



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 09:37 PM UTC

PDB ID : 2KJH / pdb_00002kjh
BMRB ID : 16321
Title : NMR based structural model of the UBCH8-UBIQUITIN complex
Authors : Serniwwka, S.A.; Shaw, G.S.
Deposited on : 2009-05-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : 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

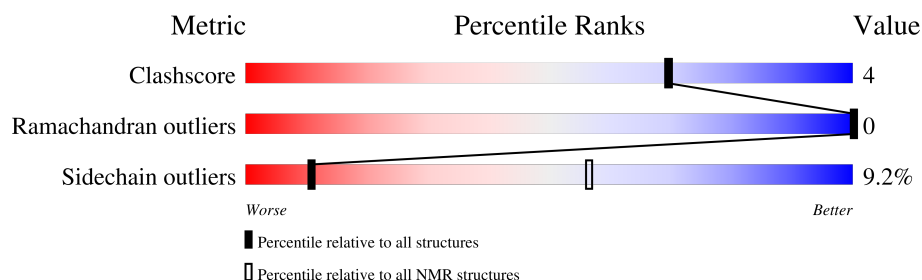
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 32%.

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 ≥ 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	152	
2	B	76	

2 Ensemble composition and analysis

This entry contains 16 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the mean structure*.

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:2-A:150 (149)	0.35	13
2	B:1-B:72 (72)	0.27	11

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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2192 atoms, of which 361 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin/ISG15-conjugating enzyme E2 L6.

Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			1459	792	232	211	218	6	

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
2	B	76	Total	C	H	N	O	S	0
			733	379	129	105	118	2	

There is a discrepancy between the modelled and reference sequences:

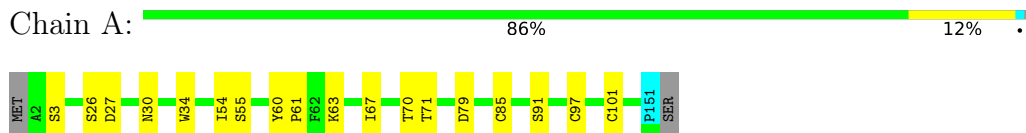
Chain	Residue	Modelled	Actual	Comment	Reference
B	76	CYS	GLY	engineered mutation	UNP P62988

4 Residue-property plots [i](#)

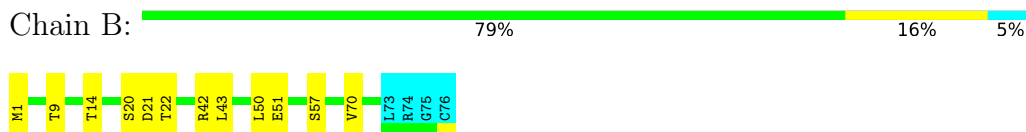
4.1 Average score per residue in the NMR ensemble

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: Ubiquitin/ISG15-conjugating enzyme E2 L6



- Molecule 2: Ubiquitin

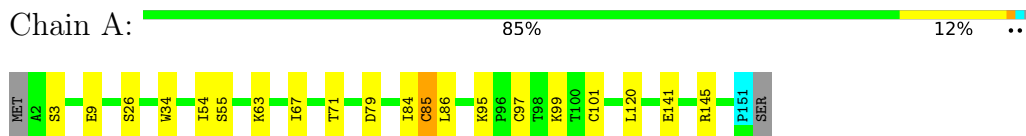


4.2 Scores per residue for each member of the ensemble

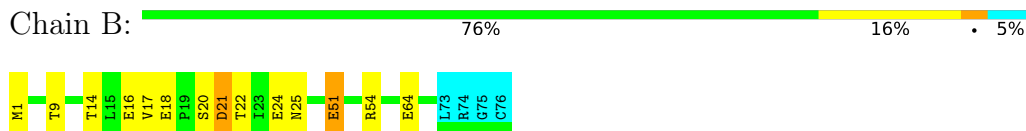
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

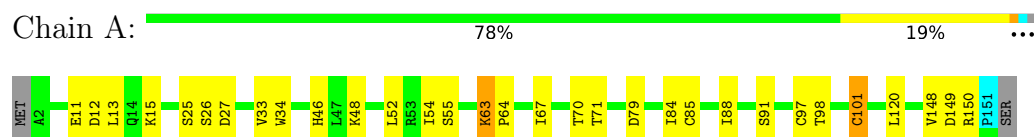


- Molecule 2: Ubiquitin

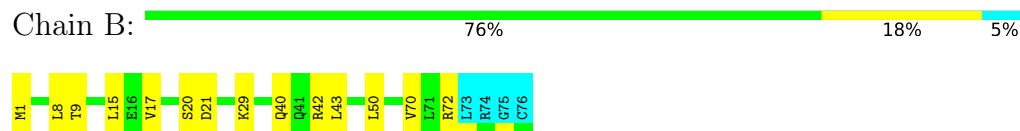


4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

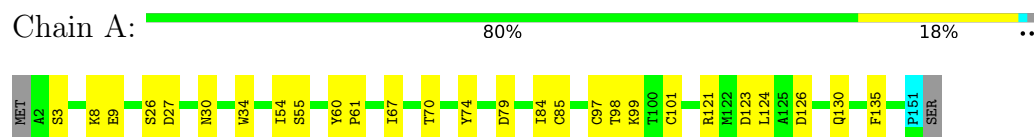


- Molecule 2: Ubiquitin

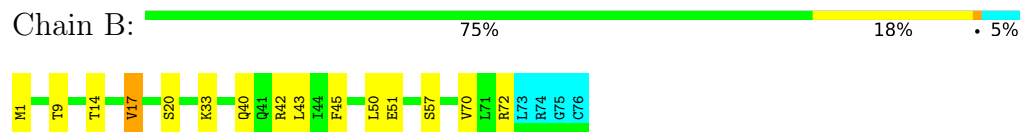


4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

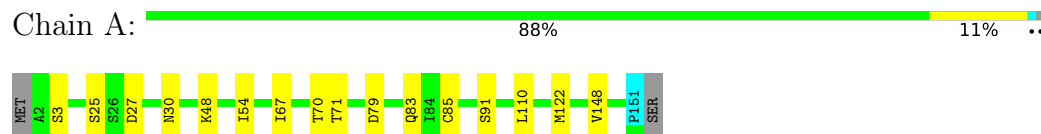


- Molecule 2: Ubiquitin

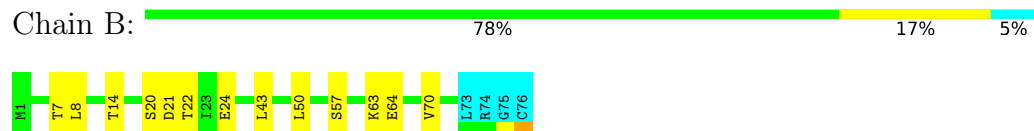


4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6



- Molecule 2: Ubiquitin



4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A:  83% 14% ...



- Molecule 2: Ubiquitin

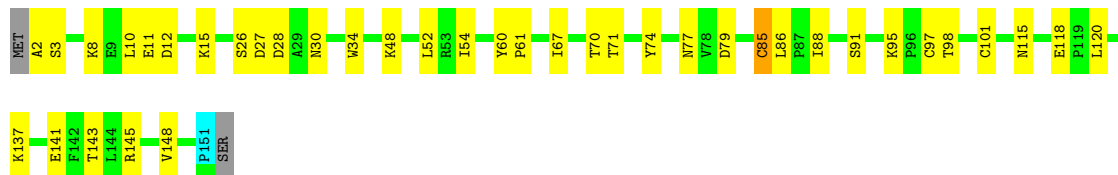
Chain B:  72% 22% 5%



4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A:  72% 25% ...



- Molecule 2: Ubiquitin

Chain B:  78% 17% 5%



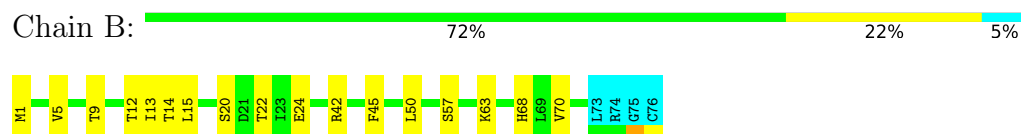
4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A:  76% 20% ...

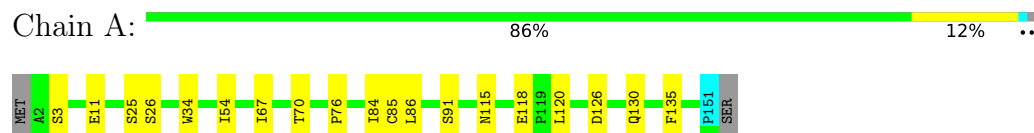


- Molecule 2: Ubiquitin

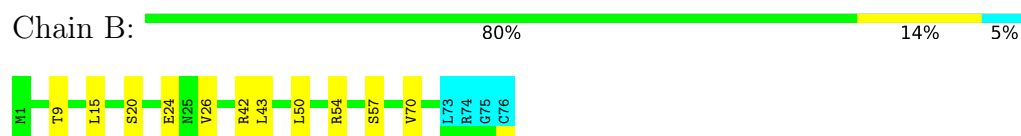


4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

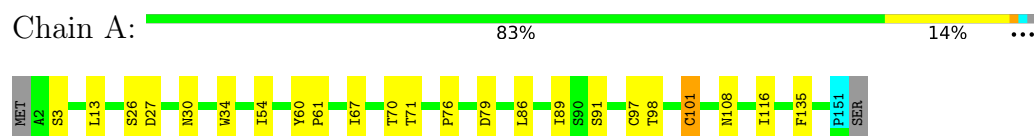


- Molecule 2: Ubiquitin

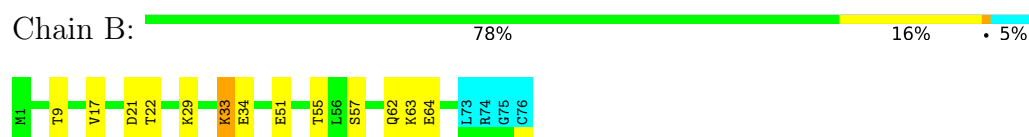


4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

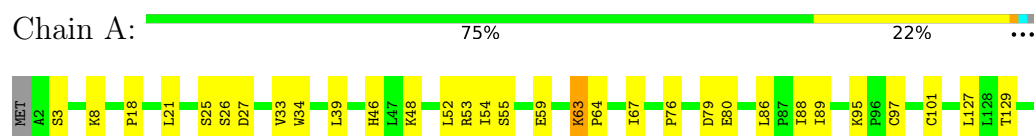


- Molecule 2: Ubiquitin



4.2.10 Score per residue for model 10

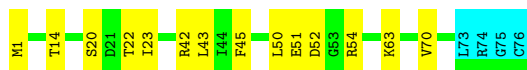
- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6





- Molecule 2: Ubiquitin

Chain B: 76% 18% 5%



4.2.11 Score per residue for model 11

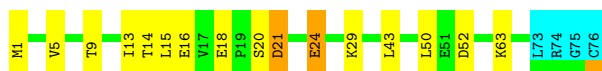
- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A: 83% 15% ..



- Molecule 2: Ubiquitin

Chain B: 74% 18% 5%



4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A: 80% 17% ...



- Molecule 2: Ubiquitin

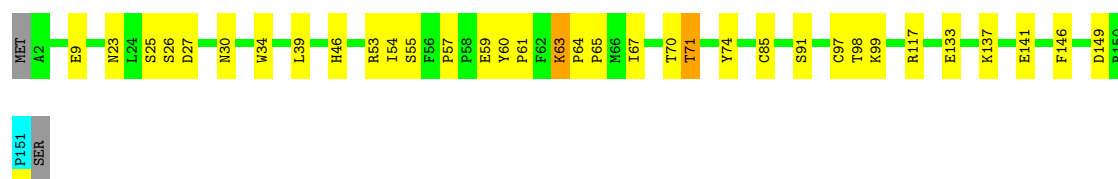
Chain B: 83% 12% 5%



4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A: 76% 21% ...



- Molecule 2: Ubiquitin

Chain B: 76% 17% 5%



4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A: 78% 20% ..



- Molecule 2: Ubiquitin

Chain B: 72% 22% 5%



4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A: 80% 18% ..



- Molecule 2: Ubiquitin

Chain B: 75% 20% 5%



4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin/ISG15-conjugating enzyme E2 L6

Chain A:  82% 16% ..



- Molecule 2: Ubiquitin

Chain B:  72% 21% • 5%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 16 were deposited, based on the following criterion: *Structures with the lowest energy in the lowest energy cluster*.

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

Software name	Classification	Version
HADDOCK	refinement	2.0
HADDOCK	structure solution	2.0
CNS	refinement	1.2

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	1046
Number of shifts mapped to atoms	717
Number of unparsed shifts	0
Number of shifts with mapping errors	329
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	32%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1220	232	1235	9±3
2	B	574	120	599	4±2
All	All	28704	5632	29355	207

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:HD21	1:A:101:CYS:HB3	0.80	1.52	2	4
2:B:1:MET:HB2	2:B:63:LYS:HB3	0.66	1.65	6	4
1:A:18:PRO:HG2	1:A:21:LEU:HB3	0.65	1.68	10	2
2:B:19:PRO:HA	2:B:56:LEU:HB2	0.64	1.67	14	2
1:A:27:ASP:HB2	1:A:33:VAL:HB	0.64	1.70	2	2
2:B:45:PHE:HB3	2:B:50:LEU:HD21	0.63	1.69	14	7
1:A:63:LYS:HD2	1:A:64:PRO:HD2	0.62	1.68	5	4
1:A:9:GLU:HG2	1:A:99:LYS:HE3	0.62	1.71	3	2
1:A:34:TRP:HB2	1:A:54:ILE:HB	0.61	1.71	15	12
2:B:17:VAL:HG12	2:B:29:LYS:HE3	0.60	1.72	9	1
1:A:27:ASP:HB3	1:A:30:ASN:O	0.60	1.96	6	9
1:A:54:ILE:HG23	1:A:67:ILE:HG12	0.60	1.72	7	14
1:A:86:LEU:HG	1:A:88:ILE:HG22	0.58	1.76	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:CYS:HB2	1:A:120:LEU:HD11	0.57	1.75	8	6
1:A:59:GLU:HB2	1:A:63:LYS:HB2	0.56	1.75	13	4
2:B:8:LEU:HD11	2:B:70:VAL:HG13	0.56	1.77	16	4
2:B:51:GLU:HB3	2:B:54:ARG:HG2	0.55	1.79	13	4
2:B:40:GLN:HA	2:B:72:ARG:HB3	0.55	1.78	14	3
2:B:23:ILE:HB	2:B:52:ASP:HA	0.54	1.79	10	2
2:B:42:ARG:HB3	2:B:70:VAL:HB	0.54	1.79	8	9
2:B:1:MET:HG2	2:B:17:VAL:O	0.53	2.02	15	5
1:A:41:ASP:HA	1:A:46:HIS:HB3	0.53	1.80	16	1
1:A:60:TYR:CD1	1:A:61:PRO:HA	0.52	2.40	13	9
2:B:43:LEU:HB3	2:B:50:LEU:HD12	0.51	1.82	13	9
1:A:77:ASN:HD21	1:A:115:ASN:HB3	0.51	1.65	6	1
2:B:15:LEU:HD11	2:B:29:LYS:HB3	0.51	1.82	2	3
2:B:51:GLU:HG2	2:B:53:GLY:H	0.50	1.66	14	1
2:B:18:GLU:O	2:B:21:ASP:HB2	0.50	2.07	16	4
1:A:81:ASN:HD22	1:A:83:GLN:HG2	0.49	1.67	15	1
1:A:48:LYS:HD2	1:A:149:ASP:HA	0.49	1.84	15	3
1:A:48:LYS:HB3	1:A:148:VAL:O	0.49	2.08	15	7
1:A:10:LEU:HB2	1:A:34:TRP:CZ2	0.48	2.42	6	1
1:A:47:LEU:HD22	1:A:144:LEU:HD21	0.48	1.85	14	1
1:A:41:ASP:HA	1:A:46:HIS:HD2	0.48	1.68	11	1
1:A:57:PRO:HD3	1:A:65:PRO:HA	0.48	1.85	13	3
1:A:79:ASP:HB3	1:A:83:GLN:HB2	0.47	1.86	4	1
2:B:5:VAL:HB	2:B:13:ILE:HG13	0.47	1.86	7	2
1:A:126:ASP:O	1:A:130:GLN:HG2	0.47	2.09	8	4
1:A:12:ASP:HA	1:A:15:LYS:HD2	0.47	1.86	6	1
1:A:133:GLU:HG3	1:A:137:LYS:HE2	0.47	1.85	13	2
1:A:88:ILE:HD11	1:A:98:THR:HG21	0.46	1.87	2	1
1:A:124:LEU:HG	1:A:135:PHE:HE1	0.46	1.70	3	3
1:A:127:LEU:HD11	1:A:134:LEU:HD23	0.46	1.88	5	3
1:A:76:PRO:HD3	1:A:135:PHE:HZ	0.46	1.70	9	3
1:A:84:ILE:HD12	1:A:86:LEU:HD13	0.46	1.87	8	2
1:A:121:ARG:HB3	1:A:123:ASP:OD1	0.46	2.10	11	3
1:A:46:HIS:HA	1:A:150:ARG:NH1	0.45	2.26	2	2
2:B:33:LYS:HD3	2:B:34:GLU:HG2	0.45	1.88	9	1
2:B:27:LYS:HB3	2:B:38:PRO:HB3	0.44	1.88	5	1
1:A:76:PRO:HD3	1:A:135:PHE:CZ	0.44	2.47	14	3
1:A:124:LEU:HG	1:A:135:PHE:CE1	0.44	2.46	15	1
1:A:9:GLU:HG2	1:A:99:LYS:HE2	0.44	1.88	1	1
1:A:141:GLU:O	1:A:145:ARG:HB2	0.44	2.12	1	2
1:A:72:LYS:HB3	1:A:142:PHE:HE2	0.44	1.72	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LYS:HG3	1:A:143:THR:O	0.44	2.13	6	1
1:A:122:MET:HE1	2:B:7:THR:HG21	0.43	1.89	4	1
1:A:95:LYS:HB2	1:A:97:CYS:SG	0.43	2.54	6	1
1:A:115:ASN:ND2	1:A:118:GLU:HB2	0.43	2.29	8	1
1:A:86:LEU:HB2	1:A:89:ILE:HG12	0.42	1.91	7	2
1:A:11:GLU:HG2	1:A:15:LYS:HE3	0.42	1.91	2	1
1:A:2:ALA:HB1	1:A:60:TYR:HB3	0.42	1.90	6	1
1:A:88:ILE:HD13	1:A:103:VAL:HA	0.42	1.90	7	1
2:B:15:LEU:HD21	2:B:26:VAL:HG13	0.42	1.92	8	1
1:A:95:LYS:HG3	1:A:98:THR:OG1	0.41	2.14	6	1
1:A:48:LYS:HB2	1:A:143:THR:HG22	0.41	1.92	15	1
1:A:71:THR:HG22	1:A:146:PHE:O	0.41	2.16	13	1
2:B:24:GLU:HB2	2:B:52:ASP:HB3	0.41	1.92	11	1
1:A:133:GLU:O	1:A:137:LYS:HG3	0.41	2.15	16	1
1:A:57:PRO:HB2	1:A:59:GLU:OE1	0.40	2.15	12	1
1:A:60:TYR:CG	1:A:61:PRO:HA	0.40	2.51	13	1
2:B:51:GLU:HB3	2:B:54:ARG:CG	0.40	2.47	1	1
1:A:95:LYS:HB3	1:A:97:CYS:SG	0.40	2.57	7	1
1:A:42:GLN:OE1	1:A:43:PRO:HD2	0.40	2.16	16	1
1:A:87:PRO:O	1:A:93:ASN:HB2	0.40	2.17	7	1
1:A:86:LEU:HB3	1:A:89:ILE:HG12	0.40	1.94	10	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	148/152 (97%)	144±1 (97±1%)	4±1 (3±1%)	0±0 (0±0%)	100	100
2	B	71/76 (93%)	70±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
All	All	3504/3648 (96%)	3424 (98%)	80 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	140/143 (98%)	128±3 (92±2%)	12±3 (8±2%)	12 59
2	B	66/69 (96%)	59±2 (89±4%)	7±2 (11±4%)	8 52
All	All	3296/3392 (97%)	2993 (91%)	303 (9%)	11 56

All 71 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	3	SER	13
2	B	9	THR	13
2	B	20	SER	13
1	A	26	SER	12
1	A	79	ASP	12
2	B	14	THR	12
2	B	22	THR	12
1	A	70	THR	12
2	B	57	SER	12
1	A	71	THR	11
1	A	97	CYS	11
1	A	91	SER	11
1	A	101	CYS	10
1	A	55	SER	9
2	B	21	ASP	9
1	A	25	SER	8
2	B	24	GLU	7
1	A	63	LYS	6
1	A	52	LEU	6
1	A	98	THR	6
2	B	51	GLU	5
2	B	64	GLU	5
1	A	84	ILE	5
1	A	74	TYR	5
1	A	8	LYS	4
2	B	55	THR	4
1	A	53	ARG	4
1	A	85	CYS	3

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Mol	Chain	Res	Type	Models (Total)
2	B	16	GLU	3
2	B	33	LYS	3
2	B	63	LYS	3
1	A	11	GLU	3
1	A	46	HIS	3
2	B	66	THR	3
1	A	95	LYS	2
1	A	110	LEU	2
1	A	142	PHE	2
2	B	12	THR	2
1	A	108	ASN	2
1	A	129	THR	2
1	A	149	ASP	2
1	A	93	ASN	2
2	B	25	ASN	1
1	A	12	ASP	1
2	B	17	VAL	1
1	A	68	LYS	1
2	B	40	GLN	1
1	A	28	ASP	1
1	A	118	GLU	1
1	A	137	LYS	1
2	B	18	GLU	1
1	A	15	LYS	1
1	A	16	LYS	1
1	A	39	LEU	1
2	B	15	LEU	1
2	B	68	HIS	1
2	B	54	ARG	1
1	A	116	ILE	1
2	B	62	GLN	1
1	A	80	GLU	1
1	A	81	ASN	1
1	A	145	ARG	1
1	A	92	GLU	1
1	A	134	LEU	1
1	A	23	ASN	1
1	A	117	ARG	1
1	A	141	GLU	1
2	B	39	ASP	1
1	A	130	GLN	1
1	A	14	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	59	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 32% for the well-defined parts and 32% 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	1046
Number of shifts mapped to atoms	717
Number of unparsed shifts	0
Number of shifts with mapping errors	329
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 329 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HA	4.419	?	1
1	A	1	MET	HB2	2.608	?	2
1	A	1	MET	C	177.128	?	1
1	A	1	MET	CA	56.828	?	1
1	A	1	MET	CB	32.757	?	1
1	A	2	ALA	HB1	1.607	?	1
1	A	2	ALA	HB2	1.607	?	1
1	A	2	ALA	HB3	1.607	?	1
1	A	3	SER	HB2	4.017	?	2
1	A	5	ARG	HA	4.221	?	1
1	A	5	ARG	HD2	2.921	?	2
1	A	6	VAL	HA	3.35	?	1
1	A	6	VAL	HB	1.886	?	1
1	A	6	VAL	HG11	1.101	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	VAL	HG12	1.101	?	2
1	A	6	VAL	HG13	1.101	?	2
1	A	7	VAL	HA	3.695	?	1
1	A	7	VAL	HG11	1.039	?	2
1	A	7	VAL	HG12	1.039	?	2
1	A	7	VAL	HG13	1.039	?	2
1	A	8	LYS	HA	4.196	?	1
1	A	9	GLU	HA	4.183	?	1
1	A	10	LEU	HA	3.931	?	1
1	A	10	LEU	HB2	1.297	?	2
1	A	11	GLU	HB2	2.157	?	2
1	A	11	GLU	HB3	2.506	?	2
1	A	12	ASP	HB2	2.775	?	2
1	A	13	LEU	HB2	1.767	?	2
1	A	13	LEU	HD11	0.924	?	4
1	A	13	LEU	HD12	0.924	?	4
1	A	13	LEU	HD13	0.924	?	4
1	A	13	LEU	HD21	1.121	?	4
1	A	13	LEU	HD22	1.121	?	4
1	A	13	LEU	HD23	1.121	?	4
1	A	14	GLN	HA	3.863	?	1
1	A	14	GLN	HB2	1.993	?	2
1	A	14	GLN	HE21	7.767	?	2
1	A	14	GLN	HE22	6.845	?	2
1	A	15	LYS	HA	4.089	?	1
1	A	15	LYS	HD2	1.674	?	2
1	A	19	PRO	HB2	2.152	?	2
1	A	20	TYR	HB2	2.849	?	2
1	A	20	TYR	HB3	3.529	?	2
1	A	21	LEU	HB2	1.175	?	2
1	A	21	LEU	HB3	1.49	?	2
1	A	21	LEU	HD11	0.865	?	2
1	A	21	LEU	HD12	0.865	?	2
1	A	21	LEU	HD13	0.865	?	2
1	A	22	ARG	HA	4.758	?	1
1	A	23	ASN	HB2	2.784	?	2
1	A	23	ASN	HB3	2.984	?	2
1	A	23	ASN	HD21	7.344	?	2
1	A	23	ASN	HD22	6.839	?	2
1	A	24	LEU	HA	4.939	?	1
1	A	24	LEU	HB2	1.597	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	24	LEU	HD11	0.558	?	4
1	A	24	LEU	HD12	0.558	?	4
1	A	24	LEU	HD13	0.558	?	4
1	A	24	LEU	HD21	0.709	?	4
1	A	24	LEU	HD22	0.709	?	4
1	A	24	LEU	HD23	0.709	?	4
1	A	25	SER	HB2	3.743	?	2
1	A	26	SER	HB2	3.832	?	2
1	A	27	ASP	HA	4.684	?	1
1	A	27	ASP	HB2	2.591	?	2
1	A	27	ASP	HB3	3.257	?	2
1	A	28	ASP	HB2	2.677	?	2
1	A	29	ALA	HB1	1.409	?	1
1	A	29	ALA	HB2	1.409	?	1
1	A	29	ALA	HB3	1.409	?	1
1	A	30	ASN	HA	4.805	?	1
1	A	31	VAL	HB	2.26	?	1
1	A	31	VAL	HG11	1.02	?	2
1	A	31	VAL	HG12	1.02	?	2
1	A	31	VAL	HG13	1.02	?	2
1	A	32	LEU	HA	4.334	?	1
1	A	32	LEU	HD11	0.637	?	4
1	A	32	LEU	HD12	0.637	?	4
1	A	32	LEU	HD13	0.637	?	4
1	A	32	LEU	HD21	0.923	?	4
1	A	32	LEU	HD22	0.923	?	4
1	A	32	LEU	HD23	0.923	?	4
1	A	35	HIS	HB2	2.993	?	2
1	A	36	ALA	HB1	1.317	?	1
1	A	36	ALA	HB2	1.317	?	1
1	A	36	ALA	HB3	1.317	?	1
1	A	37	LEU	HD11	0.737	?	4
1	A	37	LEU	HD12	0.737	?	4
1	A	37	LEU	HD13	0.737	?	4
1	A	37	LEU	HD21	1.478	?	4
1	A	37	LEU	HD22	1.478	?	4
1	A	37	LEU	HD23	1.478	?	4
1	A	38	LEU	HB2	1.848	?	2
1	A	38	LEU	HD11	0.553	?	2
1	A	38	LEU	HD12	0.553	?	2
1	A	38	LEU	HD13	0.553	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	ASP	HA	5.155	?	1
1	A	41	ASP	HB2	2.718	?	2
1	A	41	ASP	HB3	2.869	?	2
1	A	45	TYR	HB2	2.894	?	2
1	A	45	TYR	HB3	3.373	?	2
1	A	46	HIS	HB2	3.682	?	2
1	A	47	LEU	HG	1.367	?	1
1	A	48	LYS	HD2	0.828	?	2
1	A	48	LYS	HG2	1.466	?	2
1	A	49	ALA	HB1	1.209	?	1
1	A	49	ALA	HB2	1.209	?	1
1	A	49	ALA	HB3	1.209	?	1
1	A	50	PHE	HB2	2.881	?	2
1	A	50	PHE	HB3	3.176	?	2
1	A	51	ASN	HA	5.246	?	1
1	A	51	ASN	HB2	2.745	?	2
1	A	52	LEU	HA	5.029	?	1
1	A	52	LEU	HB2	1.03	?	2
1	A	52	LEU	HD11	0.087	?	2
1	A	52	LEU	HD12	0.087	?	2
1	A	52	LEU	HD13	0.087	?	2
1	A	53	ARG	HD2	3.073	?	2
1	A	54	ILE	HG12	1.392	?	9
1	A	54	ILE	HG21	-0.089	?	1
1	A	54	ILE	HG22	-0.089	?	1
1	A	54	ILE	HG23	-0.089	?	1
1	A	55	SER	HB2	3.565	?	2
1	A	58	PRO	HB2	2.169	?	2
1	A	59	GLU	HA	4.361	?	1
1	A	62	PHE	HB2	3.119	?	2
1	A	62	PHE	HB3	3.387	?	2
1	A	65	PRO	HA	4.23	?	1
1	A	66	MET	HA	4.475	?	1
1	A	66	MET	HB2	2.343	?	2
1	A	67	ILE	HA	4.699	?	1
1	A	67	ILE	HG12	1.202	?	9
1	A	67	ILE	HG21	0.464	?	1
1	A	67	ILE	HG22	0.464	?	1
1	A	67	ILE	HG23	0.464	?	1
1	A	68	LYS	HB2	1.57	?	2
1	A	68	LYS	HG2	1.271	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	PHE	HB2	2.974	?	2
1	A	69	PHE	HB3	3.586	?	2
1	A	70	THR	HA	4.481	?	1
1	A	70	THR	HG21	1.117	?	1
1	A	70	THR	HG22	1.117	?	1
1	A	70	THR	HG23	1.117	?	1
1	A	71	THR	HB	3.757	?	1
1	A	72	LYS	HA	4.222	?	1
1	A	72	LYS	HG2	1.335	?	2
1	A	74	TYR	HB2	3.14	?	2
1	A	76	PRO	HA	4.317	?	1
1	A	76	PRO	HG2	1.578	?	2
1	A	77	ASN	HB2	2.415	?	2
1	A	77	ASN	HB3	3.389	?	2
1	A	78	VAL	HA	3.56	?	1
1	A	79	ASP	HB2	2.594	?	2
1	A	80	GLU	HA	4.115	?	1
1	A	80	GLU	HB2	2.206	?	2
1	A	81	ASN	HA	4.884	?	1
1	A	81	ASN	HB2	2.908	?	2
1	A	81	ASN	HD21	7.825	?	2
1	A	81	ASN	HD22	6.988	?	2
1	A	82	GLY	HA2	3.636	?	2
1	A	82	GLY	HA3	4.791	?	2
1	A	83	GLN	HA	4.498	?	1
1	A	83	GLN	HE21	7.599	?	2
1	A	83	GLN	HE22	6.898	?	2
1	A	83	GLN	HG2	2.432	?	2
1	A	84	ILE	HB	1.6	?	1
1	A	84	ILE	HG21	0.895	?	1
1	A	84	ILE	HG22	0.895	?	1
1	A	84	ILE	HG23	0.895	?	1
1	A	85	CYS	H	8.612	?	1
1	A	85	CYS	HB2	2.769	?	2
1	A	88	ILE	HA	4.212	?	1
1	A	88	ILE	HG12	1.045	?	9
1	A	89	ILE	HG21	0.934	?	1
1	A	89	ILE	HG22	0.934	?	1
1	A	89	ILE	HG23	0.934	?	1
1	A	91	SER	HB2	4.015	?	2
1	A	92	GLU	HA	4.2	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	92	GLU	HG2	2.265	?	2
1	A	93	ASN	HA	4.884	?	1
1	A	93	ASN	HB2	2.81	?	2
1	A	93	ASN	HB3	2.962	?	2
1	A	94	TRP	HB2	3.148	?	2
1	A	96	PRO	HG2	1.684	?	2
1	A	97	SER	H	6.931	?	1
1	A	97	SER	HB2	3.652	?	2
1	A	97	SER	HB3	4.009	?	2
1	A	97	SER	C	175.127	?	1
1	A	97	SER	CA	57.955	?	1
1	A	97	SER	CB	62.92	?	1
1	A	97	SER	N	107.45	?	1
1	A	98	THR	HG21	1.146	?	1
1	A	98	THR	HG22	1.146	?	1
1	A	98	THR	HG23	1.146	?	1
1	A	99	LYS	HB2	1.672	?	2
1	A	102	GLN	HA	4.266	?	1
1	A	102	GLN	HE21	7.766	?	2
1	A	102	GLN	HE22	6.998	?	2
1	A	102	GLN	HG2	2.363	?	2
1	A	103	VAL	HA	3.567	?	1
1	A	103	VAL	HG11	1.127	?	2
1	A	103	VAL	HG12	1.127	?	2
1	A	103	VAL	HG13	1.127	?	2
1	A	105	GLU	HA	4.035	?	1
1	A	105	GLU	HG2	2.36	?	2
1	A	106	ALA	HB1	1.616	?	1
1	A	106	ALA	HB2	1.616	?	1
1	A	106	ALA	HB3	1.616	?	1
1	A	107	LEU	HD11	0.794	?	2
1	A	107	LEU	HD12	0.794	?	2
1	A	107	LEU	HD13	0.794	?	2
1	A	108	ASN	HB2	2.368	?	2
1	A	109	VAL	HA	3.632	?	1
1	A	109	VAL	HG11	1.019	?	2
1	A	109	VAL	HG12	1.019	?	2
1	A	109	VAL	HG13	1.019	?	2
1	A	110	LEU	HB2	1.894	?	2
1	A	110	LEU	HD11	1.08	?	2
1	A	110	LEU	HD12	1.08	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	110	LEU	HD13	1.08	?	2
1	A	111	VAL	HB	2.998	?	1
1	A	111	VAL	HG11	0.351	?	4
1	A	111	VAL	HG12	0.351	?	4
1	A	111	VAL	HG13	0.351	?	4
1	A	111	VAL	HG21	0.551	?	4
1	A	111	VAL	HG22	0.551	?	4
1	A	111	VAL	HG23	0.551	?	4
1	A	112	ASN	HA	4.585	?	1
1	A	112	ASN	HB2	2.757	?	2
1	A	112	ASN	HD21	7.178	?	2
1	A	112	ASN	HD22	6.778	?	2
1	A	114	PRO	HA	4.502	?	1
1	A	115	ASN	HB2	2.819	?	2
1	A	115	ASN	HD21	7.65	?	2
1	A	115	ASN	HD22	7.111	?	2
1	A	116	ILE	HA	3.743	?	1
1	A	116	ILE	HB	1.768	?	1
1	A	116	ILE	HG12	1.223	?	9
1	A	116	ILE	HG21	0.768	?	1
1	A	116	ILE	HG22	0.768	?	1
1	A	116	ILE	HG23	0.768	?	1
1	A	117	ARG	HA	4.154	?	1
1	A	117	ARG	HD2	3.197	?	2
1	A	117	ARG	HG2	1.64	?	2
1	A	119	PRO	HB2	1.75	?	2
1	A	119	PRO	HG2	1.468	?	2
1	A	120	LEU	HB2	1.385	?	2
1	A	120	LEU	HD11	0.843	?	2
1	A	120	LEU	HD12	0.843	?	2
1	A	120	LEU	HD13	0.843	?	2
1	A	122	MET	HA	3.939	?	1
1	A	122	MET	HB2	2.604	?	2
1	A	123	ASP	HB2	2.562	?	2
1	A	123	ASP	HB3	2.829	?	2
1	A	124	LEU	HB2	1.467	?	2
1	A	125	ALA	HA	4.959	?	1
1	A	125	ALA	HB1	1.482	?	1
1	A	125	ALA	HB2	1.482	?	1
1	A	125	ALA	HB3	1.482	?	1
1	A	126	ASP	HB2	2.641	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	LEU	HA	4.009	?	1
1	A	127	LEU	HD11	0.734	?	2
1	A	127	LEU	HD12	0.734	?	2
1	A	127	LEU	HD13	0.734	?	2
1	A	128	LEU	HD11	0.301	?	4
1	A	128	LEU	HD12	0.301	?	4
1	A	128	LEU	HD13	0.301	?	4
1	A	128	LEU	HD21	0.65	?	4
1	A	128	LEU	HD22	0.65	?	4
1	A	128	LEU	HD23	0.65	?	4
1	A	129	THR	HA	4.237	?	1
1	A	129	THR	HB	3.949	?	1
1	A	129	THR	HG21	1.191	?	1
1	A	129	THR	HG22	1.191	?	1
1	A	129	THR	HG23	1.191	?	1
1	A	130	GLN	HA	4.24	?	1
1	A	130	GLN	HE21	7.598	?	2
1	A	130	GLN	HE22	6.791	?	2
1	A	130	GLN	HG2	2.502	?	2
1	A	131	ASN	HD21	7.857	?	2
1	A	131	ASN	HD22	6.89	?	2
1	A	132	PRO	HA	4.393	?	1
1	A	132	PRO	HB2	2.077	?	2
1	A	133	GLU	HA	4.14	?	1
1	A	133	GLU	HG2	2.341	?	2
1	A	134	LEU	HD11	0.948	?	2
1	A	134	LEU	HD12	0.948	?	2
1	A	134	LEU	HD13	0.948	?	2
1	A	135	PHE	HB2	2.821	?	2
1	A	135	PHE	HB3	3.34	?	2
1	A	136	ARG	HB2	1.782	?	2
1	A	137	LYS	HA	3.988	?	1
1	A	137	LYS	HB2	1.897	?	2
1	A	137	LYS	HD2	1.615	?	2
1	A	138	ASN	HB2	2.604	?	2
1	A	138	ASN	HD21	7.785	?	2
1	A	138	ASN	HD22	7.274	?	2
1	A	139	ALA	HB1	1.093	?	1
1	A	139	ALA	HB2	1.093	?	1
1	A	139	ALA	HB3	1.093	?	1
1	A	140	GLU	HB2	2.152	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	141	GLU	HA	3.888	?	1
1	A	141	GLU	HB2	2.121	?	2
1	A	141	GLU	HG2	2.407	?	2
1	A	142	PHE	HB2	3.154	?	2
1	A	144	LEU	HB2	1.802	?	2
1	A	144	LEU	HD11	0.849	?	2
1	A	144	LEU	HD12	0.849	?	2
1	A	144	LEU	HD13	0.849	?	2
1	A	145	ARG	HD2	2.719	?	2
1	A	145	ARG	HG2	1.36	?	2
1	A	146	PHE	HA	4.85	?	1
1	A	146	PHE	HB2	2.641	?	2
1	A	147	GLY	HA2	3.429	?	2
1	A	147	GLY	HA3	3.848	?	2
1	A	148	VAL	HA	4.224	?	1
1	A	148	VAL	HB	1.792	?	1
1	A	148	VAL	HG11	0.958	?	2
1	A	148	VAL	HG12	0.958	?	2
1	A	148	VAL	HG13	0.958	?	2
1	A	149	ASP	HB2	2.445	?	2
1	A	151	PRO	HA	4.51	?	1
1	A	151	PRO	HB2	2.321	?	2
1	A	151	PRO	HD2	3.307	?	2
1	A	151	PRO	HG2	1.879	?	2
1	A	152	SER	H	8.109	?	1
1	A	152	SER	CA	60.559	?	1
1	A	152	SER	CB	64.463	?	1
1	A	152	SER	N	121.332	?	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
$^{13}\text{C}_\alpha$	144	-0.29 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	139	-0.18 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	127	0.03 ± 0.16	None needed (< 0.5 ppm)
^{15}N	130	0.24 ± 0.23	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 32%, i.e. 1023 atoms were assigned a chemical shift out of a possible 3170. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	573/1071 (54%)	181/428 (42%)	264/442 (60%)	128/201 (64%)
Sidechain	450/1908 (24%)	255/1236 (21%)	185/595 (31%)	10/77 (13%)
Aromatic	0/191 (0%)	0/93 (0%)	0/88 (0%)	0/10 (0%)
Overall	1023/3170 (32%)	436/1757 (25%)	449/1125 (40%)	138/288 (48%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 1030 atoms were assigned a chemical shift out of a possible 3237. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	576/1095 (53%)	182/438 (42%)	266/452 (59%)	128/205 (62%)
Sidechain	454/1951 (23%)	258/1264 (20%)	186/607 (31%)	10/80 (12%)
Aromatic	0/191 (0%)	0/93 (0%)	0/88 (0%)	0/10 (0%)
Overall	1030/3237 (32%)	440/1795 (25%)	452/1147 (39%)	138/295 (47%)

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	77	ASN	H	11.48	5.28 – 11.36	5.2

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:

