



Full wwPDB NMR Structure Validation Report ⓘ

Mar 2, 2026 – 03:01 AM UTC

PDB ID : 2LAE / pdb_00002lae
BMRB ID : 17521
Title : NMR solution structure of the C-terminal domain of the E. coli lipoprotein BamC
Authors : Pardi, A.; Warner, L.
Deposited on : 2011-03-11

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

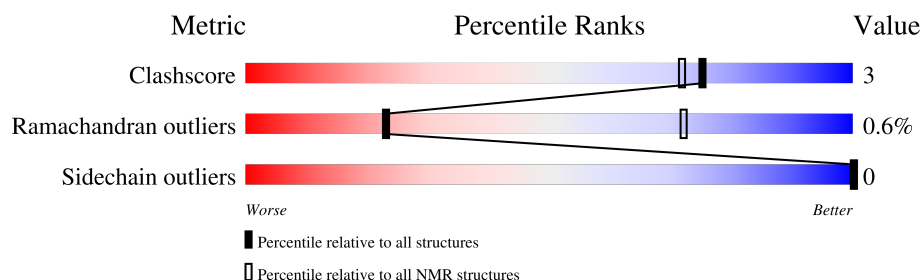
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	249	44% .. 53%

2 Ensemble composition and analysis

This entry contains 9 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:229-A:344 (116)	0.65	1

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, 3, 4, 5, 6
2	7, 8, 9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1756 atoms, of which 867 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lipoprotein 34.

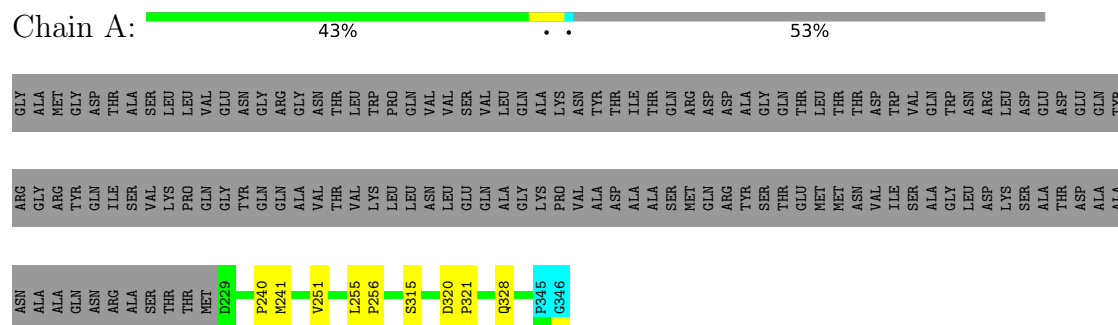
Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1756	554	867	153	179	3	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	GLY	-	expression tag	UNP P0A903
A	99	ALA	-	expression tag	UNP P0A903
A	100	MET	-	expression tag	UNP P0A903
A	345	PRO	-	expression tag	UNP P0A903
A	346	GLY	-	expression tag	UNP P0A903

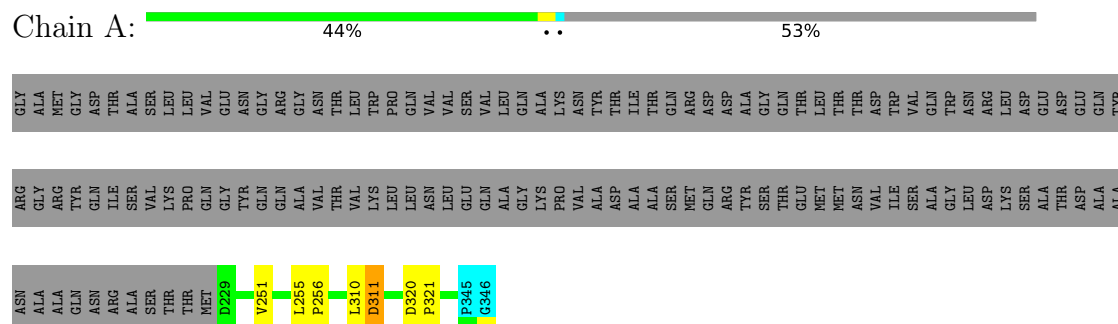
4.2.2 Score per residue for model 2

- Molecule 1: Lipoprotein 34



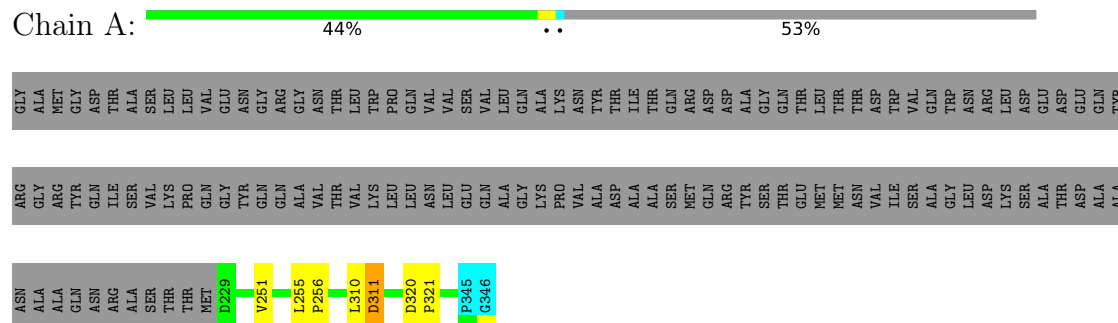
4.2.3 Score per residue for model 3

- Molecule 1: Lipoprotein 34



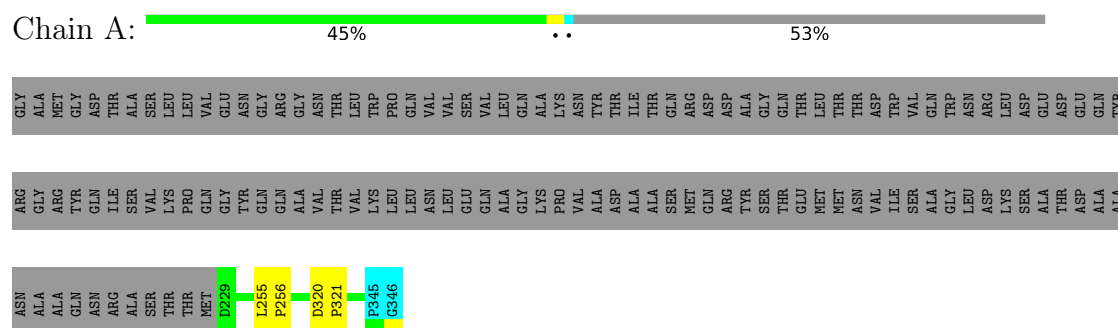
4.2.4 Score per residue for model 4

- Molecule 1: Lipoprotein 34



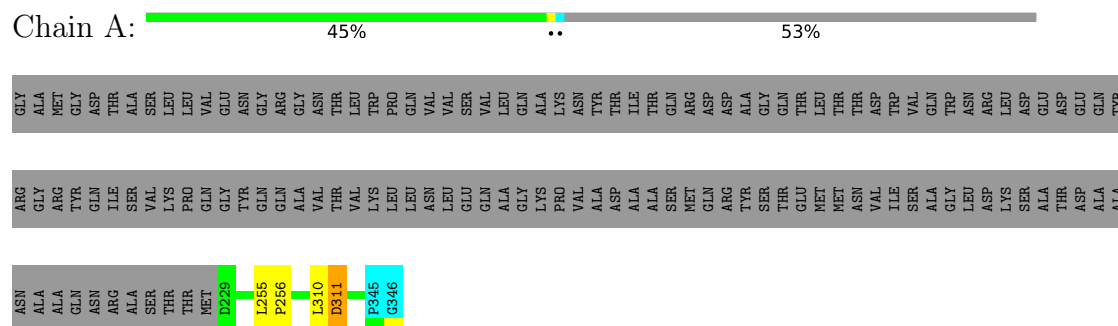
4.2.5 Score per residue for model 5

- Molecule 1: Lipoprotein 34



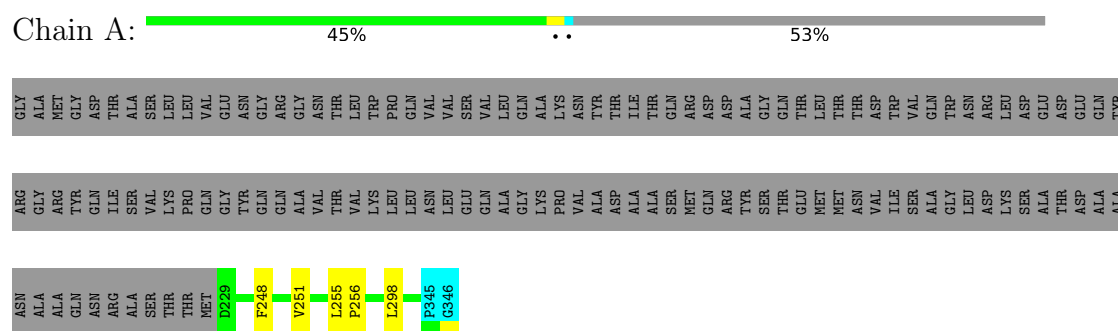
4.2.6 Score per residue for model 6

- Molecule 1: Lipoprotein 34



4.2.7 Score per residue for model 7

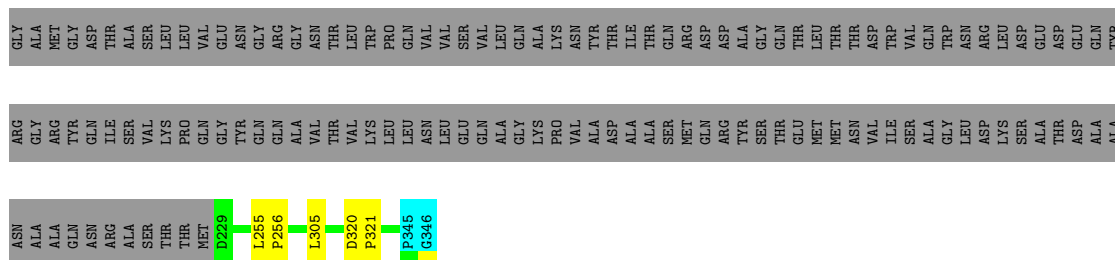
- Molecule 1: Lipoprotein 34



4.2.8 Score per residue for model 8

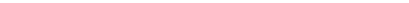
- Molecule 1: Lipoprotein 34

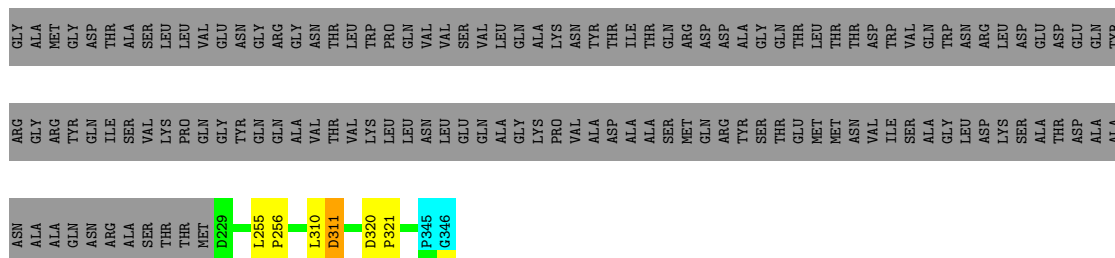




4.2.9 Score per residue for model 9

- Molecule 1: Lipoprotein 34

Chain A:  44% .. 53%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 9 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
CS-NOE-RDC Rosetta	structure solution	
CS-NOE-RDC Rosetta	refinement	

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	2539
Number of shifts mapped to atoms	1196
Number of unparsed shifts	0
Number of shifts with mapping errors	1343
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	877	857	856	5±1
All	All	7893	7713	7704	49

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:310:LEU:O	1:A:311:ASP:CB	0.70	2.39	9	5
1:A:310:LEU:O	1:A:311:ASP:HB3	0.56	2.01	9	5
1:A:255:LEU:N	1:A:256:PRO:CD	0.55	2.69	4	9
1:A:305:LEU:C	1:A:305:LEU:HD13	0.54	2.28	8	1
1:A:320:ASP:HB2	1:A:321:PRO:CD	0.51	2.36	5	7
1:A:255:LEU:N	1:A:256:PRO:HD2	0.51	2.20	7	1
1:A:320:ASP:OD1	1:A:320:ASP:C	0.46	2.57	4	7
1:A:248:PHE:CD1	1:A:248:PHE:C	0.46	2.91	7	1
1:A:255:LEU:HB3	1:A:256:PRO:HD3	0.46	1.88	5	1
1:A:251:VAL:O	1:A:255:LEU:N	0.45	2.49	1	5
1:A:248:PHE:CD1	1:A:248:PHE:O	0.44	2.70	7	1
1:A:264:MET:SD	1:A:278:VAL:HG21	0.41	2.55	1	1
1:A:320:ASP:HB2	1:A:321:PRO:HD2	0.41	1.91	9	3
1:A:241:MET:SD	1:A:315:SER:OG	0.41	2.77	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:240:PRO:HG3	1:A:328:GLN:HG3	0.40	1.93	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	115/249 (46%)	113±1 (98±1%)	2±1 (1±1%)	1±0 (1±0%)	23	72
All	All	1035/2241 (46%)	1015 (98%)	14 (1%)	6 (1%)	23	72

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	311	ASP	5
1	A	298	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	96/203 (47%)	96±0 (100±0%)	0±0 (0±0%)	100	100
All	All	864/1827 (47%)	864 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 79% for the well-defined parts and 79% 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	2539
Number of shifts mapped to atoms	1196
Number of unparsed shifts	0
Number of shifts with mapping errors	1343
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

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

- No matching atom found in the structure. All 1343 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	GLY	HA2	3.849	0.004	2
1	A	98	GLY	C	169.711	0.006	1
1	A	98	GLY	CA	43.47	0.051	1
1	A	99	ALA	H	8.594	0.007	1
1	A	99	ALA	HA	4.515	0.004	1
1	A	99	ALA	HB1	1.411	0.006	1
1	A	99	ALA	HB2	1.411	0.006	1
1	A	99	ALA	HB3	1.411	0.006	1
1	A	99	ALA	C	176.999	0.029	1
1	A	99	ALA	CA	52.237	0.019	1
1	A	99	ALA	CB	20.311	0.025	1
1	A	99	ALA	N	124.243	0.038	1
1	A	100	MET	H	8.443	0.003	1
1	A	100	MET	HA	4.456	0.009	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	MET	HB2	2.053	0.003	2
1	A	100	MET	HG2	2.607	0.000	2
1	A	100	MET	C	176.382	0.003	1
1	A	100	MET	CA	55.943	0.045	1
1	A	100	MET	CB	33.133	0.037	1
1	A	100	MET	CG	32.165	0.000	1
1	A	100	MET	N	120.185	0.014	1
1	A	101	GLY	H	8.482	0.004	1
1	A	101	GLY	HA2	4.087	0.006	2
1	A	101	GLY	HA3	3.873	0.008	2
1	A	101	GLY	C	173.248	0.007	1
1	A	101	GLY	CA	46.022	0.013	1
1	A	101	GLY	N	110.382	0.013	1
1	A	102	ASP	H	8.046	0.090	1
1	A	102	ASP	HA	4.285	0.011	1
1	A	102	ASP	HB2	3.418	0.008	2
1	A	102	ASP	HB3	2.592	0.011	2
1	A	102	ASP	C	175.405	0.006	1
1	A	102	ASP	CA	54.245	0.042	1
1	A	102	ASP	CB	41.406	0.028	1
1	A	102	ASP	N	117.064	0.024	1
1	A	103	THR	H	7.723	0.005	1
1	A	103	THR	HA	5.558	0.008	1
1	A	103	THR	HB	3.996	0.004	1
1	A	103	THR	HG21	1.088	0.002	1
1	A	103	THR	HG22	1.088	0.002	1
1	A	103	THR	HG23	1.088	0.002	1
1	A	103	THR	C	173.305	0.008	1
1	A	103	THR	CA	61.451	0.072	1
1	A	103	THR	CB	72.216	0.056	1
1	A	103	THR	CG2	21.17	0.086	1
1	A	103	THR	N	113.484	0.022	1
1	A	104	ALA	H	9.248	0.015	1
1	A	104	ALA	HA	4.784	0.006	1
1	A	104	ALA	HB1	1.303	0.013	1
1	A	104	ALA	HB2	1.303	0.013	1
1	A	104	ALA	HB3	1.303	0.013	1
1	A	104	ALA	C	175.069	0.008	1
1	A	104	ALA	CA	50.92	0.038	1
1	A	104	ALA	CB	22.05	0.022	1
1	A	104	ALA	N	129.484	0.036	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	105	SER	H	8.481	0.006	1
1	A	105	SER	HA	5.56	0.009	1
1	A	105	SER	HB2	3.61	0.023	2
1	A	105	SER	C	172.689	0.008	1
1	A	105	SER	CA	57.465	0.026	1
1	A	105	SER	CB	66.172	0.020	1
1	A	105	SER	N	114.672	0.022	1
1	A	106	LEU	H	8.893	0.004	1
1	A	106	LEU	HA	4.63	0.008	1
1	A	106	LEU	HB2	1.564	0.010	2
1	A	106	LEU	HB3	1.735	0.012	2
1	A	106	LEU	HD11	0.956	0.014	1
1	A	106	LEU	HD12	0.956	0.014	1
1	A	106	LEU	HD13	0.956	0.014	1
1	A	106	LEU	HD21	0.797	0.008	1
1	A	106	LEU	HD22	0.797	0.008	1
1	A	106	LEU	HD23	0.797	0.008	1
1	A	106	LEU	HG	1.433	0.006	1
1	A	106	LEU	C	174.585	0.010	1
1	A	106	LEU	CA	53.926	0.099	1
1	A	106	LEU	CB	46.757	0.024	1
1	A	106	LEU	CD1	23.589	0.086	2
1	A	106	LEU	CD2	26.105	0.142	2
1	A	106	LEU	N	126.664	0.025	1
1	A	107	LEU	H	8.544	0.004	1
1	A	107	LEU	HA	5.001	0.009	1
1	A	107	LEU	HB2	1.633	0.006	2
1	A	107	LEU	HB3	1.36	0.005	2
1	A	107	LEU	HD11	0.753	0.011	1
1	A	107	LEU	HD12	0.753	0.011	1
1	A	107	LEU	HD13	0.753	0.011	1
1	A	107	LEU	HD21	0.835	0.001	1
1	A	107	LEU	HD22	0.835	0.001	1
1	A	107	LEU	HD23	0.835	0.001	1
1	A	107	LEU	HG	1.511	0.000	1
1	A	107	LEU	C	176.595	0.031	1
1	A	107	LEU	CA	54.071	0.081	1
1	A	107	LEU	CB	42.711	0.034	1
1	A	107	LEU	CD1	23.856	0.030	2
1	A	107	LEU	CD2	24.755	0.015	2
1	A	107	LEU	CG	27.066	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	107	LEU	N	127.425	0.036	1
1	A	108	VAL	H	9.044	0.005	1
1	A	108	VAL	HA	4.318	0.008	1
1	A	108	VAL	HB	1.941	0.005	1
1	A	108	VAL	HG11	0.948	0.015	1
1	A	108	VAL	HG12	0.948	0.015	1
1	A	108	VAL	HG13	0.948	0.015	1
1	A	108	VAL	HG21	0.831	0.008	1
1	A	108	VAL	HG22	0.831	0.008	1
1	A	108	VAL	HG23	0.831	0.008	1
1	A	108	VAL	C	175.442	0.013	1
1	A	108	VAL	CA	60.965	0.061	1
1	A	108	VAL	CB	34.443	0.040	1
1	A	108	VAL	CG1	21.141	0.000	2
1	A	108	VAL	CG2	21.039	0.102	2
1	A	108	VAL	N	123.489	0.040	1
1	A	109	GLU	H	8.758	0.003	1
1	A	109	GLU	HA	4.376	0.009	1
1	A	109	GLU	HB2	2.15	0.020	2
1	A	109	GLU	HB3	2.022	0.015	2
1	A	109	GLU	HG2	2.358	0.000	2
1	A	109	GLU	C	176.256	0.013	1
1	A	109	GLU	CA	56.963	0.040	1
1	A	109	GLU	CB	30.362	0.021	1
1	A	109	GLU	CG	36.324	0.000	1
1	A	109	GLU	N	125.74	0.045	1
1	A	110	ASN	H	8.598	0.007	1
1	A	110	ASN	HA	4.712	0.006	1
1	A	110	ASN	HB2	2.821	0.000	2
1	A	110	ASN	HB3	2.787	0.002	2
1	A	110	ASN	C	176.052	0.011	1
1	A	110	ASN	CA	53.784	0.036	1
1	A	110	ASN	CB	39.197	0.044	1
1	A	110	ASN	N	119.602	0.032	1
1	A	111	GLY	H	8.519	0.004	1
1	A	111	GLY	HA2	4.005	0.005	2
1	A	111	GLY	HA3	3.927	0.002	2
1	A	111	GLY	C	174.496	0.003	1
1	A	111	GLY	CA	45.778	0.022	1
1	A	111	GLY	N	109.354	0.047	1
1	A	112	ARG	H	8.328	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	112	ARG	HA	4.382	0.008	1
1	A	112	ARG	HB2	1.752	0.056	2
1	A	112	ARG	HB3	1.901	0.004	2
1	A	112	ARG	HD2	3.197	0.000	1
1	A	112	ARG	C	177.357	0.006	1
1	A	112	ARG	CA	56.111	0.073	1
1	A	112	ARG	CB	30.414	0.033	1
1	A	112	ARG	CD	43.418	0.000	1
1	A	112	ARG	CG	27.239	0.000	1
1	A	112	ARG	N	120.144	0.019	1
1	A	113	GLY	H	8.513	0.005	1
1	A	113	GLY	HA2	4.011	0.018	2
1	A	113	GLY	HA3	3.845	0.017	2
1	A	113	GLY	C	174.542	0.006	1
1	A	113	GLY	CA	46.359	0.073	1
1	A	113	GLY	N	109.811	0.098	1
1	A	114	ASN	H	8.456	0.006	1
1	A	114	ASN	HA	4.817	0.009	1
1	A	114	ASN	HB2	2.917	0.017	2
1	A	114	ASN	C	175.968	0.011	1
1	A	114	ASN	CA	53.929	0.048	1
1	A	114	ASN	CB	38.286	0.015	1
1	A	114	ASN	N	118.764	0.018	1
1	A	115	THR	H	7.976	0.004	1
1	A	115	THR	HA	4.457	0.008	1
1	A	115	THR	HG21	1.249	0.000	1
1	A	115	THR	HG22	1.249	0.000	1
1	A	115	THR	HG23	1.249	0.000	1
1	A	115	THR	C	175.271	0.004	1
1	A	115	THR	CA	61.494	0.042	1
1	A	115	THR	CB	69.494	0.006	1
1	A	115	THR	CG2	21.649	0.000	1
1	A	115	THR	N	110.618	0.029	1
1	A	116	LEU	H	8.074	0.006	1
1	A	116	LEU	HA	4.296	0.006	1
1	A	116	LEU	HB2	1.573	0.009	2
1	A	116	LEU	HB3	1.783	0.005	2
1	A	116	LEU	HD11	0.927	0.009	1
1	A	116	LEU	HD12	0.927	0.009	1
1	A	116	LEU	HD13	0.927	0.009	1
1	A	116	LEU	HD21	0.8	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	LEU	HD22	0.8	0.011	1
1	A	116	LEU	HD23	0.8	0.011	1
1	A	116	LEU	C	177.787	0.009	1
1	A	116	LEU	CA	57.596	0.091	1
1	A	116	LEU	CB	42.608	0.046	1
1	A	116	LEU	CD1	24.234	0.000	2
1	A	116	LEU	CD2	26.219	0.000	2
1	A	116	LEU	N	125.26	0.029	1
1	A	117	TRP	H	8.973	0.004	1
1	A	117	TRP	HA	4.708	0.000	1
1	A	117	TRP	HE1	10.939	0.003	1
1	A	117	TRP	C	173.412	0.000	1
1	A	117	TRP	CA	61.816	0.000	1
1	A	117	TRP	CB	27.493	0.000	1
1	A	117	TRP	N	118.059	0.025	1
1	A	117	TRP	NE1	129.988	0.010	1
1	A	118	PRO	HA	3.837	0.002	1
1	A	118	PRO	HB2	1.842	0.014	2
1	A	118	PRO	HB3	2.204	0.007	2
1	A	118	PRO	HD2	3.686	0.000	2
1	A	118	PRO	HD3	3.686	0.000	2
1	A	118	PRO	C	179.667	0.012	1
1	A	118	PRO	CA	65.692	0.043	1
1	A	118	PRO	CB	30.361	0.063	1
1	A	118	PRO	CD	49.253	0.000	1
1	A	118	PRO	CG	28.091	0.000	1
1	A	119	GLN	H	7.446	0.006	1
1	A	119	GLN	HA	4.017	0.006	1
1	A	119	GLN	HB2	2.292	0.006	2
1	A	119	GLN	HB3	2.038	0.007	2
1	A	119	GLN	HG2	2.528	0.000	2
1	A	119	GLN	C	178.523	0.033	1
1	A	119	GLN	CA	59.233	0.067	1
1	A	119	GLN	CB	28.821	0.077	1
1	A	119	GLN	CG	34.654	0.000	1
1	A	119	GLN	N	117.225	0.032	1
1	A	120	VAL	H	8.204	0.005	1
1	A	120	VAL	HA	3.215	0.008	1
1	A	120	VAL	HB	2.084	0.007	1
1	A	120	VAL	HG11	0.94	0.004	1
1	A	120	VAL	HG12	0.94	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	VAL	HG13	0.94	0.004	1
1	A	120	VAL	HG21	0.606	0.007	1
1	A	120	VAL	HG22	0.606	0.007	1
1	A	120	VAL	HG23	0.606	0.007	1
1	A	120	VAL	C	177.053	0.031	1
1	A	120	VAL	CA	67.515	0.026	1
1	A	120	VAL	CB	31.173	0.036	1
1	A	120	VAL	CG1	24.0	0.114	2
1	A	120	VAL	CG2	20.938	0.036	2
1	A	120	VAL	N	121.922	0.033	1
1	A	121	VAL	H	7.493	0.005	1
1	A	121	VAL	HA	2.858	0.003	1
1	A	121	VAL	HB	1.52	0.007	1
1	A	121	VAL	HG11	-0.252	0.008	1
1	A	121	VAL	HG12	-0.252	0.008	1
1	A	121	VAL	HG13	-0.252	0.008	1
1	A	121	VAL	HG21	0.526	0.007	1
1	A	121	VAL	HG22	0.526	0.007	1
1	A	121	VAL	HG23	0.526	0.007	1
1	A	121	VAL	C	177.994	0.006	1
1	A	121	VAL	CA	67.467	0.023	1
1	A	121	VAL	CB	31.149	0.065	1
1	A	121	VAL	CG1	21.449	0.051	2
1	A	121	VAL	CG2	20.757	0.022	2
1	A	121	VAL	N	117.624	0.079	1
1	A	122	SER	H	7.839	0.005	1
1	A	122	SER	HA	4.181	0.005	1
1	A	122	SER	HB2	3.94	0.015	2
1	A	122	SER	C	177.314	0.057	1
1	A	122	SER	CA	61.943	0.056	1
1	A	122	SER	CB	62.888	0.022	1
1	A	122	SER	N	113.497	0.026	1
1	A	123	VAL	H	7.944	0.007	1
1	A	123	VAL	HA	3.653	0.010	1
1	A	123	VAL	HB	2.289	0.009	1
1	A	123	VAL	HG11	0.953	0.010	1
1	A	123	VAL	HG12	0.953	0.010	1
1	A	123	VAL	HG13	0.953	0.010	1
1	A	123	VAL	HG21	1.034	0.001	1
1	A	123	VAL	HG22	1.034	0.001	1
1	A	123	VAL	HG23	1.034	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	123	VAL	C	177.689	0.008	1
1	A	123	VAL	CA	66.173	0.032	1
1	A	123	VAL	CB	31.483	0.019	1
1	A	123	VAL	CG1	21.866	0.006	2
1	A	123	VAL	CG2	23.013	0.040	2
1	A	123	VAL	N	123.446	0.045	1
1	A	124	LEU	H	7.339	0.008	1
1	A	124	LEU	HA	3.864	0.007	1
1	A	124	LEU	HB2	1.978	0.006	2
1	A	124	LEU	HB3	1.439	0.010	2
1	A	124	LEU	HD11	0.842	0.000	1
1	A	124	LEU	HD12	0.842	0.000	1
1	A	124	LEU	HD13	0.842	0.000	1
1	A	124	LEU	HD21	0.806	0.014	1
1	A	124	LEU	HD22	0.806	0.014	1
1	A	124	LEU	HD23	0.806	0.014	1
1	A	124	LEU	C	179.307	0.005	1
1	A	124	LEU	CA	57.871	0.051	1
1	A	124	LEU	CB	41.055	0.073	1
1	A	124	LEU	CD1	23.417	0.025	2
1	A	124	LEU	CD2	28.01	0.053	2
1	A	124	LEU	N	118.275	0.032	1
1	A	125	GLN	H	8.287	0.006	1
1	A	125	GLN	HA	4.146	0.009	1
1	A	125	GLN	HB2	1.953	0.012	2
1	A	125	GLN	HB3	2.175	0.065	2
1	A	125	GLN	HG2	2.516	0.012	2
1	A	125	GLN	C	180.536	0.008	1
1	A	125	GLN	CA	58.884	0.018	1
1	A	125	GLN	CB	28.387	0.109	1
1	A	125	GLN	CG	34.638	0.000	1
1	A	125	GLN	N	117.044	0.041	1
1	A	126	ALA	H	8.251	0.006	1
1	A	126	ALA	HA	2.691	3.764	1
1	A	126	ALA	HB1	1.48	0.008	1
1	A	126	ALA	HB2	1.48	0.008	1
1	A	126	ALA	HB3	1.48	0.008	1
1	A	126	ALA	C	179.381	0.007	1
1	A	126	ALA	CA	54.522	0.034	1
1	A	126	ALA	CB	17.922	0.033	1
1	A	126	ALA	N	123.556	0.044	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	LYS	H	6.969	0.007	1
1	A	127	LYS	HA	3.988	0.006	1
1	A	127	LYS	HB2	0.925	0.009	2
1	A	127	LYS	HB3	1.062	0.040	2
1	A	127	LYS	HD2	1.506	0.000	2
1	A	127	LYS	HE2	2.954	0.000	2
1	A	127	LYS	HG2	1.506	0.000	2
1	A	127	LYS	C	175.367	0.003	1
1	A	127	LYS	CA	53.986	0.032	1
1	A	127	LYS	CB	30.165	0.022	1
1	A	127	LYS	CD	27.41	0.000	1
1	A	127	LYS	CE	42.1	0.000	1
1	A	127	LYS	CG	23.811	0.000	1
1	A	127	LYS	N	115.514	0.015	1
1	A	128	ASN	H	7.889	0.007	1
1	A	128	ASN	HA	4.27	0.004	1
1	A	128	ASN	HB2	3.115	0.011	2
1	A	128	ASN	HB3	2.756	0.005	2
1	A	128	ASN	C	174.952	0.021	1
1	A	128	ASN	CA	54.18	0.036	1
1	A	128	ASN	CB	36.929	0.063	1
1	A	128	ASN	N	113.419	0.028	1
1	A	129	TYR	H	7.348	0.006	1
1	A	129	TYR	HA	4.965	0.005	1
1	A	129	TYR	HB2	2.795	0.006	2
1	A	129	TYR	HB3	2.687	0.011	2
1	A	129	TYR	C	175.689	0.005	1
1	A	129	TYR	CA	54.302	0.037	1
1	A	129	TYR	CB	36.476	0.027	1
1	A	129	TYR	N	117.724	0.022	1
1	A	130	THR	H	8.648	0.005	1
1	A	130	THR	HA	4.171	0.008	1
1	A	130	THR	HB	4.084	0.010	1
1	A	130	THR	HG21	1.184	0.000	1
1	A	130	THR	HG22	1.184	0.000	1
1	A	130	THR	HG23	1.184	0.000	1
1	A	130	THR	C	173.483	0.006	1
1	A	130	THR	CA	63.273	0.069	1
1	A	130	THR	CB	69.272	0.025	1
1	A	130	THR	CG2	22.07	0.000	1
1	A	130	THR	N	120.322	0.024	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	ILE	H	8.838	0.006	1
1	A	131	ILE	HA	4.335	0.007	1
1	A	131	ILE	HB	1.859	0.004	1
1	A	131	ILE	HD11	0.851	0.004	1
1	A	131	ILE	HD12	0.851	0.004	1
1	A	131	ILE	HD13	0.851	0.004	1
1	A	131	ILE	HG12	1.633	0.000	1
1	A	131	ILE	HG13	1.633	0.000	1
1	A	131	ILE	HG21	0.976	0.008	1
1	A	131	ILE	HG22	0.976	0.008	1
1	A	131	ILE	HG23	0.976	0.008	1
1	A	131	ILE	C	176.427	0.008	1
1	A	131	ILE	CA	60.84	0.074	1
1	A	131	ILE	CB	39.312	0.038	1
1	A	131	ILE	CD1	13.513	0.008	1
1	A	131	ILE	CG1	27.47	0.000	1
1	A	131	ILE	CG2	19.4	0.035	1
1	A	131	ILE	N	129.574	0.031	1
1	A	132	THR	H	8.769	0.004	1
1	A	132	THR	HA	4.29	0.010	1
1	A	132	THR	HB	4.141	0.017	1
1	A	132	THR	HG21	1.065	0.002	1
1	A	132	THR	HG22	1.065	0.002	1
1	A	132	THR	HG23	1.065	0.002	1
1	A	132	THR	C	174.79	0.002	1
1	A	132	THR	CA	62.865	0.045	1
1	A	132	THR	CB	68.73	0.025	1
1	A	132	THR	CG2	22.438	0.074	1
1	A	132	THR	N	119.943	0.036	1
1	A	133	GLN	H	7.559	0.005	1
1	A	133	GLN	HA	4.525	0.010	1
1	A	133	GLN	HB2	2.01	0.004	2
1	A	133	GLN	HG2	2.353	0.000	2
1	A	133	GLN	C	173.338	0.019	1
1	A	133	GLN	CA	55.741	0.037	1
1	A	133	GLN	CB	31.16	0.062	1
1	A	133	GLN	CG	33.449	0.000	1
1	A	133	GLN	N	121.696	0.024	1
1	A	134	ARG	H	8.779	0.004	1
1	A	134	ARG	HA	4.711	0.010	1
1	A	134	ARG	HB2	1.889	0.038	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	134	ARG	HB3	1.783	0.016	2
1	A	134	ARG	HD2	3.12	0.022	1
1	A	134	ARG	HG2	1.712	0.014	2
1	A	134	ARG	C	173.059	0.001	1
1	A	134	ARG	CA	56.486	0.021	1
1	A	134	ARG	CB	34.093	0.044	1
1	A	134	ARG	CD	44.245	0.084	1
1	A	134	ARG	CG	27.475	0.000	1
1	A	134	ARG	N	124.918	0.023	1
1	A	135	ASP	H	9.036	0.009	1
1	A	135	ASP	HA	4.949	0.006	1
1	A	135	ASP	HB2	2.934	0.005	2
1	A	135	ASP	HB3	2.499	0.013	2
1	A	135	ASP	C	176.12	0.011	1
1	A	135	ASP	CA	51.969	0.038	1
1	A	135	ASP	CB	41.469	0.014	1
1	A	135	ASP	N	127.406	0.025	1
1	A	136	ASP	H	8.95	0.005	1
1	A	136	ASP	HA	4.63	0.002	1
1	A	136	ASP	HB2	2.917	0.011	2
1	A	136	ASP	HB3	2.671	0.004	2
1	A	136	ASP	C	177.818	0.003	1
1	A	136	ASP	CA	57.401	0.055	1
1	A	136	ASP	CB	40.833	0.022	1
1	A	136	ASP	N	124.226	0.031	1
1	A	137	ALA	H	8.177	0.004	1
1	A	137	ALA	HA	4.137	0.011	1
1	A	137	ALA	HB1	1.445	0.005	1
1	A	137	ALA	HB2	1.445	0.005	1
1	A	137	ALA	HB3	1.445	0.005	1
1	A	137	ALA	C	179.739	0.009	1
1	A	137	ALA	CA	54.759	0.053	1
1	A	137	ALA	CB	18.053	0.019	1
1	A	137	ALA	N	123.782	0.032	1
1	A	138	GLY	H	8.052	0.005	1
1	A	138	GLY	HA2	3.978	0.005	2
1	A	138	GLY	HA3	3.33	0.006	2
1	A	138	GLY	C	172.627	0.032	1
1	A	138	GLY	CA	45.152	0.017	1
1	A	138	GLY	N	105.127	0.026	1
1	A	139	GLN	H	7.229	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	139	GLN	HA	1.567	0.013	1
1	A	139	GLN	HB2	1.356	0.325	2
1	A	139	GLN	C	172.354	0.035	1
1	A	139	GLN	CA	55.607	0.035	1
1	A	139	GLN	CB	26.666	0.023	1
1	A	139	GLN	CG	35.086	0.000	1
1	A	139	GLN	N	118.245	0.023	1
1	A	140	THR	H	7.394	0.009	1
1	A	140	THR	HA	5.374	0.012	1
1	A	140	THR	HB	3.824	0.008	1
1	A	140	THR	HG21	1.065	0.008	1
1	A	140	THR	HG22	1.065	0.008	1
1	A	140	THR	HG23	1.065	0.008	1
1	A	140	THR	C	171.797	0.010	1
1	A	140	THR	CA	60.417	0.045	1
1	A	140	THR	CB	71.439	0.032	1
1	A	140	THR	CG2	20.234	0.000	1
1	A	140	THR	N	110.69	0.023	1
1	A	141	LEU	H	9.436	0.009	1
1	A	141	LEU	HA	5.236	0.008	1
1	A	141	LEU	HB2	2.131	0.014	2
1	A	141	LEU	HB3	2.295	0.011	2
1	A	141	LEU	HD11	0.711	0.005	1
1	A	141	LEU	HD12	0.711	0.005	1
1	A	141	LEU	HD13	0.711	0.005	1
1	A	141	LEU	HD21	0.865	0.011	1
1	A	141	LEU	HD22	0.865	0.011	1
1	A	141	LEU	HD23	0.865	0.011	1
1	A	141	LEU	C	175.035	0.007	1
1	A	141	LEU	CA	54.352	0.043	1
1	A	141	LEU	CB	44.973	0.017	1
1	A	141	LEU	CD1	28.377	0.066	2
1	A	141	LEU	CD2	25.246	0.010	2
1	A	141	LEU	CG	25.262	0.000	1
1	A	141	LEU	N	124.381	0.017	1
1	A	142	THR	H	9.02	0.009	1
1	A	142	THR	HA	5.598	0.011	1
1	A	142	THR	HB	3.879	0.007	1
1	A	142	THR	HG21	1.19	0.003	1
1	A	142	THR	HG22	1.19	0.003	1
1	A	142	THR	HG23	1.19	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	142	THR	C	174.47	0.007	1
1	A	142	THR	CA	60.905	0.027	1
1	A	142	THR	CB	71.723	0.033	1
1	A	142	THR	CG2	21.456	0.040	1
1	A	142	THR	N	116.419	0.030	1
1	A	143	THR	H	9.363	0.007	1
1	A	143	THR	HA	5.203	0.007	1
1	A	143	THR	HB	4.588	0.012	1
1	A	143	THR	HG21	1.057	0.010	1
1	A	143	THR	HG22	1.057	0.010	1
1	A	143	THR	HG23	1.057	0.010	1
1	A	143	THR	C	175.315	0.010	1
1	A	143	THR	CA	60.88	0.048	1
1	A	143	THR	CB	71.774	0.029	1
1	A	143	THR	N	115.997	0.043	1
1	A	144	ASP	H	8.129	0.004	1
1	A	144	ASP	HA	4.56	0.012	1
1	A	144	ASP	HB2	2.89	0.006	2
1	A	144	ASP	HB3	2.345	0.009	2
1	A	144	ASP	C	176.312	0.004	1
1	A	144	ASP	CA	52.461	0.014	1
1	A	144	ASP	CB	42.171	0.030	1
1	A	144	ASP	N	118.006	0.036	1
1	A	145	TRP	H	8.899	0.005	1
1	A	145	TRP	HA	4.234	0.005	1
1	A	145	TRP	HB2	2.947	0.008	2
1	A	145	TRP	HB3	2.754	0.017	2
1	A	145	TRP	HE1	10.069	0.002	1
1	A	145	TRP	C	176.589	0.003	1
1	A	145	TRP	CA	58.57	0.017	1
1	A	145	TRP	CB	30.773	0.012	1
1	A	145	TRP	N	120.338	0.023	1
1	A	145	TRP	NE1	129.644	0.012	1
1	A	146	VAL	H	9.744	0.005	1
1	A	146	VAL	HA	3.867	0.012	1
1	A	146	VAL	HB	1.794	0.010	1
1	A	146	VAL	HG11	0.512	0.005	1
1	A	146	VAL	HG12	0.512	0.005	1
1	A	146	VAL	HG13	0.512	0.005	1
1	A	146	VAL	HG21	-0.405	0.005	1
1	A	146	VAL	HG22	-0.405	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	VAL	HG23	-0.405	0.005	1
1	A	146	VAL	C	174.756	0.024	1
1	A	146	VAL	CA	61.919	0.051	1
1	A	146	VAL	CB	34.278	0.032	1
1	A	146	VAL	CG1	19.754	0.023	2
1	A	146	VAL	CG2	19.999	0.135	2
1	A	146	VAL	N	127.304	0.027	1
1	A	147	GLN	H	8.365	0.004	1
1	A	147	GLN	HA	4.426	0.008	1
1	A	147	GLN	HB2	1.922	0.005	2
1	A	147	GLN	HB3	2.06	0.018	2
1	A	147	GLN	HG2	2.281	0.000	2
1	A	147	GLN	C	175.09	0.018	1
1	A	147	GLN	CA	54.936	0.101	1
1	A	147	GLN	CB	30.23	0.049	1
1	A	147	GLN	CG	34.13	0.000	1
1	A	147	GLN	N	125.222	0.020	1
1	A	148	TRP	H	8.543	0.009	1
1	A	148	TRP	HA	5.112	0.009	1
1	A	148	TRP	HB2	3.389	0.007	2
1	A	148	TRP	HB3	3.596	0.003	2
1	A	148	TRP	HE1	9.578	0.002	1
1	A	148	TRP	C	175.563	0.025	1
1	A	148	TRP	CA	55.968	0.050	1
1	A	148	TRP	CB	31.48	0.020	1
1	A	148	TRP	N	127.821	0.043	1
1	A	148	TRP	NE1	123.327	0.024	1
1	A	149	ASN	H	8.713	0.005	1
1	A	149	ASN	HA	5.038	0.004	1
1	A	149	ASN	HB2	2.908	0.002	2
1	A	149	ASN	HB3	2.795	0.004	2
1	A	149	ASN	C	174.876	0.008	1
1	A	149	ASN	CA	53.661	0.064	1
1	A	149	ASN	CB	40.307	0.030	1
1	A	149	ASN	N	119.025	0.022	1
1	A	150	ARG	H	9.112	0.007	1
1	A	150	ARG	HA	4.631	0.004	1
1	A	150	ARG	HB2	1.81	0.027	2
1	A	150	ARG	HB3	2.219	0.008	2
1	A	150	ARG	HD2	3.297	0.000	1
1	A	150	ARG	C	177.175	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	150	ARG	CA	55.842	0.033	1
1	A	150	ARG	CB	33.177	0.015	1
1	A	150	ARG	CD	43.126	0.000	1
1	A	150	ARG	CG	27.933	0.000	1
1	A	150	ARG	N	123.518	0.040	1
1	A	151	LEU	H	8.66	0.007	1
1	A	151	LEU	HA	4.302	0.003	1
1	A	151	LEU	HB2	1.661	0.022	2
1	A	151	LEU	HB3	1.706	0.005	2
1	A	151	LEU	HD11	0.933	0.006	1
1	A	151	LEU	HD12	0.933	0.006	1
1	A	151	LEU	HD13	0.933	0.006	1
1	A	151	LEU	HD21	0.897	0.000	1
1	A	151	LEU	HD22	0.897	0.000	1
1	A	151	LEU	HD23	0.897	0.000	1
1	A	151	LEU	C	177.327	0.002	1
1	A	151	LEU	CA	56.419	0.045	1
1	A	151	LEU	CB	42.033	0.041	1
1	A	151	LEU	CD1	24.903	0.031	2
1	A	151	LEU	CD2	23.529	0.022	2
1	A	151	LEU	CG	27.136	0.000	1
1	A	151	LEU	N	122.678	0.016	1
1	A	152	ASP	H	8.395	0.004	1
1	A	152	ASP	HA	4.501	0.012	1
1	A	152	ASP	HB2	2.9	0.004	2
1	A	152	ASP	HB3	2.62	0.012	2
1	A	152	ASP	C	175.887	0.047	1
1	A	152	ASP	CA	53.992	0.064	1
1	A	152	ASP	CB	39.922	0.047	1
1	A	152	ASP	N	116.29	0.034	1
1	A	153	GLU	H	7.579	0.007	1
1	A	153	GLU	HA	4.693	0.009	1
1	A	153	GLU	HB2	1.915	0.001	2
1	A	153	GLU	HB3	2.176	0.007	2
1	A	153	GLU	HG2	2.349	0.000	2
1	A	153	GLU	C	175.983	0.005	1
1	A	153	GLU	CA	55.562	0.016	1
1	A	153	GLU	CB	31.059	0.036	1
1	A	153	GLU	CG	35.651	0.000	1
1	A	153	GLU	N	118.301	0.024	1
1	A	154	ASP	H	8.604	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	154	ASP	HA	4.609	0.007	1
1	A	154	ASP	HB2	2.75	0.012	2
1	A	154	ASP	HB3	2.665	0.008	2
1	A	154	ASP	C	176.511	0.007	1
1	A	154	ASP	CA	55.586	0.041	1
1	A	154	ASP	CB	41.487	0.019	1
1	A	154	ASP	N	121.185	0.036	1
1	A	155	GLU	H	7.994	0.004	1
1	A	155	GLU	HA	4.441	0.003	1
1	A	155	GLU	HB2	1.899	0.011	2
1	A	155	GLU	HG2	2.211	0.000	2
1	A	155	GLU	C	175.544	0.004	1
1	A	155	GLU	CA	55.672	0.027	1
1	A	155	GLU	CB	31.416	0.056	1
1	A	155	GLU	CG	36.216	0.000	1
1	A	155	GLU	N	118.937	0.020	1
1	A	156	GLN	H	8.493	0.008	1
1	A	156	GLN	HA	4.505	0.012	1
1	A	156	GLN	HB2	2.411	0.000	2
1	A	156	GLN	HB3	1.862	0.012	2
1	A	156	GLN	HG2	2.532	0.000	2
1	A	156	GLN	C	175.989	0.020	1
1	A	156	GLN	CA	55.312	0.061	1
1	A	156	GLN	CB	29.13	0.018	1
1	A	156	GLN	CG	33.337	0.000	1
1	A	156	GLN	N	119.731	0.024	1
1	A	157	TYR	H	9.164	0.006	1
1	A	157	TYR	HA	5.356	0.011	1
1	A	157	TYR	HB2	2.33	0.010	2
1	A	157	TYR	HB3	2.223	0.014	2
1	A	157	TYR	C	175.707	0.013	1
1	A	157	TYR	CA	57.325	0.017	1
1	A	157	TYR	CB	41.263	0.016	1
1	A	157	TYR	N	122.406	0.018	1
1	A	158	ARG	H	8.965	0.003	1
1	A	158	ARG	HA	5.811	0.005	1
1	A	158	ARG	HB2	1.702	0.014	2
1	A	158	ARG	HB3	1.488	0.010	2
1	A	158	ARG	HD2	2.663	0.000	2
1	A	158	ARG	HD3	2.226	0.000	2
1	A	158	ARG	HG2	1.231	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	158	ARG	C	174.891	0.006	1
1	A	158	ARG	CA	54.068	0.008	1
1	A	158	ARG	CB	34.52	0.022	1
1	A	158	ARG	CD	43.899	0.000	1
1	A	158	ARG	CG	25.392	0.000	1
1	A	158	ARG	N	115.829	0.018	1
1	A	159	GLY	H	9.07	0.004	1
1	A	159	GLY	HA2	5.827	0.007	2
1	A	159	GLY	HA3	3.495	0.007	2
1	A	159	GLY	C	171.33	0.010	1
1	A	159	GLY	CA	44.839	0.056	1
1	A	159	GLY	N	106.842	0.032	1
1	A	160	ARG	H	7.874	0.005	1
1	A	160	ARG	HA	4.307	0.006	1
1	A	160	ARG	HB2	1.138	0.012	2
1	A	160	ARG	HB3	1.051	0.000	2
1	A	160	ARG	HD2	1.988	0.000	1
1	A	160	ARG	HG2	0.428	0.000	2
1	A	160	ARG	C	175.001	0.012	1
1	A	160	ARG	CA	55.569	0.070	1
1	A	160	ARG	CB	33.409	0.019	1
1	A	160	ARG	CD	42.812	0.000	1
1	A	160	ARG	CG	27.094	0.000	1
1	A	160	ARG	N	119.297	0.023	1
1	A	161	TYR	H	7.898	0.004	1
1	A	161	TYR	HA	5.448	0.012	1
1	A	161	TYR	HB2	2.784	0.012	2
1	A	161	TYR	C	173.839	0.006	1
1	A	161	TYR	CA	57.962	0.041	1
1	A	161	TYR	CB	42.836	0.016	1
1	A	161	TYR	N	118.655	0.061	1
1	A	162	GLN	H	9.666	0.004	1
1	A	162	GLN	HA	5.654	0.009	1
1	A	162	GLN	HB2	2.145	0.013	2
1	A	162	GLN	HG2	2.395	0.000	2
1	A	162	GLN	C	175.568	0.005	1
1	A	162	GLN	CA	54.587	0.035	1
1	A	162	GLN	CB	32.358	0.037	1
1	A	162	GLN	CG	33.987	0.000	1
1	A	162	GLN	N	122.082	0.015	1
1	A	163	ILE	H	9.36	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	163	ILE	HA	5.395	0.011	1
1	A	163	ILE	HB	1.714	0.007	1
1	A	163	ILE	HD11	0.87	0.022	1
1	A	163	ILE	HD12	0.87	0.022	1
1	A	163	ILE	HD13	0.87	0.022	1
1	A	163	ILE	HG12	1.264	0.010	2
1	A	163	ILE	HG13	1.602	0.000	2
1	A	163	ILE	HG21	0.934	0.015	1
1	A	163	ILE	HG22	0.934	0.015	1
1	A	163	ILE	HG23	0.934	0.015	1
1	A	163	ILE	C	174.202	0.006	1
1	A	163	ILE	CA	59.855	0.042	1
1	A	163	ILE	CB	40.709	0.015	1
1	A	163	ILE	CD1	14.69	0.079	1
1	A	163	ILE	CG1	28.905	0.000	1
1	A	163	ILE	CG2	17.401	0.010	1
1	A	163	ILE	N	130.785	0.046	1
1	A	164	SER	H	9.019	0.005	1
1	A	164	SER	HA	5.988	0.004	1
1	A	164	SER	HB2	3.991	0.013	2
1	A	164	SER	HB3	3.871	0.014	2
1	A	164	SER	C	173.19	0.006	1
1	A	164	SER	CA	56.479	0.028	1
1	A	164	SER	CB	66.996	0.054	1
1	A	164	SER	N	119.675	0.022	1
1	A	165	VAL	H	8.203	0.005	1
1	A	165	VAL	HA	5.344	0.007	1
1	A	165	VAL	HB	2.15	0.005	1
1	A	165	VAL	HG11	1.295	0.005	1
1	A	165	VAL	HG12	1.295	0.005	1
1	A	165	VAL	HG13	1.295	0.005	1
1	A	165	VAL	HG21	0.974	0.011	1
1	A	165	VAL	HG22	0.974	0.011	1
1	A	165	VAL	HG23	0.974	0.011	1
1	A	165	VAL	C	175.321	0.006	1
1	A	165	VAL	CA	61.217	0.038	1
1	A	165	VAL	CB	35.092	0.157	1
1	A	165	VAL	CG1	23.845	0.057	2
1	A	165	VAL	CG2	22.491	0.029	2
1	A	165	VAL	N	120.811	0.028	1
1	A	166	LYS	H	8.958	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	166	LYS	HA	5.019	0.000	1
1	A	166	LYS	HB2	1.792	0.000	2
1	A	166	LYS	C	172.959	0.000	1
1	A	166	LYS	CA	52.997	0.000	1
1	A	166	LYS	N	127.55	0.025	1
1	A	167	PRO	HA	4.563	0.007	1
1	A	167	PRO	HB2	1.977	0.000	2
1	A	167	PRO	HB3	2.367	0.001	2
1	A	167	PRO	HD2	3.747	0.000	2
1	A	167	PRO	HD3	3.747	0.000	2
1	A	167	PRO	HG2	2.097	0.000	2
1	A	167	PRO	C	176.787	0.002	1
1	A	167	PRO	CA	63.2	0.022	1
1	A	167	PRO	CB	32.396	0.059	1
1	A	167	PRO	CD	50.841	0.000	1
1	A	167	PRO	CG	27.521	0.000	1
1	A	168	GLN	H	8.398	0.003	1
1	A	168	GLN	HA	4.42	0.007	1
1	A	168	GLN	HB2	1.784	0.004	2
1	A	168	GLN	HB3	1.669	0.029	2
1	A	168	GLN	HG2	2.149	0.000	2
1	A	168	GLN	HG3	1.976	0.000	2
1	A	168	GLN	C	175.27	0.001	1
1	A	168	GLN	CA	55.114	0.023	1
1	A	168	GLN	CB	30.023	0.071	1
1	A	168	GLN	CG	33.974	0.000	1
1	A	168	GLN	N	124.276	0.020	1
1	A	169	GLY	H	8.823	0.007	1
1	A	169	GLY	HA2	4.003	0.011	2
1	A	169	GLY	HA3	3.527	0.002	2
1	A	169	GLY	C	174.99	0.000	1
1	A	169	GLY	CA	46.96	0.044	1
1	A	169	GLY	N	116.253	0.036	1
1	A	170	TYR	H	8.687	0.006	1
1	A	170	TYR	HA	4.698	0.004	1
1	A	170	TYR	HB2	3.274	0.008	2
1	A	170	TYR	HB3	3.018	0.009	2
1	A	170	TYR	C	175.14	0.000	1
1	A	170	TYR	CA	58.149	0.039	1
1	A	170	TYR	CB	37.794	0.060	1
1	A	170	TYR	N	126.113	0.036	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	171	GLN	H	7.795	0.004	1
1	A	171	GLN	HA	4.78	0.006	1
1	A	171	GLN	HB2	2.007	0.007	2
1	A	171	GLN	HB3	2.104	0.011	2
1	A	171	GLN	C	174.856	0.003	1
1	A	171	GLN	CA	54.785	0.049	1
1	A	171	GLN	CB	32.019	0.081	1
1	A	171	GLN	CG	34.78	0.000	1
1	A	171	GLN	N	118.915	0.023	1
1	A	172	GLN	H	8.615	0.004	1
1	A	172	GLN	HA	4.666	0.004	1
1	A	172	GLN	HB2	1.933	0.055	2
1	A	172	GLN	HB3	1.655	0.002	2
1	A	172	GLN	HG2	2.208	0.000	2
1	A	172	GLN	C	173.41	0.008	1
1	A	172	GLN	CA	55.02	0.068	1
1	A	172	GLN	CB	32.448	0.075	1
1	A	172	GLN	CG	33.965	0.000	1
1	A	172	GLN	N	118.647	0.043	1
1	A	173	ALA	H	9.123	0.008	1
1	A	173	ALA	HA	5.329	0.008	1
1	A	173	ALA	HB1	1.177	0.007	1
1	A	173	ALA	HB2	1.177	0.007	1
1	A	173	ALA	HB3	1.177	0.007	1
1	A	173	ALA	C	177.131	0.006	1
1	A	173	ALA	CA	50.489	0.021	1
1	A	173	ALA	CB	20.898	0.021	1
1	A	173	ALA	N	123.587	0.038	1
1	A	174	VAL	H	9.316	0.008	1
1	A	174	VAL	HA	4.914	0.009	1
1	A	174	VAL	HB	2.186	0.008	1
1	A	174	VAL	HG11	0.939	0.005	1
1	A	174	VAL	HG12	0.939	0.005	1
1	A	174	VAL	HG13	0.939	0.005	1
1	A	174	VAL	C	175.531	0.010	1
1	A	174	VAL	CA	61.139	0.061	1
1	A	174	VAL	CB	32.629	0.035	1
1	A	174	VAL	CG1	21.259	0.018	2
1	A	174	VAL	N	125.348	0.033	1
1	A	175	THR	H	9.407	0.005	1
1	A	175	THR	HA	4.997	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	175	THR	HB	3.992	0.011	1
1	A	175	THR	HG21	1.105	0.004	1
1	A	175	THR	HG22	1.105	0.004	1
1	A	175	THR	HG23	1.105	0.004	1
1	A	175	THR	C	173.26	0.006	1
1	A	175	THR	CA	61.759	0.047	1
1	A	175	THR	CB	70.532	0.088	1
1	A	175	THR	CG2	21.651	0.056	1
1	A	175	THR	N	122.067	0.024	1
1	A	176	VAL	H	9.242	0.005	1
1	A	176	VAL	HA	4.525	0.009	1
1	A	176	VAL	HB	2.137	0.008	1
1	A	176	VAL	HG11	1.069	0.012	1
1	A	176	VAL	HG12	1.069	0.012	1
1	A	176	VAL	HG13	1.069	0.012	1
1	A	176	VAL	HG21	0.898	0.011	1
1	A	176	VAL	HG22	0.898	0.011	1
1	A	176	VAL	HG23	0.898	0.011	1
1	A	176	VAL	C	173.052	0.002	1
1	A	176	VAL	CA	61.377	0.067	1
1	A	176	VAL	CB	34.656	0.034	1
1	A	176	VAL	CG1	22.6	0.043	2
1	A	176	VAL	CG2	22.557	0.000	2
1	A	176	VAL	N	126.281	0.018	1
1	A	177	LYS	H	9.333	0.006	1
1	A	177	LYS	HA	5.349	0.010	1
1	A	177	LYS	HB2	1.97	0.014	2
1	A	177	LYS	HB3	1.621	0.008	2
1	A	177	LYS	HD2	1.24	0.000	2
1	A	177	LYS	HE2	2.87	0.000	2
1	A	177	LYS	HG2	1.059	0.000	2
1	A	177	LYS	C	175.486	0.007	1
1	A	177	LYS	CA	54.121	0.062	1
1	A	177	LYS	CB	35.987	0.061	1
1	A	177	LYS	CD	29.613	0.000	1
1	A	177	LYS	CE	42.207	0.000	1
1	A	177	LYS	CG	25.178	0.000	1
1	A	177	LYS	N	128.215	0.022	1
1	A	178	LEU	H	9.388	0.006	1
1	A	178	LEU	HA	4.154	0.007	1
1	A	178	LEU	HB2	1.904	0.004	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	178	LEU	HB3	1.295	0.008	2
1	A	178	LEU	HD11	1.034	0.011	1
1	A	178	LEU	HD12	1.034	0.011	1
1	A	178	LEU	HD13	1.034	0.011	1
1	A	178	LEU	HD21	0.639	0.008	1
1	A	178	LEU	HD22	0.639	0.008	1
1	A	178	LEU	HD23	0.639	0.008	1
1	A	178	LEU	HG	1.306	0.013	1
1	A	178	LEU	C	174.386	0.003	1
1	A	178	LEU	CA	54.235	0.034	1
1	A	178	LEU	CB	43.256	0.069	1
1	A	178	LEU	CD1	29.103	0.078	2
1	A	178	LEU	CD2	23.91	0.043	2
1	A	178	LEU	CG	27.13	0.021	1
1	A	178	LEU	N	130.385	0.041	1
1	A	179	LEU	H	8.583	0.006	1
1	A	179	LEU	HA	4.039	0.010	1
1	A	179	LEU	HB2	1.301	0.023	2
1	A	179	LEU	HD11	0.727	0.014	1
1	A	179	LEU	HD12	0.727	0.014	1
1	A	179	LEU	HD13	0.727	0.014	1
1	A	179	LEU	HD21	0.748	0.001	1
1	A	179	LEU	HD22	0.748	0.001	1
1	A	179	LEU	HD23	0.748	0.001	1
1	A	179	LEU	HG	1.53	0.019	1
1	A	179	LEU	C	177.325	0.011	1
1	A	179	LEU	CA	56.198	0.035	1
1	A	179	LEU	CB	43.146	0.056	1
1	A	179	LEU	CD1	21.739	0.012	2
1	A	179	LEU	CD2	26.247	0.018	2
1	A	179	LEU	CG	26.267	0.000	1
1	A	179	LEU	N	126.992	0.039	1
1	A	180	ASN	H	6.876	0.004	1
1	A	180	ASN	HA	4.825	0.006	1
1	A	180	ASN	HB2	3.015	0.003	2
1	A	180	ASN	HB3	1.954	0.005	2
1	A	180	ASN	C	171.455	0.005	1
1	A	180	ASN	CA	53.763	0.034	1
1	A	180	ASN	CB	44.761	0.057	1
1	A	180	ASN	N	110.418	0.046	1
1	A	181	LEU	H	9.096	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	181	LEU	HA	5.44	0.012	1
1	A	181	LEU	HB2	1.375	0.014	2
1	A	181	LEU	HB3	2.344	0.004	2
1	A	181	LEU	HD11	0.899	0.013	1
1	A	181	LEU	HD12	0.899	0.013	1
1	A	181	LEU	HD13	0.899	0.013	1
1	A	181	LEU	C	174.44	0.006	1
1	A	181	LEU	CA	54.137	0.016	1
1	A	181	LEU	CB	46.051	0.017	1
1	A	181	LEU	CD1	26.746	0.042	2
1	A	181	LEU	CD2	22.023	0.000	2
1	A	181	LEU	N	125.221	0.033	1
1	A	182	GLU	H	9.335	0.005	1
1	A	182	GLU	HA	5.212	0.008	1
1	A	182	GLU	HB2	1.417	0.015	2
1	A	182	GLU	HG2	2.027	0.000	2
1	A	182	GLU	HG3	1.768	0.000	2
1	A	182	GLU	C	174.426	0.005	1
1	A	182	GLU	CA	54.291	0.035	1
1	A	182	GLU	CB	35.539	0.007	1
1	A	182	GLU	CG	36.103	0.000	1
1	A	182	GLU	N	125.256	0.043	1
1	A	183	GLN	H	8.672	0.004	1
1	A	183	GLN	HA	4.255	0.011	1
1	A	183	GLN	HB2	1.684	0.007	2
1	A	183	GLN	HB3	0.933	0.023	2
1	A	183	GLN	HG2	1.395	0.000	2
1	A	183	GLN	C	175.365	0.011	1
1	A	183	GLN	CA	54.826	0.035	1
1	A	183	GLN	CB	31.259	0.019	1
1	A	183	GLN	CG	33.469	0.000	1
1	A	183	GLN	N	121.405	0.033	1
1	A	184	ALA	H	8.953	0.005	1
1	A	184	ALA	HA	3.909	0.008	1
1	A	184	ALA	HB1	1.263	0.009	1
1	A	184	ALA	HB2	1.263	0.009	1
1	A	184	ALA	HB3	1.263	0.009	1
1	A	184	ALA	C	177.05	0.005	1
1	A	184	ALA	CA	53.043	0.002	1
1	A	184	ALA	CB	17.348	0.020	1
1	A	184	ALA	N	132.33	0.046	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	185	GLY	H	8.483	0.005	1
1	A	185	GLY	HA2	3.909	0.009	2
1	A	185	GLY	HA3	3.453	0.004	2
1	A	185	GLY	C	173.659	0.003	1
1	A	185	GLY	CA	45.264	0.016	1
1	A	185	GLY	N	103.196	0.019	1
1	A	186	LYS	H	7.735	0.003	1
1	A	186	LYS	HA	4.87	0.000	1
1	A	186	LYS	HB2	1.804	0.000	2
1	A	186	LYS	C	173.586	0.000	1
1	A	186	LYS	CA	52.776	0.000	1
1	A	186	LYS	CB	33.437	0.000	1
1	A	186	LYS	N	121.425	0.021	1
1	A	187	PRO	HA	4.813	0.004	1
1	A	187	PRO	HB2	1.989	0.004	2
1	A	187	PRO	HB3	2.482	0.001	2
1	A	187	PRO	HD2	3.954	0.000	2
1	A	187	PRO	HD3	3.724	0.000	2
1	A	187	PRO	HG2	2.183	0.000	2
1	A	187	PRO	C	176.911	0.003	1
1	A	187	PRO	CA	63.291	0.023	1
1	A	187	PRO	CB	32.502	0.040	1
1	A	187	PRO	CD	50.808	0.000	1
1	A	187	PRO	CG	27.659	0.000	1
1	A	188	VAL	H	8.444	0.004	1
1	A	188	VAL	HA	4.353	0.009	1
1	A	188	VAL	HB	1.966	0.011	1
1	A	188	VAL	HG11	1.202	0.005	1
1	A	188	VAL	HG12	1.202	0.005	1
1	A	188	VAL	HG13	1.202	0.005	1
1	A	188	VAL	HG21	1.046	0.007	1
1	A	188	VAL	HG22	1.046	0.007	1
1	A	188	VAL	HG23	1.046	0.007	1
1	A	188	VAL	C	175.009	0.003	1
1	A	188	VAL	CA	61.773	0.171	1
1	A	188	VAL	CB	34.992	0.008	1
1	A	188	VAL	CG1	23.081	0.017	2
1	A	188	VAL	CG2	21.244	0.022	2
1	A	188	VAL	N	122.572	0.027	1
1	A	189	ALA	H	8.774	0.003	1
1	A	189	ALA	HA	4.859	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	189	ALA	HB1	1.392	0.008	1
1	A	189	ALA	HB2	1.392	0.008	1
1	A	189	ALA	HB3	1.392	0.008	1
1	A	189	ALA	C	176.535	0.006	1
1	A	189	ALA	CA	51.222	0.056	1
1	A	189	ALA	CB	20.428	0.038	1
1	A	189	ALA	N	126.344	0.022	1
1	A	190	ASP	H	7.688	0.007	1
1	A	190	ASP	HA	4.588	0.005	1
1	A	190	ASP	HB2	2.684	0.020	2
1	A	190	ASP	HB3	2.836	0.020	2
1	A	190	ASP	C	175.957	0.006	1
1	A	190	ASP	CA	54.217	0.048	1
1	A	190	ASP	CB	42.294	0.018	1
1	A	190	ASP	N	118.752	0.022	1
1	A	191	ALA	H	8.811	0.007	1
1	A	191	ALA	HA	4.058	0.002	1
1	A	191	ALA	HB1	1.426	0.021	1
1	A	191	ALA	HB2	1.426	0.021	1
1	A	191	ALA	HB3	1.426	0.021	1
1	A	191	ALA	C	179.788	0.004	1
1	A	191	ALA	CA	55.681	0.054	1
1	A	191	ALA	CB	18.751	0.079	1
1	A	191	ALA	N	126.914	0.024	1
1	A	192	ALA	H	8.442	0.004	1
1	A	192	ALA	HA	4.134	0.008	1
1	A	192	ALA	HB1	1.494	0.009	1
1	A	192	ALA	HB2	1.494	0.009	1
1	A	192	ALA	HB3	1.494	0.009	1
1	A	192	ALA	C	181.54	0.004	1
1	A	192	ALA	CA	55.457	0.065	1
1	A	192	ALA	CB	17.893	0.026	1
1	A	192	ALA	N	120.144	0.025	1
1	A	193	SER	H	8.11	0.006	1
1	A	193	SER	HA	4.134	0.018	1
1	A	193	SER	HB2	3.882	0.000	2
1	A	193	SER	HB3	3.714	0.000	2
1	A	193	SER	C	175.851	0.011	1
1	A	193	SER	CA	62.489	0.064	1
1	A	193	SER	N	117.567	0.034	1
1	A	194	MET	H	8.143	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	194	MET	HA	4.073	0.002	1
1	A	194	MET	HB2	2.199	0.000	2
1	A	194	MET	HB3	1.701	0.003	2
1	A	194	MET	HG2	2.609	0.000	2
1	A	194	MET	HG3	2.311	0.000	2
1	A	194	MET	C	178.206	0.011	1
1	A	194	MET	CA	58.579	0.040	1
1	A	194	MET	CB	31.52	0.024	1
1	A	194	MET	CG	32.596	0.000	1
1	A	194	MET	N	120.436	0.048	1
1	A	195	GLN	H	8.294	0.004	1
1	A	195	GLN	HA	4.26	0.005	1
1	A	195	GLN	HB2	2.082	0.008	2
1	A	195	GLN	HB3	2.198	0.000	2
1	A	195	GLN	HG2	2.398	0.000	2
1	A	195	GLN	C	178.952	0.010	1
1	A	195	GLN	CA	58.313	0.135	1
1	A	195	GLN	CB	28.701	0.046	1
1	A	195	GLN	CG	34.148	0.000	1
1	A	195	GLN	N	119.482	0.026	1
1	A	196	ARG	H	7.908	0.005	1
1	A	196	ARG	HA	3.772	0.012	1
1	A	196	ARG	HB2	1.764	0.025	2
1	A	196	ARG	HB3	1.517	0.003	2
1	A	196	ARG	HD2	2.744	0.001	2
1	A	196	ARG	HD3	2.66	0.001	2
1	A	196	ARG	HG2	0.981	0.009	2
1	A	196	ARG	HG3	0.186	0.006	2
1	A	196	ARG	C	178.897	0.011	1
1	A	196	ARG	CA	59.44	0.022	1
1	A	196	ARG	CB	29.598	0.017	1
1	A	196	ARG	CD	43.106	0.034	1
1	A	196	ARG	CG	26.032	0.000	1
1	A	196	ARG	N	120.484	0.061	1
1	A	197	TYR	H	8.003	0.005	1
1	A	197	TYR	HA	3.986	0.010	1
1	A	197	TYR	HB2	2.939	0.005	2
1	A	197	TYR	HB3	2.61	0.024	2
1	A	197	TYR	C	179.638	0.010	1
1	A	197	TYR	CA	63.273	0.049	1
1	A	197	TYR	CB	37.858	0.038	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	197	TYR	N	113.819	0.049	1
1	A	198	SER	H	8.94	0.005	1
1	A	198	SER	HA	4.52	0.006	1
1	A	198	SER	HB2	3.955	0.032	2
1	A	198	SER	C	176.005	0.025	1
1	A	198	SER	CA	63.001	0.121	1
1	A	198	SER	CB	62.039	0.075	1
1	A	198	SER	N	125.293	0.046	1
1	A	199	THR	H	7.899	0.004	1
1	A	199	THR	HA	3.634	0.014	1
1	A	199	THR	HG21	1.141	0.000	1
1	A	199	THR	HG22	1.141	0.000	1
1	A	199	THR	HG23	1.141	0.000	1
1	A	199	THR	C	175.829	0.010	1
1	A	199	THR	CA	67.188	0.029	1
1	A	199	THR	CB	68.203	0.095	1
1	A	199	THR	N	120.88	0.047	1
1	A	200	GLU	H	7.927	0.004	1
1	A	200	GLU	HA	3.703	0.005	1
1	A	200	GLU	HB2	1.234	0.005	2
1	A	200	GLU	HB3	0.843	0.019	2
1	A	200	GLU	HG2	1.239	0.000	2
1	A	200	GLU	C	178.457	0.002	1
1	A	200	GLU	CA	59.532	0.058	1
1	A	200	GLU	CB	28.849	0.028	1
1	A	200	GLU	CG	34.017	0.000	1
1	A	200	GLU	N	120.155	0.036	1
1	A	201	MET	H	6.434	0.003	1
1	A	201	MET	HA	4.726	0.010	1
1	A	201	MET	HB2	1.902	0.007	2
1	A	201	MET	HE1	1.53	0.000	1
1	A	201	MET	HE2	1.53	0.000	1
1	A	201	MET	HE3	1.53	0.000	1
1	A	201	MET	HG2	2.178	0.000	2
1	A	201	MET	C	177.337	0.016	1
1	A	201	MET	CA	56.677	0.025	1
1	A	201	MET	CB	32.908	0.023	1
1	A	201	MET	CG	32.936	0.000	1
1	A	201	MET	N	114.972	0.019	1
1	A	202	MET	H	7.834	0.004	1
1	A	202	MET	HA	4.12	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	202	MET	HB2	1.779	0.023	2
1	A	202	MET	HB3	2.397	0.000	2
1	A	202	MET	C	177.685	0.004	1
1	A	202	MET	CA	58.666	0.031	1
1	A	202	MET	CB	33.225	0.062	1
1	A	202	MET	CG	32.494	0.000	1
1	A	202	MET	N	121.002	0.029	1
1	A	203	ASN	H	8.782	0.004	1
1	A	203	ASN	HA	4.489	0.013	1
1	A	203	ASN	HB2	2.799	0.003	2
1	A	203	ASN	HB3	2.924	0.009	2
1	A	203	ASN	C	178.569	0.008	1
1	A	203	ASN	CA	55.4	0.018	1
1	A	203	ASN	CB	37.322	0.045	1
1	A	203	ASN	N	117.856	0.031	1
1	A	204	VAL	H	7.558	0.006	1
1	A	204	VAL	HA	3.771	0.007	1
1	A	204	VAL	HB	2.714	0.010	1
1	A	204	VAL	HG11	1.526	0.004	1
1	A	204	VAL	HG12	1.526	0.004	1
1	A	204	VAL	HG13	1.526	0.004	1
1	A	204	VAL	HG21	1.082	0.007	1
1	A	204	VAL	HG22	1.082	0.007	1
1	A	204	VAL	HG23	1.082	0.007	1
1	A	204	VAL	C	178.875	0.023	1
1	A	204	VAL	CA	66.679	0.074	1
1	A	204	VAL	CB	32.024	0.013	1
1	A	204	VAL	CG1	23.039	0.017	2
1	A	204	VAL	CG2	21.357	0.027	2
1	A	204	VAL	N	122.352	0.036	1
1	A	205	ILE	H	7.719	0.011	1
1	A	205	ILE	HA	3.648	0.006	1
1	A	205	ILE	HB	1.993	0.006	1
1	A	205	ILE	HD11	0.797	0.012	1
1	A	205	ILE	HD12	0.797	0.012	1
1	A	205	ILE	HD13	0.797	0.012	1
1	A	205	ILE	HG12	0.921	0.003	2
1	A	205	ILE	HG13	1.796	0.006	2
1	A	205	ILE	HG21	0.807	0.002	1
1	A	205	ILE	HG22	0.807	0.002	1
1	A	205	ILE	HG23	0.807	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	205	ILE	C	177.357	0.008	1
1	A	205	ILE	CA	65.304	0.038	1
1	A	205	ILE	CB	37.762	0.020	1
1	A	205	ILE	CD1	13.882	0.025	1
1	A	205	ILE	CG1	29.167	0.057	1
1	A	205	ILE	CG2	17.601	0.027	1
1	A	205	ILE	N	120.076	0.059	1
1	A	206	SER	H	9.106	0.006	1
1	A	206	SER	HA	3.886	0.008	1
1	A	206	SER	HB2	3.952	0.001	2
1	A	206	SER	C	177.173	0.000	1
1	A	206	SER	CA	61.737	0.075	1
1	A	206	SER	CB	62.904	0.023	1
1	A	206	SER	N	114.509	0.048	1
1	A	207	ALA	H	7.927	0.004	1
1	A	207	ALA	HA	4.233	0.009	1
1	A	207	ALA	HB1	1.509	0.005	1
1	A	207	ALA	HB2	1.509	0.005	1
1	A	207	ALA	HB3	1.509	0.005	1
1	A	207	ALA	C	180.475	0.026	1
1	A	207	ALA	CA	54.729	0.085	1
1	A	207	ALA	CB	18.163	0.030	1
1	A	207	ALA	N	121.636	0.028	1
1	A	208	GLY	H	7.876	0.005	1
1	A	208	GLY	HA2	4.063	0.006	2
1	A	208	GLY	HA3	3.672	0.001	2
1	A	208	GLY	C	175.632	0.000	1
1	A	208	GLY	CA	46.617	0.011	1
1	A	208	GLY	N	105.33	0.045	1
1	A	209	LEU	H	8.148	0.004	1
1	A	209	LEU	HA	4.187	0.007	1
1	A	209	LEU	HB2	1.872	0.008	2
1	A	209	LEU	HB3	1.459	0.008	2
1	A	209	LEU	HD11	0.675	0.001	1
1	A	209	LEU	HD12	0.675	0.001	1
1	A	209	LEU	HD13	0.675	0.001	1
1	A	209	LEU	HD21	0.724	0.000	1
1	A	209	LEU	HD22	0.724	0.000	1
1	A	209	LEU	HD23	0.724	0.000	1
1	A	209	LEU	HG	1.945	0.001	1
1	A	209	LEU	C	178.336	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	209	LEU	CA	56.194	0.000	1
1	A	209	LEU	CB	41.727	0.012	1
1	A	209	LEU	CD1	22.423	0.065	2
1	A	209	LEU	CD2	25.936	0.000	2
1	A	209	LEU	CG	26.232	0.071	1
1	A	209	LEU	N	122.005	0.030	1
1	A	210	ASP	H	7.959	0.004	1
1	A	210	ASP	HA	4.524	0.006	1
1	A	210	ASP	HB2	2.747	0.016	2
1	A	210	ASP	C	177.376	0.008	1
1	A	210	ASP	CA	55.628	0.000	1
1	A	210	ASP	CB	41.013	0.000	1
1	A	210	ASP	N	120.247	0.030	1
1	A	211	LYS	H	8.016	0.006	1
1	A	211	LYS	HA	4.264	0.008	1
1	A	211	LYS	HB2	1.935	0.000	2
1	A	211	LYS	HB3	1.844	0.009	2
1	A	211	LYS	HD2	1.728	0.000	2
1	A	211	LYS	HE2	3.035	0.000	2
1	A	211	LYS	HG2	1.502	0.000	2
1	A	211	LYS	C	177.422	0.016	1
1	A	211	LYS	CA	57.487	0.000	1
1	A	211	LYS	CB	32.556	0.054	1
1	A	211	LYS	CD	28.826	0.000	1
1	A	211	LYS	CE	42.255	0.000	1
1	A	211	LYS	CG	24.673	0.000	1
1	A	211	LYS	N	121.243	0.034	1
1	A	212	SER	H	8.182	0.007	1
1	A	212	SER	HA	4.353	0.010	1
1	A	212	SER	HB2	3.924	0.007	2
1	A	212	SER	C	175.476	0.014	1
1	A	212	SER	CA	59.723	0.028	1
1	A	212	SER	CB	63.537	0.076	1
1	A	212	SER	N	115.263	0.042	1
1	A	213	ALA	H	8.11	0.004	1
1	A	213	ALA	HA	4.341	0.004	1
1	A	213	ALA	HB1	1.488	0.008	1
1	A	213	ALA	HB2	1.488	0.008	1
1	A	213	ALA	HB3	1.488	0.008	1
1	A	213	ALA	C	178.973	0.008	1
1	A	213	ALA	CA	53.609	0.041	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	213	ALA	CB	19.002	0.064	1
1	A	213	ALA	N	125.141	0.037	1
1	A	214	THR	H	8.07	0.006	1
1	A	214	THR	HA	4.227	0.016	1
1	A	214	THR	HG21	1.234	0.000	1
1	A	214	THR	HG22	1.234	0.000	1
1	A	214	THR	HG23	1.234	0.000	1
1	A	214	THR	C	175.19	0.018	1
1	A	214	THR	CA	63.369	0.044	1
1	A	214	THR	CB	69.468	0.034	1
1	A	214	THR	CG2	21.73	0.000	1
1	A	214	THR	N	113.519	0.022	1
1	A	215	ASP	H	8.338	0.004	1
1	A	215	ASP	HA	4.545	0.003	1
1	A	215	ASP	HB2	2.697	0.005	2
1	A	215	ASP	C	177.347	0.021	1
1	A	215	ASP	CA	55.419	0.043	1
1	A	215	ASP	CB	40.855	0.031	1
1	A	215	ASP	N	122.82	0.018	1
1	A	216	ALA	H	8.141	0.004	1
1	A	216	ALA	HA	4.218	0.003	1
1	A	216	ALA	HB1	1.435	0.008	1
1	A	216	ALA	HB2	1.435	0.008	1
1	A	216	ALA	HB3	1.435	0.008	1
1	A	216	ALA	C	178.837	0.005	1
1	A	216	ALA	CA	53.715	0.089	1
1	A	216	ALA	CB	18.789	0.059	1
1	A	216	ALA	N	123.953	0.025	1
1	A	217	ALA	H	8.126	0.004	1
1	A	217	ALA	HA	4.232	0.008	1
1	A	217	ALA	HB1	1.437	0.008	1
1	A	217	ALA	HB2	1.437	0.008	1
1	A	217	ALA	HB3	1.437	0.008	1
1	A	217	ALA	C	178.723	0.007	1
1	A	217	ALA	CA	53.698	0.010	1
1	A	217	ALA	CB	18.666	0.005	1
1	A	217	ALA	N	121.836	0.033	1
1	A	218	ASN	H	8.134	0.003	1
1	A	218	ASN	HA	4.633	0.005	1
1	A	218	ASN	HB2	2.826	0.011	2
1	A	218	ASN	C	175.925	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	218	ASN	CA	53.891	0.040	1
1	A	218	ASN	CB	38.737	0.042	1
1	A	218	ASN	N	116.897	0.019	1
1	A	219	ALA	H	8.026	0.004	1
1	A	219	ALA	HA	4.25	0.007	1
1	A	219	ALA	HB1	1.439	0.007	1
1	A	219	ALA	HB2	1.439	0.007	1
1	A	219	ALA	HB3	1.439	0.007	1
1	A	219	ALA	C	178.35	0.002	1
1	A	219	ALA	CA	53.543	0.049	1
1	A	219	ALA	CB	18.891	0.015	1
1	A	219	ALA	N	123.635	0.017	1
1	A	220	ALA	H	8.079	0.004	1
1	A	220	ALA	HA	4.236	0.010	1
1	A	220	ALA	HB1	1.435	0.006	1
1	A	220	ALA	HB2	1.435	0.006	1
1	A	220	ALA	HB3	1.435	0.006	1
1	A	220	ALA	C	178.476	0.000	1
1	A	220	ALA	CA	53.343	0.042	1
1	A	220	ALA	CB	18.831	0.035	1
1	A	220	ALA	N	121.592	0.016	1
1	A	221	GLN	H	8.078	0.004	1
1	A	221	GLN	HA	4.261	0.004	1
1	A	221	GLN	HB2	2.12	0.008	2
1	A	221	GLN	HB3	2.03	0.002	2
1	A	221	GLN	HG2	2.406	0.000	2
1	A	221	GLN	C	176.228	0.023	1
1	A	221	GLN	CA	56.451	0.024	1
1	A	221	GLN	CB	29.152	0.028	1
1	A	221	GLN	CG	33.858	0.000	1
1	A	221	GLN	N	117.995	0.021	1
1	A	222	ASN	H	8.235	0.003	1
1	A	222	ASN	HA	4.693	0.006	1
1	A	222	ASN	HB2	2.873	0.000	2
1	A	222	ASN	HB3	2.781	0.000	2
1	A	222	ASN	C	175.442	0.017	1
1	A	222	ASN	CA	53.628	0.075	1
1	A	222	ASN	CB	38.801	0.017	1
1	A	222	ASN	N	118.899	0.029	1
1	A	223	ARG	H	8.162	0.020	1
1	A	223	ARG	HA	4.333	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	223	ARG	HB2	1.79	0.012	2
1	A	223	ARG	HB3	1.885	0.014	2
1	A	223	ARG	HD2	3.216	0.000	1
1	A	223	ARG	HG2	1.675	0.000	2
1	A	223	ARG	C	176.209	0.009	1
1	A	223	ARG	CA	56.452	0.040	1
1	A	223	ARG	CB	30.775	0.020	1
1	A	223	ARG	CD	43.445	0.000	1
1	A	223	ARG	CG	27.2	0.000	1
1	A	223	ARG	N	121.244	0.139	1
1	A	224	ALA	H	8.257	0.003	1
1	A	224	ALA	HA	4.368	0.012	1
1	A	224	ALA	HB1	1.43	0.004	1
1	A	224	ALA	HB2	1.43	0.004	1
1	A	224	ALA	HB3	1.43	0.004	1
1	A	224	ALA	C	177.855	0.005	1
1	A	224	ALA	CA	52.71	0.018	1
1	A	224	ALA	CB	19.266	0.033	1
1	A	224	ALA	N	124.514	0.028	1
1	A	225	SER	H	8.255	0.004	1
1	A	225	SER	HA	4.521	0.007	1
1	A	225	SER	HB2	3.925	0.007	2
1	A	225	SER	C	174.91	0.009	1
1	A	225	SER	CA	58.459	0.059	1
1	A	225	SER	CB	63.913	0.053	1
1	A	225	SER	N	114.761	0.025	1
1	A	226	THR	H	8.189	0.009	1
1	A	226	THR	HA	4.479	0.008	1
1	A	226	THR	HB	4.338	0.007	1
1	A	226	THR	HG21	1.238	0.000	1
1	A	226	THR	HG22	1.238	0.000	1
1	A	226	THR	HG23	1.238	0.000	1
1	A	226	THR	C	174.609	0.021	1
1	A	226	THR	CA	61.744	0.047	1
1	A	226	THR	CB	69.663	0.050	1
1	A	226	THR	CG2	21.774	0.000	1
1	A	226	THR	N	115.542	0.075	1
1	A	227	THR	H	8.06	0.008	1
1	A	227	THR	HA	4.344	0.002	1
1	A	227	THR	HB	4.183	0.000	1
1	A	227	THR	HG21	1.224	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	227	THR	HG22	1.224	0.000	1
1	A	227	THR	HG23	1.224	0.000	1
1	A	227	THR	C	174.379	0.020	1
1	A	227	THR	CA	62.086	0.035	1
1	A	227	THR	CB	69.869	0.028	1
1	A	227	THR	CG2	21.929	0.000	1
1	A	227	THR	N	116.815	0.030	1
1	A	228	MET	H	8.166	0.004	1
1	A	228	MET	HA	4.368	0.012	1
1	A	228	MET	HB2	1.592	0.009	2
1	A	228	MET	HB3	1.708	0.018	2
1	A	228	MET	HG2	2.235	0.000	2
1	A	228	MET	C	174.118	0.003	1
1	A	228	MET	CA	54.977	0.078	1
1	A	228	MET	CB	33.409	0.075	1
1	A	228	MET	CG	32.105	0.000	1
1	A	228	MET	N	121.746	0.064	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
$^{13}\text{C}_\alpha$	248	-0.20 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	226	0.03 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	246	-0.13 ± 0.10	None needed (< 0.5 ppm)
^{15}N	238	0.30 ± 0.19	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1183 atoms were assigned a chemical shift out of a possible 1499. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	575/577 (100%)	235/235 (100%)	230/232 (99%)	110/110 (100%)
Sidechain	604/833 (73%)	396/542 (73%)	208/260 (80%)	0/31 (0%)
Aromatic	4/89 (4%)	2/44 (5%)	0/42 (0%)	2/3 (67%)
Overall	1183/1499 (79%)	633/821 (77%)	438/534 (82%)	112/144 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1196 atoms were assigned a chemical shift out of a possible 1517. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	581/586 (99%)	238/239 (100%)	232/236 (98%)	111/111 (100%)
Sidechain	611/842 (73%)	400/548 (73%)	211/263 (80%)	0/31 (0%)
Aromatic	4/89 (4%)	2/44 (5%)	0/42 (0%)	2/3 (67%)
Overall	1196/1517 (79%)	640/831 (77%)	443/541 (82%)	113/145 (78%)

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	262	VAL	C	141.06	166.52 – 184.93	-18.8
1	A	245	ARG	HB3	4.16	0.43 – 3.11	8.9
1	A	295	ASP	HA	2.49	3.04 – 6.12	-6.8
1	A	345	PRO	HG2	3.90	0.41 – 3.45	6.5
1	A	139	GLN	HA	1.57	2.17 – 6.35	-6.4
1	A	345	PRO	HG3	3.71	0.33 – 3.48	5.7
1	A	283	LEU	HB3	-0.49	-0.26 – 3.31	-5.7
1	A	271	ARG	HG2	0.10	0.26 – 2.87	-5.6
1	A	200	GLU	HB3	0.84	0.95 – 3.05	-5.5
1	A	159	GLY	HA2	5.83	2.15 – 5.77	5.2

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

