



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2MFL  
BMRB ID : 19554  
Title : Domain 2 of E. coli ribosomal protein S1  
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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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>.

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

MolProbity : 4.02b-467  
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) : 2.40

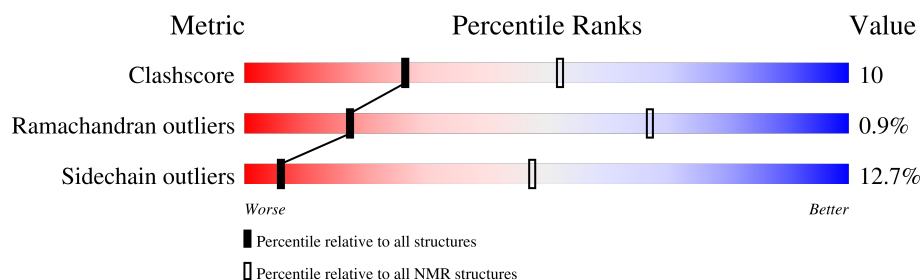
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 77%.

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  $\geq 3$ , 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	182	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 10 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:88-A:179 (92)	1.88	10

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 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1495 atoms, of which 759 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					Trace
1	A	93	Total	C	H	N	O	0
			1495	463	759	134	139	

There are 3 discrepancies between the modelled and reference sequences:

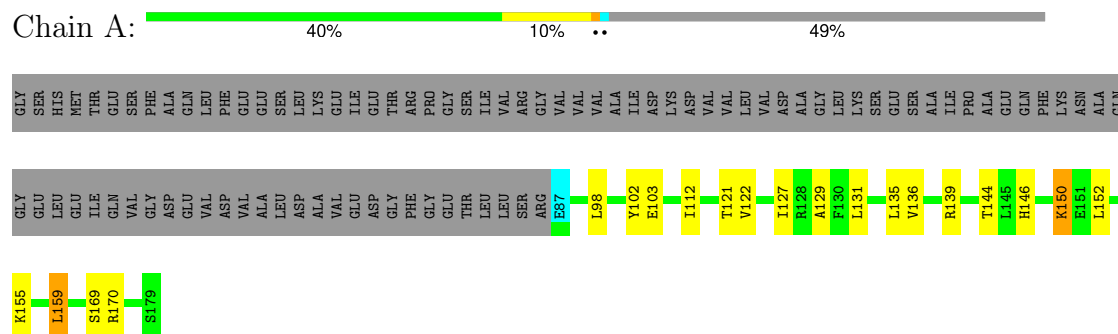
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP C9QZU1
A	-1	SER	-	expression tag	UNP C9QZU1
A	0	HIS	-	expression tag	UNP C9QZU1

## 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.

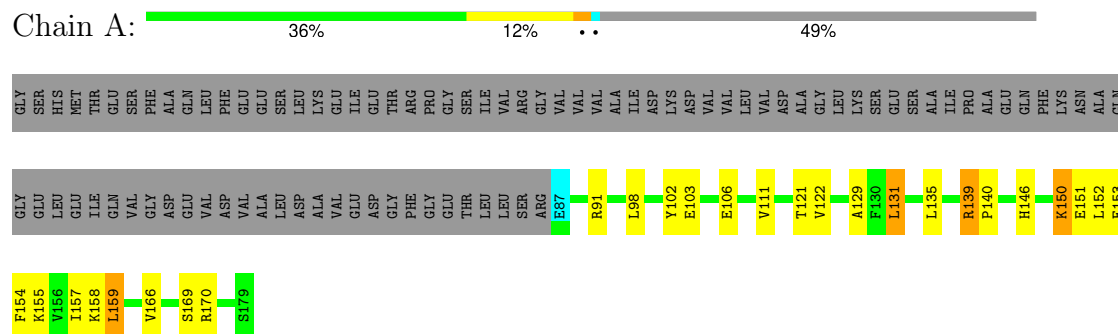
- Molecule 1: 30S ribosomal protein S1



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

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: 30S ribosomal protein S1



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 20 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
TopSpin	structure calculation	3.1
TopSpin	structure calculation	3.1
TopSpin	structure calculation	3.1
TopSpin	structure calculation	3.1
CYANA	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	1930
Number of shifts mapped to atoms	1002
Number of unparsed shifts	0
Number of shifts with mapping errors	928
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

## 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	727	753	753	14±4
All	All	7270	7530	7530	145

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 10.

5 of 108 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:VAL:HG21	1:A:124:LEU:HD13	0.63	1.70	3	1
1:A:120:PHE:CE2	1:A:136:VAL:HG11	0.63	2.28	8	1
1:A:152:LEU:HD22	1:A:176:SER:CB	0.63	2.23	6	1
1:A:152:LEU:C	1:A:152:LEU:HD22	0.63	2.13	8	1
1:A:102:TYR:CG	1:A:159:LEU:HD21	0.62	2.29	10	2

### 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	91/182 (50%)	81±1 (89±2%)	9±2 (10±2%)	1±1 (1±1%)	17	67
All	All	910/1820 (50%)	812 (89%)	90 (10%)	8 (1%)	17	67

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	138	VAL	2
1	A	112	ILE	2
1	A	178	ASN	1
1	A	117	LYS	1
1	A	142	ARG	1

### 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	79/153 (52%)	69±2 (87±2%)	10±2 (13±2%)	6	47
All	All	790/1530 (52%)	690 (87%)	100 (13%)	6	47

5 of 39 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	103	GLU	7
1	A	121	THR	7
1	A	150	LYS	7
1	A	159	LEU	7
1	A	139	ARG	6

### 6.3.3 RNA ⓘ

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 77% for the well-defined parts and 77% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list*

#### 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	1930
Number of shifts mapped to atoms	1002
Number of unparsed shifts	0
Number of shifts with mapping errors	928
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 928) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	0	HIS	H	8.33	0.02	1
1	A	0	HIS	HA	4.12	0.02	1
1	A	0	HIS	C	175.98	0.25	1
1	A	0	HIS	N	121.49	0.15	1
1	A	1	MET	H	8.52	0.02	1
1	A	1	MET	HA	4.38	0.02	1
1	A	1	MET	HB2	1.88	0.02	2
1	A	1	MET	HB3	1.97	0.02	2
1	A	1	MET	HG2	2.36	0.02	2
1	A	1	MET	HG3	2.42	0.02	2
1	A	1	MET	HE1	1.95	0.02	1
1	A	1	MET	HE2	1.95	0.02	1
1	A	1	MET	HE3	1.95	0.02	1
1	A	1	MET	C	176.27	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	CA	55.57	0.25	1
1	A	1	MET	CB	32.69	0.25	1
1	A	1	MET	CG	31.79	0.25	1
1	A	1	MET	CE	16.82	0.25	1
1	A	1	MET	N	124.69	0.15	1
1	A	2	THR	H	8.1	0.02	1
1	A	2	THR	HA	4.18	0.02	1
1	A	2	THR	HB	4.14	0.02	1
1	A	2	THR	HG21	1.09	0.02	1
1	A	2	THR	HG22	1.09	0.02	1
1	A	2	THR	HG23	1.09	0.02	1
1	A	2	THR	C	174.68	0.25	1
1	A	2	THR	CA	61.95	0.25	1
1	A	2	THR	CB	69.52	0.25	1
1	A	2	THR	CG2	21.57	0.25	1
1	A	2	THR	N	115.24	0.15	1
1	A	3	GLU	H	8.38	0.02	1
1	A	3	GLU	HA	4.14	0.02	1
1	A	3	GLU	HB2	1.82	0.02	2
1	A	3	GLU	HB3	1.94	0.02	2
1	A	3	GLU	HG2	2.11	0.02	1
1	A	3	GLU	HG3	2.11	0.02	1
1	A	3	GLU	C	176.58	0.25	1
1	A	3	GLU	CA	56.6	0.25	1
1	A	3	GLU	CB	30.04	0.25	1
1	A	3	GLU	CG	36.31	0.25	1
1	A	3	GLU	N	123.19	0.15	1
1	A	4	SER	H	8.18	0.02	1
1	A	4	SER	HA	4.39	0.02	1
1	A	4	SER	HB2	3.71	0.02	2
1	A	4	SER	HB3	3.67	0.02	2
1	A	4	SER	C	174.58	0.25	1
1	A	4	SER	CA	58.05	0.25	1
1	A	4	SER	CB	63.72	0.25	1
1	A	4	SER	N	116.25	0.15	1
1	A	5	PHE	H	8.12	0.02	1
1	A	5	PHE	HA	4.43	0.02	1
1	A	5	PHE	HB2	3.05	0.02	2
1	A	5	PHE	HB3	2.94	0.02	2
1	A	5	PHE	HD1	7.13	0.02	3
1	A	5	PHE	HD2	7.13	0.02	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	PHE	HE1	7.2	0.02	3
1	A	5	PHE	HE2	7.2	0.02	3
1	A	5	PHE	C	175.83	0.25	1
1	A	5	PHE	CA	58.22	0.25	1
1	A	5	PHE	CB	39.12	0.25	1
1	A	5	PHE	N	122.11	0.15	1
1	A	6	ALA	H	8.07	0.02	1
1	A	6	ALA	HA	4.09	0.02	1
1	A	6	ALA	HB1	1.25	0.02	1
1	A	6	ALA	HB2	1.25	0.02	1
1	A	6	ALA	HB3	1.25	0.02	1
1	A	6	ALA	C	177.95	0.25	1
1	A	6	ALA	CA	53.06	0.25	1
1	A	6	ALA	CB	18.84	0.25	1
1	A	6	ALA	N	124.0	0.15	1
1	A	7	GLN	H	8.03	0.02	1
1	A	7	GLN	HA	4.1	0.02	1
1	A	7	GLN	HB2	1.91	0.02	2
1	A	7	GLN	HB3	1.87	0.02	2
1	A	7	GLN	HG2	2.21	0.02	2
1	A	7	GLN	HG3	2.19	0.02	2
1	A	7	GLN	HE21	7.46	0.02	1
1	A	7	GLN	HE22	6.76	0.02	1
1	A	7	GLN	C	176.24	0.25	1
1	A	7	GLN	CA	56.26	0.25	1
1	A	7	GLN	CB	29.02	0.25	1
1	A	7	GLN	CG	33.7	0.25	1
1	A	7	GLN	N	118.64	0.15	1
1	A	7	GLN	NE2	112.42	0.15	1
1	A	8	LEU	H	7.96	0.02	1
1	A	8	LEU	HA	4.1	0.02	1
1	A	8	LEU	HB2	1.31	0.02	2
1	A	8	LEU	HB3	1.43	0.02	2
1	A	8	LEU	HD11	0.76	0.02	2
1	A	8	LEU	HD12	0.76	0.02	2
1	A	8	LEU	HD13	0.76	0.02	2
1	A	8	LEU	HD21	0.7	0.02	2
1	A	8	LEU	HD22	0.7	0.02	2
1	A	8	LEU	HD23	0.7	0.02	2
1	A	8	LEU	C	177.55	0.25	1
1	A	8	LEU	CA	55.66	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	LEU	CB	42.28	0.25	1
1	A	8	LEU	CG	26.77	0.25	1
1	A	8	LEU	CD1	24.96	0.25	2
1	A	8	LEU	CD2	23.28	0.25	2
1	A	8	LEU	N	122.27	0.15	1
1	A	9	PHE	H	8.12	0.02	1
1	A	9	PHE	HA	4.42	0.02	1
1	A	9	PHE	HB2	2.86	0.02	2
1	A	9	PHE	HB3	3.02	0.02	2
1	A	9	PHE	HD1	7.09	0.02	3
1	A	9	PHE	HD2	7.09	0.02	3
1	A	9	PHE	HE1	7.18	0.02	3
1	A	9	PHE	HE2	7.18	0.02	3
1	A	9	PHE	C	176.07	0.25	1
1	A	9	PHE	CA	58.24	0.25	1
1	A	9	PHE	CB	39.23	0.25	1
1	A	9	PHE	N	120.29	0.15	1
1	A	10	GLU	H	8.15	0.02	1
1	A	10	GLU	HA	4.04	0.02	1
1	A	10	GLU	HB2	1.91	0.02	2
1	A	10	GLU	HB3	1.84	0.02	2
1	A	10	GLU	HG2	2.12	0.02	1
1	A	10	GLU	C	176.96	0.25	1
1	A	10	GLU	CA	56.9	0.25	1
1	A	10	GLU	CB	29.68	0.25	1
1	A	10	GLU	N	121.66	0.15	1
1	A	11	GLU	H	8.17	0.02	1
1	A	11	GLU	HA	4.18	0.02	1
1	A	11	GLU	N	122.51	0.15	1
1	A	12	SER	HA	4.26	0.02	1
1	A	12	SER	HB2	3.73	0.02	2
1	A	12	SER	HB3	3.68	0.02	2
1	A	12	SER	C	174.84	0.25	1
1	A	12	SER	CA	58.37	0.25	1
1	A	12	SER	CB	63.45	0.25	1
1	A	13	LEU	H	7.95	0.02	1
1	A	13	LEU	HA	4.15	0.02	1
1	A	13	LEU	HB2	1.51	0.02	2
1	A	13	LEU	HB3	1.44	0.02	2
1	A	13	LEU	HD11	0.74	0.02	1
1	A	13	LEU	HD12	0.74	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	LEU	HD13	0.74	0.02	1
1	A	13	LEU	C	177.56	0.25	1
1	A	13	LEU	CA	55.51	0.25	1
1	A	13	LEU	CB	42.19	0.25	1
1	A	13	LEU	CG	26.94	0.25	1
1	A	13	LEU	CD1	23.57	0.25	2
1	A	13	LEU	CD2	24.99	0.25	2
1	A	13	LEU	N	123.28	0.15	1
1	A	14	LYS	H	7.93	0.02	1
1	A	14	LYS	HA	4.13	0.02	1
1	A	14	LYS	HB2	1.72	0.02	2
1	A	14	LYS	HB3	1.66	0.02	2
1	A	14	LYS	HG2	1.3	0.02	2
1	A	14	LYS	HG3	1.36	0.02	2
1	A	14	LYS	HE3	2.87	0.02	1
1	A	14	LYS	C	176.74	0.25	1
1	A	14	LYS	CA	56.82	0.25	1
1	A	14	LYS	CB	32.78	0.25	1
1	A	14	LYS	CG	24.67	0.25	1
1	A	14	LYS	CD	29.0	0.25	1
1	A	14	LYS	CE	41.9	0.25	1
1	A	14	LYS	N	120.9	0.15	1
1	A	15	GLU	H	8.13	0.02	1
1	A	15	GLU	HA	4.16	0.02	1
1	A	15	GLU	C	176.49	0.25	1
1	A	15	GLU	CA	56.9	0.25	1
1	A	15	GLU	CB	29.45	0.25	1
1	A	15	GLU	CG	36.31	0.25	1
1	A	15	GLU	N	121.14	0.15	1
1	A	16	ILE	H	8.01	0.02	1
1	A	16	ILE	HA	4.0	0.02	1
1	A	16	ILE	HB	1.75	0.02	1
1	A	16	ILE	HG12	1.07	0.02	2
1	A	16	ILE	HG13	1.37	0.02	2
1	A	16	ILE	HG21	0.78	0.02	1
1	A	16	ILE	HG22	0.78	0.02	1
1	A	16	ILE	HG23	0.78	0.02	1
1	A	16	ILE	HD11	0.73	0.02	1
1	A	16	ILE	HD12	0.73	0.02	1
1	A	16	ILE	HD13	0.73	0.02	1
1	A	16	ILE	C	175.69	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	ILE	CA	61.2	0.25	1
1	A	16	ILE	CB	38.62	0.25	1
1	A	16	ILE	CG1	27.27	0.25	1
1	A	16	ILE	CG2	17.45	0.25	1
1	A	16	ILE	CD1	13.01	0.25	1
1	A	16	ILE	N	120.71	0.15	1
1	A	17	GLU	H	8.3	0.02	1
1	A	17	GLU	HA	4.21	0.02	1
1	A	17	GLU	HB2	1.89	0.02	2
1	A	17	GLU	HB3	1.91	0.02	2
1	A	17	GLU	HG2	2.15	0.02	1
1	A	17	GLU	C	176.39	0.25	1
1	A	17	GLU	CA	56.52	0.25	1
1	A	17	GLU	CB	29.59	0.25	1
1	A	17	GLU	CG	36.32	0.25	1
1	A	17	GLU	N	124.38	0.15	1
1	A	18	THR	H	8.06	0.02	1
1	A	18	THR	HA	4.2	0.02	1
1	A	18	THR	HB	4.04	0.02	1
1	A	18	THR	HG21	1.06	0.02	1
1	A	18	THR	HG22	1.06	0.02	1
1	A	18	THR	HG23	1.06	0.02	1
1	A	18	THR	C	174.2	0.25	1
1	A	18	THR	CA	61.56	0.25	1
1	A	18	THR	CB	69.61	0.25	1
1	A	18	THR	CG2	21.58	0.25	1
1	A	18	THR	N	115.78	0.15	1
1	A	19	ARG	H	8.33	0.02	1
1	A	19	ARG	HA	4.52	0.02	1
1	A	19	ARG	HB2	1.63	0.02	2
1	A	19	ARG	HB3	1.73	0.02	2
1	A	19	ARG	HG2	1.54	0.02	2
1	A	19	ARG	HG3	1.55	0.02	2
1	A	19	ARG	HD2	3.07	0.02	1
1	A	19	ARG	HD3	3.07	0.02	1
1	A	19	ARG	C	174.15	0.25	1
1	A	19	ARG	CA	53.86	0.25	1
1	A	19	ARG	CB	30.1	0.25	1
1	A	19	ARG	CG	26.73	0.25	1
1	A	19	ARG	CD	43.17	0.25	1
1	A	19	ARG	N	124.8	0.15	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	PRO	HA	4.31	0.02	1
1	A	20	PRO	HB2	1.82	0.02	2
1	A	20	PRO	HB3	2.19	0.02	2
1	A	20	PRO	HG2	1.88	0.02	2
1	A	20	PRO	HG3	1.95	0.02	2
1	A	20	PRO	HD2	3.71	0.02	2
1	A	20	PRO	HD3	3.52	0.02	2
1	A	20	PRO	C	177.35	0.25	1
1	A	20	PRO	CA	63.38	0.25	1
1	A	20	PRO	CB	32.01	0.25	1
1	A	20	PRO	CG	27.36	0.25	1
1	A	20	PRO	CD	50.56	0.25	1
1	A	21	GLY	H	8.47	0.02	1
1	A	21	GLY	HA2	3.86	0.02	1
1	A	21	GLY	HA3	3.86	0.02	1
1	A	21	GLY	C	174.04	0.25	1
1	A	21	GLY	CA	45.11	0.25	1
1	A	21	GLY	N	109.79	0.15	1
1	A	22	SER	H	8.1	0.02	1
1	A	22	SER	HA	4.38	0.02	1
1	A	22	SER	HB2	3.75	0.02	2
1	A	22	SER	HB3	3.74	0.02	2
1	A	22	SER	C	173.11	0.25	1
1	A	22	SER	CA	58.35	0.25	1
1	A	22	SER	CB	63.85	0.25	1
1	A	22	SER	N	115.12	0.15	1
1	A	23	ILE	H	7.95	0.02	1
1	A	23	ILE	HA	4.67	0.02	1
1	A	23	ILE	HB	1.61	0.02	1
1	A	23	ILE	HG12	0.98	0.02	2
1	A	23	ILE	HG13	1.33	0.02	2
1	A	23	ILE	HG21	0.64	0.02	1
1	A	23	ILE	HG22	0.64	0.02	1
1	A	23	ILE	HG23	0.64	0.02	1
1	A	23	ILE	HD11	0.63	0.02	1
1	A	23	ILE	HD12	0.63	0.02	1
1	A	23	ILE	HD13	0.63	0.02	1
1	A	23	ILE	C	176.0	0.25	1
1	A	23	ILE	CA	59.64	0.25	1
1	A	23	ILE	CB	39.31	0.25	1
1	A	23	ILE	CG1	27.14	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	23	ILE	CG2	17.7	0.25	1
1	A	23	ILE	CD1	12.21	0.25	1
1	A	23	ILE	N	122.51	0.15	1
1	A	24	VAL	H	8.94	0.02	1
1	A	24	VAL	HA	4.45	0.02	1
1	A	24	VAL	HB	2.03	0.02	1
1	A	24	VAL	HG11	0.75	0.02	2
1	A	24	VAL	HG12	0.75	0.02	2
1	A	24	VAL	HG13	0.75	0.02	2
1	A	24	VAL	HG21	0.78	0.02	2
1	A	24	VAL	HG22	0.78	0.02	2
1	A	24	VAL	HG23	0.78	0.02	2
1	A	24	VAL	C	173.38	0.25	1
1	A	24	VAL	CA	59.48	0.25	1
1	A	24	VAL	CB	34.95	0.25	1
1	A	24	VAL	CG1	19.85	0.25	2
1	A	24	VAL	CG2	21.44	0.25	2
1	A	24	VAL	N	123.65	0.15	1
1	A	25	ARG	H	8.19	0.02	1
1	A	25	ARG	HA	5.03	0.02	1
1	A	25	ARG	HB2	1.7	0.02	2
1	A	25	ARG	HB3	1.6	0.02	2
1	A	25	ARG	HD2	3.03	0.02	1
1	A	25	ARG	C	176.19	0.25	1
1	A	25	ARG	CA	54.22	0.25	1
1	A	25	ARG	CB	30.7	0.25	1
1	A	25	ARG	CG	26.5	0.25	1
1	A	25	ARG	CD	42.77	0.25	1
1	A	25	ARG	N	123.42	0.15	1
1	A	26	GLY	H	8.89	0.02	1
1	A	26	GLY	HA2	3.17	0.02	2
1	A	26	GLY	HA3	4.67	0.02	2
1	A	26	GLY	C	171.1	0.25	1
1	A	26	GLY	CA	43.93	0.25	1
1	A	26	GLY	N	111.49	0.15	1
1	A	27	VAL	H	7.75	0.02	1
1	A	27	VAL	HA	4.79	0.02	1
1	A	27	VAL	HB	1.79	0.02	1
1	A	27	VAL	HG11	0.74	0.02	2
1	A	27	VAL	HG12	0.74	0.02	2
1	A	27	VAL	HG13	0.74	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	VAL	HG21	0.82	0.02	2
1	A	27	VAL	HG22	0.82	0.02	2
1	A	27	VAL	HG23	0.82	0.02	2
1	A	27	VAL	C	175.67	0.25	1
1	A	27	VAL	CA	59.72	0.25	1
1	A	27	VAL	CB	35.04	0.25	1
1	A	27	VAL	CG1	20.68	0.25	2
1	A	27	VAL	CG2	21.49	0.25	2
1	A	27	VAL	N	117.64	0.15	1
1	A	28	VAL	H	8.89	0.02	1
1	A	28	VAL	HA	3.78	0.02	1
1	A	28	VAL	HB	2.08	0.02	1
1	A	28	VAL	HG11	0.58	0.02	2
1	A	28	VAL	HG12	0.58	0.02	2
1	A	28	VAL	HG13	0.58	0.02	2
1	A	28	VAL	HG21	0.54	0.02	2
1	A	28	VAL	HG22	0.54	0.02	2
1	A	28	VAL	HG23	0.54	0.02	2
1	A	28	VAL	C	176.99	0.25	1
1	A	28	VAL	CA	63.89	0.25	1
1	A	28	VAL	CB	31.5	0.25	1
1	A	28	VAL	CG1	22.15	0.25	2
1	A	28	VAL	CG2	22.17	0.25	2
1	A	28	VAL	N	126.69	0.15	1
1	A	29	VAL	H	9.18	0.02	1
1	A	29	VAL	HA	4.31	0.02	1
1	A	29	VAL	HB	1.98	0.02	1
1	A	29	VAL	HG11	0.75	0.02	2
1	A	29	VAL	HG12	0.75	0.02	2
1	A	29	VAL	HG13	0.75	0.02	2
1	A	29	VAL	HG21	0.89	0.02	2
1	A	29	VAL	HG22	0.89	0.02	2
1	A	29	VAL	HG23	0.89	0.02	2
1	A	29	VAL	C	175.62	0.25	1
1	A	29	VAL	CA	62.17	0.25	1
1	A	29	VAL	CB	33.2	0.25	1
1	A	29	VAL	CG1	19.96	0.25	2
1	A	29	VAL	CG2	21.67	0.25	2
1	A	29	VAL	N	126.29	0.15	1
1	A	30	ALA	H	7.65	0.02	1
1	A	30	ALA	HA	4.32	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	ALA	HB1	1.29	0.02	1
1	A	30	ALA	HB2	1.29	0.02	1
1	A	30	ALA	HB3	1.29	0.02	1
1	A	30	ALA	C	174.35	0.25	1
1	A	30	ALA	CA	52.39	0.25	1
1	A	30	ALA	CB	21.91	0.25	1
1	A	30	ALA	N	121.33	0.15	1
1	A	31	ILE	H	8.46	0.02	1
1	A	31	ILE	HA	4.27	0.02	1
1	A	31	ILE	HB	1.44	0.02	1
1	A	31	ILE	HG12	1.17	0.02	2
1	A	31	ILE	HG13	0.65	0.02	2
1	A	31	ILE	HG21	0.65	0.02	1
1	A	31	ILE	HG22	0.65	0.02	1
1	A	31	ILE	HG23	0.65	0.02	1
1	A	31	ILE	HD11	0.58	0.02	1
1	A	31	ILE	HD12	0.58	0.02	1
1	A	31	ILE	HD13	0.58	0.02	1
1	A	31	ILE	C	174.34	0.25	1
1	A	31	ILE	CA	61.52	0.25	1
1	A	31	ILE	CB	41.19	0.25	1
1	A	31	ILE	CG1	27.96	0.25	1
1	A	31	ILE	CG2	17.58	0.25	1
1	A	31	ILE	CD1	14.65	0.25	1
1	A	31	ILE	N	120.33	0.15	1
1	A	32	ASP	H	8.51	0.02	1
1	A	32	ASP	HA	4.72	0.02	1
1	A	32	ASP	HB2	2.63	0.02	2
1	A	32	ASP	HB3	2.57	0.02	2
1	A	32	ASP	C	174.69	0.25	1
1	A	32	ASP	CA	52.63	0.25	1
1	A	32	ASP	CB	42.84	0.25	1
1	A	32	ASP	N	128.17	0.15	1
1	A	33	LYS	H	8.44	0.02	1
1	A	33	LYS	HA	3.75	0.02	1
1	A	33	LYS	HB2	1.79	0.02	2
1	A	33	LYS	HB3	1.69	0.02	2
1	A	33	LYS	HG2	1.3	0.02	2
1	A	33	LYS	HG3	1.36	0.02	2
1	A	33	LYS	HD2	1.6	0.02	2
1	A	33	LYS	HD3	1.57	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	33	LYS	HE2	2.91	0.02	2
1	A	33	LYS	HE3	2.85	0.02	2
1	A	33	LYS	C	175.88	0.25	1
1	A	33	LYS	CA	58.7	0.25	1
1	A	33	LYS	CB	31.1	0.25	1
1	A	33	LYS	CG	24.49	0.25	1
1	A	33	LYS	CD	28.83	0.25	1
1	A	33	LYS	CE	41.7	0.25	1
1	A	33	LYS	N	118.54	0.15	1
1	A	34	ASP	H	8.61	0.02	1
1	A	34	ASP	HA	4.68	0.02	1
1	A	34	ASP	HB2	2.73	0.02	2
1	A	34	ASP	HB3	2.63	0.02	2
1	A	34	ASP	C	176.51	0.25	1
1	A	34	ASP	CA	55.07	0.25	1
1	A	34	ASP	CB	42.0	0.25	1
1	A	34	ASP	N	116.09	0.15	1
1	A	35	VAL	H	8.1	0.02	1
1	A	35	VAL	HA	4.55	0.02	1
1	A	35	VAL	HB	1.81	0.02	1
1	A	35	VAL	HG11	0.74	0.02	2
1	A	35	VAL	HG12	0.74	0.02	2
1	A	35	VAL	HG13	0.74	0.02	2
1	A	35	VAL	HG21	0.69	0.02	2
1	A	35	VAL	HG22	0.69	0.02	2
1	A	35	VAL	HG23	0.69	0.02	2
1	A	35	VAL	C	172.77	0.25	1
1	A	35	VAL	CA	61.1	0.25	1
1	A	35	VAL	CB	36.11	0.25	1
1	A	35	VAL	CG1	20.56	0.25	2
1	A	35	VAL	CG2	21.74	0.25	2
1	A	35	VAL	N	120.83	0.15	1
1	A	36	VAL	H	9.04	0.02	1
1	A	36	VAL	HA	4.18	0.02	1
1	A	36	VAL	HG11	0.69	0.02	2
1	A	36	VAL	HG12	0.69	0.02	2
1	A	36	VAL	HG13	0.69	0.02	2
1	A	36	VAL	HG21	0.44	0.02	2
1	A	36	VAL	HG22	0.44	0.02	2
1	A	36	VAL	HG23	0.44	0.02	2
1	A	36	VAL	C	174.14	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	36	VAL	CA	61.02	0.25	1
1	A	36	VAL	CB	33.61	0.25	1
1	A	36	VAL	CG2	21.79	0.25	1
1	A	36	VAL	N	125.49	0.15	1
1	A	37	LEU	H	8.68	0.02	1
1	A	37	LEU	HA	5.07	0.02	1
1	A	37	LEU	HB2	1.5	0.02	2
1	A	37	LEU	HB3	1.13	0.02	2
1	A	37	LEU	HG	1.34	0.02	1
1	A	37	LEU	HD11	0.65	0.02	2
1	A	37	LEU	HD12	0.65	0.02	2
1	A	37	LEU	HD13	0.65	0.02	2
1	A	37	LEU	HD21	0.67	0.02	2
1	A	37	LEU	HD22	0.67	0.02	2
1	A	37	LEU	HD23	0.67	0.02	2
1	A	37	LEU	C	176.61	0.25	1
1	A	37	LEU	CA	53.29	0.25	1
1	A	37	LEU	CB	43.28	0.25	1
1	A	37	LEU	CG	27.11	0.25	1
1	A	37	LEU	CD1	23.75	0.25	2
1	A	37	LEU	CD2	24.41	0.25	2
1	A	37	LEU	N	127.38	0.15	1
1	A	38	VAL	H	9.11	0.02	1
1	A	38	VAL	HA	4.65	0.02	1
1	A	38	VAL	HB	1.66	0.02	1
1	A	38	VAL	HG11	0.51	0.02	2
1	A	38	VAL	HG12	0.51	0.02	2
1	A	38	VAL	HG13	0.51	0.02	2
1	A	38	VAL	HG21	0.66	0.02	2
1	A	38	VAL	HG22	0.66	0.02	2
1	A	38	VAL	HG23	0.66	0.02	2
1	A	38	VAL	C	174.48	0.25	1
1	A	38	VAL	CA	59.79	0.25	1
1	A	38	VAL	CB	35.4	0.25	1
1	A	38	VAL	CG1	21.07	0.25	2
1	A	38	VAL	CG2	21.84	0.25	2
1	A	38	VAL	N	123.21	0.15	1
1	A	39	ASP	H	9.13	0.02	1
1	A	39	ASP	HA	4.86	0.02	1
1	A	39	ASP	HB2	2.83	0.02	2
1	A	39	ASP	HB3	2.44	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	39	ASP	C	175.67	0.25	1
1	A	39	ASP	CA	52.62	0.25	1
1	A	39	ASP	CB	41.03	0.25	1
1	A	39	ASP	N	124.79	0.15	1
1	A	40	ALA	H	9.2	0.02	1
1	A	40	ALA	HA	4.73	0.02	1
1	A	40	ALA	HB1	1.13	0.02	1
1	A	40	ALA	HB2	1.13	0.02	1
1	A	40	ALA	HB3	1.13	0.02	1
1	A	40	ALA	C	176.4	0.25	1
1	A	40	ALA	CA	50.24	0.25	1
1	A	40	ALA	CB	19.27	0.25	1
1	A	40	ALA	N	131.94	0.15	1
1	A	41	GLY	H	8.47	0.02	1
1	A	41	GLY	HA2	3.73	0.02	2
1	A	41	GLY	HA3	4.0	0.02	2
1	A	41	GLY	C	174.97	0.25	1
1	A	41	GLY	CA	45.74	0.25	1
1	A	41	GLY	N	106.93	0.15	1
1	A	42	LEU	H	7.52	0.02	1
1	A	42	LEU	HA	4.48	0.02	1
1	A	42	LEU	HB2	1.69	0.02	2
1	A	42	LEU	HB3	1.9	0.02	2
1	A	42	LEU	HG	1.41	0.02	1
1	A	42	LEU	HD11	0.79	0.02	2
1	A	42	LEU	HD12	0.79	0.02	2
1	A	42	LEU	HD13	0.79	0.02	2
1	A	42	LEU	HD21	0.72	0.02	2
1	A	42	LEU	HD22	0.72	0.02	2
1	A	42	LEU	HD23	0.72	0.02	2
1	A	42	LEU	C	177.17	0.25	1
1	A	42	LEU	CA	53.97	0.25	1
1	A	42	LEU	CB	40.96	0.25	1
1	A	42	LEU	CG	27.39	0.25	1
1	A	42	LEU	CD1	25.51	0.25	2
1	A	42	LEU	CD2	22.52	0.25	2
1	A	42	LEU	N	119.15	0.15	1
1	A	43	LYS	H	8.36	0.02	1
1	A	43	LYS	HA	3.9	0.02	1
1	A	43	LYS	HB2	1.69	0.02	2
1	A	43	LYS	HB3	1.79	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	43	LYS	HG2	1.37	0.02	2
1	A	43	LYS	HG3	1.34	0.02	2
1	A	43	LYS	HD2	1.57	0.02	2
1	A	43	LYS	HD3	1.57	0.02	2
1	A	43	LYS	HE3	2.88	0.02	1
1	A	43	LYS	C	176.42	0.25	1
1	A	43	LYS	CA	58.63	0.25	1
1	A	43	LYS	CB	31.69	0.25	1
1	A	43	LYS	CG	24.75	0.25	1
1	A	43	LYS	CD	28.8	0.25	1
1	A	43	LYS	CE	41.74	0.25	1
1	A	43	LYS	N	119.01	0.15	1
1	A	44	SER	H	7.41	0.02	1
1	A	44	SER	HA	4.48	0.02	1
1	A	44	SER	HB2	3.62	0.02	2
1	A	44	SER	HB3	3.66	0.02	2
1	A	44	SER	C	173.65	0.25	1
1	A	44	SER	CA	56.37	0.25	1
1	A	44	SER	CB	64.94	0.25	1
1	A	44	SER	N	110.68	0.15	1
1	A	45	GLU	H	8.83	0.02	1
1	A	45	GLU	HA	4.3	0.02	1
1	A	45	GLU	HB2	1.78	0.02	2
1	A	45	GLU	HB3	1.64	0.02	2
1	A	45	GLU	HG2	2.12	0.02	2
1	A	45	GLU	HG3	2.08	0.02	2
1	A	45	GLU	C	176.52	0.25	1
1	A	45	GLU	CA	57.8	0.25	1
1	A	45	GLU	CB	29.77	0.25	1
1	A	45	GLU	CG	36.63	0.25	1
1	A	45	GLU	N	122.64	0.15	1
1	A	46	SER	H	8.99	0.02	1
1	A	46	SER	HA	4.54	0.02	1
1	A	46	SER	HB2	3.48	0.02	2
1	A	46	SER	HB3	3.67	0.02	2
1	A	46	SER	C	172.15	0.25	1
1	A	46	SER	CA	58.37	0.25	1
1	A	46	SER	CB	64.46	0.25	1
1	A	46	SER	N	119.33	0.15	1
1	A	47	ALA	H	8.53	0.02	1
1	A	47	ALA	HA	4.82	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	47	ALA	HB1	1.13	0.02	1
1	A	47	ALA	HB2	1.13	0.02	1
1	A	47	ALA	HB3	1.13	0.02	1
1	A	47	ALA	C	176.19	0.25	1
1	A	47	ALA	CA	50.93	0.25	1
1	A	47	ALA	CB	19.5	0.25	1
1	A	47	ALA	N	128.62	0.15	1
1	A	48	ILE	H	9.19	0.02	1
1	A	48	ILE	HA	4.65	0.02	1
1	A	48	ILE	HB	1.9	0.02	1
1	A	48	ILE	HG12	1.2	0.02	1
1	A	48	ILE	HG21	0.91	0.02	1
1	A	48	ILE	HG22	0.91	0.02	1
1	A	48	ILE	HG23	0.91	0.02	1
1	A	48	ILE	HD11	0.66	0.02	1
1	A	48	ILE	HD12	0.66	0.02	1
1	A	48	ILE	HD13	0.66	0.02	1
1	A	48	ILE	CA	57.37	0.25	1
1	A	48	ILE	CB	40.82	0.25	1
1	A	48	ILE	CG1	27.1	0.25	1
1	A	48	ILE	CG2	17.58	0.25	1
1	A	48	ILE	CD1	13.0	0.25	1
1	A	48	ILE	N	125.71	0.15	1
1	A	49	PRO	HA	4.44	0.02	1
1	A	49	PRO	HG2	2.07	0.02	1
1	A	49	PRO	HD2	3.81	0.02	2
1	A	49	PRO	HD3	3.55	0.02	2
1	A	49	PRO	C	177.67	0.25	1
1	A	49	PRO	CA	63.85	0.25	1
1	A	49	PRO	CB	32.49	0.25	1
1	A	49	PRO	CG	28.01	0.25	1
1	A	49	PRO	CD	51.06	0.25	1
1	A	50	ALA	H	8.22	0.02	1
1	A	50	ALA	HA	3.97	0.02	1
1	A	50	ALA	HB1	1.18	0.02	1
1	A	50	ALA	HB2	1.18	0.02	1
1	A	50	ALA	HB3	1.18	0.02	1
1	A	50	ALA	C	178.92	0.25	1
1	A	50	ALA	CA	54.77	0.25	1
1	A	50	ALA	CB	17.92	0.25	1
1	A	50	ALA	N	125.73	0.15	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	GLU	H	8.56	0.02	1
1	A	51	GLU	HA	3.69	0.02	1
1	A	51	GLU	HB2	1.92	0.02	2
1	A	51	GLU	HB3	2.04	0.02	2
1	A	51	GLU	HG2	2.22	0.02	2
1	A	51	GLU	HG3	2.16	0.02	2
1	A	51	GLU	C	177.85	0.25	1
1	A	51	GLU	CA	58.99	0.25	1
1	A	51	GLU	CB	29.12	0.25	1
1	A	51	GLU	CG	35.42	0.25	1
1	A	51	GLU	N	115.15	0.15	1
1	A	52	GLN	H	7.44	0.02	1
1	A	52	GLN	HA	3.88	0.02	1
1	A	52	GLN	HB3	1.55	0.02	1
1	A	52	GLN	HG3	1.92	0.02	1
1	A	52	GLN	C	175.84	0.25	1
1	A	52	GLN	CA	57.46	0.25	1
1	A	52	GLN	CB	27.89	0.25	1
1	A	52	GLN	CG	33.6	0.25	1
1	A	52	GLN	N	115.78	0.15	1
1	A	53	PHE	H	7.84	0.02	1
1	A	53	PHE	HA	4.69	0.02	1
1	A	53	PHE	HD1	7.13	0.02	3
1	A	53	PHE	HD2	7.13	0.02	3
1	A	53	PHE	HE1	7.04	0.02	3
1	A	53	PHE	HE2	7.04	0.02	3
1	A	53	PHE	HZ	6.87	0.02	1
1	A	53	PHE	C	174.78	0.25	1
1	A	53	PHE	CA	56.68	0.25	1
1	A	53	PHE	CB	40.23	0.25	1
1	A	53	PHE	N	115.82	0.15	1
1	A	54	LYS	H	7.01	0.02	1
1	A	54	LYS	HA	4.67	0.02	1
1	A	54	LYS	HB2	1.49	0.02	2
1	A	54	LYS	HB3	1.65	0.02	2
1	A	54	LYS	HG3	0.87	0.02	1
1	A	54	LYS	HD2	1.44	0.02	1
1	A	54	LYS	HE2	2.5	0.02	2
1	A	54	LYS	HE3	2.72	0.02	2
1	A	54	LYS	C	176.79	0.25	1
1	A	54	LYS	CA	55.82	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	LYS	CB	34.93	0.25	1
1	A	54	LYS	CG	26.46	0.25	1
1	A	54	LYS	CE	41.94	0.25	1
1	A	54	LYS	N	119.72	0.15	1
1	A	55	ASN	H	8.53	0.02	1
1	A	55	ASN	HA	4.66	0.02	1
1	A	55	ASN	HB2	2.92	0.02	2
1	A	55	ASN	HB3	3.44	0.02	2
1	A	55	ASN	HD21	7.88	0.02	1
1	A	55	ASN	HD22	7.34	0.02	1
1	A	55	ASN	C	177.67	0.25	1
1	A	55	ASN	CA	50.67	0.25	1
1	A	55	ASN	CB	38.57	0.25	1
1	A	55	ASN	N	120.17	0.15	1
1	A	55	ASN	ND2	112.8	0.15	1
1	A	56	ALA	H	8.43	0.02	1
1	A	56	ALA	HA	4.03	0.02	1
1	A	56	ALA	HB1	1.34	0.02	1
1	A	56	ALA	HB2	1.34	0.02	1
1	A	56	ALA	HB3	1.34	0.02	1
1	A	56	ALA	C	178.59	0.25	1
1	A	56	ALA	CA	54.54	0.25	1
1	A	56	ALA	CB	17.98	0.25	1
1	A	56	ALA	N	120.74	0.15	1
1	A	57	GLN	H	7.58	0.02	1
1	A	57	GLN	HA	4.3	0.02	1
1	A	57	GLN	HB2	2.21	0.02	2
1	A	57	GLN	HB3	1.95	0.02	2
1	A	57	GLN	HG2	2.33	0.02	2
1	A	57	GLN	HG3	2.2	0.02	2
1	A	57	GLN	HE21	7.43	0.02	1
1	A	57	GLN	HE22	6.72	0.02	1
1	A	57	GLN	C	176.13	0.25	1
1	A	57	GLN	CA	55.73	0.25	1
1	A	57	GLN	CB	28.54	0.25	1
1	A	57	GLN	CG	34.74	0.25	1
1	A	57	GLN	N	114.92	0.15	1
1	A	57	GLN	NE2	112.05	0.15	1
1	A	58	GLY	H	8.16	0.02	1
1	A	58	GLY	HA2	4.12	0.02	2
1	A	58	GLY	HA3	3.56	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	GLY	C	173.66	0.25	1
1	A	58	GLY	CA	45.42	0.25	1
1	A	58	GLY	N	107.93	0.15	1
1	A	59	GLU	H	7.72	0.02	1
1	A	59	GLU	HA	4.33	0.02	1
1	A	59	GLU	HB2	1.86	0.02	2
1	A	59	GLU	HB3	1.81	0.02	2
1	A	59	GLU	HG2	2.0	0.02	2
1	A	59	GLU	HG3	2.08	0.02	2
1	A	59	GLU	C	175.84	0.25	1
1	A	59	GLU	CA	54.31	0.25	1
1	A	59	GLU	CB	30.74	0.25	1
1	A	59	GLU	CG	35.69	0.25	1
1	A	59	GLU	N	119.72	0.15	1
1	A	60	LEU	H	8.71	0.02	1
1	A	60	LEU	HA	4.29	0.02	1
1	A	60	LEU	HB3	1.51	0.02	1
1	A	60	LEU	HG	1.56	0.02	1
1	A	60	LEU	HD11	0.76	0.02	2
1	A	60	LEU	HD12	0.76	0.02	2
1	A	60	LEU	HD13	0.76	0.02	2
1	A	60	LEU	HD21	0.75	0.02	2
1	A	60	LEU	HD22	0.75	0.02	2
1	A	60	LEU	HD23	0.75	0.02	2
1	A	60	LEU	C	177.68	0.25	1
1	A	60	LEU	CA	55.14	0.25	1
1	A	60	LEU	CB	43.05	0.25	1
1	A	60	LEU	CG	27.73	0.25	1
1	A	60	LEU	CD1	25.49	0.25	2
1	A	60	LEU	CD2	25.3	0.25	2
1	A	60	LEU	N	123.06	0.15	1
1	A	61	GLU	H	8.81	0.02	1
1	A	61	GLU	HA	4.39	0.02	1
1	A	61	GLU	HB2	1.86	0.02	2
1	A	61	GLU	HB3	2.13	0.02	2
1	A	61	GLU	HG2	2.21	0.02	2
1	A	61	GLU	HG3	2.08	0.02	2
1	A	61	GLU	C	175.52	0.25	1
1	A	61	GLU	CA	55.78	0.25	1
1	A	61	GLU	CB	30.24	0.25	1
1	A	61	GLU	CG	36.72	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	GLU	N	123.55	0.15	1
1	A	62	ILE	H	6.78	0.02	1
1	A	62	ILE	HA	4.42	0.02	1
1	A	62	ILE	HB	1.53	0.02	1
1	A	62	ILE	HG12	0.68	0.02	2
1	A	62	ILE	HG13	1.2	0.02	2
1	A	62	ILE	HG21	0.64	0.02	1
1	A	62	ILE	HG22	0.64	0.02	1
1	A	62	ILE	HG23	0.64	0.02	1
1	A	62	ILE	HD11	0.29	0.02	1
1	A	62	ILE	HD12	0.29	0.02	1
1	A	62	ILE	HD13	0.29	0.02	1
1	A	62	ILE	C	172.66	0.25	1
1	A	62	ILE	CA	58.94	0.25	1
1	A	62	ILE	CB	41.9	0.25	1
1	A	62	ILE	CG1	27.04	0.25	1
1	A	62	ILE	CG2	18.4	0.25	1
1	A	62	ILE	CD1	14.93	0.25	1
1	A	62	ILE	N	113.6	0.15	1
1	A	63	GLN	H	8.37	0.02	1
1	A	63	GLN	HA	4.37	0.02	1
1	A	63	GLN	HB2	1.71	0.02	2
1	A	63	GLN	HB3	1.88	0.02	2
1	A	63	GLN	HG2	2.13	0.02	2
1	A	63	GLN	HG3	2.19	0.02	2
1	A	63	GLN	HE21	6.64	0.02	1
1	A	63	GLN	HE22	7.58	0.02	1
1	A	63	GLN	C	175.17	0.25	1
1	A	63	GLN	CA	53.16	0.25	1
1	A	63	GLN	CB	32.8	0.25	1
1	A	63	GLN	CG	33.29	0.25	1
1	A	63	GLN	N	119.37	0.15	1
1	A	63	GLN	NE2	112.89	0.15	1
1	A	64	VAL	H	8.37	0.02	1
1	A	64	VAL	HA	3.09	0.02	1
1	A	64	VAL	HB	1.75	0.02	1
1	A	64	VAL	HG11	0.77	0.02	2
1	A	64	VAL	HG12	0.77	0.02	2
1	A	64	VAL	HG13	0.77	0.02	2
1	A	64	VAL	HG21	0.79	0.02	2
1	A	64	VAL	HG22	0.79	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	VAL	HG23	0.79	0.02	2
1	A	64	VAL	C	177.19	0.25	1
1	A	64	VAL	CA	65.59	0.25	1
1	A	64	VAL	CB	31.02	0.25	1
1	A	64	VAL	CG1	21.23	0.25	2
1	A	64	VAL	CG2	22.61	0.25	2
1	A	64	VAL	N	120.76	0.15	1
1	A	65	GLY	H	8.87	0.02	1
1	A	65	GLY	HA2	3.36	0.02	2
1	A	65	GLY	HA3	4.36	0.02	2
1	A	65	GLY	C	174.19	0.25	1
1	A	65	GLY	CA	44.38	0.25	1
1	A	65	GLY	N	116.75	0.15	1
1	A	66	ASP	H	7.8	0.02	1
1	A	66	ASP	HA	4.48	0.02	1
1	A	66	ASP	HB2	2.46	0.02	2
1	A	66	ASP	HB3	2.65	0.02	2
1	A	66	ASP	C	175.24	0.25	1
1	A	66	ASP	CA	54.73	0.25	1
1	A	66	ASP	CB	40.93	0.25	1
1	A	66	ASP	N	121.36	0.15	1
1	A	67	GLU	H	8.32	0.02	1
1	A	67	GLU	HA	5.13	0.02	1
1	A	67	GLU	HB2	1.82	0.02	2
1	A	67	GLU	HB3	1.77	0.02	2
1	A	67	GLU	HG2	2.24	0.02	2
1	A	67	GLU	HG3	1.99	0.02	2
1	A	67	GLU	C	176.5	0.25	1
1	A	67	GLU	CA	54.99	0.25	1
1	A	67	GLU	CB	31.19	0.25	1
1	A	67	GLU	CG	36.99	0.25	1
1	A	67	GLU	N	119.51	0.15	1
1	A	68	VAL	H	8.68	0.02	1
1	A	68	VAL	HA	4.51	0.02	1
1	A	68	VAL	HB	2.0	0.02	1
1	A	68	VAL	HG11	0.48	0.02	2
1	A	68	VAL	HG12	0.48	0.02	2
1	A	68	VAL	HG13	0.48	0.02	2
1	A	68	VAL	HG21	0.58	0.02	2
1	A	68	VAL	HG22	0.58	0.02	2
1	A	68	VAL	HG23	0.58	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	VAL	CA	58.83	0.25	1
1	A	68	VAL	CB	35.82	0.25	1
1	A	68	VAL	CG1	19.07	0.25	2
1	A	68	VAL	CG2	22.25	0.25	2
1	A	68	VAL	N	116.48	0.15	1
1	A	69	ASP	HA	5.12	0.02	1
1	A	69	ASP	HB2	2.25	0.02	2
1	A	69	ASP	HB3	2.43	0.02	2
1	A	69	ASP	CA	53.79	0.25	1
1	A	69	ASP	CB	41.68	0.25	1
1	A	70	VAL	H	9.07	0.02	1
1	A	70	VAL	HA	4.24	0.02	1
1	A	70	VAL	HB	1.85	0.02	1
1	A	70	VAL	HG11	0.69	0.02	2
1	A	70	VAL	HG12	0.69	0.02	2
1	A	70	VAL	HG13	0.69	0.02	2
1	A	70	VAL	HG21	0.72	0.02	2
1	A	70	VAL	HG22	0.72	0.02	2
1	A	70	VAL	HG23	0.72	0.02	2
1	A	70	VAL	CA	60.09	0.25	1
1	A	70	VAL	CB	34.77	0.25	1
1	A	70	VAL	CG1	20.79	0.25	2
1	A	70	VAL	CG2	21.66	0.25	2
1	A	70	VAL	N	120.66	0.15	1
1	A	71	ALA	H	8.47	0.02	1
1	A	71	ALA	HA	4.64	0.02	1
1	A	71	ALA	HB1	1.22	0.02	1
1	A	71	ALA	HB2	1.22	0.02	1
1	A	71	ALA	HB3	1.22	0.02	1
1	A	71	ALA	C	177.38	0.25	1
1	A	71	ALA	CA	50.81	0.25	1
1	A	71	ALA	CB	18.96	0.25	1
1	A	71	ALA	N	127.65	0.15	1
1	A	72	LEU	H	8.39	0.02	1
1	A	72	LEU	HA	4.18	0.02	1
1	A	72	LEU	HB2	1.5	0.02	2
1	A	72	LEU	HB3	1.45	0.02	2
1	A	72	LEU	HD11	0.7	0.02	1
1	A	72	LEU	HD12	0.7	0.02	1
1	A	72	LEU	HD13	0.7	0.02	1
1	A	72	LEU	CA	55.2	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	LEU	CB	42.77	0.25	1
1	A	72	LEU	N	124.33	0.15	1
1	A	73	ASP	HA	4.34	0.02	1
1	A	73	ASP	HB3	2.56	0.02	1
1	A	73	ASP	CA	54.8	0.25	1
1	A	73	ASP	CB	42.01	0.25	1
1	A	74	ALA	H	7.91	0.02	1
1	A	74	ALA	HA	4.25	0.02	1
1	A	74	ALA	HB1	1.28	0.02	1
1	A	74	ALA	HB2	1.28	0.02	1
1	A	74	ALA	HB3	1.28	0.02	1
1	A	74	ALA	CA	52.18	0.25	1
1	A	74	ALA	CB	19.2	0.25	1
1	A	74	ALA	N	122.62	0.15	1
1	A	75	VAL	H	7.84	0.02	1
1	A	75	VAL	HA	3.96	0.02	1
1	A	75	VAL	HB	2.0	0.02	1
1	A	75	VAL	HG11	0.8	0.02	2
1	A	75	VAL	HG12	0.8	0.02	2
1	A	75	VAL	HG13	0.8	0.02	2
1	A	75	VAL	HG21	0.81	0.02	2
1	A	75	VAL	HG22	0.81	0.02	2
1	A	75	VAL	HG23	0.81	0.02	2
1	A	75	VAL	C	176.46	0.25	1
1	A	75	VAL	CA	62.26	0.25	1
1	A	75	VAL	CB	32.64	0.25	1
1	A	75	VAL	CG1	20.68	0.25	2
1	A	75	VAL	CG2	21.25	0.25	2
1	A	75	VAL	N	118.41	0.15	1
1	A	76	GLU	H	8.38	0.02	1
1	A	76	GLU	HA	4.14	0.02	1
1	A	76	GLU	HB2	1.94	0.02	2
1	A	76	GLU	HB3	1.81	0.02	2
1	A	76	GLU	HG2	2.13	0.02	1
1	A	76	GLU	HG3	2.13	0.02	1
1	A	76	GLU	C	176.41	0.25	1
1	A	76	GLU	CA	56.91	0.25	1
1	A	76	GLU	CB	29.89	0.25	1
1	A	76	GLU	CG	36.35	0.25	1
1	A	76	GLU	N	123.87	0.15	1
1	A	77	ASP	H	8.27	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	ASP	HA	4.44	0.02	1
1	A	77	ASP	HB2	2.58	0.02	2
1	A	77	ASP	HB3	2.56	0.02	2
1	A	77	ASP	C	176.86	0.25	1
1	A	77	ASP	CA	54.52	0.25	1
1	A	77	ASP	CB	41.08	0.25	1
1	A	77	ASP	N	121.3	0.15	1
1	A	78	GLY	H	8.18	0.02	1
1	A	78	GLY	HA2	3.77	0.02	2
1	A	78	GLY	HA3	3.78	0.02	2
1	A	78	GLY	C	174.46	0.25	1
1	A	78	GLY	CA	45.54	0.25	1
1	A	78	GLY	N	108.55	0.15	1
1	A	79	PHE	H	8.08	0.02	1
1	A	79	PHE	HA	4.49	0.02	1
1	A	79	PHE	HB2	2.98	0.02	2
1	A	79	PHE	HB3	3.1	0.02	2
1	A	79	PHE	HD1	7.15	0.02	3
1	A	79	PHE	HD2	7.15	0.02	3
1	A	79	PHE	HE1	7.22	0.02	3
1	A	79	PHE	HE2	7.22	0.02	3
1	A	79	PHE	HZ	7.02	0.02	1
1	A	79	PHE	C	176.52	0.25	1
1	A	79	PHE	CA	58.22	0.25	1
1	A	79	PHE	CB	39.41	0.25	1
1	A	79	PHE	N	120.13	0.15	1
1	A	80	GLY	H	8.32	0.02	1
1	A	80	GLY	HA2	3.83	0.02	2
1	A	80	GLY	HA3	3.74	0.02	2
1	A	80	GLY	C	174.29	0.25	1
1	A	80	GLY	CA	45.33	0.25	1
1	A	80	GLY	N	110.02	0.15	1
1	A	81	GLU	H	8.17	0.02	1
1	A	81	GLU	HA	4.2	0.02	1
1	A	81	GLU	HB2	1.88	0.02	2
1	A	81	GLU	HB3	1.94	0.02	2
1	A	81	GLU	HG2	2.12	0.02	2
1	A	81	GLU	HG3	2.18	0.02	2
1	A	81	GLU	C	177.14	0.25	1
1	A	81	GLU	CA	56.9	0.25	1
1	A	81	GLU	CB	29.52	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	GLU	CG	36.3	0.25	1
1	A	81	GLU	N	120.56	0.15	1
1	A	82	THR	H	8.19	0.02	1
1	A	82	THR	HA	4.21	0.02	1
1	A	82	THR	HB	4.21	0.02	1
1	A	82	THR	HG21	1.11	0.02	1
1	A	82	THR	HG22	1.11	0.02	1
1	A	82	THR	HG23	1.11	0.02	1
1	A	82	THR	CA	62.2	0.25	1
1	A	82	THR	CB	69.61	0.25	1
1	A	82	THR	CG2	21.57	0.25	1
1	A	82	THR	N	114.98	0.15	1

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	167	$0.17 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	147	$0.15 \pm 0.21$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	160	$0.11 \pm 0.22$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	163	$-0.00 \pm 0.46$	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 77%, i.e. 1002 atoms were assigned a chemical shift out of a possible 1296. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	437/463 (94%)	180/189 (95%)	172/184 (93%)	85/90 (94%)
Sidechain	523/768 (68%)	351/496 (71%)	166/236 (70%)	6/36 (17%)
Aromatic	42/65 (65%)	29/33 (88%)	12/29 (41%)	1/3 (33%)
Overall	1002/1296 (77%)	560/718 (78%)	350/449 (78%)	92/129 (71%)

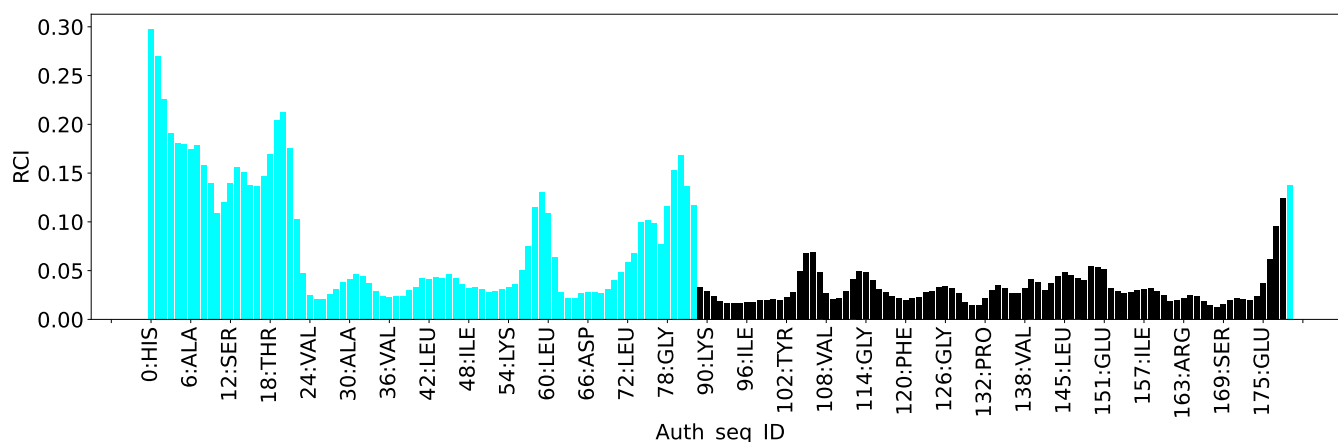
### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

### 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	619
Intra-residue ( $ i-j =0$ )	175
Sequential ( $ i-j =1$ )	193
Medium range ( $ i-j >1$ and $ i-j <5$ )	63
Long range ( $ i-j \geq 5$ )	188
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	3.4
Number of long range restraints per residue <sup>1</sup>	1.0

<sup>1</sup>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)	0.7	0.17
0.2-0.5 (Medium)	0.5	0.26
>0.5 (Large)	None	None

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

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis ⓘ

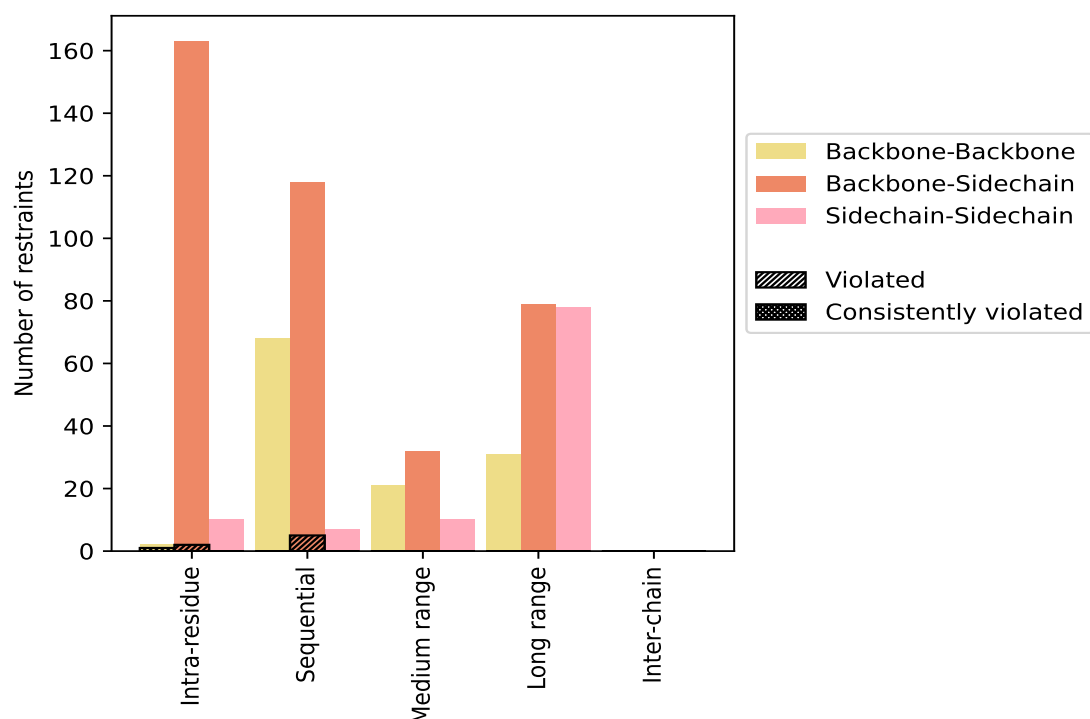
### 9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">175</a>	<a href="#">28.3</a>	<a href="#">3</a>	<a href="#">1.7</a>	<a href="#">0.5</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	2	0.3	1	50.0	0.2	0	0.0	0.0
Backbone-Sidechain	163	26.3	2	1.2	0.3	0	0.0	0.0
Sidechain-Sidechain	10	1.6	0	0.0	0.0	0	0.0	0.0
<a href="#">Sequential ( i-j =1)</a>	<a href="#">193</a>	<a href="#">31.2</a>	<a href="#">5</a>	<a href="#">2.6</a>	<a href="#">0.8</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	68	11.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	118	19.1	5	4.2	0.8	0	0.0	0.0
Sidechain-Sidechain	7	1.1	0	0.0	0.0	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">63</a>	<a href="#">10.2</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	21	3.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	32	5.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	10	1.6	0	0.0	0.0	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">188</a>	<a href="#">30.4</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	31	5.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	79	12.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	78	12.6	0	0.0	0.0	0	0.0	0.0
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
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
<a href="#">Hydrogen bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">619</a>	<a href="#">100.0</a>	<a href="#">8</a>	<a href="#">1.3</a>	<a href="#">1.3</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	122	19.7	1	0.8	0.2	0	0.0	0.0
Backbone-Sidechain	392	63.3	7	1.8	1.1	0	0.0	0.0
Sidechain-Sidechain	105	17.0	0	0.0	0.0	0	0.0	0.0

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

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



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

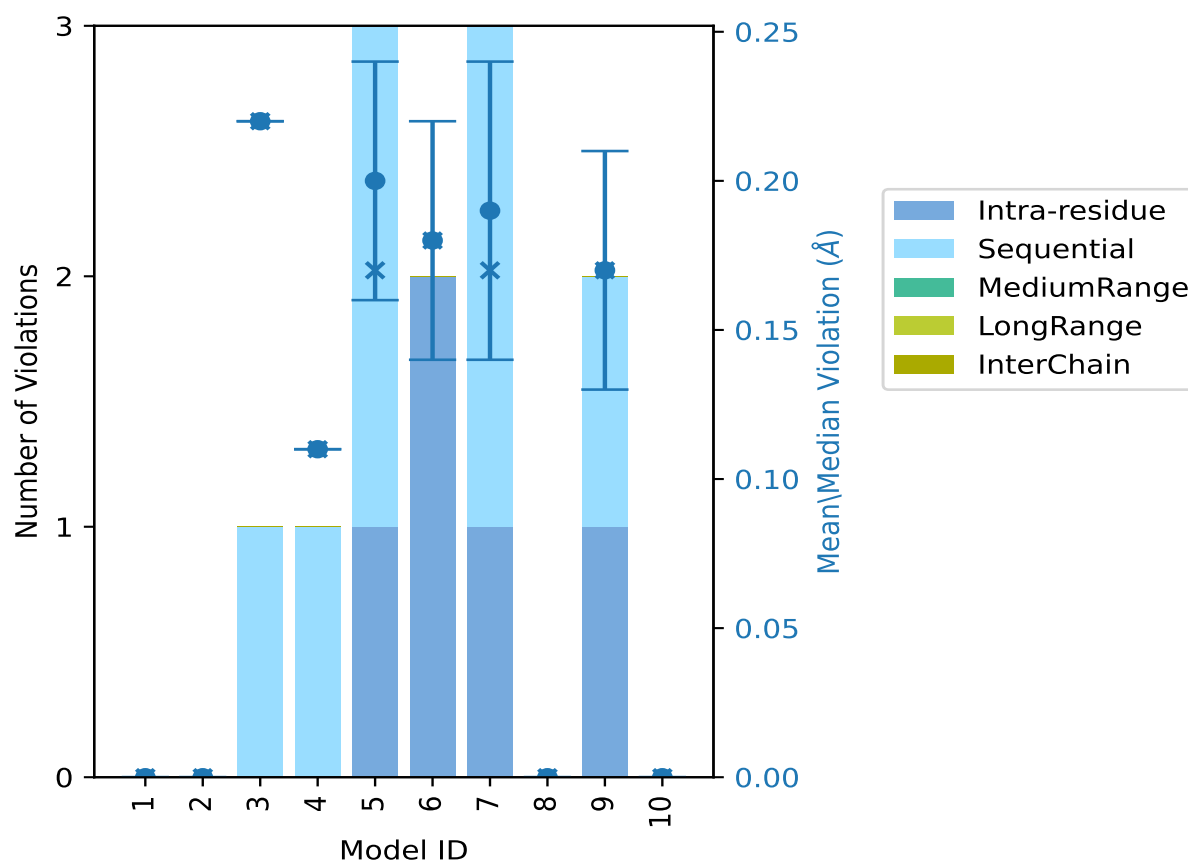
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	1	0	0	0	1	0.22	0.22	0.0	0.22
4	0	1	0	0	0	1	0.11	0.11	0.0	0.11
5	1	2	0	0	0	3	0.2	0.26	0.04	0.17
6	2	0	0	0	0	2	0.18	0.22	0.04	0.18
7	1	2	0	0	0	3	0.19	0.26	0.05	0.17
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	1	1	0	0	0	2	0.17	0.21	0.04	0.17
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance 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

### 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, 611(IR:172, SQ:188, MR:63, LR:188, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
2	3	0	0	0	5	1	10.0
0	2	0	0	0	2	2	20.0
1	0	0	0	0	1	3	30.0

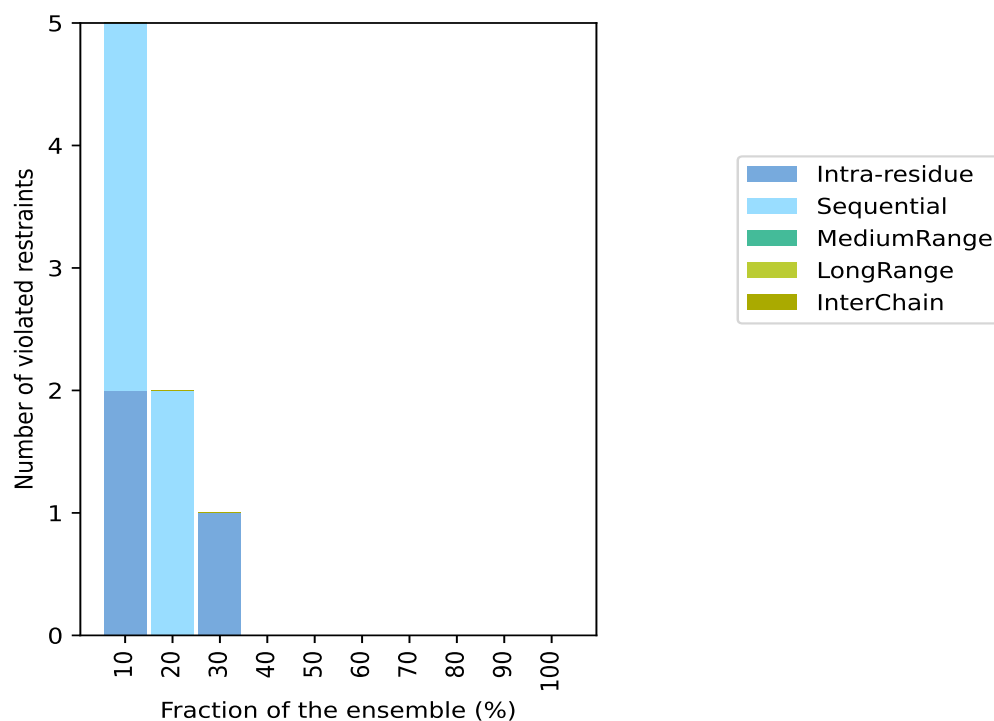
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
0	0	0	0	0	0	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

### 9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



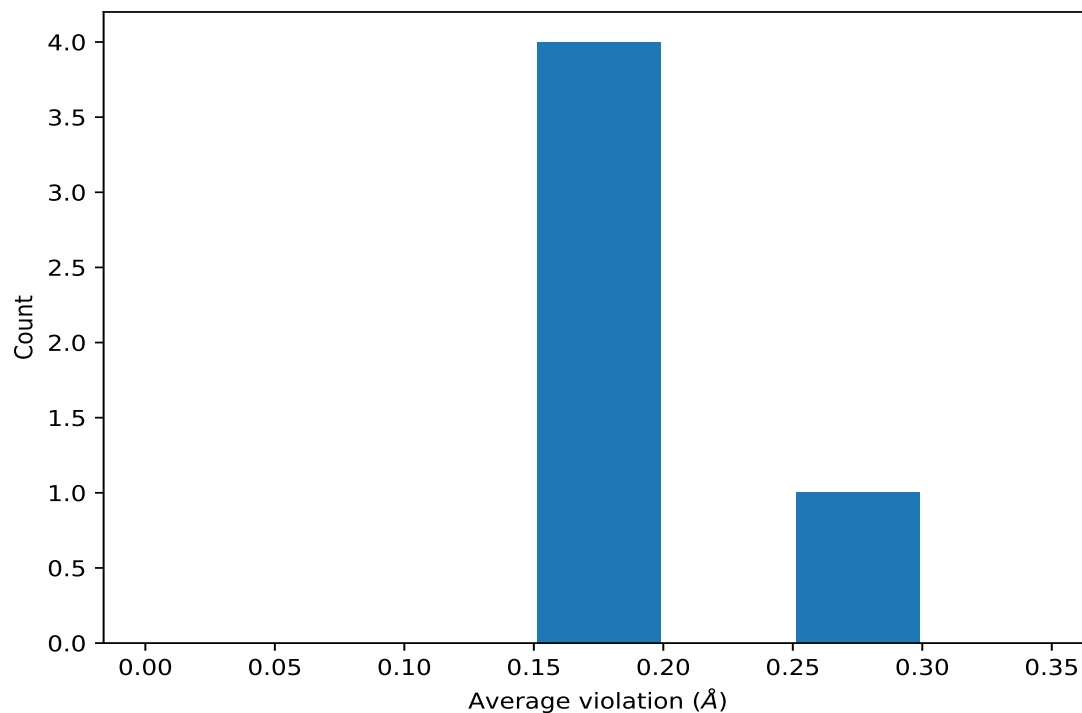
## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

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



in the ensemble



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

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean 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.

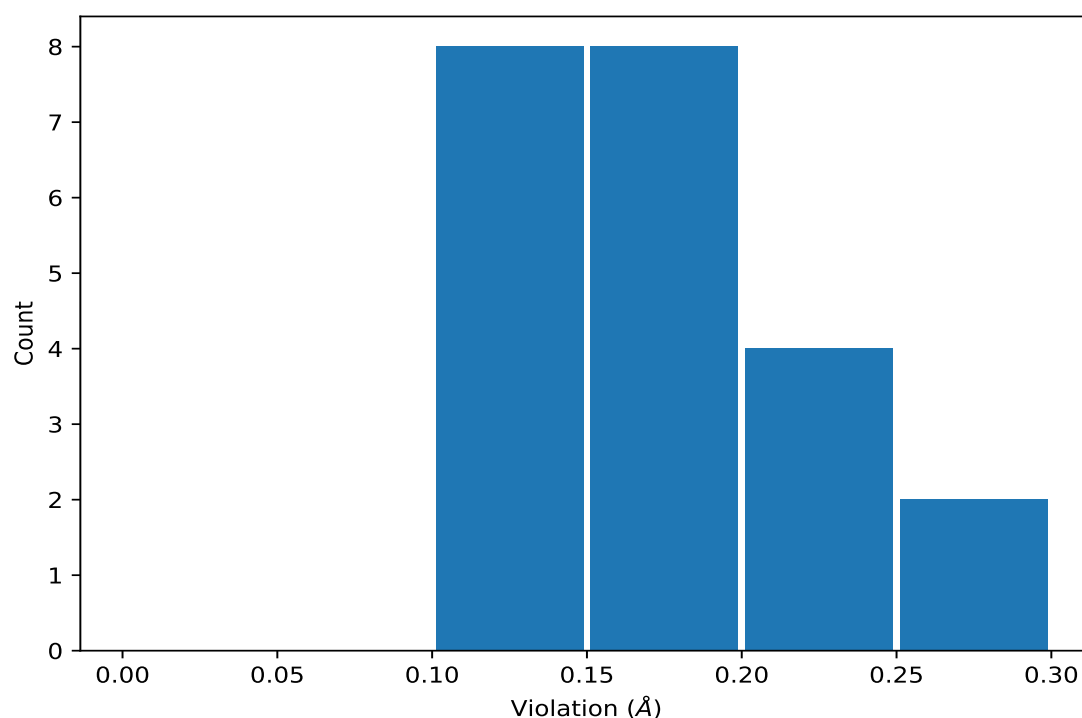
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,424)	1:99:A:GLU:H	1:99:A:GLU:HG2	3	0.18	0.03	0.16
(1,424)	1:99:A:GLU:H	1:99:A:GLU:HG3	3	0.18	0.03	0.16
(1,149)	1:177:A:GLU:HB3	1:178:A:ASN:H	2	0.26	0.0	0.26
(1,614)	1:177:A:GLU:HB2	1:178:A:ASN:H	2	0.17	0.0	0.17
(1,614)	1:177:A:GLU:HB3	1:178:A:ASN:H	2	0.17	0.0	0.17

<sup>1</sup>Number of violated models, <sup>2</sup>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)
(1,149)	1:177:A:GLU:HB3	1:178:A:ASN:H	5	0.26
(1,149)	1:177:A:GLU:HB3	1:178:A:ASN:H	7	0.26
(1,424)	1:99:A:GLU:H	1:99:A:GLU:HG2	6	0.22
(1,424)	1:99:A:GLU:H	1:99:A:GLU:HG3	6	0.22
(1,179)	1:174:A:ILE:HG13	1:175:A:GLU:H	3	0.22
(1,104)	1:136:A:VAL:H	1:136:A:VAL:HB	9	0.21
(1,614)	1:177:A:GLU:HB2	1:178:A:ASN:H	5	0.17
(1,614)	1:177:A:GLU:HB3	1:178:A:ASN:H	5	0.17
(1,614)	1:177:A:GLU:HB2	1:178:A:ASN:H	7	0.17
(1,614)	1:177:A:GLU:HB3	1:178:A:ASN:H	7	0.17
(1,424)	1:99:A:GLU:H	1:99:A:GLU:HG2	5	0.16
(1,424)	1:99:A:GLU:H	1:99:A:GLU:HG3	5	0.16
(1,424)	1:99:A:GLU:H	1:99:A:GLU:HG2	7	0.15
(1,424)	1:99:A:GLU:H	1:99:A:GLU:HG3	7	0.15
(1,147)	1:179:A:SER:H	1:179:A:SER:HA	6	0.13

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found