (82%)	369/431 (86%)	165/203 (81%)	6/28 (21%)
Aromatic	30/49 (61%)	17/24 (71%)	11/22 (50%)	2/3 (67%)
Overall	975/1126 (87%)	552/624 (88%)	337/391 (86%)	86/111 (77%)

7.1.4 Statistically unusual chemical shifts (i)

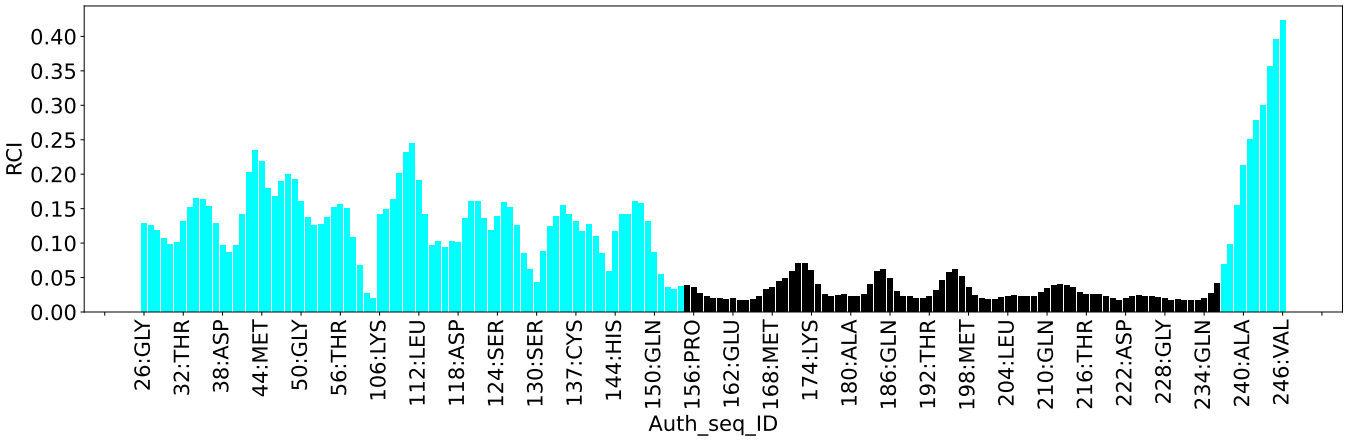
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	216	THR	CB	59.33	61.12 – 78.27	-6.0
1	A	171	GLU	CG	29.29	30.20 – 42.01	-5.8

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	627
Intra-residue (|i-j|=0)	169
Sequential (|i-j|=1)	159
Medium range (|i-j|>1 and |i-j|<5)	121
Long range (|i-j|≥5)	34
Inter-chain	0
Hydrogen bond restraints	144
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	2.5
Number of long range restraints per residue[1]	0.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	3.3	0.2
0.2-0.5 (Medium)	7.2	0.5
>0.5 (Large)	8.2	9.47

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

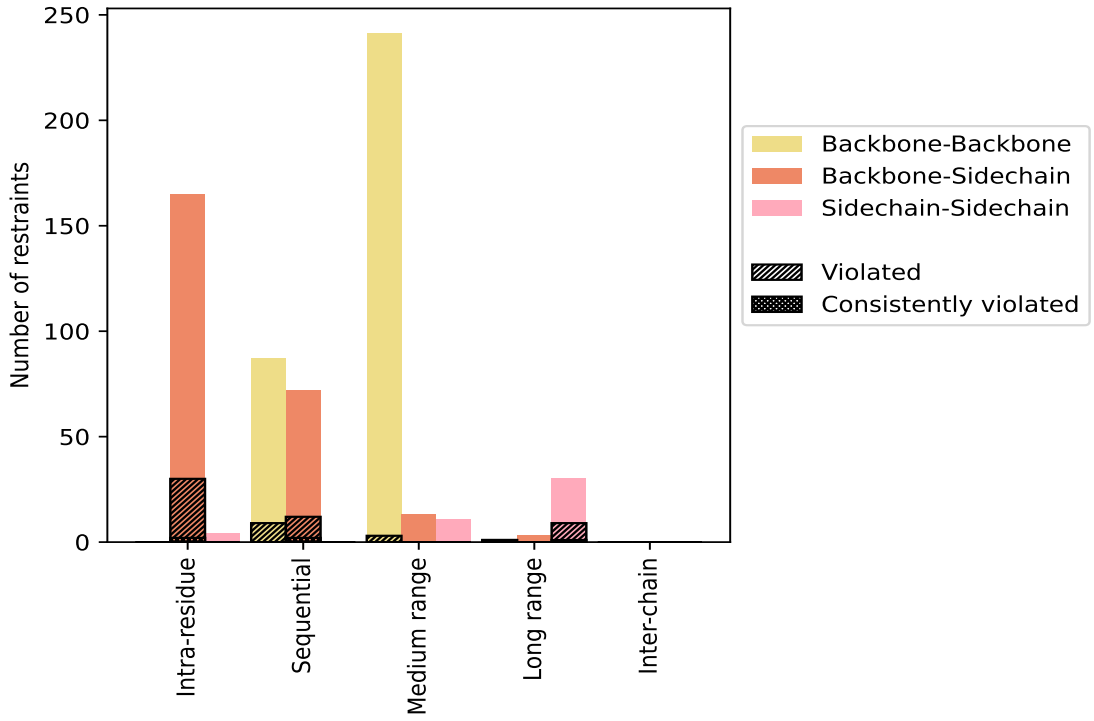
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	169	27.0	30	17.8	4.8	2	1.2	0.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	165	26.3	30	18.2	4.8	2	1.2	0.3
Sidechain-Sidechain	4	0.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	159	25.4	21	13.2	3.3	2	1.3	0.3
Backbone-Backbone	87	13.9	9	10.3	1.4	0	0.0	0.0
Backbone-Sidechain	72	11.5	12	16.7	1.9	2	2.8	0.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	121	19.3	3	2.5	0.5	0	0.0	0.0
Backbone-Backbone	97	15.5	3	3.1	0.5	0	0.0	0.0
Backbone-Sidechain	13	2.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	11	1.8	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	34	5.4	10	29.4	1.6	2	5.9	0.3
Backbone-Backbone	1	0.2	1	100.0	0.2	1	100.0	0.2
Backbone-Sidechain	3	0.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	30	4.8	9	30.0	1.4	1	3.3	0.2
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	144	23.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	627	100.0	64	10.2	10.2	6	1.0	1.0
Backbone-Backbone	329	52.5	13	4.0	2.1	1	0.3	0.2
Backbone-Sidechain	253	40.4	42	16.6	6.7	4	1.6	0.6
Sidechain-Sidechain	45	7.2	9	20.0	1.4	1	2.2	0.2

[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	4	4	1	6	0	15	1.01	5.99	1.44	0.36
2	3	5	0	5	0	13	1.15	7.48	1.89	0.43
3	7	5	1	8	0	21	0.91	7.54	1.59	0.3
4	7	5	1	5	0	18	0.89	4.89	1.08	0.59
5	8	4	1	3	0	16	0.85	6.62	1.54	0.36
6	8	4	1	7	0	20	0.89	6.04	1.26	0.57
7	10	8	1	9	0	28	0.69	6.72	1.23	0.31
8	6	6	2	5	0	19	0.84	6.76	1.46	0.32
9	5	6	1	5	0	17	1.04	5.62	1.26	0.67
10	8	5	0	8	0	21	0.75	4.94	1.04	0.37
11	6	5	0	6	0	17	1.04	5.2	1.15	0.88

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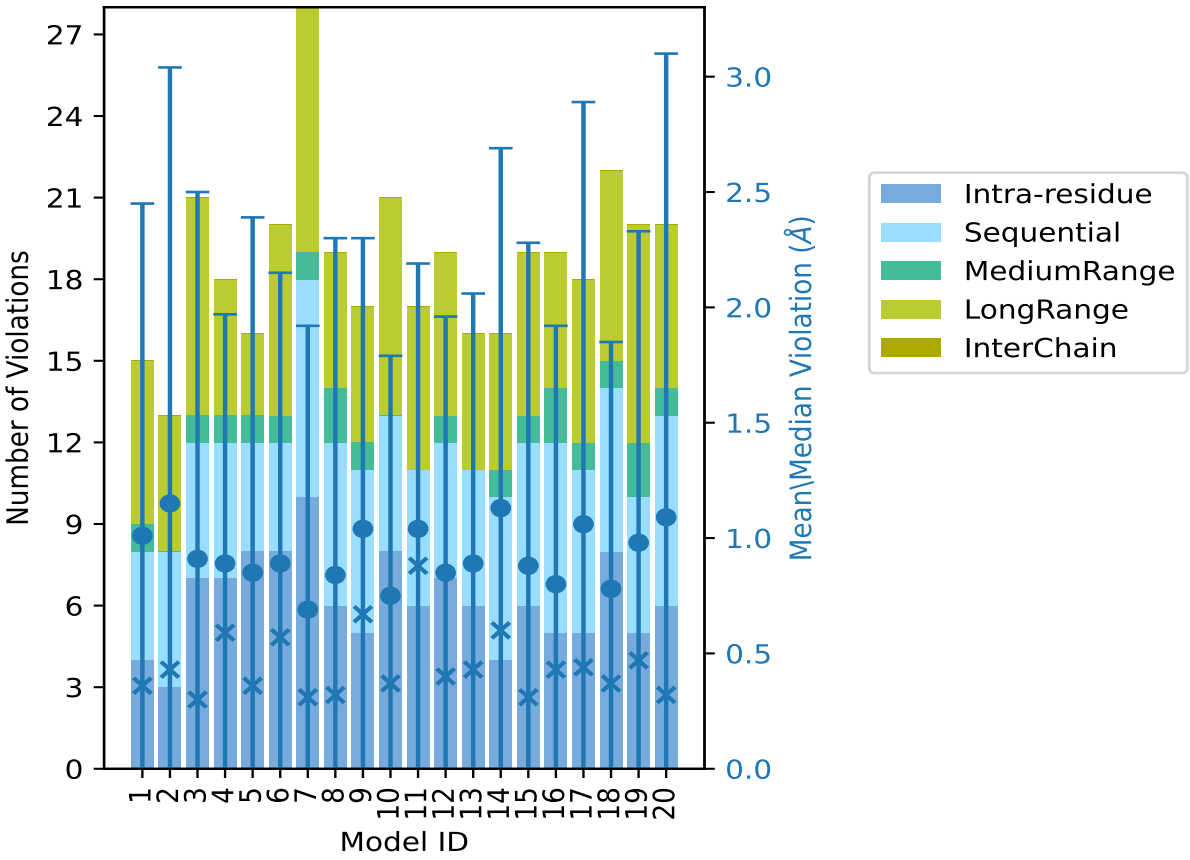
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	7	5	1	6	0	19	0.85	5.03	1.11	0.4
13	6	5	0	5	0	16	0.89	5.02	1.17	0.43
14	4	6	1	5	0	16	1.13	6.87	1.56	0.6
15	6	6	1	6	0	19	0.88	6.36	1.4	0.31
16	5	7	2	5	0	19	0.8	5.19	1.12	0.43
17	5	6	1	6	0	18	1.06	8.29	1.83	0.44
18	8	6	1	7	0	22	0.78	5.26	1.07	0.37
19	5	5	2	8	0	20	0.98	6.18	1.35	0.47
20	6	7	1	6	0	20	1.09	9.47	2.01	0.32

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

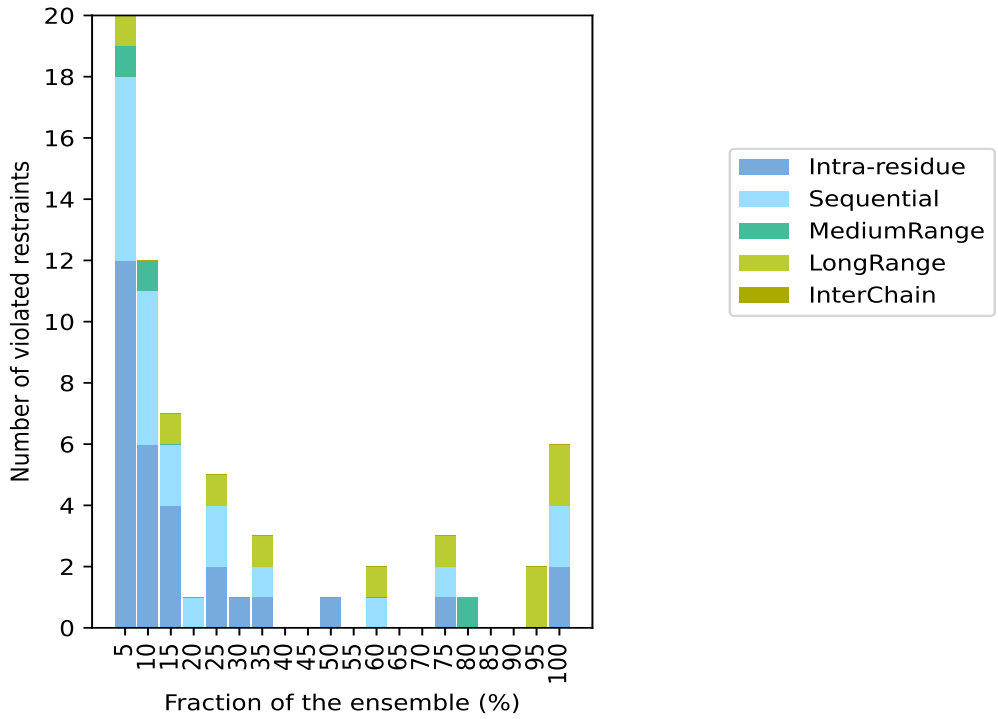
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 419(IR:139, SQ:138, MR:118, LR:24, 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]	%
12	6	1	1	0	20	1	5.0
6	5	1	0	0	12	2	10.0
4	2	0	1	0	7	3	15.0
0	1	0	0	0	1	4	20.0
2	2	0	1	0	5	5	25.0
1	0	0	0	0	1	6	30.0
1	1	0	1	0	3	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
1	0	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	1	0	1	0	2	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
1	1	0	1	0	3	15	75.0
0	0	1	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	2	0	2	19	95.0
2	2	0	2	0	6	20	100.0

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

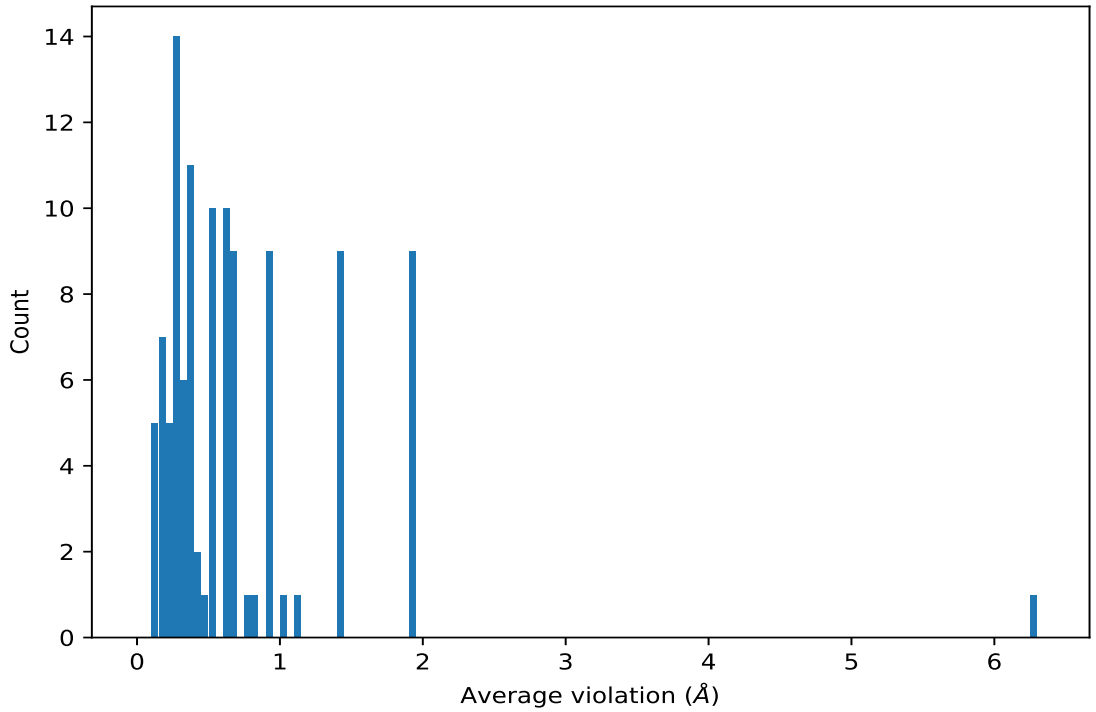
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	20	6.27	1.2	6.11
(3,27)	1:A:183:LEU:HD21	1:A:224:LEU:HD21	20	0.65	0.29	0.75
(3,27)	1:A:183:LEU:HD21	1:A:224:LEU:HD22	20	0.65	0.29	0.75
(3,27)	1:A:183:LEU:HD21	1:A:224:LEU:HD23	20	0.65	0.29	0.75
(3,27)	1:A:183:LEU:HD22	1:A:224:LEU:HD21	20	0.65	0.29	0.75
(3,27)	1:A:183:LEU:HD22	1:A:224:LEU:HD22	20	0.65	0.29	0.75
(3,27)	1:A:183:LEU:HD22	1:A:224:LEU:HD23	20	0.65	0.29	0.75
(3,27)	1:A:183:LEU:HD23	1:A:224:LEU:HD21	20	0.65	0.29	0.75
(3,27)	1:A:183:LEU:HD23	1:A:224:LEU:HD22	20	0.65	0.29	0.75
(3,27)	1:A:183:LEU:HD23	1:A:224:LEU:HD23	20	0.65	0.29	0.75
(1,128)	1:A:185:TYR:HB2	1:A:186:GLN:H	20	0.53	0.16	0.61
(1,5)	1:A:232:VAL:HB	1:A:233:VAL:H	20	0.39	0.08	0.39
(1,226)	1:A:232:VAL:H	1:A:232:VAL:HB	20	0.28	0.0	0.28
(3,42)	1:A:203:LEU:HA	1:A:203:LEU:HD21	20	0.25	0.04	0.25
(3,42)	1:A:203:LEU:HA	1:A:203:LEU:HD22	20	0.25	0.04	0.25
(3,42)	1:A:203:LEU:HA	1:A:203:LEU:HD23	20	0.25	0.04	0.25

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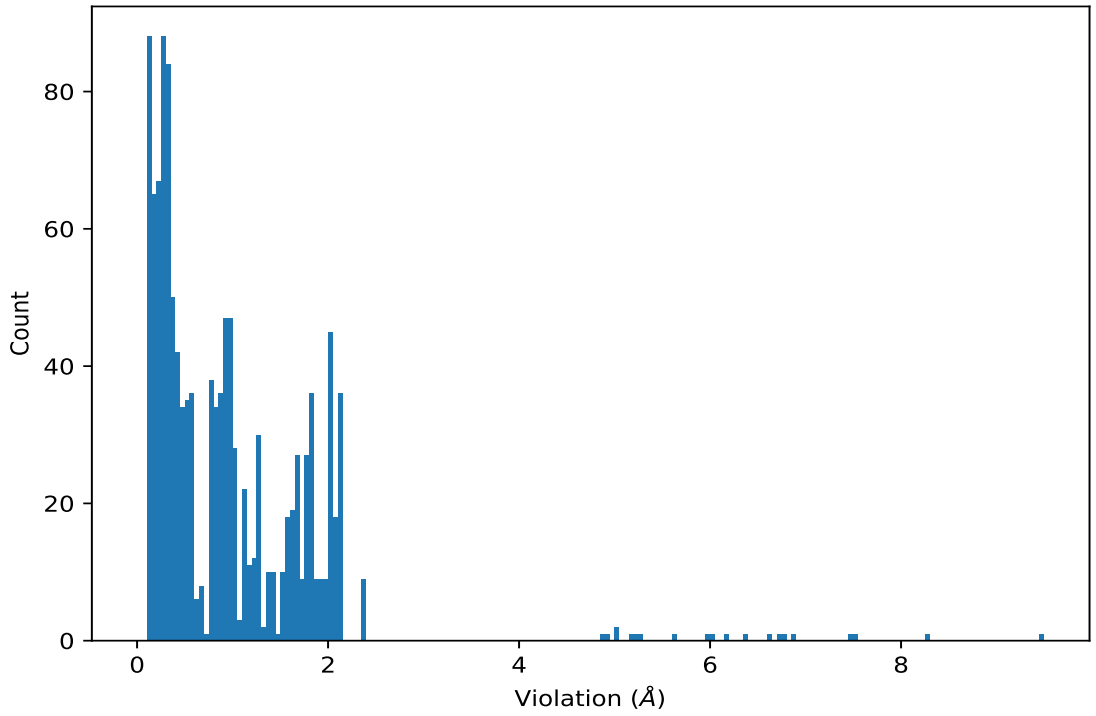
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,2)	1:A:224:LEU:HD11	1:A:233:VAL:HG11	19	1.9	0.27	2.0
(3,2)	1:A:224:LEU:HD11	1:A:233:VAL:HG12	19	1.9	0.27	2.0
(3,2)	1:A:224:LEU:HD11	1:A:233:VAL:HG13	19	1.9	0.27	2.0
(3,2)	1:A:224:LEU:HD12	1:A:233:VAL:HG11	19	1.9	0.27	2.0
(3,2)	1:A:224:LEU:HD12	1:A:233:VAL:HG12	19	1.9	0.27	2.0
(3,2)	1:A:224:LEU:HD12	1:A:233:VAL:HG13	19	1.9	0.27	2.0
(3,2)	1:A:224:LEU:HD13	1:A:233:VAL:HG11	19	1.9	0.27	2.0
(3,2)	1:A:224:LEU:HD13	1:A:233:VAL:HG12	19	1.9	0.27	2.0
(3,2)	1:A:224:LEU:HD13	1:A:233:VAL:HG13	19	1.9	0.27	2.0
(3,34)	1:A:179:LEU:HD11	1:A:203:LEU:HD11	19	1.43	0.38	1.56
(3,34)	1:A:179:LEU:HD11	1:A:203:LEU:HD12	19	1.43	0.38	1.56
(3,34)	1:A:179:LEU:HD11	1:A:203:LEU:HD13	19	1.43	0.38	1.56
(3,34)	1:A:179:LEU:HD12	1:A:203:LEU:HD11	19	1.43	0.38	1.56
(3,34)	1:A:179:LEU:HD12	1:A:203:LEU:HD12	19	1.43	0.38	1.56
(3,34)	1:A:179:LEU:HD12	1:A:203:LEU:HD13	19	1.43	0.38	1.56
(3,34)	1:A:179:LEU:HD13	1:A:203:LEU:HD11	19	1.43	0.38	1.56
(3,34)	1:A:179:LEU:HD13	1:A:203:LEU:HD12	19	1.43	0.38	1.56
(3,34)	1:A:179:LEU:HD13	1:A:203:LEU:HD13	19	1.43	0.38	1.56
(1,183)	1:A:192:THR:HA	1:A:196:ASP:H	16	1.02	0.31	1.08
(1,182)	1:A:196:ASP:H	1:A:197:GLN:H	15	0.84	0.03	0.85

[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)
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	20	9.47
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	17	8.29
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	3	7.54
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	2	7.48
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	14	6.87
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	8	6.76
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	7	6.72
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	5	6.62
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	15	6.36
(1,206)	1:A:167:LEU:HA	1:A:175:GLY:H	19	6.18

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value