wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2MU2
BMRB ID	:	25127
Title	:	NMR structure of the cap domain of NP_346487.1, a putative phosphoglycolate phosphatase from Streptococcus pneumoniae TIGR4
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Deposited on	:	2014-09-03

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:

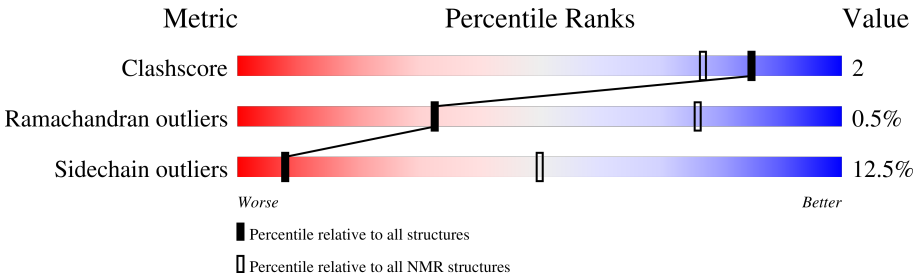
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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	208	23% · 8% 66%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:21-A:74 (54)	0.53	7

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1156 atoms, of which 578 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hydrolase, haloacid dehalogenase-like family.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	71	1156	369	578	95	114	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0H2URV7
A	0	HIS	-	expression tag	UNP A0A0H2URV7

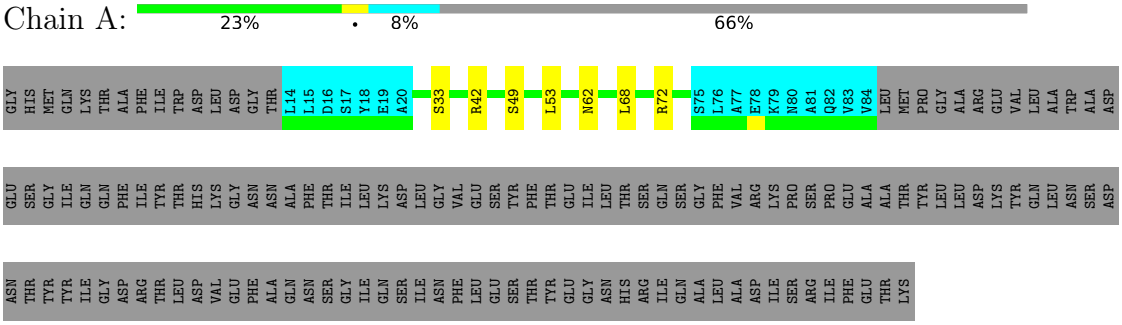
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain A:

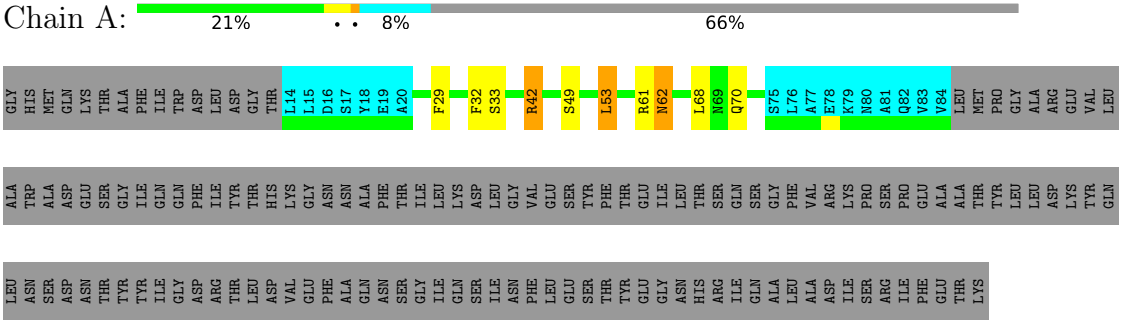


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 7. Colouring as in section 4.1 above.

• Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
CYANA	structure solution	3.0
OPAL	refinement	
UNIO-ATNOS/CANDID	structure solution	
CYANA	refinement	3.0

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	2213
Number of shifts mapped to atoms	798
Number of unparsed shifts	0
Number of shifts with mapping errors	1415
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.61±0.01	0±0/456 (0.0± 0.0%)	1.05±0.06	2±1/616 (0.2± 0.2%)
All	All	0.61	0/9120 (0.0%)	1.05	30/12320 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.8
All	All	0	16

There are no bond-length outliers.

5 of 12 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	42	ARG	NE-CZ-NH2	-8.12	116.24	120.30	15	4
1	A	68	LEU	CB-CG-CD1	7.00	122.89	111.00	13	7
1	A	72	ARG	NE-CZ-NH2	-6.72	116.94	120.30	4	3
1	A	61	ARG	CD-NE-CZ	6.34	132.47	123.60	3	1
1	A	71	VAL	CG1-CB-CG2	-6.27	100.86	110.90	17	1

There are no chirality outliers.

5 of 6 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	42	ARG	Sidechain	6
1	A	72	ARG	Sidechain	3
1	A	36	TYR	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	48	TYR	Sidechain	2
1	A	61	ARG	Sidechain	2

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	449	450	450	2±1
All	All	8980	9000	9000	40

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 2.

5 of 19 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LEU:HD11	1:A:65:VAL:HG23	0.58	1.76	14	1
1:A:29:PHE:CZ	1:A:53:LEU:HD11	0.54	2.36	12	10
1:A:34:ILE:HD13	1:A:57:VAL:HG11	0.54	1.79	16	1
1:A:32:PHE:CZ	1:A:68:LEU:HD12	0.53	2.39	17	3
1:A:54:LEU:HD12	1:A:54:LEU:H	0.52	1.63	3	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	54/208 (26%)	49±1 (90±2%)	5±1 (9±2%)	0±1 (0±1%)	32	76
All	All	1080/4160 (26%)	974 (90%)	101 (9%)	5 (0%)	32	76

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occur-

rence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	62	ASN	3
1	A	49	SER	1
1	A	33	SER	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	50/181 (28%)	44±1 (88±3%)	6±1 (12±3%)	8 50
All	All	1000/3620 (28%)	875 (88%)	125 (12%)	8 50

5 of 26 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	33	SER	12
1	A	53	LEU	11
1	A	49	SER	10
1	A	62	ASN	10
1	A	72	ARG	9

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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

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 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	2213
Number of shifts mapped to atoms	798
Number of unparsed shifts	0
Number of shifts with mapping errors	1415
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

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 1415) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-1	GLY	CA	43.22	0.3	1
1	A	-1	GLY	HA2	3.73	0.020	1
1	A	-1	GLY	HA3	3.73	0.020	1
1	A	0	HIS	CA	55.898	0.3	1
1	A	0	HIS	CB	30.061	0.3	1
1	A	0	HIS	CD2	119.624	0.3	1
1	A	0	HIS	CE1	137.421	0.3	1
1	A	0	HIS	HA	4.648	0.020	1
1	A	0	HIS	HB2	3.039	0.020	2
1	A	0	HIS	HB3	3.086	0.020	2
1	A	0	HIS	HD2	7.051	0.020	1
1	A	0	HIS	HE1	8.099	0.020	1
1	A	1	MET	CA	55.481	0.3	1
1	A	1	MET	CB	32.606	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	CG	31.763	0.3	1
1	A	1	MET	CE	16.81	0.3	1
1	A	1	MET	HA	4.365	0.020	1
1	A	1	MET	HB2	1.741	0.020	2
1	A	1	MET	HB3	1.908	0.020	2
1	A	1	MET	HG2	2.356	0.020	1
1	A	1	MET	HG3	2.356	0.020	1
1	A	1	MET	N	122.414	0.3	1
1	A	1	MET	HE1	1.843	0.020	1
1	A	1	MET	HE2	1.843	0.020	1
1	A	1	MET	HE3	1.843	0.020	1
1	A	2	GLN	CA	55.83	0.3	1
1	A	2	GLN	CB	29.136	0.3	1
1	A	2	GLN	CG	33.72	0.3	1
1	A	2	GLN	HA	4.247	0.020	1
1	A	2	GLN	HB2	1.878	0.020	2
1	A	2	GLN	HB3	1.992	0.020	2
1	A	2	GLN	HG2	2.292	0.020	1
1	A	2	GLN	HG3	2.292	0.020	1
1	A	2	GLN	HE21	7.463	0.020	1
1	A	2	GLN	HE22	6.807	0.020	1
1	A	2	GLN	N	120.814	0.3	1
1	A	2	GLN	NE2	112.396	0.3	1
1	A	3	LYS	CA	56.803	0.3	1
1	A	3	LYS	CB	32.088	0.3	1
1	A	3	LYS	CG	24.651	0.3	1
1	A	3	LYS	CD	29.032	0.3	1
1	A	3	LYS	CE	42.226	0.3	1
1	A	3	LYS	HA	4.184	0.020	1
1	A	3	LYS	HB2	1.715	0.020	2
1	A	3	LYS	HB3	1.85	0.020	2
1	A	3	LYS	HG2	1.347	0.020	2
1	A	3	LYS	HG3	1.422	0.020	2
1	A	3	LYS	HD2	1.668	0.020	1
1	A	3	LYS	HD3	1.668	0.020	1
1	A	3	LYS	HE2	2.943	0.020	1
1	A	3	LYS	HE3	2.943	0.020	1
1	A	3	LYS	N	122.403	0.3	1
1	A	4	THR	CA	62.39	0.3	1
1	A	4	THR	CB	70.75	0.3	1
1	A	4	THR	CG2	21.241	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	THR	HA	5.06	0.020	1
1	A	4	THR	HB	3.585	0.020	1
1	A	4	THR	N	122.564	0.3	1
1	A	4	THR	HG21	0.992	0.020	1
1	A	4	THR	HG22	0.992	0.020	1
1	A	4	THR	HG23	0.992	0.020	1
1	A	5	ALA	CA	50.324	0.3	1
1	A	5	ALA	CB	24.441	0.3	1
1	A	5	ALA	HA	5.577	0.020	1
1	A	5	ALA	N	127.062	0.3	1
1	A	5	ALA	HB1	1.514	0.020	1
1	A	5	ALA	HB2	1.514	0.020	1
1	A	5	ALA	HB3	1.514	0.020	1
1	A	6	PHE	CA	51.706	0.3	1
1	A	6	PHE	CB	41.224	0.3	1
1	A	6	PHE	CD1	129.228	0.3	1
1	A	6	PHE	CE1	129.969	0.3	1
1	A	6	PHE	CZ	128.581	0.3	1
1	A	6	PHE	HA	5.576	0.020	1
1	A	6	PHE	HB2	2.418	0.020	2
1	A	6	PHE	HB3	3.077	0.020	2
1	A	6	PHE	HD1	7.17	0.020	1
1	A	6	PHE	HD2	7.17	0.020	1
1	A	6	PHE	HE1	6.7	0.020	1
1	A	6	PHE	HE2	6.7	0.020	1
1	A	6	PHE	HZ	6.546	0.020	1
1	A	6	PHE	N	121.363	0.3	1
1	A	7	ILE	CA	59.953	0.3	1
1	A	7	ILE	CB	39.488	0.3	1
1	A	7	ILE	CG1	26.468	0.3	1
1	A	7	ILE	CG2	18.833	0.3	1
1	A	7	ILE	CD1	13.92	0.3	1
1	A	7	ILE	HA	4.56	0.020	1
1	A	7	ILE	HB	2.027	0.020	1
1	A	7	ILE	HG12	0.766	0.020	2
1	A	7	ILE	HG13	1.587	0.020	2
1	A	7	ILE	N	123.065	0.3	1
1	A	7	ILE	HG21	0.979	0.020	1
1	A	7	ILE	HG22	0.979	0.020	1
1	A	7	ILE	HG23	0.979	0.020	1
1	A	7	ILE	HD11	0.588	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ILE	HD12	0.588	0.020	1
1	A	7	ILE	HD13	0.588	0.020	1
1	A	8	TRP	CA	58.419	0.3	1
1	A	8	TRP	CB	30.679	0.3	1
1	A	8	TRP	CD1	126.46	0.3	1
1	A	8	TRP	CE3	120.177	0.3	1
1	A	8	TRP	CZ2	113.856	0.3	1
1	A	8	TRP	CZ3	121.37	0.3	1
1	A	8	TRP	CH2	123.178	0.3	1
1	A	8	TRP	HA	4.349	0.020	1
1	A	8	TRP	HB2	3.0	0.020	2
1	A	8	TRP	HB3	3.473	0.020	2
1	A	8	TRP	HD1	7.588	0.020	1
1	A	8	TRP	HE1	11.173	0.020	1
1	A	8	TRP	HE3	7.397	0.020	1
1	A	8	TRP	HZ2	7.239	0.020	1
1	A	8	TRP	HZ3	6.603	0.020	1
1	A	8	TRP	HH2	6.78	0.020	1
1	A	8	TRP	N	127.163	0.3	1
1	A	8	TRP	NE1	130.001	0.3	1
1	A	9	ASP	CA	52.65	0.3	1
1	A	9	ASP	CB	42.458	0.3	1
1	A	9	ASP	HA	5.008	0.020	1
1	A	9	ASP	HB2	2.912	0.020	1
1	A	9	ASP	HB3	2.912	0.020	1
1	A	9	ASP	N	119.77	0.3	1
1	A	10	LEU	CB	44.069	0.3	1
1	A	10	LEU	CG	26.362	0.3	1
1	A	10	LEU	CD1	26.081	0.3	1
1	A	10	LEU	CD2	25.122	0.3	1
1	A	10	LEU	HB2	1.474	0.020	2
1	A	10	LEU	HB3	1.348	0.020	2
1	A	10	LEU	HG	1.336	0.020	1
1	A	10	LEU	HD11	0.652	0.020	1
1	A	10	LEU	HD12	0.652	0.020	1
1	A	10	LEU	HD13	0.652	0.020	1
1	A	10	LEU	HD21	0.59	0.020	1
1	A	10	LEU	HD22	0.59	0.020	1
1	A	10	LEU	HD23	0.59	0.020	1
1	A	11	ASP	CA	57.21	0.3	1
1	A	11	ASP	CB	40.58	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ASP	HA	4.17	0.020	1
1	A	11	ASP	HB2	2.599	0.020	1
1	A	11	ASP	HB3	2.599	0.020	1
1	A	12	GLY	CA	45.817	0.3	1
1	A	12	GLY	HA2	3.609	0.020	1
1	A	12	GLY	N	113.46	0.3	1
1	A	13	THR	CA	64.702	0.3	1
1	A	13	THR	CB	68.325	0.3	1
1	A	13	THR	CG2	22.127	0.3	1
1	A	13	THR	HA	4.28	0.020	1
1	A	13	THR	HB	3.697	0.020	1
1	A	13	THR	N	114.9	0.3	1
1	A	13	THR	HG21	1.249	0.020	1
1	A	13	THR	HG22	1.249	0.020	1
1	A	13	THR	HG23	1.249	0.020	1
1	A	85	LEU	CA	54.538	0.3	1
1	A	85	LEU	CB	42.554	0.3	1
1	A	85	LEU	CG	26.979	0.3	1
1	A	85	LEU	CD1	22.899	0.3	1
1	A	85	LEU	CD2	26.44	0.3	1
1	A	85	LEU	HA	4.584	0.020	1
1	A	85	LEU	HB2	1.588	0.020	2
1	A	85	LEU	HB3	1.74	0.020	2
1	A	85	LEU	HG	1.753	0.020	1
1	A	85	LEU	N	119.969	0.3	1
1	A	85	LEU	HD11	0.604	0.020	1
1	A	85	LEU	HD12	0.604	0.020	1
1	A	85	LEU	HD13	0.604	0.020	1
1	A	85	LEU	HD21	0.841	0.020	1
1	A	85	LEU	HD22	0.841	0.020	1
1	A	85	LEU	HD23	0.841	0.020	1
1	A	86	MET	CA	53.201	0.3	1
1	A	86	MET	CB	31.619	0.3	1
1	A	86	MET	CG	32.408	0.3	1
1	A	86	MET	CE	16.795	0.3	1
1	A	86	MET	HA	4.493	0.020	1
1	A	86	MET	HB2	1.684	0.020	2
1	A	86	MET	HB3	1.894	0.020	2
1	A	86	MET	HG2	1.898	0.020	2
1	A	86	MET	HG3	2.395	0.020	2
1	A	86	MET	N	120.935	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	MET	HE1	1.988	0.020	1
1	A	86	MET	HE2	1.988	0.020	1
1	A	86	MET	HE3	1.988	0.020	1
1	A	87	PRO	CA	64.058	0.3	1
1	A	87	PRO	CB	31.414	0.3	1
1	A	87	PRO	CG	27.949	0.3	1
1	A	87	PRO	CD	50.754	0.3	1
1	A	87	PRO	HA	4.343	0.020	1
1	A	87	PRO	HB2	1.838	0.020	2
1	A	87	PRO	HB3	2.301	0.020	2
1	A	87	PRO	HG2	2.001	0.020	2
1	A	87	PRO	HG3	2.116	0.020	2
1	A	87	PRO	HD2	3.554	0.020	2
1	A	87	PRO	HD3	4.053	0.020	2
1	A	88	GLY	CA	45.567	0.3	1
1	A	88	GLY	HA2	3.864	0.020	1
1	A	88	GLY	N	113.384	0.3	1
1	A	89	ALA	CA	55.435	0.3	1
1	A	89	ALA	CB	20.206	0.3	1
1	A	89	ALA	HA	3.863	0.020	1
1	A	89	ALA	N	123.112	0.3	1
1	A	89	ALA	HB1	1.367	0.020	1
1	A	89	ALA	HB2	1.367	0.020	1
1	A	89	ALA	HB3	1.367	0.020	1
1	A	90	ARG	CA	60.278	0.3	1
1	A	90	ARG	CB	29.361	0.3	1
1	A	90	ARG	CG	28.376	0.3	1
1	A	90	ARG	CD	42.824	0.3	1
1	A	90	ARG	HA	3.524	0.020	1
1	A	90	ARG	HB2	1.623	0.020	2
1	A	90	ARG	HB3	1.689	0.020	2
1	A	90	ARG	HG2	1.497	0.020	2
1	A	90	ARG	HG3	1.578	0.020	2
1	A	90	ARG	HD2	3.083	0.020	2
1	A	90	ARG	HD3	3.216	0.020	2
1	A	90	ARG	HE	7.309	0.020	1
1	A	90	ARG	N	116.517	0.3	1
1	A	90	ARG	NE	83.561	0.3	1
1	A	91	GLU	CA	60.71	0.3	1
1	A	91	GLU	CB	28.357	0.3	1
1	A	91	GLU	CG	37.58	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	GLU	HA	3.904	0.020	1
1	A	91	GLU	HB2	1.833	0.020	2
1	A	91	GLU	HB3	2.106	0.020	2
1	A	91	GLU	HG2	2.154	0.020	2
1	A	91	GLU	HG3	2.476	0.020	2
1	A	91	GLU	N	117.674	0.3	1
1	A	92	VAL	CA	65.955	0.3	1
1	A	92	VAL	CB	31.11	0.3	1
1	A	92	VAL	CG1	23.551	0.3	1
1	A	92	VAL	CG2	22.05	0.3	1
1	A	92	VAL	HA	4.231	0.020	1
1	A	92	VAL	HB	2.101	0.020	1
1	A	92	VAL	N	121.435	0.3	1
1	A	92	VAL	HG11	1.203	0.020	1
1	A	92	VAL	HG12	1.203	0.020	1
1	A	92	VAL	HG13	1.203	0.020	1
1	A	92	VAL	HG21	1.311	0.020	1
1	A	92	VAL	HG22	1.311	0.020	1
1	A	92	VAL	HG23	1.311	0.020	1
1	A	93	LEU	CA	58.084	0.3	1
1	A	93	LEU	CB	40.955	0.3	1
1	A	93	LEU	CG	26.18	0.3	1
1	A	93	LEU	CD1	23.202	0.3	1
1	A	93	LEU	CD2	25.006	0.3	1
1	A	93	LEU	HA	3.958	0.020	1
1	A	93	LEU	HB2	-0.141	0.020	2
1	A	93	LEU	HB3	1.266	0.020	2
1	A	93	LEU	HG	1.412	0.020	1
1	A	93	LEU	N	122.574	0.3	1
1	A	93	LEU	HD11	0.182	0.020	1
1	A	93	LEU	HD12	0.182	0.020	1
1	A	93	LEU	HD13	0.182	0.020	1
1	A	93	LEU	HD21	0.405	0.020	1
1	A	93	LEU	HD22	0.405	0.020	1
1	A	93	LEU	HD23	0.405	0.020	1
1	A	94	ALA	CA	54.93	0.3	1
1	A	94	ALA	CB	18.285	0.3	1
1	A	94	ALA	HA	3.922	0.020	1
1	A	94	ALA	N	118.71	0.3	1
1	A	94	ALA	HB1	1.431	0.020	1
1	A	94	ALA	HB2	1.431	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	ALA	HB3	1.431	0.020	1
1	A	95	TRP	CA	61.147	0.3	1
1	A	95	TRP	CB	27.769	0.3	1
1	A	95	TRP	CD1	126.914	0.3	1
1	A	95	TRP	CE3	120.079	0.3	1
1	A	95	TRP	CZ2	114.275	0.3	1
1	A	95	TRP	CZ3	120.115	0.3	1
1	A	95	TRP	CH2	123.612	0.3	1
1	A	95	TRP	HA	4.073	0.020	1
1	A	95	TRP	HB2	3.329	0.020	2
1	A	95	TRP	HB3	3.53	0.020	2
1	A	95	TRP	HD1	7.221	0.020	1
1	A	95	TRP	HE1	10.052	0.020	1
1	A	95	TRP	HE3	7.68	0.020	1
1	A	95	TRP	HZ2	7.261	0.020	1
1	A	95	TRP	HZ3	6.681	0.020	1
1	A	95	TRP	HH2	6.607	0.020	1
1	A	95	TRP	N	121.304	0.3	1
1	A	95	TRP	NE1	130.9	0.3	1
1	A	96	ALA	CA	54.953	0.3	1
1	A	96	ALA	CB	17.74	0.3	1
1	A	96	ALA	HA	2.621	0.020	1
1	A	96	ALA	N	125.853	0.3	1
1	A	96	ALA	HB1	1.169	0.020	1
1	A	96	ALA	HB2	1.169	0.020	1
1	A	96	ALA	HB3	1.169	0.020	1
1	A	97	ASP	CA	57.55	0.3	1
1	A	97	ASP	CB	43.189	0.3	1
1	A	97	ASP	HA	4.162	0.020	1
1	A	97	ASP	HB2	2.658	0.020	2
1	A	97	ASP	HB3	2.719	0.020	2
1	A	97	ASP	N	118.094	0.3	1
1	A	98	GLU	CA	58.62	0.3	1
1	A	98	GLU	CB	29.005	0.3	1
1	A	98	GLU	CG	36.04	0.3	1
1	A	98	GLU	HA	3.828	0.020	1
1	A	98	GLU	HB2	1.896	0.020	2
1	A	98	GLU	HB3	1.995	0.020	2
1	A	98	GLU	HG2	2.243	0.020	1
1	A	98	GLU	HG3	2.243	0.020	1
1	A	98	GLU	N	120.13	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	SER	CA	58.908	0.3	1
1	A	99	SER	CB	62.867	0.3	1
1	A	99	SER	HA	4.021	0.020	1
1	A	99	SER	HB2	2.928	0.020	2
1	A	99	SER	HB3	3.265	0.020	2
1	A	99	SER	N	112.957	0.3	1
1	A	100	GLY	CA	45.374	0.3	1
1	A	100	GLY	HA2	3.571	0.020	1
1	A	100	GLY	N	108.185	0.3	1
1	A	101	ILE	CA	61.293	0.3	1
1	A	101	ILE	CB	37.746	0.3	1
1	A	101	ILE	CG1	28.102	0.3	1
1	A	101	ILE	CG2	14.762	0.3	1
1	A	101	ILE	CD1	12.944	0.3	1
1	A	101	ILE	HA	3.415	0.020	1
1	A	101	ILE	HB	0.861	0.020	1
1	A	101	ILE	HG12	-0.051	0.020	2
1	A	101	ILE	HG13	0.72	0.020	2
1	A	101	ILE	N	123.259	0.3	1
1	A	101	ILE	HG21	-0.533	0.020	1
1	A	101	ILE	HG22	-0.533	0.020	1
1	A	101	ILE	HG23	-0.533	0.020	1
1	A	101	ILE	HD11	-0.482	0.020	1
1	A	101	ILE	HD12	-0.482	0.020	1
1	A	101	ILE	HD13	-0.482	0.020	1
1	A	102	GLN	CA	56.172	0.3	1
1	A	102	GLN	CB	30.265	0.3	1
1	A	102	GLN	CG	34.847	0.3	1
1	A	102	GLN	HA	3.988	0.020	1
1	A	102	GLN	HB2	1.805	0.020	1
1	A	102	GLN	HB3	1.805	0.020	1
1	A	102	GLN	HG2	1.944	0.020	2
1	A	102	GLN	HG3	2.198	0.020	2
1	A	102	GLN	HE21	6.609	0.020	1
1	A	102	GLN	HE22	7.104	0.020	1
1	A	102	GLN	N	128.828	0.3	1
1	A	102	GLN	NE2	109.481	0.3	1
1	A	103	GLN	CA	55.881	0.3	1
1	A	103	GLN	CB	33.253	0.3	1
1	A	103	GLN	CG	37.391	0.3	1
1	A	103	GLN	HA	5.871	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	GLN	HB2	2.068	0.020	1
1	A	103	GLN	HB3	2.068	0.020	1
1	A	103	GLN	HG2	1.624	0.020	2
1	A	103	GLN	HG3	2.515	0.020	2
1	A	103	GLN	HE21	8.13	0.020	1
1	A	103	GLN	HE22	5.658	0.020	1
1	A	103	GLN	N	121.585	0.3	1
1	A	103	GLN	NE2	107.655	0.3	1
1	A	104	PHE	CA	55.957	0.3	1
1	A	104	PHE	CB	44.324	0.3	1
1	A	104	PHE	CD1	131.781	0.3	1
1	A	104	PHE	CE1	131.285	0.3	1
1	A	104	PHE	CZ	129.005	0.3	1
1	A	104	PHE	HA	5.377	0.020	1
1	A	104	PHE	HB2	2.763	0.020	2
1	A	104	PHE	HB3	3.265	0.020	2
1	A	104	PHE	HD1	7.133	0.020	1
1	A	104	PHE	HD2	7.133	0.020	1
1	A	104	PHE	HE1	6.403	0.020	1
1	A	104	PHE	HE2	6.403	0.020	1
1	A	104	PHE	HZ	6.247	0.020	1
1	A	104	PHE	N	120.327	0.3	1
1	A	105	ILE	CA	59.076	0.3	1
1	A	105	ILE	CB	43.036	0.3	1
1	A	105	ILE	CG1	28.768	0.3	1
1	A	105	ILE	CG2	17.37	0.3	1
1	A	105	ILE	CD1	13.676	0.3	1
1	A	105	ILE	HA	5.277	0.020	1
1	A	105	ILE	HB	1.373	0.020	1
1	A	105	ILE	HG12	0.525	0.020	2
1	A	105	ILE	HG13	0.803	0.020	2
1	A	105	ILE	N	120.427	0.3	1
1	A	105	ILE	HG21	0.713	0.020	1
1	A	105	ILE	HG22	0.713	0.020	1
1	A	105	ILE	HG23	0.713	0.020	1
1	A	105	ILE	HD11	-0.389	0.020	1
1	A	105	ILE	HD12	-0.389	0.020	1
1	A	105	ILE	HD13	-0.389	0.020	1
1	A	106	TYR	CA	56.801	0.3	1
1	A	106	TYR	CB	38.8	0.3	1
1	A	106	TYR	CD1	131.621	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	TYR	CE1	118.688	0.3	1
1	A	106	TYR	HA	5.706	0.020	1
1	A	106	TYR	HB2	2.676	0.020	2
1	A	106	TYR	HB3	2.803	0.020	2
1	A	106	TYR	HD1	6.598	0.020	1
1	A	106	TYR	HD2	6.598	0.020	1
1	A	106	TYR	HE1	6.3	0.020	1
1	A	106	TYR	HE2	6.3	0.020	1
1	A	106	TYR	N	123.027	0.3	1
1	A	107	THR	CA	57.45	0.3	1
1	A	107	THR	CB	70.58	0.3	1
1	A	107	THR	CG2	18.51	0.3	1
1	A	107	THR	HA	4.737	0.020	1
1	A	107	THR	HB	3.772	0.020	1
1	A	107	THR	N	124.164	0.3	1
1	A	107	THR	HG21	1.091	0.020	1
1	A	107	THR	HG22	1.091	0.020	1
1	A	107	THR	HG23	1.091	0.020	1
1	A	108	HIS	CB	29.242	0.3	1
1	A	108	HIS	CD2	122.623	0.3	1
1	A	108	HIS	CE1	137.76	0.3	1
1	A	108	HIS	HB2	3.165	0.020	2
1	A	108	HIS	HB3	3.202	0.020	2
1	A	108	HIS	HD2	6.412	0.020	1
1	A	108	HIS	HE1	7.642	0.020	1
1	A	109	LYS	CA	57.887	0.3	1
1	A	109	LYS	CB	33.884	0.3	1
1	A	109	LYS	CG	24.759	0.3	1
1	A	109	LYS	CD	29.091	0.3	1
1	A	109	LYS	CE	40.76	0.3	1
1	A	109	LYS	HA	4.124	0.020	1
1	A	109	LYS	HB2	1.704	0.020	2
1	A	109	LYS	HB3	1.778	0.020	2
1	A	109	LYS	HG2	1.598	0.020	2
1	A	109	LYS	HG3	1.669	0.020	2
1	A	109	LYS	HD2	1.239	0.020	2
1	A	109	LYS	HD3	1.62	0.020	2
1	A	109	LYS	HE2	2.614	0.020	2
1	A	109	LYS	HE3	2.667	0.020	2
1	A	109	LYS	N	125.156	0.3	1
1	A	110	GLY	CA	44.252	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	110	GLY	HA2	3.773	0.020	1
1	A	110	GLY	N	107.585	0.3	1
1	A	111	ASN	CA	55.173	0.3	1
1	A	111	ASN	CB	37.272	0.3	1
1	A	111	ASN	HA	4.577	0.020	1
1	A	111	ASN	HB2	2.831	0.020	2
1	A	111	ASN	HB3	3.002	0.020	2
1	A	111	ASN	HD21	6.931	0.020	1
1	A	111	ASN	HD22	7.576	0.020	1
1	A	111	ASN	N	116.521	0.3	1
1	A	111	ASN	ND2	111.195	0.3	1
1	A	112	ASN	CA	55.348	0.3	1
1	A	112	ASN	CB	35.821	0.3	1
1	A	112	ASN	HA	4.578	0.020	1
1	A	112	ASN	HB2	2.784	0.020	2
1	A	112	ASN	HB3	2.876	0.020	2
1	A	112	ASN	HD21	7.683	0.020	1
1	A	112	ASN	HD22	6.87	0.020	1
1	A	112	ASN	N	119.869	0.3	1
1	A	112	ASN	ND2	112.464	0.3	1
1	A	113	ALA	CA	55.663	0.3	1
1	A	113	ALA	CB	18.456	0.3	1
1	A	113	ALA	HA	3.547	0.020	1
1	A	113	ALA	N	120.951	0.3	1
1	A	113	ALA	HB1	0.967	0.020	1
1	A	113	ALA	HB2	0.967	0.020	1
1	A	113	ALA	HB3	0.967	0.020	1
1	A	114	PHE	CA	62.38	0.3	1
1	A	114	PHE	CB	38.583	0.3	1
1	A	114	PHE	CD1	131.108	0.3	1
1	A	114	PHE	CE1	130.37	0.3	1
1	A	114	PHE	HA	3.822	0.020	1
1	A	114	PHE	HB2	3.02	0.020	2
1	A	114	PHE	HB3	3.132	0.020	2
1	A	114	PHE	HD1	7.388	0.020	1
1	A	114	PHE	HD2	7.388	0.020	1
1	A	114	PHE	HE1	7.389	0.020	1
1	A	114	PHE	HE2	7.389	0.020	1
1	A	114	PHE	N	112.128	0.3	1
1	A	115	THR	CA	65.689	0.3	1
1	A	115	THR	CB	68.577	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	115	THR	CG2	22.292	0.3	1
1	A	115	THR	HA	3.789	0.020	1
1	A	115	THR	HB	4.21	0.020	1
1	A	115	THR	N	114.082	0.3	1
1	A	115	THR	HG21	1.209	0.020	1
1	A	115	THR	HG22	1.209	0.020	1
1	A	115	THR	HG23	1.209	0.020	1
1	A	116	ILE	CA	64.654	0.3	1
1	A	116	ILE	CB	38.977	0.3	1
1	A	116	ILE	CG1	28.434	0.3	1
1	A	116	ILE	CG2	17.845	0.3	1
1	A	116	ILE	CD1	14.14	0.3	1
1	A	116	ILE	HA	3.758	0.020	1
1	A	116	ILE	HB	1.496	0.020	1
1	A	116	ILE	HG12	0.95	0.020	2
1	A	116	ILE	HG13	1.658	0.020	2
1	A	116	ILE	N	121.065	0.3	1
1	A	116	ILE	HG21	0.687	0.020	1
1	A	116	ILE	HG22	0.687	0.020	1
1	A	116	ILE	HG23	0.687	0.020	1
1	A	116	ILE	HD11	0.607	0.020	1
1	A	116	ILE	HD12	0.607	0.020	1
1	A	116	ILE	HD13	0.607	0.020	1
1	A	117	LEU	CA	57.642	0.3	1
1	A	117	LEU	CB	41.196	0.3	1
1	A	117	LEU	CG	26.221	0.3	1
1	A	117	LEU	CD1	21.555	0.3	1
1	A	117	LEU	CD2	26.653	0.3	1
1	A	117	LEU	HA	3.735	0.020	1
1	A	117	LEU	HB2	0.947	0.020	2
1	A	117	LEU	HB3	1.756	0.020	2
1	A	117	LEU	HG	1.787	0.020	1
1	A	117	LEU	N	116.126	0.3	1
1	A	117	LEU	HD11	0.436	0.020	1
1	A	117	LEU	HD12	0.436	0.020	1
1	A	117	LEU	HD13	0.436	0.020	1
1	A	117	LEU	HD21	0.403	0.020	1
1	A	117	LEU	HD22	0.403	0.020	1
1	A	117	LEU	HD23	0.403	0.020	1
1	A	118	LYS	CA	59.008	0.3	1
1	A	118	LYS	CB	32.072	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	118	LYS	CG	24.683	0.3	1
1	A	118	LYS	CD	29.14	0.3	1
1	A	118	LYS	CE	41.805	0.3	1
1	A	118	LYS	HA	4.26	0.020	1
1	A	118	LYS	HB2	1.783	0.020	2
1	A	118	LYS	HB3	1.876	0.020	2
1	A	118	LYS	HG2	1.342	0.020	2
1	A	118	LYS	HG3	1.431	0.020	2
1	A	118	LYS	HD2	1.619	0.020	1
1	A	118	LYS	HD3	1.619	0.020	1
1	A	118	LYS	HE2	2.907	0.020	1
1	A	118	LYS	HE3	2.907	0.020	1
1	A	118	LYS	N	119.753	0.3	1
1	A	119	ASP	CA	57.456	0.3	1
1	A	119	ASP	CB	39.937	0.3	1
1	A	119	ASP	HA	4.318	0.020	1
1	A	119	ASP	HB2	2.6	0.020	2
1	A	119	ASP	HB3	2.84	0.020	2
1	A	119	ASP	N	123.294	0.3	1
1	A	120	LEU	CA	54.787	0.3	1
1	A	120	LEU	CB	42.807	0.3	1
1	A	120	LEU	CG	26.325	0.3	1
1	A	120	LEU	CD1	21.956	0.3	1
1	A	120	LEU	CD2	26.181	0.3	1
1	A	120	LEU	HA	4.339	0.020	1
1	A	120	LEU	HB2	1.477	0.020	2
1	A	120	LEU	HB3	1.67	0.020	2
1	A	120	LEU	HG	1.872	0.020	1
1	A	120	LEU	N	116.265	0.3	1
1	A	120	LEU	HD11	0.906	0.020	1
1	A	120	LEU	HD12	0.906	0.020	1
1	A	120	LEU	HD13	0.906	0.020	1
1	A	120	LEU	HD21	0.534	0.020	1
1	A	120	LEU	HD22	0.534	0.020	1
1	A	120	LEU	HD23	0.534	0.020	1
1	A	121	GLY	CA	46.536	0.3	1
1	A	121	GLY	HA2	4.087	0.020	1
1	A	121	GLY	HA3	4.087	0.020	1
1	A	121	GLY	N	107.679	0.3	1
1	A	122	VAL	CA	59.678	0.3	1
1	A	122	VAL	CB	33.131	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	VAL	CG1	19.35	0.3	1
1	A	122	VAL	CG2	21.544	0.3	1
1	A	122	VAL	HA	4.736	0.020	1
1	A	122	VAL	HB	2.687	0.020	1
1	A	122	VAL	N	106.458	0.3	1
1	A	122	VAL	HG11	0.723	0.020	1
1	A	122	VAL	HG12	0.723	0.020	1
1	A	122	VAL	HG13	0.723	0.020	1
1	A	122	VAL	HG21	0.808	0.020	1
1	A	122	VAL	HG22	0.808	0.020	1
1	A	122	VAL	HG23	0.808	0.020	1
1	A	123	GLU	CA	59.787	0.3	1
1	A	123	GLU	CB	28.359	0.3	1
1	A	123	GLU	CG	35.445	0.3	1
1	A	123	GLU	HA	3.903	0.020	1
1	A	123	GLU	HB2	1.814	0.020	1
1	A	123	GLU	HB3	1.814	0.020	1
1	A	123	GLU	HG2	2.172	0.020	2
1	A	123	GLU	HG3	2.246	0.020	2
1	A	123	GLU	N	123.57	0.3	1
1	A	124	SER	CA	59.945	0.3	1
1	A	124	SER	CB	62.342	0.3	1
1	A	124	SER	HA	4.054	0.020	1
1	A	124	SER	HB2	3.597	0.020	1
1	A	124	SER	HB3	3.597	0.020	1
1	A	124	SER	N	111.925	0.3	1
1	A	125	TYR	CA	59.927	0.3	1
1	A	125	TYR	CB	37.344	0.3	1
1	A	125	TYR	CD1	132.46	0.3	1
1	A	125	TYR	CE1	117.404	0.3	1
1	A	125	TYR	HA	3.901	0.020	1
1	A	125	TYR	HB2	1.388	0.020	2
1	A	125	TYR	HB3	2.247	0.020	2
1	A	125	TYR	HD1	6.937	0.020	1
1	A	125	TYR	HD2	6.937	0.020	1
1	A	125	TYR	HE1	6.547	0.020	1
1	A	125	TYR	HE2	6.547	0.020	1
1	A	125	TYR	N	116.799	0.3	1
1	A	126	PHE	CA	56.868	0.3	1
1	A	126	PHE	CB	40.104	0.3	1
1	A	126	PHE	CD1	131.378	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	126	PHE	CE1	129.685	0.3	1
1	A	126	PHE	HA	4.437	0.020	1
1	A	126	PHE	HB2	2.672	0.020	1
1	A	126	PHE	HB3	2.672	0.020	1
1	A	126	PHE	HD1	6.913	0.020	1
1	A	126	PHE	HD2	6.913	0.020	1
1	A	126	PHE	HE1	6.501	0.020	1
1	A	126	PHE	HE2	6.501	0.020	1
1	A	126	PHE	N	114.9	0.3	1
1	A	127	THR	CA	66.202	0.3	1
1	A	127	THR	CB	69.043	0.3	1
1	A	127	THR	CG2	21.552	0.3	1
1	A	127	THR	HA	3.89	0.020	1
1	A	127	THR	HB	3.149	0.020	1
1	A	127	THR	N	123.007	0.3	1
1	A	127	THR	HG21	1.153	0.020	1
1	A	127	THR	HG22	1.153	0.020	1
1	A	127	THR	HG23	1.153	0.020	1
1	A	128	GLU	CA	57.061	0.3	1
1	A	128	GLU	CB	32.666	0.3	1
1	A	128	GLU	CG	36.308	0.3	1
1	A	128	GLU	HA	4.632	0.020	1
1	A	128	GLU	HB2	2.081	0.020	2
1	A	128	GLU	HB3	2.414	0.020	2
1	A	128	GLU	HG2	2.475	0.020	2
1	A	128	GLU	HG3	2.712	0.020	2
1	A	128	GLU	N	116.25	0.3	1
1	A	129	ILE	CA	61.41	0.3	1
1	A	129	ILE	CB	39.038	0.3	1
1	A	129	ILE	CG1	27.193	0.3	1
1	A	129	ILE	CG2	15.148	0.3	1
1	A	129	ILE	CD1	13.914	0.3	1
1	A	129	ILE	HA	4.182	0.020	1
1	A	129	ILE	HB	1.872	0.020	1
1	A	129	ILE	HG12	0.475	0.020	2
1	A	129	ILE	HG13	1.498	0.020	2
1	A	129	ILE	N	127.17	0.3	1
1	A	129	ILE	HG21	0.056	0.020	1
1	A	129	ILE	HG22	0.056	0.020	1
1	A	129	ILE	HG23	0.056	0.020	1
1	A	129	ILE	HD11	0.808	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	ILE	HD12	0.808	0.020	1
1	A	129	ILE	HD13	0.808	0.020	1
1	A	130	LEU	CA	53.385	0.3	1
1	A	130	LEU	CB	44.029	0.3	1
1	A	130	LEU	CG	27.582	0.3	1
1	A	130	LEU	CD1	25.797	0.3	1
1	A	130	LEU	CD2	23.946	0.3	1
1	A	130	LEU	HA	5.085	0.020	1
1	A	130	LEU	HB2	1.497	0.020	2
1	A	130	LEU	HB3	2.487	0.020	2
1	A	130	LEU	HG	1.94	0.020	1
1	A	130	LEU	N	128.197	0.3	1
1	A	130	LEU	HD11	0.806	0.020	1
1	A	130	LEU	HD12	0.806	0.020	1
1	A	130	LEU	HD13	0.806	0.020	1
1	A	130	LEU	HD21	1.131	0.020	1
1	A	130	LEU	HD22	1.131	0.020	1
1	A	130	LEU	HD23	1.131	0.020	1
1	A	131	THR	CA	59.538	0.3	1
1	A	131	THR	CB	71.719	0.3	1
1	A	131	THR	CG2	21.587	0.3	1
1	A	131	THR	HA	5.45	0.020	1
1	A	131	THR	HB	5.064	0.020	1
1	A	131	THR	N	113.134	0.3	1
1	A	131	THR	HG21	0.745	0.020	1
1	A	131	THR	HG22	0.745	0.020	1
1	A	131	THR	HG23	0.745	0.020	1
1	A	132	SER	CA	60.584	0.3	1
1	A	132	SER	CB	62.613	0.3	1
1	A	132	SER	HA	4.563	0.020	1
1	A	132	SER	HB2	3.884	0.020	2
1	A	132	SER	HB3	3.989	0.020	2
1	A	132	SER	N	117.025	0.3	1
1	A	133	GLN	CA	55.509	0.3	1
1	A	133	GLN	CB	29.113	0.3	1
1	A	133	GLN	CG	35.246	0.3	1
1	A	133	GLN	HA	4.42	0.020	1
1	A	133	GLN	HB2	1.823	0.020	2
1	A	133	GLN	HB3	2.344	0.020	2
1	A	133	GLN	HG2	2.282	0.020	1
1	A	133	GLN	HG3	2.282	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	GLN	HE21	6.874	0.020	1
1	A	133	GLN	HE22	7.543	0.020	1
1	A	133	GLN	N	119.901	0.3	1
1	A	133	GLN	NE2	112.862	0.3	1
1	A	134	SER	CA	60.999	0.3	1
1	A	134	SER	CB	63.306	0.3	1
1	A	134	SER	HA	4.29	0.020	1
1	A	134	SER	HB2	4.169	0.020	1
1	A	134	SER	HB3	4.169	0.020	1
1	A	134	SER	N	115.961	0.3	1
1	A	135	GLY	CA	45.304	0.3	1
1	A	135	GLY	HA2	3.436	0.020	1
1	A	135	GLY	N	106.469	0.3	1
1	A	136	PHE	CA	56.865	0.3	1
1	A	136	PHE	CB	40.494	0.3	1
1	A	136	PHE	CD1	130.506	0.3	1
1	A	136	PHE	CE1	130.694	0.3	1
1	A	136	PHE	CZ	129.77	0.3	1
1	A	136	PHE	HA	4.72	0.020	1
1	A	136	PHE	HB2	2.737	0.020	2
1	A	136	PHE	HB3	2.897	0.020	2
1	A	136	PHE	HD1	6.898	0.020	1
1	A	136	PHE	HD2	6.898	0.020	1
1	A	136	PHE	HE1	6.825	0.020	1
1	A	136	PHE	HE2	6.825	0.020	1
1	A	136	PHE	HZ	5.694	0.020	1
1	A	136	PHE	N	119.126	0.3	1
1	A	137	VAL	CA	63.511	0.3	1
1	A	137	VAL	CB	31.403	0.3	1
1	A	137	VAL	CG1	22.237	0.3	1
1	A	137	VAL	CG2	22.435	0.3	1
1	A	137	VAL	HA	3.781	0.020	1
1	A	137	VAL	HB	1.934	0.020	1
1	A	137	VAL	N	123.508	0.3	1
1	A	137	VAL	HG11	1.037	0.020	1
1	A	137	VAL	HG12	1.037	0.020	1
1	A	137	VAL	HG13	1.037	0.020	1
1	A	137	VAL	HG21	1.173	0.020	1
1	A	137	VAL	HG22	1.173	0.020	1
1	A	137	VAL	HG23	1.173	0.020	1
1	A	138	ARG	CA	56.883	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	ARG	CB	31.299	0.3	1
1	A	138	ARG	CG	27.623	0.3	1
1	A	138	ARG	CD	43.178	0.3	1
1	A	138	ARG	HA	4.088	0.020	1
1	A	138	ARG	HB2	1.534	0.020	2
1	A	138	ARG	HB3	1.876	0.020	2
1	A	138	ARG	HG2	1.165	0.020	2
1	A	138	ARG	HG3	1.545	0.020	2
1	A	138	ARG	HD2	2.916	0.020	1
1	A	138	ARG	HD3	2.916	0.020	1
1	A	138	ARG	HE	7.146	0.020	1
1	A	138	ARG	N	125.266	0.3	1
1	A	138	ARG	NE	83.794	0.3	1
1	A	140	PRO	CA	63.902	0.3	1
1	A	140	PRO	CB	32.508	0.3	1
1	A	140	PRO	CG	23.76	0.3	1
1	A	140	PRO	CD	49.11	0.3	1
1	A	140	PRO	HA	4.171	0.020	1
1	A	140	PRO	HB2	2.089	0.020	2
1	A	140	PRO	HB3	2.25	0.020	2
1	A	140	PRO	HG2	1.56	0.020	2
1	A	140	PRO	HG3	1.99	0.020	2
1	A	140	PRO	HD2	3.43	0.020	1
1	A	140	PRO	HD3	3.43	0.020	1
1	A	141	SER	CA	57.046	0.3	1
1	A	141	SER	CB	63.59	0.3	1
1	A	141	SER	HA	4.647	0.020	1
1	A	141	SER	HB2	3.732	0.020	2
1	A	141	SER	HB3	3.937	0.020	2
1	A	141	SER	N	122.628	0.3	1
1	A	142	PRO	CA	63.582	0.3	1
1	A	142	PRO	CB	33.353	0.3	1
1	A	142	PRO	CG	26.25	0.3	1
1	A	142	PRO	CD	50.98	0.3	1
1	A	142	PRO	HA	4.53	0.020	1
1	A	142	PRO	HB2	1.579	0.020	2
1	A	142	PRO	HB3	1.95	0.020	2
1	A	142	PRO	HG2	1.763	0.020	1
1	A	142	PRO	HG3	1.763	0.020	1
1	A	142	PRO	HD2	3.602	0.020	2
1	A	142	PRO	HD3	3.895	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	143	GLU	CA	61.767	0.3	1
1	A	143	GLU	CB	30.363	0.3	1
1	A	143	GLU	CG	37.186	0.3	1
1	A	143	GLU	HA	3.756	0.020	1
1	A	143	GLU	HB2	2.072	0.020	1
1	A	143	GLU	HB3	2.072	0.020	1
1	A	143	GLU	HG2	2.332	0.020	2
1	A	143	GLU	HG3	2.383	0.020	2
1	A	143	GLU	N	122.858	0.3	1
1	A	144	ALA	CA	54.814	0.3	1
1	A	144	ALA	CB	18.091	0.3	1
1	A	144	ALA	HA	2.565	0.020	1
1	A	144	ALA	N	119.464	0.3	1
1	A	144	ALA	HB1	0.157	0.020	1
1	A	144	ALA	HB2	0.157	0.020	1
1	A	144	ALA	HB3	0.157	0.020	1
1	A	145	ALA	CA	55.01	0.3	1
1	A	145	ALA	CB	17.786	0.3	1
1	A	145	ALA	HA	3.714	0.020	1
1	A	145	ALA	N	115.442	0.3	1
1	A	145	ALA	HB1	1.07	0.020	1
1	A	145	ALA	HB2	1.07	0.020	1
1	A	145	ALA	HB3	1.07	0.020	1
1	A	146	THR	CA	66.495	0.3	1
1	A	146	THR	CB	68.3	0.3	1
1	A	146	THR	CG2	22.029	0.3	1
1	A	146	THR	HA	3.557	0.020	1
1	A	146	THR	HB	3.977	0.020	1
1	A	146	THR	N	114.397	0.3	1
1	A	146	THR	HG21	1.115	0.020	1
1	A	146	THR	HG22	1.115	0.020	1
1	A	146	THR	HG23	1.115	0.020	1
1	A	147	TYR	CA	60.17	0.3	1
1	A	147	TYR	CB	37.54	0.3	1
1	A	147	TYR	CD1	133.952	0.3	1
1	A	147	TYR	CE1	117.557	0.3	1
1	A	147	TYR	HA	4.234	0.020	1
1	A	147	TYR	HB2	2.601	0.020	2
1	A	147	TYR	HB3	3.032	0.020	2
1	A	147	TYR	HD1	6.961	0.020	1
1	A	147	TYR	HD2	6.961	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	TYR	HE1	6.811	0.020	1
1	A	147	TYR	HE2	6.811	0.020	1
1	A	147	TYR	N	119.928	0.3	1
1	A	148	LEU	CA	57.7	0.3	1
1	A	148	LEU	CB	42.129	0.3	1
1	A	148	LEU	CG	25.98	0.3	1
1	A	148	LEU	CD1	25.078	0.3	1
1	A	148	LEU	CD2	22.875	0.3	1
1	A	148	LEU	HA	3.527	0.020	1
1	A	148	LEU	HB2	0.509	0.020	2
1	A	148	LEU	HB3	1.628	0.020	2
1	A	148	LEU	HG	1.826	0.020	1
1	A	148	LEU	N	120.501	0.3	1
1	A	148	LEU	HD11	0.376	0.020	1
1	A	148	LEU	HD12	0.376	0.020	1
1	A	148	LEU	HD13	0.376	0.020	1
1	A	148	LEU	HD21	0.516	0.020	1
1	A	148	LEU	HD22	0.516	0.020	1
1	A	148	LEU	HD23	0.516	0.020	1
1	A	149	LEU	CA	58.605	0.3	1
1	A	149	LEU	CB	41.636	0.3	1
1	A	149	LEU	CG	27.182	0.3	1
1	A	149	LEU	CD1	24.058	0.3	1
1	A	149	LEU	CD2	25.054	0.3	1
1	A	149	LEU	HA	3.523	0.020	1
1	A	149	LEU	HB2	1.353	0.020	2
1	A	149	LEU	HB3	1.729	0.020	2
1	A	149	LEU	HG	1.6	0.020	1
1	A	149	LEU	N	117.961	0.3	1
1	A	149	LEU	HD11	0.559	0.020	1
1	A	149	LEU	HD12	0.559	0.020	1
1	A	149	LEU	HD13	0.559	0.020	1
1	A	149	LEU	HD21	0.587	0.020	1
1	A	149	LEU	HD22	0.587	0.020	1
1	A	149	LEU	HD23	0.587	0.020	1
1	A	150	ASP	CA	56.308	0.3	1
1	A	150	ASP	CB	41.28	0.3	1
1	A	150	ASP	HA	4.273	0.020	1
1	A	150	ASP	HB2	2.453	0.020	2
1	A	150	ASP	HB3	2.639	0.020	2
1	A	150	ASP	N	115.806	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	LYS	CA	59.473	0.3	1
1	A	151	LYS	CB	32.847	0.3	1
1	A	151	LYS	CG	24.445	0.3	1
1	A	151	LYS	CD	30.796	0.3	1
1	A	151	LYS	CE	42.31	0.3	1
1	A	151	LYS	HA	3.548	0.020	1
1	A	151	LYS	HB2	0.991	0.020	2
1	A	151	LYS	HB3	1.195	0.020	2
1	A	151	LYS	HG2	-0.366	0.020	2
1	A	151	LYS	HG3	0.718	0.020	2
1	A	151	LYS	HD2	1.106	0.020	2
1	A	151	LYS	HD3	1.261	0.020	2
1	A	151	LYS	HE2	2.722	0.020	2
1	A	151	LYS	HE3	2.563	0.020	2
1	A	151	LYS	N	120.627	0.3	1
1	A	152	TYR	CA	58.205	0.3	1
1	A	152	TYR	CB	37.017	0.3	1
1	A	152	TYR	HA	4.338	0.020	1
1	A	152	TYR	HB2	2.423	0.020	2
1	A	152	TYR	HB3	3.294	0.020	2
1	A	152	TYR	N	111.882	0.3	1
1	A	153	GLN	CA	56.255	0.3	1
1	A	153	GLN	CB	25.78	0.3	1
1	A	153	GLN	CG	34.217	0.3	1
1	A	153	GLN	HA	3.935	0.020	1
1	A	153	GLN	HB2	2.018	0.020	2
1	A	153	GLN	HB3	2.077	0.020	2
1	A	153	GLN	HG2	2.135	0.020	2
1	A	153	GLN	HG3	2.202	0.020	2
1	A	153	GLN	HE21	7.619	0.020	1
1	A	153	GLN	HE22	6.688	0.020	1
1	A	153	GLN	N	117.831	0.3	1
1	A	153	GLN	NE2	113.706	0.3	1
1	A	154	LEU	CA	53.615	0.3	1
1	A	154	LEU	CB	41.724	0.3	1
1	A	154	LEU	CG	26.512	0.3	1
1	A	154	LEU	CD1	21.774	0.3	1
1	A	154	LEU	CD2	24.198	0.3	1
1	A	154	LEU	HA	4.148	0.020	1
1	A	154	LEU	HB2	1.503	0.020	2
1	A	154	LEU	HB3	1.558	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	154	LEU	HG	1.45	0.020	1
1	A	154	LEU	N	117.373	0.3	1
1	A	154	LEU	HD11	0.748	0.020	1
1	A	154	LEU	HD12	0.748	0.020	1
1	A	154	LEU	HD13	0.748	0.020	1
1	A	154	LEU	HD21	0.389	0.020	1
1	A	154	LEU	HD22	0.389	0.020	1
1	A	154	LEU	HD23	0.389	0.020	1
1	A	155	ASN	CA	51.682	0.3	1
1	A	155	ASN	CB	40.198	0.3	1
1	A	155	ASN	HA	4.881	0.020	1
1	A	155	ASN	HB2	2.751	0.020	2
1	A	155	ASN	HB3	2.896	0.020	2
1	A	155	ASN	HD21	7.592	0.020	1
1	A	155	ASN	HD22	7.13	0.020	1
1	A	155	ASN	N	118.564	0.3	1
1	A	155	ASN	ND2	112.934	0.3	1
1	A	156	SER	CA	62.952	0.3	1
1	A	156	SER	CB	62.077	0.3	1
1	A	156	SER	HA	3.732	0.020	1
1	A	156	SER	HB2	3.863	0.020	2
1	A	156	SER	HB3	3.947	0.020	2
1	A	156	SER	N	127.297	0.3	1
1	A	157	ASP	CA	55.867	0.3	1
1	A	157	ASP	CB	40.399	0.3	1
1	A	157	ASP	HA	4.421	0.020	1
1	A	157	ASP	HB2	2.461	0.020	2
1	A	157	ASP	HB3	2.56	0.020	2
1	A	157	ASP	N	117.391	0.3	1
1	A	158	ASN	CA	51.617	0.3	1
1	A	158	ASN	CB	40.756	0.3	1
1	A	158	ASN	HA	5.069	0.020	1
1	A	158	ASN	HB2	2.602	0.020	2
1	A	158	ASN	HB3	3.466	0.020	2
1	A	158	ASN	HD21	7.308	0.020	1
1	A	158	ASN	HD22	6.877	0.020	1
1	A	158	ASN	N	114.852	0.3	1
1	A	158	ASN	ND2	112.961	0.3	1
1	A	159	THR	CA	62.577	0.3	1
1	A	159	THR	CB	69.772	0.3	1
1	A	159	THR	CG2	21.068	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	159	THR	HA	5.324	0.020	1
1	A	159	THR	HB	3.659	0.020	1
1	A	159	THR	N	117.228	0.3	1
1	A	159	THR	HG21	0.974	0.020	1
1	A	159	THR	HG22	0.974	0.020	1
1	A	159	THR	HG23	0.974	0.020	1
1	A	160	TYR	CA	55.231	0.3	1
1	A	160	TYR	CB	40.746	0.3	1
1	A	160	TYR	CD1	133.647	0.3	1
1	A	160	TYR	CE1	117.119	0.3	1
1	A	160	TYR	HA	4.612	0.020	1
1	A	160	TYR	HB2	2.144	0.020	2
1	A	160	TYR	HB3	2.824	0.020	2
1	A	160	TYR	HD1	6.993	0.020	1
1	A	160	TYR	HD2	6.993	0.020	1
1	A	160	TYR	HE1	6.449	0.020	1
1	A	160	TYR	HE2	6.449	0.020	1
1	A	160	TYR	N	124.03	0.3	1
1	A	161	TYR	CA	56.462	0.3	1
1	A	161	TYR	CB	40.141	0.3	1
1	A	161	TYR	CD1	133.651	0.3	1
1	A	161	TYR	CE1	117.113	0.3	1
1	A	161	TYR	HA	5.806	0.020	1
1	A	161	TYR	HB2	2.833	0.020	2
1	A	161	TYR	HB3	3.014	0.020	2
1	A	161	TYR	HD1	7.161	0.020	1
1	A	161	TYR	HD2	7.161	0.020	1
1	A	161	TYR	HE1	6.756	0.020	1
1	A	161	TYR	HE2	6.756	0.020	1
1	A	161	TYR	N	124.249	0.3	1
1	A	162	ILE	CA	60.034	0.3	1
1	A	162	ILE	CB	37.221	0.3	1
1	A	162	ILE	CG1	27.151	0.3	1
1	A	162	ILE	CG2	17.272	0.3	1
1	A	162	ILE	CD1	10.746	0.3	1
1	A	162	ILE	HA	4.972	0.020	1
1	A	162	ILE	HB	0.94	0.020	1
1	A	162	ILE	HG12	-0.168	0.020	2
1	A	162	ILE	HG13	0.473	0.020	2
1	A	162	ILE	N	131.645	0.3	1
1	A	162	ILE	HG21	0.226	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	162	ILE	HG22	0.226	0.020	1
1	A	162	ILE	HG23	0.226	0.020	1
1	A	162	ILE	HD11	-1.468	0.020	1
1	A	162	ILE	HD12	-1.468	0.020	1
1	A	162	ILE	HD13	-1.468	0.020	1
1	A	163	GLY	CA	45.523	0.3	1
1	A	163	GLY	HA2	3.764	0.020	1
1	A	163	GLY	N	109.681	0.3	1
1	A	164	ASP	CA	53.345	0.3	1
1	A	164	ASP	CB	41.876	0.3	1
1	A	164	ASP	HA	5.064	0.020	1
1	A	164	ASP	HB2	2.576	0.020	2
1	A	164	ASP	HB3	2.864	0.020	2
1	A	164	ASP	N	113.822	0.3	1
1	A	165	ARG	CA	54.305	0.3	1
1	A	165	ARG	CB	34.387	0.3	1
1	A	165	ARG	CG	26.003	0.3	1
1	A	165	ARG	CD	43.546	0.3	1
1	A	165	ARG	HA	5.091	0.020	1
1	A	165	ARG	HB2	1.82	0.020	2
1	A	165	ARG	HB3	1.999	0.020	2
1	A	165	ARG	HG2	1.703	0.020	1
1	A	165	ARG	HG3	1.703	0.020	1
1	A	165	ARG	HD2	3.127	0.020	1
1	A	165	ARG	HD3	3.127	0.020	1
1	A	165	ARG	HE	7.628	0.020	1
1	A	165	ARG	N	119.576	0.3	1
1	A	165	ARG	NE	85.496	0.3	1
1	A	166	THR	CA	66.995	0.3	1
1	A	166	THR	CB	67.943	0.3	1
1	A	166	THR	CG2	22.558	0.3	1
1	A	166	THR	HA	3.715	0.020	1
1	A	166	THR	HB	4.09	0.020	1
1	A	166	THR	N	120.316	0.3	1
1	A	166	THR	HG21	1.204	0.020	1
1	A	166	THR	HG22	1.204	0.020	1
1	A	166	THR	HG23	1.204	0.020	1
1	A	167	LEU	CA	57.541	0.3	1
1	A	167	LEU	CB	42.12	0.3	1
1	A	167	LEU	CG	26.85	0.3	1
1	A	167	LEU	CD1	25.856	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	167	LEU	CD2	24.588	0.3	1
1	A	167	LEU	HA	4.106	0.020	1
1	A	167	LEU	HB2	1.42	0.020	2
1	A	167	LEU	HB3	1.566	0.020	2
1	A	167	LEU	HG	1.42	0.020	1
1	A	167	LEU	N	120.408	0.3	1
1	A	167	LEU	HD11	0.801	0.020	1
1	A	167	LEU	HD12	0.801	0.020	1
1	A	167	LEU	HD13	0.801	0.020	1
1	A	167	LEU	HD21	0.758	0.020	1
1	A	167	LEU	HD22	0.758	0.020	1
1	A	167	LEU	HD23	0.758	0.020	1
1	A	168	ASP	CA	57.24	0.3	1
1	A	168	ASP	CB	40.862	0.3	1
1	A	168	ASP	HA	4.431	0.020	1
1	A	168	ASP	HB2	2.907	0.020	2
1	A	168	ASP	HB3	3.069	0.020	2
1	A	168	ASP	N	118.8	0.3	1
1	A	169	VAL	CA	65.98	0.3	1
1	A	169	VAL	CB	31.171	0.3	1
1	A	169	VAL	CG1	21.408	0.3	1
1	A	169	VAL	CG2	22.152	0.3	1
1	A	169	VAL	HA	3.62	0.020	1
1	A	169	VAL	HB	2.161	0.020	1
1	A	169	VAL	N	119.82	0.3	1
1	A	169	VAL	HG11	0.845	0.020	1
1	A	169	VAL	HG12	0.845	0.020	1
1	A	169	VAL	HG13	0.845	0.020	1
1	A	169	VAL	HG21	0.957	0.020	1
1	A	169	VAL	HG22	0.957	0.020	1
1	A	169	VAL	HG23	0.957	0.020	1
1	A	170	GLU	CA	59.353	0.3	1
1	A	170	GLU	CB	29.208	0.3	1
1	A	170	GLU	CG	36.245	0.3	1
1	A	170	GLU	HA	3.749	0.020	1
1	A	170	GLU	HB2	1.887	0.020	2
1	A	170	GLU	HB3	1.972	0.020	2
1	A	170	GLU	HG2	2.059	0.020	2
1	A	170	GLU	HG3	2.27	0.020	2
1	A	170	GLU	N	118.557	0.3	1
1	A	171	PHE	CA	59.306	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	171	PHE	CB	39.393	0.3	1
1	A	171	PHE	CD1	131.823	0.3	1
1	A	171	PHE	CE1	130.665	0.3	1
1	A	171	PHE	CZ	129.598	0.3	1
1	A	171	PHE	HA	4.4	0.020	1
1	A	171	PHE	HB2	2.876	0.020	2
1	A	171	PHE	HB3	3.111	0.020	2
1	A	171	PHE	HD1	6.406	0.020	1
1	A	171	PHE	HD2	6.406	0.020	1
1	A	171	PHE	HE1	6.991	0.020	1
1	A	171	PHE	HE2	6.991	0.020	1
1	A	171	PHE	HZ	6.665	0.020	1
1	A	171	PHE	N	119.706	0.3	1
1	A	172	ALA	CA	54.638	0.3	1
1	A	172	ALA	CB	18.505	0.3	1
1	A	172	ALA	HA	3.343	0.020	1
1	A	172	ALA	N	123.752	0.3	1
1	A	172	ALA	HB1	1.492	0.020	1
1	A	172	ALA	HB2	1.492	0.020	1
1	A	172	ALA	HB3	1.492	0.020	1
1	A	173	GLN	CA	58.85	0.3	1
1	A	173	GLN	CB	27.69	0.3	1
1	A	173	GLN	CG	33.151	0.3	1
1	A	173	GLN	HA	3.263	0.020	1
1	A	173	GLN	HB2	0.587	0.020	2
1	A	173	GLN	HB3	1.559	0.020	2
1	A	173	GLN	HG2	1.652	0.020	2
1	A	173	GLN	HG3	1.756	0.020	2
1	A	173	GLN	HE21	6.556	0.020	1
1	A	173	GLN	HE22	7.292	0.020	1
1	A	173	GLN	N	118.543	0.3	1
1	A	173	GLN	NE2	110.091	0.3	1
1	A	174	ASN	CA	54.632	0.3	1
1	A	174	ASN	CB	37.06	0.3	1
1	A	174	ASN	HA	4.259	0.020	1
1	A	174	ASN	HB2	2.581	0.020	2
1	A	174	ASN	HB3	2.938	0.020	2
1	A	174	ASN	HD21	7.219	0.020	1
1	A	174	ASN	HD22	7.183	0.020	1
1	A	174	ASN	N	118.639	0.3	1
1	A	174	ASN	ND2	109.759	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	175	SER	CA	58.692	0.3	1
1	A	175	SER	CB	63.575	0.3	1
1	A	175	SER	HA	4.065	0.020	1
1	A	175	SER	HB2	3.194	0.020	2
1	A	175	SER	HB3	3.352	0.020	2
1	A	175	SER	N	113.373	0.3	1
1	A	176	GLY	CA	45.692	0.3	1
1	A	176	GLY	HA2	3.765	0.020	1
1	A	176	GLY	N	109.599	0.3	1
1	A	177	ILE	CA	58.893	0.3	1
1	A	177	ILE	CB	38.635	0.3	1
1	A	177	ILE	CG1	24.513	0.3	1
1	A	177	ILE	CG2	17.151	0.3	1
1	A	177	ILE	CD1	13.854	0.3	1
1	A	177	ILE	HA	5.041	0.020	1
1	A	177	ILE	HB	2.065	0.020	1
1	A	177	ILE	HG12	1.429	0.020	1
1	A	177	ILE	HG13	1.429	0.020	1
1	A	177	ILE	N	110.604	0.3	1
1	A	177	ILE	HG21	0.589	0.020	1
1	A	177	ILE	HG22	0.589	0.020	1
1	A	177	ILE	HG23	0.589	0.020	1
1	A	177	ILE	HD11	0.521	0.020	1
1	A	177	ILE	HD12	0.521	0.020	1
1	A	177	ILE	HD13	0.521	0.020	1
1	A	178	GLN	CA	54.267	0.3	1
1	A	178	GLN	CB	31.266	0.3	1
1	A	178	GLN	CG	33.464	0.3	1
1	A	178	GLN	HA	4.319	0.020	1
1	A	178	GLN	HB2	1.928	0.020	1
1	A	178	GLN	HB3	1.928	0.020	1
1	A	178	GLN	HG2	1.721	0.020	2
1	A	178	GLN	HG3	2.046	0.020	2
1	A	178	GLN	HE21	7.627	0.020	1
1	A	178	GLN	HE22	6.853	0.020	1
1	A	178	GLN	N	117.813	0.3	1
1	A	178	GLN	NE2	116.252	0.3	1
1	A	179	SER	CA	55.517	0.3	1
1	A	179	SER	CB	64.547	0.3	1
1	A	179	SER	HA	5.601	0.020	1
1	A	179	SER	HB2	3.635	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	179	SER	HB3	3.797	0.020	2
1	A	179	SER	N	113.682	0.3	1
1	A	180	ILE	CA	60.73	0.3	1
1	A	180	ILE	CB	39.28	0.3	1
1	A	180	ILE	CG1	28.111	0.3	1
1	A	180	ILE	CG2	18.452	0.3	1
1	A	180	ILE	CD1	12.364	0.3	1
1	A	180	ILE	HA	4.904	0.020	1
1	A	180	ILE	HB	1.365	0.020	1
1	A	180	ILE	HG12	0.665	0.020	2
1	A	180	ILE	HG13	1.535	0.020	2
1	A	180	ILE	N	130.824	0.3	1
1	A	180	ILE	HG21	0.508	0.020	1
1	A	180	ILE	HG22	0.508	0.020	1
1	A	180	ILE	HG23	0.508	0.020	1
1	A	180	ILE	HD11	0.115	0.020	1
1	A	180	ILE	HD12	0.115	0.020	1
1	A	180	ILE	HD13	0.115	0.020	1
1	A	181	ASN	CA	51.075	0.3	1
1	A	181	ASN	CB	43.432	0.3	1
1	A	181	ASN	HA	5.671	0.020	1
1	A	181	ASN	HB2	2.319	0.020	2
1	A	181	ASN	HB3	2.674	0.020	2
1	A	181	ASN	HD21	8.078	0.020	1
1	A	181	ASN	HD22	6.321	0.020	1
1	A	181	ASN	N	125.98	0.3	1
1	A	181	ASN	ND2	113.2	0.3	1
1	A	182	PHE	CA	59.022	0.3	1
1	A	182	PHE	CB	40.331	0.3	1
1	A	182	PHE	CD1	131.955	0.3	1
1	A	182	PHE	CE1	130.494	0.3	1
1	A	182	PHE	CZ	129.346	0.3	1
1	A	182	PHE	HA	5.109	0.020	1
1	A	182	PHE	HB2	2.722	0.020	2
1	A	182	PHE	HB3	3.374	0.020	2
1	A	182	PHE	HD1	7.237	0.020	1
1	A	182	PHE	HD2	7.237	0.020	1
1	A	182	PHE	HE1	7.033	0.020	1
1	A	182	PHE	HE2	7.033	0.020	1
1	A	182	PHE	HZ	7.149	0.020	1
1	A	182	PHE	N	123.613	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	183	LEU	CA	53.821	0.3	1
1	A	183	LEU	CB	42.719	0.3	1
1	A	183	LEU	CG	26.315	0.3	1
1	A	183	LEU	CD1	26.554	0.3	1
1	A	183	LEU	CD2	22.639	0.3	1
1	A	183	LEU	HA	4.4	0.020	1
1	A	183	LEU	HB2	1.329	0.020	2
1	A	183	LEU	HB3	1.359	0.020	2
1	A	183	LEU	HG	1.715	0.020	1
1	A	183	LEU	N	122.398	0.3	1
1	A	183	LEU	HD11	0.805	0.020	1
1	A	183	LEU	HD12	0.805	0.020	1
1	A	183	LEU	HD13	0.805	0.020	1
1	A	183	LEU	HD21	0.823	0.020	1
1	A	183	LEU	HD22	0.823	0.020	1
1	A	183	LEU	HD23	0.823	0.020	1
1	A	184	GLU	CA	55.43	0.3	1
1	A	184	GLU	CB	30.78	0.3	1
1	A	184	GLU	CG	36.012	0.3	1
1	A	184	GLU	HA	3.94	0.020	1
1	A	184	GLU	HB2	1.743	0.020	2
1	A	184	GLU	HB3	1.839	0.020	2
1	A	184	GLU	HG2	2.125	0.020	1
1	A	184	GLU	HG3	2.125	0.020	1
1	A	184	GLU	N	116.574	0.3	1
1	A	185	SER	CA	56.629	0.3	1
1	A	185	SER	CB	64.665	0.3	1
1	A	185	SER	HA	4.601	0.020	1
1	A	185	SER	HB2	3.071	0.020	2
1	A	185	SER	HB3	3.734	0.020	2
1	A	185	SER	N	114.82	0.3	1
1	A	186	THR	CA	62.539	0.3	1
1	A	186	THR	CB	68.705	0.3	1
1	A	186	THR	CG2	21.769	0.3	1
1	A	186	THR	HA	4.152	0.020	1
1	A	186	THR	HB	4.344	0.020	1
1	A	186	THR	N	115.455	0.3	1
1	A	186	THR	HG21	1.187	0.020	1
1	A	186	THR	HG22	1.187	0.020	1
1	A	186	THR	HG23	1.187	0.020	1
1	A	187	TYR	CA	56.24	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	187	TYR	CB	37.176	0.3	1
1	A	187	TYR	CD1	132.785	0.3	1
1	A	187	TYR	CE1	117.715	0.3	1
1	A	187	TYR	HA	4.615	0.020	1
1	A	187	TYR	HB2	2.496	0.020	2
1	A	187	TYR	HB3	2.986	0.020	2
1	A	187	TYR	HD1	7.053	0.020	1
1	A	187	TYR	HD2	7.053	0.020	1
1	A	187	TYR	HE1	6.754	0.020	1
1	A	187	TYR	HE2	6.754	0.020	1
1	A	187	TYR	N	123.322	0.3	1
1	A	188	GLU	CA	58.389	0.3	1
1	A	188	GLU	CB	28.479	0.3	1
1	A	188	GLU	CG	35.786	0.3	1
1	A	188	GLU	HA	3.8	0.020	1
1	A	188	GLU	HB2	1.803	0.020	2
1	A	188	GLU	HB3	1.892	0.020	2
1	A	188	GLU	HG2	2.12	0.020	2
1	A	188	GLU	HG3	2.207	0.020	2
1	A	188	GLU	N	133.693	0.3	1
1	A	189	GLY	CA	45.383	0.3	1
1	A	189	GLY	HA2	2.483	0.020	1
1	A	190	ASN	CA	52.942	0.3	1
1	A	190	ASN	CB	42.01	0.3	1
1	A	190	ASN	HA	5.371	0.020	1
1	A	190	ASN	HB2	2.164	0.020	2
1	A	190	ASN	HB3	2.761	0.020	2
1	A	190	ASN	HD21	6.488	0.020	1
1	A	190	ASN	HD22	7.948	0.020	1
1	A	190	ASN	N	117.76	0.3	1
1	A	190	ASN	ND2	113.55	0.3	1
1	A	191	HIS	CA	54.051	0.3	1
1	A	191	HIS	CB	28.771	0.3	1
1	A	191	HIS	CD2	121.053	0.3	1
1	A	191	HIS	CE1	137.135	0.3	1
1	A	191	HIS	HA	4.436	0.020	1
1	A	191	HIS	HB2	2.927	0.020	2
1	A	191	HIS	HB3	3.137	0.020	2
1	A	191	HIS	HD2	7.526	0.020	1
1	A	191	HIS	HE1	8.578	0.020	1
1	A	191	HIS	N	125.92	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	192	ARG	CA	55.781	0.3	1
1	A	192	ARG	CB	30.357	0.3	1
1	A	192	ARG	CG	27.442	0.3	1
1	A	192	ARG	CD	43.811	0.3	1
1	A	192	ARG	HA	5.029	0.020	1
1	A	192	ARG	HB2	1.348	0.020	2
1	A	192	ARG	HB3	1.532	0.020	2
1	A	192	ARG	HG2	1.342	0.020	1
1	A	192	ARG	HG3	1.342	0.020	1
1	A	192	ARG	HD2	2.776	0.020	1
1	A	192	ARG	HD3	2.776	0.020	1
1	A	192	ARG	HE	6.734	0.020	1
1	A	192	ARG	N	125.626	0.3	1
1	A	192	ARG	NE	85.549	0.3	1
1	A	193	ILE	CA	59.286	0.3	1
1	A	193	ILE	CB	41.468	0.3	1
1	A	193	ILE	CG1	23.624	0.3	1
1	A	193	ILE	CG2	18.581	0.3	1
1	A	193	ILE	CD1	13.291	0.3	1
1	A	193	ILE	HA	4.508	0.020	1
1	A	193	ILE	HB	1.78	0.020	1
1	A	193	ILE	HG12	0.089	0.020	2
1	A	193	ILE	HG13	0.236	0.020	2
1	A	193	ILE	N	120.996	0.3	1
1	A	193	ILE	HG21	0.492	0.020	1
1	A	193	ILE	HG22	0.492	0.020	1
1	A	193	ILE	HG23	0.492	0.020	1
1	A	193	ILE	HD11	-0.06	0.020	1
1	A	193	ILE	HD12	-0.06	0.020	1
1	A	193	ILE	HD13	-0.06	0.020	1
1	A	194	GLN	CA	55.862	0.3	1
1	A	194	GLN	CB	30.379	0.3	1
1	A	194	GLN	CG	34.321	0.3	1
1	A	194	GLN	HA	4.619	0.020	1
1	A	194	GLN	HB2	1.989	0.020	2
1	A	194	GLN	HB3	2.14	0.020	2
1	A	194	GLN	HG2	2.273	0.020	1
1	A	194	GLN	HG3	2.273	0.020	1
1	A	194	GLN	HE21	7.541	0.020	1
1	A	194	GLN	HE22	6.705	0.020	1
1	A	194	GLN	N	116.823	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	194	GLN	NE2	111.954	0.3	1
1	A	195	ALA	CA	50.744	0.3	1
1	A	195	ALA	CB	21.711	0.3	1
1	A	195	ALA	HA	4.649	0.020	1
1	A	195	ALA	N	121.893	0.3	1
1	A	195	ALA	HB1	1.394	0.020	1
1	A	195	ALA	HB2	1.394	0.020	1
1	A	195	ALA	HB3	1.394	0.020	1
1	A	196	LEU	CA	58.151	0.3	1
1	A	196	LEU	CB	40.945	0.3	1
1	A	196	LEU	CG	27.136	0.3	1
1	A	196	LEU	CD1	22.139	0.3	1
1	A	196	LEU	CD2	24.911	0.3	1
1	A	196	LEU	HA	3.931	0.020	1
1	A	196	LEU	HB2	1.306	0.020	2
1	A	196	LEU	HB3	1.864	0.020	2
1	A	196	LEU	HG	2.061	0.020	1
1	A	196	LEU	N	122.418	0.3	1
1	A	196	LEU	HD11	0.959	0.020	1
1	A	196	LEU	HD12	0.959	0.020	1
1	A	196	LEU	HD13	0.959	0.020	1
1	A	196	LEU	HD21	0.975	0.020	1
1	A	196	LEU	HD22	0.975	0.020	1
1	A	196	LEU	HD23	0.975	0.020	1
1	A	197	ALA	CA	53.997	0.3	1
1	A	197	ALA	CB	18.263	0.3	1
1	A	197	ALA	HA	3.933	0.020	1
1	A	197	ALA	N	117.953	0.3	1
1	A	197	ALA	HB1	1.246	0.020	1
1	A	197	ALA	HB2	1.246	0.020	1
1	A	197	ALA	HB3	1.246	0.020	1
1	A	198	ASP	CA	55.874	0.3	1
1	A	198	ASP	CB	41.095	0.3	1
1	A	198	ASP	HA	4.177	0.020	1
1	A	198	ASP	HB2	2.731	0.020	2
1	A	198	ASP	HB3	2.794	0.020	2
1	A	198	ASP	N	115.994	0.3	1
1	A	199	ILE	CA	66.489	0.3	1
1	A	199	ILE	CB	37.038	0.3	1
1	A	199	ILE	CG1	32.062	0.3	1
1	A	199	ILE	CG2	17.151	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	199	ILE	CD1	14.425	0.3	1
1	A	199	ILE	HA	3.184	0.020	1
1	A	199	ILE	HB	1.776	0.020	1
1	A	199	ILE	HG12	0.558	0.020	2
1	A	199	ILE	HG13	1.767	0.020	2
1	A	199	ILE	N	120.35	0.3	1
1	A	199	ILE	HG21	0.678	0.020	1
1	A	199	ILE	HG22	0.678	0.020	1
1	A	199	ILE	HG23	0.678	0.020	1
1	A	199	ILE	HD11	0.768	0.020	1
1	A	199	ILE	HD12	0.768	0.020	1
1	A	199	ILE	HD13	0.768	0.020	1
1	A	200	SER	CA	60.718	0.3	1
1	A	200	SER	CB	60.653	0.3	1
1	A	200	SER	HA	2.845	0.020	1
1	A	200	SER	HB2	2.119	0.020	2
1	A	200	SER	HB3	2.612	0.020	2
1	A	200	SER	N	111.475	0.3	1
1	A	201	ARG	CA	57.621	0.3	1
1	A	201	ARG	CB	29.644	0.3	1
1	A	201	ARG	CG	27.395	0.3	1
1	A	201	ARG	CD	43.096	0.3	1
1	A	201	ARG	HA	3.981	0.020	1
1	A	201	ARG	HB2	1.713	0.020	2
1	A	201	ARG	HB3	1.788	0.020	2
1	A	201	ARG	HG2	1.496	0.020	2
1	A	201	ARG	HG3	1.549	0.020	2
1	A	201	ARG	HD2	3.072	0.020	1
1	A	201	ARG	HD3	3.072	0.020	1
1	A	201	ARG	HE	7.153	0.020	1
1	A	201	ARG	N	119.614	0.3	1
1	A	201	ARG	NE	84.304	0.3	1
1	A	202	ILE	CA	64.107	0.3	1
1	A	202	ILE	CB	37.519	0.3	1
1	A	202	ILE	CG1	28.218	0.3	1
1	A	202	ILE	CG2	15.147	0.3	1
1	A	202	ILE	CD1	13.829	0.3	1
1	A	202	ILE	HA	3.388	0.020	1
1	A	202	ILE	HB	1.438	0.020	1
1	A	202	ILE	HG12	0.698	0.020	2
1	A	202	ILE	HG13	1.372	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	202	ILE	N	119.347	0.3	1
1	A	202	ILE	HG21	-0.256	0.020	1
1	A	202	ILE	HG22	-0.256	0.020	1
1	A	202	ILE	HG23	-0.256	0.020	1
1	A	202	ILE	HD11	0.387	0.020	1
1	A	202	ILE	HD12	0.387	0.020	1
1	A	202	ILE	HD13	0.387	0.020	1
1	A	203	PHE	CA	58.686	0.3	1
1	A	203	PHE	CB	40.07	0.3	1
1	A	203	PHE	CD1	132.149	0.3	1
1	A	203	PHE	CE1	131.016	0.3	1
1	A	203	PHE	CZ	128.906	0.3	1
1	A	203	PHE	HA	4.26	0.020	1
1	A	203	PHE	HB2	2.86	0.020	2
1	A	203	PHE	HB3	3.529	0.020	2
1	A	203	PHE	HD1	7.358	0.020	1
1	A	203	PHE	HD2	7.358	0.020	1
1	A	203	PHE	HE1	6.933	0.020	1
1	A	203	PHE	HE2	6.933	0.020	1
1	A	203	PHE	HZ	5.776	0.020	1
1	A	203	PHE	N	115.479	0.3	1
1	A	204	GLU	CA	56.706	0.3	1
1	A	204	GLU	CB	30.363	0.3	1
1	A	204	GLU	CG	36.125	0.3	1
1	A	204	GLU	HA	4.385	0.020	1
1	A	204	GLU	HB2	1.95	0.020	2
1	A	204	GLU	HB3	2.02	0.020	2
1	A	204	GLU	HG2	2.281	0.020	2
1	A	204	GLU	HG3	2.345	0.020	2
1	A	204	GLU	N	120.316	0.3	1
1	A	205	THR	CA	61.673	0.3	1
1	A	205	THR	CB	69.606	0.3	1
1	A	205	THR	CG2	21.391	0.3	1
1	A	205	THR	HA	4.308	0.020	1
1	A	205	THR	HB	4.192	0.020	1
1	A	205	THR	N	114.855	0.3	1
1	A	205	THR	HG21	1.141	0.020	1
1	A	205	THR	HG22	1.141	0.020	1
1	A	205	THR	HG23	1.141	0.020	1
1	A	206	LYS	CA	57.498	0.3	1
1	A	206	LYS	CB	33.549	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	206	LYS	CG	24.632	0.3	1
1	A	206	LYS	HA	4.107	0.020	1
1	A	206	LYS	HB2	1.654	0.020	2
1	A	206	LYS	HB3	1.774	0.020	2
1	A	206	LYS	HG2	1.317	0.020	1
1	A	206	LYS	HG3	1.317	0.020	1
1	A	206	LYS	N	129.024	0.3	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	205	-0.02 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	196	0.41 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	196	0.36 ± 0.46	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 78%, i.e. 619 atoms were assigned a chemical shift out of a possible 791. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	160/269 (59%)	54/108 (50%)	54/108 (50%)	52/53 (98%)
Sidechain	417/464 (90%)	283/299 (95%)	124/144 (86%)	10/21 (48%)
Aromatic	42/58 (72%)	27/28 (96%)	15/30 (50%)	0/0 (—%)
Overall	619/791 (78%)	364/435 (84%)	193/282 (68%)	62/74 (84%)

7.1.4 Statistically unusual chemical shifts

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	162	ILE	HD11	-1.47	-0.72 – 2.09	-7.7
1	A	162	ILE	HD12	-1.47	-0.72 – 2.09	-7.7

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	162	ILE	HD13	-1.47	-0.72 – 2.09	-7.7
1	A	151	LYS	HG2	-0.37	0.13 – 2.61	-7.0
1	A	200	SER	HB2	2.12	2.61 – 5.13	-7.0
1	A	173	GLN	HB2	0.59	0.80 – 3.29	-5.9
1	A	93	LEU	HB2	-0.14	-0.07 – 3.30	-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: