Full wwPDB NMR Structure Validation Report (i)

Jan 25, 2024 – 12:02 AM EST

PDB ID	:	2KGS
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 (i) 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 (i)) were used in the production of this report:

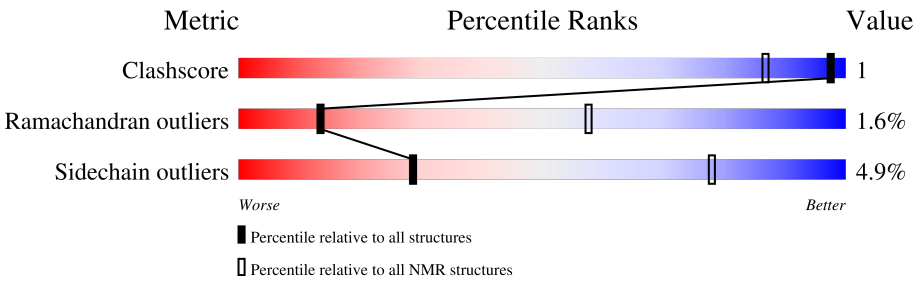
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	132	84% • 13%

2 Ensemble composition and analysis (i)

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
			Total	C	H	N	O	S	
1	A	132	1927	602	970	161	192	2	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A:

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

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A: 83% 5% 13%

4.2.4 Score per residue for model 4 (medoid)

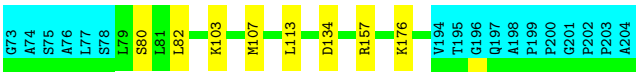
• Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A: 82% • • 13%

4.2.5 Score per residue for model 5

• Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A: 81% 6% 13%



4.2.6 Score per residue for model 6

• Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A: 81% 5% • 13%

4.2.7 Score per residue for model 7

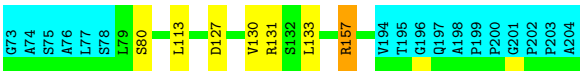
• Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A: 84% • 13%

4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A:

4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A:

5 Refinement protocol and experimental data overview (i)

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	2296
Number of shifts mapped to atoms	1291
Number of unparsed shifts	0
Number of shifts with mapping errors	1005
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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	0.61±0.02	0±0/869 (0.0± 0.0%)	1.13±0.40	2±2/1190 (0.1± 0.2%)
All	All	0.61	1/8690 (0.0%)	1.20	15/11900 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	193	GLU	CG-CD	6.67	1.61	1.51	10	1

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	185	ASP	CB-CG-OD1	-38.90	83.29	118.30	10	1
1	A	193	GLU	OE1-CD-OE2	37.04	167.74	123.30	10	1
1	A	185	ASP	CB-CG-OD2	-36.70	85.27	118.30	10	1
1	A	185	ASP	OD1-CG-OD2	23.82	168.56	123.30	10	1
1	A	193	GLU	CG-CD-OE1	-17.34	83.62	118.30	10	1
1	A	193	GLU	CG-CD-OE2	-17.08	84.13	118.30	10	1
1	A	177	ARG	NE-CZ-NH1	6.39	123.50	120.30	1	3
1	A	157	ARG	NE-CZ-NH1	6.26	123.43	120.30	4	2
1	A	86	ARG	NE-CZ-NH1	5.42	123.01	120.30	9	2
1	A	177	ARG	NE-CZ-NH2	-5.32	117.64	120.30	1	2

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 (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	115/132 (87%)	106±1 (92±1%)	7±1 (6±1%)	2±0 (2±0%)	13	57
All	All	1150/1320 (87%)	1063 (92%)	69 (6%)	18 (2%)	13	57

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 (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	97/107 (91%)	92±2 (95±2%)	5±2 (5±2%)	29	78
All	All	970/1070 (91%)	922 (95%)	48 (5%)	29	78

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	8
1	A	133	LEU	5
1	A	127	ASP	4
1	A	134	ASP	4
1	A	80	SER	3
1	A	82	LEU	3
1	A	103	LYS	3
1	A	153	LEU	3
1	A	130	VAL	2
1	A	156	GLU	2
1	A	154	LYS	1
1	A	172	LYS	1
1	A	107	MET	1
1	A	176	LYS	1
1	A	84	ILE	1
1	A	131	ARG	1
1	A	157	ARG	1
1	A	100	GLU	1
1	A	123	GLN	1
1	A	132	SER	1
1	A	188	ILE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 74% 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 (i)

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	2296
Number of shifts mapped to atoms	1291
Number of unparsed shifts	0
Number of shifts with mapping errors	1005
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 54 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	VAL	H	7.488	.	1
1	A	146	VAL	HA	3.994	.	1
1	A	146	VAL	HB	2.355	.	1
1	A	146	VAL	HG11	1.061	.	2
1	A	146	VAL	HG12	1.061	.	2
1	A	146	VAL	HG13	1.061	.	2
1	A	146	VAL	HG21	0.977	.	2
1	A	146	VAL	HG22	0.977	.	2
1	A	146	VAL	HG23	0.977	.	2
1	A	146	VAL	N	115.4	.	1
1	A	173	ASP	H	7.690	.	1
1	A	173	ASP	HA	4.353	.	1
1	A	173	ASP	HB2	2.791	.	2
1	A	173	ASP	HB3	2.648	.	2
1	A	173	ASP	C	177.1	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	173	ASP	CA	55.44	.	1
1	A	173	ASP	CB	37.90	.	1
1	A	173	ASP	N	116.0	.	1
1	A	176	LYS	H	8.588	.	1
1	A	176	LYS	HA	3.913	.	1
1	A	176	LYS	HB2	1.786	.	2
1	A	176	LYS	HB3	1.754	.	2
1	A	176	LYS	HD2	1.604	.	4
1	A	176	LYS	HD3	1.604	.	4
1	A	176	LYS	HG2	1.357	.	4
1	A	176	LYS	HG3	1.357	.	4
1	A	176	LYS	C	175.5	.	1
1	A	176	LYS	CA	56.85	.	1
1	A	176	LYS	CB	29.65	.	1
1	A	176	LYS	N	117.7	.	1
1	A	191	ASN	H	7.000	.	1
1	A	191	ASN	HA	4.791	.	1
1	A	191	ASN	HB2	3.183	.	2
1	A	191	ASN	HB3	2.632	.	2
1	A	191	ASN	C	174.3	.	1
1	A	191	ASN	CA	50.06	.	1
1	A	191	ASN	CB	35.72	.	1
1	A	191	ASN	N	113.2	.	1
1	A	196	GLY	H	8.362	.	1
1	A	196	GLY	HA2	3.878	.	2
1	A	196	GLY	HA3	3.825	.	2
1	A	196	GLY	C	173.0	.	1
1	A	196	GLY	CA	43.87	.	1
1	A	196	GLY	N	104.5	.	1
1	A	200	PRO	HA	4.439	.	1
1	A	200	PRO	HB2	2.261	.	2
1	A	200	PRO	HB3	1.939	.	2
1	A	200	PRO	HD2	3.519	.	2
1	A	200	PRO	HD3	3.519	.	2
1	A	200	PRO	HG2	2.033	.	2
1	A	200	PRO	HG3	2.033	.	2
1	A	200	PRO	C	177.2	.	1
1	A	200	PRO	CA	63.66	.	1
1	A	200	PRO	CB	27.92	.	1

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

- No matching atom found in the structure. All 1005 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	SER	H	8.179	.	1
1	A	133	SER	HA	4.502	.	1
1	A	133	SER	HB2	3.843	.	2
1	A	133	SER	HB3	3.843	.	2
1	A	133	SER	C	172.2	.	1
1	A	133	SER	CA	55.47	.	1
1	A	133	SER	CB	62.13	.	1
1	A	133	SER	N	114.0	.	1
1	A	134	GLY	H	8.332	.	1
1	A	134	GLY	HA2	4.284	.	2
1	A	134	GLY	HA3	4.078	.	2
1	A	134	GLY	N	110.0	.	1
1	A	135	PRO	HA	4.446	.	1
1	A	135	PRO	HB2	2.07	.	2
1	A	135	PRO	HB3	1.996	.	2
1	A	135	PRO	HD2	3.777	.	2
1	A	135	PRO	HD3	3.635	.	2
1	A	135	PRO	HG2	2.298	.	2
1	A	135	PRO	HG3	2.298	.	2
1	A	135	PRO	C	175.8	.	1
1	A	135	PRO	CA	62.09	.	1
1	A	135	PRO	CB	29.68	.	1
1	A	136	CYS	H	8.54	.	1
1	A	136	CYS	HA	4.731	.	1
1	A	136	CYS	HB2	3.289	.	2
1	A	136	CYS	HB3	2.895	.	2
1	A	136	CYS	C	173.0	.	1
1	A	136	CYS	CA	52.67	.	1
1	A	136	CYS	CB	38.32	.	1
1	A	136	CYS	N	115.9	.	1
1	A	137	ALA	H	7.537	.	1
1	A	137	ALA	HA	4.196	.	1
1	A	137	ALA	HB1	1.336	.	1
1	A	137	ALA	HB2	1.336	.	1
1	A	137	ALA	HB3	1.336	.	1
1	A	137	ALA	C	175.1	.	1
1	A	137	ALA	CA	51.08	.	1
1	A	137	ALA	CB	16.46	.	1
1	A	137	ALA	N	123.8	.	1
1	A	138	ASP	H	8.405	.	1
1	A	138	ASP	HA	4.711	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	ASP	HB2	2.861	.	2
1	A	138	ASP	HB3	2.5	.	2
1	A	138	ASP	C	174.3	.	1
1	A	138	ASP	CA	51.17	.	1
1	A	138	ASP	CB	37.5	.	1
1	A	138	ASP	N	119.2	.	1
1	A	139	LEU	H	7.653	.	1
1	A	139	LEU	HA	4.114	.	1
1	A	139	LEU	HB2	1.691	.	2
1	A	139	LEU	HB3	1.691	.	2
1	A	139	LEU	HD11	0.942	.	2
1	A	139	LEU	HD12	0.942	.	2
1	A	139	LEU	HD13	0.942	.	2
1	A	139	LEU	HD21	0.912	.	2
1	A	139	LEU	HD22	0.912	.	2
1	A	139	LEU	HD23	0.912	.	2
1	A	139	LEU	HG	1.547	.	1
1	A	139	LEU	C	176.2	.	1
1	A	139	LEU	CA	55.48	.	1
1	A	139	LEU	CB	40.25	.	1
1	A	139	LEU	N	121.0	.	1
1	A	140	GLN	H	9.108	.	1
1	A	140	GLN	HA	3.807	.	1
1	A	140	GLN	HB2	2.25	.	2
1	A	140	GLN	HB3	2.153	.	2
1	A	140	GLN	HG2	2.461	.	2
1	A	140	GLN	HG3	2.275	.	2
1	A	140	GLN	C	176.2	.	1
1	A	140	GLN	CA	56.91	.	1
1	A	140	GLN	CB	26.55	.	1
1	A	140	GLN	N	118.0	.	1
1	A	141	SER	H	7.861	.	1
1	A	141	SER	HA	4.186	.	1
1	A	141	SER	HB2	3.897	.	2
1	A	141	SER	HB3	3.897	.	2
1	A	141	SER	C	174.7	.	1
1	A	141	SER	CA	59.9	.	1
1	A	141	SER	CB	59.9	.	1
1	A	141	SER	N	114.2	.	1
1	A	142	ALA	H	7.904	.	1
1	A	142	ALA	HA	4.211	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	142	ALA	HB1	1.548	.	1
1	A	142	ALA	HB2	1.548	.	1
1	A	142	ALA	HB3	1.548	.	1
1	A	142	ALA	C	178.6	.	1
1	A	142	ALA	CA	52.86	.	1
1	A	142	ALA	CB	16.27	.	1
1	A	142	ALA	N	125.1	.	1
1	A	143	ILE	H	8.643	.	1
1	A	143	ILE	HA	3.699	.	1
1	A	143	ILE	HB	2.024	.	1
1	A	143	ILE	HD11	0.941	.	1
1	A	143	ILE	HD12	0.941	.	1
1	A	143	ILE	HD13	0.941	.	1
1	A	143	ILE	HG12	1.655	.	2
1	A	143	ILE	HG13	1.655	.	2
1	A	143	ILE	HG21	1.178	.	1
1	A	143	ILE	HG22	1.178	.	1
1	A	143	ILE	HG23	1.178	.	1
1	A	143	ILE	C	175.8	.	1
1	A	143	ILE	CA	62.53	.	1
1	A	143	ILE	CB	34.76	.	1
1	A	143	ILE	N	118.0	.	1
1	A	144	ASN	H	8.753	.	1
1	A	144	ASN	HA	4.58	.	1
1	A	144	ASN	HB2	3.005	.	2
1	A	144	ASN	HB3	2.871	.	2
1	A	144	ASN	C	176.2	.	1
1	A	144	ASN	CA	53.05	.	1
1	A	144	ASN	CB	34.58	.	1
1	A	144	ASN	N	120.7	.	1
1	A	145	ALA	H	7.977	.	1
1	A	145	ALA	HA	4.21	.	1
1	A	145	ALA	HB1	1.535	.	1
1	A	145	ALA	HB2	1.535	.	1
1	A	145	ALA	HB3	1.535	.	1
1	A	145	ALA	C	177.4	.	1
1	A	145	ALA	CA	52.21	.	1
1	A	145	ALA	CB	15.64	.	1
1	A	145	ALA	N	122.1	.	1
1	A	147	THR	H	8.533	.	1
1	A	147	THR	HA	4.153	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	THR	HB	4.502	.	1
1	A	147	THR	HG21	1.11	.	1
1	A	147	THR	HG22	1.11	.	1
1	A	147	THR	HG23	1.11	.	1
1	A	147	THR	C	175.0	.	1
1	A	147	THR	CA	61.1	.	1
1	A	147	THR	CB	66.32	.	1
1	A	147	THR	N	108.5	.	1
1	A	148	GLY	H	8.265	.	1
1	A	148	GLY	HA2	4.026	.	2
1	A	148	GLY	HA3	3.848	.	2
1	A	148	GLY	C	171.5	.	1
1	A	148	GLY	CA	43.97	.	1
1	A	148	GLY	N	110.6	.	1
1	A	149	GLY	H	7.953	.	1
1	A	149	GLY	HA2	4.664	.	2
1	A	149	GLY	HA3	3.629	.	2
1	A	149	GLY	N	107.5	.	1
1	A	150	PRO	HA	4.623	.	1
1	A	150	PRO	HB2	1.96	.	2
1	A	150	PRO	HB3	1.85	.	2
1	A	150	PRO	HG2	2.18	.	2
1	A	150	PRO	HG3	2.11	.	2
1	A	150	PRO	C	174.0	.	1
1	A	150	PRO	CA	60.29	.	1
1	A	150	PRO	CB	30.4	.	1
1	A	151	ILE	H	9.157	.	1
1	A	151	ILE	HA	3.966	.	1
1	A	151	ILE	HB	1.546	.	1
1	A	151	ILE	HD11	0.692	.	1
1	A	151	ILE	HD12	0.692	.	1
1	A	151	ILE	HD13	0.692	.	1
1	A	151	ILE	HG12	1.317	.	2
1	A	151	ILE	HG13	1.317	.	2
1	A	151	ILE	HG21	0.778	.	1
1	A	151	ILE	HG22	0.778	.	1
1	A	151	ILE	HG23	0.778	.	1
1	A	151	ILE	C	172.2	.	1
1	A	151	ILE	N	122.7	.	1
1	A	152	ALA	H	8.356	.	1
1	A	152	ALA	HA	4.79	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	152	ALA	HB1	1.376	.	1
1	A	152	ALA	HB2	1.376	.	1
1	A	152	ALA	HB3	1.376	.	1
1	A	152	ALA	N	130.3	.	1
1	A	153	PHE	H	8.986	.	1
1	A	153	PHE	C	174.2	.	1
1	A	153	PHE	CA	54.81	.	1
1	A	153	PHE	CB	39.18	.	1
1	A	153	PHE	N	120.7	.	1
1	A	154	GLY	H	8.417	.	1
1	A	154	GLY	HA2	4.106	.	2
1	A	154	GLY	HA3	3.951	.	2
1	A	154	GLY	N	107.7	.	1
1	A	155	ASN	H	8.527	.	1
1	A	155	ASN	HA	4.718	.	1
1	A	155	ASN	HB2	2.838	.	2
1	A	155	ASN	HB3	2.719	.	2
1	A	155	ASN	C	173.2	.	1
1	A	155	ASN	CA	51.01	.	1
1	A	155	ASN	CB	36.43	.	1
1	A	155	ASN	N	118.0	.	1
1	A	156	ASP	H	8.356	.	1
1	A	156	ASP	HA	4.552	.	1
1	A	156	ASP	HB2	2.714	.	2
1	A	156	ASP	HB3	2.714	.	2
1	A	156	ASP	N	119.2	.	1
1	A	157	GLY	H	8.106	.	1
1	A	157	GLY	N	106.6	.	1
1	A	158	ALA	H	8.313	.	1
1	A	158	ALA	HA	4.367	.	1
1	A	158	ALA	HB1	1.4	.	1
1	A	158	ALA	HB2	1.4	.	1
1	A	158	ALA	HB3	1.4	.	1
1	A	158	ALA	N	123.7	.	1
1	A	159	SER	H	8.185	.	1
1	A	159	SER	HA	4.205	.	1
1	A	159	SER	HB2	3.772	.	2
1	A	159	SER	HB3	3.772	.	2
1	A	159	SER	N	106.5	.	1
1	A	160	LEU	H	8.485	.	1
1	A	160	LEU	N	121.9	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	161	ILE	H	6.523	.	1
1	A	161	ILE	N	114.8	.	1
1	A	163	ALA	H	8.326	.	1
1	A	163	ALA	N	118.0	.	1
1	A	164	ASP	H	8.142	.	1
1	A	164	ASP	N	111.4	.	1
1	A	165	TYR	H	7.293	.	1
1	A	165	TYR	N	119.4	.	1
1	A	166	GLU	H	8.136	.	1
1	A	166	GLU	HB2	2.148	.	2
1	A	166	GLU	HB3	1.916	.	2
1	A	166	GLU	HG2	2.333	.	2
1	A	166	GLU	HG3	2.333	.	2
1	A	166	GLU	N	117.2	.	1
1	A	167	ILE	H	7.116	.	1
1	A	167	ILE	HA	3.536	.	1
1	A	167	ILE	HB	1.679	.	1
1	A	167	ILE	HD11	0.83	.	1
1	A	167	ILE	HD12	0.83	.	1
1	A	167	ILE	HD13	0.83	.	1
1	A	167	ILE	HG12	1.679	.	2
1	A	167	ILE	HG13	1.155	.	2
1	A	167	ILE	HG21	0.946	.	1
1	A	167	ILE	HG22	0.946	.	1
1	A	167	ILE	HG23	0.946	.	1
1	A	167	ILE	N	117.7	.	1
1	A	168	LEU	H	8.46	.	1
1	A	168	LEU	CA	55.52	.	1
1	A	168	LEU	CB	25.03	.	1
1	A	168	LEU	N	117.5	.	1
1	A	169	ASN	H	8.662	.	1
1	A	169	ASN	HA	4.393	.	1
1	A	169	ASN	HB2	3.283	.	2
1	A	169	ASN	HB3	3.048	.	2
1	A	169	ASN	C	176.0	.	1
1	A	169	ASN	CA	53.89	.	1
1	A	169	ASN	CB	34.57	.	1
1	A	169	ASN	N	120.3	.	1
1	A	170	ARG	H	7.77	.	1
1	A	170	ARG	HA	4.241	.	1
1	A	170	ARG	HB2	1.815	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	170	ARG	HB3	1.815	.	2
1	A	170	ARG	HG2	2.061	.	2
1	A	170	ARG	HG3	2.061	.	2
1	A	170	ARG	C	177.8	.	1
1	A	170	ARG	CA	57.06	.	1
1	A	170	ARG	CB	28.85	.	1
1	A	170	ARG	N	119.7	.	1
1	A	171	VAL	H	8.375	.	1
1	A	171	VAL	HA	3.359	.	1
1	A	171	VAL	HB	2.307	.	1
1	A	171	VAL	HG11	1.002	.	2
1	A	171	VAL	HG12	1.002	.	2
1	A	171	VAL	HG13	1.002	.	2
1	A	171	VAL	HG21	0.857	.	2
1	A	171	VAL	HG22	0.857	.	2
1	A	171	VAL	HG23	0.857	.	2
1	A	171	VAL	C	175.2	.	1
1	A	171	VAL	CA	65.1	.	1
1	A	171	VAL	CB	28.96	.	1
1	A	171	VAL	N	121.0	.	1
1	A	172	ALA	H	8.601	.	1
1	A	172	ALA	HA	3.762	.	1
1	A	172	ALA	HB1	1.523	.	1
1	A	172	ALA	HB2	1.523	.	1
1	A	172	ALA	HB3	1.523	.	1
1	A	172	ALA	C	176.3	.	1
1	A	172	ALA	CA	53.32	.	1
1	A	172	ALA	CB	15.78	.	1
1	A	172	ALA	N	120.4	.	1
1	A	174	LYS	H	7.47	.	1
1	A	174	LYS	HA	4.101	.	1
1	A	174	LYS	HB2	2.063	.	2
1	A	174	LYS	HB3	1.666	.	2
1	A	174	LYS	HD2	1.803	.	4
1	A	174	LYS	HD3	1.803	.	4
1	A	174	LYS	HG2	1.518	.	4
1	A	174	LYS	HG3	1.312	.	4
1	A	174	LYS	C	176.3	.	1
1	A	174	LYS	CA	55.42	.	1
1	A	174	LYS	CB	29.21	.	1
1	A	174	LYS	N	118.4	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	175	LEU	H	7.892	.	1
1	A	175	LEU	HA	3.933	.	1
1	A	175	LEU	HB2	1.806	.	2
1	A	175	LEU	HB3	1.806	.	2
1	A	175	LEU	HD11	0.745	.	2
1	A	175	LEU	HD12	0.745	.	2
1	A	175	LEU	HD13	0.745	.	2
1	A	175	LEU	HD21	0.718	.	2
1	A	175	LEU	HD22	0.718	.	2
1	A	175	LEU	HD23	0.718	.	2
1	A	175	LEU	C	177.7	.	1
1	A	175	LEU	CA	55.27	.	1
1	A	175	LEU	CB	39.18	.	1
1	A	175	LEU	N	117.0	.	1
1	A	177	ALA	H	6.896	.	1
1	A	177	ALA	HA	4.274	.	1
1	A	177	ALA	HB1	1.522	.	1
1	A	177	ALA	HB2	1.522	.	1
1	A	177	ALA	HB3	1.522	.	1
1	A	177	ALA	C	174.5	.	1
1	A	177	ALA	CA	50.48	.	1
1	A	177	ALA	CB	16.62	.	1
1	A	177	ALA	N	117.9	.	1
1	A	178	CYS	H	7.323	.	1
1	A	178	CYS	HA	5.16	.	1
1	A	178	CYS	HB2	3.244	.	2
1	A	178	CYS	HB3	2.636	.	2
1	A	178	CYS	N	116.4	.	1
1	A	179	PRO	HA	4.337	.	1
1	A	179	PRO	HB2	1.978	.	2
1	A	179	PRO	HB3	1.901	.	2
1	A	179	PRO	HD2	3.705	.	2
1	A	179	PRO	HD3	3.406	.	2
1	A	179	PRO	HG2	2.271	.	2
1	A	179	PRO	HG3	2.271	.	2
1	A	179	PRO	C	174.5	.	1
1	A	179	PRO	CA	62.2	.	1
1	A	179	PRO	CB	29.61	.	1
1	A	180	ASP	H	8.399	.	1
1	A	180	ASP	HA	4.802	.	1
1	A	180	ASP	HB2	2.781	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	180	ASP	HB3	2.575	.	2
1	A	180	ASP	C	174.5	.	1
1	A	180	ASP	CA	52.25	.	1
1	A	180	ASP	CB	38.79	.	1
1	A	180	ASP	N	115.1	.	1
1	A	181	ALA	H	8.093	.	1
1	A	181	ALA	HA	4.268	.	1
1	A	181	ALA	HB1	1.384	.	1
1	A	181	ALA	HB2	1.384	.	1
1	A	181	ALA	HB3	1.384	.	1
1	A	181	ALA	CB	17.26	.	1
1	A	181	ALA	N	123.7	.	1
1	A	182	ARG	H	8.65	.	1
1	A	182	ARG	HA	5.084	.	1
1	A	182	ARG	HB2	1.838	.	2
1	A	182	ARG	HB3	1.545	.	2
1	A	182	ARG	C	173.2	.	1
1	A	182	ARG	CA	52.36	.	1
1	A	182	ARG	CB	29.78	.	1
1	A	182	ARG	N	121.4	.	1
1	A	183	VAL	H	8.436	.	1
1	A	183	VAL	HA	5.238	.	1
1	A	183	VAL	HB	1.93	.	1
1	A	183	VAL	HG11	0.773	.	2
1	A	183	VAL	HG12	0.773	.	2
1	A	183	VAL	HG13	0.773	.	2
1	A	183	VAL	HG21	0.773	.	2
1	A	183	VAL	HG22	0.773	.	2
1	A	183	VAL	HG23	0.773	.	2
1	A	183	VAL	C	173.0	.	1
1	A	183	VAL	CA	56.76	.	1
1	A	183	VAL	CB	33.23	.	1
1	A	183	VAL	N	113.6	.	1
1	A	184	THR	H	9.584	.	1
1	A	184	THR	HA	4.853	.	1
1	A	184	THR	HB	3.874	.	1
1	A	184	THR	HG21	1.008	.	1
1	A	184	THR	HG22	1.008	.	1
1	A	184	THR	HG23	1.008	.	1
1	A	184	THR	C	169.7	.	1
1	A	184	THR	CA	59.69	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	184	THR	CB	68.31	.	1
1	A	184	THR	N	122.6	.	1
1	A	185	ILE	H	9.175	.	1
1	A	185	ILE	HA	4.565	.	1
1	A	185	ILE	HB	2.073	.	1
1	A	185	ILE	HG12	1.401	.	2
1	A	185	ILE	HG13	1.353	.	2
1	A	185	ILE	HG21	1.229	.	1
1	A	185	ILE	HG22	1.229	.	1
1	A	185	ILE	HG23	1.229	.	1
1	A	185	ILE	C	171.2	.	1
1	A	185	ILE	CA	57.04	.	1
1	A	185	ILE	CB	34.38	.	1
1	A	185	ILE	N	126.7	.	1
1	A	186	ASN	H	8.802	.	1
1	A	186	ASN	HA	5.476	.	1
1	A	186	ASN	HB2	2.684	.	2
1	A	186	ASN	HB3	2.074	.	2
1	A	186	ASN	C	172.7	.	1
1	A	186	ASN	CA	49.33	.	1
1	A	186	ASN	CB	39.04	.	1
1	A	186	ASN	N	125.5	.	1
1	A	187	GLY	H	9.236	.	1
1	A	187	GLY	HA2	4.89	.	2
1	A	187	GLY	HA3	3.809	.	2
1	A	187	GLY	C	169.2	.	1
1	A	187	GLY	CA	41.96	.	1
1	A	187	GLY	N	109.5	.	1
1	A	188	TYR	H	8.546	.	1
1	A	188	TYR	HA	5.565	.	1
1	A	188	TYR	HB2	3.582	.	2
1	A	188	TYR	HB3	2.715	.	2
1	A	188	TYR	C	174.0	.	1
1	A	188	TYR	CA	54.89	.	1
1	A	188	TYR	CB	42.49	.	1
1	A	188	TYR	N	118.3	.	1
1	A	189	THR	H	8.344	.	1
1	A	189	THR	HA	4.344	.	1
1	A	189	THR	HB	3.87	.	1
1	A	189	THR	HG21	1.201	.	1
1	A	189	THR	HG22	1.201	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	189	THR	HG23	1.201	.	1
1	A	189	THR	C	171.3	.	1
1	A	189	THR	N	111.5	.	1
1	A	190	ASP	H	7.855	.	1
1	A	190	ASP	HA	4.661	.	1
1	A	190	ASP	HB2	3.151	.	2
1	A	190	ASP	HB3	3.027	.	2
1	A	190	ASP	C	171.7	.	1
1	A	190	ASP	CA	51.74	.	1
1	A	190	ASP	CB	39.1	.	1
1	A	190	ASP	N	117.0	.	1
1	A	192	THR	H	8.216	.	1
1	A	192	THR	HA	4.188	.	1
1	A	192	THR	HB	4.08	.	1
1	A	192	THR	HG21	1.192	.	1
1	A	192	THR	HG22	1.192	.	1
1	A	192	THR	HG23	1.192	.	1
1	A	192	THR	C	173.0	.	1
1	A	192	THR	CA	61.11	.	1
1	A	192	THR	CB	67.49	.	1
1	A	192	THR	N	114.1	.	1
1	A	193	GLY	H	8.234	.	1
1	A	193	GLY	HA2	3.962	.	2
1	A	193	GLY	HA3	3.962	.	2
1	A	193	GLY	C	171.4	.	1
1	A	193	GLY	CA	42.36	.	1
1	A	193	GLY	N	108.6	.	1
1	A	194	SER	H	7.806	.	1
1	A	194	SER	HA	4.63	.	1
1	A	194	SER	HB2	4.035	.	2
1	A	194	SER	HB3	3.886	.	2
1	A	194	SER	N	114.3	.	1
1	A	195	GLU	H	9.334	.	1
1	A	195	GLU	HA	4.223	.	1
1	A	195	GLU	HB2	2.075	.	2
1	A	195	GLU	HB3	2.075	.	2
1	A	195	GLU	HG2	2.425	.	2
1	A	195	GLU	HG3	2.425	.	2
1	A	195	GLU	N	126.4	.	1
1	A	197	ILE	H	7.195	.	1
1	A	197	ILE	HA	4.213	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	197	ILE	HB	1.964	.	1
1	A	197	ILE	HD11	0.837	.	1
1	A	197	ILE	HD12	0.837	.	1
1	A	197	ILE	HD13	0.837	.	1
1	A	197	ILE	HG12	1.481	.	2
1	A	197	ILE	HG13	1.24	.	2
1	A	197	ILE	HG21	0.909	.	1
1	A	197	ILE	HG22	0.909	.	1
1	A	197	ILE	HG23	0.909	.	1
1	A	197	ILE	C	175.4	.	1
1	A	197	ILE	CA	59.27	.	1
1	A	197	ILE	CB	36.25	.	1
1	A	197	ILE	N	118.2	.	1
1	A	198	ASN	H	8.411	.	1
1	A	198	ASN	HA	4.543	.	1
1	A	198	ASN	HB2	2.768	.	2
1	A	198	ASN	HB3	2.768	.	2
1	A	198	ASN	C	176.1	.	1
1	A	198	ASN	CA	53.47	.	1
1	A	198	ASN	CB	35.85	.	1
1	A	198	ASN	N	119.9	.	1
1	A	199	ILE	H	8.637	.	1
1	A	199	ILE	HA	3.58	.	1
1	A	199	ILE	HB	2.07	.	1
1	A	199	ILE	HD11	0.847	.	1
1	A	199	ILE	HD12	0.847	.	1
1	A	199	ILE	HD13	0.847	.	1
1	A	199	ILE	HG12	1.775	.	2
1	A	199	ILE	HG13	1.775	.	2
1	A	199	ILE	HG21	0.873	.	1
1	A	199	ILE	HG22	0.873	.	1
1	A	199	ILE	HG23	0.873	.	1
1	A	199	ILE	N	119.8	.	1
1	A	201	LEU	H	7.66	.	1
1	A	201	LEU	HA	4.221	.	1
1	A	201	LEU	HB2	1.743	.	2
1	A	201	LEU	HB3	1.654	.	2
1	A	201	LEU	HD11	0.899	.	2
1	A	201	LEU	HD12	0.899	.	2
1	A	201	LEU	HD13	0.899	.	2
1	A	201	LEU	HD21	0.899	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	201	LEU	HD22	0.899	.	2
1	A	201	LEU	HD23	0.899	.	2
1	A	201	LEU	HG	1.497	.	1
1	A	201	LEU	C	176.9	.	1
1	A	201	LEU	CA	56.05	.	1
1	A	201	LEU	CB	40.06	.	1
1	A	201	LEU	N	119.5	.	1
1	A	202	SER	H	8.35	.	1
1	A	202	SER	HA	3.746	.	1
1	A	202	SER	HB2	3.848	.	2
1	A	202	SER	HB3	3.848	.	2
1	A	202	SER	C	173.6	.	1
1	A	202	SER	CA	59.89	.	1
1	A	202	SER	CB	59.89	.	1
1	A	202	SER	N	114.8	.	1
1	A	203	ALA	H	8.026	.	1
1	A	203	ALA	HA	3.82	.	1
1	A	203	ALA	HB1	1.485	.	1
1	A	203	ALA	HB2	1.485	.	1
1	A	203	ALA	HB3	1.485	.	1
1	A	203	ALA	C	177.4	.	1
1	A	203	ALA	CA	52.51	.	1
1	A	203	ALA	CB	15.36	.	1
1	A	203	ALA	N	126.7	.	1
1	A	204	GLN	H	8.069	.	1
1	A	204	GLN	HA	4.07	.	1
1	A	204	GLN	HB2	2.247	.	2
1	A	204	GLN	HB3	2.247	.	2
1	A	204	GLN	HG2	2.491	.	2
1	A	204	GLN	HG3	2.359	.	2
1	A	204	GLN	C	176.3	.	1
1	A	204	GLN	CA	56.59	.	1
1	A	204	GLN	CB	25.59	.	1
1	A	204	GLN	N	120.2	.	1
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

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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
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	210	ALA	H	8.613	.	1
1	A	210	ALA	HA	3.814	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	210	ALA	HB1	1.466	.	1
1	A	210	ALA	HB2	1.466	.	1
1	A	210	ALA	HB3	1.466	.	1
1	A	210	ALA	C	176.3	.	1
1	A	210	ALA	CA	53.94	.	1
1	A	210	ALA	CB	17.44	.	1
1	A	210	ALA	N	122.8	.	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	214	VAL	H	8.423	.	1
1	A	214	VAL	HA	4.404	.	1
1	A	214	VAL	HB	2.091	.	1
1	A	214	VAL	HG11	1.038	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	214	VAL	HG12	1.038	.	2
1	A	214	VAL	HG13	1.038	.	2
1	A	214	VAL	HG21	0.953	.	2
1	A	214	VAL	HG22	0.953	.	2
1	A	214	VAL	HG23	0.953	.	2
1	A	214	VAL	C	178.7	.	1
1	A	214	VAL	CA	62.84	.	1
1	A	214	VAL	CB	29.43	.	1
1	A	214	VAL	N	120.4	.	1
1	A	215	ALA	H	7.953	.	1
1	A	215	ALA	HA	4.084	.	1
1	A	215	ALA	HB1	1.368	.	1
1	A	215	ALA	HB2	1.368	.	1
1	A	215	ALA	HB3	1.368	.	1
1	A	215	ALA	C	177.4	.	1
1	A	215	ALA	CA	52.46	.	1
1	A	215	ALA	CB	14.81	.	1
1	A	215	ALA	N	125.2	.	1
1	A	216	ARG	H	7.372	.	1
1	A	216	ARG	HA	4.175	.	1
1	A	216	ARG	HB2	2.114	.	2
1	A	216	ARG	HB3	1.764	.	2
1	A	216	ARG	HD2	2.88	.	2
1	A	216	ARG	HD3	2.84	.	2
1	A	216	ARG	HG2	1.477	.	2
1	A	216	ARG	HG3	1.477	.	2
1	A	216	ARG	C	173.8	.	1
1	A	216	ARG	CA	51.46	.	1
1	A	216	ARG	CB	26.76	.	1
1	A	216	ARG	N	114.4	.	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	218	VAL	H	7.947	.	1
1	A	218	VAL	HA	3.65	.	1
1	A	218	VAL	HB	1.452	.	1
1	A	218	VAL	HG11	0.915	.	2
1	A	218	VAL	HG12	0.915	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	218	VAL	HG13	0.915	.	2
1	A	218	VAL	HG21	0.915	.	2
1	A	218	VAL	HG22	0.915	.	2
1	A	218	VAL	HG23	0.915	.	2
1	A	218	VAL	C	172.7	.	1
1	A	218	VAL	CA	60.93	.	1
1	A	218	VAL	CB	28.9	.	1
1	A	218	VAL	N	123.7	.	1
1	A	219	ALA	H	8.313	.	1
1	A	219	ALA	HA	4.141	.	1
1	A	219	ALA	HB1	1.243	.	1
1	A	219	ALA	HB2	1.243	.	1
1	A	219	ALA	HB3	1.243	.	1
1	A	219	ALA	C	177.5	.	1
1	A	219	ALA	CA	50.69	.	1
1	A	219	ALA	CB	16.19	.	1
1	A	219	ALA	N	130.2	.	1
1	A	220	GLY	H	8.869	.	1
1	A	220	GLY	HA2	3.916	.	2
1	A	220	GLY	HA3	3.674	.	2
1	A	220	GLY	C	173.4	.	1
1	A	220	GLY	CA	45.5	.	1
1	A	220	GLY	N	111.6	.	1
1	A	221	ASP	H	8.338	.	1
1	A	221	ASP	HA	4.675	.	1
1	A	221	ASP	HB2	2.997	.	2
1	A	221	ASP	HB3	2.695	.	2
1	A	221	ASP	C	174.8	.	1
1	A	221	ASP	CA	51.83	.	1
1	A	221	ASP	CB	36.64	.	1
1	A	221	ASP	N	115.3	.	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	H	7.342	.	1
1	A	223	ILE	HA	4.835	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	223	ILE	HB	1.71	.	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	223	ILE	C	172.1	.	1
1	A	223	ILE	CA	58.21	.	1
1	A	223	ILE	CB	38.77	.	1
1	A	223	ILE	N	117.9	.	1
1	A	224	ALA	H	8.607	.	1
1	A	224	ALA	HA	4.888	.	1
1	A	224	ALA	HB1	1.417	.	1
1	A	224	ALA	HB2	1.417	.	1
1	A	224	ALA	HB3	1.417	.	1
1	A	224	ALA	C	174.0	.	1
1	A	224	ALA	CA	48.05	.	1
1	A	224	ALA	CB	19.37	.	1
1	A	224	ALA	N	130.2	.	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	226	VAL	H	8.686	.	1
1	A	226	VAL	HA	4.191	.	1
1	A	226	VAL	HB	2.282	.	1
1	A	226	VAL	HG11	0.749	.	2
1	A	226	VAL	HG12	0.749	.	2
1	A	226	VAL	HG13	0.749	.	2
1	A	226	VAL	HG21	0.749	.	2
1	A	226	VAL	HG22	0.749	.	2
1	A	226	VAL	HG23	0.749	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	226	VAL	C	172.0	.	1
1	A	226	VAL	CA	59.42	.	1
1	A	226	VAL	CB	32.97	.	1
1	A	226	VAL	N	123.5	.	1
1	A	227	GLY	H	8.564	.	1
1	A	227	GLY	HA2	4.134	.	2
1	A	227	GLY	HA3	3.219	.	2
1	A	227	GLY	C	170.4	.	1
1	A	227	GLY	CA	43.34	.	1
1	A	227	GLY	N	113.2	.	1
1	A	228	LEU	H	8.491	.	1
1	A	228	LEU	HA	4.321	.	1
1	A	228	LEU	HB2	1.42	.	2
1	A	228	LEU	HB3	1.19	.	2
1	A	228	LEU	HD11	0.669	.	2
1	A	228	LEU	HD12	0.669	.	2
1	A	228	LEU	HD13	0.669	.	2
1	A	228	LEU	HD21	0.555	.	2
1	A	228	LEU	HD22	0.555	.	2
1	A	228	LEU	HD23	0.555	.	2
1	A	228	LEU	HG	1.104	.	1
1	A	228	LEU	C	176.0	.	1
1	A	228	LEU	CA	52.05	.	1
1	A	228	LEU	CB	39.52	.	1
1	A	228	LEU	N	125.1	.	1
1	A	229	GLY	H	8.698	.	1
1	A	229	GLY	HA2	4.076	.	2
1	A	229	GLY	HA3	3.09	.	2
1	A	229	GLY	C	171.7	.	1
1	A	229	GLY	CA	44.06	.	1
1	A	229	GLY	N	108.6	.	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
1	A	230	SER	CB	55.73	.	1
1	A	230	SER	N	119.8	.	1
1	A	231	VAL	H	6.939	.	1
1	A	231	VAL	HA	4.129	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	231	VAL	HB	2.288	.	1
1	A	231	VAL	HG11	1.099	.	2
1	A	231	VAL	HG12	1.099	.	2
1	A	231	VAL	HG13	1.099	.	2
1	A	231	VAL	HG21	1.099	.	2
1	A	231	VAL	HG22	1.099	.	2
1	A	231	VAL	HG23	1.099	.	2
1	A	231	VAL	C	171.1	.	1
1	A	231	VAL	CA	59.19	.	1
1	A	231	VAL	CB	30.04	.	1
1	A	231	VAL	N	117.7	.	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	234	ILE	H	7.66	.	1
1	A	234	ILE	HA	4.244	.	1
1	A	234	ILE	HB	2.172	.	1
1	A	234	ILE	HD11	0.727	.	1
1	A	234	ILE	HD12	0.727	.	1
1	A	234	ILE	HD13	0.727	.	1
1	A	234	ILE	HG12	1.792	.	2
1	A	234	ILE	HG13	1.111	.	2
1	A	234	ILE	HG21	0.852	.	1
1	A	234	ILE	HG22	0.852	.	1
1	A	234	ILE	HG23	0.852	.	1
1	A	234	ILE	C	172.7	.	1
1	A	234	ILE	CA	58.57	.	1
1	A	234	ILE	CB	36.69	.	1
1	A	234	ILE	N	116.1	.	1
1	A	235	ALA	H	8.619	.	1
1	A	235	ALA	HA	4.532	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	235	ALA	HB1	1.291	.	1
1	A	235	ALA	HB2	1.291	.	1
1	A	235	ALA	HB3	1.291	.	1
1	A	235	ALA	N	126.9	.	1
1	A	236	SER	H	8.411	.	1
1	A	236	SER	HA	4.24	.	1
1	A	236	SER	HB2	4.019	.	2
1	A	236	SER	HB3	3.751	.	2
1	A	236	SER	N	113.0	.	1
1	A	237	ASN	H	8.515	.	1
1	A	237	ASN	HA	4.783	.	1
1	A	237	ASN	HB2	3.151	.	2
1	A	237	ASN	HB3	2.481	.	2
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	237	ASN	N	123.3	.	1
1	A	238	ALA	H	8.466	.	1
1	A	238	ALA	HA	4.24	.	1
1	A	238	ALA	HB1	1.426	.	1
1	A	238	ALA	HB2	1.426	.	1
1	A	238	ALA	HB3	1.426	.	1
1	A	238	ALA	C	175.0	.	1
1	A	238	ALA	CA	51.41	.	1
1	A	238	ALA	CB	17.1	.	1
1	A	238	ALA	N	121.8	.	1
1	A	239	THR	H	7.14	.	1
1	A	239	THR	HA	5.023	.	1
1	A	239	THR	HB	4.632	.	1
1	A	239	THR	HG21	1.196	.	1
1	A	239	THR	HG22	1.196	.	1
1	A	239	THR	HG23	1.196	.	1
1	A	239	THR	N	105.0	.	1
1	A	240	PRO	HA	4.142	.	1
1	A	240	PRO	HD2	4.023	.	2
1	A	240	PRO	HD3	3.85	.	2
1	A	240	PRO	C	177.5	.	1
1	A	240	PRO	CA	62.93	.	1
1	A	240	PRO	CB	29.2	.	1
1	A	241	GLU	H	9.041	.	1
1	A	241	GLU	HA	4.032	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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	242	GLY	H	8.106	.	1
1	A	242	GLY	HA2	4.365	.	2
1	A	242	GLY	HA3	3.534	.	2
1	A	242	GLY	C	173.6	.	1
1	A	242	GLY	CA	44.64	.	1
1	A	242	GLY	N	111.5	.	1
1	A	243	ARG	H	8.014	.	1
1	A	243	ARG	HA	4.048	.	1
1	A	243	ARG	HB2	1.951	.	2
1	A	243	ARG	HB3	1.904	.	2
1	A	243	ARG	HD2	3.146	.	2
1	A	243	ARG	HD3	3.04	.	2
1	A	243	ARG	HG2	2.127	.	2
1	A	243	ARG	HG3	2.127	.	2
1	A	243	ARG	C	176.7	.	1
1	A	243	ARG	CA	58.34	.	1
1	A	243	ARG	CB	28.24	.	1
1	A	243	ARG	N	118.6	.	1
1	A	244	ALA	H	7.55	.	1
1	A	244	ALA	HA	3.913	.	1
1	A	244	ALA	HB1	1.458	.	1
1	A	244	ALA	HB2	1.458	.	1
1	A	244	ALA	HB3	1.458	.	1
1	A	244	ALA	C	178.1	.	1
1	A	244	ALA	CA	52.56	.	1
1	A	244	ALA	CB	15.71	.	1
1	A	244	ALA	N	116.2	.	1
1	A	245	LYS	H	7.262	.	1
1	A	245	LYS	HA	4.016	.	1
1	A	245	LYS	HB2	1.83	.	2
1	A	245	LYS	HB3	1.596	.	2
1	A	245	LYS	HD2	1.377	.	4
1	A	245	LYS	HD3	1.377	.	4

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	245	LYS	HG2	1.291	.	4
1	A	245	LYS	HG3	1.291	.	4
1	A	245	LYS	C	175.2	.	1
1	A	245	LYS	CA	55.36	.	1
1	A	245	LYS	CB	29.83	.	1
1	A	245	LYS	N	116.7	.	1
1	A	246	ASN	H	7.33	.	1
1	A	246	ASN	HA	4.559	.	1
1	A	246	ASN	HB2	2.546	.	2
1	A	246	ASN	HB3	2.487	.	2
1	A	246	ASN	C	173.8	.	1
1	A	246	ASN	CA	52.43	.	1
1	A	246	ASN	CB	35.72	.	1
1	A	246	ASN	N	113.6	.	1
1	A	247	ARG	H	6.798	.	1
1	A	247	ARG	HA	4.153	.	1
1	A	247	ARG	HB2	2.285	.	2
1	A	247	ARG	HB3	2.165	.	2
1	A	247	ARG	HD2	3.307	.	2
1	A	247	ARG	HD3	3.078	.	2
1	A	247	ARG	HG2	1.375	.	2
1	A	247	ARG	HG3	1.264	.	2
1	A	247	ARG	C	170.1	.	1
1	A	247	ARG	CA	53.78	.	1
1	A	247	ARG	CB	26.82	.	1
1	A	247	ARG	N	117.7	.	1
1	A	248	ARG	H	7.415	.	1
1	A	248	ARG	HA	5.576	.	1
1	A	248	ARG	HB2	1.746	.	2
1	A	248	ARG	HB3	1.746	.	2
1	A	248	ARG	C	171.4	.	1
1	A	248	ARG	CA	52.23	.	1
1	A	248	ARG	CB	29.65	.	1
1	A	248	ARG	N	121.2	.	1
1	A	249	VAL	H	8.65	.	1
1	A	249	VAL	HA	5.625	.	1
1	A	249	VAL	HB	1.962	.	1
1	A	249	VAL	HG11	0.948	.	2
1	A	249	VAL	HG12	0.948	.	2
1	A	249	VAL	HG13	0.948	.	2
1	A	249	VAL	HG21	0.948	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	249	VAL	HG22	0.948	.	2
1	A	249	VAL	HG23	0.948	.	2
1	A	249	VAL	C	172.1	.	1
1	A	249	VAL	CA	57.12	.	1
1	A	249	VAL	CB	33.76	.	1
1	A	249	VAL	N	115.4	.	1
1	A	250	GLU	H	9.45	.	1
1	A	250	GLU	HA	5.032	.	1
1	A	250	GLU	HB2	2.135	.	2
1	A	250	GLU	HB3	2.06	.	2
1	A	250	GLU	HG2	2.296	.	2
1	A	250	GLU	HG3	2.296	.	2
1	A	250	GLU	C	172.4	.	1
1	A	250	GLU	CA	52.39	.	1
1	A	250	GLU	CB	30.76	.	1
1	A	250	GLU	N	123.1	.	1
1	A	251	ILE	H	8.613	.	1
1	A	251	ILE	HA	4.48	.	1
1	A	251	ILE	HB	1.787	.	1
1	A	251	ILE	HD11	0.68	.	1
1	A	251	ILE	HD12	0.68	.	1
1	A	251	ILE	HD13	0.68	.	1
1	A	251	ILE	HG12	1.659	.	2
1	A	251	ILE	HG13	1.659	.	2
1	A	251	ILE	HG21	0.779	.	1
1	A	251	ILE	HG22	0.779	.	1
1	A	251	ILE	HG23	0.779	.	1
1	A	251	ILE	C	172.6	.	1
1	A	251	ILE	CA	59.03	.	1
1	A	251	ILE	CB	36.3	.	1
1	A	251	ILE	N	121.7	.	1
1	A	252	VAL	H	9.236	.	1
1	A	252	VAL	HA	4.702	.	1
1	A	252	VAL	HB	2.001	.	1
1	A	252	VAL	HG11	0.871	.	2
1	A	252	VAL	HG12	0.871	.	2
1	A	252	VAL	HG13	0.871	.	2
1	A	252	VAL	HG21	0.68	.	2
1	A	252	VAL	HG22	0.68	.	2
1	A	252	VAL	HG23	0.68	.	2
1	A	252	VAL	C	173.0	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	252	VAL	CA	58.88	.	1
1	A	252	VAL	CB	32.04	.	1
1	A	252	VAL	N	130.5	.	1
1	A	253	VAL	H	8.955	.	1
1	A	253	VAL	HA	4.361	.	1
1	A	253	VAL	HB	1.963	.	1
1	A	253	VAL	HG11	1.083	.	2
1	A	253	VAL	HG12	1.083	.	2
1	A	253	VAL	HG13	1.083	.	2
1	A	253	VAL	HG21	0.725	.	2
1	A	253	VAL	HG22	0.725	.	2
1	A	253	VAL	HG23	0.725	.	2
1	A	253	VAL	C	172.8	.	1
1	A	253	VAL	CA	59.7	.	1
1	A	253	VAL	CB	30.33	.	1
1	A	253	VAL	N	126.7	.	1
1	A	254	ASN	H	8.753	.	1
1	A	254	ASN	HA	4.416	.	1
1	A	254	ASN	HB2	2.771	.	2
1	A	254	ASN	HB3	2.464	.	2
1	A	254	ASN	N	131.7	.	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	191	2.14 ± 0.08	Should be checked
$^{13}C_{\beta}$	181	2.73 ± 0.15	Should be checked
$^{13}C'$	193	2.43 ± 0.13	Should be applied
^{15}N	230	-0.69 ± 0.35	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 74%, i.e. 1111 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	^{1}H	^{13}C	^{15}N
Backbone	525/565 (93%)	228/228 (100%)	190/230 (83%)	107/107 (100%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	586/861 (68%)	494/568 (87%)	92/270 (34%)	0/23 (0%)
Aromatic	0/68 (0%)	0/34 (0%)	0/29 (0%)	0/5 (0%)
Overall	1111/1494 (74%)	722/830 (87%)	282/529 (53%)	107/135 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1236 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	^{1}H	^{13}C	^{15}N
Backbone	588/645 (91%)	260/261 (100%)	208/264 (79%)	120/120 (100%)
Sidechain	648/958 (68%)	548/634 (86%)	100/300 (33%)	0/24 (0%)
Aromatic	0/68 (0%)	0/34 (0%)	0/29 (0%)	0/5 (0%)
Overall	1236/1671 (74%)	808/929 (87%)	308/593 (52%)	120/149 (81%)

7.1.4 Statistically unusual chemical shifts (i)

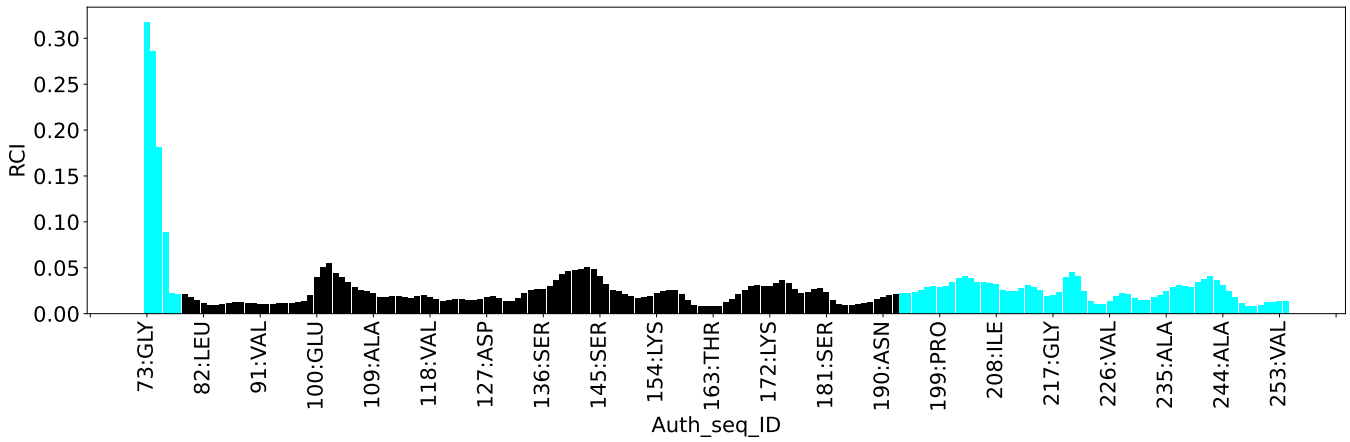
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	168	LEU	CB	25.03	33.11 – 51.34	-9.4
1	A	225	THR	CB	57.32	61.12 – 78.27	-7.2
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

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:


RCI
0.30
0.25
0.20
0.15
0.10
0.05
0.00
73:GLY
82:LEU
91:VAL
100:GLU
109:ALA
118:VAL
127:ASP
136:SER
145:SER
154:LYS
163:THR
172:LYS
181:SER
190:ASN
199:PRO
208:ILE
217:GLY
226:VAL
235:ALA
244:ALA
253:VAL
Auth_seq_ID