



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2KGS / pdb_00002kgs
BMRB ID : 16237
Title : Solution structure of the amino-terminal domain of OmpATb, a pore forming protein from Mycobacterium tuberculosis
Authors : Yang, Y.; Auguin, D.; Delbecq, S.; Dumas, E.; Molle, V.; Saint, N.
Deposited on : 2009-03-18

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

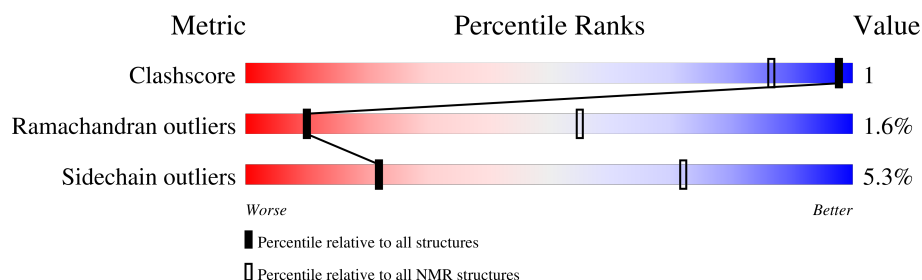
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

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	132	 83% . 13%

2 Ensemble composition and analysis

This entry contains 10 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:79-A:193 (115)	0.40	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 2 clusters and 6 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1927 atoms, of which 970 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein Rv0899/MT0922.

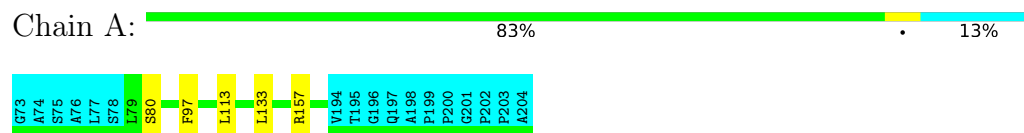
Mol	Chain	Residues	Atoms						Trace
1	A	132	Total	C	H	N	O	S	0
			1927	602	970	161	192	2	

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: Uncharacterized protein Rv0899/MT0922

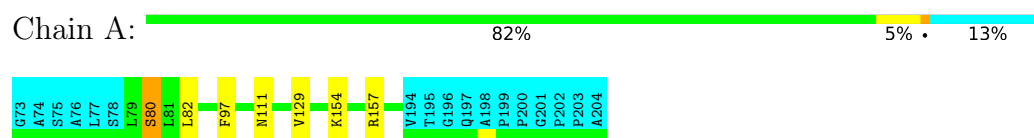


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

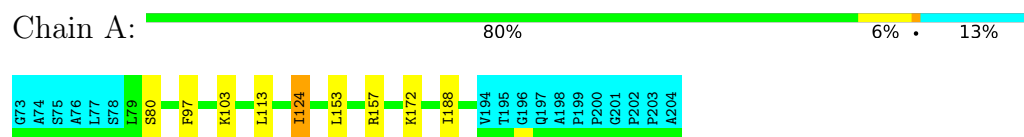
4.2.1 Score per residue for model 1

- Molecule 1: Uncharacterized protein Rv0899/MT0922



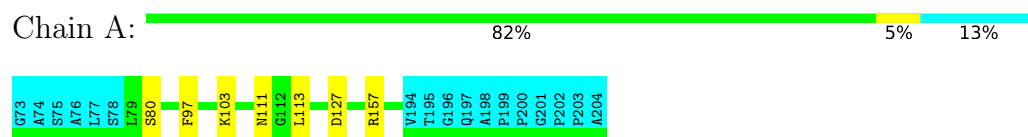
4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein Rv0899/MT0922



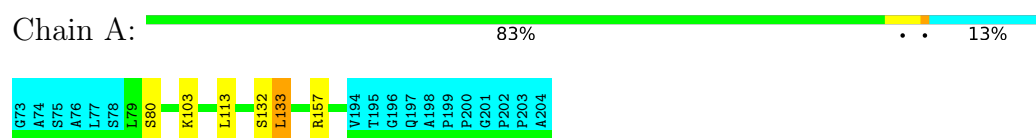
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein Rv0899/MT0922



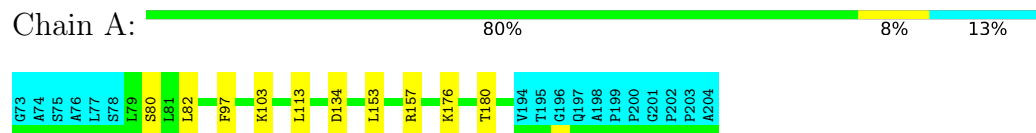
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Uncharacterized protein Rv0899/MT0922



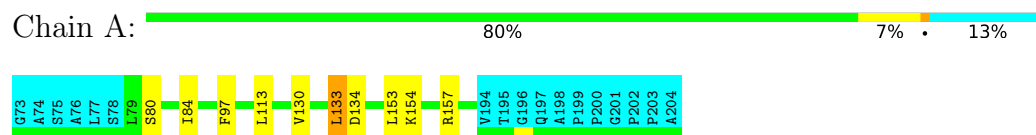
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein Rv0899/MT0922



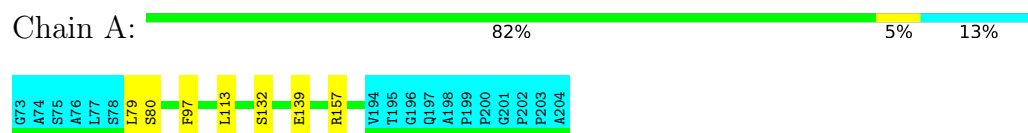
4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein Rv0899/MT0922



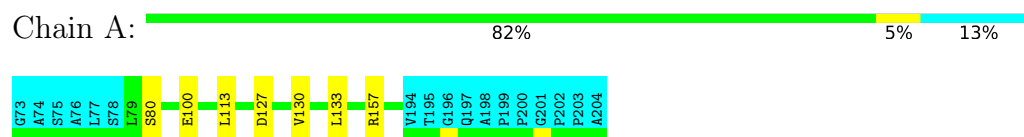
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein Rv0899/MT0922



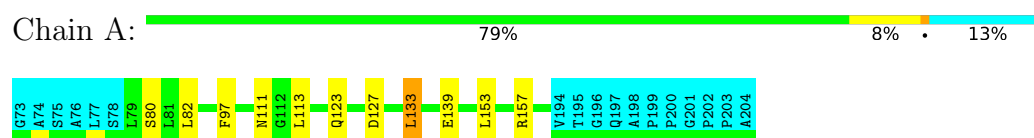
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein Rv0899/MT0922



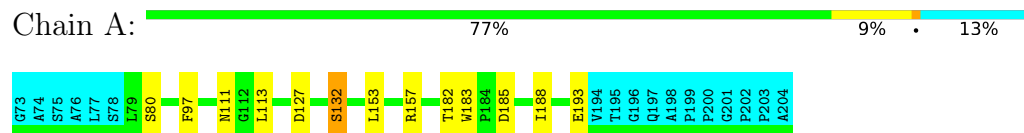
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein Rv0899/MT0922



4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein Rv0899/MT0922



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, minimization*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Amber	refinement	8
CYANA	structure solution	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	1574
Number of shifts mapped to atoms	1284
Number of unparsed shifts	0
Number of shifts with mapping errors	290
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.82±0.01	0±0/869 (0.0± 0.0%)	1.51±0.12	3±3/1190 (0.2± 0.2%)
All	All	0.82	0/8690 (0.0%)	1.51	29/11900 (0.2%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	185	ASP	OD1-CG-OD2	19.02	168.56	122.90	10	1
1	A	193	GLU	OE1-CD-OE2	18.68	167.74	122.90	10	1
1	A	185	ASP	CB-CG-OD1	-15.27	83.29	118.40	10	1
1	A	193	GLU	CG-CD-OE1	-15.12	83.62	118.40	10	1
1	A	193	GLU	CG-CD-OE2	-14.90	84.13	118.40	10	1
1	A	185	ASP	CB-CG-OD2	-14.40	85.27	118.40	10	1
1	A	97	PHE	CA-CB-CG	6.69	120.49	113.80	5	7
1	A	111	ASN	CA-C-N	5.85	126.58	120.03	3	4
1	A	111	ASN	C-N-CA	5.85	126.58	120.03	3	4
1	A	132	SER	N-CA-C	5.55	117.06	109.18	4	2
1	A	97	PHE	N-CA-C	5.54	113.00	108.07	3	2
1	A	132	SER	CA-C-N	5.10	130.16	121.29	4	1
1	A	132	SER	C-N-CA	5.10	130.16	121.29	4	1
1	A	79	LEU	CA-C-N	5.01	131.11	121.54	7	1
1	A	79	LEU	C-N-CA	5.01	131.11	121.54	7	1

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	853	866	864	1±1
All	All	8530	8660	8640	9

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HD12	1:A:133:LEU:H	0.64	1.51	9	3
1:A:182:THR:HG23	1:A:183:TRP:CD2	0.54	2.37	10	1
1:A:124:ILE:HD12	1:A:124:ILE:H	0.49	1.67	2	1
1:A:133:LEU:H	1:A:133:LEU:CD1	0.45	2.25	4	3
1:A:103:LYS:HD2	1:A:124:ILE:HD13	0.43	1.91	2	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	115/132 (87%)	106±1 (92±1%)	7±1 (6±1%)	2±0 (2±0%)	10	55
All	All	1150/1320 (87%)	1063 (92%)	69 (6%)	18 (2%)	10	55

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	157	ARG	10
1	A	80	SER	8

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	97/107 (91%)	92±2 (95±2%)	5±2 (5±2%)	22	72
All	All	970/1070 (91%)	919 (95%)	51 (5%)	22	72

All 21 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	113	LEU	9
1	A	153	LEU	5
1	A	127	ASP	4
1	A	133	LEU	4
1	A	80	SER	3
1	A	82	LEU	3
1	A	103	LYS	3
1	A	154	LYS	2
1	A	188	ILE	2
1	A	134	ASP	2
1	A	130	VAL	2
1	A	132	SER	2
1	A	139	GLU	2
1	A	129	VAL	1
1	A	124	ILE	1
1	A	172	LYS	1
1	A	176	LYS	1
1	A	180	THR	1
1	A	84	ILE	1
1	A	100	GLU	1
1	A	123	GLN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 76% 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	1574
Number of shifts mapped to atoms	1284
Number of unparsed shifts	0
Number of shifts with mapping errors	290
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	21

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

- No matching atom found in the structure. All 290 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	134	ASP	HA2	4.284	?	2
1	A	134	ASP	HA3	4.078	?	2
1	A	135	PHE	HG2	2.298	?	2
1	A	135	PHE	HG3	2.298	?	2
1	A	139	GLU	HD11	0.942	?	2
1	A	139	GLU	HD12	0.942	?	2
1	A	139	GLU	HD13	0.942	?	2
1	A	139	GLU	HD21	0.912	?	2
1	A	139	GLU	HD22	0.912	?	2
1	A	139	GLU	HD23	0.912	?	2
1	A	140	PRO	H	9.108	?	1
1	A	141	VAL	HB2	3.897	?	2
1	A	141	VAL	HB3	3.897	?	2
1	A	143	THR	HD11	0.941	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	143	THR	HD12	0.941	?	1
1	A	143	THR	HD13	0.941	?	1
1	A	143	THR	HG12	1.655	?	2
1	A	143	THR	HG13	1.655	?	2
1	A	147	PRO	H	8.533	?	1
1	A	147	PRO	HG21	1.11	?	1
1	A	147	PRO	HG22	1.11	?	1
1	A	147	PRO	HG23	1.11	?	1
1	A	148	ILE	HA2	4.026	?	2
1	A	148	ILE	HA3	3.848	?	2
1	A	149	PRO	H	7.953	?	1
1	A	149	PRO	HA2	4.664	?	2
1	A	149	PRO	HA3	3.629	?	2
1	A	150	ASP	HG2	2.18	?	2
1	A	150	ASP	HG3	2.11	?	2
1	A	151	PHE	HD11	0.692	?	1
1	A	151	PHE	HD12	0.692	?	1
1	A	151	PHE	HD13	0.692	?	1
1	A	151	PHE	HG12	1.317	?	2
1	A	151	PHE	HG13	1.317	?	2
1	A	151	PHE	HG21	0.778	?	1
1	A	151	PHE	HG22	0.778	?	1
1	A	151	PHE	HG23	0.778	?	1
1	A	152	GLY	HB1	1.376	?	1
1	A	152	GLY	HB2	1.376	?	1
1	A	152	GLY	HB3	1.376	?	1
1	A	154	LYS	HA2	4.106	?	2
1	A	154	LYS	HA3	3.951	?	2
1	A	155	VAL	HB2	2.838	?	2
1	A	155	VAL	HB3	2.719	?	2
1	A	159	THR	HB2	3.772	?	2
1	A	159	THR	HB3	3.772	?	2
1	A	166	ALA	HG2	2.333	?	2
1	A	166	ALA	HG3	2.333	?	2
1	A	167	PRO	H	7.116	?	1
1	A	167	PRO	HD11	0.83	?	1
1	A	167	PRO	HD12	0.83	?	1
1	A	167	PRO	HD13	0.83	?	1
1	A	167	PRO	HG12	1.679	?	2
1	A	167	PRO	HG13	1.155	?	2
1	A	167	PRO	HG21	0.946	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	167	PRO	HG22	0.946	?	1
1	A	167	PRO	HG23	0.946	?	1
1	A	171	HIS	HG11	1.002	?	2
1	A	171	HIS	HG12	1.002	?	2
1	A	171	HIS	HG13	1.002	?	2
1	A	171	HIS	HG21	0.857	?	2
1	A	171	HIS	HG22	0.857	?	2
1	A	171	HIS	HG23	0.857	?	2
1	A	174	ALA	HD2	1.803	?	4
1	A	174	ALA	HD3	1.803	?	4
1	A	174	ALA	HG2	1.518	?	4
1	A	174	ALA	HG3	1.312	?	4
1	A	175	VAL	HB2	1.806	?	2
1	A	175	VAL	HB3	1.806	?	2
1	A	175	VAL	HD11	0.745	?	2
1	A	175	VAL	HD12	0.745	?	2
1	A	175	VAL	HD13	0.745	?	2
1	A	175	VAL	HD21	0.718	?	2
1	A	175	VAL	HD22	0.718	?	2
1	A	175	VAL	HD23	0.718	?	2
1	A	179	ALA	HD2	3.705	?	2
1	A	179	ALA	HD3	3.406	?	2
1	A	179	ALA	HG2	2.271	?	2
1	A	179	ALA	HG3	2.271	?	2
1	A	180	THR	HB2	2.781	?	2
1	A	180	THR	HB3	2.575	?	2
1	A	182	THR	HB2	1.838	?	2
1	A	182	THR	HB3	1.545	?	2
1	A	183	TRP	HG11	0.773	?	2
1	A	183	TRP	HG12	0.773	?	2
1	A	183	TRP	HG13	0.773	?	2
1	A	183	TRP	HG21	0.773	?	2
1	A	183	TRP	HG22	0.773	?	2
1	A	183	TRP	HG23	0.773	?	2
1	A	184	PRO	H	9.584	?	1
1	A	184	PRO	HG21	1.008	?	1
1	A	184	PRO	HG22	1.008	?	1
1	A	184	PRO	HG23	1.008	?	1
1	A	185	ASP	HG12	1.401	?	2
1	A	185	ASP	HG13	1.353	?	2
1	A	185	ASP	HG21	1.229	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	185	ASP	HG22	1.229	?	1
1	A	185	ASP	HG23	1.229	?	1
1	A	187	LYS	HA2	4.89	?	2
1	A	187	LYS	HA3	3.809	?	2
1	A	188	ILE	HB2	3.582	?	2
1	A	188	ILE	HB3	2.715	?	2
1	A	193	GLU	HA2	3.962	?	2
1	A	193	GLU	HA3	3.962	?	2
1	A	194	VAL	HB2	4.035	?	2
1	A	194	VAL	HB3	3.886	?	2
1	A	195	THR	HB2	2.075	?	4
1	A	195	THR	HB3	2.075	?	2
1	A	195	THR	HG3	2.425	?	2
1	A	197	GLN	HD11	0.837	?	1
1	A	197	GLN	HD12	0.837	?	1
1	A	197	GLN	HD13	0.837	?	1
1	A	197	GLN	HG12	1.481	?	2
1	A	197	GLN	HG13	1.24	?	2
1	A	197	GLN	HG21	0.909	?	1
1	A	197	GLN	HG22	0.909	?	1
1	A	197	GLN	HG23	0.909	?	1
1	A	199	PRO	H	8.637	?	1
1	A	199	PRO	HD11	0.847	?	1
1	A	199	PRO	HD12	0.847	?	1
1	A	199	PRO	HD13	0.847	?	1
1	A	199	PRO	HG12	1.775	?	2
1	A	199	PRO	HG13	1.775	?	2
1	A	199	PRO	HG21	0.873	?	1
1	A	199	PRO	HG22	0.873	?	1
1	A	199	PRO	HG23	0.873	?	1
1	A	201	GLY	HB2	1.743	?	2
1	A	201	GLY	HB3	1.654	?	2
1	A	201	GLY	HD11	0.899	?	2
1	A	201	GLY	HD12	0.899	?	2
1	A	201	GLY	HD13	0.899	?	2
1	A	201	GLY	HD21	0.899	?	2
1	A	201	GLY	HD22	0.899	?	2
1	A	201	GLY	HD23	0.899	?	2
1	A	201	GLY	HG	1.497	?	1
1	A	201	GLY	CB	40.06	?	1
1	A	202	PRO	H	8.35	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	203	PRO	H	8.026	?	1
1	A	204	ALA	HG2	2.491	?	2
1	A	204	ALA	HG3	2.359	?	2
1	A	205	ARG	H	7.58	?	1
1	A	205	ARG	HA	3.733	?	1
1	A	205	ARG	HB2	1.517	?	2
1	A	205	ARG	HB3	1.175	?	2
1	A	205	ARG	C	174.8	?	1
1	A	205	ARG	CB	26.85	?	1
1	A	205	ARG	N	117.7	?	1
1	A	206	ALA	H	7.293	?	1
1	A	206	ALA	HA	3.926	?	1
1	A	206	ALA	HB1	1.33	?	1
1	A	206	ALA	HB2	1.33	?	1
1	A	206	ALA	HB3	1.33	?	1
1	A	206	ALA	C	176.4	?	1
1	A	206	ALA	CA	53.01	?	1
1	A	206	ALA	CB	15.98	?	1
1	A	206	ALA	N	118.5	?	1
1	A	207	LYS	H	8.173	?	1
1	A	207	LYS	HA	3.964	?	1
1	A	207	LYS	HB2	2.053	?	2
1	A	207	LYS	HB3	1.872	?	2
1	A	207	LYS	HG2	1.483	?	4
1	A	207	LYS	HG3	1.483	?	4
1	A	207	LYS	C	175.1	?	1
1	A	207	LYS	CA	57.11	?	1
1	A	207	LYS	CB	30.08	?	1
1	A	207	LYS	N	118.9	?	1
1	A	208	ILE	H	8.173	?	1
1	A	208	ILE	HA	3.97	?	1
1	A	208	ILE	HB	2.232	?	1
1	A	208	ILE	C	177.3	?	1
1	A	208	ILE	CA	62.48	?	1
1	A	208	ILE	CB	35.62	?	1
1	A	208	ILE	N	119.3	?	1
1	A	209	VAL	H	7.207	?	1
1	A	209	VAL	HA	3.627	?	1
1	A	209	VAL	HB	2.317	?	1
1	A	209	VAL	HG11	1.166	?	2
1	A	209	VAL	HG12	1.166	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	209	VAL	HG13	1.166	?	2
1	A	209	VAL	HG21	0.957	?	2
1	A	209	VAL	HG22	0.957	?	2
1	A	209	VAL	HG23	0.957	?	2
1	A	209	VAL	C	174.5	?	1
1	A	209	VAL	CA	64.85	?	1
1	A	209	VAL	CB	29.02	?	1
1	A	209	VAL	N	119.0	?	1
1	A	211	ASP	H	9.291	?	1
1	A	211	ASP	HA	4.281	?	1
1	A	211	ASP	HB2	2.844	?	2
1	A	211	ASP	HB3	2.597	?	2
1	A	211	ASP	C	177.2	?	1
1	A	211	ASP	CA	54.78	?	1
1	A	211	ASP	CB	37.33	?	1
1	A	211	ASP	N	115.9	?	1
1	A	212	TYR	H	7.733	?	1
1	A	212	TYR	HA	4.177	?	1
1	A	212	TYR	HB2	3.288	?	2
1	A	212	TYR	HB3	3.173	?	2
1	A	212	TYR	C	174.9	?	1
1	A	212	TYR	CA	60.21	?	1
1	A	212	TYR	CB	36.31	?	1
1	A	212	TYR	N	122.5	?	1
1	A	213	LEU	H	8.21	?	1
1	A	213	LEU	HA	3.813	?	1
1	A	213	LEU	HB2	2.192	?	2
1	A	213	LEU	HB3	1.459	?	2
1	A	213	LEU	HD11	0.866	?	2
1	A	213	LEU	HD12	0.866	?	2
1	A	213	LEU	HD13	0.866	?	2
1	A	213	LEU	HD21	0.741	?	2
1	A	213	LEU	HD22	0.741	?	2
1	A	213	LEU	HD23	0.741	?	2
1	A	213	LEU	C	177.5	?	1
1	A	213	LEU	CA	56.22	?	1
1	A	213	LEU	CB	38.29	?	1
1	A	213	LEU	N	117.5	?	1
1	A	216	ARG	HD2	2.88	?	2
1	A	216	ARG	HD3	2.84	?	2
1	A	216	ARG	HG2	1.477	?	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	216	ARG	HG3	1.477	?	2
1	A	216	ARG	CA	51.46	?	1
1	A	217	GLY	H	7.843	?	1
1	A	217	GLY	HA2	4.326	?	2
1	A	217	GLY	HA3	3.648	?	2
1	A	217	GLY	C	172.4	?	1
1	A	217	GLY	CA	43.03	?	1
1	A	217	GLY	N	105.4	?	1
1	A	222	HIS	H	8.21	?	1
1	A	222	HIS	HA	4.665	?	1
1	A	222	HIS	HB2	4.098	?	2
1	A	222	HIS	HB3	3.268	?	2
1	A	222	HIS	C	169.7	?	1
1	A	222	HIS	CA	53.25	?	1
1	A	222	HIS	CB	25.85	?	1
1	A	222	HIS	N	117.5	?	1
1	A	223	ILE	HD11	0.651	?	1
1	A	223	ILE	HD12	0.651	?	1
1	A	223	ILE	HD13	0.651	?	1
1	A	223	ILE	HG12	1.642	?	2
1	A	223	ILE	HG13	1.642	?	2
1	A	223	ILE	HG21	0.746	?	1
1	A	223	ILE	HG22	0.746	?	1
1	A	223	ILE	HG23	0.746	?	1
1	A	225	THR	H	8.448	?	1
1	A	225	THR	HA	5.135	?	1
1	A	225	THR	HB	3.956	?	1
1	A	225	THR	HG21	0.979	?	1
1	A	225	THR	HG22	0.979	?	1
1	A	225	THR	HG23	0.979	?	1
1	A	225	THR	C	171.9	?	1
1	A	225	THR	CA	68.53	?	1
1	A	225	THR	CB	57.32	?	1
1	A	225	THR	N	112.0	?	1
1	A	228	LEU	HG	1.104	?	1
1	A	230	SER	H	9.646	?	1
1	A	230	SER	HA	4.665	?	1
1	A	230	SER	HB2	3.676	?	2
1	A	230	SER	HB3	3.598	?	2
1	A	230	SER	C	173.7	?	1
1	A	230	SER	CA	62.13	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	230	SER	CB	55.73	?	1
1	A	230	SER	N	119.8	?	1
1	A	232	ASN	H	8.662	?	1
1	A	232	ASN	HA	4.342	?	1
1	A	232	ASN	HB2	2.978	?	2
1	A	232	ASN	HB3	2.64	?	2
1	A	232	ASN	N	114.3	?	1
1	A	233	PRO	HA	4.325	?	1
1	A	233	PRO	HB2	1.921	?	2
1	A	233	PRO	HB3	1.921	?	2
1	A	233	PRO	HD2	3.656	?	2
1	A	233	PRO	HD3	3.656	?	2
1	A	233	PRO	C	176.0	?	1
1	A	233	PRO	CA	61.53	?	1
1	A	233	PRO	CB	28.63	?	1
1	A	237	ASN	C	173.1	?	1
1	A	237	ASN	CA	52.27	?	1
1	A	237	ASN	CB	37.15	?	1
1	A	241	GLU	H	9.041	?	1
1	A	241	GLU	HA	4.032	?	1
1	A	241	GLU	HB2	2.006	?	2
1	A	241	GLU	HB3	1.898	?	2
1	A	241	GLU	HG2	2.4	?	2
1	A	241	GLU	HG3	2.252	?	2
1	A	241	GLU	C	176.7	?	1
1	A	241	GLU	CA	57.43	?	1
1	A	241	GLU	CB	25.99	?	1
1	A	241	GLU	N	118.0	?	1
1	A	245	LYS	HD2	1.377	?	4
1	A	245	LYS	HD3	1.377	?	4

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	130	2.06 ± 0.13	Should be checked
$^{13}\text{C}_\beta$	122	2.68 ± 0.14	Should be checked
$^{13}\text{C}'$	131	2.46 ± 0.09	Should be applied
^{15}N	142	-0.76 ± 0.47	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 76%, i.e. 1138 atoms were assigned a chemical shift out of a possible 1494. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	542/565 (96%)	228/228 (100%)	207/230 (90%)	107/107 (100%)
Sidechain	594/861 (69%)	496/568 (87%)	98/270 (36%)	0/23 (0%)
Aromatic	2/68 (3%)	2/34 (6%)	0/29 (0%)	0/5 (0%)
Overall	1138/1494 (76%)	726/830 (87%)	305/529 (58%)	107/135 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1275 atoms were assigned a chemical shift out of a possible 1671. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	611/645 (95%)	260/261 (100%)	231/264 (88%)	120/120 (100%)
Sidechain	662/958 (69%)	554/634 (87%)	108/300 (36%)	0/24 (0%)
Aromatic	2/68 (3%)	2/34 (6%)	0/29 (0%)	0/5 (0%)
Overall	1275/1671 (76%)	816/929 (88%)	339/593 (57%)	120/149 (81%)

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	168	SER	CB	25.03	56.28 – 71.32	-25.8
1	A	202	PRO	CB	59.89	26.06 – 37.61	24.3
1	A	169	SER	CB	34.57	56.28 – 71.32	-19.4
1	A	135	PHE	HD1	3.63	5.51 – 8.60	-11.1
1	A	135	PHE	HD2	3.78	5.52 – 8.61	-10.6
1	A	198	ALA	CB	35.85	10.19 – 27.75	9.6
1	A	201	GLY	CA	56.05	38.93 – 51.79	8.3
1	A	193	GLU	CA	42.36	47.03 – 67.62	-7.3
1	A	225	THR	CB	57.32	61.12 – 78.27	-7.2
1	A	147	PRO	HB3	4.50	0.25 – 3.76	7.1
1	A	147	PRO	HB2	4.50	0.37 – 3.78	7.1
1	A	148	ILE	CA	43.97	48.30 – 75.08	-6.6
1	A	139	GLU	CB	40.25	21.56 – 38.37	6.1
1	A	195	THR	HG3	2.42	0.08 – 2.19	6.1

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	83	SER	CB	54.64	56.28 – 71.32	-6.1
1	A	161	THR	CB	59.80	61.12 – 78.27	-5.8
1	A	230	SER	CB	55.73	56.28 – 71.32	-5.4
1	A	202	PRO	HB3	3.85	0.25 – 3.76	5.2
1	A	149	PRO	N	107.50	108.67 – 162.11	-5.2
1	A	202	PRO	HB2	3.85	0.37 – 3.78	5.2
1	A	147	PRO	N	108.50	108.67 – 162.11	-5.0

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:

