



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 12:19 PM UTC

PDB ID : 6HKA / pdb_00006hka
BMRB ID : 27167
Title : The solution structure of the micelle-associated FATC domain of the human protein kinase ataxia telangiectasia mutated (ATM)
Authors : Abd Rahim, M.S.; Dames, S.A.
Deposited on : 2018-09-06

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

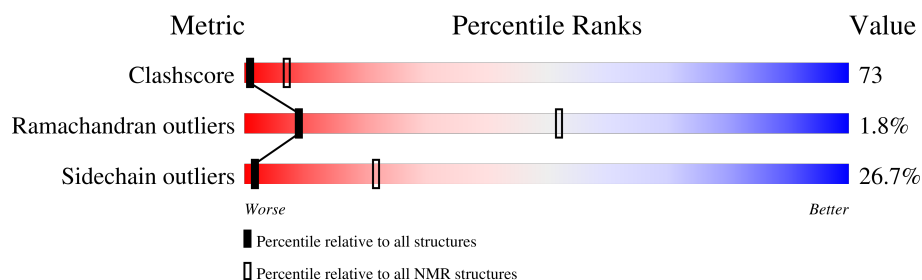
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	100	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 8 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:72-A:82 (11)	0.38	8

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition

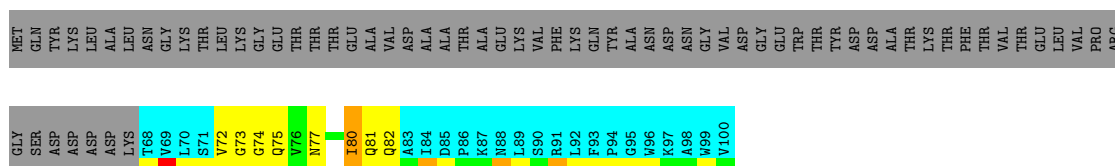
There is only 1 type of molecule in this entry. The entry contains 530 atoms, of which 271 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Immunoglobulin G-binding protein G,Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					Trace
1	A	33	Total	C	H	N	O	0
			530	170	271	45	44	

There are 14 discrepancies between the modelled and reference sequences:

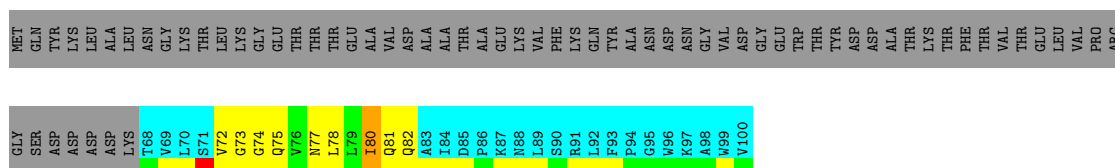
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P19909
A	2	GLN	-	expression tag	UNP P19909
A	6	ALA	ILE	conflict	UNP P19909
A	57	LEU	-	linker	UNP P19909
A	58	VAL	-	linker	UNP P19909
A	59	PRO	-	linker	UNP P19909
A	60	ARG	-	linker	UNP P19909
A	61	GLY	-	linker	UNP P19909
A	62	SER	-	linker	UNP P19909
A	63	ASP	-	linker	UNP P19909
A	64	ASP	-	linker	UNP P19909
A	65	ASP	-	linker	UNP P19909
A	66	ASP	-	linker	UNP P19909
A	67	LYS	-	linker	UNP P19909



4.2.3 Score per residue for model 3

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

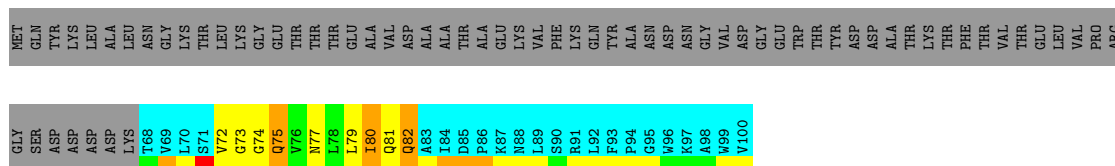
Chain A: 8% 22% 67%



4.2.4 Score per residue for model 4

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

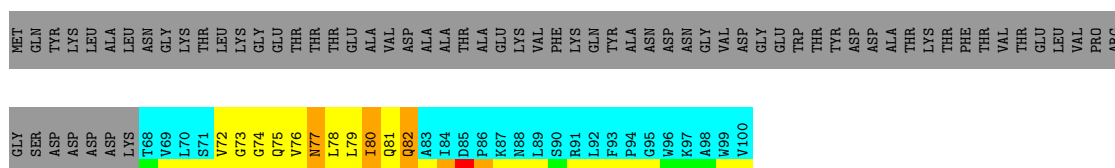
Chain A: 6% 22% 67%



4.2.5 Score per residue for model 5

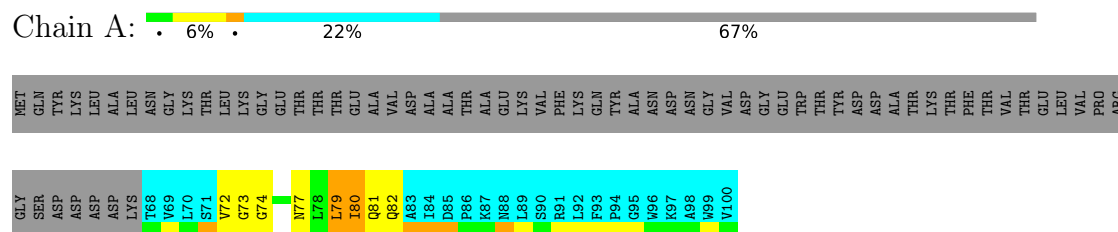
- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

Chain A: 8% 22% 67%



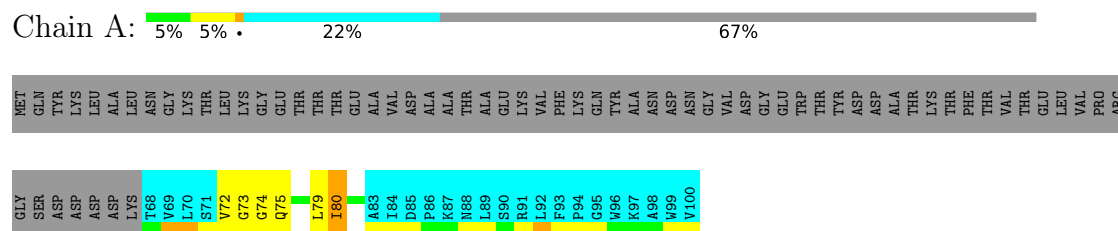
4.2.6 Score per residue for model 6

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM



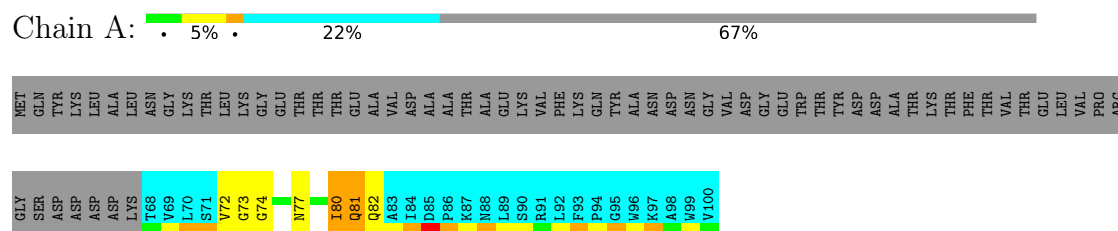
4.2.7 Score per residue for model 7

- Molecule 1: Immunoglobulin G-binding protein G, Serine-protein kinase ATM



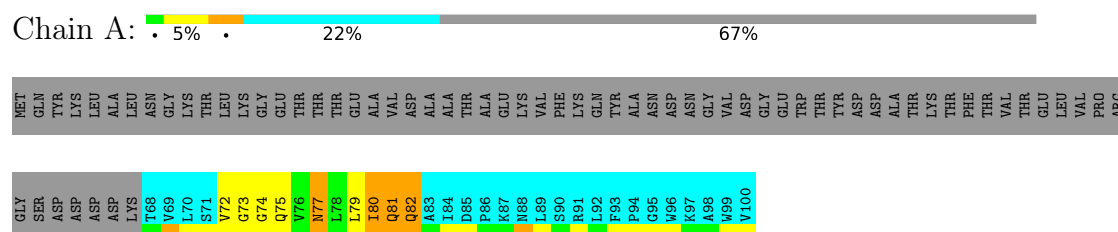
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Immunoglobulin G-binding protein G, Serine-protein kinase ATM



4.2.9 Score per residue for model 9

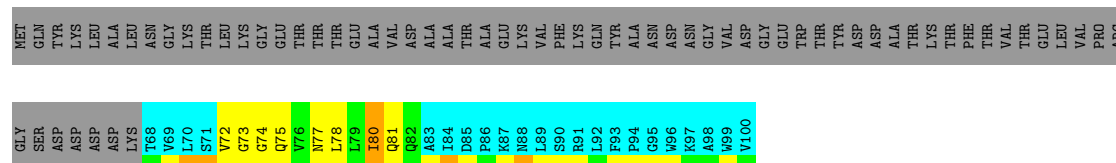
- Molecule 1: Immunoglobulin G-binding protein G, Serine-protein kinase ATM



4.2.10 Score per residue for model 10

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

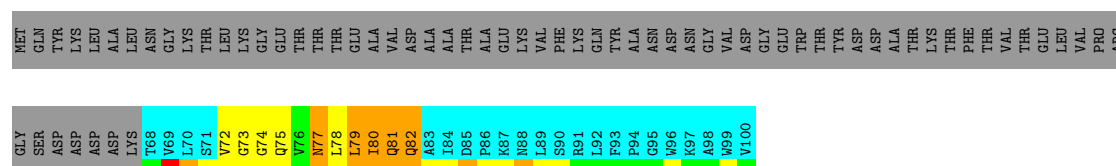
Chain A:  7% 22% 67%



4.2.11 Score per residue for model 11

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

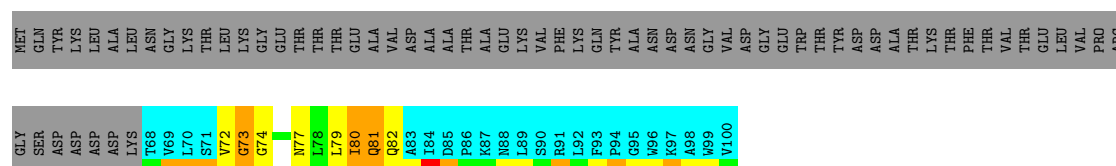
Chain A:  5% 5% 22% 67%



4.2.12 Score per residue for model 12

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

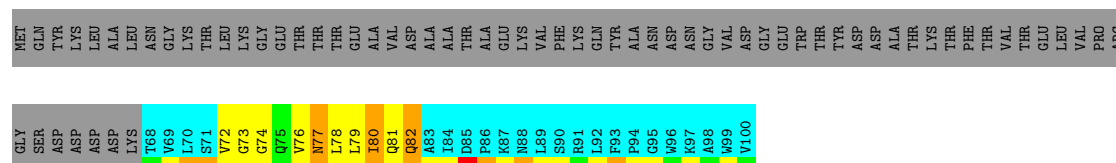
Chain A:  5% 22% 67%



4.2.13 Score per residue for model 13

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

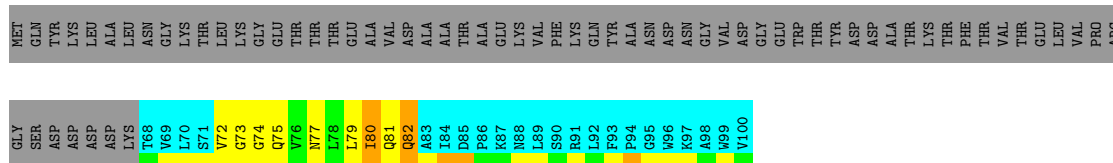
Chain A:  7% 22% 67%



4.2.14 Score per residue for model 14

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

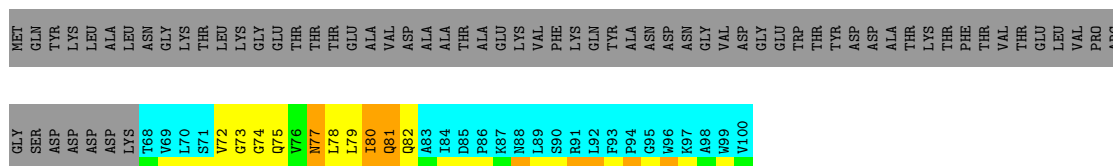
Chain A:  7% 22% 67%



4.2.15 Score per residue for model 15

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

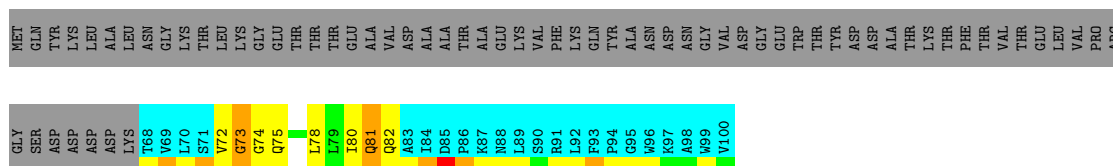
Chain A:  7% 22% 67%



4.2.16 Score per residue for model 16

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

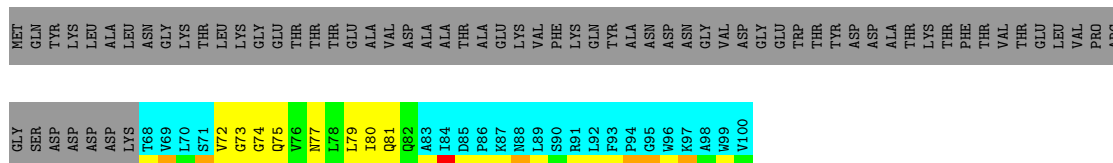
Chain A:  6% 22% 67%



4.2.17 Score per residue for model 17

- Molecule 1: Immunoglobulin G-binding protein G,Serine-protein kinase ATM

Chain A:  8% 22% 67%



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 lowest energy*.

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

Software name	Classification	Version
Xplor-NIH	structure calculation	

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	1103
Number of shifts mapped to atoms	406
Number of unparsed shifts	0
Number of shifts with mapping errors	697
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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	81	87	87	12±5
All	All	1620	1740	1740	245

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 73.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ILE:O	1:A:80:ILE:HD12	0.71	1.86	7	3
1:A:82:GLN:NE2	1:A:82:GLN:H	0.70	1.84	1	1
1:A:82:GLN:H	1:A:82:GLN:HE21	0.68	1.27	1	2
1:A:82:GLN:NE2	1:A:82:GLN:N	0.64	2.46	1	2
1:A:81:GLN:NE2	1:A:82:GLN:N	0.64	2.45	16	2
1:A:77:ASN:HD22	1:A:81:GLN:HE22	0.63	1.34	6	2
1:A:77:ASN:ND2	1:A:81:GLN:NE2	0.63	2.47	14	6
1:A:77:ASN:ND2	1:A:78:LEU:N	0.62	2.47	13	4
1:A:77:ASN:ND2	1:A:81:GLN:HE22	0.61	1.93	6	2
1:A:81:GLN:N	1:A:81:GLN:HE21	0.60	1.94	9	2
1:A:75:GLN:NE2	1:A:75:GLN:H	0.59	1.95	9	3
1:A:77:ASN:HD22	1:A:78:LEU:N	0.59	1.94	13	2
1:A:78:LEU:O	1:A:82:GLN:NE2	0.58	2.37	1	2
1:A:82:GLN:H	1:A:82:GLN:NE2	0.58	1.95	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:VAL:HG23	1:A:73:GLY:N	0.57	2.14	7	10
1:A:78:LEU:O	1:A:81:GLN:NE2	0.57	2.37	16	1
1:A:75:GLN:NE2	1:A:75:GLN:N	0.57	2.53	2	6
1:A:72:VAL:O	1:A:74:GLY:N	0.56	2.39	12	17
1:A:77:ASN:O	1:A:81:GLN:NE2	0.56	2.39	18	10
1:A:82:GLN:HE21	1:A:82:GLN:C	0.56	2.09	18	3
1:A:79:LEU:C	1:A:82:GLN:HE22	0.55	2.09	19	1
1:A:74:GLY:O	1:A:77:ASN:ND2	0.55	2.40	5	2
1:A:82:GLN:NE2	1:A:82:GLN:C	0.54	2.65	9	3
1:A:77:ASN:ND2	1:A:77:ASN:C	0.54	2.66	11	5
1:A:75:GLN:O	1:A:79:LEU:HD23	0.54	2.03	11	2
1:A:77:ASN:CG	1:A:81:GLN:NE2	0.53	2.66	18	5
1:A:77:ASN:C	1:A:81:GLN:HE21	0.53	2.11	10	4
1:A:78:LEU:O	1:A:80:ILE:N	0.53	2.42	13	2
1:A:72:VAL:C	1:A:74:GLY:N	0.52	2.67	13	19
1:A:77:ASN:C	1:A:81:GLN:NE2	0.52	2.68	19	2
1:A:80:ILE:HD13	1:A:80:ILE:O	0.52	2.05	18	8
1:A:80:ILE:HD12	1:A:80:ILE:C	0.52	2.30	7	2
1:A:80:ILE:CG2	1:A:81:GLN:NE2	0.51	2.73	8	2
1:A:82:GLN:O	1:A:82:GLN:NE2	0.51	2.44	11	1
1:A:77:ASN:CG	1:A:78:LEU:N	0.50	2.68	15	1
1:A:82:GLN:HE21	1:A:82:GLN:N	0.50	2.01	1	2
1:A:80:ILE:O	1:A:80:ILE:HD13	0.49	2.07	14	2
1:A:77:ASN:ND2	1:A:81:GLN:HE21	0.49	2.02	19	1
1:A:80:ILE:CG2	1:A:81:GLN:N	0.49	2.75	5	5
1:A:80:ILE:C	1:A:82:GLN:N	0.49	2.70	5	2
1:A:80:ILE:HD13	1:A:80:ILE:C	0.49	2.32	18	3
1:A:77:ASN:HD22	1:A:81:GLN:NE2	0.48	2.04	6	1
1:A:75:GLN:N	1:A:75:GLN:OE1	0.48	2.46	15	1
1:A:75:GLN:N	1:A:75:GLN:CD	0.48	2.71	2	2
1:A:81:GLN:N	1:A:81:GLN:NE2	0.48	2.60	9	2
1:A:72:VAL:HG23	1:A:73:GLY:H	0.48	1.68	14	1
1:A:81:GLN:NE2	1:A:82:GLN:CB	0.47	2.76	5	1
1:A:72:VAL:C	1:A:74:GLY:H	0.47	2.17	4	9
1:A:77:ASN:OD1	1:A:81:GLN:NE2	0.47	2.47	2	2
1:A:78:LEU:C	1:A:80:ILE:N	0.47	2.71	13	2
1:A:72:VAL:CG2	1:A:73:GLY:N	0.47	2.77	7	7
1:A:79:LEU:HD13	1:A:79:LEU:O	0.46	2.10	6	1
1:A:80:ILE:HG23	1:A:81:GLN:NE2	0.46	2.25	11	2
1:A:73:GLY:O	1:A:77:ASN:OD1	0.46	2.34	11	3
1:A:75:GLN:O	1:A:79:LEU:HD13	0.45	2.12	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ASN:O	1:A:81:GLN:CD	0.45	2.60	11	2
1:A:76:VAL:C	1:A:78:LEU:N	0.45	2.74	5	2
1:A:72:VAL:O	1:A:73:GLY:C	0.45	2.60	20	10
1:A:81:GLN:CD	1:A:81:GLN:C	0.44	2.84	16	1
1:A:80:ILE:C	1:A:80:ILE:HD13	0.44	2.37	5	1
1:A:82:GLN:CD	1:A:82:GLN:C	0.44	2.86	16	7
1:A:72:VAL:O	1:A:75:GLN:N	0.44	2.51	20	2
1:A:80:ILE:O	1:A:81:GLN:C	0.44	2.60	12	2
1:A:77:ASN:O	1:A:78:LEU:C	0.44	2.61	1	5
1:A:72:VAL:O	1:A:76:VAL:HG23	0.44	2.12	13	1
1:A:77:ASN:O	1:A:80:ILE:N	0.44	2.48	15	1
1:A:77:ASN:HD22	1:A:78:LEU:H	0.43	1.53	13	1
1:A:73:GLY:O	1:A:77:ASN:CG	0.43	2.62	13	1
1:A:75:GLN:CD	1:A:75:GLN:N	0.43	2.77	1	4
1:A:80:ILE:HG23	1:A:81:GLN:N	0.42	2.29	5	1
1:A:77:ASN:O	1:A:77:ASN:OD1	0.42	2.38	8	1
1:A:81:GLN:NE2	1:A:81:GLN:C	0.42	2.78	16	1
1:A:82:GLN:CD	1:A:82:GLN:O	0.42	2.63	15	1
1:A:78:LEU:C	1:A:80:ILE:H	0.41	2.23	13	1
1:A:80:ILE:CG2	1:A:81:GLN:HE22	0.41	2.27	18	1
1:A:82:GLN:C	1:A:82:GLN:HE21	0.41	2.23	9	1
1:A:80:ILE:C	1:A:80:ILE:CD1	0.41	2.93	18	3
1:A:80:ILE:HG23	1:A:81:GLN:HE22	0.40	1.77	11	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	11/100 (11%)	9±1 (85±9%)	1±1 (12±8%)	0±0 (2±4%)	9	52
All	All	219/2000 (11%)	188 (86%)	27 (12%)	4 (2%)	9	52

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	73	GLY	3
1	A	79	LEU	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	9/83 (11%)	7±1 (73±12%)	2±1 (27±12%)	2	22
All	All	180/1660 (11%)	132 (73%)	48 (27%)	2	22

All 6 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	80	ILE	20
1	A	82	GLN	10
1	A	81	GLN	6
1	A	77	ASN	5
1	A	79	LEU	5
1	A	75	GLN	2

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 89% 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: *output*

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	1103
Number of shifts mapped to atoms	406
Number of unparsed shifts	0
Number of shifts with mapping errors	697
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. All 697 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HA	4.231	?	1
1	A	1	MET	HB2	2.141	?	2
1	A	1	MET	HB3	2.276	?	2
1	A	1	MET	HE1	2.173	?	1
1	A	1	MET	HE2	2.173	?	1
1	A	1	MET	HE3	2.173	?	1
1	A	1	MET	HG2	2.219	?	2
1	A	1	MET	HG3	2.47	?	2
1	A	1	MET	CA	54.777	?	1
1	A	1	MET	CB	32.772	?	1
1	A	1	MET	CE	16.413	?	1
1	A	1	MET	CG	30.795	?	1
1	A	2	GLN	H	8.391	?	1
1	A	2	GLN	HA	5.02	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	GLN	HB2	2.022	?	2
1	A	2	GLN	HB3	2.075	?	2
1	A	2	GLN	HE21	7.88	?	2
1	A	2	GLN	HE22	6.954	?	2
1	A	2	GLN	HG2	2.147	?	2
1	A	2	GLN	HG3	2.42	?	2
1	A	2	GLN	CA	56.041	?	1
1	A	2	GLN	CB	30.522	?	1
1	A	2	GLN	CG	35.226	?	1
1	A	2	GLN	N	123.863	?	1
1	A	2	GLN	NE2	112.632	?	1
1	A	3	TYR	H	9.126	?	1
1	A	3	TYR	HA	5.399	?	1
1	A	3	TYR	HB2	2.775	?	2
1	A	3	TYR	HB3	3.465	?	2
1	A	3	TYR	HD1	7.183	?	3
1	A	3	TYR	HE1	6.946	?	3
1	A	3	TYR	CA	57.366	?	1
1	A	3	TYR	CB	43.59	?	1
1	A	3	TYR	CD1	133.674	?	3
1	A	3	TYR	CE1	118.145	?	3
1	A	3	TYR	N	124.692	?	1
1	A	4	LYS	H	9.218	?	1
1	A	4	LYS	HA	5.294	?	1
1	A	4	LYS	HB2	2.004	?	2
1	A	4	LYS	HB3	2.004	?	2
1	A	4	LYS	HD2	1.662	?	2
1	A	4	LYS	HD3	1.662	?	2
1	A	4	LYS	HE2	2.938	?	2
1	A	4	LYS	HE3	2.938	?	2
1	A	4	LYS	HG2	1.367	?	2
1	A	4	LYS	HG3	1.503	?	2
1	A	4	LYS	CA	55.342	?	1
1	A	4	LYS	CB	36.065	?	1
1	A	4	LYS	CD	29.236	?	1
1	A	4	LYS	CE	42.133	?	1
1	A	4	LYS	CG	25.577	?	1
1	A	4	LYS	N	121.737	?	1
1	A	5	LEU	H	8.582	?	1
1	A	5	LEU	HA	4.983	?	1
1	A	5	LEU	HB2	-1.055	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LEU	HB3	0.865	?	2
1	A	5	LEU	HD11	0.608	?	4
1	A	5	LEU	HD12	0.608	?	4
1	A	5	LEU	HD13	0.608	?	4
1	A	5	LEU	HD21	0.535	?	4
1	A	5	LEU	HD22	0.535	?	4
1	A	5	LEU	HD23	0.535	?	4
1	A	5	LEU	HG	0.913	?	1
1	A	5	LEU	CA	52.825	?	1
1	A	5	LEU	CB	42.565	?	1
1	A	5	LEU	CD1	26.048	?	2
1	A	5	LEU	CD2	24.419	?	2
1	A	5	LEU	CG	27.228	?	1
1	A	5	LEU	N	125.83	?	1
1	A	6	ALA	H	9.312	?	1
1	A	6	ALA	HA	4.852	?	1
1	A	6	ALA	HB1	1.339	?	1
1	A	6	ALA	HB2	1.339	?	1
1	A	6	ALA	HB3	1.339	?	1
1	A	6	ALA	CA	50.685	?	1
1	A	6	ALA	CB	19.959	?	1
1	A	6	ALA	N	130.084	?	1
1	A	7	LEU	H	8.595	?	1
1	A	7	LEU	HA	4.544	?	1
1	A	7	LEU	HB2	1.471	?	2
1	A	7	LEU	HB3	1.471	?	2
1	A	7	LEU	HD11	0.813	?	4
1	A	7	LEU	HD12	0.813	?	4
1	A	7	LEU	HD13	0.813	?	4
1	A	7	LEU	HD21	0.765	?	4
1	A	7	LEU	HD22	0.765	?	4
1	A	7	LEU	HD23	0.765	?	4
1	A	7	LEU	HG	1.384	?	1
1	A	7	LEU	CA	54.451	?	1
1	A	7	LEU	CB	42.746	?	1
1	A	7	LEU	CD1	25.9	?	2
1	A	7	LEU	CD2	25.453	?	2
1	A	7	LEU	CG	27.449	?	1
1	A	7	LEU	N	122.407	?	1
1	A	8	ASN	H	8.845	?	1
1	A	8	ASN	HA	5.221	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	ASN	HB2	2.656	?	2
1	A	8	ASN	HB3	2.951	?	2
1	A	8	ASN	HD21	7.172	?	2
1	A	8	ASN	HD22	6.901	?	2
1	A	8	ASN	CA	51.735	?	1
1	A	8	ASN	CB	38.79	?	1
1	A	8	ASN	N	125.342	?	1
1	A	8	ASN	ND2	111.803	?	1
1	A	9	GLY	H	8.043	?	1
1	A	9	GLY	HA2	4.07	?	2
1	A	9	GLY	HA3	4.481	?	2
1	A	9	GLY	CA	44.825	?	1
1	A	9	GLY	N	110.527	?	1
1	A	10	LYS	H	9.119	?	1
1	A	10	LYS	HA	4.118	?	1
1	A	10	LYS	HB2	1.877	?	2
1	A	10	LYS	HB3	1.877	?	2
1	A	10	LYS	HD2	1.701	?	2
1	A	10	LYS	HD3	1.701	?	2
1	A	10	LYS	HE3	3.044	?	2
1	A	10	LYS	HG3	1.498	?	2
1	A	10	LYS	CA	59.03	?	1
1	A	10	LYS	CB	32.762	?	1
1	A	10	LYS	CD	29.301	?	1
1	A	10	LYS	CE	42.183	?	1
1	A	10	LYS	CG	25.059	?	1
1	A	10	LYS	N	121.262	?	1
1	A	11	THR	H	8.815	?	1
1	A	11	THR	HA	4.408	?	1
1	A	11	THR	HB	4.27	?	1
1	A	11	THR	HG21	1.207	?	1
1	A	11	THR	HG22	1.207	?	1
1	A	11	THR	HG23	1.207	?	1
1	A	11	THR	CA	62.184	?	1
1	A	11	THR	CB	69.764	?	1
1	A	11	THR	CG2	22.012	?	1
1	A	11	THR	N	109.687	?	1
1	A	12	LEU	H	7.449	?	1
1	A	12	LEU	HA	4.454	?	1
1	A	12	LEU	HB2	1.499	?	2
1	A	12	LEU	HB3	1.559	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	LEU	HD11	0.848	?	4
1	A	12	LEU	HD12	0.848	?	4
1	A	12	LEU	HD13	0.848	?	4
1	A	12	LEU	HD21	0.922	?	4
1	A	12	LEU	HD22	0.922	?	4
1	A	12	LEU	HD23	0.922	?	4
1	A	12	LEU	HG	1.47	?	1
1	A	12	LEU	CA	55.157	?	1
1	A	12	LEU	CB	43.716	?	1
1	A	12	LEU	CD1	25.12	?	2
1	A	12	LEU	CD2	24.262	?	2
1	A	12	LEU	CG	27.3	?	1
1	A	12	LEU	N	124.735	?	1
1	A	13	LYS	H	8.202	?	1
1	A	13	LYS	HA	5.055	?	1
1	A	13	LYS	HB2	1.792	?	2
1	A	13	LYS	HB3	1.913	?	2
1	A	13	LYS	HD3	1.767	?	2
1	A	13	LYS	HE2	3.013	?	2
1	A	13	LYS	HE3	3.036	?	2
1	A	13	LYS	HG3	1.498	?	2
1	A	13	LYS	CA	54.378	?	1
1	A	13	LYS	CB	35.137	?	1
1	A	13	LYS	CD	29.373	?	1
1	A	13	LYS	CE	42.622	?	1
1	A	13	LYS	CG	25.11	?	1
1	A	13	LYS	N	123.828	?	1
1	A	14	GLY	H	8.429	?	1
1	A	14	GLY	HA3	4.251	?	2
1	A	14	GLY	CA	45.222	?	1
1	A	14	GLY	N	109.873	?	1
1	A	15	GLU	H	8.492	?	1
1	A	15	GLU	HA	5.638	?	1
1	A	15	GLU	HB2	1.985	?	2
1	A	15	GLU	HB3	2.044	?	2
1	A	15	GLU	HG3	2.209	?	2
1	A	15	GLU	CA	54.835	?	1
1	A	15	GLU	CB	33.686	?	1
1	A	15	GLU	CG	36.115	?	1
1	A	15	GLU	N	119.542	?	1
1	A	16	THR	H	8.667	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	THR	HA	4.779	?	1
1	A	16	THR	HB	4.012	?	1
1	A	16	THR	HG21	0.613	?	1
1	A	16	THR	HG22	0.613	?	1
1	A	16	THR	HG23	0.613	?	1
1	A	16	THR	CA	60.544	?	1
1	A	16	THR	CB	69.787	?	1
1	A	16	THR	CG2	19.531	?	1
1	A	16	THR	N	116.085	?	1
1	A	17	THR	H	8.175	?	1
1	A	17	THR	HA	5.87	?	1
1	A	17	THR	HB	4.333	?	1
1	A	17	THR	HG21	1.227	?	1
1	A	17	THR	HG22	1.227	?	1
1	A	17	THR	HG23	1.227	?	1
1	A	17	THR	CA	60.063	?	1
1	A	17	THR	CB	73.266	?	1
1	A	17	THR	CG2	21.571	?	1
1	A	17	THR	N	112.314	?	1
1	A	18	THR	H	9.043	?	1
1	A	18	THR	HA	4.724	?	1
1	A	18	THR	HB	3.899	?	1
1	A	18	THR	HG21	0.55	?	1
1	A	18	THR	HG22	0.55	?	1
1	A	18	THR	HG23	0.55	?	1
1	A	18	THR	CA	62.428	?	1
1	A	18	THR	CB	70.241	?	1
1	A	18	THR	CG2	19.189	?	1
1	A	18	THR	N	115.158	?	1
1	A	19	GLU	H	7.999	?	1
1	A	19	GLU	HA	5.221	?	1
1	A	19	GLU	HB2	1.988	?	2
1	A	19	GLU	HB3	2.003	?	2
1	A	19	GLU	HG2	2.116	?	2
1	A	19	GLU	HG3	2.346	?	2
1	A	19	GLU	CA	54.53	?	1
1	A	19	GLU	CB	30.44	?	1
1	A	19	GLU	CG	35.646	?	1
1	A	19	GLU	N	126.278	?	1
1	A	20	ALA	H	9.383	?	1
1	A	20	ALA	HA	4.985	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	ALA	HB1	1.397	?	1
1	A	20	ALA	HB2	1.397	?	1
1	A	20	ALA	HB3	1.397	?	1
1	A	20	ALA	CA	50.95	?	1
1	A	20	ALA	CB	23.753	?	1
1	A	20	ALA	N	127.705	?	1
1	A	21	VAL	H	8.545	?	1
1	A	21	VAL	HA	4.161	?	1
1	A	21	VAL	HB	2.243	?	1
1	A	21	VAL	HG11	1.048	?	4
1	A	21	VAL	HG12	1.048	?	4
1	A	21	VAL	HG13	1.048	?	4
1	A	21	VAL	HG21	1.056	?	4
1	A	21	VAL	HG22	1.056	?	4
1	A	21	VAL	HG23	1.056	?	4
1	A	21	VAL	CA	63.695	?	1
1	A	21	VAL	CB	32.083	?	1
1	A	21	VAL	CG1	20.118	?	2
1	A	21	VAL	CG2	21.009	?	2
1	A	21	VAL	N	116.082	?	1
1	A	22	ASP	H	7.378	?	1
1	A	22	ASP	HA	4.827	?	1
1	A	22	ASP	HB2	3.034	?	2
1	A	22	ASP	HB3	3.09	?	2
1	A	22	ASP	CA	52.539	?	1
1	A	22	ASP	CB	42.22	?	1
1	A	22	ASP	N	115.392	?	1
1	A	23	ALA	H	8.332	?	1
1	A	23	ALA	HA	3.318	?	1
1	A	23	ALA	HB1	1.228	?	1
1	A	23	ALA	HB2	1.228	?	1
1	A	23	ALA	HB3	1.228	?	1
1	A	23	ALA	CA	54.667	?	1
1	A	23	ALA	CB	17.557	?	1
1	A	23	ALA	N	121.755	?	1
1	A	24	ALA	H	8.108	?	1
1	A	24	ALA	HA	4.014	?	1
1	A	24	ALA	HB1	1.346	?	1
1	A	24	ALA	HB2	1.346	?	1
1	A	24	ALA	HB3	1.346	?	1
1	A	24	ALA	CA	54.869	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	24	ALA	CB	17.965	?	1
1	A	24	ALA	N	120.731	?	1
1	A	25	THR	H	8.325	?	1
1	A	25	THR	HA	3.747	?	1
1	A	25	THR	HB	4.074	?	1
1	A	25	THR	HG21	1.279	?	1
1	A	25	THR	HG22	1.279	?	1
1	A	25	THR	HG23	1.279	?	1
1	A	25	THR	CA	66.974	?	1
1	A	25	THR	CB	67.992	?	1
1	A	25	THR	CG2	21.155	?	1
1	A	25	THR	N	116.624	?	1
1	A	26	ALA	H	7.224	?	1
1	A	26	ALA	HA	3.159	?	1
1	A	26	ALA	HB1	0.624	?	1
1	A	26	ALA	HB2	0.624	?	1
1	A	26	ALA	HB3	0.624	?	1
1	A	26	ALA	CA	54.947	?	1
1	A	26	ALA	CB	17.671	?	1
1	A	26	ALA	N	123.943	?	1
1	A	27	GLU	H	8.379	?	1
1	A	27	GLU	HA	2.697	?	1
1	A	27	GLU	HB2	1.714	?	2
1	A	27	GLU	HB3	1.986	?	2
1	A	27	GLU	HG3	1.692	?	2
1	A	27	GLU	CA	59.704	?	1
1	A	27	GLU	CB	29.08	?	1
1	A	27	GLU	CG	35.489	?	1
1	A	27	GLU	N	116.893	?	1
1	A	28	LYS	H	6.995	?	1
1	A	28	LYS	HA	3.774	?	1
1	A	28	LYS	HB3	1.887	?	2
1	A	28	LYS	HD3	1.662	?	2
1	A	28	LYS	HE3	2.937	?	2
1	A	28	LYS	HG2	1.374	?	2
1	A	28	LYS	HG3	1.595	?	2
1	A	28	LYS	CA	59.826	?	1
1	A	28	LYS	CB	32.361	?	1
1	A	28	LYS	CD	29.256	?	1
1	A	28	LYS	CG	25.111	?	1
1	A	28	LYS	N	116.775	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	VAL	H	7.372	?	1
1	A	29	VAL	HA	3.658	?	1
1	A	29	VAL	HB	1.798	?	1
1	A	29	VAL	HG11	0.825	?	4
1	A	29	VAL	HG12	0.825	?	4
1	A	29	VAL	HG13	0.825	?	4
1	A	29	VAL	HG21	0.95	?	4
1	A	29	VAL	HG22	0.95	?	4
1	A	29	VAL	HG23	0.95	?	4
1	A	29	VAL	CA	66.134	?	1
1	A	29	VAL	CB	31.803	?	1
1	A	29	VAL	CG1	20.45	?	2
1	A	29	VAL	CG2	21.79	?	2
1	A	29	VAL	N	120.895	?	1
1	A	30	PHE	H	8.534	?	1
1	A	30	PHE	HA	4.84	?	1
1	A	30	PHE	HB2	2.909	?	2
1	A	30	PHE	HB3	3.398	?	2
1	A	30	PHE	HD1	6.625	?	3
1	A	30	PHE	HE1	7.136	?	3
1	A	30	PHE	HZ	7.83	?	1
1	A	30	PHE	CA	56.854	?	1
1	A	30	PHE	CB	37.57	?	1
1	A	30	PHE	CD1	130.035	?	3
1	A	30	PHE	CE1	130.443	?	3
1	A	30	PHE	CZ	132.303	?	1
1	A	30	PHE	N	120.757	?	1
1	A	31	LYS	H	9.151	?	1
1	A	31	LYS	HA	4.192	?	1
1	A	31	LYS	HB2	1.604	?	2
1	A	31	LYS	HB3	1.73	?	2
1	A	31	LYS	HD2	1.088	?	2
1	A	31	LYS	HD3	1.168	?	2
1	A	31	LYS	HE2	1.716	?	2
1	A	31	LYS	HE3	1.968	?	2
1	A	31	LYS	HG2	0.546	?	2
1	A	31	LYS	HG3	0.903	?	2
1	A	31	LYS	CA	59.881	?	1
1	A	31	LYS	CB	31.727	?	1
1	A	31	LYS	CD	28.944	?	1
1	A	31	LYS	CE	41.461	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	31	LYS	CG	25.794	?	1
1	A	31	LYS	N	122.973	?	1
1	A	32	GLN	H	7.523	?	1
1	A	32	GLN	HA	4.102	?	1
1	A	32	GLN	HB2	2.25	?	2
1	A	32	GLN	HB3	2.294	?	2
1	A	32	GLN	HE21	6.933	?	2
1	A	32	GLN	HE22	7.976	?	2
1	A	32	GLN	HG2	2.469	?	2
1	A	32	GLN	HG3	2.495	?	2
1	A	32	GLN	CA	58.787	?	1
1	A	32	GLN	CB	28.225	?	1
1	A	32	GLN	CG	33.543	?	1
1	A	32	GLN	N	120.03	?	1
1	A	32	GLN	NE2	115.48	?	1
1	A	33	TYR	H	8.249	?	1
1	A	33	TYR	HA	4.352	?	1
1	A	33	TYR	HB3	3.369	?	2
1	A	33	TYR	HD1	7.03	?	3
1	A	33	TYR	HE1	6.773	?	3
1	A	33	TYR	CA	61.764	?	1
1	A	33	TYR	CB	38.568	?	1
1	A	33	TYR	CD1	132.881	?	3
1	A	33	TYR	CE1	118.332	?	3
1	A	33	TYR	N	120.647	?	1
1	A	34	ALA	H	9.215	?	1
1	A	34	ALA	HA	3.862	?	1
1	A	34	ALA	HB1	1.893	?	1
1	A	34	ALA	HB2	1.893	?	1
1	A	34	ALA	HB3	1.893	?	1
1	A	34	ALA	CA	56.267	?	1
1	A	34	ALA	CB	17.929	?	1
1	A	34	ALA	N	122.922	?	1
1	A	35	ASN	H	8.338	?	1
1	A	35	ASN	HA	4.504	?	1
1	A	35	ASN	HB3	2.987	?	2
1	A	35	ASN	HD21	7.662	?	2
1	A	35	ASN	HD22	7.011	?	2
1	A	35	ASN	CA	56.975	?	1
1	A	35	ASN	CB	38.923	?	1
1	A	35	ASN	N	117.921	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	ASN	ND2	112.526	?	1
1	A	36	ASP	H	8.934	?	1
1	A	36	ASP	HA	4.426	?	1
1	A	36	ASP	HB2	2.632	?	2
1	A	36	ASP	HB3	2.79	?	2
1	A	36	ASP	CA	56.985	?	1
1	A	36	ASP	CB	40.114	?	1
1	A	36	ASP	N	121.417	?	1
1	A	37	ASN	H	7.46	?	1
1	A	37	ASN	HA	4.684	?	1
1	A	37	ASN	HB2	2.15	?	2
1	A	37	ASN	HB3	2.744	?	2
1	A	37	ASN	HD21	6.732	?	2
1	A	37	ASN	HD22	6.434	?	2
1	A	37	ASN	CA	53.835	?	1
1	A	37	ASN	CB	40.206	?	1
1	A	37	ASN	N	115.465	?	1
1	A	37	ASN	ND2	115.452	?	1
1	A	38	GLY	H	7.841	?	1
1	A	38	GLY	HA3	3.986	?	2
1	A	38	GLY	CA	47.057	?	1
1	A	38	GLY	N	108.595	?	1
1	A	39	VAL	H	8.193	?	1
1	A	39	VAL	HA	4.229	?	1
1	A	39	VAL	HB	1.85	?	1
1	A	39	VAL	HG11	0.86	?	4
1	A	39	VAL	HG12	0.86	?	4
1	A	39	VAL	HG13	0.86	?	4
1	A	39	VAL	HG21	0.727	?	4
1	A	39	VAL	HG22	0.727	?	4
1	A	39	VAL	HG23	0.727	?	4
1	A	39	VAL	CA	61.918	?	1
1	A	39	VAL	CB	33.39	?	1
1	A	39	VAL	CG1	21.36	?	2
1	A	39	VAL	CG2	21.414	?	2
1	A	39	VAL	N	120.582	?	1
1	A	40	ASP	H	8.537	?	1
1	A	40	ASP	HA	4.959	?	1
1	A	40	ASP	HB2	2.669	?	2
1	A	40	ASP	HB3	2.772	?	2
1	A	40	ASP	CA	52.566	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	40	ASP	CB	43.37	?	1
1	A	40	ASP	N	127.235	?	1
1	A	41	GLY	H	8.136	?	1
1	A	41	GLY	HA2	3.89	?	2
1	A	41	GLY	HA3	4.216	?	2
1	A	41	GLY	CA	45.632	?	1
1	A	41	GLY	N	107.889	?	1
1	A	42	GLU	H	8.343	?	1
1	A	42	GLU	HA	4.779	?	1
1	A	42	GLU	HB2	2.03	?	2
1	A	42	GLU	HB3	2.105	?	2
1	A	42	GLU	HG2	2.292	?	2
1	A	42	GLU	HG3	2.39	?	2
1	A	42	GLU	CA	55.549	?	1
1	A	42	GLU	CB	31.403	?	1
1	A	42	GLU	CG	36.194	?	1
1	A	42	GLU	N	121.131	?	1
1	A	43	TRP	H	9.362	?	1
1	A	43	TRP	HA	5.393	?	1
1	A	43	TRP	HB2	3.224	?	2
1	A	43	TRP	HB3	3.394	?	2
1	A	43	TRP	HD1	7.61	?	1
1	A	43	TRP	HE1	10.541	?	4
1	A	43	TRP	HE3	7.637	?	4
1	A	43	TRP	HH2	6.781	?	4
1	A	43	TRP	HZ2	7.349	?	4
1	A	43	TRP	HZ3	7.038	?	4
1	A	43	TRP	CA	57.894	?	1
1	A	43	TRP	CB	30.454	?	1
1	A	43	TRP	CD1	127.166	?	4
1	A	43	TRP	CE3	121.136	?	4
1	A	43	TRP	CH2	123.145	?	1
1	A	43	TRP	CZ2	114.436	?	4
1	A	43	TRP	CZ3	121.369	?	4
1	A	43	TRP	N	128.502	?	1
1	A	43	TRP	NE1	130.794	?	1
1	A	44	THR	H	9.278	?	1
1	A	44	THR	HA	4.859	?	1
1	A	44	THR	HB	4.282	?	1
1	A	44	THR	HG21	1.254	?	1
1	A	44	THR	HG22	1.254	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	44	THR	HG23	1.254	?	1
1	A	44	THR	CA	60.711	?	1
1	A	44	THR	CB	72.36	?	1
1	A	44	THR	CG2	22.053	?	1
1	A	44	THR	N	115.104	?	1
1	A	45	TYR	H	8.66	?	1
1	A	45	TYR	HA	5.045	?	1
1	A	45	TYR	HB2	2.565	?	2
1	A	45	TYR	HB3	2.936	?	2
1	A	45	TYR	HD1	7.222	?	3
1	A	45	TYR	HE1	6.388	?	3
1	A	45	TYR	CA	57.024	?	1
1	A	45	TYR	CB	41.646	?	1
1	A	45	TYR	CD1	132.112	?	3
1	A	45	TYR	CE1	117.475	?	3
1	A	45	TYR	N	121.325	?	1
1	A	46	ASP	H	7.508	?	1
1	A	46	ASP	HA	4.648	?	1
1	A	46	ASP	HB2	2.325	?	2
1	A	46	ASP	HB3	2.668	?	2
1	A	46	ASP	CA	51.866	?	1
1	A	46	ASP	CB	43.215	?	1
1	A	46	ASP	N	128.475	?	1
1	A	47	ASP	H	8.648	?	1
1	A	47	ASP	HA	4.213	?	1
1	A	47	ASP	HB2	2.889	?	2
1	A	47	ASP	HB3	2.588	?	2
1	A	47	ASP	CA	56.368	?	1
1	A	47	ASP	CB	42.221	?	1
1	A	47	ASP	N	125.145	?	1
1	A	48	ALA	H	8.4	?	1
1	A	48	ALA	HA	4.176	?	1
1	A	48	ALA	HB1	1.556	?	1
1	A	48	ALA	HB2	1.556	?	1
1	A	48	ALA	HB3	1.556	?	1
1	A	48	ALA	CA	55.147	?	1
1	A	48	ALA	CB	18.36	?	1
1	A	48	ALA	N	120.179	?	1
1	A	49	THR	H	7.064	?	1
1	A	49	THR	HA	4.434	?	1
1	A	49	THR	HB	4.444	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	THR	HG21	1.128	?	1
1	A	49	THR	HG22	1.128	?	1
1	A	49	THR	HG23	1.128	?	1
1	A	49	THR	CA	60.53	?	1
1	A	49	THR	CB	70.277	?	1
1	A	49	THR	CG2	21.292	?	1
1	A	49	THR	N	103.662	?	1
1	A	50	LYS	H	7.908	?	1
1	A	50	LYS	HA	4.246	?	1
1	A	50	LYS	HB3	2.132	?	2
1	A	50	LYS	HD2	1.474	?	2
1	A	50	LYS	HD3	1.767	?	2
1	A	50	LYS	HE3	3.023	?	2
1	A	50	LYS	HG2	1.284	?	2
1	A	50	LYS	HG3	1.456	?	2
1	A	50	LYS	CA	56.508	?	1
1	A	50	LYS	CB	29.455	?	1
1	A	50	LYS	CD	28.478	?	1
1	A	50	LYS	CE	43.05	?	1
1	A	50	LYS	CG	24.566	?	1
1	A	50	LYS	N	123.189	?	1
1	A	51	THR	H	7.4	?	1
1	A	51	THR	HA	5.515	?	1
1	A	51	THR	HB	3.801	?	1
1	A	51	THR	HG21	0.979	?	1
1	A	51	THR	HG22	0.979	?	1
1	A	51	THR	HG23	0.979	?	1
1	A	51	THR	CA	62.225	?	1
1	A	51	THR	CB	72.143	?	1
1	A	51	THR	CG2	20.369	?	1
1	A	51	THR	N	111.09	?	1
1	A	52	PHE	H	10.312	?	1
1	A	52	PHE	HA	5.648	?	1
1	A	52	PHE	HB2	3.209	?	2
1	A	52	PHE	HB3	3.331	?	2
1	A	52	PHE	HD1	7.83	?	3
1	A	52	PHE	HE1	7.193	?	3
1	A	52	PHE	HZ	6.982	?	1
1	A	52	PHE	CA	57.414	?	1
1	A	52	PHE	CB	42.108	?	1
1	A	52	PHE	CD1	132.643	?	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	PHE	CE1	132.566	?	3
1	A	52	PHE	CZ	128.717	?	1
1	A	52	PHE	N	131.285	?	1
1	A	53	THR	H	9.234	?	1
1	A	53	THR	HA	5.276	?	1
1	A	53	THR	HB	3.88	?	1
1	A	53	THR	HG21	1.04	?	1
1	A	53	THR	HG22	1.04	?	1
1	A	53	THR	HG23	1.04	?	1
1	A	53	THR	CA	61.651	?	1
1	A	53	THR	CB	70.665	?	1
1	A	53	THR	CG2	20.99	?	1
1	A	53	THR	N	118.766	?	1
1	A	54	VAL	H	8.175	?	1
1	A	54	VAL	HA	4.52	?	1
1	A	54	VAL	HB	0.216	?	1
1	A	54	VAL	HG11	0.326	?	4
1	A	54	VAL	HG12	0.326	?	4
1	A	54	VAL	HG13	0.326	?	4
1	A	54	VAL	HG21	-0.435	?	4
1	A	54	VAL	HG22	-0.435	?	4
1	A	54	VAL	HG23	-0.435	?	4
1	A	54	VAL	CA	58.647	?	1
1	A	54	VAL	CB	32.433	?	1
1	A	54	VAL	CG1	19.934	?	2
1	A	54	VAL	CG2	20.32	?	2
1	A	54	VAL	N	124.27	?	1
1	A	55	THR	H	8.482	?	1
1	A	55	THR	HA	4.745	?	1
1	A	55	THR	HB	3.967	?	1
1	A	55	THR	HG21	1.227	?	1
1	A	55	THR	HG22	1.227	?	1
1	A	55	THR	HG23	1.227	?	1
1	A	55	THR	CA	60.871	?	1
1	A	55	THR	CB	70.537	?	1
1	A	55	THR	CG2	21.473	?	1
1	A	55	THR	N	123.648	?	1
1	A	56	GLU	H	8.171	?	1
1	A	56	GLU	HA	4.466	?	1
1	A	56	GLU	HB2	2.063	?	2
1	A	56	GLU	HB3	2.16	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	56	GLU	HG2	2.363	?	2
1	A	56	GLU	HG3	2.441	?	2
1	A	56	GLU	CA	56.573	?	1
1	A	56	GLU	CB	31.289	?	1
1	A	56	GLU	CG	36.458	?	1
1	A	56	GLU	N	127.224	?	1
1	A	57	LEU	H	8.644	?	1
1	A	57	LEU	HA	4.48	?	1
1	A	57	LEU	HB2	1.688	?	2
1	A	57	LEU	HB3	1.575	?	2
1	A	57	LEU	HD11	0.946	?	4
1	A	57	LEU	HD12	0.946	?	4
1	A	57	LEU	HD13	0.946	?	4
1	A	57	LEU	HD21	0.896	?	4
1	A	57	LEU	HD22	0.896	?	4
1	A	57	LEU	HD23	0.896	?	4
1	A	57	LEU	HG	1.642	?	1
1	A	57	LEU	CA	55.157	?	1
1	A	57	LEU	CB	42.485	?	1
1	A	57	LEU	CD1	25.04	?	2
1	A	57	LEU	CD2	23.599	?	2
1	A	57	LEU	CG	27.171	?	1
1	A	57	LEU	N	125.852	?	1
1	A	58	VAL	H	8.291	?	1
1	A	58	VAL	HA	4.496	?	1
1	A	58	VAL	HB	2.116	?	1
1	A	58	VAL	HG11	0.965	?	4
1	A	58	VAL	HG12	0.965	?	4
1	A	58	VAL	HG13	0.965	?	4
1	A	58	VAL	HG21	1.005	?	4
1	A	58	VAL	HG22	1.005	?	4
1	A	58	VAL	HG23	1.005	?	4
1	A	58	VAL	CA	59.666	?	1
1	A	58	VAL	CB	32.905	?	1
1	A	58	VAL	CG1	20.386	?	2
1	A	58	VAL	CG2	20.901	?	2
1	A	58	VAL	N	123.305	?	1
1	A	59	PRO	HA	4.479	?	1
1	A	59	PRO	HB2	1.942	?	2
1	A	59	PRO	HB3	2.347	?	2
1	A	59	PRO	HD2	3.738	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	59	PRO	HD3	3.9	?	2
1	A	59	PRO	HG2	2.02	?	2
1	A	59	PRO	HG3	2.106	?	2
1	A	59	PRO	CA	63.087	?	1
1	A	59	PRO	CB	32.171	?	1
1	A	59	PRO	CD	51.103	?	1
1	A	59	PRO	CG	27.468	?	1
1	A	60	ARG	H	8.553	?	1
1	A	60	ARG	HA	4.381	?	1
1	A	60	ARG	HB2	1.841	?	2
1	A	60	ARG	HB3	1.916	?	2
1	A	60	ARG	HD3	3.271	?	2
1	A	60	ARG	HG3	1.756	?	2
1	A	60	ARG	CA	56.391	?	1
1	A	60	ARG	CB	31.074	?	1
1	A	60	ARG	CD	43.433	?	1
1	A	60	ARG	CG	27.13	?	1
1	A	60	ARG	N	122.358	?	1
1	A	61	GLY	H	8.606	?	1
1	A	61	GLY	HA2	4.113	?	2
1	A	61	GLY	HA3	4.012	?	2
1	A	61	GLY	CA	45.219	?	1
1	A	61	GLY	N	110.998	?	1
1	A	62	SER	H	8.366	?	1
1	A	62	SER	HA	4.527	?	1
1	A	62	SER	HB2	3.893	?	2
1	A	62	SER	HB3	3.954	?	2
1	A	62	SER	CA	58.475	?	1
1	A	62	SER	CB	64.103	?	1
1	A	62	SER	N	115.855	?	1
1	A	63	ASP	H	8.565	?	1
1	A	63	ASP	HA	4.679	?	1
1	A	63	ASP	HB2	2.68	?	2
1	A	63	ASP	HB3	2.765	?	2
1	A	63	ASP	CA	54.672	?	1
1	A	63	ASP	CB	41.064	?	1
1	A	63	ASP	N	122.358	?	1
1	A	64	ASP	H	8.248	?	1
1	A	64	ASP	HA	4.611	?	1
1	A	64	ASP	HB2	2.683	?	2
1	A	64	ASP	HB3	2.723	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	ASP	CA	54.693	?	1
1	A	64	ASP	CB	41.069	?	1
1	A	64	ASP	N	120.092	?	1
1	A	65	ASP	H	8.24	?	1
1	A	65	ASP	HA	4.639	?	1
1	A	65	ASP	HB3	2.768	?	2
1	A	65	ASP	CA	54.693	?	1
1	A	65	ASP	CB	41.045	?	1
1	A	65	ASP	N	120.092	?	1
1	A	66	ASP	H	8.313	?	1
1	A	66	ASP	HA	4.605	?	1
1	A	66	ASP	HB3	2.734	?	2
1	A	66	ASP	CA	54.691	?	1
1	A	66	ASP	CB	40.747	?	1
1	A	66	ASP	N	120.514	?	1
1	A	67	LYS	H	8.266	?	1
1	A	67	LYS	HA	4.381	?	1
1	A	67	LYS	HB3	1.853	?	2
1	A	67	LYS	HD3	1.884	?	2
1	A	67	LYS	HE3	3.063	?	2
1	A	67	LYS	HG3	1.499	?	2
1	A	67	LYS	CA	56.504	?	1
1	A	67	LYS	CB	32.638	?	1
1	A	67	LYS	CD	29.081	?	1
1	A	67	LYS	CE	41.794	?	1
1	A	67	LYS	CG	24.758	?	1
1	A	67	LYS	N	121.478	?	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
$^{13}\text{C}_\alpha$	100	-0.53 ± 0.40	None needed (imprecise)
$^{13}\text{C}_\beta$	92	0.02 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	96	1.21 ± 0.59	Should be applied

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 89%, i.e. 136 atoms were assigned a chemical shift out of a possible 153. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	44/57 (77%)	22/24 (92%)	11/22 (50%)	11/11 (100%)
Sidechain	92/96 (96%)	63/63 (100%)	25/29 (86%)	4/4 (100%)
Overall	136/153 (89%)	85/87 (98%)	36/51 (71%)	15/15 (100%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 406 atoms were assigned a chemical shift out of a possible 468. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	129/164 (79%)	65/67 (97%)	33/66 (50%)	31/31 (100%)
Sidechain	249/270 (92%)	169/178 (95%)	75/82 (91%)	5/10 (50%)
Aromatic	28/34 (82%)	14/17 (82%)	12/15 (80%)	2/2 (100%)
Overall	406/468 (87%)	248/262 (95%)	120/163 (74%)	38/43 (88%)

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	5	LEU	HB2	-1.05	-0.07 – 3.30	-7.9
1	A	31	LYS	HE2	1.72	1.95 – 3.88	-6.2
1	A	54	VAL	HB	0.22	0.43 – 3.54	-5.7

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:

