



wwPDB NMR Structure Validation Summary Report ⓘ

Sep 24, 2025 – 06:52 pm BST

PDB ID : 9IEW / pdb_00009iew
BMRB ID : 34982
Title : The solution NMR structure of OB domain of ComEC from Moorella glycerini
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Deposited on : 2025-02-15

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

We welcome your comments at validation@mail.wwpdb.org

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

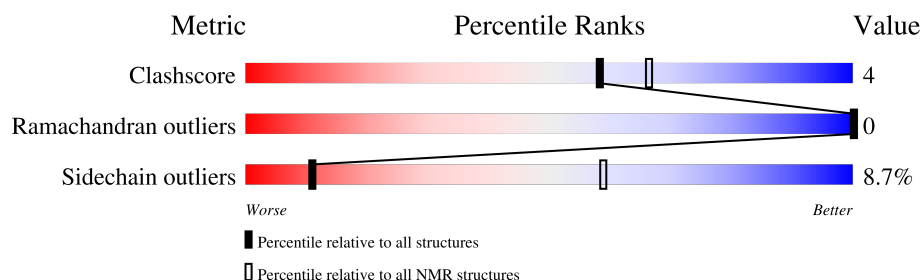
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	124	<div> <div>40%</div> <div>9%</div> <div>52%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:89-A:113, A:124-A:132, A:140-A:152, A:184-A:196 (60)	0.14	6

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2028 atoms, of which 1019 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Competence protein.

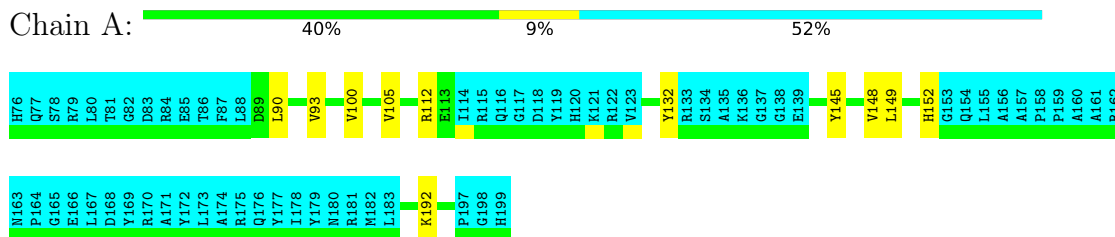
Mol	Chain	Residues	Atoms						Trace
1	A	124	Total	C	H	N	O	S	0
			2028	636	1019	193	179	1	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

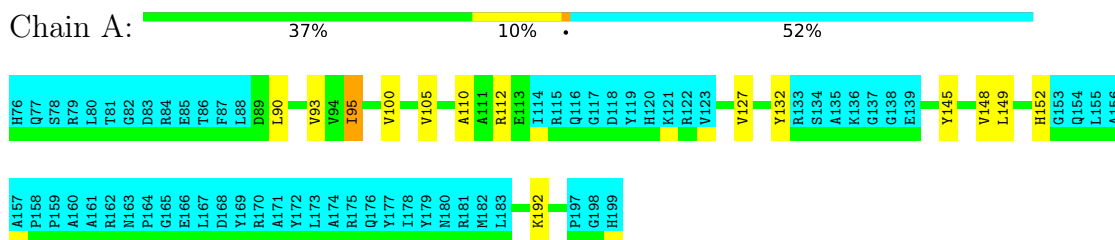
- Molecule 1: Competence protein



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

The representative model is number 6. Colouring as in section 4.1 above.

- Molecule 1: Competence protein



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	
Amber	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	660
Number of shifts mapped to atoms	17
Number of unparsed shifts	0
Number of shifts with mapping errors	643
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	491	511	511	4±1
All	All	9820	10220	10220	90

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 4.

5 of 10 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:VAL:HA	1:A:105:VAL:HG22	0.56	1.77	15	19
1:A:93:VAL:CG2	1:A:148:VAL:HG22	0.53	2.34	12	20
1:A:152:HIS:CD2	1:A:152:HIS:C	0.52	2.87	18	20
1:A:95:ILE:HG21	1:A:110:ALA:HB2	0.50	1.83	6	4
1:A:90:LEU:HD13	1:A:90:LEU:C	0.45	2.37	12	14

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	60/124 (48%)	57±1 (94±1%)	3±1 (6±1%)	0±0 (0±0%)	100	100
All	All	1200/2480 (48%)	1131 (94%)	69 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	54/104 (52%)	49±1 (91±3%)	5±1 (9±3%)	11	59
All	All	1080/2080 (52%)	986 (91%)	94 (9%)	11	59

5 of 9 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	149	LEU	20
1	A	145	TYR	16
1	A	112	ARG	14
1	A	132	TYR	14
1	A	192	LYS	13

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	660
Number of shifts mapped to atoms	17
Number of unparsed shifts	0
Number of shifts with mapping errors	643
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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 643) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	GLY	H	8.398	0.020	1
1	A	7	GLY	HA2	3.702	0.020	2
1	A	7	GLY	HA3	4.063	0.020	2
1	A	7	GLY	CA	47.497	0.3	1
1	A	7	GLY	N	110.787	0.3	1
1	A	8	ASP	H	8.282	0.020	1
1	A	8	ASP	HA	4.685	0.020	1
1	A	8	ASP	HB2	2.594	0.020	2
1	A	8	ASP	HB3	2.863	0.020	2
1	A	8	ASP	CA	54.628	0.3	1
1	A	8	ASP	CB	41.119	0.3	1
1	A	8	ASP	N	120.63	0.3	1
1	A	42	GLY	H	8.018	0.020	1
1	A	42	GLY	HA2	3.073	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	GLY	HA3	3.075	0.020	2
1	A	42	GLY	CA	43.807	0.3	1
1	A	42	GLY	N	112.653	0.3	1
1	A	46	LYS	H	8.421	0.020	1
1	A	46	LYS	HA	4.382	0.020	1
1	A	46	LYS	HB2	1.464	0.020	2
1	A	46	LYS	HB3	1.536	0.020	2
1	A	46	LYS	HD2	1.608	0.020	2
1	A	46	LYS	HD3	1.637	0.020	2
1	A	46	LYS	HE2	2.825	0.020	2
1	A	46	LYS	HE3	2.867	0.020	2
1	A	46	LYS	HG2	1.153	0.020	2
1	A	46	LYS	HG3	1.242	0.020	2
1	A	46	LYS	CA	55.18	0.3	1
1	A	46	LYS	CB	35.86	0.3	1
1	A	46	LYS	CD	29.47	0.3	1
1	A	46	LYS	CE	42.088	0.3	1
1	A	46	LYS	CG	24.134	0.3	1
1	A	46	LYS	N	122.655	0.3	1
1	A	47	ARG	H	8.566	0.020	1
1	A	47	ARG	HA	5.265	0.020	1
1	A	47	ARG	HB2	1.792	0.020	2
1	A	47	ARG	HB3	1.795	0.020	2
1	A	47	ARG	HD2	3.239	0.020	2
1	A	47	ARG	HD3	3.267	0.020	2
1	A	47	ARG	HG2	1.671	0.020	2
1	A	47	ARG	HG3	1.666	0.020	2
1	A	47	ARG	CA	55.542	0.3	1
1	A	47	ARG	CB	30.246	0.3	1
1	A	47	ARG	CD	43.576	0.3	1
1	A	47	ARG	CG	27.462	0.3	1
1	A	47	ARG	N	124.939	0.3	1
1	A	48	VAL	H	7.683	0.020	1
1	A	48	VAL	HA	4.515	0.020	1
1	A	48	VAL	HB	2.062	0.020	1
1	A	48	VAL	HG11	0.732	0.020	2
1	A	48	VAL	HG12	0.732	0.020	2
1	A	48	VAL	HG13	0.732	0.020	2
1	A	48	VAL	HG21	0.505	0.020	2
1	A	48	VAL	HG22	0.505	0.020	2
1	A	48	VAL	HG23	0.505	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	VAL	CA	59.301	0.3	1
1	A	48	VAL	CB	35.464	0.3	1
1	A	48	VAL	CG1	21.594	0.3	1
1	A	48	VAL	CG2	18.201	0.3	1
1	A	48	VAL	N	117.251	0.3	1
1	A	49	ARG	H	8.632	0.020	1
1	A	49	ARG	HA	4.844	0.020	1
1	A	49	ARG	HB2	1.683	0.020	2
1	A	49	ARG	HB3	1.841	0.020	2
1	A	49	ARG	HD2	3.231	0.020	2
1	A	49	ARG	HD3	3.257	0.020	2
1	A	49	ARG	HG2	1.546	0.020	2
1	A	49	ARG	HG3	1.687	0.020	2
1	A	49	ARG	CA	55.256	0.3	1
1	A	49	ARG	CB	30.683	0.3	1
1	A	49	ARG	CD	43.236	0.3	1
1	A	49	ARG	CG	26.829	0.3	1
1	A	49	ARG	N	120.829	0.3	1
1	A	50	GLU	H	7.229	0.020	1
1	A	50	GLU	HA	4.678	0.020	1
1	A	50	GLU	HB2	2.066	0.020	2
1	A	50	GLU	HB3	2.076	0.020	2
1	A	50	GLU	HG2	1.807	0.020	2
1	A	50	GLU	HG3	2.334	0.020	2
1	A	50	GLU	CA	55.391	0.3	1
1	A	50	GLU	CB	33.155	0.3	1
1	A	50	GLU	CG	35.918	0.3	1
1	A	50	GLU	N	120.465	0.3	1
1	A	51	LYS	H	8.881	0.020	1
1	A	51	LYS	HA	5.336	0.020	1
1	A	51	LYS	HB2	1.498	0.020	2
1	A	51	LYS	HB3	1.796	0.020	2
1	A	51	LYS	HD2	1.225	0.020	2
1	A	51	LYS	HD3	1.465	0.020	2
1	A	51	LYS	HE2	3.18	0.020	2
1	A	51	LYS	HE3	3.075	0.020	2
1	A	51	LYS	HG2	0.749	0.020	2
1	A	51	LYS	HG3	0.762	0.020	2
1	A	51	LYS	CA	56.045	0.3	1
1	A	51	LYS	CB	34.254	0.3	1
1	A	51	LYS	CD	27.354	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	LYS	CE	43.966	0.3	1
1	A	51	LYS	CG	24.871	0.3	1
1	A	51	LYS	N	123.112	0.3	1
1	A	52	VAL	H	9.221	0.020	1
1	A	52	VAL	HA	4.599	0.020	1
1	A	52	VAL	HB	1.678	0.020	1
1	A	52	VAL	HG11	0.753	0.020	2
1	A	52	VAL	HG12	0.753	0.020	2
1	A	52	VAL	HG13	0.753	0.020	2
1	A	52	VAL	HG21	0.699	0.020	2
1	A	52	VAL	HG22	0.699	0.020	2
1	A	52	VAL	HG23	0.699	0.020	2
1	A	52	VAL	CA	60.313	0.3	1
1	A	52	VAL	CB	36.821	0.3	1
1	A	52	VAL	CG1	21.069	0.3	1
1	A	52	VAL	CG2	20.768	0.3	1
1	A	52	VAL	N	119.449	0.3	1
1	A	55	VAL	H	9.153	0.020	1
1	A	55	VAL	HA	4.567	0.020	1
1	A	55	VAL	HB	2.091	0.020	1
1	A	55	VAL	HG11	0.852	0.020	2
1	A	55	VAL	HG12	0.852	0.020	2
1	A	55	VAL	HG13	0.852	0.020	2
1	A	55	VAL	HG21	0.404	0.020	2
1	A	55	VAL	HG22	0.404	0.020	2
1	A	55	VAL	HG23	0.404	0.020	2
1	A	55	VAL	CA	64.786	0.3	1
1	A	55	VAL	CB	31.31	0.3	1
1	A	55	VAL	CG1	20.765	0.3	1
1	A	55	VAL	CG2	21.259	0.3	1
1	A	55	VAL	N	128.74	0.3	1
1	A	56	LEU	H	9.147	0.020	1
1	A	56	LEU	HA	5.284	0.020	1
1	A	56	LEU	HB2	1.215	0.020	2
1	A	56	LEU	HB3	2.1	0.020	2
1	A	56	LEU	HD11	1.086	0.020	2
1	A	56	LEU	HD12	1.086	0.020	2
1	A	56	LEU	HD13	1.086	0.020	2
1	A	56	LEU	HD21	0.859	0.020	2
1	A	56	LEU	HD22	0.859	0.020	2
1	A	56	LEU	HD23	0.859	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	56	LEU	HG	1.103	0.020	1
1	A	56	LEU	CA	52.378	0.3	1
1	A	56	LEU	CB	43.881	0.3	1
1	A	56	LEU	CD1	21.474	0.3	1
1	A	56	LEU	CD2	23.039	0.3	1
1	A	56	LEU	CG	26.651	0.3	1
1	A	56	LEU	N	128.711	0.3	1
1	A	57	TYR	H	8.798	0.020	1
1	A	57	TYR	HA	4.62	0.020	1
1	A	57	TYR	HB2	2.876	0.020	2
1	A	57	TYR	HB3	3.204	0.020	2
1	A	57	TYR	HD1	7.196	0.020	3
1	A	57	TYR	HD2	7.2	0.020	3
1	A	57	TYR	HE1	6.699	0.020	3
1	A	57	TYR	HE2	6.686	0.020	3
1	A	57	TYR	CA	59.567	0.3	1
1	A	57	TYR	CB	38.749	0.3	1
1	A	57	TYR	CD1	132.748	0.3	1
1	A	57	TYR	CE1	117.889	0.3	1
1	A	57	TYR	N	127.11	0.3	1
1	A	58	ARG	H	7.972	0.020	1
1	A	58	ARG	HA	5.192	0.020	1
1	A	58	ARG	HB2	1.996	0.020	2
1	A	58	ARG	HB3	1.561	0.020	2
1	A	58	ARG	HD2	3.066	0.020	2
1	A	58	ARG	HD3	3.214	0.020	2
1	A	58	ARG	HG2	1.55	0.020	2
1	A	58	ARG	HG3	1.496	0.020	2
1	A	58	ARG	CA	55.292	0.3	1
1	A	58	ARG	CB	32.14	0.3	1
1	A	58	ARG	CD	43.206	0.3	1
1	A	58	ARG	CG	26.557	0.3	1
1	A	58	ARG	N	121.601	0.3	1
1	A	59	SER	H	8.632	0.020	1
1	A	59	SER	HA	4.649	0.020	1
1	A	59	SER	HB2	3.943	0.020	2
1	A	59	SER	HB3	4.089	0.020	2
1	A	59	SER	CA	57.465	0.3	1
1	A	59	SER	CB	64.51	0.3	1
1	A	59	SER	N	117.74	0.3	1
1	A	60	ALA	H	8.746	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	ALA	HA	4.31	0.020	1
1	A	60	ALA	HB1	1.469	0.020	1
1	A	60	ALA	HB2	1.469	0.020	1
1	A	60	ALA	HB3	1.469	0.020	1
1	A	60	ALA	CA	53.654	0.3	1
1	A	60	ALA	CB	18.577	0.3	1
1	A	60	ALA	N	126.998	0.3	1
1	A	61	LYS	H	8.239	0.020	1
1	A	61	LYS	HA	4.307	0.020	1
1	A	61	LYS	HB2	1.772	0.020	2
1	A	61	LYS	HB3	1.93	0.020	2
1	A	61	LYS	HD2	1.694	0.020	2
1	A	61	LYS	HD3	1.701	0.020	2
1	A	61	LYS	HE2	3.03	0.020	2
1	A	61	LYS	HE3	3.059	0.020	2
1	A	61	LYS	HG2	1.419	0.020	2
1	A	61	LYS	HG3	1.472	0.020	2
1	A	61	LYS	CA	56.343	0.3	1
1	A	61	LYS	CB	32.445	0.3	1
1	A	61	LYS	CD	29.221	0.3	1
1	A	61	LYS	CE	42.301	0.3	1
1	A	61	LYS	CG	24.722	0.3	1
1	A	61	LYS	N	117.536	0.3	1
1	A	62	GLY	H	8.073	0.020	1
1	A	62	GLY	HA2	4.012	0.020	2
1	A	62	GLY	HA3	3.983	0.020	2
1	A	62	GLY	CA	45.203	0.3	1
1	A	62	GLY	N	108.5	0.3	1
1	A	63	GLY	H	8.165	0.020	1
1	A	63	GLY	HA2	3.954	0.020	2
1	A	63	GLY	HA3	4.046	0.020	2
1	A	63	GLY	CA	44.477	0.3	1
1	A	63	GLY	N	108.45	0.3	1
1	A	64	GLU	H	8.523	0.020	1
1	A	64	GLU	HA	4.504	0.020	1
1	A	64	GLU	HB2	1.882	0.020	2
1	A	64	GLU	HB3	2.011	0.020	2
1	A	64	GLU	HG2	2.294	0.020	2
1	A	64	GLU	HG3	2.305	0.020	2
1	A	64	GLU	CA	54.22	0.3	1
1	A	64	GLU	CB	29.402	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	GLU	CG	35.744	0.3	1
1	A	64	GLU	N	122.301	0.3	1
1	A	65	PRO	HA	4.444	0.020	1
1	A	65	PRO	HB2	2.157	0.020	2
1	A	65	PRO	HB3	1.808	0.020	2
1	A	65	PRO	HD2	3.798	0.020	2
1	A	65	PRO	HD3	3.7	0.020	2
1	A	65	PRO	HG2	1.93	0.020	2
1	A	65	PRO	HG3	1.873	0.020	2
1	A	65	PRO	CA	62.519	0.3	1
1	A	65	PRO	CB	31.845	0.3	1
1	A	65	PRO	CD	50.395	0.3	1
1	A	65	PRO	CG	26.957	0.3	1
1	A	66	VAL	H	8.283	0.020	1
1	A	66	VAL	HA	3.834	0.020	1
1	A	66	VAL	HB	1.809	0.020	1
1	A	66	VAL	HG11	0.625	0.020	2
1	A	66	VAL	HG12	0.625	0.020	2
1	A	66	VAL	HG13	0.625	0.020	2
1	A	66	VAL	HG21	0.887	0.020	2
1	A	66	VAL	HG22	0.887	0.020	2
1	A	66	VAL	HG23	0.887	0.020	2
1	A	66	VAL	CA	62.384	0.3	1
1	A	66	VAL	CB	31.803	0.3	1
1	A	66	VAL	CG1	20.753	0.3	1
1	A	66	VAL	CG2	20.986	0.3	1
1	A	66	VAL	N	122.281	0.3	1
1	A	67	LEU	H	8.282	0.020	1
1	A	67	LEU	HA	4.374	0.020	1
1	A	67	LEU	HB2	1.451	0.020	2
1	A	67	LEU	HB3	1.439	0.020	2
1	A	67	LEU	HD11	0.752	0.020	2
1	A	67	LEU	HD12	0.752	0.020	2
1	A	67	LEU	HD13	0.752	0.020	2
1	A	67	LEU	HD21	0.864	0.020	2
1	A	67	LEU	HD22	0.864	0.020	2
1	A	67	LEU	HD23	0.864	0.020	2
1	A	67	LEU	HG	1.568	0.020	1
1	A	67	LEU	CA	54.085	0.3	1
1	A	67	LEU	CB	42.611	0.3	1
1	A	67	LEU	CD1	23.948	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	67	LEU	CD2	25.073	0.3	1
1	A	67	LEU	CG	26.521	0.3	1
1	A	67	LEU	N	128.288	0.3	1
1	A	68	TYR	H	7.812	0.020	1
1	A	68	TYR	HA	4.686	0.020	1
1	A	68	TYR	HB2	2.396	0.020	2
1	A	68	TYR	HB3	3.602	0.020	2
1	A	68	TYR	HD1	6.783	0.020	1
1	A	68	TYR	HE1	6.616	0.020	1
1	A	68	TYR	CA	58.403	0.3	1
1	A	68	TYR	CB	38.293	0.3	1
1	A	68	TYR	CD1	132.751	0.3	1
1	A	68	TYR	CE1	117.709	0.3	1
1	A	68	TYR	N	122.904	0.3	1
1	A	69	ARG	H	9.067	0.020	1
1	A	69	ARG	HA	4.782	0.020	1
1	A	69	ARG	HB2	1.834	0.020	2
1	A	69	ARG	HB3	1.816	0.020	2
1	A	69	ARG	HD2	3.274	0.020	2
1	A	69	ARG	HD3	3.28	0.020	2
1	A	69	ARG	HG2	1.711	0.020	2
1	A	69	ARG	HG3	1.685	0.020	2
1	A	69	ARG	CA	53.939	0.3	1
1	A	69	ARG	CB	34.623	0.3	1
1	A	69	ARG	CD	43.374	0.3	1
1	A	69	ARG	CG	26.6	0.3	1
1	A	69	ARG	N	117.52	0.3	1
1	A	70	TYR	H	8.652	0.020	1
1	A	70	TYR	HA	3.773	0.020	1
1	A	70	TYR	HB2	2.813	0.020	2
1	A	70	TYR	HB3	2.875	0.020	2
1	A	70	TYR	HD1	6.808	0.020	3
1	A	70	TYR	HD2	6.788	0.020	3
1	A	70	TYR	HE1	6.846	0.020	3
1	A	70	TYR	HE2	7.143	0.020	3
1	A	70	TYR	CA	59.964	0.3	1
1	A	70	TYR	CB	38.748	0.3	1
1	A	70	TYR	CD1	132.762	0.3	1
1	A	70	TYR	CE1	118.02	0.3	1
1	A	70	TYR	N	119.656	0.3	1
1	A	71	GLY	H	8.76	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	GLY	HA2	3.082	0.020	2
1	A	71	GLY	HA3	4.214	0.020	2
1	A	71	GLY	CA	44.691	0.3	1
1	A	71	GLY	N	117.906	0.3	1
1	A	72	ASP	H	8.387	0.020	1
1	A	72	ASP	HA	4.792	0.020	1
1	A	72	ASP	HB2	2.225	0.020	2
1	A	72	ASP	HB3	2.941	0.020	2
1	A	72	ASP	CA	55.585	0.3	1
1	A	72	ASP	CB	40.77	0.3	1
1	A	72	ASP	N	121.655	0.3	1
1	A	73	VAL	H	8.721	0.020	1
1	A	73	VAL	HA	4.335	0.020	1
1	A	73	VAL	HB	1.68	0.020	1
1	A	73	VAL	HG11	0.817	0.020	2
1	A	73	VAL	HG12	0.817	0.020	2
1	A	73	VAL	HG13	0.817	0.020	2
1	A	73	VAL	HG21	0.672	0.020	2
1	A	73	VAL	HG22	0.672	0.020	2
1	A	73	VAL	HG23	0.672	0.020	2
1	A	73	VAL	CA	61.567	0.3	1
1	A	73	VAL	CB	31.267	0.3	1
1	A	73	VAL	CG1	20.66	0.3	1
1	A	73	VAL	CG2	21.227	0.3	1
1	A	73	VAL	N	122.842	0.3	1
1	A	74	LEU	H	8.94	0.020	1
1	A	74	LEU	HA	5.1	0.020	1
1	A	74	LEU	HB2	0.829	0.020	2
1	A	74	LEU	HB3	1.279	0.020	2
1	A	74	LEU	HD11	-0.015	0.020	2
1	A	74	LEU	HD12	-0.015	0.020	2
1	A	74	LEU	HD13	-0.015	0.020	2
1	A	74	LEU	HD21	-0.124	0.020	2
1	A	74	LEU	HD22	-0.124	0.020	2
1	A	74	LEU	HD23	-0.124	0.020	2
1	A	74	LEU	HG	1.219	0.020	1
1	A	74	LEU	CA	52.201	0.3	1
1	A	74	LEU	CB	44.633	0.3	1
1	A	74	LEU	CD1	23.967	0.3	1
1	A	74	LEU	CD2	20.958	0.3	1
1	A	74	LEU	CG	25.946	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	LEU	N	126.214	0.3	1
1	A	75	ARG	H	9.029	0.020	1
1	A	75	ARG	HA	5.3	0.020	1
1	A	75	ARG	HB2	1.492	0.020	2
1	A	75	ARG	HB3	1.743	0.020	2
1	A	75	ARG	HD2	3.086	0.020	2
1	A	75	ARG	HD3	3.077	0.020	2
1	A	75	ARG	HE	9.243	0.020	1
1	A	75	ARG	HG2	1.291	0.020	2
1	A	75	ARG	HG3	1.307	0.020	2
1	A	75	ARG	CA	54.445	0.3	1
1	A	75	ARG	CB	32.556	0.3	1
1	A	75	ARG	CD	43.621	0.3	1
1	A	75	ARG	CG	26.963	0.3	1
1	A	75	ARG	N	121.504	0.3	1
1	A	76	VAL	H	9.756	0.020	1
1	A	76	VAL	HA	4.872	0.020	1
1	A	76	VAL	HB	1.968	0.020	1
1	A	76	VAL	HG11	0.883	0.020	2
1	A	76	VAL	HG12	0.883	0.020	2
1	A	76	VAL	HG13	0.883	0.020	2
1	A	76	VAL	HG21	0.76	0.020	2
1	A	76	VAL	HG22	0.76	0.020	2
1	A	76	VAL	HG23	0.76	0.020	2
1	A	76	VAL	CA	60.344	0.3	1
1	A	76	VAL	CB	34.21	0.3	1
1	A	76	VAL	CG1	21.849	0.3	1
1	A	76	VAL	CG2	20.565	0.3	1
1	A	76	VAL	N	128.82	0.3	1
1	A	77	HIS	H	8.907	0.020	1
1	A	77	HIS	HA	5.858	0.020	1
1	A	77	HIS	HB2	3.139	0.020	2
1	A	77	HIS	HB3	2.996	0.020	2
1	A	77	HIS	HD2	7.019	0.020	1
1	A	77	HIS	HE1	7.689	0.020	1
1	A	77	HIS	CA	54.337	0.3	1
1	A	77	HIS	CB	30.92	0.3	1
1	A	77	HIS	CD2	122.785	0.3	1
1	A	77	HIS	CE1	137.369	0.3	1
1	A	77	HIS	N	127.788	0.3	1
1	A	78	GLY	H	8.608	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	78	GLY	HA2	3.975	0.020	2
1	A	78	GLY	HA3	3.976	0.020	2
1	A	78	GLY	CA	46.098	0.3	1
1	A	78	GLY	N	111.595	0.3	1
1	A	79	GLN	H	8.331	0.020	1
1	A	79	GLN	HA	4.704	0.020	1
1	A	79	GLN	HB2	1.562	0.020	2
1	A	79	GLN	HB3	1.42	0.020	2
1	A	79	GLN	HG2	1.437	0.020	2
1	A	79	GLN	HG3	1.409	0.020	2
1	A	79	GLN	CA	53.493	0.3	1
1	A	79	GLN	CB	31.452	0.3	1
1	A	79	GLN	CG	33.162	0.3	1
1	A	79	GLN	N	117.944	0.3	1
1	A	89	PRO	HA	4.311	0.020	1
1	A	89	PRO	HB2	2.18	0.020	2
1	A	89	PRO	HB3	2.558	0.020	2
1	A	89	PRO	HD2	4.076	0.020	2
1	A	89	PRO	HD3	4.079	0.020	2
1	A	89	PRO	HG2	2.164	0.020	2
1	A	89	PRO	HG3	2.089	0.020	2
1	A	89	PRO	CA	64.964	0.3	1
1	A	89	PRO	CB	32.416	0.3	1
1	A	89	PRO	CD	51.015	0.3	1
1	A	89	PRO	CG	27.322	0.3	1
1	A	90	GLY	H	9.172	0.020	1
1	A	90	GLY	HA2	3.949	0.020	2
1	A	90	GLY	HA3	4.025	0.020	2
1	A	90	GLY	CA	47.514	0.3	1
1	A	90	GLY	N	117.571	0.3	1
1	A	91	GLU	H	8.95	0.020	1
1	A	91	GLU	HA	4.236	0.020	1
1	A	91	GLU	HB2	1.87	0.020	2
1	A	91	GLU	HB3	1.971	0.020	2
1	A	91	GLU	HG2	2.253	0.020	2
1	A	91	GLU	HG3	2.269	0.020	2
1	A	91	GLU	CA	54.829	0.3	1
1	A	91	GLU	CB	41.215	0.3	1
1	A	91	GLU	CG	35.98	0.3	1
1	A	91	GLU	N	126.897	0.3	1
1	A	92	LEU	H	8.143	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	92	LEU	HA	4.571	0.020	1
1	A	92	LEU	HB2	1.58	0.020	2
1	A	92	LEU	HB3	1.465	0.020	2
1	A	92	LEU	HD11	0.75	0.020	2
1	A	92	LEU	HD12	0.75	0.020	2
1	A	92	LEU	HD13	0.75	0.020	2
1	A	92	LEU	HD21	0.699	0.020	2
1	A	92	LEU	HD22	0.699	0.020	2
1	A	92	LEU	HD23	0.699	0.020	2
1	A	92	LEU	HG	1.447	0.020	1
1	A	92	LEU	CA	57.632	0.3	1
1	A	92	LEU	CB	39.184	0.3	1
1	A	92	LEU	CD1	23.662	0.3	1
1	A	92	LEU	CD2	24.717	0.3	1
1	A	92	LEU	CG	27.768	0.3	1
1	A	92	LEU	N	122.034	0.3	1
1	A	93	ASP	H	8.147	0.020	1
1	A	93	ASP	HA	4.358	0.020	1
1	A	93	ASP	HB2	1.695	0.020	2
1	A	93	ASP	HB3	1.925	0.020	2
1	A	93	ASP	HD2	3.258	0.020	1
1	A	93	ASP	CA	56.29	0.3	1
1	A	93	ASP	CB	30.949	0.3	1
1	A	93	ASP	CG	27.699	0.3	1
1	A	93	ASP	N	126.259	0.3	1
1	A	107	MET	H	8.803	0.020	1
1	A	107	MET	HA	4.547	0.020	1
1	A	107	MET	HB2	1.936	0.020	2
1	A	107	MET	HB3	1.778	0.020	2
1	A	107	MET	HE1	1.66	0.020	1
1	A	107	MET	HE2	1.66	0.020	1
1	A	107	MET	HE3	1.66	0.020	1
1	A	107	MET	HG2	2.252	0.020	2
1	A	107	MET	HG3	2.224	0.020	2
1	A	107	MET	CA	54.46	0.3	1
1	A	107	MET	CB	36.87	0.3	1
1	A	107	MET	CE	16.744	0.3	1
1	A	107	MET	CG	32.174	0.3	1
1	A	107	MET	N	119.67	0.3	1
1	A	108	LEU	H	9.223	0.020	1
1	A	108	LEU	HA	4.98	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	LEU	HB2	1.909	0.020	2
1	A	108	LEU	HB3	1.594	0.020	2
1	A	108	LEU	HD11	0.927	0.020	2
1	A	108	LEU	HD12	0.927	0.020	2
1	A	108	LEU	HD13	0.927	0.020	2
1	A	108	LEU	HD21	0.861	0.020	2
1	A	108	LEU	HD22	0.861	0.020	2
1	A	108	LEU	HD23	0.861	0.020	2
1	A	108	LEU	HG	1.707	0.020	1
1	A	108	LEU	CA	54.336	0.3	1
1	A	108	LEU	CB	41.45	0.3	1
1	A	108	LEU	CD1	24.735	0.3	1
1	A	108	LEU	CD2	23.322	0.3	1
1	A	108	LEU	CG	27.458	0.3	1
1	A	108	LEU	N	126.295	0.3	1
1	A	109	ILE	H	9.541	0.020	1
1	A	109	ILE	HA	4.758	0.020	1
1	A	109	ILE	HB	2.222	0.020	1
1	A	109	ILE	HD11	0.826	0.020	1
1	A	109	ILE	HD12	0.826	0.020	1
1	A	109	ILE	HD13	0.826	0.020	1
1	A	109	ILE	HG12	1.413	0.020	2
1	A	109	ILE	HG13	1.221	0.020	2
1	A	109	ILE	HG21	1.082	0.020	1
1	A	109	ILE	HG22	1.082	0.020	1
1	A	109	ILE	HG23	1.082	0.020	1
1	A	109	ILE	CA	58.61	0.3	1
1	A	109	ILE	CB	39.222	0.3	1
1	A	109	ILE	CD1	11.708	0.3	1
1	A	109	ILE	CG1	26.698	0.3	1
1	A	109	ILE	CG2	19.53	0.3	1
1	A	109	ILE	N	125.04	0.3	1
1	A	112	PRO	HA	4.3	0.020	1
1	A	112	PRO	HB2	2.158	0.020	2
1	A	112	PRO	HB3	2.545	0.020	2
1	A	112	PRO	HD2	4.03	0.020	2
1	A	112	PRO	HD3	4.071	0.020	2
1	A	112	PRO	HG2	1.805	0.020	2
1	A	112	PRO	HG3	2.127	0.020	2
1	A	112	PRO	CA	64.684	0.3	1
1	A	112	PRO	CB	32.238	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	112	PRO	CD	51.156	0.3	1
1	A	112	PRO	CG	27.556	0.3	1
1	A	113	ARG	H	8.024	0.020	1
1	A	113	ARG	HA	4.365	0.020	1
1	A	113	ARG	HB2	1.986	0.020	2
1	A	113	ARG	HB3	1.809	0.020	2
1	A	113	ARG	HD2	3.273	0.020	2
1	A	113	ARG	HD3	3.265	0.020	2
1	A	113	ARG	HG2	1.72	0.020	2
1	A	113	ARG	HG3	1.761	0.020	2
1	A	113	ARG	CA	56.917	0.3	1
1	A	113	ARG	CB	29.088	0.3	1
1	A	113	ARG	CD	43.037	0.3	1
1	A	113	ARG	CG	27.535	0.3	1
1	A	113	ARG	N	115.034	0.3	1
1	A	114	ALA	H	8.019	0.020	1
1	A	114	ALA	HA	4.43	0.020	1
1	A	114	ALA	HB1	2.029	0.020	1
1	A	114	ALA	HB2	2.029	0.020	1
1	A	114	ALA	HB3	2.029	0.020	1
1	A	114	ALA	CA	53.167	0.3	1
1	A	114	ALA	CB	19.102	0.3	1
1	A	114	ALA	N	121.002	0.3	1
1	A	115	ILE	H	7.57	0.020	1
1	A	115	ILE	HA	4.795	0.020	1
1	A	115	ILE	HB	1.93	0.020	1
1	A	115	ILE	HD11	0.908	0.020	1
1	A	115	ILE	HD12	0.908	0.020	1
1	A	115	ILE	HD13	0.908	0.020	1
1	A	115	ILE	HG12	1.667	0.020	2
1	A	115	ILE	HG13	1.684	0.020	2
1	A	115	ILE	HG21	0.582	0.020	1
1	A	115	ILE	HG22	0.582	0.020	1
1	A	115	ILE	HG23	0.582	0.020	1
1	A	115	ILE	CA	60.654	0.3	1
1	A	115	ILE	CB	39.985	0.3	1
1	A	115	ILE	CD1	14.258	0.3	1
1	A	115	ILE	CG1	27.558	0.3	1
1	A	115	ILE	CG2	19.336	0.3	1
1	A	115	ILE	N	117.917	0.3	1
1	A	116	VAL	H	8.653	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	VAL	HA	4.39	0.020	1
1	A	116	VAL	HB	1.915	0.020	1
1	A	116	VAL	HG11	0.898	0.020	2
1	A	116	VAL	HG12	0.898	0.020	2
1	A	116	VAL	HG13	0.898	0.020	2
1	A	116	VAL	HG21	0.861	0.020	2
1	A	116	VAL	HG22	0.861	0.020	2
1	A	116	VAL	HG23	0.861	0.020	2
1	A	116	VAL	CA	59.891	0.3	1
1	A	116	VAL	CB	35.561	0.3	1
1	A	116	VAL	CG1	20.763	0.3	1
1	A	116	VAL	CG2	20.787	0.3	1
1	A	116	VAL	N	123.8	0.3	1
1	A	117	LYS	H	8.567	0.020	1
1	A	117	LYS	HA	4.703	0.020	1
1	A	117	LYS	HB2	1.49	0.020	2
1	A	117	LYS	HB3	1.875	0.020	2
1	A	117	LYS	HD2	1.705	0.020	2
1	A	117	LYS	HD3	1.73	0.020	2
1	A	117	LYS	HE2	2.894	0.020	2
1	A	117	LYS	HE3	2.895	0.020	2
1	A	117	LYS	HG2	1.466	0.020	2
1	A	117	LYS	HG3	1.167	0.020	2
1	A	117	LYS	CA	55.43	0.3	1
1	A	117	LYS	CB	33.433	0.3	1
1	A	117	LYS	CD	29.862	0.3	1
1	A	117	LYS	CE	41.954	0.3	1
1	A	117	LYS	CG	25.931	0.3	1
1	A	117	LYS	N	125.812	0.3	1
1	A	118	LEU	H	9.25	0.020	1
1	A	118	LEU	HA	4.399	0.020	1
1	A	118	LEU	HB2	1.386	0.020	2
1	A	118	LEU	HB3	1.512	0.020	2
1	A	118	LEU	HD11	0.782	0.020	2
1	A	118	LEU	HD12	0.782	0.020	2
1	A	118	LEU	HD13	0.782	0.020	2
1	A	118	LEU	HD21	0.707	0.020	2
1	A	118	LEU	HD22	0.707	0.020	2
1	A	118	LEU	HD23	0.707	0.020	2
1	A	118	LEU	HG	1.509	0.020	1
1	A	118	LEU	CA	54.583	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	118	LEU	CB	42.616	0.3	1
1	A	118	LEU	CD1	25.994	0.3	1
1	A	118	LEU	CD2	21.961	0.3	1
1	A	118	LEU	CG	26.226	0.3	1
1	A	118	LEU	N	128.211	0.3	1
1	A	119	GLY	H	7.577	0.020	1
1	A	119	GLY	HA2	4.03	0.020	2
1	A	119	GLY	HA3	4.263	0.020	2
1	A	119	GLY	CA	44.813	0.3	1
1	A	119	GLY	N	106.164	0.3	1
1	A	120	THR	H	8.388	0.020	1
1	A	120	THR	HA	5.055	0.020	1
1	A	120	THR	HB	4.038	0.020	1
1	A	120	THR	HG21	1.24	0.020	1
1	A	120	THR	HG22	1.24	0.020	1
1	A	120	THR	HG23	1.24	0.020	1
1	A	120	THR	CA	60.73	0.3	1
1	A	120	THR	CB	71.567	0.3	1
1	A	120	THR	CG2	21.632	0.3	1
1	A	120	THR	N	113.721	0.3	1
1	A	121	GLU	H	9.038	0.020	1
1	A	121	GLU	HA	4.728	0.020	1
1	A	121	GLU	HB2	1.779	0.020	2
1	A	121	GLU	HB3	1.956	0.020	2
1	A	121	GLU	HG2	2.211	0.020	2
1	A	121	GLU	HG3	2.21	0.020	2
1	A	121	GLU	CA	53.784	0.3	1
1	A	121	GLU	CB	30.503	0.3	1
1	A	121	GLU	CG	35.945	0.3	1
1	A	121	GLU	N	126.031	0.3	1
1	A	122	PRO	HA	4.446	0.020	1
1	A	122	PRO	HB2	1.937	0.020	2
1	A	122	PRO	HB3	2.297	0.020	2
1	A	122	PRO	HD2	3.809	0.020	2
1	A	122	PRO	HD3	3.7	0.020	2
1	A	122	PRO	HG2	2.038	0.020	2
1	A	122	PRO	HG3	2.009	0.020	2
1	A	122	PRO	CA	63.205	0.3	1
1	A	122	PRO	CB	32.046	0.3	1
1	A	122	PRO	CD	50.2	0.3	1
1	A	122	PRO	CG	27.074	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	123	GLY	H	8.484	0.020	1
1	A	123	GLY	HA2	3.87	0.020	2
1	A	123	GLY	HA3	3.928	0.020	2
1	A	123	GLY	CA	45.232	0.3	1
1	A	123	GLY	N	108.906	0.3	1
1	A	124	HIS	H	7.831	0.020	1
1	A	124	HIS	HA	4.447	0.020	1
1	A	124	HIS	HB2	3.054	0.020	2
1	A	124	HIS	HB3	3.173	0.020	2
1	A	124	HIS	HD2	6.96	0.020	1
1	A	124	HIS	CA	57.24	0.3	1
1	A	124	HIS	CB	30.619	0.3	1
1	A	124	HIS	CD2	120.658	0.3	1
1	A	124	HIS	N	123.926	0.3	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	57	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	48	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	53	0.00 \pm 0.00	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 891. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/295 (0%)	0/119 (0%)	0/120 (0%)	0/56 (0%)
Sidechain	0/544 (0%)	0/355 (0%)	0/163 (0%)	0/26 (0%)
Aromatic	0/52 (0%)	0/24 (0%)	0/27 (0%)	0/1 (0%)
Overall	0/891 (0%)	0/498 (0%)	0/310 (0%)	0/83 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

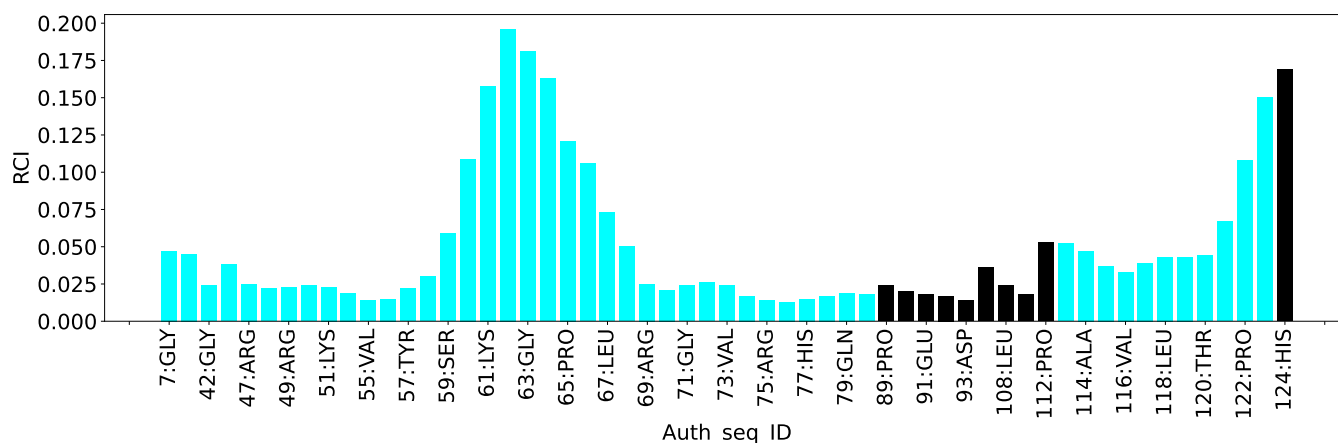
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	93	ASP	CG	27.70	149.18 – 208.82	-25.4
1	A	91	GLU	CB	41.22	21.56 – 38.37	6.7
1	A	93	ASP	CB	30.95	32.98 – 48.76	-6.3

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis [i](#)

8.1 Conformationally restricting restraints [i](#)

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	2070
Intra-residue ($ i-j =0$)	368
Sequential ($ i-j =1$)	501
Medium range ($ i-j >1$ and $ i-j <5$)	212
Long range ($ i-j \geq 5$)	989
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	2070
Number of restraints per residue	16.7
Number of long range restraints per residue ¹	8.0

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

8.2 Residual restraint violations [i](#)

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 [i](#)

Distance violations less than 0.1 Å are not included in the calculation. There are no distance violations

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 ⓘ

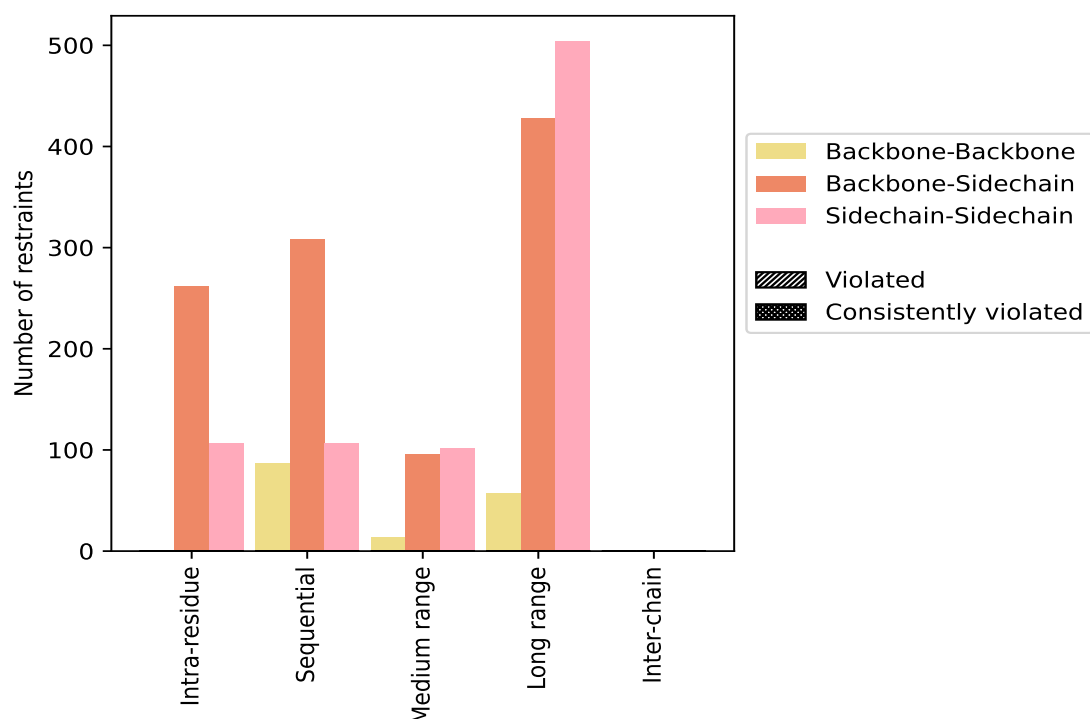
9.1 Summary of distance violations ⓘ

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)	368	17.8	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	262	12.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	106	5.1	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	501	24.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	87	4.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	308	14.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	106	5.1	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	212	10.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	14	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	96	4.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	102	4.9	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	989	47.8	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	57	2.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	428	20.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	504	24.3	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	0	0.0	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	2070	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	158	7.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1094	52.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	818	39.5	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 [i](#)



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

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

No violations found

9.3 Distance violation statistics for the ensemble [i](#)

No violations found

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

No violations found

9.5 All violated distance restraints [i](#)

No violations found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found