wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2LAF
BMRB ID	:	17522
Title	:	NMR solution structure of the N-terminal domain of the E. coli lipoprotein BamC
Authors	:	Pardi, A.; Warner, L.
Deposited on	:	2011-03-11

This is a wwPDB NMR Structure Validation Summary 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:

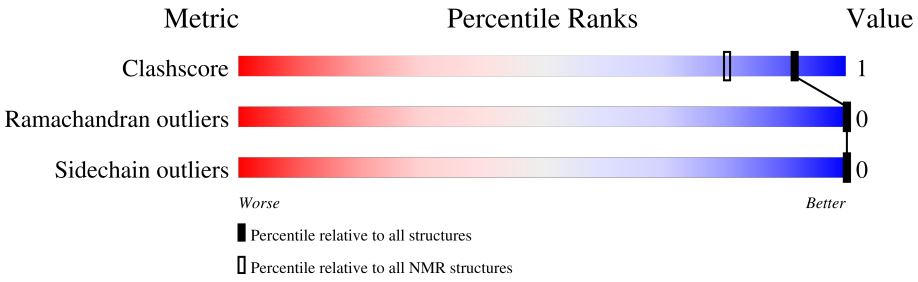
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 78%.

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	249	44% · 55%

2 Ensemble composition and analysis

This entry contains 9 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:101-A:212 (112)	1.72	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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1739 atoms, of which 860 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lipoprotein 34.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	112	1739	543	860	156	177	3	0

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

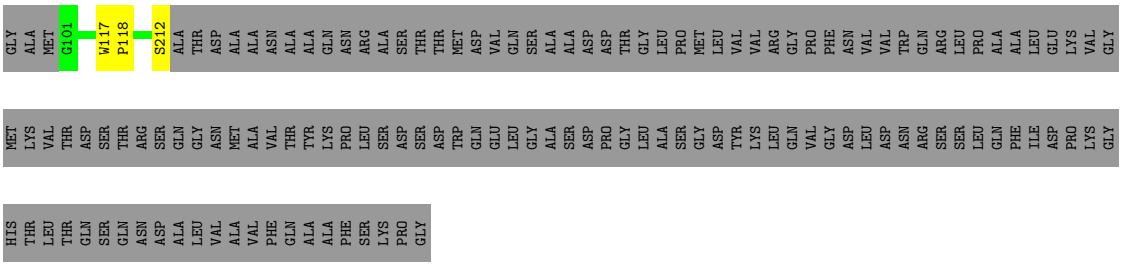
4 Residue-property plots (i)

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: Lipoprotein 34

Chain A: 

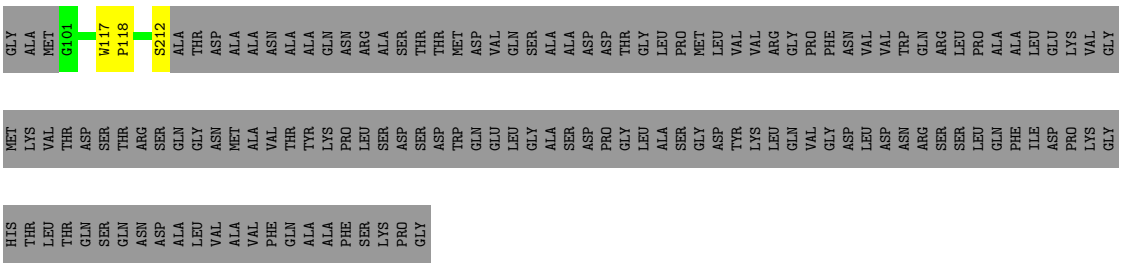


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: Lipoprotein 34

Chain A: 



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	1175
Number of unparsed shifts	0
Number of shifts with mapping errors	1364
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality

6.1 Standard geometry

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	0.73±0.00	1±0/892 (0.1± 0.0%)	0.50±0.00	0±0/1211 (0.0± 0.0%)
All	All	0.73	9/8028 (0.1%)	0.50	0/10899 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	212	SER	C-O	-12.10	1.00	1.23	3	9

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	879	860	859	3±1
All	All	7911	7740	7731	23

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.

5 of 8 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:TRP:N	1:A:118:PRO:HD2	0.54	2.18	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:TRP:N	1:A:118:PRO:CD	0.51	2.74	2	7
1:A:141:LEU:C	1:A:141:LEU:HD12	0.51	2.26	7	2
1:A:181:LEU:C	1:A:181:LEU:CD2	0.47	2.83	1	1
1:A:183:GLN:HG3	1:A:183:GLN:O	0.45	2.10	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	110/249 (44%)	107±1 (97±1%)	3±1 (3±1%)	0±0 (0±0%)	100	100
All	All	990/2241 (44%)	962 (97%)	28 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	95/203 (47%)	95±0 (100±0%)	0±0 (0±0%)	100	100
All	All	855/1827 (47%)	855 (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 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

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 78% 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	1175
Number of unparsed shifts	0
Number of shifts with mapping errors	1364
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. First 5 (of 1364) 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	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
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

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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
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

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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
1	A	223	ARG	HB2	1.79	0.012	2
1	A	223	ARG	HB3	1.885	0.014	2
1	A	223	ARG	HG2	1.675	0.000	2
1	A	223	ARG	HD2	3.216	0.000	1
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	CG	27.2	0.000	1
1	A	223	ARG	CD	43.445	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

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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
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
1	A	229	ASP	H	8.02	0.011	1
1	A	229	ASP	HA	4.787	0.008	1
1	A	229	ASP	HB2	2.539	0.006	2
1	A	229	ASP	HB3	2.643	0.006	2
1	A	229	ASP	C	175.141	0.012	1
1	A	229	ASP	CA	54.627	0.069	1
1	A	229	ASP	CB	42.485	0.024	1
1	A	229	ASP	N	121.341	0.068	1
1	A	230	VAL	H	8.293	0.007	1
1	A	230	VAL	HA	5.074	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	230	VAL	HB	2.035	0.011	1
1	A	230	VAL	HG11	1.076	0.005	1
1	A	230	VAL	HG12	1.076	0.005	1
1	A	230	VAL	HG13	1.076	0.005	1
1	A	230	VAL	HG21	1.082	0.002	1
1	A	230	VAL	HG22	1.082	0.002	1
1	A	230	VAL	HG23	1.082	0.002	1
1	A	230	VAL	C	174.256	0.008	1
1	A	230	VAL	CA	60.871	0.049	1
1	A	230	VAL	CB	34.688	0.075	1
1	A	230	VAL	CG1	21.84	0.000	2
1	A	230	VAL	CG2	23.215	0.015	2
1	A	230	VAL	N	121.534	0.028	1
1	A	231	GLN	H	8.93	0.004	1
1	A	231	GLN	HA	4.846	0.001	1
1	A	231	GLN	HB2	1.949	0.034	2
1	A	231	GLN	HB3	2.2	0.009	2
1	A	231	GLN	HG2	2.405	0.000	2
1	A	231	GLN	C	174.405	0.013	1
1	A	231	GLN	CA	53.92	0.028	1
1	A	231	GLN	CB	33.708	0.044	1
1	A	231	GLN	CG	33.784	0.000	1
1	A	231	GLN	N	122.539	0.011	1
1	A	232	SER	H	8.872	0.003	1
1	A	232	SER	HA	4.78	0.004	1
1	A	232	SER	HB2	3.836	0.006	2
1	A	232	SER	C	173.975	0.010	1
1	A	232	SER	CA	57.642	0.065	1
1	A	232	SER	CB	63.922	0.030	1
1	A	232	SER	N	116.356	0.024	1
1	A	233	ALA	H	8.708	0.005	1
1	A	233	ALA	HA	4.634	0.013	1
1	A	233	ALA	HB1	1.292	0.010	1
1	A	233	ALA	HB2	1.292	0.010	1
1	A	233	ALA	HB3	1.292	0.010	1
1	A	233	ALA	C	174.804	0.004	1
1	A	233	ALA	CA	51.511	0.061	1
1	A	233	ALA	CB	23.203	0.012	1
1	A	233	ALA	N	127.509	0.020	1
1	A	234	ALA	H	8.059	0.005	1
1	A	234	ALA	HA	5.13	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	234	ALA	HB1	1.206	0.006	1
1	A	234	ALA	HB2	1.206	0.006	1
1	A	234	ALA	HB3	1.206	0.006	1
1	A	234	ALA	C	176.891	0.011	1
1	A	234	ALA	CA	50.694	0.048	1
1	A	234	ALA	CB	21.63	0.012	1
1	A	234	ALA	N	122.3	0.019	1
1	A	235	ASP	H	9.082	0.004	1
1	A	235	ASP	HA	4.557	0.010	1
1	A	235	ASP	HB2	3.364	0.006	2
1	A	235	ASP	HB3	2.865	0.008	2
1	A	235	ASP	C	178.008	0.007	1
1	A	235	ASP	CA	52.748	0.006	1
1	A	235	ASP	CB	41.433	0.019	1
1	A	235	ASP	N	121.815	0.031	1
1	A	236	ASP	H	8.447	0.006	1
1	A	236	ASP	HA	4.412	0.009	1
1	A	236	ASP	HB2	2.722	0.013	2
1	A	236	ASP	C	177.505	0.009	1
1	A	236	ASP	CA	57.009	0.027	1
1	A	236	ASP	CB	40.392	0.016	1
1	A	236	ASP	N	116.81	0.022	1
1	A	237	THR	H	8.566	0.003	1
1	A	237	THR	HA	4.54	0.011	1
1	A	237	THR	HB	4.409	0.037	1
1	A	237	THR	HG21	1.183	0.001	1
1	A	237	THR	HG22	1.183	0.001	1
1	A	237	THR	HG23	1.183	0.001	1
1	A	237	THR	C	174.691	0.008	1
1	A	237	THR	CA	61.22	0.045	1
1	A	237	THR	CB	69.404	0.017	1
1	A	237	THR	CG2	22.03	0.000	1
1	A	237	THR	N	110.717	0.022	1
1	A	238	GLY	H	8.217	0.073	1
1	A	238	GLY	HA2	4.327	0.020	2
1	A	238	GLY	HA3	3.59	0.003	2
1	A	238	GLY	C	174.548	0.065	1
1	A	238	GLY	CA	45.199	0.013	1
1	A	238	GLY	N	110.176	0.022	1
1	A	239	LEU	H	8.408	0.004	1
1	A	239	LEU	HA	4.732	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	239	LEU	HB2	2.015	0.005	2
1	A	239	LEU	HB3	1.313	0.008	2
1	A	239	LEU	HG	1.666	0.000	1
1	A	239	LEU	HD11	0.887	0.009	1
1	A	239	LEU	HD12	0.887	0.009	1
1	A	239	LEU	HD13	0.887	0.009	1
1	A	239	LEU	HD21	0.993	0.011	1
1	A	239	LEU	HD22	0.993	0.011	1
1	A	239	LEU	HD23	0.993	0.011	1
1	A	239	LEU	CA	52.742	0.000	1
1	A	239	LEU	CB	40.322	0.047	1
1	A	239	LEU	N	125.145	0.032	1
1	A	240	PRO	HA	4.794	0.009	1
1	A	240	PRO	HB2	1.728	0.012	2
1	A	240	PRO	HB3	2.399	0.019	2
1	A	240	PRO	HG2	2.088	0.000	2
1	A	240	PRO	HG3	1.948	0.000	2
1	A	240	PRO	HD2	4.075	0.000	2
1	A	240	PRO	HD3	3.634	0.000	2
1	A	240	PRO	C	176.548	0.003	1
1	A	240	PRO	CA	63.354	0.061	1
1	A	240	PRO	CB	32.742	0.073	1
1	A	240	PRO	CG	27.212	0.000	1
1	A	240	PRO	CD	51.017	0.000	1
1	A	241	MET	H	8.607	0.004	1
1	A	241	MET	HA	4.972	0.008	1
1	A	241	MET	HB2	2.101	0.009	2
1	A	241	MET	HB3	1.986	0.002	2
1	A	241	MET	HG2	2.191	0.000	2
1	A	241	MET	C	173.925	0.017	1
1	A	241	MET	CA	55.57	0.072	1
1	A	241	MET	CB	35.67	0.048	1
1	A	241	MET	CG	31.024	0.000	1
1	A	241	MET	N	119.163	0.026	1
1	A	242	LEU	H	9.222	0.003	1
1	A	242	LEU	HA	5.24	0.017	1
1	A	242	LEU	HB2	1.76	0.000	2
1	A	242	LEU	HB3	1.165	0.016	2
1	A	242	LEU	HG	1.856	0.002	1
1	A	242	LEU	HD11	0.736	0.000	1
1	A	242	LEU	HD12	0.736	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	242	LEU	HD13	0.736	0.000	1
1	A	242	LEU	HD21	0.78	0.001	1
1	A	242	LEU	HD22	0.78	0.001	1
1	A	242	LEU	HD23	0.78	0.001	1
1	A	242	LEU	C	176.502	0.008	1
1	A	242	LEU	CA	53.587	0.007	1
1	A	242	LEU	CB	44.785	0.035	1
1	A	242	LEU	CG	27.048	0.011	1
1	A	242	LEU	CD1	26.285	0.000	2
1	A	242	LEU	CD2	25.497	0.032	2
1	A	242	LEU	N	120.982	0.025	1
1	A	243	VAL	H	9.241	0.005	1
1	A	243	VAL	HA	4.794	0.006	1
1	A	243	VAL	HB	1.723	0.011	1
1	A	243	VAL	HG11	0.761	0.003	1
1	A	243	VAL	HG12	0.761	0.003	1
1	A	243	VAL	HG13	0.761	0.003	1
1	A	243	VAL	HG21	0.761	0.004	1
1	A	243	VAL	HG22	0.761	0.004	1
1	A	243	VAL	HG23	0.761	0.004	1
1	A	243	VAL	C	174.683	0.005	1
1	A	243	VAL	CA	61.215	0.052	1
1	A	243	VAL	CB	34.522	0.039	1
1	A	243	VAL	CG1	22.124	0.000	2
1	A	243	VAL	CG2	22.124	0.000	2
1	A	243	VAL	N	119.886	0.019	1
1	A	244	VAL	H	9.354	0.005	1
1	A	244	VAL	HA	4.782	0.005	1
1	A	244	VAL	HB	1.724	0.005	1
1	A	244	VAL	HG11	0.439	0.004	1
1	A	244	VAL	HG12	0.439	0.004	1
1	A	244	VAL	HG13	0.439	0.004	1
1	A	244	VAL	HG21	0.732	0.008	1
1	A	244	VAL	HG22	0.732	0.008	1
1	A	244	VAL	HG23	0.732	0.008	1
1	A	244	VAL	C	176.648	0.009	1
1	A	244	VAL	CA	59.856	0.075	1
1	A	244	VAL	CB	34.093	0.010	1
1	A	244	VAL	CG1	22.037	0.062	2
1	A	244	VAL	CG2	21.376	0.032	2
1	A	244	VAL	N	127.044	0.024	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	245	ARG	H	8.862	0.008	1
1	A	245	ARG	HA	4.31	0.011	1
1	A	245	ARG	HB2	2.153	0.013	2
1	A	245	ARG	HB3	4.163	3.326	2
1	A	245	ARG	HG2	1.587	0.003	2
1	A	245	ARG	HG3	1.903	0.000	2
1	A	245	ARG	HD2	3.226	0.004	1
1	A	245	ARG	C	174.122	0.005	1
1	A	245	ARG	CA	56.319	0.027	1
1	A	245	ARG	CB	28.329	0.116	1
1	A	245	ARG	CD	43.181	0.000	1
1	A	245	ARG	N	129.566	0.017	1
1	A	246	GLY	H	8.353	0.004	1
1	A	246	GLY	HA2	4.29	0.000	2
1	A	246	GLY	HA3	3.553	0.000	2
1	A	246	GLY	C	169.103	0.000	1
1	A	246	GLY	CA	44.704	0.000	1
1	A	246	GLY	N	113.385	0.020	1
1	A	247	PRO	HA	4.365	0.015	1
1	A	247	PRO	HB2	2.155	0.009	2
1	A	247	PRO	HB3	2.477	0.004	2
1	A	247	PRO	HG2	2.055	0.000	2
1	A	247	PRO	HD2	3.699	0.000	2
1	A	247	PRO	HD3	3.38	0.000	2
1	A	247	PRO	C	176.627	0.015	1
1	A	247	PRO	CA	61.985	0.038	1
1	A	247	PRO	CB	32.602	0.012	1
1	A	247	PRO	CG	27.508	0.000	1
1	A	247	PRO	CD	49.82	0.000	1
1	A	248	PHE	H	9.221	0.003	1
1	A	248	PHE	HA	4.205	0.005	1
1	A	248	PHE	HB2	2.981	0.007	2
1	A	248	PHE	C	176.411	0.006	1
1	A	248	PHE	CA	62.266	0.040	1
1	A	248	PHE	CB	39.964	0.049	1
1	A	248	PHE	N	125.189	0.020	1
1	A	249	ASN	H	9.205	0.005	1
1	A	249	ASN	HA	4.221	0.004	1
1	A	249	ASN	HB2	2.832	0.005	2
1	A	249	ASN	C	177.831	0.007	1
1	A	249	ASN	CA	56.781	0.025	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	249	ASN	CB	37.724	0.014	1
1	A	249	ASN	N	114.069	0.020	1
1	A	250	VAL	H	7.049	0.017	1
1	A	250	VAL	HA	3.801	0.004	1
1	A	250	VAL	HB	1.905	0.018	1
1	A	250	VAL	HG11	1.007	0.004	1
1	A	250	VAL	HG12	1.007	0.004	1
1	A	250	VAL	HG13	1.007	0.004	1
1	A	250	VAL	HG21	0.895	0.017	1
1	A	250	VAL	HG22	0.895	0.017	1
1	A	250	VAL	HG23	0.895	0.017	1
1	A	250	VAL	C	177.31	0.002	1
1	A	250	VAL	CA	65.159	0.041	1
1	A	250	VAL	CB	32.727	0.056	1
1	A	250	VAL	CG1	22.177	0.021	2
1	A	250	VAL	CG2	20.897	0.000	2
1	A	250	VAL	N	119.115	0.022	1
1	A	251	VAL	H	8.148	0.005	1
1	A	251	VAL	HA	3.069	0.004	1
1	A	251	VAL	HB	1.846	0.002	1
1	A	251	VAL	HG11	0.547	0.003	1
1	A	251	VAL	HG12	0.547	0.003	1
1	A	251	VAL	HG13	0.547	0.003	1
1	A	251	VAL	HG21	0.665	0.007	1
1	A	251	VAL	HG22	0.665	0.007	1
1	A	251	VAL	HG23	0.665	0.007	1
1	A	251	VAL	C	177.109	0.001	1
1	A	251	VAL	CA	68.011	0.016	1
1	A	251	VAL	CB	31.574	0.047	1
1	A	251	VAL	CG1	23.898	0.022	2
1	A	251	VAL	CG2	20.489	0.029	2
1	A	251	VAL	N	121.47	0.026	1
1	A	252	TRP	H	9.22	0.006	1
1	A	252	TRP	HA	3.681	0.005	1
1	A	252	TRP	HB2	2.751	0.000	2
1	A	252	TRP	HB3	2.367	0.004	2
1	A	252	TRP	HE1	10.214	0.004	1
1	A	252	TRP	C	177.968	0.005	1
1	A	252	TRP	CA	61.201	0.048	1
1	A	252	TRP	CB	28.791	0.024	1
1	A	252	TRP	N	117.685	0.026	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	252	TRP	NE1	128.894	0.007	1
1	A	253	GLN	H	6.957	0.003	1
1	A	253	GLN	HA	4.027	0.007	1
1	A	253	GLN	HB2	2.29	0.004	2
1	A	253	GLN	HG2	2.582	0.000	2
1	A	253	GLN	C	178.183	0.007	1
1	A	253	GLN	CA	58.34	0.023	1
1	A	253	GLN	CB	29.029	0.068	1
1	A	253	GLN	CG	34.226	0.000	1
1	A	253	GLN	N	113.779	0.025	1
1	A	254	ARG	H	7.954	0.004	1
1	A	254	ARG	HA	4.253	0.010	1
1	A	254	ARG	HB2	2.067	0.013	2
1	A	254	ARG	HB3	1.853	0.016	2
1	A	254	ARG	HD2	3.194	0.000	1
1	A	254	ARG	C	177.675	0.014	1
1	A	254	ARG	CA	56.692	0.074	1
1	A	254	ARG	CB	31.166	0.035	1
1	A	254	ARG	CG	27.544	0.000	1
1	A	254	ARG	CD	42.759	0.000	1
1	A	254	ARG	N	117.006	0.031	1
1	A	255	LEU	H	7.909	0.009	1
1	A	255	LEU	HA	3.999	0.002	1
1	A	255	LEU	HB2	1.841	0.012	2
1	A	255	LEU	HB3	0.908	0.001	2
1	A	255	LEU	C	174.641	0.000	1
1	A	255	LEU	CA	59.977	0.000	1
1	A	255	LEU	CB	40.691	0.018	1
1	A	255	LEU	N	121.277	0.036	1
1	A	256	PRO	HA	3.931	0.006	1
1	A	256	PRO	HB2	1.857	0.004	2
1	A	256	PRO	HB3	2.218	0.011	2
1	A	256	PRO	HD2	3.438	0.000	2
1	A	256	PRO	HD3	3.438	0.000	2
1	A	256	PRO	C	178.43	0.006	1
1	A	256	PRO	CA	67.821	0.050	1
1	A	256	PRO	CB	30.664	0.072	1
1	A	256	PRO	CG	29.182	0.000	1
1	A	256	PRO	CD	49.518	0.000	1
1	A	257	ALA	H	8.038	0.005	1
1	A	257	ALA	HA	4.187	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	257	ALA	HB1	1.428	0.004	1
1	A	257	ALA	HB2	1.428	0.004	1
1	A	257	ALA	HB3	1.428	0.004	1
1	A	257	ALA	C	180.029	0.005	1
1	A	257	ALA	CA	54.587	0.029	1
1	A	257	ALA	CB	18.73	0.030	1
1	A	257	ALA	N	117.838	0.028	1
1	A	258	ALA	H	7.424	0.004	1
1	A	258	ALA	HA	3.854	0.004	1
1	A	258	ALA	HB1	0.855	0.009	1
1	A	258	ALA	HB2	0.855	0.009	1
1	A	258	ALA	HB3	0.855	0.009	1
1	A	258	ALA	C	178.758	0.003	1
1	A	258	ALA	CA	55.18	0.030	1
1	A	258	ALA	CB	18.416	0.029	1
1	A	258	ALA	N	121.393	0.024	1
1	A	259	LEU	H	8.902	0.004	1
1	A	259	LEU	HA	3.831	0.007	1
1	A	259	LEU	HB2	1.682	0.031	2
1	A	259	LEU	HB3	1.724	0.011	2
1	A	259	LEU	HD21	0.549	0.000	1
1	A	259	LEU	HD22	0.549	0.000	1
1	A	259	LEU	HD23	0.549	0.000	1
1	A	259	LEU	C	179.466	0.028	1
1	A	259	LEU	CA	57.366	0.057	1
1	A	259	LEU	CB	39.831	0.014	1
1	A	259	LEU	CG	27.542	0.000	1
1	A	259	LEU	CD1	24.387	0.000	2
1	A	259	LEU	N	116.127	0.019	1
1	A	260	GLU	H	7.652	0.003	1
1	A	260	GLU	HA	3.943	0.019	1
1	A	260	GLU	HB2	2.172	0.023	2
1	A	260	GLU	HB3	2.043	0.017	2
1	A	260	GLU	HG2	2.358	0.000	2
1	A	260	GLU	C	179.807	0.004	1
1	A	260	GLU	CA	59.402	0.037	1
1	A	260	GLU	CB	29.366	0.041	1
1	A	260	GLU	CG	36.512	0.000	1
1	A	260	GLU	N	118.337	0.018	1
1	A	261	LYS	H	7.287	0.004	1
1	A	261	LYS	HA	3.986	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	261	LYS	HB2	1.826	0.006	2
1	A	261	LYS	HB3	2.011	0.014	2
1	A	261	LYS	HG2	1.59	0.000	2
1	A	261	LYS	HD2	1.755	0.000	2
1	A	261	LYS	HE2	2.962	0.000	2
1	A	261	LYS	C	176.308	0.003	1
1	A	261	LYS	CA	58.037	0.040	1
1	A	261	LYS	CB	32.604	0.030	1
1	A	261	LYS	CG	25.234	0.000	1
1	A	261	LYS	CD	29.162	0.000	1
1	A	261	LYS	CE	42.331	0.000	1
1	A	261	LYS	N	117.168	0.025	1
1	A	262	VAL	H	7.227	0.005	1
1	A	262	VAL	HA	4.229	0.004	1
1	A	262	VAL	HB	2.304	0.004	1
1	A	262	VAL	HG11	0.586	0.000	1
1	A	262	VAL	HG12	0.586	0.000	1
1	A	262	VAL	HG13	0.586	0.000	1
1	A	262	VAL	HG21	0.629	0.001	1
1	A	262	VAL	HG22	0.629	0.001	1
1	A	262	VAL	HG23	0.629	0.001	1
1	A	262	VAL	C	141.06	.	1
1	A	262	VAL	CA	59.317	0.027	1
1	A	262	VAL	CB	31.212	0.011	1
1	A	262	VAL	CG1	22.74	0.006	2
1	A	262	VAL	CG2	19.217	0.030	2
1	A	262	VAL	N	109.464	0.025	1
1	A	263	GLY	H	7.018	0.004	1
1	A	263	GLY	HA2	4.423	0.007	2
1	A	263	GLY	HA3	3.501	0.008	2
1	A	263	GLY	C	175.074	0.009	1
1	A	263	GLY	CA	45.299	0.061	1
1	A	263	GLY	N	102.002	0.013	1
1	A	264	MET	H	8.163	0.004	1
1	A	264	MET	HA	5.066	0.006	1
1	A	264	MET	HB2	2.005	0.005	2
1	A	264	MET	HB3	1.418	0.007	2
1	A	264	MET	HG2	2.71	0.000	2
1	A	264	MET	HE1	2.203	0.000	1
1	A	264	MET	HE2	2.203	0.000	1
1	A	264	MET	HE3	2.203	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	264	MET	C	173.479	0.008	1
1	A	264	MET	CA	55.335	0.062	1
1	A	264	MET	CB	34.299	0.042	1
1	A	264	MET	CG	35.682	0.000	1
1	A	264	MET	N	120.427	0.031	1
1	A	265	LYS	H	8.445	0.004	1
1	A	265	LYS	HA	4.389	0.003	1
1	A	265	LYS	HB2	1.752	0.014	2
1	A	265	LYS	HG2	1.336	0.000	2
1	A	265	LYS	HD2	1.566	0.000	2
1	A	265	LYS	HE2	2.944	0.000	2
1	A	265	LYS	C	176.057	0.008	1
1	A	265	LYS	CA	54.604	0.030	1
1	A	265	LYS	CB	34.348	0.037	1
1	A	265	LYS	CG	24.661	0.000	1
1	A	265	LYS	CD	28.961	0.000	1
1	A	265	LYS	CE	42.081	0.000	1
1	A	265	LYS	N	123.242	0.030	1
1	A	266	VAL	H	8.333	0.005	1
1	A	266	VAL	HA	4.457	0.002	1
1	A	266	VAL	HB	2.002	0.014	1
1	A	266	VAL	HG11	0.905	0.009	1
1	A	266	VAL	HG12	0.905	0.009	1
1	A	266	VAL	HG13	0.905	0.009	1
1	A	266	VAL	HG21	0.922	0.004	1
1	A	266	VAL	HG22	0.922	0.004	1
1	A	266	VAL	HG23	0.922	0.004	1
1	A	266	VAL	C	177.409	0.004	1
1	A	266	VAL	CA	62.931	0.065	1
1	A	266	VAL	CB	32.345	0.016	1
1	A	266	VAL	CG1	23.582	0.002	2
1	A	266	VAL	CG2	21.657	0.000	2
1	A	266	VAL	N	126.036	0.021	1
1	A	267	THR	H	9.306	0.004	1
1	A	267	THR	HA	4.43	0.009	1
1	A	267	THR	HB	4.318	0.010	1
1	A	267	THR	HG21	1.177	0.000	1
1	A	267	THR	HG22	1.177	0.000	1
1	A	267	THR	HG23	1.177	0.000	1
1	A	267	THR	C	174.661	0.017	1
1	A	267	THR	CA	62.303	0.063	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	267	THR	CB	69.097	0.042	1
1	A	267	THR	CG2	21.232	0.000	1
1	A	267	THR	N	121.022	0.026	1
1	A	268	ASP	H	7.78	0.004	1
1	A	268	ASP	HA	4.85	0.004	1
1	A	268	ASP	HB2	2.878	0.009	2
1	A	268	ASP	HB3	2.444	0.012	2
1	A	268	ASP	C	174.191	0.005	1
1	A	268	ASP	CA	54.321	0.023	1
1	A	268	ASP	CB	43.848	0.007	1
1	A	268	ASP	N	120.149	0.033	1
1	A	269	SER	H	8.392	0.005	1
1	A	269	SER	HA	5.242	0.004	1
1	A	269	SER	HB2	4.027	0.010	2
1	A	269	SER	HB3	4.113	0.006	2
1	A	269	SER	C	173.458	0.005	1
1	A	269	SER	CA	58.322	0.027	1
1	A	269	SER	CB	65.936	0.046	1
1	A	269	SER	N	115.107	0.014	1
1	A	270	THR	H	9.169	0.005	1
1	A	270	THR	HA	4.752	0.000	1
1	A	270	THR	HB	4.168	0.000	1
1	A	270	THR	C	175.18	0.002	1
1	A	270	THR	CA	60.798	0.031	1
1	A	270	THR	CB	70.183	0.006	1
1	A	270	THR	N	117.819	0.021	1
1	A	271	ARG	H	9.306	0.003	1
1	A	271	ARG	HA	2.962	0.006	1
1	A	271	ARG	HB2	1.649	0.005	2
1	A	271	ARG	HB3	1.189	0.013	2
1	A	271	ARG	HG2	0.098	0.006	2
1	A	271	ARG	HD2	2.797	0.000	1
1	A	271	ARG	C	178.792	0.016	1
1	A	271	ARG	CA	60.104	0.052	1
1	A	271	ARG	CB	29.88	0.045	1
1	A	271	ARG	CG	26.676	0.084	1
1	A	271	ARG	CD	43.064	0.000	1
1	A	271	ARG	N	132.424	0.013	1
1	A	272	SER	H	8.796	0.005	1
1	A	272	SER	HA	3.986	0.003	1
1	A	272	SER	HB2	3.878	0.021	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	272	SER	C	174.958	0.002	1
1	A	272	SER	CA	60.859	0.051	1
1	A	272	SER	CB	62.094	0.054	1
1	A	272	SER	N	113.329	0.034	1
1	A	273	GLN	H	6.807	0.005	1
1	A	273	GLN	HA	4.519	0.007	1
1	A	273	GLN	HB2	2.394	0.019	2
1	A	273	GLN	HB3	1.72	0.007	2
1	A	273	GLN	HG2	2.379	0.000	2
1	A	273	GLN	C	175.812	0.006	1
1	A	273	GLN	CA	54.826	0.024	1
1	A	273	GLN	CB	30.776	0.029	1
1	A	273	GLN	CG	34.007	0.000	1
1	A	273	GLN	N	116.554	0.023	1
1	A	274	GLY	H	7.861	0.005	1
1	A	274	GLY	HA2	4.403	0.002	2
1	A	274	GLY	HA3	3.666	0.005	2
1	A	274	GLY	C	172.654	0.007	1
1	A	274	GLY	CA	46.792	0.015	1
1	A	274	GLY	N	109.054	0.021	1
1	A	275	ASN	H	7.584	0.004	1
1	A	275	ASN	HA	5.908	0.005	1
1	A	275	ASN	HB2	2.688	0.009	2
1	A	275	ASN	C	174.314	0.008	1
1	A	275	ASN	CA	52.56	0.053	1
1	A	275	ASN	CB	43.064	0.008	1
1	A	275	ASN	N	115.042	0.027	1
1	A	276	MET	H	9.275	0.003	1
1	A	276	MET	HA	4.965	0.005	1
1	A	276	MET	HB2	1.865	0.014	2
1	A	276	MET	HB3	1.671	0.009	2
1	A	276	MET	HG2	2.311	0.000	2
1	A	276	MET	C	173.209	0.004	1
1	A	276	MET	CA	55.528	0.092	1
1	A	276	MET	CB	36.896	0.015	1
1	A	276	MET	CG	33.445	0.000	1
1	A	276	MET	N	120.517	0.031	1
1	A	277	ALA	H	8.699	0.005	1
1	A	277	ALA	HA	4.975	0.005	1
1	A	277	ALA	HB1	1.438	0.008	1
1	A	277	ALA	HB2	1.438	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	277	ALA	HB3	1.438	0.008	1
1	A	277	ALA	C	176.257	0.004	1
1	A	277	ALA	CA	51.555	0.038	1
1	A	277	ALA	CB	20.617	0.021	1
1	A	277	ALA	N	127.483	0.024	1
1	A	278	VAL	H	8.551	0.004	1
1	A	278	VAL	HA	5.613	0.017	1
1	A	278	VAL	HB	1.855	0.007	1
1	A	278	VAL	HG11	0.855	0.009	1
1	A	278	VAL	HG12	0.855	0.009	1
1	A	278	VAL	HG13	0.855	0.009	1
1	A	278	VAL	HG21	0.962	0.000	1
1	A	278	VAL	HG22	0.962	0.000	1
1	A	278	VAL	HG23	0.962	0.000	1
1	A	278	VAL	C	175.277	0.006	1
1	A	278	VAL	CA	58.313	0.037	1
1	A	278	VAL	CB	36.282	0.035	1
1	A	278	VAL	CG1	22.228	0.034	2
1	A	278	VAL	CG2	20.264	0.031	2
1	A	278	VAL	N	116.129	0.026	1
1	A	279	THR	H	9.079	0.006	1
1	A	279	THR	HA	5.194	0.005	1
1	A	279	THR	HB	3.807	0.007	1
1	A	279	THR	HG21	1.248	0.008	1
1	A	279	THR	HG22	1.248	0.008	1
1	A	279	THR	HG23	1.248	0.008	1
1	A	279	THR	C	173.793	0.009	1
1	A	279	THR	CA	62.264	0.037	1
1	A	279	THR	CB	71.48	0.032	1
1	A	279	THR	CG2	21.905	0.060	1
1	A	279	THR	N	120.995	0.026	1
1	A	280	TYR	H	9.794	0.005	1
1	A	280	TYR	HA	5.508	0.006	1
1	A	280	TYR	HB2	2.751	0.010	2
1	A	280	TYR	HB3	3.227	0.012	2
1	A	280	TYR	C	174.599	0.005	1
1	A	280	TYR	CA	55.65	0.041	1
1	A	280	TYR	CB	41.675	0.031	1
1	A	280	TYR	N	129.611	0.019	1
1	A	281	LYS	H	8.262	0.004	1
1	A	281	LYS	HA	4.398	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	281	LYS	HB2	1.638	0.000	2
1	A	281	LYS	C	171.763	0.000	1
1	A	281	LYS	CA	52.977	0.000	1
1	A	281	LYS	CB	34.53	0.000	1
1	A	281	LYS	N	133.081	0.025	1
1	A	282	PRO	HA	4.141	0.010	1
1	A	282	PRO	HB2	2.666	0.000	2
1	A	282	PRO	HB3	2.928	0.000	2
1	A	282	PRO	HG2	2.023	0.000	2
1	A	282	PRO	HD2	3.538	0.000	2
1	A	282	PRO	HD3	3.538	0.000	2
1	A	282	PRO	C	176.726	0.010	1
1	A	282	PRO	CA	63.009	0.036	1
1	A	282	PRO	CB	32.724	0.012	1
1	A	282	PRO	CG	26.998	0.000	1
1	A	282	PRO	CD	50.622	0.000	1
1	A	283	LEU	H	5.929	0.006	1
1	A	283	LEU	HA	4.013	0.005	1
1	A	283	LEU	HB2	0.995	0.005	2
1	A	283	LEU	HB3	-0.49	0.005	2
1	A	283	LEU	HG	0.679	0.011	1
1	A	283	LEU	HD11	-0.011	0.008	1
1	A	283	LEU	HD12	-0.011	0.008	1
1	A	283	LEU	HD13	-0.011	0.008	1
1	A	283	LEU	HD21	0.305	0.009	1
1	A	283	LEU	HD22	0.305	0.009	1
1	A	283	LEU	HD23	0.305	0.009	1
1	A	283	LEU	C	176.333	0.006	1
1	A	283	LEU	CA	53.992	0.047	1
1	A	283	LEU	CB	40.737	0.016	1
1	A	283	LEU	CG	26.993	0.200	1
1	A	283	LEU	CD1	24.218	0.044	2
1	A	283	LEU	CD2	21.86	0.037	2
1	A	283	LEU	N	119.309	0.013	1
1	A	284	SER	H	8.568	0.003	1
1	A	284	SER	HA	4.495	0.008	1
1	A	284	SER	HB2	3.993	0.001	2
1	A	284	SER	HB3	4.224	0.019	2
1	A	284	SER	C	174.659	0.006	1
1	A	284	SER	CA	57.513	0.043	1
1	A	284	SER	CB	64.775	0.024	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	284	SER	N	115.13	0.025	1
1	A	285	ASP	H	8.933	0.004	1
1	A	285	ASP	HA	4.684	0.014	1
1	A	285	ASP	HB2	2.794	0.007	2
1	A	285	ASP	C	179.244	0.008	1
1	A	285	ASP	CA	58.673	0.021	1
1	A	285	ASP	CB	40.623	0.026	1
1	A	285	ASP	N	121.191	0.040	1
1	A	286	SER	H	8.511	0.004	1
1	A	286	SER	HA	4.203	0.008	1
1	A	286	SER	HB2	3.852	0.002	2
1	A	286	SER	C	176.699	0.005	1
1	A	286	SER	CA	61.474	0.059	1
1	A	286	SER	CB	62.357	0.084	1
1	A	286	SER	N	113.906	0.022	1
1	A	287	ASP	H	7.697	0.006	1
1	A	287	ASP	HA	4.489	0.004	1
1	A	287	ASP	HB2	2.702	0.009	2
1	A	287	ASP	HB3	2.349	0.005	2
1	A	287	ASP	C	180.222	0.004	1
1	A	287	ASP	CA	57.277	0.031	1
1	A	287	ASP	CB	40.495	0.037	1
1	A	287	ASP	N	124.33	0.032	1
1	A	288	TRP	H	8.506	0.005	1
1	A	288	TRP	HA	4.578	0.008	1
1	A	288	TRP	HB2	3.694	0.012	2
1	A	288	TRP	HB3	3.293	0.015	2
1	A	288	TRP	HE1	9.19	0.002	1
1	A	288	TRP	C	179.006	0.013	1
1	A	288	TRP	CA	60.764	0.027	1
1	A	288	TRP	CB	29.16	0.064	1
1	A	288	TRP	N	123.206	0.028	1
1	A	288	TRP	NE1	128.094	0.017	1
1	A	289	GLN	H	7.939	0.005	1
1	A	289	GLN	HA	4.15	0.003	1
1	A	289	GLN	HB2	2.233	0.014	2
1	A	289	GLN	HG2	2.525	0.000	2
1	A	289	GLN	C	179.383	0.005	1
1	A	289	GLN	CA	59.089	0.036	1
1	A	289	GLN	CB	28.135	0.051	1
1	A	289	GLN	CG	34.089	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	289	GLN	N	118.148	0.031	1
1	A	290	GLU	H	7.894	0.004	1
1	A	290	GLU	HA	4.033	0.006	1
1	A	290	GLU	HB2	2.093	0.008	2
1	A	290	GLU	HG2	2.376	0.000	2
1	A	290	GLU	C	178.18	0.004	1
1	A	290	GLU	CA	58.907	0.028	1
1	A	290	GLU	CB	29.431	0.035	1
1	A	290	GLU	CG	36.072	0.000	1
1	A	290	GLU	N	119.951	0.036	1
1	A	291	LEU	H	7.751	0.005	1
1	A	291	LEU	HA	4.077	0.005	1
1	A	291	LEU	HB2	2.034	0.008	2
1	A	291	LEU	HB3	1.672	0.004	2
1	A	291	LEU	HD11	0.786	0.000	1
1	A	291	LEU	HD12	0.786	0.000	1
1	A	291	LEU	HD13	0.786	0.000	1
1	A	291	LEU	C	176.769	0.014	1
1	A	291	LEU	CA	56.856	0.049	1
1	A	291	LEU	CB	42.353	0.058	1
1	A	291	LEU	CG	26.363	0.000	1
1	A	291	LEU	CD1	23.879	0.000	2
1	A	291	LEU	N	119.785	0.031	1
1	A	292	GLY	H	8.003	0.004	1
1	A	292	GLY	HA2	4.232	0.004	2
1	A	292	GLY	HA3	3.764	0.009	2
1	A	292	GLY	C	173.95	0.000	1
1	A	292	GLY	CA	44.919	0.069	1
1	A	292	GLY	N	103.869	0.041	1
1	A	293	ALA	H	7.77	0.004	1
1	A	293	ALA	HA	4.673	0.005	1
1	A	293	ALA	HB1	1.27	0.008	1
1	A	293	ALA	HB2	1.27	0.008	1
1	A	293	ALA	HB3	1.27	0.008	1
1	A	293	ALA	C	174.208	0.005	1
1	A	293	ALA	CA	50.491	0.036	1
1	A	293	ALA	CB	22.422	0.013	1
1	A	293	ALA	N	121.819	0.018	1
1	A	294	SER	H	7.629	0.004	1
1	A	294	SER	HA	4.202	0.006	1
1	A	294	SER	HB2	3.595	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	294	SER	HB3	3.471	0.015	2
1	A	294	SER	C	172.156	0.005	1
1	A	294	SER	CA	57.383	0.035	1
1	A	294	SER	CB	64.376	0.031	1
1	A	294	SER	N	112.916	0.019	1
1	A	295	ASP	H	7.724	0.004	1
1	A	295	ASP	HA	2.494	0.000	1
1	A	295	ASP	HB2	2.299	0.000	2
1	A	295	ASP	HB3	1.925	0.000	2
1	A	295	ASP	C	176.275	0.000	1
1	A	295	ASP	CA	51.368	0.000	1
1	A	295	ASP	CB	41.47	0.000	1
1	A	295	ASP	N	122.458	0.028	1
1	A	296	PRO	HA	4.22	0.007	1
1	A	296	PRO	HB2	1.565	0.018	2
1	A	296	PRO	HB3	1.8	0.004	2
1	A	296	PRO	HD2	3.432	0.000	2
1	A	296	PRO	HD3	3.432	0.000	2
1	A	296	PRO	C	176.631	0.002	1
1	A	296	PRO	CA	63.123	0.040	1
1	A	296	PRO	CB	32.027	0.018	1
1	A	296	PRO	CG	26.407	0.000	1
1	A	296	PRO	CD	51.135	0.000	1
1	A	297	GLY	H	8.799	0.003	1
1	A	297	GLY	HA2	3.822	0.008	2
1	A	297	GLY	HA3	3.624	0.005	2
1	A	297	GLY	C	174.949	0.002	1
1	A	297	GLY	CA	46.314	0.017	1
1	A	297	GLY	N	110.033	0.022	1
1	A	298	LEU	H	7.252	0.005	1
1	A	298	LEU	HA	4.337	0.005	1
1	A	298	LEU	HB2	1.657	0.011	2
1	A	298	LEU	HB3	1.196	0.006	2
1	A	298	LEU	HG	1.34	0.011	1
1	A	298	LEU	HD11	0.921	2.112	1
1	A	298	LEU	HD12	0.921	2.112	1
1	A	298	LEU	HD13	0.921	2.112	1
1	A	298	LEU	HD21	0.257	0.000	1
1	A	298	LEU	HD22	0.257	0.000	1
1	A	298	LEU	HD23	0.257	0.000	1
1	A	298	LEU	C	177.44	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	298	LEU	CA	54.566	0.049	1
1	A	298	LEU	CB	43.685	0.042	1
1	A	298	LEU	CG	28.303	0.096	1
1	A	298	LEU	CD1	23.796	0.011	2
1	A	298	LEU	CD2	24.256	0.017	2
1	A	298	LEU	N	121.289	0.021	1
1	A	299	ALA	H	8.568	0.004	1
1	A	299	ALA	HA	4.477	0.008	1
1	A	299	ALA	HB1	1.521	0.008	1
1	A	299	ALA	HB2	1.521	0.008	1
1	A	299	ALA	HB3	1.521	0.008	1
1	A	299	ALA	C	179.03	0.007	1
1	A	299	ALA	CA	51.834	0.042	1
1	A	299	ALA	CB	19.442	0.017	1
1	A	299	ALA	N	125.737	0.024	1
1	A	300	SER	H	8.826	0.003	1
1	A	300	SER	HA	4.435	0.006	1
1	A	300	SER	HB2	3.903	0.000	2
1	A	300	SER	HB3	4.02	0.000	2
1	A	300	SER	C	173.579	0.004	1
1	A	300	SER	CA	59.237	0.019	1
1	A	300	SER	CB	63.956	0.021	1
1	A	300	SER	N	117.238	0.034	1
1	A	301	GLY	H	8.554	0.005	1
1	A	301	GLY	HA2	4.588	0.002	2
1	A	301	GLY	HA3	3.941	0.008	2
1	A	301	GLY	C	171.624	0.004	1
1	A	301	GLY	CA	44.746	0.013	1
1	A	301	GLY	N	108.567	0.028	1
1	A	302	ASP	H	8.395	0.008	1
1	A	302	ASP	HA	5.575	0.005	1
1	A	302	ASP	HB2	2.919	0.004	2
1	A	302	ASP	HB3	2.533	0.002	2
1	A	302	ASP	C	175.289	0.012	1
1	A	302	ASP	CA	54.321	0.038	1
1	A	302	ASP	CB	40.719	0.064	1
1	A	302	ASP	N	122.239	0.026	1
1	A	303	TYR	H	9.341	0.005	1
1	A	303	TYR	HA	4.928	0.004	1
1	A	303	TYR	HB2	3.038	0.016	2
1	A	303	TYR	HB3	2.823	0.003	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	303	TYR	C	176.104	0.004	1
1	A	303	TYR	CA	57.009	0.062	1
1	A	303	TYR	CB	42.79	0.029	1
1	A	303	TYR	N	120.909	0.030	1
1	A	304	LYS	H	9.214	0.004	1
1	A	304	LYS	HA	5.08	0.009	1
1	A	304	LYS	HB2	1.858	0.004	2
1	A	304	LYS	HB3	1.768	0.003	2
1	A	304	LYS	HG2	1.404	0.000	2
1	A	304	LYS	HD2	1.599	0.000	2
1	A	304	LYS	HE2	2.926	0.000	2
1	A	304	LYS	C	174.041	0.004	1
1	A	304	LYS	CA	55.025	0.047	1
1	A	304	LYS	CB	34.771	0.039	1
1	A	304	LYS	CG	25.008	0.000	1
1	A	304	LYS	CD	29.086	0.000	1
1	A	304	LYS	CE	42.226	0.000	1
1	A	304	LYS	N	121.585	0.035	1
1	A	305	LEU	H	9.059	0.005	1
1	A	305	LEU	HA	4.713	0.012	1
1	A	305	LEU	HB2	1.533	0.008	2
1	A	305	LEU	HB3	0.85	0.014	2
1	A	305	LEU	HG	1.044	0.018	1
1	A	305	LEU	HD11	0.555	0.010	1
1	A	305	LEU	HD12	0.555	0.010	1
1	A	305	LEU	HD13	0.555	0.010	1
1	A	305	LEU	HD21	-0.178	0.009	1
1	A	305	LEU	HD22	-0.178	0.009	1
1	A	305	LEU	HD23	-0.178	0.009	1
1	A	305	LEU	C	174.014	0.000	1
1	A	305	LEU	CA	53.347	0.035	1
1	A	305	LEU	CB	44.225	0.031	1
1	A	305	LEU	CG	26.866	0.051	1
1	A	305	LEU	CD1	26.835	0.125	2
1	A	305	LEU	CD2	21.84	0.059	2
1	A	305	LEU	N	125.224	0.014	1
1	A	306	GLN	H	8.804	0.005	1
1	A	306	GLN	HA	5.063	0.007	1
1	A	306	GLN	HB2	2.047	0.013	2
1	A	306	GLN	HB3	2.025	0.002	2
1	A	306	GLN	HG2	2.335	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	306	GLN	HG3	2.199	0.009	2
1	A	306	GLN	C	175.476	0.025	1
1	A	306	GLN	CA	54.064	0.032	1
1	A	306	GLN	CB	30.75	0.020	1
1	A	306	GLN	CG	34.237	0.030	1
1	A	306	GLN	N	125.589	0.035	1
1	A	307	VAL	H	9.889	0.006	1
1	A	307	VAL	HA	5.375	0.005	1
1	A	307	VAL	HB	2.454	0.001	1
1	A	307	VAL	HG11	0.859	0.006	1
1	A	307	VAL	HG12	0.859	0.006	1
1	A	307	VAL	HG13	0.859	0.006	1
1	A	307	VAL	HG21	1.057	0.006	1
1	A	307	VAL	HG22	1.057	0.006	1
1	A	307	VAL	HG23	1.057	0.006	1
1	A	307	VAL	C	175.797	0.008	1
1	A	307	VAL	CA	60.442	0.042	1
1	A	307	VAL	CB	32.736	0.034	1
1	A	307	VAL	CG1	21.396	0.049	2
1	A	307	VAL	CG2	21.654	0.064	2
1	A	307	VAL	N	131.31	0.031	1
1	A	308	GLY	H	9.369	0.011	1
1	A	308	GLY	HA2	4.534	0.006	2
1	A	308	GLY	HA3	3.641	0.004	2
1	A	308	GLY	C	172.864	0.004	1
1	A	308	GLY	CA	43.952	0.032	1
1	A	308	GLY	N	116.874	0.019	1
1	A	309	ASP	H	8.543	0.006	1
1	A	309	ASP	HA	4.882	0.005	1
1	A	309	ASP	HB2	2.865	0.003	2
1	A	309	ASP	HB3	2.011	0.009	2
1	A	309	ASP	C	175.802	0.006	1
1	A	309	ASP	CA	53.772	0.023	1
1	A	309	ASP	CB	41.114	0.086	1
1	A	309	ASP	N	121.894	0.027	1
1	A	310	LEU	H	8.18	0.005	1
1	A	310	LEU	HA	4.751	0.011	1
1	A	310	LEU	HB2	1.249	0.008	2
1	A	310	LEU	HB3	1.691	0.012	2
1	A	310	LEU	HG	1.457	0.007	1
1	A	310	LEU	HD11	0.752	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	310	LEU	HD12	0.752	0.002	1
1	A	310	LEU	HD13	0.752	0.002	1
1	A	310	LEU	HD21	0.79	0.005	1
1	A	310	LEU	HD22	0.79	0.005	1
1	A	310	LEU	HD23	0.79	0.005	1
1	A	310	LEU	C	178.107	0.003	1
1	A	310	LEU	CA	53.807	0.038	1
1	A	310	LEU	CB	41.758	0.023	1
1	A	310	LEU	CG	27.295	0.061	1
1	A	310	LEU	CD1	26.151	0.007	2
1	A	310	LEU	CD2	23.483	0.076	2
1	A	310	LEU	N	129.563	0.018	1
1	A	311	ASP	H	8.834	0.005	1
1	A	311	ASP	HA	4.234	0.008	1
1	A	311	ASP	HB2	2.806	0.007	2
1	A	311	ASP	HB3	3.266	0.007	2
1	A	311	ASP	C	175.099	0.001	1
1	A	311	ASP	CA	58.089	0.030	1
1	A	311	ASP	CB	38.882	0.055	1
1	A	311	ASP	N	116.168	0.033	1
1	A	312	ASN	H	8.801	0.003	1
1	A	312	ASN	HA	4.501	0.010	1
1	A	312	ASN	HB2	2.996	0.014	2
1	A	312	ASN	HB3	2.82	0.016	2
1	A	312	ASN	C	173.364	0.012	1
1	A	312	ASN	CA	53.674	0.069	1
1	A	312	ASN	CB	37.726	0.020	1
1	A	312	ASN	N	119.607	0.028	1
1	A	313	ARG	H	7.49	0.004	1
1	A	313	ARG	HA	4.88	0.003	1
1	A	313	ARG	HB2	1.694	0.009	2
1	A	313	ARG	HG2	1.508	0.004	2
1	A	313	ARG	HD2	3.143	0.010	2
1	A	313	ARG	HD3	2.958	0.000	2
1	A	313	ARG	C	174.499	0.003	1
1	A	313	ARG	CA	54.56	0.028	1
1	A	313	ARG	CB	33.37	0.032	1
1	A	313	ARG	CG	27.185	0.000	1
1	A	313	ARG	CD	43.715	0.038	1
1	A	313	ARG	N	117.254	0.020	1
1	A	314	SER	H	8.814	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	314	SER	HA	5.665	0.005	1
1	A	314	SER	HB2	3.82	0.005	2
1	A	314	SER	HB3	3.447	0.007	2
1	A	314	SER	C	172.443	0.007	1
1	A	314	SER	CA	58.085	0.031	1
1	A	314	SER	CB	67.138	0.063	1
1	A	314	SER	N	113.76	0.031	1
1	A	315	SER	H	9.387	0.006	1
1	A	315	SER	HA	5.645	0.006	1
1	A	315	SER	HB2	4.296	0.013	2
1	A	315	SER	HB3	3.614	0.013	2
1	A	315	SER	C	173.614	0.009	1
1	A	315	SER	CA	55.703	0.009	1
1	A	315	SER	CB	66.948	0.013	1
1	A	315	SER	N	118.892	0.019	1
1	A	316	LEU	H	9.32	0.008	1
1	A	316	LEU	HA	4.966	0.012	1
1	A	316	LEU	HB2	1.631	0.007	2
1	A	316	LEU	HB3	1.023	0.012	2
1	A	316	LEU	HG	1.427	0.009	1
1	A	316	LEU	HD11	0.721	0.022	1
1	A	316	LEU	HD12	0.721	0.022	1
1	A	316	LEU	HD13	0.721	0.022	1
1	A	316	LEU	HD21	0.443	0.006	1
1	A	316	LEU	HD22	0.443	0.006	1
1	A	316	LEU	HD23	0.443	0.006	1
1	A	316	LEU	C	175.347	0.011	1
1	A	316	LEU	CA	53.738	0.050	1
1	A	316	LEU	CB	44.535	0.038	1
1	A	316	LEU	CG	27.558	0.016	1
1	A	316	LEU	CD1	21.73	0.000	2
1	A	316	LEU	CD2	24.848	0.105	2
1	A	316	LEU	N	119.297	0.015	1
1	A	317	GLN	H	8.351	0.005	1
1	A	317	GLN	HA	4.989	0.005	1
1	A	317	GLN	HB2	1.836	0.046	2
1	A	317	GLN	HB3	2.147	0.013	2
1	A	317	GLN	HG2	2.645	0.000	2
1	A	317	GLN	C	173.875	0.008	1
1	A	317	GLN	CA	55.417	0.008	1
1	A	317	GLN	CB	34.264	0.096	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	317	GLN	CG	35.675	0.000	1
1	A	317	GLN	N	122.665	0.039	1
1	A	318	PHE	H	9.022	0.004	1
1	A	318	PHE	HA	5.305	0.006	1
1	A	318	PHE	HB2	3.018	0.009	2
1	A	318	PHE	HB3	2.719	0.021	2
1	A	318	PHE	C	174.968	0.005	1
1	A	318	PHE	CA	58.093	0.050	1
1	A	318	PHE	CB	42.464	0.082	1
1	A	318	PHE	N	126.094	0.035	1
1	A	319	ILE	H	9.317	0.004	1
1	A	319	ILE	HA	4.473	0.005	1
1	A	319	ILE	HB	1.76	0.010	1
1	A	319	ILE	HG12	1.471	0.013	2
1	A	319	ILE	HG13	1.123	0.038	2
1	A	319	ILE	HG21	0.935	0.000	1
1	A	319	ILE	HG22	0.935	0.000	1
1	A	319	ILE	HG23	0.935	0.000	1
1	A	319	ILE	HD11	0.805	0.000	1
1	A	319	ILE	HD12	0.805	0.000	1
1	A	319	ILE	HD13	0.805	0.000	1
1	A	319	ILE	C	175.37	0.012	1
1	A	319	ILE	CA	60.219	0.091	1
1	A	319	ILE	CB	40.039	0.011	1
1	A	319	ILE	CG1	28.107	0.055	1
1	A	319	ILE	CG2	18.015	0.000	1
1	A	319	ILE	CD1	12.918	0.000	1
1	A	319	ILE	N	121.34	0.040	1
1	A	320	ASP	H	9.104	0.004	1
1	A	320	ASP	HA	4.482	0.000	1
1	A	320	ASP	HB2	3.211	0.000	2
1	A	320	ASP	HB3	2.708	0.000	2
1	A	320	ASP	C	176.167	0.000	1
1	A	320	ASP	CA	53.177	0.000	1
1	A	320	ASP	N	127.859	0.020	1
1	A	321	PRO	HA	4.455	0.007	1
1	A	321	PRO	HB2	1.72	0.007	2
1	A	321	PRO	HB3	2.556	0.008	2
1	A	321	PRO	HD2	3.367	0.000	2
1	A	321	PRO	HD3	3.367	0.000	2
1	A	321	PRO	C	178.019	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	321	PRO	CA	65.022	0.016	1
1	A	321	PRO	CB	32.355	0.011	1
1	A	321	PRO	CG	27.436	0.000	1
1	A	321	PRO	CD	50.771	0.000	1
1	A	322	LYS	H	7.954	0.005	1
1	A	322	LYS	HA	4.327	0.006	1
1	A	322	LYS	HB2	1.786	0.027	2
1	A	322	LYS	HG2	1.378	0.000	2
1	A	322	LYS	HD2	1.667	0.000	2
1	A	322	LYS	HE2	2.998	0.000	2
1	A	322	LYS	C	176.46	0.006	1
1	A	322	LYS	CA	55.027	0.030	1
1	A	322	LYS	CB	32.289	0.015	1
1	A	322	LYS	CG	25.262	0.000	1
1	A	322	LYS	CD	28.861	0.000	1
1	A	322	LYS	CE	42.269	0.000	1
1	A	322	LYS	N	115.356	0.028	1
1	A	323	GLY	H	8.429	0.003	1
1	A	323	GLY	HA2	4.045	0.006	2
1	A	323	GLY	HA3	3.49	0.005	2
1	A	323	GLY	C	174.505	0.006	1
1	A	323	GLY	CA	45.49	0.032	1
1	A	323	GLY	N	107.803	0.019	1
1	A	324	HIS	H	8.371	0.004	1
1	A	324	HIS	HA	5.075	0.017	1
1	A	324	HIS	HB2	3.315	0.014	2
1	A	324	HIS	C	175.192	0.004	1
1	A	324	HIS	CA	53.811	0.040	1
1	A	324	HIS	CB	30.257	0.027	1
1	A	324	HIS	N	120.489	0.028	1
1	A	325	THR	H	8.261	0.004	1
1	A	325	THR	HA	4.882	0.004	1
1	A	325	THR	HB	4.646	0.013	1
1	A	325	THR	HG21	1.329	0.002	1
1	A	325	THR	HG22	1.329	0.002	1
1	A	325	THR	HG23	1.329	0.002	1
1	A	325	THR	C	175.861	0.000	1
1	A	325	THR	CA	62.024	0.045	1
1	A	325	THR	CB	69.481	0.020	1
1	A	325	THR	CG2	22.848	0.000	1
1	A	325	THR	N	115.322	0.044	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	326	LEU	H	7.872	0.005	1
1	A	326	LEU	HA	4.469	0.013	1
1	A	326	LEU	HB2	1.873	0.005	2
1	A	326	LEU	HB3	1.753	0.003	2
1	A	326	LEU	HG	1.948	0.000	1
1	A	326	LEU	HD21	0.772	0.001	1
1	A	326	LEU	HD22	0.772	0.001	1
1	A	326	LEU	HD23	0.772	0.001	1
1	A	326	LEU	C	178.749	0.009	1
1	A	326	LEU	CA	55.461	0.046	1
1	A	326	LEU	CB	41.226	0.026	1
1	A	326	LEU	CG	27.11	0.000	1
1	A	326	LEU	CD1	21.984	0.000	2
1	A	326	LEU	CD2	27.193	0.059	2
1	A	326	LEU	N	120.291	0.030	1
1	A	327	THR	H	8.42	0.004	1
1	A	327	THR	HA	4.31	0.011	1
1	A	327	THR	HB	4.723	0.012	1
1	A	327	THR	HG21	1.376	0.000	1
1	A	327	THR	HG22	1.376	0.000	1
1	A	327	THR	HG23	1.376	0.000	1
1	A	327	THR	C	175.106	0.002	1
1	A	327	THR	CA	61.169	0.036	1
1	A	327	THR	CB	70.816	0.064	1
1	A	327	THR	CG2	21.981	0.000	1
1	A	327	THR	N	111.05	0.016	1
1	A	328	GLN	H	9.121	0.004	1
1	A	328	GLN	HA	3.778	0.010	1
1	A	328	GLN	HB2	2.227	0.000	2
1	A	328	GLN	HB3	2.151	0.010	2
1	A	328	GLN	HG2	2.427	0.000	2
1	A	328	GLN	C	177.76	0.000	1
1	A	328	GLN	CA	59.862	0.056	1
1	A	328	GLN	CB	28.584	0.028	1
1	A	328	GLN	CG	33.338	0.000	1
1	A	328	GLN	N	121.167	0.024	1
1	A	329	SER	H	8.47	0.004	1
1	A	329	SER	HA	4.221	0.014	1
1	A	329	SER	HB2	3.846	0.000	2
1	A	329	SER	C	177.651	0.009	1
1	A	329	SER	CA	61.77	0.081	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	329	SER	CB	62.363	0.000	1
1	A	329	SER	N	112.023	0.014	1
1	A	330	GLN	H	7.466	0.008	1
1	A	330	GLN	HA	4.07	0.006	1
1	A	330	GLN	HB2	2.355	0.017	2
1	A	330	GLN	HB3	1.731	0.012	2
1	A	330	GLN	HG2	2.267	0.000	2
1	A	330	GLN	C	177.166	0.003	1
1	A	330	GLN	CA	58.704	0.040	1
1	A	330	GLN	CB	29.965	0.047	1
1	A	330	GLN	CG	34.832	0.000	1
1	A	330	GLN	N	122.477	0.023	1
1	A	331	ASN	H	8.531	0.004	1
1	A	331	ASN	HA	4.076	0.003	1
1	A	331	ASN	HB2	2.821	0.006	2
1	A	331	ASN	HB3	2.334	0.014	2
1	A	331	ASN	C	177.225	0.002	1
1	A	331	ASN	CA	57.888	0.024	1
1	A	331	ASN	CB	41.655	0.037	1
1	A	331	ASN	N	117.438	0.022	1
1	A	332	ASP	H	8.788	0.003	1
1	A	332	ASP	HA	4.425	0.012	1
1	A	332	ASP	HB2	2.804	0.001	2
1	A	332	ASP	HB3	2.7	0.010	2
1	A	332	ASP	C	179.893	0.009	1
1	A	332	ASP	CA	57.36	0.026	1
1	A	332	ASP	CB	39.701	0.036	1
1	A	332	ASP	N	116.884	0.032	1
1	A	333	ALA	H	7.693	0.004	1
1	A	333	ALA	HA	4.2	0.002	1
1	A	333	ALA	HB1	1.524	0.008	1
1	A	333	ALA	HB2	1.524	0.008	1
1	A	333	ALA	HB3	1.524	0.008	1
1	A	333	ALA	C	179.051	0.003	1
1	A	333	ALA	CA	54.441	0.058	1
1	A	333	ALA	CB	18.904	0.017	1
1	A	333	ALA	N	123.117	0.026	1
1	A	334	LEU	H	7.771	0.003	1
1	A	334	LEU	HA	4.139	0.011	1
1	A	334	LEU	HB2	2.315	0.015	2
1	A	334	LEU	HB3	1.536	0.012	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	334	LEU	HG	1.781	0.005	1
1	A	334	LEU	HD11	0.401	0.000	1
1	A	334	LEU	HD12	0.401	0.000	1
1	A	334	LEU	HD13	0.401	0.000	1
1	A	334	LEU	HD21	0.444	0.000	1
1	A	334	LEU	HD22	0.444	0.000	1
1	A	334	LEU	HD23	0.444	0.000	1
1	A	334	LEU	C	178.356	0.008	1
1	A	334	LEU	CA	55.58	0.039	1
1	A	334	LEU	CB	42.531	0.016	1
1	A	334	LEU	CG	26.106	0.000	1
1	A	334	LEU	CD1	26.072	0.003	2
1	A	334	LEU	CD2	22.508	0.014	2
1	A	334	LEU	N	116.464	0.016	1
1	A	335	VAL	H	7.69	0.004	1
1	A	335	VAL	HA	3.465	0.008	1
1	A	335	VAL	HB	2.266	0.016	1
1	A	335	VAL	HG11	0.913	0.005	1
1	A	335	VAL	HG12	0.913	0.005	1
1	A	335	VAL	HG13	0.913	0.005	1
1	A	335	VAL	HG21	1.107	0.008	1
1	A	335	VAL	HG22	1.107	0.008	1
1	A	335	VAL	HG23	1.107	0.008	1
1	A	335	VAL	C	177.487	0.011	1
1	A	335	VAL	CA	67.719	0.041	1
1	A	335	VAL	CB	31.266	0.040	1
1	A	335	VAL	CG1	21.279	0.035	2
1	A	335	VAL	CG2	24.366	0.037	2
1	A	335	VAL	N	122.325	0.023	1
1	A	336	ALA	H	8.212	0.005	1
1	A	336	ALA	HA	4.26	0.005	1
1	A	336	ALA	HB1	1.54	0.005	1
1	A	336	ALA	HB2	1.54	0.005	1
1	A	336	ALA	HB3	1.54	0.005	1
1	A	336	ALA	C	180.995	0.004	1
1	A	336	ALA	CA	54.851	0.015	1
1	A	336	ALA	CB	18.674	0.023	1
1	A	336	ALA	N	118.605	0.023	1
1	A	337	VAL	H	6.772	0.004	1
1	A	337	VAL	HA	3.423	0.006	1
1	A	337	VAL	HB	2.154	0.009	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	337	VAL	HG11	0.94	0.003	1
1	A	337	VAL	HG12	0.94	0.003	1
1	A	337	VAL	HG13	0.94	0.003	1
1	A	337	VAL	HG21	0.742	0.009	1
1	A	337	VAL	HG22	0.742	0.009	1
1	A	337	VAL	HG23	0.742	0.009	1
1	A	337	VAL	C	176.89	0.001	1
1	A	337	VAL	CA	66.011	0.053	1
1	A	337	VAL	CB	32.078	0.018	1
1	A	337	VAL	CG1	22.336	0.000	2
1	A	337	VAL	CG2	22.336	0.000	2
1	A	337	VAL	N	116.286	0.013	1
1	A	338	PHE	H	8.602	0.012	1
1	A	338	PHE	HA	4.065	0.004	1
1	A	338	PHE	HB2	3.004	0.006	2
1	A	338	PHE	C	177.821	0.007	1
1	A	338	PHE	CA	63.249	0.020	1
1	A	338	PHE	CB	38.519	0.016	1
1	A	338	PHE	N	116.884	0.025	1
1	A	339	GLN	H	9.059	0.004	1
1	A	339	GLN	HA	4.18	0.004	1
1	A	339	GLN	HB2	2.127	0.005	2
1	A	339	GLN	HB3	2.419	0.022	2
1	A	339	GLN	C	179.177	0.002	1
1	A	339	GLN	CA	59.738	0.030	1
1	A	339	GLN	CB	28.448	0.041	1
1	A	339	GLN	CG	33.891	0.000	1
1	A	339	GLN	N	121.479	0.038	1
1	A	340	ALA	H	7.526	0.004	1
1	A	340	ALA	HA	4.248	0.000	1
1	A	340	ALA	HB1	1.513	0.006	1
1	A	340	ALA	HB2	1.513	0.006	1
1	A	340	ALA	HB3	1.513	0.006	1
1	A	340	ALA	C	180.724	0.007	1
1	A	340	ALA	CA	54.879	0.025	1
1	A	340	ALA	CB	18.221	0.044	1
1	A	340	ALA	N	120.165	0.065	1
1	A	341	ALA	H	8.409	0.004	1
1	A	341	ALA	HA	3.788	0.011	1
1	A	341	ALA	HB1	1.226	0.009	1
1	A	341	ALA	HB2	1.226	0.009	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	341	ALA	HB3	1.226	0.009	1
1	A	341	ALA	C	179.711	0.007	1
1	A	341	ALA	CA	55.71	0.010	1
1	A	341	ALA	CB	18.926	0.015	1
1	A	341	ALA	N	121.207	0.028	1
1	A	342	PHE	H	8.468	0.005	1
1	A	342	PHE	HA	4.584	0.004	1
1	A	342	PHE	HB2	3.405	0.007	2
1	A	342	PHE	HB3	3.198	0.004	2
1	A	342	PHE	C	176.504	0.007	1
1	A	342	PHE	CA	59.692	0.016	1
1	A	342	PHE	CB	39.064	0.006	1
1	A	342	PHE	N	112.735	0.036	1
1	A	343	SER	H	7.582	0.003	1
1	A	343	SER	HA	4.582	0.003	1
1	A	343	SER	HB2	4.116	0.007	2
1	A	343	SER	C	174.125	0.007	1
1	A	343	SER	CA	59.65	0.046	1
1	A	343	SER	CB	64.287	0.024	1
1	A	343	SER	N	113.796	0.035	1
1	A	344	LYS	H	7.542	0.011	1
1	A	344	LYS	HA	4.694	0.000	1
1	A	344	LYS	HB2	1.834	0.000	2
1	A	344	LYS	C	174.389	0.000	1
1	A	344	LYS	N	123.073	0.026	1
1	A	345	PRO	HA	4.46	0.004	1
1	A	345	PRO	HB2	1.996	0.015	2
1	A	345	PRO	HB3	2.295	0.012	2
1	A	345	PRO	HG2	3.897	0.005	2
1	A	345	PRO	HG3	3.71	0.000	2
1	A	345	PRO	CA	63.448	0.047	1
1	A	345	PRO	CB	32.268	0.018	1
1	A	345	PRO	CG	27.34	0.000	1
1	A	345	PRO	CD	50.701	0.000	1
1	A	346	GLY	H	7.994	0.004	1
1	A	346	GLY	HA2	3.731	0.000	1
1	A	346	GLY	CA	46.312	0.000	1
1	A	346	GLY	N	115.149	0.018	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
$^{13}C_{\alpha}$	248	-0.49 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	226	0.15 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	246	-0.20 ± 0.08	None needed (< 0.5 ppm)
^{15}N	238	-0.35 ± 0.24	None needed (< 0.5 ppm)

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 78%, i.e. 1175 atoms were assigned a chemical shift out of a possible 1506. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	562/562 (100%)	229/229 (100%)	224/224 (100%)	109/109 (100%)
Sidechain	607/863 (70%)	397/557 (71%)	210/265 (79%)	0/41 (0%)
Aromatic	6/81 (7%)	3/38 (8%)	0/40 (0%)	3/3 (100%)
Overall	1175/1506 (78%)	629/824 (76%)	434/529 (82%)	112/153 (73%)

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: