



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 05:36 PM UTC

PDB ID : 2MX2 / pdb\_00002mx2  
BMRB ID : 25382  
Title : UBX-L domain of VCIP135  
Authors : Iwazu, T.; Murayama, S.; Igarashi, R.; Hrioaki, H.; Shirakawa, M.; Tochio, H.  
Deposited on : 2014-12-07

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

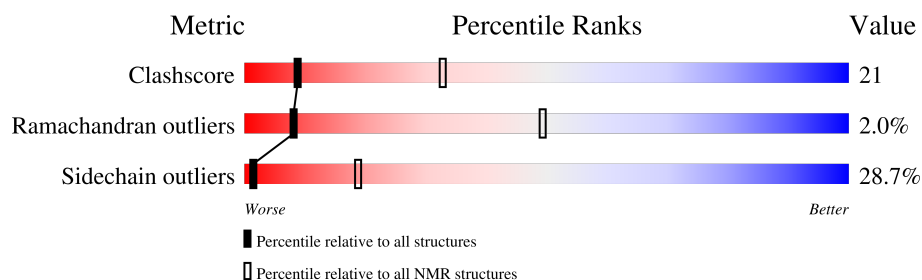
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	86	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:7-A:86 (80)	0.34	15

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 5 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1327 atoms, of which 673 are hydrogens and 0 are deuteriums.

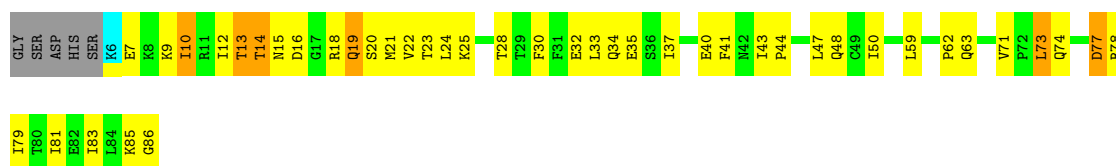
- Molecule 1 is a protein called Deubiquitinating protein VCIP135.

Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1327	417	673	112	121	4	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8CF97
A	2	SER	-	expression tag	UNP Q8CF97
A	3	ASP	-	expression tag	UNP Q8CF97
A	4	HIS	-	expression tag	UNP Q8CF97
A	5	SER	-	expression tag	UNP Q8CF97

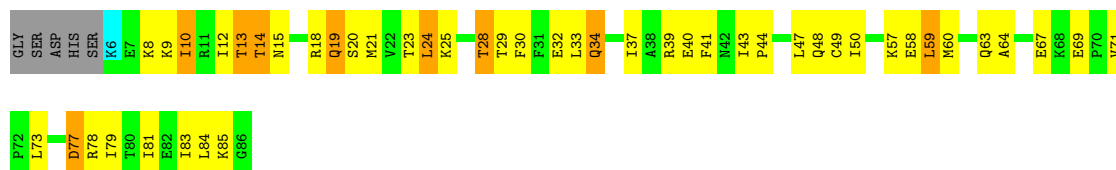




### 4.2.3 Score per residue for model 3

- Molecule 1: Deubiquitinating protein VCIP135

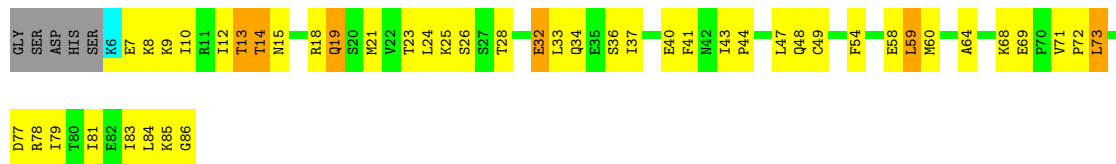
Chain A: 38% 44% 10% • 6%



### 4.2.4 Score per residue for model 4

- Molecule 1: Deubiquitinating protein VCIP135

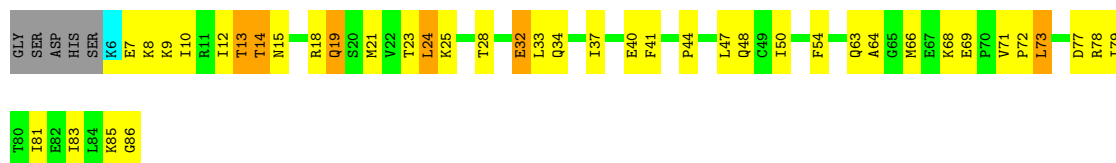
Chain A: 40% 47% 7% • 6%



### 4.2.5 Score per residue for model 5

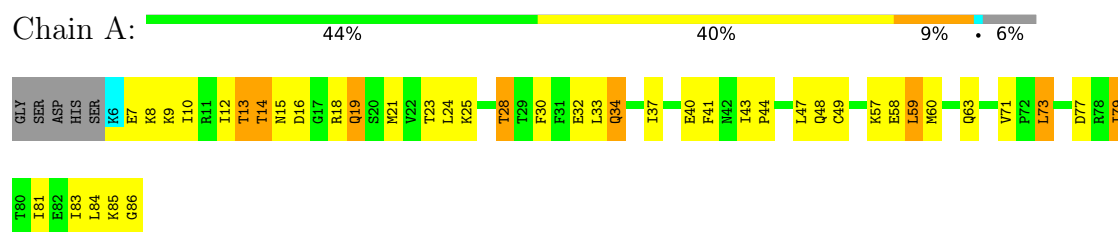
- Molecule 1: Deubiquitinating protein VCIP135

Chain A: 45% 41% 7% • 6%



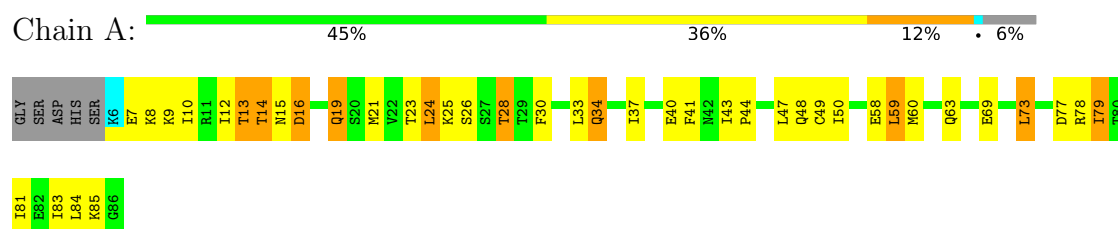
### 4.2.6 Score per residue for model 6

- Molecule 1: Deubiquitinating protein VCIP135



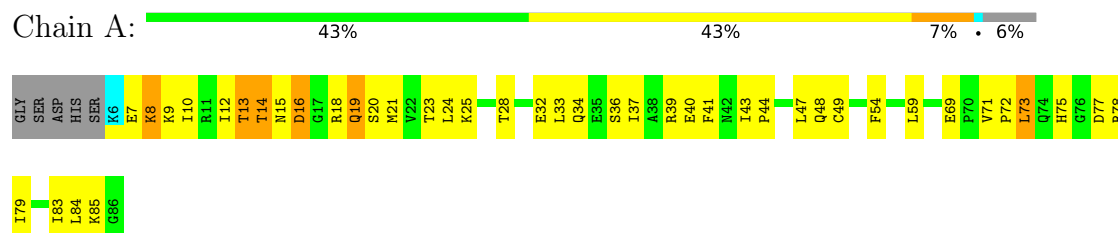
#### 4.2.7 Score per residue for model 7

- Molecule 1: Deubiquitinating protein VCIP135



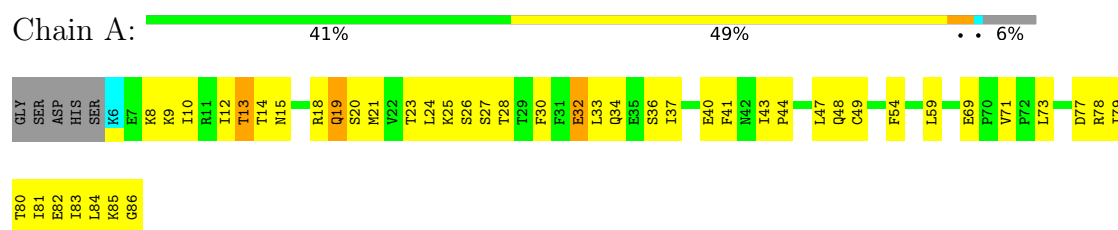
#### 4.2.8 Score per residue for model 8

- Molecule 1: Deubiquitinating protein VCIP135



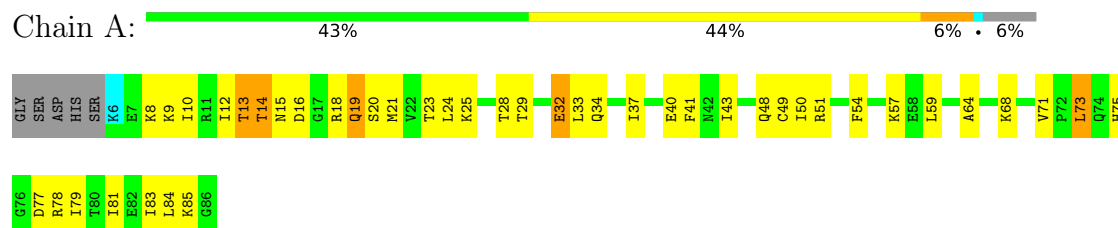
#### 4.2.9 Score per residue for model 9

- Molecule 1: Deubiquitinating protein VCIP135



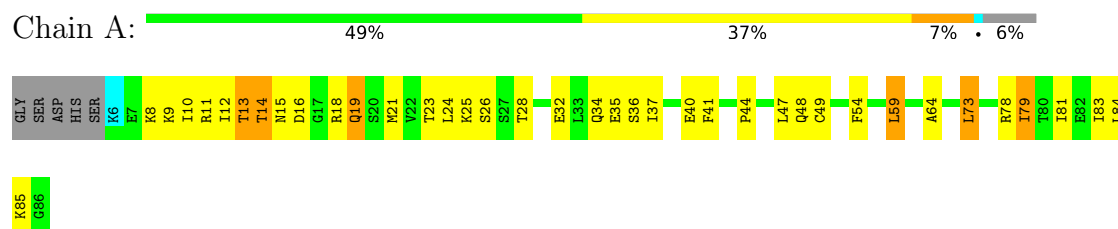
#### 4.2.10 Score per residue for model 10

- Molecule 1: Deubiquitinating protein VCIP135



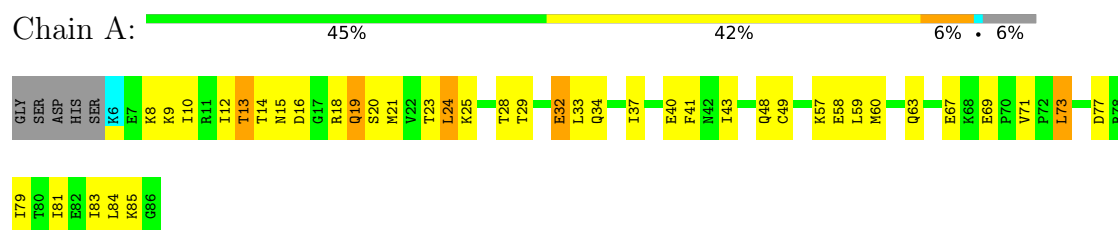
#### 4.2.11 Score per residue for model 11

- Molecule 1: Deubiquitinating protein VCIP135



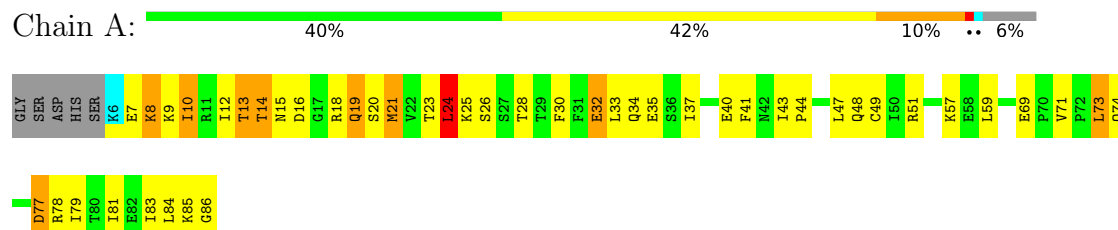
#### 4.2.12 Score per residue for model 12

- Molecule 1: Deubiquitinating protein VCIP135



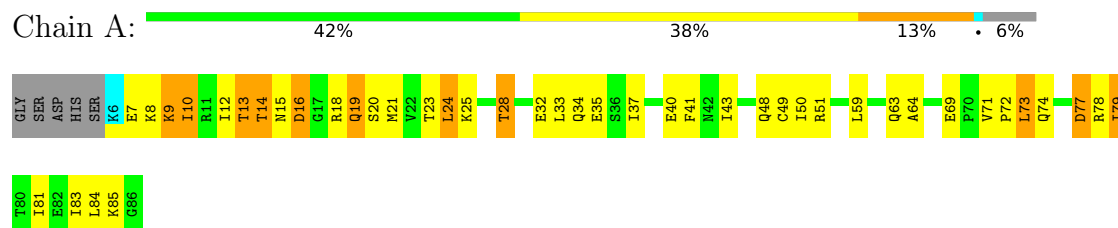
#### 4.2.13 Score per residue for model 13

- Molecule 1: Deubiquitinating protein VCIP135



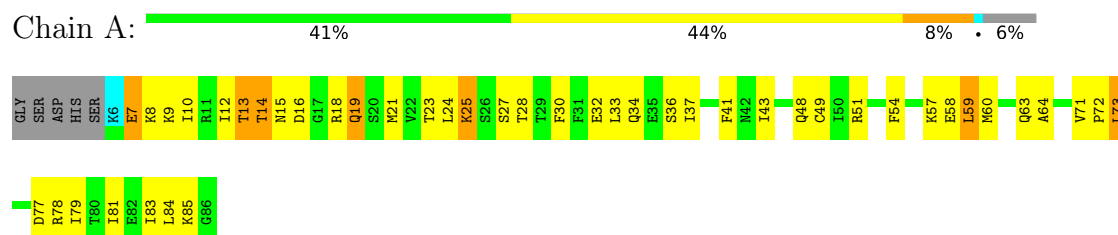
#### 4.2.14 Score per residue for model 14

- Molecule 1: Deubiquitinating protein VCIP135



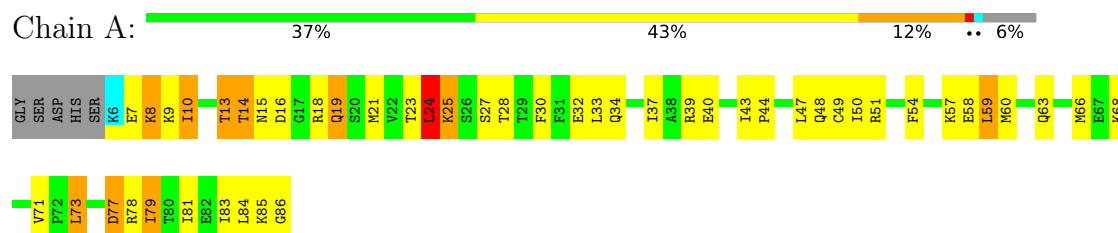
#### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Deubiquitinating protein VCIP135



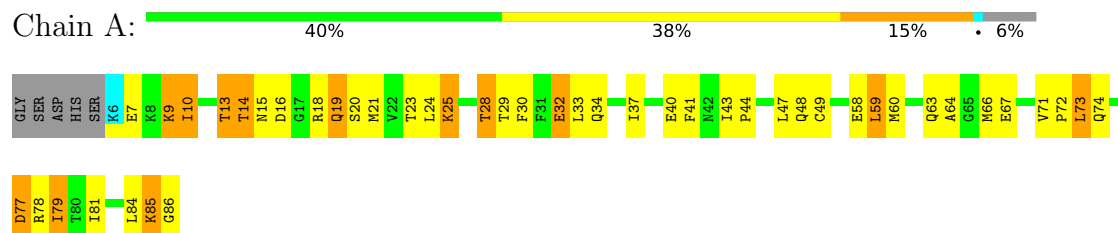
#### 4.2.16 Score per residue for model 16

- Molecule 1: Deubiquitinating protein VCIP135



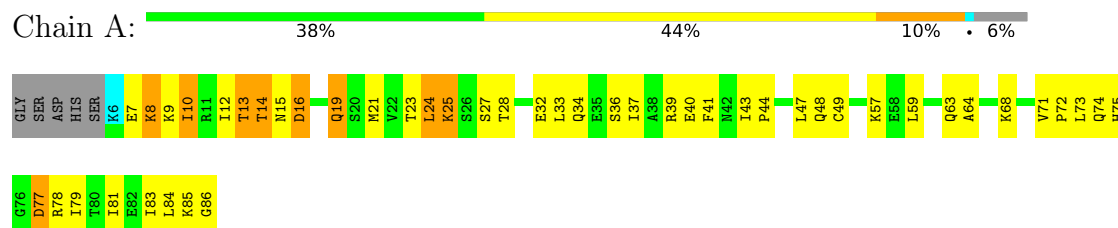
#### 4.2.17 Score per residue for model 17

- Molecule 1: Deubiquitinating protein VCIP135



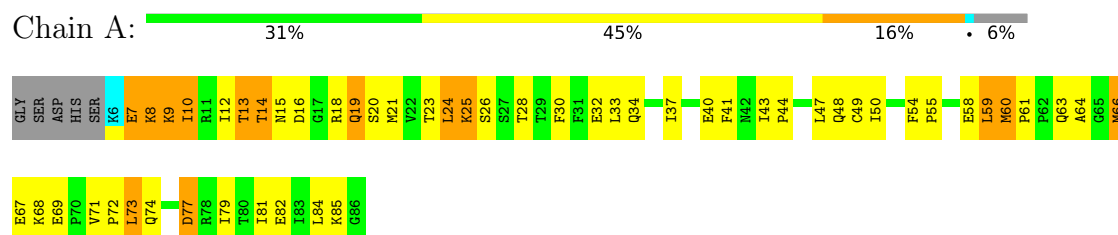
### 4.2.18 Score per residue for model 18

- Molecule 1: Deubiquitinating protein VCIP135



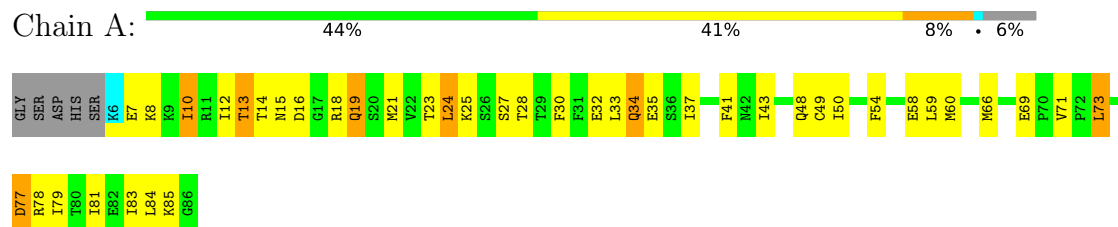
### 4.2.19 Score per residue for model 19

- Molecule 1: Deubiquitinating protein VCIP135



### 4.2.20 Score per residue for model 20

- Molecule 1: Deubiquitinating protein VCIP135



## 5 Refinement protocol and experimental data overview

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

Of the 200 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 solution	
CYANA	refinement	
CNS	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	1033
Number of shifts mapped to atoms	1006
Number of unparsed shifts	0
Number of shifts with mapping errors	27
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

## 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	645	660	659	27±5
All	All	12900	13200	13180	548

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD22	1:A:84:LEU:O	0.79	1.77	17	1
1:A:8:LYS:HG3	1:A:10:ILE:HD11	0.75	1.57	19	4
1:A:15:ASN:OD1	1:A:83:ILE:HD12	0.73	1.82	20	13
1:A:49:CYS:HB2	1:A:84:LEU:HD21	0.72	1.61	17	18
1:A:9:LYS:C	1:A:10:ILE:HD13	0.72	2.08	19	6
1:A:13:THR:HG23	1:A:19:GLN:HB3	0.70	1.61	14	20
1:A:44:PRO:CG	1:A:47:LEU:HD12	0.69	2.18	13	15
1:A:24:LEU:CD2	1:A:71:VAL:HG21	0.68	2.18	17	12
1:A:47:LEU:HD21	1:A:86:GLY:HA3	0.68	1.63	2	5
1:A:10:ILE:HD12	1:A:74:GLN:O	0.64	1.93	2	6
1:A:37:ILE:HG22	1:A:48:GLN:OE1	0.64	1.93	11	20
1:A:23:THR:HG23	1:A:23:THR:O	0.63	1.93	19	18
1:A:16:ASP:OD1	1:A:83:ILE:HD13	0.62	1.94	1	4
1:A:10:ILE:HG22	1:A:77:ASP:C	0.61	2.21	16	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:THR:HG21	1:A:18:ARG:NH2	0.60	2.11	20	1
1:A:18:ARG:NH2	1:A:43:ILE:CD1	0.60	2.65	20	1
1:A:24:LEU:HD21	1:A:71:VAL:HG21	0.59	1.73	19	6
1:A:28:THR:HG23	1:A:32:GLU:HB3	0.59	1.75	9	14
1:A:37:ILE:HG21	1:A:81:ILE:HG13	0.59	1.73	16	19
1:A:8:LYS:CD	1:A:10:ILE:HD11	0.58	2.27	16	1
1:A:24:LEU:HD23	1:A:71:VAL:HG21	0.58	1.76	6	6
1:A:33:LEU:HD22	1:A:71:VAL:HG11	0.58	1.75	6	13
1:A:47:LEU:HD21	1:A:86:GLY:CA	0.58	2.28	16	6
1:A:66:MET:HE3	1:A:69:GLU:OE1	0.58	1.98	19	1
1:A:73:LEU:CD1	1:A:79:ILE:HD13	0.57	2.30	17	7
1:A:14:THR:OG1	1:A:18:ARG:HG2	0.57	1.99	5	10
1:A:14:THR:OG1	1:A:18:ARG:CZ	0.56	2.53	20	1
1:A:28:THR:HG23	1:A:32:GLU:CB	0.56	2.31	17	19
1:A:24:LEU:HG	1:A:28:THR:HG21	0.56	1.78	5	18
1:A:33:LEU:O	1:A:37:ILE:HD12	0.56	2.01	9	1
1:A:24:LEU:CD1	1:A:28:THR:HG21	0.54	2.32	19	1
1:A:12:ILE:HG21	1:A:41:PHE:CE1	0.54	2.37	19	12
1:A:25:LYS:N	1:A:25:LYS:CE	0.53	2.71	16	3
1:A:23:THR:O	1:A:24:LEU:C	0.53	2.51	13	8
1:A:49:CYS:CB	1:A:84:LEU:HD21	0.53	2.33	17	4
1:A:8:LYS:HE2	1:A:10:ILE:HD11	0.53	1.80	16	1
1:A:58:GLU:O	1:A:60:MET:N	0.53	2.41	4	11
1:A:12:ILE:O	1:A:19:GLN:HA	0.52	2.04	20	1
1:A:18:ARG:NH2	1:A:43:ILE:HD13	0.52	2.19	20	1
1:A:59:LEU:HD21	1:A:72:PRO:CD	0.52	2.35	4	1
1:A:9:LYS:O	1:A:10:ILE:HD13	0.52	2.05	19	6
1:A:29:THR:HG22	1:A:32:GLU:OE2	0.52	2.05	12	2
1:A:10:ILE:HD12	1:A:24:LEU:HD22	0.51	1.81	1	1
1:A:37:ILE:HG23	1:A:41:PHE:CD1	0.51	2.40	4	5
1:A:33:LEU:CD2	1:A:71:VAL:HG11	0.51	2.36	6	11
1:A:23:THR:O	1:A:23:THR:HG23	0.50	2.05	11	2
1:A:12:ILE:HG21	1:A:41:PHE:CE2	0.50	2.42	20	1
1:A:25:LYS:N	1:A:25:LYS:HE2	0.50	2.22	18	1
1:A:73:LEU:CD1	1:A:79:ILE:HG21	0.50	2.37	20	17
1:A:14:THR:CG2	1:A:41:PHE:CD2	0.49	2.96	7	9
1:A:14:THR:HG21	1:A:18:ARG:HH21	0.49	1.67	20	1
1:A:29:THR:HG21	1:A:67:GLU:O	0.49	2.07	3	3
1:A:73:LEU:HD11	1:A:79:ILE:HG21	0.49	1.85	17	11
1:A:33:LEU:HD21	1:A:50:ILE:HD13	0.49	1.85	3	1
1:A:12:ILE:CG2	1:A:41:PHE:CE1	0.48	2.96	19	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:GLU:HB3	1:A:25:LYS:HA	0.48	1.86	15	1
1:A:44:PRO:HG2	1:A:47:LEU:HD12	0.48	1.85	13	3
1:A:24:LEU:HD21	1:A:33:LEU:HD13	0.48	1.85	16	3
1:A:10:ILE:HG22	1:A:77:ASP:O	0.48	2.09	16	4
1:A:12:ILE:HD11	1:A:22:VAL:CG2	0.48	2.39	2	1
1:A:8:LYS:CE	1:A:10:ILE:HD11	0.48	2.39	16	1
1:A:51:ARG:O	1:A:79:ILE:HG22	0.48	2.09	13	1
1:A:14:THR:HG23	1:A:41:PHE:CE2	0.47	2.45	5	7
1:A:15:ASN:OD1	1:A:15:ASN:N	0.47	2.47	20	4
1:A:50:ILE:HA	1:A:81:ILE:HD13	0.47	1.87	2	3
1:A:33:LEU:CD2	1:A:50:ILE:HD13	0.47	2.40	5	8
1:A:12:ILE:CG2	1:A:41:PHE:CZ	0.47	2.98	7	6
1:A:18:ARG:NH1	1:A:43:ILE:HD11	0.47	2.25	4	1
1:A:54:PHE:HA	1:A:55:PRO:C	0.46	2.34	19	1
1:A:12:ILE:CG2	1:A:41:PHE:CE2	0.46	2.99	20	1
1:A:43:ILE:HG22	1:A:48:GLN:HG3	0.46	1.87	9	17
1:A:59:LEU:HD21	1:A:72:PRO:HD2	0.45	1.87	4	2
1:A:37:ILE:HG23	1:A:41:PHE:CD2	0.45	2.46	20	1
1:A:18:ARG:HH12	1:A:83:ILE:HD11	0.45	1.71	12	12
1:A:13:THR:O	1:A:81:ILE:N	0.45	2.50	16	6
1:A:25:LYS:N	1:A:25:LYS:HE3	0.45	2.27	19	1
1:A:41:PHE:CD1	1:A:41:PHE:N	0.45	2.84	11	4
1:A:11:ARG:HG2	1:A:12:ILE:N	0.45	2.26	11	1
1:A:85:LYS:O	1:A:85:LYS:CG	0.44	2.65	17	1
1:A:30:PHE:CE1	1:A:50:ILE:HD12	0.44	2.47	7	1
1:A:71:VAL:HB	1:A:72:PRO:HD2	0.43	1.90	18	6
1:A:14:THR:CB	1:A:18:ARG:NH2	0.43	2.81	20	1
1:A:14:THR:CG2	1:A:18:ARG:NH2	0.43	2.80	20	1
1:A:18:ARG:NH1	1:A:83:ILE:HD11	0.43	2.28	4	2
1:A:8:LYS:HD2	1:A:10:ILE:HD11	0.43	1.90	16	1
1:A:85:LYS:CE	1:A:85:LYS:H	0.43	2.27	17	1
1:A:24:LEU:HD11	1:A:28:THR:HG21	0.43	1.90	19	1
1:A:18:ARG:NH2	1:A:43:ILE:HD11	0.43	2.28	20	1
1:A:14:THR:OG1	1:A:18:ARG:CG	0.43	2.67	4	2
1:A:13:THR:O	1:A:80:THR:HG23	0.42	2.14	9	1
1:A:28:THR:O	1:A:71:VAL:N	0.42	2.52	19	1
1:A:30:PHE:CE1	1:A:59:LEU:O	0.42	2.73	15	11
1:A:7:GLU:HB2	1:A:25:LYS:HA	0.42	1.91	17	1
1:A:21:MET:O	1:A:21:MET:HE2	0.42	2.14	13	1
1:A:8:LYS:HB2	1:A:75:HIS:CA	0.41	2.45	18	3
1:A:51:ARG:CB	1:A:57:LYS:O	0.41	2.68	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ILE:HG22	1:A:51:ARG:N	0.41	2.31	14	2
1:A:16:ASP:CB	1:A:18:ARG:NH1	0.41	2.83	20	1
1:A:8:LYS:HG2	1:A:24:LEU:O	0.41	2.15	1	1
1:A:81:ILE:HG22	1:A:82:GLU:N	0.41	2.30	19	2
1:A:16:ASP:CB	1:A:18:ARG:NH2	0.41	2.84	14	2
1:A:60:MET:HB2	1:A:61:PRO:HD2	0.41	1.93	19	1
1:A:30:PHE:CZ	1:A:34:GLN:OE1	0.41	2.74	20	2
1:A:24:LEU:CD1	1:A:33:LEU:HD13	0.41	2.45	17	2
1:A:13:THR:HG23	1:A:19:GLN:CB	0.40	2.43	16	1
1:A:14:THR:N	1:A:18:ARG:O	0.40	2.54	6	2
1:A:51:ARG:CG	1:A:57:LYS:O	0.40	2.69	15	1
1:A:30:PHE:CE2	1:A:34:GLN:OE1	0.40	2.75	6	2
1:A:85:LYS:O	1:A:85:LYS:HG2	0.40	2.16	17	1

## 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	79/86 (92%)	69±1 (87±2%)	9±1 (11±2%)	2±1 (2±1%)	8	49
All	All	1580/1720 (92%)	1376 (87%)	172 (11%)	32 (2%)	8	49

All 5 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	59	LEU	16
1	A	64	ALA	10
1	A	24	LEU	3
1	A	7	GLU	2
1	A	62	PRO	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	73/78 (94%)	52±2 (71±3%)	21±2 (29±3%)	1	19
All	All	1460/1560 (94%)	1041 (71%)	419 (29%)	1	19

All 36 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	10	ILE	20
1	A	13	THR	20
1	A	19	GLN	20
1	A	21	MET	20
1	A	25	LYS	20
1	A	34	GLN	20
1	A	73	LEU	20
1	A	85	LYS	20
1	A	14	THR	19
1	A	77	ASP	19
1	A	40	GLU	18
1	A	9	LYS	16
1	A	78	ARG	16
1	A	8	LYS	15
1	A	16	ASP	14
1	A	63	GLN	13
1	A	7	GLU	12
1	A	69	GLU	11
1	A	24	LEU	10
1	A	79	ILE	10
1	A	20	SER	10
1	A	54	PHE	9
1	A	32	GLU	7
1	A	15	ASN	7
1	A	66	MET	6
1	A	57	LYS	6
1	A	26	SER	6
1	A	36	SER	6
1	A	68	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	39	ARG	5
1	A	35	GLU	5
1	A	28	THR	5
1	A	27	SER	5
1	A	59	LEU	1
1	A	60	MET	1
1	A	67	GLU	1

### 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 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: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1033
Number of shifts mapped to atoms	1006
Number of unparsed shifts	0
Number of shifts with mapping errors	27
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	227

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

- No matching atom found in the structure. All 27 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	GLY	HA2	3.791	0.000	.
1	A	1	GLY	HA3	3.791	0.000	.
1	A	1	GLY	CA	71.841	0.000	1
1	A	2	SER	HA	4.428	0.000	1
1	A	2	SER	HB2	3.759	0.000	.
1	A	2	SER	HB3	3.759	0.000	.
1	A	2	SER	CA	58.26	0.000	1
1	A	2	SER	CB	63.819	0.000	1
1	A	3	ASP	HA	4.55	0.000	1
1	A	3	ASP	HB2	2.636	0.000	.
1	A	3	ASP	HB3	2.551	0.000	.
1	A	3	ASP	CA	54.107	0.000	1
1	A	3	ASP	CB	68.941	0.000	1
1	A	4	HIS	HA	4.584	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	HIS	HB2	3.135	0.000	.
1	A	4	HIS	HB3	3.002	0.000	.
1	A	4	HIS	HD2	6.955	0.000	1
1	A	4	HIS	HE1	7.815	0.000	1
1	A	4	HIS	CA	56.572	0.000	1
1	A	4	HIS	CB	58.172	0.000	1
1	A	4	HIS	CD2	64.111	0.000	1
1	A	4	HIS	CE1	54.216	0.000	1
1	A	5	SER	HA	4.324	0.000	1
1	A	5	SER	HB2	3.852	0.000	.
1	A	5	SER	HB3	3.805	0.000	.
1	A	5	SER	CA	59.114	0.000	1
1	A	5	SER	CB	63.63	0.000	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
$^{13}\text{C}_\alpha$	86	$0.32 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	80	$0.00 \pm 0.00$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	70	$-0.07 \pm 0.65$	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. 987 atoms were assigned a chemical shift out of a possible 1135. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	305/389 (78%)	155/157 (99%)	80/160 (50%)	70/72 (97%)
Sidechain	621/680 (91%)	422/440 (96%)	190/212 (90%)	9/28 (32%)
Aromatic	61/66 (92%)	31/32 (97%)	30/32 (94%)	0/2 (0%)
Overall	987/1135 (87%)	608/629 (97%)	300/404 (74%)	79/102 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1001 atoms were assigned a chemical shift out of a possible 1153. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	307/394 (78%)	156/159 (98%)	81/162 (50%)	70/73 (96%)
Sidechain	633/693 (91%)	430/448 (96%)	194/216 (90%)	9/29 (31%)
Aromatic	61/66 (92%)	31/32 (97%)	30/32 (94%)	0/2 (0%)
Overall	1001/1153 (87%)	617/639 (97%)	305/410 (74%)	79/104 (76%)

### 7.1.4 Statistically unusual chemical shifts ⓘ

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	46	TYR	CD1	49.37	125.84 – 139.60	-60.6
1	A	52	TYR	CD1	49.44	125.84 – 139.60	-60.5
1	A	46	TYR	CD2	49.37	125.28 – 140.14	-56.1
1	A	52	TYR	CD2	49.44	125.28 – 140.14	-56.0
1	A	54	PHE	CE2	73.94	124.80 – 136.72	-47.7
1	A	41	PHE	CE2	74.73	124.80 – 136.72	-47.0
1	A	41	PHE	CD2	75.03	125.53 – 137.61	-46.8
1	A	30	PHE	CD2	75.21	125.53 – 137.61	-46.7
1	A	54	PHE	CD2	75.56	125.53 – 137.61	-46.4
1	A	30	PHE	CE2	75.56	124.80 – 136.72	-46.3
1	A	31	PHE	CD2	75.75	125.53 – 137.61	-46.2
1	A	31	PHE	CE2	75.78	124.80 – 136.72	-46.1
1	A	41	PHE	CD1	75.03	125.33 – 137.83	-45.2
1	A	30	PHE	CD1	75.21	125.33 – 137.83	-45.1
1	A	52	TYR	CE2	61.69	111.68 – 124.17	-45.0
1	A	54	PHE	CD1	75.56	125.33 – 137.83	-44.8
1	A	31	PHE	CD1	75.75	125.33 – 137.83	-44.7
1	A	46	TYR	CE2	62.64	111.68 – 124.17	-44.3
1	A	79	ILE	CG2	75.14	10.93 – 24.12	43.7
1	A	12	ILE	CG2	74.92	10.93 – 24.12	43.5
1	A	50	ILE	CG2	74.88	10.93 – 24.12	43.5
1	A	43	ILE	CG2	74.68	10.93 – 24.12	43.3
1	A	54	PHE	CE1	73.94	124.17 – 137.29	-43.3
1	A	37	ILE	CG2	74.26	10.93 – 24.12	43.0
1	A	10	ILE	CG2	73.87	10.93 – 24.12	42.7
1	A	41	PHE	CE1	74.73	124.17 – 137.29	-42.7
1	A	83	ILE	CG2	73.76	10.93 – 24.12	42.6
1	A	81	ILE	CG2	73.65	10.93 – 24.12	42.6
1	A	30	PHE	CE1	75.56	124.17 – 137.29	-42.0
1	A	52	TYR	CE1	61.69	111.24 – 124.66	-41.9
1	A	31	PHE	CE1	75.78	124.17 – 137.29	-41.9

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	46	TYR	CE1	62.64	111.24 – 124.66	-41.2
1	A	41	PHE	CZ	73.48	121.82 – 136.66	-37.6
1	A	30	PHE	CZ	74.03	121.82 – 136.66	-37.2
1	A	31	PHE	CZ	74.45	121.82 – 136.66	-36.9
1	A	22	VAL	CG2	76.26	13.71 – 28.88	36.2
1	A	4	HIS	CE1	54.22	126.08 – 149.12	-36.2
1	A	54	PHE	CZ	75.56	121.82 – 136.66	-36.2
1	A	75	HIS	CE1	54.81	126.08 – 149.12	-35.9
1	A	71	VAL	CG2	75.66	13.71 – 28.88	35.8
1	A	43	ILE	CD1	70.99	5.18 – 21.60	35.1
1	A	37	ILE	CD1	70.72	5.18 – 21.60	34.9
1	A	12	ILE	CD1	70.50	5.18 – 21.60	34.8
1	A	50	ILE	CD1	70.09	5.18 – 21.60	34.5
1	A	81	ILE	CD1	70.02	5.18 – 21.60	34.5
1	A	79	ILE	CD1	69.95	5.18 – 21.60	34.4
1	A	83	ILE	CD1	69.86	5.18 – 21.60	34.4
1	A	10	ILE	CD1	69.75	5.18 – 21.60	34.3
1	A	8	LYS	CE	70.47	37.57 – 46.21	33.1
1	A	85	LYS	CE	70.17	37.57 – 46.21	32.7
1	A	6	LYS	CE	70.16	37.57 – 46.21	32.7
1	A	25	LYS	CE	70.11	37.57 – 46.21	32.7
1	A	68	LYS	CE	70.08	37.57 – 46.21	32.6
1	A	9	LYS	CE	70.07	37.57 – 46.21	32.6
1	A	57	LYS	CE	70.06	37.57 – 46.21	32.6
1	A	60	MET	CE	73.32	8.39 – 25.85	32.2
1	A	66	MET	CE	73.04	8.39 – 25.85	32.0
1	A	21	MET	CE	72.48	8.39 – 25.85	31.7
1	A	38	ALA	CB	74.48	10.19 – 27.75	31.6
1	A	18	ARG	CD	72.01	38.57 – 47.75	31.4
1	A	64	ALA	CB	73.96	10.19 – 27.75	31.3
1	A	78	ARG	CD	71.74	38.57 – 47.75	31.1
1	A	11	ARG	CD	71.60	38.57 – 47.75	31.0
1	A	51	ARG	CD	71.53	38.57 – 47.75	30.9
1	A	39	ARG	CD	71.40	38.57 – 47.75	30.8
1	A	8	LYS	CD	58.10	23.50 – 34.42	26.7
1	A	34	GLN	CG	62.73	28.36 – 39.21	26.7
1	A	73	LEU	CG	55.31	21.37 – 32.19	26.4
1	A	29	THR	CG2	50.28	16.06 – 27.03	26.2
1	A	70	PRO	CG	56.00	21.69 – 32.72	26.1
1	A	23	THR	CG2	50.16	16.06 – 27.03	26.1
1	A	59	LEU	CG	55.01	21.37 – 32.19	26.1
1	A	28	THR	CG2	50.15	16.06 – 27.03	26.1

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	62	PRO	CG	55.90	21.69 – 32.72	26.0
1	A	63	GLN	CG	61.99	28.36 – 39.21	26.0
1	A	33	LEU	CG	54.88	21.37 – 32.19	26.0
1	A	45	PRO	CG	55.84	21.69 – 32.72	26.0
1	A	25	LYS	CD	57.21	23.50 – 34.42	25.9
1	A	84	LEU	CG	54.75	21.37 – 32.19	25.9
1	A	56	PRO	CG	55.71	21.69 – 32.72	25.8
1	A	57	LYS	CD	57.10	23.50 – 34.42	25.8
1	A	9	LYS	CD	57.07	23.50 – 34.42	25.7
1	A	44	PRO	CG	55.59	21.69 – 32.72	25.7
1	A	14	THR	CG2	49.77	16.06 – 27.03	25.7
1	A	68	LYS	CD	57.06	23.50 – 34.42	25.7
1	A	6	LYS	CD	57.00	23.50 – 34.42	25.7
1	A	74	GLN	CG	61.59	28.36 – 39.21	25.6
1	A	61	PRO	CG	55.39	21.69 – 32.72	25.6
1	A	13	THR	CG2	49.54	16.06 – 27.03	25.5
1	A	24	LEU	CG	54.38	21.37 – 32.19	25.5
1	A	68	LYS	CG	53.22	19.35 – 30.45	25.5
1	A	85	LYS	CD	56.83	23.50 – 34.42	25.5
1	A	19	GLN	CG	61.41	28.36 – 39.21	25.5
1	A	25	LYS	CG	53.11	19.35 – 30.45	25.4
1	A	48	GLN	CG	61.33	28.36 – 39.21	25.4
1	A	72	PRO	CG	55.20	21.69 – 32.72	25.4
1	A	80	THR	CG2	49.29	16.06 – 27.03	25.3
1	A	9	LYS	CG	52.89	19.35 – 30.45	25.2
1	A	6	LYS	CG	52.88	19.35 – 30.45	25.2
1	A	47	LEU	CG	53.92	21.37 – 32.19	25.1
1	A	85	LYS	CG	52.70	19.35 – 30.45	25.1
1	A	8	LYS	CG	52.65	19.35 – 30.45	25.0
1	A	32	GLU	CG	65.60	30.20 – 42.01	25.0
1	A	51	ARG	CG	56.80	21.24 – 33.19	24.8
1	A	55	PRO	CB	60.38	26.06 – 37.61	24.7
1	A	45	PRO	CB	60.21	26.06 – 37.61	24.6
1	A	62	PRO	CB	60.19	26.06 – 37.61	24.6
1	A	56	PRO	CB	60.18	26.06 – 37.61	24.5
1	A	28	THR	HG1	6.29	0.08 – 2.19	24.4
1	A	70	PRO	CB	60.03	26.06 – 37.61	24.4
1	A	57	LYS	CG	51.86	19.35 – 30.45	24.3
1	A	58	GLU	CG	64.78	30.20 – 42.01	24.3
1	A	67	GLU	CG	64.76	30.20 – 42.01	24.3
1	A	35	GLU	CG	64.54	30.20 – 42.01	24.1
1	A	44	PRO	CB	59.58	26.06 – 37.61	24.0

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	7	GLU	CG	64.45	30.20 – 42.01	24.0
1	A	55	PRO	CG	53.48	21.69 – 32.72	23.8
1	A	39	ARG	CG	55.59	21.24 – 33.19	23.7
1	A	69	GLU	CG	64.01	30.20 – 42.01	23.6
1	A	11	ARG	CG	55.44	21.24 – 33.19	23.6
1	A	78	ARG	CG	55.41	21.24 – 33.19	23.6
1	A	82	GLU	CG	63.70	30.20 – 42.01	23.4
1	A	18	ARG	NE	122.10	76.53 – 92.65	23.3
1	A	18	ARG	CG	54.95	21.24 – 33.19	23.2
1	A	61	PRO	CB	58.36	26.06 – 37.61	23.0
1	A	39	ARG	NE	121.22	76.53 – 92.65	22.7
1	A	40	GLU	CG	62.75	30.20 – 42.01	22.6
1	A	29	THR	HG1	5.90	0.08 – 2.19	22.6
1	A	86	GLY	CA	74.18	38.93 – 51.79	22.4
1	A	17	GLY	CA	73.92	38.93 – 51.79	22.2
1	A	65	GLY	CA	73.46	38.93 – 51.79	21.9
1	A	72	PRO	CB	56.95	26.06 – 37.61	21.7
1	A	66	MET	CG	60.53	25.46 – 38.60	21.7
1	A	60	MET	CG	60.28	25.46 – 38.60	21.5
1	A	76	GLY	CA	72.79	38.93 – 51.79	21.3
1	A	21	MET	CG	59.45	25.46 – 38.60	20.9
1	A	53	GLY	CA	72.15	38.93 – 51.79	20.8
1	A	71	VAL	CG1	49.66	14.71 – 28.29	20.7
1	A	1	GLY	CA	71.84	38.93 – 51.79	20.6
1	A	22	VAL	CG1	49.23	14.71 – 28.29	20.4
1	A	33	LEU	CD1	55.31	16.71 – 32.55	19.4
1	A	73	LEU	CD1	54.85	16.71 – 32.55	19.1
1	A	59	LEU	CD1	54.61	16.71 – 32.55	18.9
1	A	77	ASP	CB	69.99	32.98 – 48.76	18.4
1	A	19	GLN	CB	60.95	20.34 – 37.98	18.0
1	A	84	LEU	CD1	53.11	16.71 – 32.55	18.0
1	A	37	ILE	CG1	58.32	19.24 – 36.26	18.0
1	A	47	LEU	CD1	52.90	16.71 – 32.55	17.9
1	A	3	ASP	CB	68.94	32.98 – 48.76	17.8
1	A	75	HIS	CD2	62.20	103.95 – 136.66	-17.8
1	A	7	GLU	CB	59.74	21.56 – 38.37	17.7
1	A	8	LYS	CB	63.56	24.03 – 41.47	17.7
1	A	51	ARG	CB	61.99	21.74 – 39.52	17.6
1	A	57	LYS	CB	63.50	24.03 – 41.47	17.6
1	A	16	ASP	CB	68.44	32.98 – 48.76	17.5
1	A	82	GLU	CB	59.20	21.56 – 38.37	17.4
1	A	22	VAL	CB	63.11	23.86 – 41.50	17.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	18	ARG	CB	61.28	21.74 – 39.52	17.2
1	A	74	GLN	CB	59.54	20.34 – 37.98	17.2
1	A	4	HIS	CD2	64.11	103.95 – 136.66	-17.2
1	A	58	GLU	CB	58.63	21.56 – 38.37	17.1
1	A	83	ILE	CG1	56.73	19.24 – 36.26	17.0
1	A	32	GLU	CB	58.48	21.56 – 38.37	17.0
1	A	25	LYS	CB	61.90	24.03 – 41.47	16.7
1	A	9	LYS	CB	61.90	24.03 – 41.47	16.7
1	A	11	ARG	CB	60.33	21.74 – 39.52	16.7
1	A	50	ILE	CG1	56.17	19.24 – 36.26	16.7
1	A	40	GLU	CB	57.92	21.56 – 38.37	16.6
1	A	78	ARG	CB	60.21	21.74 – 39.52	16.6
1	A	24	LEU	CD1	50.94	16.71 – 32.55	16.6
1	A	73	LEU	CB	72.50	33.11 – 51.34	16.6
1	A	81	ILE	CG1	55.84	19.24 – 36.26	16.5
1	A	69	GLU	CB	57.46	21.56 – 38.37	16.4
1	A	35	GLU	CB	57.44	21.56 – 38.37	16.3
1	A	59	LEU	CD2	51.45	15.73 – 32.47	16.3
1	A	15	ASN	CB	65.39	30.50 – 46.89	16.3
1	A	48	GLN	CB	57.87	20.34 – 37.98	16.3
1	A	63	GLN	CB	57.87	20.34 – 37.98	16.3
1	A	85	LYS	CB	61.10	24.03 – 41.47	16.3
1	A	24	LEU	CB	71.80	33.11 – 51.34	16.2
1	A	6	LYS	CB	60.97	24.03 – 41.47	16.2
1	A	34	GLN	CB	57.62	20.34 – 37.98	16.1
1	A	73	LEU	CD2	50.99	15.73 – 32.47	16.1
1	A	24	LEU	CD2	50.94	15.73 – 32.47	16.0
1	A	79	ILE	CG1	54.98	19.24 – 36.26	16.0
1	A	10	ILE	CG1	54.93	19.24 – 36.26	16.0
1	A	33	LEU	CD2	50.81	15.73 – 32.47	16.0
1	A	42	ASN	CB	64.81	30.50 – 46.89	15.9
1	A	67	GLU	CB	56.68	21.56 – 38.37	15.9
1	A	84	LEU	CD2	50.42	15.73 – 32.47	15.7
1	A	47	LEU	CD2	50.27	15.73 – 32.47	15.6
1	A	12	ILE	CG1	54.33	19.24 – 36.26	15.6
1	A	39	ARG	CB	58.36	21.74 – 39.52	15.6
1	A	43	ILE	CB	69.21	28.63 – 48.45	15.5
1	A	71	VAL	CB	59.91	23.86 – 41.50	15.4
1	A	84	LEU	CB	70.35	33.11 – 51.34	15.4
1	A	68	LYS	CB	59.52	24.03 – 41.47	15.3
1	A	43	ILE	CG1	53.81	19.24 – 36.26	15.3
1	A	79	ILE	CB	68.71	28.63 – 48.45	15.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	59	LEU	CB	69.88	33.11 – 51.34	15.2
1	A	10	ILE	CB	68.56	28.63 – 48.45	15.1
1	A	47	LEU	CB	69.74	33.11 – 51.34	15.1
1	A	12	ILE	CB	68.11	28.63 – 48.45	14.9
1	A	52	TYR	CB	70.58	28.67 – 49.81	14.8
1	A	54	PHE	CB	70.01	29.72 – 50.07	14.8
1	A	33	LEU	CB	69.05	33.11 – 51.34	14.7
1	A	50	ILE	CB	67.67	28.63 – 48.45	14.7
1	A	41	PHE	CB	69.76	29.72 – 50.07	14.7
1	A	81	ILE	CB	66.89	28.63 – 48.45	14.3
1	A	75	HIS	CB	59.56	19.76 – 40.75	14.0
1	A	37	ILE	CB	65.94	28.63 – 48.45	13.8
1	A	83	ILE	CB	65.93	28.63 – 48.45	13.8
1	A	13	THR	HG1	4.01	0.08 – 2.19	13.6
1	A	30	PHE	CB	67.56	29.72 – 50.07	13.6
1	A	21	MET	CB	61.69	22.22 – 43.61	13.4
1	A	4	HIS	CB	58.17	19.76 – 40.75	13.3
1	A	31	PHE	CB	66.85	29.72 – 50.07	13.2
1	A	66	MET	CB	59.68	22.22 – 43.61	12.5
1	A	60	MET	CB	59.47	22.22 – 43.61	12.4
1	A	46	TYR	CB	64.34	28.67 – 49.81	11.9
1	A	80	THR	HG1	3.52	0.08 – 2.19	11.3
1	A	63	GLN	NE2	125.14	103.38 – 120.35	7.8
1	A	74	GLN	NE2	124.93	103.38 – 120.35	7.7
1	A	34	GLN	NE2	124.72	103.38 – 120.35	7.6
1	A	19	GLN	NE2	123.81	103.38 – 120.35	7.0
1	A	15	ASN	ND2	125.31	101.55 – 123.95	5.6
1	A	61	PRO	HA	2.70	2.78 – 6.00	-5.2

### 7.1.5 Random Coil Index (RCI) plots

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

Random coil index (RCI) for chain A:

