



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 07:34 PM UTC

PDB ID : 2LJ9 / pdb_00002lj9
BMRB ID : 17926
Title : Partial 3d structure of the c-terminal part of the free arabidopsis thaliana cp12-2 in its oxidized form
Authors : Trivelli, X.; Sparla, F.; Marri, L.; Trost, P.
Deposited on : 2011-09-09

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

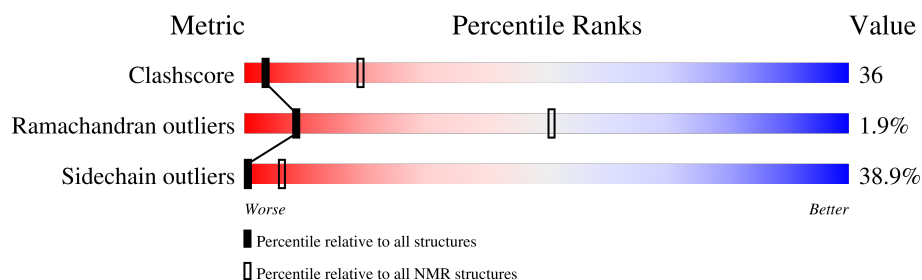
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	99	 • 9% • 8% 78%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:57-A:70 (14)	0.85	4

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 300 atoms, of which 117 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CP12 domain-containing protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	22	Total	C	H	N	O	S	0
			300	107	117	29	45	2	

There are 21 discrepancies between the modelled and reference sequences:

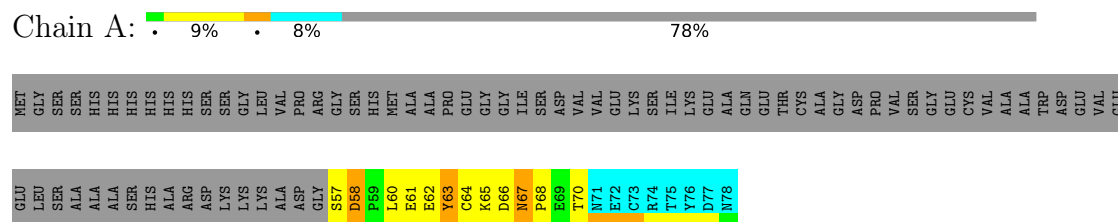
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9LZP9
A	-19	GLY	-	expression tag	UNP Q9LZP9
A	-18	SER	-	expression tag	UNP Q9LZP9
A	-17	SER	-	expression tag	UNP Q9LZP9
A	-16	HIS	-	expression tag	UNP Q9LZP9
A	-15	HIS	-	expression tag	UNP Q9LZP9
A	-14	HIS	-	expression tag	UNP Q9LZP9
A	-13	HIS	-	expression tag	UNP Q9LZP9
A	-12	HIS	-	expression tag	UNP Q9LZP9
A	-11	HIS	-	expression tag	UNP Q9LZP9
A	-10	SER	-	expression tag	UNP Q9LZP9
A	-9	SER	-	expression tag	UNP Q9LZP9
A	-8	GLY	-	expression tag	UNP Q9LZP9
A	-7	LEU	-	expression tag	UNP Q9LZP9
A	-6	VAL	-	expression tag	UNP Q9LZP9
A	-5	PRO	-	expression tag	UNP Q9LZP9
A	-4	ARG	-	expression tag	UNP Q9LZP9
A	-3	GLY	-	expression tag	UNP Q9LZP9
A	-2	SER	-	expression tag	UNP Q9LZP9
A	-1	HIS	-	expression tag	UNP Q9LZP9
A	0	MET	-	expression tag	UNP Q9LZP9

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: CP12 domain-containing protein 2

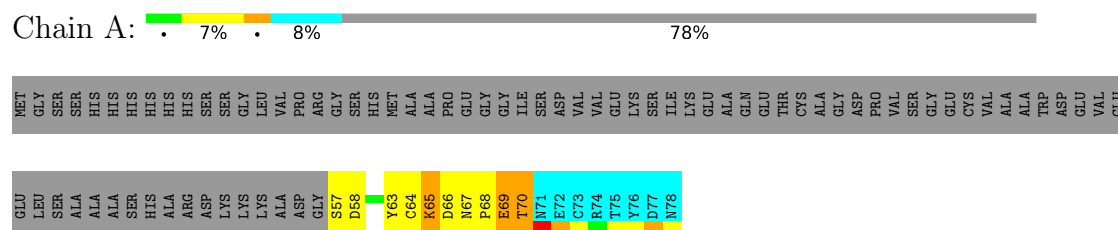


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

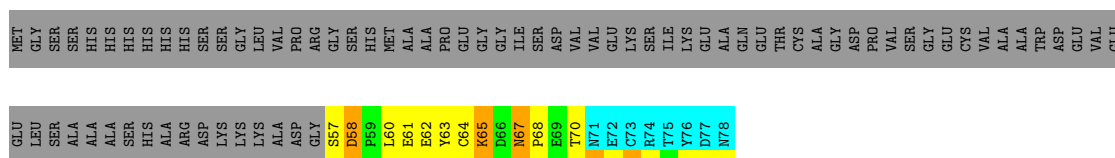
- Molecule 1: CP12 domain-containing protein 2



4.2.2 Score per residue for model 2

- Molecule 1: CP12 domain-containing protein 2

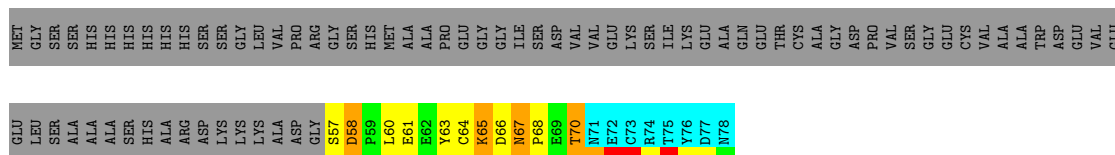




4.2.3 Score per residue for model 3

- Molecule 1: CP12 domain-containing protein 2

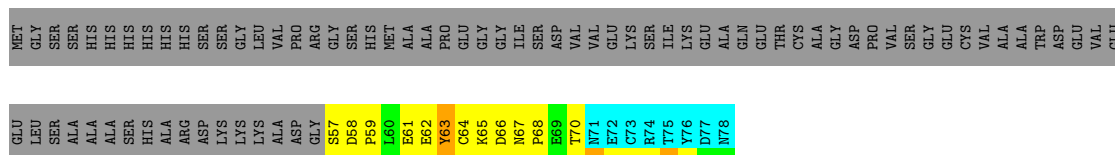
Chain A: . 7% . 8% 78%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: CP12 domain-containing protein 2

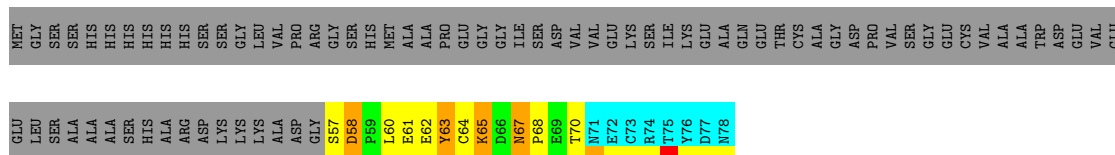
Chain A: . 11% . 8% 78%



4.2.5 Score per residue for model 5

- Molecule 1: CP12 domain-containing protein 2

Chain A: . 7% . 8% 78%



4.2.6 Score per residue for model 6

- Molecule 1: CP12 domain-containing protein 2

Chain A: . 9% . 8% 78%

4.2.7 Score per residue for model 7

- Molecule 1: CP12 domain-containing protein 2



4.2.8 Score per residue for model 8

- Molecule 1: CP12 domain-containing protein 2



4.2.9 Score per residue for model 9

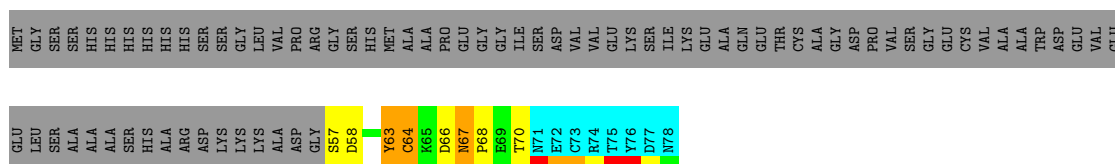
- Molecule 1: CP12 domain-containing protein 2



4.2.10 Score per residue for model 10

- Molecule 1: CP12 domain-containing protein 2

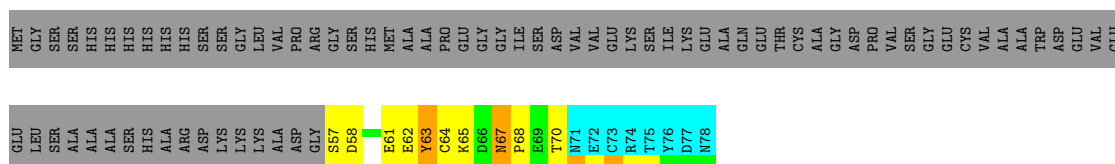




4.2.11 Score per residue for model 11

- Molecule 1: CP12 domain-containing protein 2

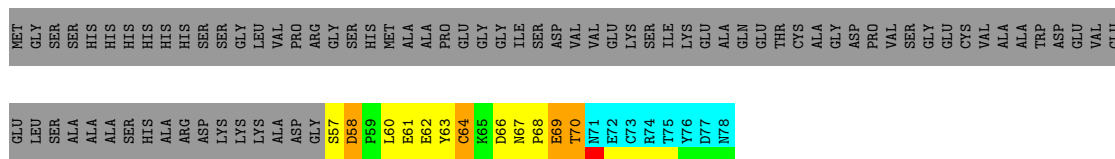
Chain A: . 8% . 8% 78%



4.2.12 Score per residue for model 12

- Molecule 1: CP12 domain-containing protein 2

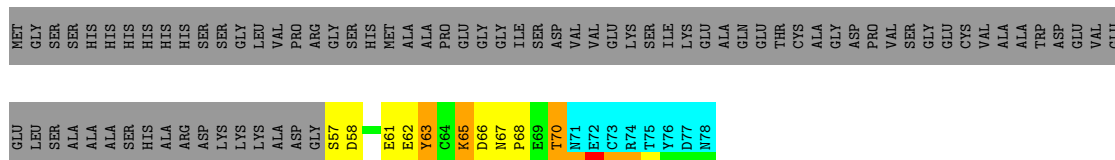
Chain A: . 8% . 8% 78%



4.2.13 Score per residue for model 13

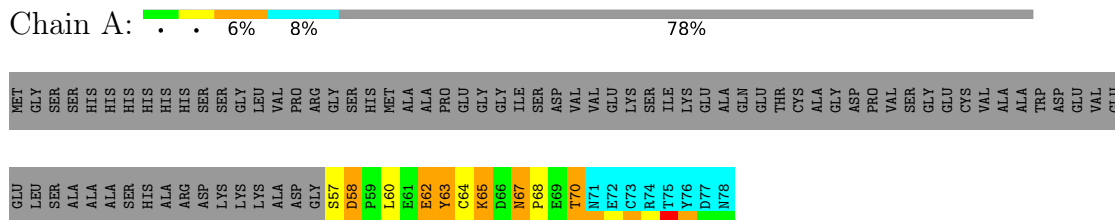
- Molecule 1: CP12 domain-containing protein 2

Chain A: . 7% . 8% 78%



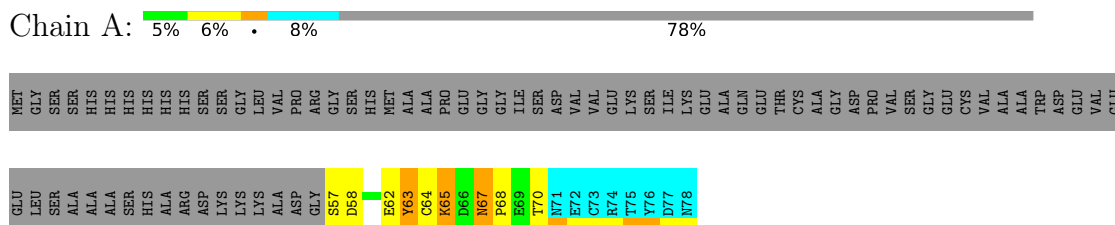
4.2.14 Score per residue for model 14

- Molecule 1: CP12 domain-containing protein 2



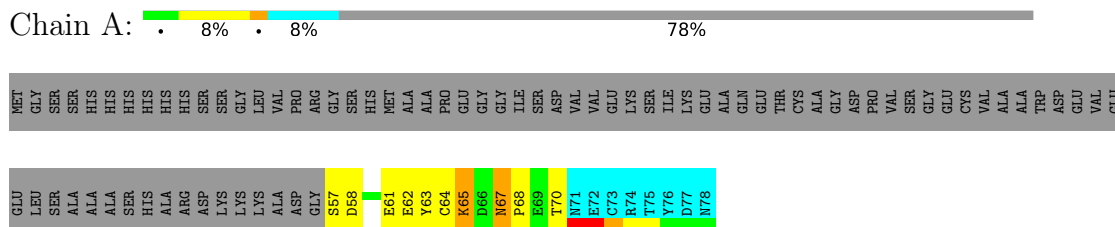
4.2.15 Score per residue for model 15

- Molecule 1: CP12 domain-containing protein 2



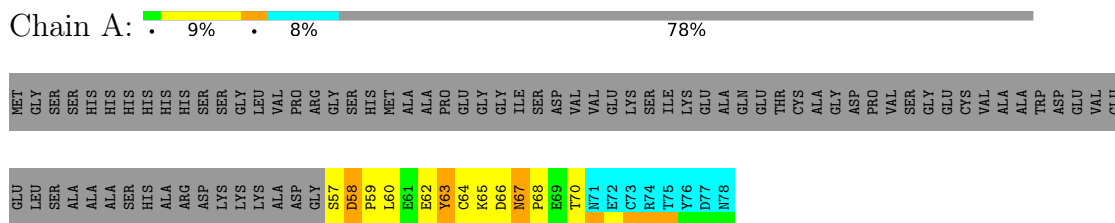
4.2.16 Score per residue for model 16

- Molecule 1: CP12 domain-containing protein 2



4.2.17 Score per residue for model 17

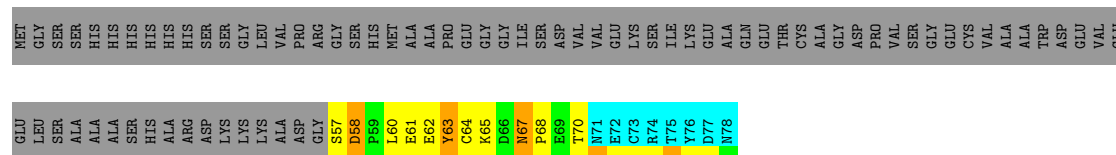
- Molecule 1: CP12 domain-containing protein 2



4.2.18 Score per residue for model 18

- Molecule 1: CP12 domain-containing protein 2

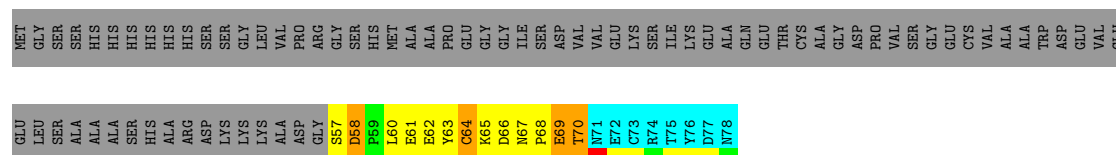
Chain A:  78%



4.2.19 Score per residue for model 19

- Molecule 1: CP12 domain-containing protein 2

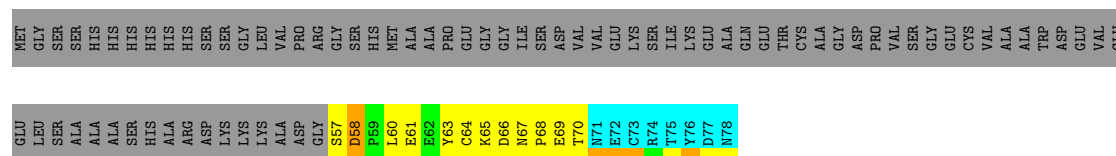
Chain A:  78%



4.2.20 Score per residue for model 20

- Molecule 1: CP12 domain-containing protein 2

Chain A:  78%



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 20 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
PROCHECK	refinement	
CNSSOLVE	structure solution	1.2.1
CNSSOLVE	refinement	1.2.1

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	518
Number of shifts mapped to atoms	202
Number of unparsed shifts	0
Number of shifts with mapping errors	316
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	113	72	94	7±6
All	All	2260	1440	1880	149

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ASN:HB3	1:A:70:THR:C	0.78	2.03	3	2
1:A:60:LEU:HD12	1:A:61:GLU:N	0.66	2.05	8	1
1:A:63:TYR:O	1:A:67:ASN:N	0.66	2.28	3	7
1:A:67:ASN:OD1	1:A:70:THR:HB	0.62	1.94	3	1
1:A:66:ASP:O	1:A:68:PRO:HD3	0.60	1.96	20	6
1:A:67:ASN:CB	1:A:70:THR:HG23	0.60	2.27	13	1
1:A:64:CYS:HA	1:A:67:ASN:HB2	0.59	1.73	3	1
1:A:64:CYS:HA	1:A:67:ASN:O	0.58	1.98	4	9
1:A:63:TYR:O	1:A:67:ASN:ND2	0.58	2.36	3	2
1:A:63:TYR:HB2	1:A:67:ASN:ND2	0.58	2.14	20	1
1:A:67:ASN:HB3	1:A:70:THR:HG23	0.56	1.77	13	1
1:A:67:ASN:HB3	1:A:70:THR:H	0.56	1.59	1	4
1:A:66:ASP:C	1:A:68:PRO:HD3	0.56	2.25	6	2
1:A:64:CYS:O	1:A:68:PRO:HA	0.54	2.01	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ASN:HB3	1:A:70:THR:CB	0.53	2.33	13	5
1:A:65:LYS:HG3	1:A:66:ASP:N	0.53	2.18	13	1
1:A:67:ASN:CB	1:A:70:THR:C	0.53	2.81	13	1
1:A:64:CYS:O	1:A:68:PRO:CA	0.53	2.57	15	10
1:A:63:TYR:HB2	1:A:67:ASN:HD22	0.51	1.66	20	1
1:A:63:TYR:C	1:A:67:ASN:ND2	0.51	2.69	13	3
1:A:67:ASN:CA	1:A:70:THR:HG23	0.51	2.36	13	1
1:A:62:GLU:O	1:A:65:LYS:HG3	0.50	2.07	16	2
1:A:63:TYR:O	1:A:66:ASP:N	0.49	2.45	3	2
1:A:67:ASN:HB3	1:A:70:THR:N	0.49	2.22	1	4
1:A:66:ASP:O	1:A:68:PRO:CD	0.49	2.61	13	6
1:A:60:LEU:HA	1:A:63:TYR:CE2	0.49	2.43	20	1
1:A:62:GLU:O	1:A:65:LYS:HB3	0.49	2.08	14	10
1:A:62:GLU:HA	1:A:65:LYS:HG2	0.48	1.85	19	1
1:A:67:ASN:HB3	1:A:70:THR:CG2	0.48	2.39	13	1
1:A:67:ASN:HB3	1:A:70:THR:O	0.48	2.08	3	1
1:A:67:ASN:O	1:A:70:THR:N	0.46	2.48	12	3
1:A:67:ASN:HB2	1:A:70:THR:C	0.46	2.35	12	4
1:A:64:CYS:HA	1:A:70:THR:O	0.46	2.10	12	3
1:A:63:TYR:C	1:A:67:ASN:HD22	0.46	2.18	12	4
1:A:67:ASN:HB3	1:A:70:THR:CA	0.45	2.41	1	2
1:A:64:CYS:SG	1:A:70:THR:O	0.45	2.75	8	3
1:A:64:CYS:O	1:A:67:ASN:C	0.44	2.60	9	2
1:A:64:CYS:O	1:A:68:PRO:N	0.43	2.51	15	1
1:A:63:TYR:CD1	1:A:64:CYS:N	0.43	2.86	20	1
1:A:67:ASN:HA	1:A:70:THR:OG1	0.43	2.13	3	1
1:A:67:ASN:O	1:A:69:GLU:N	0.43	2.52	1	4
1:A:67:ASN:HA	1:A:70:THR:HG23	0.43	1.89	13	1
1:A:67:ASN:C	1:A:69:GLU:N	0.42	2.75	1	3
1:A:67:ASN:O	1:A:68:PRO:C	0.42	2.61	12	3
1:A:63:TYR:C	1:A:65:LYS:N	0.42	2.76	1	3
1:A:62:GLU:O	1:A:65:LYS:CG	0.42	2.68	19	2
1:A:58:ASP:C	1:A:60:LEU:N	0.42	2.78	17	12
1:A:62:GLU:O	1:A:65:LYS:HG2	0.42	2.14	19	1
1:A:67:ASN:CB	1:A:70:THR:CB	0.41	2.98	12	2
1:A:58:ASP:O	1:A:60:LEU:N	0.41	2.54	7	1
1:A:60:LEU:O	1:A:63:TYR:CZ	0.41	2.74	20	1
1:A:58:ASP:C	1:A:60:LEU:H	0.40	2.24	9	1

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	13/99 (13%)	10±1 (78±6%)	3±1 (20±7%)	0±0 (2±3%)	8	51
All	All	260/1980 (13%)	202 (78%)	53 (20%)	5 (2%)	8	51

All 2 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	PRO	4
1	A	67	ASN	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	14/80 (18%)	9±1 (61±6%)	5±1 (39±6%)	0	6
All	All	280/1600 (18%)	171 (61%)	109 (39%)	0	6

All 11 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	57	SER	20
1	A	58	ASP	20
1	A	65	LYS	12
1	A	61	GLU	12
1	A	67	ASN	10
1	A	63	TYR	10
1	A	70	THR	9
1	A	69	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	66	ASP	5
1	A	62	GLU	3
1	A	64	CYS	3

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 84% for the well-defined parts and 84% 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	518
Number of shifts mapped to atoms	202
Number of unparsed shifts	0
Number of shifts with mapping errors	316
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. All 316 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	ALA	H	8.31	0.02	1
1	A	1	ALA	HA	4.3	0.02	1
1	A	1	ALA	HB1	1.38	0.02	1
1	A	1	ALA	HB2	1.38	0.02	1
1	A	1	ALA	HB3	1.38	0.02	1
1	A	1	ALA	C	176.81	0.15	1
1	A	1	ALA	CA	52.11	0.08	1
1	A	1	ALA	CB	19.34	0.08	1
1	A	1	ALA	N	125.39	0.13	1
1	A	2	ALA	H	8.33	0.02	1
1	A	2	ALA	HA	4.59	0.02	1
1	A	2	ALA	C	175.58	0.15	1
1	A	2	ALA	CA	50.42	0.08	1
1	A	2	ALA	CB	18.14	0.08	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ALA	N	124.75	0.13	1
1	A	3	PRO	HA	4.44	0.02	1
1	A	3	PRO	HB2	2.29	0.02	2
1	A	3	PRO	HB3	2.29	0.02	2
1	A	3	PRO	HG2	1.93	0.02	2
1	A	3	PRO	HG3	1.93	0.02	2
1	A	3	PRO	C	177.11	0.15	1
1	A	3	PRO	CA	63.13	0.08	1
1	A	3	PRO	CB	32.01	0.08	1
1	A	3	PRO	CG	27.5	0.08	1
1	A	4	GLU	H	8.66	0.02	1
1	A	4	GLU	HA	4.27	0.02	1
1	A	4	GLU	HB2	2.03	0.02	1
1	A	4	GLU	HB3	2.03	0.02	1
1	A	4	GLU	HG2	2.32	0.02	1
1	A	4	GLU	HG3	2.32	0.02	1
1	A	4	GLU	C	177.1	0.15	1
1	A	4	GLU	CA	56.94	0.08	1
1	A	4	GLU	CB	30.06	0.08	1
1	A	4	GLU	CG	36.41	0.08	1
1	A	4	GLU	N	121.31	0.13	1
1	A	5	GLY	H	8.53	0.02	1
1	A	5	GLY	HA2	4.0	0.02	1
1	A	5	GLY	HA3	4.0	0.02	1
1	A	5	GLY	C	174.6	0.15	1
1	A	5	GLY	CA	45.33	0.08	1
1	A	5	GLY	N	110.23	0.13	1
1	A	6	GLY	H	8.3	0.02	1
1	A	6	GLY	HA2	3.98	0.02	1
1	A	6	GLY	HA3	3.98	0.02	1
1	A	6	GLY	C	174.06	0.15	1
1	A	6	GLY	CA	45.17	0.08	1
1	A	6	GLY	N	108.69	0.13	1
1	A	7	ILE	H	8.16	0.02	1
1	A	7	ILE	HA	4.26	0.02	1
1	A	7	ILE	HB	1.9	0.02	1
1	A	7	ILE	HG12	1.47	0.02	2
1	A	7	ILE	HG13	1.2	0.02	2
1	A	7	ILE	HG21	0.96	0.02	1
1	A	7	ILE	HG22	0.96	0.02	1
1	A	7	ILE	HG23	0.96	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ILE	C	176.25	0.15	1
1	A	7	ILE	CA	61.17	0.08	1
1	A	7	ILE	CB	38.87	0.08	1
1	A	7	ILE	CD1	12.96	0.08	1
1	A	7	ILE	CG1	27.26	0.08	1
1	A	7	ILE	CG2	17.74	0.08	1
1	A	7	ILE	N	119.75	0.13	1
1	A	8	SER	H	8.46	0.02	1
1	A	8	SER	HA	4.53	0.02	1
1	A	8	SER	HB2	3.91	0.02	1
1	A	8	SER	HB3	3.91	0.02	1
1	A	8	SER	C	174.45	0.15	1
1	A	8	SER	CA	58.33	0.08	1
1	A	8	SER	CB	63.95	0.08	1
1	A	8	SER	N	119.63	0.13	1
1	A	13	LYS	HA	4.27	0.02	1
1	A	13	LYS	HB2	1.83	0.02	1
1	A	13	LYS	HB3	1.83	0.02	1
1	A	13	LYS	HG2	1.47	0.02	1
1	A	13	LYS	HG3	1.47	0.02	1
1	A	13	LYS	C	176.97	0.15	1
1	A	13	LYS	CA	56.9	0.08	1
1	A	13	LYS	CB	33.07	0.08	1
1	A	13	LYS	CG	25.03	0.08	1
1	A	14	SER	H	8.39	0.02	1
1	A	14	SER	HA	4.45	0.02	1
1	A	14	SER	HB2	3.92	0.02	1
1	A	14	SER	HB3	3.92	0.02	1
1	A	14	SER	C	174.97	0.15	1
1	A	14	SER	CA	58.54	0.08	1
1	A	14	SER	CB	63.67	0.08	1
1	A	14	SER	N	117.05	0.13	1
1	A	17	GLU	C	175.42	0.15	1
1	A	17	GLU	CA	55.24	0.08	1
1	A	17	GLU	CB	32.99	0.08	1
1	A	18	ALA	H	8.37	0.02	1
1	A	18	ALA	N	125.78	0.13	1
1	A	19	GLN	HB2	2.19	0.02	1
1	A	19	GLN	HB3	2.19	0.02	1
1	A	19	GLN	HE21	6.9	0.02	1
1	A	19	GLN	HE22	7.53	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	GLN	HG2	2.42	0.02	1
1	A	19	GLN	HG3	2.42	0.02	1
1	A	19	GLN	CD	180.3	0.15	1
1	A	19	GLN	CG	33.87	0.08	1
1	A	19	GLN	NE2	111.77	0.13	1
1	A	20	GLU	HB2	2.08	0.02	2
1	A	20	GLU	HB3	1.93	0.02	2
1	A	20	GLU	C	176.96	0.15	1
1	A	20	GLU	CA	57.01	0.08	1
1	A	20	GLU	CB	30.17	0.08	1
1	A	20	GLU	CG	36.56	0.08	1
1	A	21	THR	H	8.24	0.02	1
1	A	21	THR	HA	4.37	0.02	1
1	A	21	THR	HB	3.87	0.02	1
1	A	21	THR	C	174.84	0.15	1
1	A	21	THR	CA	62.54	0.08	1
1	A	21	THR	CB	69.84	0.08	1
1	A	21	THR	N	115.0	0.13	1
1	A	23	ALA	HA	4.47	0.02	1
1	A	23	ALA	HB1	1.41	0.02	1
1	A	23	ALA	HB2	1.41	0.02	1
1	A	23	ALA	HB3	1.41	0.02	1
1	A	23	ALA	C	177.41	0.15	1
1	A	23	ALA	CA	52.41	0.08	1
1	A	23	ALA	CB	19.9	0.08	1
1	A	24	GLY	H	8.13	0.02	1
1	A	24	GLY	HA2	3.99	0.02	2
1	A	24	GLY	HA3	3.88	0.02	2
1	A	24	GLY	C	171.93	0.15	1
1	A	24	GLY	CA	44.67	0.08	1
1	A	24	GLY	N	108.06	0.13	1
1	A	25	ASP	H	7.93	0.02	1
1	A	25	ASP	HA	4.79	0.02	1
1	A	25	ASP	HB2	2.58	0.02	1
1	A	25	ASP	HB3	2.58	0.02	1
1	A	25	ASP	CA	51.87	0.08	1
1	A	25	ASP	CB	42.81	0.08	1
1	A	25	ASP	N	118.59	0.13	1
1	A	27	VAL	HA	4.92	0.02	1
1	A	27	VAL	HB	2.11	0.02	1
1	A	27	VAL	C	176.35	0.15	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	VAL	CA	62.7	0.08	1
1	A	27	VAL	CB	32.61	0.08	1
1	A	28	SER	H	8.42	0.02	1
1	A	28	SER	HA	4.52	0.02	1
1	A	28	SER	HB2	4.04	0.02	2
1	A	28	SER	HB3	3.91	0.02	2
1	A	28	SER	C	175.35	0.15	1
1	A	28	SER	CA	57.77	0.08	1
1	A	28	SER	CB	64.17	0.08	1
1	A	28	SER	N	119.87	0.13	1
1	A	29	GLY	H	8.63	0.02	1
1	A	29	GLY	C	174.57	0.15	1
1	A	29	GLY	CA	46.0	0.08	1
1	A	29	GLY	N	111.27	0.13	1
1	A	30	GLU	H	8.49	0.02	1
1	A	30	GLU	CA	56.98	0.08	1
1	A	30	GLU	CB	29.49	0.08	1
1	A	30	GLU	N	120.23	0.13	1
1	A	35	TRP	HA	4.65	0.02	1
1	A	35	TRP	HB2	3.35	0.02	2
1	A	35	TRP	HB3	3.25	0.02	2
1	A	35	TRP	HD1	7.29	0.02	1
1	A	35	TRP	HE1	10.13	0.02	1
1	A	35	TRP	HE3	7.61	0.02	1
1	A	35	TRP	HH2	7.19	0.02	1
1	A	35	TRP	HZ2	7.43	0.02	1
1	A	35	TRP	HZ3	7.11	0.02	1
1	A	35	TRP	NE1	129.52	0.13	1
1	A	41	LEU	HA	4.3	0.02	1
1	A	41	LEU	HB2	1.69	0.02	1
1	A	41	LEU	HB3	1.69	0.02	1
1	A	41	LEU	HD11	0.9	0.02	1
1	A	41	LEU	HD12	0.9	0.02	1
1	A	41	LEU	HD13	0.9	0.02	1
1	A	41	LEU	HD21	0.9	0.02	1
1	A	41	LEU	HD22	0.9	0.02	1
1	A	41	LEU	HD23	0.9	0.02	1
1	A	41	LEU	C	178.17	0.15	1
1	A	41	LEU	CA	55.91	0.08	1
1	A	41	LEU	CB	42.21	0.08	1
1	A	42	SER	H	8.31	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	SER	HA	4.37	0.02	1
1	A	42	SER	HB2	3.93	0.02	1
1	A	42	SER	HB3	3.93	0.02	1
1	A	42	SER	C	175.27	0.15	1
1	A	42	SER	CA	58.95	0.08	1
1	A	42	SER	CB	63.67	0.08	1
1	A	42	SER	N	116.28	0.13	1
1	A	45	ALA	HA	4.27	0.02	1
1	A	45	ALA	HB1	1.46	0.02	1
1	A	45	ALA	HB2	1.46	0.02	1
1	A	45	ALA	HB3	1.46	0.02	1
1	A	45	ALA	C	178.84	0.15	1
1	A	45	ALA	CA	53.48	0.08	1
1	A	45	ALA	CB	18.76	0.08	1
1	A	46	SER	H	8.12	0.02	1
1	A	46	SER	C	175.13	0.15	1
1	A	46	SER	CA	59.55	0.08	1
1	A	46	SER	CB	63.4	0.08	1
1	A	46	SER	N	114.22	0.13	1
1	A	47	HIS	HA	4.63	0.02	1
1	A	47	HIS	HB2	3.25	0.02	1
1	A	47	HIS	HB3	3.25	0.02	1
1	A	47	HIS	C	175.43	0.15	1
1	A	47	HIS	CA	56.66	0.08	1
1	A	47	HIS	CB	29.65	0.08	1
1	A	48	ALA	H	8.11	0.02	1
1	A	48	ALA	HA	4.25	0.02	1
1	A	48	ALA	HB1	1.45	0.02	1
1	A	48	ALA	HB2	1.45	0.02	1
1	A	48	ALA	HB3	1.45	0.02	1
1	A	48	ALA	C	178.32	0.15	1
1	A	48	ALA	CA	53.46	0.08	1
1	A	48	ALA	CB	18.87	0.08	1
1	A	48	ALA	N	123.6	0.13	1
1	A	49	ARG	H	8.25	0.02	1
1	A	49	ARG	HB2	1.88	0.02	1
1	A	49	ARG	HB3	1.88	0.02	1
1	A	49	ARG	HD2	3.23	0.02	5
1	A	49	ARG	HD3	3.23	0.02	5
1	A	49	ARG	HE	7.19	0.02	5
1	A	49	ARG	HG2	1.67	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	ARG	HG3	1.67	0.02	1
1	A	49	ARG	CA	56.71	0.08	1
1	A	49	ARG	CB	30.44	0.08	1
1	A	49	ARG	CG	27.28	0.08	1
1	A	49	ARG	CZ	175.12	0.15	1
1	A	49	ARG	N	119.24	0.13	1
1	A	49	ARG	NE	84.52	0.13	1
1	A	50	ASP	H	8.21	0.02	1
1	A	50	ASP	HA	4.58	0.02	1
1	A	50	ASP	HB2	2.71	0.02	1
1	A	50	ASP	HB3	2.71	0.02	1
1	A	50	ASP	C	176.48	0.15	1
1	A	50	ASP	CA	54.77	0.08	1
1	A	50	ASP	CB	40.92	0.08	1
1	A	50	ASP	N	120.56	0.13	1
1	A	51	LYS	H	8.16	0.02	1
1	A	51	LYS	HA	4.28	0.02	1
1	A	51	LYS	HB2	1.8	0.02	1
1	A	51	LYS	HB3	1.8	0.02	1
1	A	51	LYS	HG2	1.46	0.02	1
1	A	51	LYS	HG3	1.46	0.02	1
1	A	51	LYS	C	176.64	0.15	1
1	A	51	LYS	CA	56.55	0.08	1
1	A	51	LYS	CB	32.79	0.08	1
1	A	51	LYS	CG	24.83	0.08	1
1	A	51	LYS	N	121.55	0.13	1
1	A	52	LYS	H	8.28	0.02	1
1	A	52	LYS	HA	4.29	0.02	1
1	A	52	LYS	HB2	1.82	0.02	1
1	A	52	LYS	HB3	1.82	0.02	1
1	A	52	LYS	HG2	1.46	0.02	1
1	A	52	LYS	HG3	1.46	0.02	1
1	A	52	LYS	C	176.8	0.15	1
1	A	52	LYS	CA	56.49	0.08	1
1	A	52	LYS	CB	32.92	0.08	1
1	A	52	LYS	CG	24.91	0.08	1
1	A	52	LYS	N	122.06	0.13	1
1	A	53	LYS	H	8.38	0.02	1
1	A	53	LYS	HA	4.29	0.02	1
1	A	53	LYS	HB2	1.82	0.02	1
1	A	53	LYS	HB3	1.82	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	LYS	HG2	1.47	0.02	1
1	A	53	LYS	HG3	1.47	0.02	1
1	A	53	LYS	C	176.65	0.15	1
1	A	53	LYS	CB	32.99	0.08	1
1	A	53	LYS	CG	24.91	0.08	1
1	A	53	LYS	N	122.69	0.13	1
1	A	54	ALA	H	8.5	0.02	1
1	A	54	ALA	HA	4.32	0.02	1
1	A	54	ALA	HB1	1.42	0.02	1
1	A	54	ALA	HB2	1.42	0.02	1
1	A	54	ALA	HB3	1.42	0.02	1
1	A	54	ALA	C	177.56	0.15	1
1	A	54	ALA	CA	52.62	0.08	1
1	A	54	ALA	CB	19.0	0.08	1
1	A	54	ALA	N	125.58	0.13	1
1	A	55	ASP	H	8.32	0.02	1
1	A	55	ASP	HA	4.6	0.02	1
1	A	55	ASP	HB2	2.74	0.02	1
1	A	55	ASP	HB3	2.74	0.02	1
1	A	55	ASP	C	176.95	0.15	1
1	A	55	ASP	CA	54.24	0.08	1
1	A	55	ASP	CB	41.07	0.08	1
1	A	55	ASP	N	119.45	0.13	1
1	A	56	GLY	H	8.4	0.02	1
1	A	56	GLY	HA2	4.06	0.02	2
1	A	56	GLY	HA3	3.94	0.02	2
1	A	56	GLY	C	174.21	0.15	1
1	A	56	GLY	CA	45.41	0.08	1
1	A	56	GLY	N	109.36	0.13	1
1	A	57	SER	HB2	3.87	0.02	1
1	A	58	ASP	HB2	2.87	0.02	2
1	A	59	PRO	HB2	2.36	0.02	2
1	A	60	LEU	HB2	1.7	0.02	1
1	A	61	GLU	HB2	2.11	0.02	1
1	A	62	GLU	HB2	2.06	0.02	1
1	A	63	TYR	HB2	3.21	0.02	2
1	A	64	CYS	HB2	3.07	0.02	2
1	A	65	LYS	HB2	1.9	0.02	1
1	A	65	LYS	HD2	1.62	0.02	1
1	A	65	LYS	HG2	1.44	0.02	1
1	A	66	ASP	HB2	2.67	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	67	ASN	HB2	2.4	0.02	2
1	A	68	PRO	HB2	2.35	0.02	2
1	A	68	PRO	HD2	3.57	0.02	2
1	A	68	PRO	HG2	2.03	0.02	2
1	A	69	GLU	HB2	2.22	0.02	2
1	A	69	GLU	HG2	2.29	0.02	1
1	A	71	ASN	HB2	2.86	0.02	1
1	A	72	GLU	HB2	2.12	0.02	1
1	A	73	CYS	HB2	3.17	0.02	2
1	A	74	ARG	HB2	1.84	0.02	1
1	A	74	ARG	HD2	3.23	0.02	5
1	A	74	ARG	HG2	1.68	0.02	1
1	A	76	TYR	HB2	3.16	0.02	2
1	A	77	ASP	HB2	2.74	0.02	2
1	A	78	ASN	HB2	2.74	0.02	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	55	-0.32 ± 0.31	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	51	0.10 ± 0.27	None needed (< 0.5 ppm)
$^{13}\text{C}'$	50	-0.55 ± 0.25	Should be applied
^{15}N	46	0.96 ± 0.86	None needed (imprecise)

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 84%, i.e. 143 atoms were assigned a chemical shift out of a possible 170. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	64/66 (97%)	26/26 (100%)	26/28 (93%)	12/12 (100%)
Sidechain	75/95 (79%)	48/59 (81%)	26/34 (76%)	1/2 (50%)
Aromatic	4/9 (44%)	4/4 (100%)	0/5 (0%)	0/0 (—%)
Overall	143/170 (84%)	78/89 (88%)	52/67 (78%)	13/14 (93%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 229 atoms were assigned a chemical shift out of a possible

274. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	103/106 (97%)	42/42 (100%)	41/44 (93%)	20/20 (100%)
Sidechain	118/150 (79%)	75/92 (82%)	39/51 (76%)	4/7 (57%)
Aromatic	8/18 (44%)	8/8 (100%)	0/10 (0%)	0/0 (—%)
Overall	229/274 (84%)	125/142 (88%)	80/105 (76%)	24/27 (89%)

7.1.4 Statistically unusual chemical shifts [i](#)

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:

