



# wwPDB NMR Structure Validation Summary Report ⓘ

Feb 4, 2025 – 02:22 PM EST

PDB ID : 8EPY  
BMRB ID : 31046  
Title : The solution structure of abxF in complex with its product (-)-ABX, an enzyme catalyzing the formation of the chiral spiroketal of an anthrabenzoxocinone antibiotic, (-)-ABX  
Authors : Jia, X.; Yan, X.; Qu, X.; Mobli, M.  
Deposited on : 2022-10-06

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

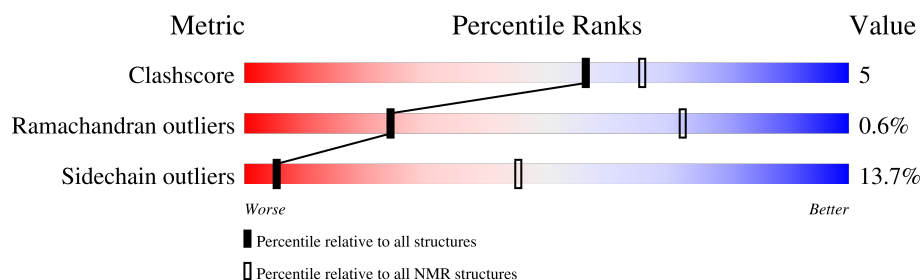
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 4%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	245	 69% 10% • 20%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:16-A:41, A:51-A:132, A:141-A:166, A:183-A:245 (197)	0.42	2

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 4 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3521 atoms, of which 1714 are hydrogens and 0 are deuteriums.

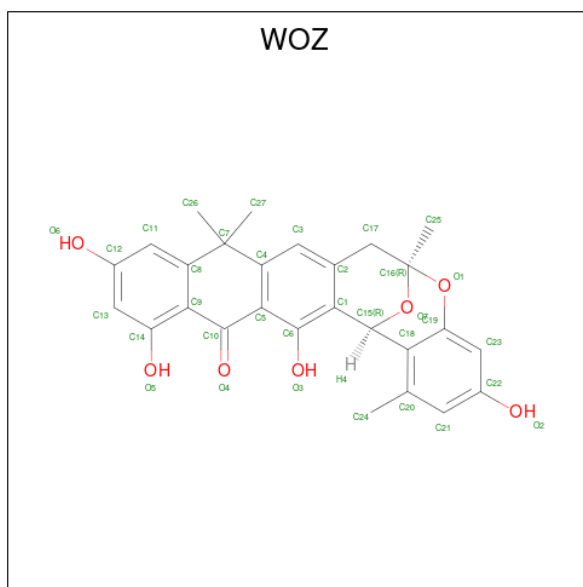
- Molecule 1 is a protein called Glyoxalase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	245	3463	1110	1690	307	348	8	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A2I6B3F9
A	2	SER	-	expression tag	UNP A0A2I6B3F9
A	3	HIS	-	expression tag	UNP A0A2I6B3F9

- Molecule 2 is (6R,16R)-3,11,13,15-tetrahydroxy-1,6,9,9-tetramethyl-6,7,9,16-tetrahydro-14H-6,16-epoxyanthra[2,3-e]benzo[b]oxocin-14-one (three-letter code: WOZ) (formula:  $C_{27}H_{24}O_7$ ) (labeled as "Ligand of Interest" by depositor).



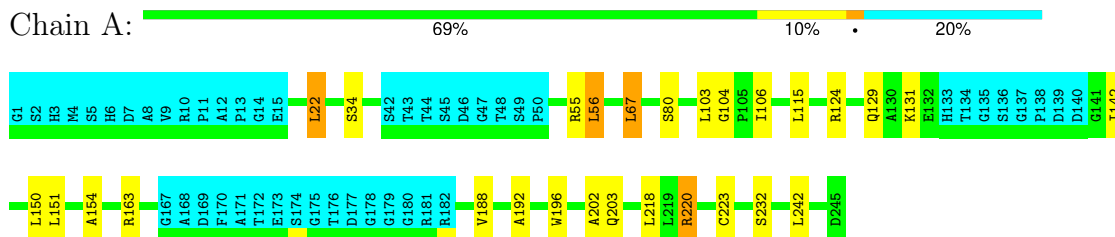
Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	A	1	58	27	24	7

## 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.

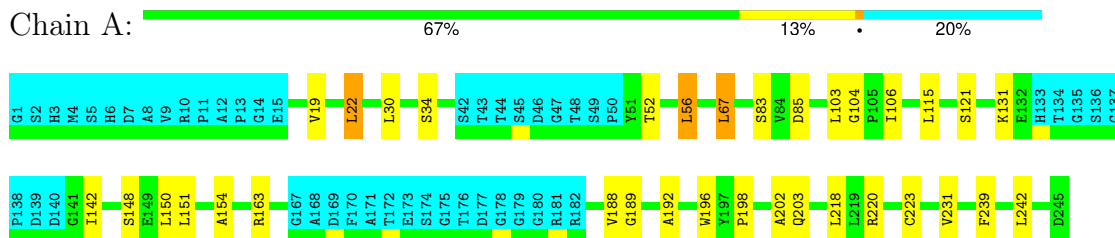
- Molecule 1: Glyoxalase



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

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: Glyoxalase



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 200 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 calculation	
XTB	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	2684
Number of shifts mapped to atoms	140
Number of unparsed shifts	0
Number of shifts with mapping errors	2544
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WOZ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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	1446	1410	1410	14±2
All	All	29600	28680	28200	274

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 5.

5 of 47 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:HD23	1:A:67:LEU:HD12	0.72	1.62	13	15
1:A:22:LEU:HD23	1:A:67:LEU:HD22	0.62	1.72	15	1
1:A:22:LEU:HD22	1:A:22:LEU:C	0.58	2.19	15	20
1:A:67:LEU:HD13	1:A:67:LEU:N	0.57	2.14	16	15
1:A:188:VAL:HB	1:A:192:ALA:HB3	0.56	1.78	11	19

## 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	196/245 (80%)	179±2 (91±1%)	16±2 (8±1%)	1±1 (1±0%)	24	72
All	All	3920/4900 (80%)	3581 (91%)	316 (8%)	23 (1%)	24	72

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	154	ALA	17
1	A	189	GLY	6

### 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	142/176 (81%)	123±2 (86±2%)	19±2 (14±2%)	5	45
All	All	2840/3520 (81%)	2451 (86%)	389 (14%)	5	45

5 of 47 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	22	LEU	20
1	A	56	LEU	20
1	A	131	LYS	20
1	A	218	LEU	20
1	A	220	ARG	20



### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	WOZ	A	246	-	39,39,39	0.69±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	WOZ	A	246	-	54,65,65	0.90±0.04	3±0 (5±0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	246	WOZ	C25-C16	2.16	1.53	1.51	16	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	246	WOZ	C18-C15-C1	3.06	114.83	110.08	4	20
2	A	246	WOZ	C16-O1-C19	2.67	114.13	118.47	13	20
2	A	246	WOZ	C8-C7-C4	2.28	114.07	108.98	9	19
2	A	246	WOZ	C25-C16-C17	2.05	111.04	113.32	17	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 4% for the well-defined parts and 5% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 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	2684
Number of shifts mapped to atoms	140
Number of unparsed shifts	0
Number of shifts with mapping errors	2544
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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 2544) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	0	HIS	CA	56.215	0.000	.
1	A	0	HIS	CB	30.083	0.000	.
1	A	0	HIS	CD2	119.954	0.000	.
1	A	0	HIS	HD2	7.128	0.000	.
1	A	0	HIS	C	174.962	0.000	.
1	A	1	MET	N	121.713	0.000	.
1	A	1	MET	H	8.382	0.000	.
1	A	1	MET	CA	55.446	0.000	.
1	A	1	MET	HA	4.479	0.000	.
1	A	1	MET	CB	32.985	0.001	.
1	A	1	MET	HB2	1.941	0.000	.
1	A	1	MET	HB3	2.042	0.000	.
1	A	1	MET	CG	31.873	0.000	.
1	A	1	MET	HG2	2.443	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HG3	2.512	0.000	.
1	A	1	MET	C	176.041	0.001	.
1	A	4	ASP	N	120.948	0.000	.
1	A	4	ASP	H	8.284	0.000	.
1	A	4	ASP	CA	54.433	0.000	.
1	A	4	ASP	HA	4.572	0.000	.
1	A	4	ASP	CB	41.249	0.000	.
1	A	4	ASP	HB2	2.574	0.000	.
1	A	4	ASP	HB3	2.672	0.000	.
1	A	4	ASP	C	175.69	0.000	.
1	A	5	ALA	N	124.02	0.000	.
1	A	5	ALA	H	8.143	0.000	.
1	A	5	ALA	CA	52.416	0.000	.
1	A	5	ALA	HA	4.353	0.000	.
1	A	5	ALA	HB1	1.377	0.000	.
1	A	5	ALA	HB2	1.377	0.000	.
1	A	5	ALA	HB3	1.377	0.000	.
1	A	5	ALA	CB	19.401	0.000	.
1	A	5	ALA	C	177.369	0.002	.
1	A	6	VAL	N	120.034	0.000	.
1	A	6	VAL	H	8.157	0.000	.
1	A	6	VAL	CA	62.237	0.000	.
1	A	6	VAL	HA	4.118	0.000	.
1	A	6	VAL	CB	32.741	0.000	.
1	A	6	VAL	HB	2.069	0.000	.
1	A	6	VAL	HG11	0.937	0.005	.
1	A	6	VAL	HG12	0.937	0.005	.
1	A	6	VAL	HG13	0.937	0.005	.
1	A	6	VAL	HG21	0.935	0.000	.
1	A	6	VAL	HG22	0.935	0.000	.
1	A	6	VAL	HG23	0.935	0.000	.
1	A	6	VAL	CG1	20.654	0.000	.
1	A	6	VAL	CG2	21.284	0.000	.
1	A	6	VAL	C	175.675	0.000	.
1	A	7	ARG	N	125.536	0.000	.
1	A	7	ARG	H	8.348	0.000	.
1	A	7	ARG	CA	53.951	0.000	.
1	A	7	ARG	HA	4.656	0.000	.
1	A	7	ARG	CB	30.577	0.000	.
1	A	7	ARG	HB2	1.758	0.000	.
1	A	7	ARG	HB3	1.928	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ARG	CG	27.184	0.000	.
1	A	7	ARG	HG2	1.683	0.000	.
1	A	7	ARG	HG3	1.683	0.000	.
1	A	7	ARG	CD	43.35	0.000	.
1	A	7	ARG	HD2	3.247	0.000	.
1	A	7	ARG	HD3	3.247	0.000	.
1	A	7	ARG	C	173.819	0.000	.
1	A	8	PRO	CD	50.761	0.000	.
1	A	8	PRO	CA	63.053	0.000	.
1	A	8	PRO	HA	4.464	0.000	.
1	A	8	PRO	CB	31.987	0.000	.
1	A	8	PRO	HB2	2.209	0.000	.
1	A	8	PRO	HB3	2.209	0.000	.
1	A	8	PRO	CG	27.482	0.000	.
1	A	8	PRO	HG2	2.017	0.000	.
1	A	8	PRO	HG3	2.017	0.000	.
1	A	8	PRO	HD2	3.688	0.000	.
1	A	8	PRO	HD3	3.688	0.000	.
1	A	8	PRO	C	176.288	0.000	.
1	A	9	ALA	N	127.952	0.004	.
1	A	9	ALA	H	8.455	0.002	.
1	A	9	ALA	CA	50.229	0.000	.
1	A	9	ALA	HA	4.63	0.000	.
1	A	9	ALA	HB1	1.481	0.000	.
1	A	9	ALA	HB2	1.481	0.000	.
1	A	9	ALA	HB3	1.481	0.000	.
1	A	9	ALA	CB	18.177	0.000	.
1	A	9	ALA	C	174.697	0.000	.
1	A	10	PRO	CD	50.18	0.001	.
1	A	10	PRO	CA	63.786	0.001	.
1	A	10	PRO	HA	4.29	0.000	.
1	A	10	PRO	CB	31.684	0.000	.
1	A	10	PRO	HB2	2.591	0.000	.
1	A	10	PRO	HB3	2.591	0.000	.
1	A	10	PRO	CG	28.595	0.000	.
1	A	10	PRO	HG2	2.28	0.000	.
1	A	10	PRO	HG3	2.055	0.000	.
1	A	10	PRO	HD2	3.664	0.000	.
1	A	10	PRO	HD3	3.968	0.001	.
1	A	10	PRO	C	178.249	0.000	.
1	A	11	GLY	N	116.178	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	GLY	H	9.682	0.000	.
1	A	11	GLY	CA	43.888	0.000	.
1	A	11	GLY	HA2	3.451	0.000	.
1	A	11	GLY	HA3	3.451	0.000	.
1	A	11	GLY	C	173.865	0.000	.
1	A	12	GLU	N	123.511	0.001	.
1	A	12	GLU	H	8.336	0.000	.
1	A	12	GLU	CA	55.292	0.000	.
1	A	12	GLU	HA	4.428	0.000	.
1	A	12	GLU	CB	31.489	0.001	.
1	A	12	GLU	HB2	2.153	0.000	.
1	A	12	GLU	HB3	2.285	0.000	.
1	A	12	GLU	CG	35.817	0.000	.
1	A	12	GLU	HG2	2.65	0.000	.
1	A	12	GLU	HG3	2.65	0.000	.
1	A	12	GLU	C	176.888	0.000	.
1	A	14	THR	N	122.262	0.000	.
1	A	14	THR	H	9.159	0.000	.
1	A	14	THR	CA	64.237	0.000	.
1	A	14	THR	HA	4.833	0.000	.
1	A	14	THR	CB	72.28	0.004	.
1	A	14	THR	HB	4.05	0.001	.
1	A	14	THR	HG21	1.476	0.000	.
1	A	14	THR	HG22	1.476	0.000	.
1	A	14	THR	HG23	1.476	0.000	.
1	A	14	THR	CG2	21.34	0.001	.
1	A	14	THR	C	171.334	0.000	.
1	A	15	TRP	N	121.304	0.000	.
1	A	15	TRP	H	7.928	0.000	.
1	A	15	TRP	CA	56.34	0.000	.
1	A	15	TRP	HA	4.6	0.000	.
1	A	15	TRP	CB	33.925	0.001	.
1	A	15	TRP	HB2	2.639	0.000	.
1	A	15	TRP	HB3	2.129	0.003	.
1	A	15	TRP	C	172.683	0.000	.
1	A	16	VAL	N	118.896	0.000	.
1	A	16	VAL	H	8.409	0.000	.
1	A	16	VAL	CA	58.355	0.000	.
1	A	16	VAL	HA	5.314	0.000	.
1	A	16	VAL	CB	34.946	0.000	.
1	A	16	VAL	HB	1.959	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	VAL	HG11	-0.077	0.000	.
1	A	16	VAL	HG12	-0.077	0.000	.
1	A	16	VAL	HG13	-0.077	0.000	.
1	A	16	VAL	HG21	0.556	0.000	.
1	A	16	VAL	HG22	0.556	0.000	.
1	A	16	VAL	HG23	0.556	0.000	.
1	A	16	VAL	CG1	17.85	0.000	.
1	A	16	VAL	CG2	24.136	0.000	.
1	A	18	LEU	N	130.414	0.000	.
1	A	18	LEU	H	8.182	0.000	.
1	A	18	LEU	CA	52.747	0.000	.
1	A	18	LEU	HA	4.262	0.000	.
1	A	18	LEU	CB	40.951	0.006	.
1	A	18	LEU	HB2	-1.652	0.000	.
1	A	18	LEU	HB3	-0.96	0.000	.
1	A	18	LEU	CG	26.787	0.002	.
1	A	18	LEU	HG	0.649	0.000	.
1	A	18	LEU	HD11	-0.1	0.000	.
1	A	18	LEU	HD12	-0.1	0.000	.
1	A	18	LEU	HD13	-0.1	0.000	.
1	A	18	LEU	HD21	0.371	0.001	.
1	A	18	LEU	HD22	0.371	0.001	.
1	A	18	LEU	HD23	0.371	0.001	.
1	A	18	LEU	CD1	22.315	0.000	.
1	A	18	LEU	CD2	25.602	0.000	.
1	A	18	LEU	C	173.802	0.000	.
1	A	19	LEU	N	124.941	0.000	.
1	A	19	LEU	H	7.217	0.004	.
1	A	19	LEU	CA	53.207	0.000	.
1	A	19	LEU	HA	4.826	0.000	.
1	A	19	LEU	CB	43.233	0.001	.
1	A	19	LEU	HB2	0.813	0.000	.
1	A	19	LEU	HB3	1.897	0.000	.
1	A	19	LEU	CG	26.129	0.000	.
1	A	19	LEU	HG	1.606	0.000	.
1	A	19	LEU	HD11	0.659	0.000	.
1	A	19	LEU	HD12	0.659	0.000	.
1	A	19	LEU	HD13	0.659	0.000	.
1	A	19	LEU	HD21	0.845	0.000	.
1	A	19	LEU	HD22	0.845	0.000	.
1	A	19	LEU	HD23	0.845	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	LEU	CD1	23.84	0.003	.
1	A	19	LEU	CD2	26.169	0.000	.
1	A	19	LEU	C	175.962	0.005	.
1	A	20	THR	N	117.663	0.000	.
1	A	20	THR	H	8.394	0.000	.
1	A	20	THR	CA	55.202	0.000	.
1	A	20	THR	HA	5.319	0.002	.
1	A	20	THR	CB	69.828	0.000	.
1	A	20	THR	HB	3.781	0.000	.
1	A	20	THR	HG21	0.981	0.000	.
1	A	20	THR	HG22	0.981	0.000	.
1	A	20	THR	HG23	0.981	0.000	.
1	A	20	THR	CG2	19.055	0.000	.
1	A	21	PRO	CD	52.418	0.000	.
1	A	21	PRO	CA	63.741	0.000	.
1	A	21	PRO	HA	4.803	0.001	.
1	A	21	PRO	CB	32.204	0.001	.
1	A	21	PRO	HB2	2.064	0.000	.
1	A	21	PRO	HB3	2.33	0.001	.
1	A	21	PRO	CG	26.639	0.002	.
1	A	21	PRO	HG2	2.064	0.000	.
1	A	21	PRO	HG3	2.064	0.000	.
1	A	21	PRO	HD2	3.692	0.000	.
1	A	21	PRO	HD3	4.157	0.001	.
1	A	21	PRO	C	175.371	0.000	.
1	A	22	ASP	N	119.544	0.000	.
1	A	22	ASP	H	8.117	0.000	.
1	A	22	ASP	CA	52.41	0.000	.
1	A	22	ASP	HA	4.863	0.000	.
1	A	22	ASP	CB	40.808	0.000	.
1	A	22	ASP	HB2	2.322	0.001	.
1	A	22	ASP	HB3	2.836	0.002	.
1	A	22	ASP	C	175.17	0.000	.
1	A	23	ARG	N	127.795	0.000	.
1	A	23	ARG	H	9.074	0.000	.
1	A	23	ARG	CA	60.065	0.000	.
1	A	23	ARG	HA	3.723	0.000	.
1	A	23	ARG	CB	30.82	0.000	.
1	A	23	ARG	HB2	1.925	0.000	.
1	A	23	ARG	HB3	1.627	0.000	.
1	A	23	ARG	CG	26.652	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	23	ARG	HG2	1.199	0.000	.
1	A	23	ARG	HG3	1.421	0.001	.
1	A	23	ARG	CD	44.39	0.001	.
1	A	23	ARG	HD2	2.639	0.000	.
1	A	23	ARG	HD3	3.219	0.001	.
1	A	23	ARG	C	177.08	0.000	.
1	A	24	GLY	N	106.757	0.000	.
1	A	24	GLY	H	8.928	0.000	.
1	A	24	GLY	CA	47.63	0.001	.
1	A	24	GLY	HA2	3.605	0.003	.
1	A	24	GLY	HA3	3.924	0.000	.
1	A	24	GLY	C	176.839	0.000	.
1	A	25	ALA	N	123.627	0.001	.
1	A	25	ALA	H	7.673	0.000	.
1	A	25	ALA	CA	54.372	0.000	.
1	A	25	ALA	HA	4.187	0.000	.
1	A	25	ALA	HB1	1.34	0.000	.
1	A	25	ALA	HB2	1.34	0.000	.
1	A	25	ALA	HB3	1.34	0.000	.
1	A	25	ALA	CB	18.564	0.000	.
1	A	25	ALA	C	181.046	0.000	.
1	A	26	ALA	N	123.192	0.000	.
1	A	26	ALA	H	7.885	0.000	.
1	A	26	ALA	CA	55.447	0.000	.
1	A	26	ALA	HA	4.342	0.000	.
1	A	26	ALA	HB1	1.662	0.000	.
1	A	26	ALA	HB2	1.662	0.000	.
1	A	26	ALA	HB3	1.662	0.000	.
1	A	26	ALA	CB	17.907	0.000	.
1	A	26	ALA	C	179.291	0.000	.
1	A	27	LEU	N	117.307	0.000	.
1	A	27	LEU	H	8.729	0.000	.
1	A	27	LEU	CA	58.367	0.001	.
1	A	27	LEU	HA	3.783	0.000	.
1	A	27	LEU	CB	39.284	0.000	.
1	A	27	LEU	HB2	1.105	0.000	.
1	A	27	LEU	HB3	1.643	0.000	.
1	A	27	LEU	CG	25.807	0.000	.
1	A	27	LEU	HG	1.486	0.000	.
1	A	27	LEU	HD11	0.043	0.000	.
1	A	27	LEU	HD12	0.043	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	LEU	HD13	0.043	0.000	.
1	A	27	LEU	HD21	0.483	0.000	.
1	A	27	LEU	HD22	0.483	0.000	.
1	A	27	LEU	HD23	0.483	0.000	.
1	A	27	LEU	CD1	22.051	0.000	.
1	A	27	LEU	CD2	24.415	0.000	.
1	A	27	LEU	C	180.064	0.008	.
1	A	28	GLN	N	116.385	0.001	.
1	A	28	GLN	H	7.249	0.000	.
1	A	28	GLN	CA	59.239	0.000	.
1	A	28	GLN	HA	4.03	0.000	.
1	A	28	GLN	CB	28.705	0.000	.
1	A	28	GLN	HB2	2.205	0.000	.
1	A	28	GLN	HB3	2.205	0.000	.
1	A	28	GLN	CG	33.918	0.002	.
1	A	28	GLN	HG2	2.442	0.000	.
1	A	28	GLN	HG3	2.553	0.000	.
1	A	28	GLN	NE2	111.986	0.001	.
1	A	28	GLN	HE21	6.842	0.000	.
1	A	28	GLN	HE22	7.469	0.000	.
1	A	28	GLN	C	177.913	0.000	.
1	A	29	PHE	N	120.866	0.001	.
1	A	29	PHE	H	7.699	0.000	.
1	A	29	PHE	CA	61.602	0.001	.
1	A	29	PHE	HA	4.16	0.000	.
1	A	29	PHE	CB	39.247	0.000	.
1	A	29	PHE	HB2	2.897	0.000	.
1	A	29	PHE	HB3	3.185	0.002	.
1	A	29	PHE	HD1	6.298	0.000	.
1	A	29	PHE	HD2	6.298	0.000	.
1	A	29	PHE	HE1	7.021	0.000	.
1	A	29	PHE	HE2	7.021	0.000	.
1	A	29	PHE	CD1	132.466	0.000	.
1	A	29	PHE	CE1	130.932	0.000	.
1	A	29	PHE	CZ	129.466	0.001	.
1	A	29	PHE	HZ	7.423	0.000	.
1	A	29	PHE	CE2	130.932	0.000	.
1	A	29	PHE	CD2	132.466	0.000	.
1	A	29	PHE	C	175.685	0.000	.
1	A	30	TYR	N	115.423	0.000	.
1	A	30	TYR	H	8.764	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	TYR	CA	63.628	0.000	.
1	A	30	TYR	HA	3.329	0.000	.
1	A	30	TYR	CB	39.219	0.000	.
1	A	30	TYR	HB2	2.676	0.000	.
1	A	30	TYR	HB3	2.911	0.000	.
1	A	30	TYR	HD1	6.19	0.000	.
1	A	30	TYR	HD2	6.19	0.000	.
1	A	30	TYR	HH	12.3	0.000	.
1	A	30	TYR	C	179.327	0.000	.
1	A	31	SER	N	113.142	0.000	.
1	A	31	SER	H	8.429	0.000	.
1	A	31	SER	CA	61.595	0.000	.
1	A	31	SER	HA	4.092	0.000	.
1	A	31	SER	CB	63.023	0.000	.
1	A	31	SER	HB2	4.231	0.000	.
1	A	31	SER	HB3	4.303	0.000	.
1	A	31	SER	C	177.549	0.000	.
1	A	32	ALA	N	124.159	0.000	.
1	A	32	ALA	H	7.296	0.000	.
1	A	32	ALA	CA	54.808	0.000	.
1	A	32	ALA	HA	3.983	0.000	.
1	A	32	ALA	HB1	1.388	0.000	.
1	A	32	ALA	HB2	1.388	0.000	.
1	A	32	ALA	HB3	1.388	0.000	.
1	A	32	ALA	CB	18.512	0.000	.
1	A	32	ALA	C	179.317	0.000	.
1	A	33	LEU	N	116.441	0.000	.
1	A	33	LEU	H	7.423	0.000	.
1	A	33	LEU	CA	56.722	0.000	.
1	A	33	LEU	HA	3.606	0.000	.
1	A	33	LEU	CB	42.451	0.000	.
1	A	33	LEU	HB2	0.114	0.000	.
1	A	33	LEU	HB3	0.198	0.000	.
1	A	33	LEU	CG	25.9	0.000	.
1	A	33	LEU	HG	0.191	0.000	.
1	A	33	LEU	HD11	0.362	0.000	.
1	A	33	LEU	HD12	0.362	0.000	.
1	A	33	LEU	HD13	0.362	0.000	.
1	A	33	LEU	HD21	0.106	0.000	.
1	A	33	LEU	HD22	0.106	0.000	.
1	A	33	LEU	HD23	0.106	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	33	LEU	CD1	23.513	0.000	.
1	A	33	LEU	CD2	26.209	0.000	.
1	A	33	LEU	C	177.539	0.000	.
1	A	34	PHE	N	111.581	0.001	.
1	A	34	PHE	H	7.45	0.000	.
1	A	34	PHE	CA	55.796	0.000	.
1	A	34	PHE	HA	4.761	0.000	.
1	A	34	PHE	CB	41.298	0.000	.
1	A	34	PHE	HB2	1.153	0.000	.
1	A	34	PHE	HB3	2.723	0.000	.
1	A	34	PHE	HD1	6.129	0.000	.
1	A	34	PHE	HD2	6.129	0.000	.
1	A	34	PHE	HE1	6.476	0.000	.
1	A	34	PHE	HE2	6.476	0.000	.
1	A	34	PHE	CD1	130.824	0.000	.
1	A	34	PHE	CE1	129.585	0.000	.
1	A	34	PHE	CZ	129.397	0.006	.
1	A	34	PHE	HZ	6.897	0.003	.
1	A	34	PHE	CE2	129.585	0.000	.
1	A	34	PHE	CD2	130.824	0.000	.
1	A	34	PHE	C	176.881	0.000	.
1	A	35	GLY	N	107.358	0.001	.
1	A	35	GLY	H	7.97	0.000	.
1	A	35	GLY	CA	45.825	0.000	.
1	A	35	GLY	HA2	3.944	0.000	.
1	A	35	GLY	HA3	4.095	0.000	.
1	A	35	GLY	C	174.241	0.000	.
1	A	36	TRP	N	116.638	0.000	.
1	A	36	TRP	H	6.177	0.000	.
1	A	36	TRP	CA	55.387	0.000	.
1	A	36	TRP	HA	4.732	0.000	.
1	A	36	TRP	CB	30.984	0.000	.
1	A	36	TRP	HB2	2.752	0.000	.
1	A	36	TRP	HB3	2.772	0.000	.
1	A	36	TRP	CD1	122.774	0.000	.
1	A	36	TRP	CE3	119.7	0.000	.
1	A	36	TRP	NE1	129.181	0.000	.
1	A	36	TRP	HD1	6.714	0.000	.
1	A	36	TRP	HE3	7.312	0.000	.
1	A	36	TRP	CZ3	121.81	0.005	.
1	A	36	TRP	CZ2	115.722	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	36	TRP	HE1	10.46	0.000	.
1	A	36	TRP	HZ3	6.341	0.002	.
1	A	36	TRP	CH2	125.482	0.001	.
1	A	36	TRP	HZ2	5.912	0.000	.
1	A	36	TRP	HH2	5.856	0.003	.
1	A	36	TRP	C	173.96	0.000	.
1	A	37	GLU	N	119.397	0.000	.
1	A	37	GLU	H	9.109	0.000	.
1	A	37	GLU	CA	54.174	0.001	.
1	A	37	GLU	HA	4.148	0.000	.
1	A	37	GLU	CB	32.445	0.000	.
1	A	37	GLU	HB2	1.792	0.001	.
1	A	37	GLU	HB3	1.943	0.000	.
1	A	37	GLU	CG	36.62	0.003	.
1	A	37	GLU	HG2	2.139	0.000	.
1	A	37	GLU	HG3	2.31	0.000	.
1	A	37	GLU	C	176.001	0.003	.
1	A	38	PHE	N	120.741	0.000	.
1	A	38	PHE	H	8.491	0.000	.
1	A	38	PHE	CA	55.995	0.002	.
1	A	38	PHE	HA	5.712	0.000	.
1	A	38	PHE	CB	41.996	0.001	.
1	A	38	PHE	HB2	2.891	0.000	.
1	A	38	PHE	HB3	3.241	0.000	.
1	A	38	PHE	HD1	7.27	0.000	.
1	A	38	PHE	HD2	7.27	0.000	.
1	A	38	PHE	CD1	131.912	0.000	.
1	A	38	PHE	CD2	131.912	0.002	.
1	A	38	PHE	C	176.294	0.000	.
1	A	39	SER	N	117.062	0.000	.
1	A	39	SER	H	8.879	0.000	.
1	A	39	SER	CA	57.323	0.000	.
1	A	39	SER	HA	4.814	0.000	.
1	A	39	SER	CB	65.143	0.000	.
1	A	39	SER	HB2	3.831	0.000	.
1	A	39	SER	HB3	3.831	0.000	.
1	A	39	SER	C	173.603	0.000	.
1	A	40	THR	N	122.348	0.000	.
1	A	40	THR	H	8.892	0.000	.
1	A	40	THR	CA	62.89	0.001	.
1	A	40	THR	HA	4.721	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	40	THR	CB	69.362	0.005	.
1	A	40	THR	HB	4.083	0.000	.
1	A	40	THR	HG21	1.239	0.000	.
1	A	40	THR	HG22	1.239	0.000	.
1	A	40	THR	HG23	1.239	0.000	.
1	A	40	THR	CG2	21.873	0.000	.
1	A	41	THR	N	123.272	0.000	.
1	A	41	THR	H	8.796	0.000	.
1	A	41	THR	CA	60.24	0.000	.
1	A	41	THR	HA	4.491	0.000	.
1	A	41	THR	CB	69.724	0.001	.
1	A	41	THR	HB	3.682	0.001	.
1	A	41	THR	HG21	0.733	0.000	.
1	A	41	THR	HG22	0.733	0.000	.
1	A	41	THR	HG23	0.733	0.000	.
1	A	41	THR	CG2	21.619	0.000	.
1	A	41	THR	C	172.696	0.000	.
1	A	43	ASP	N	123.551	0.000	.
1	A	43	ASP	H	8.579	0.000	.
1	A	43	ASP	CA	54.126	0.000	.
1	A	43	ASP	HA	4.868	0.000	.
1	A	43	ASP	CB	41.328	0.002	.
1	A	43	ASP	HB2	2.904	0.000	.
1	A	43	ASP	HB3	2.737	0.001	.
1	A	43	ASP	C	176.289	0.000	.
1	A	44	GLY	N	109.288	0.000	.
1	A	44	GLY	H	8.697	0.000	.
1	A	44	GLY	CA	45.353	0.003	.
1	A	44	GLY	HA2	3.835	0.000	.
1	A	44	GLY	HA3	4.369	0.000	.
1	A	44	GLY	C	174.513	0.006	.
1	A	45	THR	N	114.17	0.000	.
1	A	45	THR	H	8.375	0.000	.
1	A	45	THR	CA	63.078	0.000	.
1	A	45	THR	HA	4.443	0.000	.
1	A	45	THR	CB	70.499	0.001	.
1	A	45	THR	HB	4.358	0.000	.
1	A	45	THR	HG21	1.263	0.000	.
1	A	45	THR	HG22	1.263	0.000	.
1	A	45	THR	HG23	1.263	0.000	.
1	A	45	THR	CG2	21.675	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	46	SER	CA	55.881	0.000	.
1	A	46	SER	HA	4.875	0.000	.
1	A	46	SER	CB	64.2	0.000	.
1	A	46	SER	HB2	3.861	0.000	.
1	A	46	SER	HB3	3.861	0.000	.
1	A	48	TYR	CA	56.442	0.000	.
1	A	48	TYR	HA	4.794	0.000	.
1	A	48	TYR	CB	39.358	0.001	.
1	A	48	TYR	HB2	3.159	0.000	.
1	A	48	TYR	HB3	3.159	0.000	.
1	A	48	TYR	HD1	7.062	0.001	.
1	A	48	TYR	HD2	7.062	0.001	.
1	A	48	TYR	HE1	6.692	0.004	.
1	A	48	TYR	HE2	6.692	0.004	.
1	A	48	TYR	CD1	134.56	0.005	.
1	A	48	TYR	CE1	118.176	0.007	.
1	A	48	TYR	CE2	118.176	0.000	.
1	A	48	TYR	CD2	134.56	0.000	.
1	A	49	THR	N	118.084	0.000	.
1	A	49	THR	H	9.447	0.000	.
1	A	49	THR	CA	63.309	0.001	.
1	A	49	THR	HA	4.678	0.000	.
1	A	49	THR	CB	71.62	0.001	.
1	A	49	THR	HB	4.049	0.000	.
1	A	49	THR	HG21	1.305	0.000	.
1	A	49	THR	HG22	1.305	0.000	.
1	A	49	THR	HG23	1.305	0.000	.
1	A	49	THR	CG2	23.706	0.008	.
1	A	50	MET	N	126.406	0.000	.
1	A	50	MET	H	9.006	0.000	.
1	A	50	MET	CA	53.625	0.001	.
1	A	50	MET	HA	5.062	0.002	.
1	A	50	MET	CB	33.455	0.000	.
1	A	50	MET	HB2	2.027	0.000	.
1	A	50	MET	HB3	2.027	0.000	.
1	A	50	MET	CG	32.5	0.001	.
1	A	50	MET	HG2	2.453	0.000	.
1	A	50	MET	HG3	2.731	0.000	.
1	A	50	MET	HE1	2.05	0.000	.
1	A	50	MET	HE2	2.05	0.000	.
1	A	50	MET	HE3	2.05	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	50	MET	CE	16.962	0.000	.
1	A	50	MET	C	175.409	0.000	.
1	A	51	CYS	N	125.134	0.005	.
1	A	51	CYS	H	8.743	0.001	.
1	A	51	CYS	CA	56.817	0.000	.
1	A	51	CYS	HA	5.112	0.000	.
1	A	51	CYS	CB	28.266	0.003	.
1	A	51	CYS	HB2	1.904	0.000	.
1	A	51	CYS	HB3	2.607	0.000	.
1	A	51	CYS	C	174.058	0.004	.
1	A	52	ARG	N	123.912	0.001	.
1	A	52	ARG	H	9.473	0.000	.
1	A	52	ARG	CA	54.459	0.000	.
1	A	52	ARG	HA	5.278	0.000	.
1	A	52	ARG	CB	35.04	0.000	.
1	A	52	ARG	HB2	1.451	0.000	.
1	A	52	ARG	HB3	1.511	0.000	.
1	A	52	ARG	CG	28.193	0.000	.
1	A	52	ARG	HG2	1.307	0.000	.
1	A	52	ARG	HG3	1.407	0.000	.
1	A	52	ARG	CD	43.422	0.001	.
1	A	52	ARG	HD2	2.951	0.000	.
1	A	52	ARG	HD3	3.129	0.000	.
1	A	52	ARG	NE	84.14	0.000	.
1	A	52	ARG	HE	7.338	0.000	.
1	A	52	ARG	C	174.196	0.000	.
1	A	53	LEU	N	120.396	0.000	.
1	A	53	LEU	H	8.771	0.000	.
1	A	53	LEU	CA	54.666	0.000	.
1	A	53	LEU	HA	4.636	0.000	.
1	A	53	LEU	CB	45.926	0.000	.
1	A	53	LEU	HB2	1.365	0.000	.
1	A	53	LEU	HB3	1.606	0.000	.
1	A	53	LEU	CG	27.604	0.000	.
1	A	53	LEU	HG	1.291	0.000	.
1	A	53	LEU	HD11	1.122	0.000	.
1	A	53	LEU	HD12	1.122	0.000	.
1	A	53	LEU	HD13	1.122	0.000	.
1	A	53	LEU	HD21	1.085	0.000	.
1	A	53	LEU	HD22	1.085	0.000	.
1	A	53	LEU	HD23	1.085	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	LEU	CD1	22.928	0.000	.
1	A	53	LEU	CD2	26.406	0.000	.
1	A	53	LEU	C	176.473	0.004	.
1	A	54	ARG	N	126.897	0.000	.
1	A	54	ARG	H	9.74	0.000	.
1	A	54	ARG	CA	57.675	0.000	.
1	A	54	ARG	HA	3.871	0.000	.
1	A	54	ARG	CB	28.496	0.000	.
1	A	54	ARG	HB2	1.923	0.000	.
1	A	54	ARG	HB3	1.923	0.000	.
1	A	54	ARG	C	176.38	0.000	.
1	A	55	GLY	N	103.009	0.001	.
1	A	55	GLY	H	8.823	0.000	.
1	A	55	GLY	CA	45.428	0.000	.
1	A	55	GLY	HA2	3.601	0.001	.
1	A	55	GLY	HA3	4.174	0.000	.
1	A	55	GLY	C	174.135	0.000	.
1	A	56	ARG	N	119.717	0.000	.
1	A	56	ARG	H	7.794	0.000	.
1	A	56	ARG	CA	53.551	0.000	.
1	A	56	ARG	HA	4.749	0.000	.
1	A	56	ARG	CB	32.528	0.000	.
1	A	56	ARG	HB2	1.995	0.000	.
1	A	56	ARG	HB3	1.825	0.000	.
1	A	56	ARG	CG	27.373	0.001	.
1	A	56	ARG	HG2	1.701	0.001	.
1	A	56	ARG	HG3	1.701	0.001	.
1	A	56	ARG	CD	42.997	0.000	.
1	A	56	ARG	HD2	3.21	0.001	.
1	A	56	ARG	HD3	3.21	0.001	.
1	A	56	ARG	NE	85.286	0.000	.
1	A	56	ARG	HE	7.341	0.000	.
1	A	56	ARG	C	175.553	0.000	.
1	A	57	GLU	N	120.572	0.001	.
1	A	57	GLU	H	8.874	0.000	.
1	A	57	GLU	CA	57.226	0.000	.
1	A	57	GLU	HA	4.317	0.000	.
1	A	57	GLU	CB	29.895	0.000	.
1	A	57	GLU	HB2	2.212	0.000	.
1	A	57	GLU	HB3	2.212	0.000	.
1	A	57	GLU	C	175.672	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	VAL	N	122.747	0.000	.
1	A	58	VAL	H	8.99	0.000	.
1	A	58	VAL	CA	63.673	0.000	.
1	A	58	VAL	HA	3.943	0.000	.
1	A	58	VAL	CB	34.455	0.000	.
1	A	58	VAL	HB	0.832	0.000	.
1	A	58	VAL	HG11	0.492	0.000	.
1	A	58	VAL	HG12	0.492	0.000	.
1	A	58	VAL	HG13	0.492	0.000	.
1	A	58	VAL	HG21	0.586	0.000	.
1	A	58	VAL	HG22	0.586	0.000	.
1	A	58	VAL	HG23	0.586	0.000	.
1	A	58	VAL	CG1	20.593	0.000	.
1	A	58	VAL	CG2	21.54	0.000	.
1	A	58	VAL	C	174.902	0.000	.
1	A	59	CYS	N	109.691	0.000	.
1	A	59	CYS	H	6.905	0.000	.
1	A	59	CYS	CA	56.121	0.000	.
1	A	59	CYS	HA	2.357	0.000	.
1	A	59	CYS	CB	28.554	0.000	.
1	A	59	CYS	HB2	2.745	0.000	.
1	A	59	CYS	HB3	2.211	0.000	.
1	A	59	CYS	C	170.685	0.000	.
1	A	60	SER	N	108.236	0.000	.
1	A	60	SER	H	7.254	0.000	.
1	A	60	SER	CA	56.623	0.000	.
1	A	60	SER	HA	5.564	0.000	.
1	A	60	SER	CB	66.289	0.002	.
1	A	60	SER	HB2	4.034	0.000	.
1	A	60	SER	HB3	4.089	0.000	.
1	A	61	ILE	N	117.918	0.000	.
1	A	61	ILE	H	8.836	0.000	.
1	A	61	ILE	CA	60.69	0.000	.
1	A	61	ILE	HA	4.73	0.000	.
1	A	61	ILE	CB	42.335	0.002	.
1	A	61	ILE	HB	1.236	0.000	.
1	A	61	ILE	HG21	0.628	0.000	.
1	A	61	ILE	HG22	0.628	0.000	.
1	A	61	ILE	HG23	0.628	0.000	.
1	A	61	ILE	CG2	17.202	0.000	.
1	A	61	ILE	CG1	26.934	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	ILE	HG12	1.439	0.000	.
1	A	61	ILE	HG13	1.439	0.000	.
1	A	61	ILE	HD11	0.725	0.000	.
1	A	61	ILE	HD12	0.725	0.000	.
1	A	61	ILE	HD13	0.725	0.000	.
1	A	61	ILE	CD1	14.265	0.005	.
1	A	61	ILE	C	174.227	0.000	.
1	A	62	GLY	N	115.062	0.000	.
1	A	62	GLY	H	9.563	0.000	.
1	A	62	GLY	CA	43.994	0.000	.
1	A	62	GLY	HA2	3.982	0.000	.
1	A	62	GLY	HA3	3.982	0.000	.
1	A	63	ASP	CA	54.092	0.000	.
1	A	63	ASP	HA	4.96	0.007	.
1	A	63	ASP	CB	41.514	0.001	.
1	A	63	ASP	HB2	2.569	0.000	.
1	A	63	ASP	HB3	2.73	0.000	.
1	A	63	ASP	C	175.806	0.000	.
1	A	64	LEU	N	124.619	0.000	.
1	A	64	LEU	H	7.635	0.000	.
1	A	64	LEU	CA	55.946	0.000	.
1	A	64	LEU	HA	4.055	0.000	.
1	A	64	LEU	CB	43.459	0.001	.
1	A	64	LEU	HB2	0.827	0.002	.
1	A	64	LEU	HB3	1.484	0.000	.
1	A	64	LEU	CG	26.299	0.001	.
1	A	64	LEU	HG	0.83	0.000	.
1	A	64	LEU	HD11	0.721	0.000	.
1	A	64	LEU	HD12	0.721	0.000	.
1	A	64	LEU	HD13	0.721	0.000	.
1	A	64	LEU	HD21	0.826	0.000	.
1	A	64	LEU	HD22	0.826	0.000	.
1	A	64	LEU	HD23	0.826	0.000	.
1	A	64	LEU	CD1	23.912	0.000	.
1	A	64	LEU	CD2	25.945	0.000	.
1	A	64	LEU	C	176.877	0.002	.
1	A	66	GLU	CA	56.365	0.000	.
1	A	66	GLU	HA	4.282	0.000	.
1	A	66	GLU	CB	30.032	0.000	.
1	A	66	GLU	HB2	1.873	0.000	.
1	A	66	GLU	HB3	2.108	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	66	GLU	CG	36.307	0.001	.
1	A	66	GLU	HG2	2.275	0.000	.
1	A	66	GLU	HG3	2.213	0.000	.
1	A	66	GLU	C	176.388	0.000	.
1	A	67	ASN	N	118.803	0.000	.
1	A	67	ASN	H	8.291	0.000	.
1	A	67	ASN	CA	51.983	0.001	.
1	A	67	ASN	HA	4.867	0.000	.
1	A	67	ASN	CB	39.192	0.002	.
1	A	67	ASN	HB2	2.653	0.000	.
1	A	67	ASN	HB3	2.654	0.001	.
1	A	67	ASN	ND2	114.317	0.000	.
1	A	67	ASN	HD21	6.879	0.000	.
1	A	67	ASN	HD22	7.593	0.000	.
1	A	67	ASN	C	172.678	0.000	.
1	A	68	PRO	CD	50.406	0.000	.
1	A	68	PRO	CA	63.915	0.005	.
1	A	68	PRO	HA	4.43	0.000	.
1	A	68	PRO	CB	32.232	0.000	.
1	A	68	PRO	HB2	2.012	0.000	.
1	A	68	PRO	HB3	2.193	0.000	.
1	A	68	PRO	CG	27.152	0.003	.
1	A	68	PRO	HG2	1.963	0.000	.
1	A	68	PRO	HG3	2.036	0.000	.
1	A	68	PRO	HD2	3.676	0.000	.
1	A	68	PRO	HD3	3.676	0.000	.
1	A	68	PRO	C	176.33	0.000	.
1	A	69	GLY	N	111.249	0.000	.
1	A	69	GLY	H	7.911	0.000	.
1	A	69	GLY	CA	45.383	0.001	.
1	A	69	GLY	HA2	4.167	0.000	.
1	A	69	GLY	HA3	3.963	0.000	.
1	A	70	PRO	CD	49.879	0.000	.
1	A	70	PRO	CA	63.646	0.000	.
1	A	70	PRO	HA	4.405	0.000	.
1	A	70	PRO	CB	32.058	0.000	.
1	A	70	PRO	HB2	1.885	0.000	.
1	A	70	PRO	HB3	2.314	0.000	.
1	A	70	PRO	CG	27.12	0.000	.
1	A	70	PRO	HG2	2.008	0.000	.
1	A	70	PRO	HG3	2.008	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	70	PRO	HD2	3.626	0.000	.
1	A	70	PRO	HD3	3.626	0.000	.
1	A	71	ALA	N	121.048	0.000	.
1	A	71	ALA	H	7.979	0.000	.
1	A	71	ALA	CA	53.004	0.002	.
1	A	71	ALA	HA	4.303	0.000	.
1	A	71	ALA	HB1	1.394	0.002	.
1	A	71	ALA	HB2	1.394	0.002	.
1	A	71	ALA	HB3	1.394	0.002	.
1	A	71	ALA	CB	19.094	0.000	.
1	A	71	ALA	C	177.069	0.000	.
1	A	72	LEU	N	118.512	0.000	.
1	A	72	LEU	H	7.676	0.000	.
1	A	72	LEU	CA	54.13	0.005	.
1	A	72	LEU	HA	4.448	0.000	.
1	A	72	LEU	CB	44.351	0.000	.
1	A	72	LEU	HB2	1.511	0.000	.
1	A	72	LEU	HB3	1.555	0.000	.
1	A	72	LEU	CG	26.873	0.000	.
1	A	72	LEU	HG	1.568	0.000	.
1	A	72	LEU	HD11	0.809	0.001	.
1	A	72	LEU	HD12	0.809	0.001	.
1	A	72	LEU	HD13	0.809	0.001	.
1	A	72	LEU	HD21	0.855	0.000	.
1	A	72	LEU	HD22	0.855	0.000	.
1	A	72	LEU	HD23	0.855	0.000	.
1	A	72	LEU	CD1	23.268	0.001	.
1	A	72	LEU	CD2	25.451	0.002	.
1	A	72	LEU	C	176.665	0.000	.
1	A	73	GLY	N	107.479	0.000	.
1	A	73	GLY	H	8.453	0.000	.
1	A	73	GLY	CA	45.772	0.005	.
1	A	73	GLY	HA2	4.015	0.000	.
1	A	73	GLY	HA3	4.015	0.000	.
1	A	74	GLY	N	108.942	0.000	.
1	A	74	GLY	H	8.497	0.000	.
1	A	74	GLY	CA	44.341	0.000	.
1	A	74	GLY	HA2	3.624	0.000	.
1	A	74	GLY	HA3	4.631	0.000	.
1	A	74	GLY	C	174.947	0.000	.
1	A	75	TRP	N	122.612	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	75	TRP	H	9.481	0.000	.
1	A	75	TRP	CA	57.784	0.000	.
1	A	75	TRP	HA	5.19	0.000	.
1	A	75	TRP	CB	30.639	0.000	.
1	A	75	TRP	HB2	2.967	0.000	.
1	A	75	TRP	HB3	3.661	0.000	.
1	A	75	TRP	CD1	126.642	0.000	.
1	A	75	TRP	CE3	119.583	0.001	.
1	A	75	TRP	NE1	127.867	0.000	.
1	A	75	TRP	HD1	7.493	0.001	.
1	A	75	TRP	HE3	7.209	0.001	.
1	A	75	TRP	CZ2	114.468	0.001	.
1	A	75	TRP	HE1	9.884	0.000	.
1	A	75	TRP	CH2	126.008	0.000	.
1	A	75	TRP	HZ2	6.446	0.000	.
1	A	75	TRP	HH2	7.044	0.000	.
1	A	75	TRP	C	178.743	0.000	.
1	A	76	SER	CA	58.797	0.000	.
1	A	76	SER	HA	4.925	0.000	.
1	A	76	SER	CB	64.837	0.000	.
1	A	76	SER	HB2	3.419	0.000	.
1	A	76	SER	HB3	4.208	0.000	.
1	A	77	SER	N	120.114	0.000	.
1	A	77	SER	H	8.461	0.000	.
1	A	77	SER	CA	58.798	0.000	.
1	A	77	SER	HA	4.935	0.000	.
1	A	77	SER	CB	64.913	0.000	.
1	A	77	SER	HB2	3.404	0.000	.
1	A	77	SER	HB3	3.404	0.000	.
1	A	77	SER	C	170.989	0.000	.
1	A	78	TYR	N	120.186	0.000	.
1	A	78	TYR	H	8.928	0.000	.
1	A	78	TYR	CA	56.702	0.000	.
1	A	78	TYR	HA	4.664	0.000	.
1	A	78	TYR	CB	39.653	0.002	.
1	A	78	TYR	HB2	2.556	0.005	.
1	A	78	TYR	HB3	2.984	0.000	.
1	A	78	TYR	HD1	6.855	0.001	.
1	A	78	TYR	HD2	6.855	0.001	.
1	A	78	TYR	HE1	6.868	0.000	.
1	A	78	TYR	HE2	6.868	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	78	TYR	CD1	132.326	0.000	.
1	A	78	TYR	CE1	118.298	0.000	.
1	A	78	TYR	CE2	118.298	0.000	.
1	A	78	TYR	CD2	132.326	0.000	.
1	A	78	TYR	C	175.037	0.000	.
1	A	79	LEU	N	125.78	0.000	.
1	A	79	LEU	H	8.904	0.000	.
1	A	79	LEU	CA	52.472	0.000	.
1	A	79	LEU	HA	4.895	0.000	.
1	A	79	LEU	CB	43.296	0.001	.
1	A	79	LEU	HB2	0.89	0.000	.
1	A	79	LEU	HB3	1.706	0.000	.
1	A	79	LEU	CG	27.791	0.000	.
1	A	79	LEU	HG	1.265	0.000	.
1	A	79	LEU	HD11	0.338	0.000	.
1	A	79	LEU	HD12	0.338	0.000	.
1	A	79	LEU	HD13	0.338	0.000	.
1	A	79	LEU	HD21	0.471	0.000	.
1	A	79	LEU	HD22	0.471	0.000	.
1	A	79	LEU	HD23	0.471	0.000	.
1	A	79	LEU	CD1	21.824	0.000	.
1	A	79	LEU	CD2	25.322	0.000	.
1	A	79	LEU	C	176.876	0.001	.
1	A	81	VAL	N	116.916	0.000	.
1	A	81	VAL	H	8.608	0.000	.
1	A	81	VAL	CA	59.255	0.000	.
1	A	81	VAL	HA	4.862	0.000	.
1	A	81	VAL	CB	36.027	0.000	.
1	A	81	VAL	HB	2.113	0.000	.
1	A	81	VAL	HG11	0.661	0.000	.
1	A	81	VAL	HG12	0.661	0.000	.
1	A	81	VAL	HG13	0.661	0.000	.
1	A	81	VAL	HG21	1.083	0.000	.
1	A	81	VAL	HG22	1.083	0.000	.
1	A	81	VAL	HG23	1.083	0.000	.
1	A	81	VAL	CG1	18.683	0.000	.
1	A	81	VAL	CG2	23.869	0.000	.
1	A	81	VAL	C	175.037	0.000	.
1	A	82	ASP	N	121.088	0.000	.
1	A	82	ASP	H	8.836	0.000	.
1	A	82	ASP	CA	56.166	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	ASP	HA	4.636	0.000	.
1	A	82	ASP	CB	40.809	0.000	.
1	A	82	ASP	HB2	2.577	0.000	.
1	A	82	ASP	HB3	2.645	0.003	.
1	A	82	ASP	C	177.354	0.000	.
1	A	83	ASP	N	116.398	0.000	.
1	A	83	ASP	H	7.269	0.000	.
1	A	83	ASP	CA	53.031	0.001	.
1	A	83	ASP	HA	4.495	0.000	.
1	A	83	ASP	CB	42.722	0.001	.
1	A	83	ASP	HB2	2.397	0.000	.
1	A	83	ASP	HB3	2.72	0.000	.
1	A	83	ASP	C	176.095	0.000	.
1	A	84	ALA	N	129.069	0.000	.
1	A	84	ALA	H	9.428	0.000	.
1	A	84	ALA	CA	55.492	0.000	.
1	A	84	ALA	HA	3.794	0.000	.
1	A	84	ALA	HB1	1.113	0.000	.
1	A	84	ALA	HB2	1.113	0.000	.
1	A	84	ALA	HB3	1.113	0.000	.
1	A	84	ALA	CB	17.837	0.000	.
1	A	84	ALA	C	177.911	0.000	.
1	A	86	ALA	N	125.185	0.000	.
1	A	86	ALA	H	8.244	0.000	.
1	A	86	ALA	CA	54.341	0.000	.
1	A	86	ALA	HA	4.074	0.000	.
1	A	86	ALA	HB1	1.363	0.000	.
1	A	86	ALA	HB2	1.363	0.000	.
1	A	86	ALA	HB3	1.363	0.000	.
1	A	86	ALA	CB	17.79	0.001	.
1	A	86	ALA	C	181.312	0.000	.
1	A	88	ALA	N	118.62	0.000	.
1	A	88	ALA	H	8.226	0.000	.
1	A	88	ALA	CA	54.988	0.000	.
1	A	88	ALA	HA	3.706	0.000	.
1	A	88	ALA	HB1	1.516	0.000	.
1	A	88	ALA	HB2	1.516	0.000	.
1	A	88	ALA	HB3	1.516	0.000	.
1	A	88	ALA	CB	18.015	0.000	.
1	A	88	ALA	C	179.01	0.000	.
1	A	91	VAL	N	115.357	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	VAL	H	7.819	0.000	.
1	A	91	VAL	CA	69.345	0.000	.
1	A	91	VAL	HA	3.529	0.000	.
1	A	91	VAL	CB	30.295	0.003	.
1	A	91	VAL	HB	2.089	0.000	.
1	A	91	VAL	HG11	0.795	0.000	.
1	A	91	VAL	HG12	0.795	0.000	.
1	A	91	VAL	HG13	0.795	0.000	.
1	A	91	VAL	HG21	0.927	0.000	.
1	A	91	VAL	HG22	0.927	0.000	.
1	A	91	VAL	HG23	0.927	0.000	.
1	A	91	VAL	CG1	22.189	0.000	.
1	A	91	VAL	CG2	24.321	0.000	.
1	A	91	VAL	C	175.819	0.000	.
1	A	92	PRO	CD	50.422	0.000	.
1	A	92	PRO	CA	64.867	0.000	.
1	A	92	PRO	HA	4.685	0.000	.
1	A	92	PRO	CB	30.951	0.000	.
1	A	92	PRO	HB2	1.94	0.000	.
1	A	92	PRO	HB3	2.395	0.000	.
1	A	92	PRO	CG	28.567	0.000	.
1	A	92	PRO	HG2	1.921	0.000	.
1	A	92	PRO	HG3	2.154	0.000	.
1	A	92	PRO	HD2	3.46	0.000	.
1	A	92	PRO	HD3	3.768	0.000	.
1	A	92	PRO	C	181.031	0.000	.
1	A	93	GLU	N	118.774	0.000	.
1	A	93	GLU	H	6.947	0.000	.
1	A	93	GLU	CA	58.384	0.001	.
1	A	93	GLU	HA	4.139	0.000	.
1	A	93	GLU	CB	29.144	0.000	.
1	A	93	GLU	HB2	2.166	0.000	.
1	A	93	GLU	HB3	2.166	0.000	.
1	A	93	GLU	CG	35.909	0.000	.
1	A	93	GLU	HG2	2.293	0.000	.
1	A	93	GLU	HG3	2.431	0.000	.
1	A	93	GLU	C	178.236	0.000	.
1	A	94	LEU	N	117.709	0.000	.
1	A	94	LEU	H	7.571	0.000	.
1	A	94	LEU	CA	54.416	0.000	.
1	A	94	LEU	HA	4.405	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	LEU	CB	44.032	0.000	.
1	A	94	LEU	HB2	1.767	0.000	.
1	A	94	LEU	HB3	1.806	0.000	.
1	A	94	LEU	CG	25.737	0.001	.
1	A	94	LEU	HG	1.601	0.000	.
1	A	94	LEU	HD11	0.801	0.000	.
1	A	94	LEU	HD12	0.801	0.000	.
1	A	94	LEU	HD13	0.801	0.000	.
1	A	94	LEU	HD21	0.362	0.000	.
1	A	94	LEU	HD22	0.362	0.000	.
1	A	94	LEU	HD23	0.362	0.000	.
1	A	94	LEU	CD1	22.627	0.000	.
1	A	94	LEU	CD2	25.452	0.000	.
1	A	94	LEU	C	176.915	0.000	.
1	A	95	GLY	N	105.091	0.000	.
1	A	95	GLY	H	7.617	0.000	.
1	A	95	GLY	CA	45.247	0.000	.
1	A	95	GLY	HA2	3.822	0.000	.
1	A	95	GLY	HA3	4.393	0.000	.
1	A	95	GLY	C	175.124	0.000	.
1	A	96	GLY	N	107.985	0.001	.
1	A	96	GLY	H	8.023	0.000	.
1	A	96	GLY	CA	43.291	0.006	.
1	A	96	GLY	HA2	3.435	0.000	.
1	A	96	GLY	HA3	4.044	0.000	.
1	A	96	GLY	C	171.448	0.000	.
1	A	97	ALA	N	120.487	0.000	.
1	A	97	ALA	H	8.488	0.000	.
1	A	97	ALA	CA	50.784	0.000	.
1	A	97	ALA	HA	4.618	0.000	.
1	A	97	ALA	HB1	1.187	0.000	.
1	A	97	ALA	HB2	1.187	0.000	.
1	A	97	ALA	HB3	1.187	0.000	.
1	A	97	ALA	CB	22.369	0.000	.
1	A	97	ALA	C	176.403	0.000	.
1	A	98	VAL	N	122.906	0.000	.
1	A	98	VAL	H	9.189	0.000	.
1	A	98	VAL	CA	64.258	0.000	.
1	A	98	VAL	HA	3.971	0.000	.
1	A	98	VAL	CB	31.575	0.001	.
1	A	98	VAL	HB	2.091	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	VAL	HG11	0.891	0.000	.
1	A	98	VAL	HG12	0.891	0.000	.
1	A	98	VAL	HG13	0.891	0.000	.
1	A	98	VAL	HG21	0.995	0.000	.
1	A	98	VAL	HG22	0.995	0.000	.
1	A	98	VAL	HG23	0.995	0.000	.
1	A	98	VAL	CG1	21.759	0.001	.
1	A	98	VAL	CG2	22.839	0.000	.
1	A	98	VAL	C	175.76	0.002	.
1	A	99	LEU	N	128.5	0.000	.
1	A	99	LEU	H	9.138	0.000	.
1	A	99	LEU	CA	55.559	0.000	.
1	A	99	LEU	HA	4.415	0.000	.
1	A	99	LEU	CB	42.813	0.000	.
1	A	99	LEU	HB2	1.398	0.000	.
1	A	99	LEU	HB3	1.398	0.000	.
1	A	99	LEU	CG	27.377	0.000	.
1	A	99	LEU	HG	1.504	0.000	.
1	A	99	LEU	HD11	0.739	0.000	.
1	A	99	LEU	HD12	0.739	0.000	.
1	A	99	LEU	HD13	0.739	0.000	.
1	A	99	LEU	HD21	0.747	0.000	.
1	A	99	LEU	HD22	0.747	0.000	.
1	A	99	LEU	HD23	0.747	0.000	.
1	A	99	LEU	CD1	21.93	0.000	.
1	A	99	LEU	CD2	25.183	0.000	.
1	A	99	LEU	C	176.934	0.000	.
1	A	100	LEU	N	119.087	0.000	.
1	A	100	LEU	H	7.729	0.000	.
1	A	100	LEU	CA	55.884	0.001	.
1	A	100	LEU	HA	4.518	0.000	.
1	A	100	LEU	CB	46.089	0.001	.
1	A	100	LEU	HB2	1.623	0.000	.
1	A	100	LEU	HB3	1.684	0.000	.
1	A	100	LEU	CG	27.532	0.000	.
1	A	100	LEU	HG	1.59	0.000	.
1	A	100	LEU	HD11	0.996	0.000	.
1	A	100	LEU	HD12	0.996	0.000	.
1	A	100	LEU	HD13	0.996	0.000	.
1	A	100	LEU	HD21	1.055	0.000	.
1	A	100	LEU	HD22	1.055	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	LEU	HD23	1.055	0.000	.
1	A	100	LEU	CD1	26.054	0.004	.
1	A	100	LEU	CD2	24.403	0.000	.
1	A	100	LEU	C	175.288	0.006	.
1	A	101	GLY	N	111.994	0.000	.
1	A	101	GLY	H	8.833	0.000	.
1	A	101	GLY	CA	44.121	0.000	.
1	A	101	GLY	HA2	3.474	0.000	.
1	A	101	GLY	HA3	4.567	0.000	.
1	A	102	PRO	CD	50.354	0.001	.
1	A	102	PRO	CA	61.934	0.002	.
1	A	102	PRO	HA	5.223	0.000	.
1	A	102	PRO	CB	34.625	0.001	.
1	A	102	PRO	HB2	1.876	0.000	.
1	A	102	PRO	HB3	1.876	0.000	.
1	A	102	PRO	CG	26.225	0.000	.
1	A	102	PRO	HG2	1.611	0.000	.
1	A	102	PRO	HG3	1.611	0.000	.
1	A	102	PRO	HD2	3.462	0.000	.
1	A	102	PRO	HD3	3.618	0.000	.
1	A	102	PRO	C	175.935	0.000	.
1	A	103	ILE	N	121.901	0.000	.
1	A	103	ILE	H	9.367	0.000	.
1	A	103	ILE	CA	59.492	0.000	.
1	A	103	ILE	HA	4.575	0.000	.
1	A	103	ILE	CB	42.655	0.000	.
1	A	103	ILE	HB	1.78	0.000	.
1	A	103	ILE	HG21	0.904	0.000	.
1	A	103	ILE	HG22	0.904	0.000	.
1	A	103	ILE	HG23	0.904	0.000	.
1	A	103	ILE	CG2	17.807	0.000	.
1	A	103	ILE	CG1	27.152	0.000	.
1	A	103	ILE	HG12	1.44	0.000	.
1	A	103	ILE	HG13	1.084	0.000	.
1	A	103	ILE	HD11	0.842	0.002	.
1	A	103	ILE	HD12	0.842	0.002	.
1	A	103	ILE	HD13	0.842	0.002	.
1	A	103	ILE	CD1	13.793	0.001	.
1	A	103	ILE	C	173.813	0.002	.
1	A	104	ASP	N	124.544	0.000	.
1	A	104	ASP	H	8.545	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	ASP	CA	54.375	0.000	.
1	A	104	ASP	HA	4.83	0.000	.
1	A	104	ASP	CB	41.725	0.000	.
1	A	104	ASP	HB2	2.497	0.000	.
1	A	104	ASP	HB3	2.497	0.000	.
1	A	104	ASP	C	175.894	0.001	.
1	A	105	ILE	N	123.84	0.000	.
1	A	105	ILE	H	8.022	0.000	.
1	A	105	ILE	CA	60.233	0.001	.
1	A	105	ILE	HA	4.017	0.000	.
1	A	105	ILE	CB	36.586	0.000	.
1	A	105	ILE	HB	1.36	0.000	.
1	A	105	ILE	HG21	0.357	0.002	.
1	A	105	ILE	HG22	0.357	0.002	.
1	A	105	ILE	HG23	0.357	0.002	.
1	A	105	ILE	CG2	16.459	0.007	.
1	A	105	ILE	CG1	26.547	0.000	.
1	A	105	ILE	HG12	0.829	0.000	.
1	A	105	ILE	HG13	0.507	0.000	.
1	A	105	ILE	HD11	-0.473	0.003	.
1	A	105	ILE	HD12	-0.473	0.003	.
1	A	105	ILE	HD13	-0.473	0.003	.
1	A	105	ILE	CD1	10.553	0.003	.
1	A	105	ILE	C	173.603	0.000	.
1	A	106	LEU	N	124.681	0.000	.
1	A	106	LEU	H	8.63	0.000	.
1	A	106	LEU	CA	56.461	0.002	.
1	A	106	LEU	HA	3.827	0.000	.
1	A	106	LEU	CB	40.531	0.000	.
1	A	106	LEU	HB2	1.605	0.000	.
1	A	106	LEU	HB3	1.872	0.000	.
1	A	106	LEU	CG	27.171	0.000	.
1	A	106	LEU	HG	1.661	0.000	.
1	A	106	LEU	HD11	0.92	0.000	.
1	A	106	LEU	HD12	0.92	0.000	.
1	A	106	LEU	HD13	0.92	0.000	.
1	A	106	LEU	HD21	0.985	0.000	.
1	A	106	LEU	HD22	0.985	0.000	.
1	A	106	LEU	HD23	0.985	0.000	.
1	A	106	LEU	CD1	22.951	0.000	.
1	A	106	LEU	CD2	25.894	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	107	ALA	CA	52.704	0.000	.
1	A	107	ALA	HA	4.294	0.000	.
1	A	107	ALA	HB1	1.369	0.000	.
1	A	107	ALA	HB2	1.369	0.000	.
1	A	107	ALA	HB3	1.369	0.000	.
1	A	107	ALA	CB	19.222	0.002	.
1	A	108	GLN	N	118.676	0.008	.
1	A	108	GLN	H	8.964	0.000	.
1	A	108	GLN	CA	57.066	0.000	.
1	A	108	GLN	HA	4.406	0.000	.
1	A	108	GLN	CB	30.733	0.000	.
1	A	108	GLN	HB2	1.915	0.000	.
1	A	108	GLN	HB3	1.915	0.000	.
1	A	108	GLN	CG	34.22	0.001	.
1	A	108	GLN	HG2	2.326	0.000	.
1	A	108	GLN	HG3	2.447	0.000	.
1	A	108	GLN	NE2	110.206	0.009	.
1	A	108	GLN	HE21	6.656	0.008	.
1	A	108	GLN	HE22	7.22	0.003	.
1	A	109	GLY	N	104.669	0.000	.
1	A	109	GLY	H	7.087	0.000	.
1	A	109	GLY	CA	45.046	0.002	.
1	A	109	GLY	HA2	2.959	0.000	.
1	A	109	GLY	HA3	3.083	0.000	.
1	A	110	ARG	N	120.975	0.000	.
1	A	110	ARG	H	7.705	0.000	.
1	A	110	ARG	CA	54.196	0.000	.
1	A	110	ARG	HA	4.827	0.000	.
1	A	110	ARG	CB	33.214	0.000	.
1	A	110	ARG	HB2	1.74	0.000	.
1	A	110	ARG	HB3	1.613	0.000	.
1	A	110	ARG	CG	26.905	0.000	.
1	A	110	ARG	HG2	1.558	0.000	.
1	A	110	ARG	HG3	1.558	0.000	.
1	A	110	ARG	CD	43.239	0.000	.
1	A	110	ARG	HD2	2.812	0.000	.
1	A	110	ARG	HD3	3.098	0.000	.
1	A	110	ARG	NE	83.458	0.000	.
1	A	110	ARG	HE	7.577	0.000	.
1	A	110	ARG	C	172.539	0.000	.
1	A	111	MET	N	124.764	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	MET	H	9.06	0.000	.
1	A	111	MET	CA	54.05	0.001	.
1	A	111	MET	HA	5.612	0.000	.
1	A	111	MET	CB	37.608	0.000	.
1	A	111	MET	HB2	1.993	0.000	.
1	A	111	MET	HB3	2.159	0.000	.
1	A	111	MET	CG	32.43	0.001	.
1	A	111	MET	HG2	2.486	0.000	.
1	A	111	MET	HG3	2.597	0.000	.
1	A	111	MET	HE1	1.754	0.005	.
1	A	111	MET	HE2	1.754	0.005	.
1	A	111	MET	HE3	1.754	0.005	.
1	A	111	MET	CE	17.974	0.000	.
1	A	111	MET	C	174.643	0.000	.
1	A	112	LEU	N	121.783	0.000	.
1	A	112	LEU	H	9.114	0.000	.
1	A	112	LEU	CA	55.554	0.000	.
1	A	112	LEU	HA	5.044	0.000	.
1	A	112	LEU	CB	45.949	0.000	.
1	A	112	LEU	HB2	1.622	0.000	.
1	A	112	LEU	HB3	1.9	0.000	.
1	A	112	LEU	CG	26.421	0.000	.
1	A	112	LEU	HG	1.757	0.000	.
1	A	112	LEU	HD11	0.87	0.000	.
1	A	112	LEU	HD12	0.87	0.000	.
1	A	112	LEU	HD13	0.87	0.000	.
1	A	112	LEU	HD21	0.965	0.000	.
1	A	112	LEU	HD22	0.965	0.000	.
1	A	112	LEU	HD23	0.965	0.000	.
1	A	112	LEU	CD1	27.013	0.000	.
1	A	112	LEU	CD2	27.558	0.000	.
1	A	112	LEU	C	174.261	0.000	.
1	A	113	LEU	N	121.676	0.000	.
1	A	113	LEU	H	8.904	0.000	.
1	A	113	LEU	CA	53.975	0.001	.
1	A	113	LEU	HA	5.312	0.000	.
1	A	113	LEU	CB	46.056	0.000	.
1	A	113	LEU	HB2	1.45	0.000	.
1	A	113	LEU	HB3	1.702	0.000	.
1	A	113	LEU	CG	27.359	0.000	.
1	A	113	LEU	HG	1.847	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	LEU	HD11	0.964	0.001	.
1	A	113	LEU	HD12	0.964	0.001	.
1	A	113	LEU	HD13	0.964	0.001	.
1	A	113	LEU	HD21	1.006	0.005	.
1	A	113	LEU	HD22	1.006	0.005	.
1	A	113	LEU	HD23	1.006	0.005	.
1	A	113	LEU	CD1	24.138	0.000	.
1	A	113	LEU	CD2	25.334	0.000	.
1	A	113	LEU	C	175.18	0.000	.
1	A	114	ALA	N	127.385	0.000	.
1	A	114	ALA	H	9.738	0.000	.
1	A	114	ALA	CA	49.837	0.000	.
1	A	114	ALA	HA	5.376	0.000	.
1	A	114	ALA	HB1	1.367	0.000	.
1	A	114	ALA	HB2	1.367	0.000	.
1	A	114	ALA	HB3	1.367	0.000	.
1	A	114	ALA	CB	22.961	0.000	.
1	A	114	ALA	C	174.191	0.000	.
1	A	115	GLY	N	107.004	0.000	.
1	A	115	GLY	H	9.436	0.000	.
1	A	115	GLY	CA	43.264	0.000	.
1	A	115	GLY	HA2	3.319	0.000	.
1	A	115	GLY	HA3	5.095	0.001	.
1	A	115	GLY	C	173.094	0.000	.
1	A	116	ASP	N	122.539	0.001	.
1	A	116	ASP	H	8.051	0.000	.
1	A	116	ASP	CA	51.67	0.000	.
1	A	116	ASP	HA	3.17	0.000	.
1	A	116	ASP	CB	39.263	0.002	.
1	A	116	ASP	HB2	2.472	0.000	.
1	A	116	ASP	HB3	2.633	0.000	.
1	A	116	ASP	C	175.339	0.000	.
1	A	117	PRO	CD	50.391	0.000	.
1	A	117	PRO	CA	65.75	0.001	.
1	A	117	PRO	HA	4.127	0.000	.
1	A	117	PRO	CB	31.598	0.000	.
1	A	117	PRO	HB2	2.393	0.000	.
1	A	117	PRO	HB3	2.393	0.000	.
1	A	117	PRO	CG	28.429	0.000	.
1	A	117	PRO	HG2	1.498	0.000	.
1	A	117	PRO	HG3	1.498	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	117	PRO	HD2	3.114	0.000	.
1	A	117	PRO	HD3	2.17	0.000	.
1	A	117	PRO	C	177.796	0.000	.
1	A	118	SER	N	111.97	0.000	.
1	A	118	SER	H	7.469	0.000	.
1	A	118	SER	CA	58.902	0.000	.
1	A	118	SER	HA	4.308	0.000	.
1	A	118	SER	CB	62.924	0.000	.
1	A	118	SER	HB2	3.455	0.000	.
1	A	118	SER	HB3	3.664	0.000	.
1	A	118	SER	C	173.708	0.005	.
1	A	119	GLY	N	109.116	0.000	.
1	A	119	GLY	H	8.295	0.000	.
1	A	119	GLY	CA	44.71	0.002	.
1	A	119	GLY	HA2	3.426	0.008	.
1	A	119	GLY	HA3	4.05	0.000	.
1	A	119	GLY	C	175.185	0.000	.
1	A	120	HIS	N	120.766	0.000	.
1	A	120	HIS	H	8.155	0.000	.
1	A	120	HIS	CA	55.657	0.000	.
1	A	120	HIS	HA	4.792	0.000	.
1	A	120	HIS	CB	27.043	0.000	.
1	A	120	HIS	HB2	3.421	0.000	.
1	A	120	HIS	HB3	3.617	0.000	.
1	A	120	HIS	CD2	120.461	0.000	.
1	A	120	HIS	HD2	7.396	0.000	.
1	A	120	HIS	C	174.599	0.002	.
1	A	121	ARG	N	124.265	0.000	.
1	A	121	ARG	H	8.577	0.000	.
1	A	121	ARG	CA	56.012	0.001	.
1	A	121	ARG	HA	5.114	0.000	.
1	A	121	ARG	CB	31.887	0.000	.
1	A	121	ARG	HB2	1.871	0.000	.
1	A	121	ARG	HB3	1.994	0.000	.
1	A	121	ARG	CG	27.272	0.000	.
1	A	121	ARG	HG2	1.517	0.000	.
1	A	121	ARG	HG3	1.698	0.000	.
1	A	121	ARG	CD	43.925	0.000	.
1	A	121	ARG	HD2	3.226	0.000	.
1	A	121	ARG	HD3	3.38	0.000	.
1	A	121	ARG	NE	84.359	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	121	ARG	HE	7.18	0.000	.
1	A	121	ARG	C	176.311	0.000	.
1	A	122	VAL	N	128.718	0.000	.
1	A	122	VAL	H	10.054	0.000	.
1	A	122	VAL	CA	60.966	0.000	.
1	A	122	VAL	HA	4.231	0.000	.
1	A	122	VAL	CB	35.842	0.000	.
1	A	122	VAL	HB	2.2	0.000	.
1	A	122	VAL	HG11	1.106	0.000	.
1	A	122	VAL	HG12	1.106	0.000	.
1	A	122	VAL	HG13	1.106	0.000	.
1	A	122	VAL	HG21	0.552	0.000	.
1	A	122	VAL	HG22	0.552	0.000	.
1	A	122	VAL	HG23	0.552	0.000	.
1	A	122	VAL	CG1	17.732	0.003	.
1	A	122	VAL	CG2	20.96	0.000	.
1	A	123	GLY	N	115.491	0.000	.
1	A	123	GLY	H	8.436	0.000	.
1	A	123	GLY	CA	44.853	0.000	.
1	A	123	GLY	HA2	3.06	0.000	.
1	A	123	GLY	HA3	4.987	0.000	.
1	A	123	GLY	C	172.619	0.000	.
1	A	124	LEU	N	124.02	0.000	.
1	A	124	LEU	H	9.463	0.000	.
1	A	124	LEU	CA	53.506	0.001	.
1	A	124	LEU	HA	5.906	0.000	.
1	A	124	LEU	CB	43.339	0.000	.
1	A	124	LEU	HB2	1.451	0.000	.
1	A	124	LEU	HB3	1.878	0.000	.
1	A	124	LEU	CG	27.393	0.000	.
1	A	124	LEU	HG	1.712	0.000	.
1	A	124	LEU	HD11	1.074	0.000	.
1	A	124	LEU	HD12	1.074	0.000	.
1	A	124	LEU	HD13	1.074	0.000	.
1	A	124	LEU	HD21	0.795	0.000	.
1	A	124	LEU	HD22	0.795	0.000	.
1	A	124	LEU	HD23	0.795	0.000	.
1	A	124	LEU	CD1	24.634	0.000	.
1	A	124	LEU	CD2	25.83	0.000	.
1	A	124	LEU	C	175.119	0.001	.
1	A	125	TRP	N	123.117	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	TRP	H	8.951	0.000	.
1	A	125	TRP	CA	54.988	0.000	.
1	A	125	TRP	HA	5.442	0.000	.
1	A	125	TRP	CB	33.97	0.000	.
1	A	125	TRP	HB2	2.953	0.005	.
1	A	125	TRP	HB3	3.16	0.000	.
1	A	125	TRP	CD1	126.321	0.000	.
1	A	125	TRP	NE1	126.843	0.001	.
1	A	125	TRP	HD1	7.001	0.000	.
1	A	125	TRP	CZ2	113.163	0.000	.
1	A	125	TRP	HE1	9.141	0.000	.
1	A	125	TRP	CH2	121.943	0.001	.
1	A	125	TRP	HZ2	6.515	0.000	.
1	A	125	TRP	HH2	5.745	0.000	.
1	A	125	TRP	C	174.13	0.001	.
1	A	126	GLN	N	130.329	0.000	.
1	A	126	GLN	H	8.935	0.000	.
1	A	126	GLN	CA	52.527	0.001	.
1	A	126	GLN	HA	4.942	0.000	.
1	A	126	GLN	CB	29.882	0.000	.
1	A	126	GLN	HB2	1.738	0.000	.
1	A	126	GLN	HB3	1.738	0.000	.
1	A	126	GLN	CG	32.328	0.000	.
1	A	126	GLN	HG2	2.3	0.000	.
1	A	126	GLN	HG3	2.3	0.000	.
1	A	126	GLN	NE2	112.115	0.005	.
1	A	126	GLN	HE21	7.091	0.000	.
1	A	126	GLN	HE22	7.61	0.000	.
1	A	126	GLN	C	173.921	0.000	.
1	A	127	ALA	N	130.025	0.000	.
1	A	127	ALA	H	8.684	0.000	.
1	A	127	ALA	CA	54.019	0.001	.
1	A	127	ALA	HA	3.776	0.000	.
1	A	127	ALA	HB1	1.475	0.000	.
1	A	127	ALA	HB2	1.475	0.000	.
1	A	127	ALA	HB3	1.475	0.000	.
1	A	127	ALA	CB	20.127	0.000	.
1	A	127	ALA	C	178.23	0.002	.
1	A	128	LYS	N	124.63	0.000	.
1	A	128	LYS	H	7.917	0.000	.
1	A	128	LYS	CA	57.384	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	128	LYS	HA	4.394	0.000	.
1	A	128	LYS	CB	31.67	0.000	.
1	A	128	LYS	HB2	1.161	0.000	.
1	A	128	LYS	HB3	1.737	0.000	.
1	A	128	LYS	CG	25.297	0.001	.
1	A	128	LYS	HG2	1.027	0.000	.
1	A	128	LYS	HG3	1.285	0.000	.
1	A	128	LYS	CD	29.067	0.002	.
1	A	128	LYS	HD2	1.342	0.000	.
1	A	128	LYS	HD3	1.436	0.000	.
1	A	128	LYS	CE	41.937	0.000	.
1	A	128	LYS	HE2	2.571	0.000	.
1	A	128	LYS	HE3	2.731	0.000	.
1	A	128	LYS	C	175.219	0.000	.
1	A	129	GLU	N	117.681	0.000	.
1	A	129	GLU	H	8.038	0.000	.
1	A	129	GLU	CA	58.287	0.000	.
1	A	129	GLU	HA	4.245	0.000	.
1	A	129	GLU	CB	30.322	0.000	.
1	A	129	GLU	HB2	1.95	0.000	.
1	A	129	GLU	HB3	2.158	0.000	.
1	A	129	GLU	CG	36.964	0.002	.
1	A	129	GLU	HG2	2.265	0.000	.
1	A	129	GLU	HG3	2.51	0.000	.
1	A	129	GLU	C	176.084	0.000	.
1	A	130	HIS	N	122.206	0.000	.
1	A	130	HIS	H	9.053	0.000	.
1	A	130	HIS	CA	58.02	0.000	.
1	A	130	HIS	HA	4.89	0.000	.
1	A	130	HIS	CB	33.531	0.000	.
1	A	130	HIS	HB2	3.138	0.000	.
1	A	130	HIS	HB3	3.208	0.000	.
1	A	130	HIS	C	175.619	0.000	.
1	A	131	THR	N	113.61	0.000	.
1	A	131	THR	H	8.123	0.000	.
1	A	131	THR	CA	61.485	0.001	.
1	A	131	THR	HA	4.43	0.000	.
1	A	131	THR	CB	68.666	0.000	.
1	A	131	THR	HB	4.609	0.000	.
1	A	131	THR	HG21	1.102	0.000	.
1	A	131	THR	HG22	1.102	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	THR	HG23	1.102	0.000	.
1	A	131	THR	CG2	21.633	0.000	.
1	A	131	THR	C	174.424	0.000	.
1	A	132	GLY	N	108.736	0.000	.
1	A	132	GLY	H	7.569	0.000	.
1	A	132	GLY	CA	45.322	0.000	.
1	A	132	GLY	HA2	3.92	0.000	.
1	A	132	GLY	HA3	4.927	0.000	.
1	A	132	GLY	C	174.071	0.000	.
1	A	133	SER	N	116.53	0.000	.
1	A	133	SER	H	8.93	0.000	.
1	A	133	SER	CA	60.143	0.000	.
1	A	133	SER	HA	4.565	0.000	.
1	A	133	SER	CB	64.226	0.001	.
1	A	133	SER	HB2	3.925	0.000	.
1	A	133	SER	HB3	4.113	0.000	.
1	A	133	SER	C	176.838	0.000	.
1	A	134	GLY	N	113.363	0.000	.
1	A	134	GLY	H	8.939	0.000	.
1	A	134	GLY	CA	45.326	0.000	.
1	A	134	GLY	HA2	3.845	0.000	.
1	A	134	GLY	HA3	4.381	0.000	.
1	A	135	PRO	CD	49.565	0.000	.
1	A	135	PRO	CA	63.277	0.001	.
1	A	135	PRO	HA	4.333	0.000	.
1	A	135	PRO	CB	32.039	0.000	.
1	A	135	PRO	HB2	1.777	0.000	.
1	A	135	PRO	HB3	2.27	0.000	.
1	A	135	PRO	CG	27.116	0.000	.
1	A	135	PRO	HG2	1.995	0.000	.
1	A	135	PRO	HG3	1.995	0.000	.
1	A	135	PRO	HD2	3.669	0.000	.
1	A	135	PRO	HD3	3.669	0.000	.
1	A	136	ASP	N	121.766	0.000	.
1	A	136	ASP	H	8.537	0.000	.
1	A	136	ASP	CA	53.927	0.005	.
1	A	136	ASP	HA	4.323	0.001	.
1	A	136	ASP	CB	39.842	0.002	.
1	A	136	ASP	HB2	2.625	0.000	.
1	A	136	ASP	HB3	2.777	0.000	.
1	A	136	ASP	C	176.298	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	ASP	N	125.584	0.000	.
1	A	137	ASP	H	8.18	0.000	.
1	A	137	ASP	CA	52.789	0.005	.
1	A	137	ASP	HA	4.63	0.000	.
1	A	137	ASP	CB	41.229	0.001	.
1	A	137	ASP	HB2	2.334	0.001	.
1	A	137	ASP	HB3	2.891	0.000	.
1	A	137	ASP	C	176.128	0.001	.
1	A	138	GLY	N	107.164	0.000	.
1	A	138	GLY	H	7.732	0.000	.
1	A	138	GLY	CA	44.28	0.001	.
1	A	138	GLY	HA2	3.688	0.001	.
1	A	138	GLY	HA3	4.325	0.001	.
1	A	138	GLY	C	172.669	0.000	.
1	A	139	ILE	N	117.904	0.000	.
1	A	139	ILE	H	8.319	0.000	.
1	A	139	ILE	CA	62.849	0.000	.
1	A	139	ILE	HA	3.408	0.004	.
1	A	139	ILE	CB	37.482	0.000	.
1	A	139	ILE	HB	1.862	0.000	.
1	A	139	ILE	HG21	1.062	0.001	.
1	A	139	ILE	HG22	1.062	0.001	.
1	A	139	ILE	HG23	1.062	0.001	.
1	A	139	ILE	CG2	18.229	0.000	.
1	A	139	ILE	CG1	27.46	0.000	.
1	A	139	ILE	HG12	1.219	0.000	.
1	A	139	ILE	HG13	1.576	0.000	.
1	A	139	ILE	HD11	0.816	0.000	.
1	A	139	ILE	HD12	0.816	0.000	.
1	A	139	ILE	HD13	0.816	0.000	.
1	A	139	ILE	CD1	12.733	0.000	.
1	A	139	ILE	C	177.906	0.000	.
1	A	140	GLY	N	116.622	0.000	.
1	A	140	GLY	H	9.652	0.000	.
1	A	140	GLY	CA	45.083	0.004	.
1	A	140	GLY	HA2	3.227	0.001	.
1	A	140	GLY	HA3	4.381	0.000	.
1	A	140	GLY	C	171.946	0.000	.
1	A	141	ALA	N	118.824	0.001	.
1	A	141	ALA	H	7.543	0.000	.
1	A	141	ALA	CA	51.235	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	141	ALA	HA	4.344	0.000	.
1	A	141	ALA	HB1	1.559	0.000	.
1	A	141	ALA	HB2	1.559	0.000	.
1	A	141	ALA	HB3	1.559	0.000	.
1	A	141	ALA	CB	19.958	0.000	.
1	A	141	ALA	C	176.261	0.001	.
1	A	142	TYR	N	119.136	0.000	.
1	A	142	TYR	H	8.694	0.000	.
1	A	142	TYR	CA	56.285	0.000	.
1	A	142	TYR	HA	4.549	0.000	.
1	A	142	TYR	CB	38.207	0.003	.
1	A	142	TYR	HB2	2.868	0.000	.
1	A	142	TYR	HB3	2.582	0.000	.
1	A	142	TYR	HD1	6.311	0.000	.
1	A	142	TYR	HD2	6.311	0.000	.
1	A	142	TYR	HE1	7.053	0.000	.
1	A	142	TYR	HE2	7.053	0.000	.
1	A	142	TYR	CD1	130.631	0.000	.
1	A	142	TYR	CE1	118.169	0.000	.
1	A	142	TYR	CE2	118.169	0.000	.
1	A	142	TYR	CD2	130.631	0.000	.
1	A	142	TYR	C	175.106	0.000	.
1	A	143	THR	N	127.833	0.000	.
1	A	143	THR	H	8.534	0.000	.
1	A	143	THR	CA	65.489	0.000	.
1	A	143	THR	HA	4.195	0.000	.
1	A	143	THR	CB	69.488	0.001	.
1	A	143	THR	HB	3.363	0.000	.
1	A	143	THR	HG21	0.98	0.000	.
1	A	143	THR	HG22	0.98	0.000	.
1	A	143	THR	HG23	0.98	0.000	.
1	A	143	THR	CG2	22.471	0.002	.
1	A	143	THR	C	174.2	0.000	.
1	A	144	ARG	N	109.282	0.000	.
1	A	144	ARG	H	6.832	0.000	.
1	A	144	ARG	CA	55.32	0.000	.
1	A	144	ARG	HA	3.644	0.000	.
1	A	144	ARG	CB	30.234	0.000	.
1	A	144	ARG	C	173.593	0.000	.
1	A	145	SER	N	110.089	0.000	.
1	A	145	SER	H	6.303	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	145	SER	CA	58.23	0.001	.
1	A	145	SER	HA	5.798	0.001	.
1	A	145	SER	CB	66.655	0.000	.
1	A	145	SER	HB2	3.462	0.002	.
1	A	145	SER	HB3	4.197	0.000	.
1	A	145	SER	C	171.576	0.000	.
1	A	146	GLU	N	119.046	0.000	.
1	A	146	GLU	H	8.525	0.000	.
1	A	146	GLU	CA	55.092	0.000	.
1	A	146	GLU	HA	5.059	0.007	.
1	A	146	GLU	CB	33.335	0.000	.
1	A	146	GLU	HB2	1.7	0.000	.
1	A	146	GLU	HB3	1.7	0.000	.
1	A	146	GLU	CG	37.66	0.001	.
1	A	146	GLU	HG2	2.683	0.000	.
1	A	146	GLU	HG3	2.683	0.000	.
1	A	146	GLU	C	173.09	0.005	.
1	A	147	LEU	N	124.825	0.000	.
1	A	147	LEU	H	7.983	0.000	.
1	A	147	LEU	CA	52.423	0.000	.
1	A	147	LEU	HA	3.602	0.000	.
1	A	147	LEU	CB	40.321	0.002	.
1	A	147	LEU	HB2	-1.791	0.000	.
1	A	147	LEU	HB3	-1.791	0.000	.
1	A	147	LEU	CG	26.282	0.000	.
1	A	147	LEU	HG	0.519	0.000	.
1	A	147	LEU	HD11	-0.554	0.000	.
1	A	147	LEU	HD12	-0.554	0.000	.
1	A	147	LEU	HD13	-0.554	0.000	.
1	A	147	LEU	HD21	0.598	0.000	.
1	A	147	LEU	HD22	0.598	0.000	.
1	A	147	LEU	HD23	0.598	0.000	.
1	A	147	LEU	CD1	19.992	0.000	.
1	A	147	LEU	CD2	26.07	0.000	.
1	A	147	LEU	C	173.274	0.002	.
1	A	148	LEU	N	130.321	0.000	.
1	A	148	LEU	H	8.352	0.000	.
1	A	148	LEU	CA	53.631	0.000	.
1	A	148	LEU	HA	4.721	0.000	.
1	A	148	LEU	CB	40.328	0.000	.
1	A	148	LEU	HB2	1.528	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	148	LEU	HB3	1.783	0.000	.
1	A	148	LEU	CG	28.864	0.000	.
1	A	148	LEU	HG	1.495	0.000	.
1	A	148	LEU	HD11	0.414	0.000	.
1	A	148	LEU	HD12	0.414	0.000	.
1	A	148	LEU	HD13	0.414	0.000	.
1	A	148	LEU	HD21	0.637	0.000	.
1	A	148	LEU	HD22	0.637	0.000	.
1	A	148	LEU	HD23	0.637	0.000	.
1	A	148	LEU	CD1	22.959	0.000	.
1	A	148	LEU	CD2	24.122	0.000	.
1	A	148	LEU	C	175.405	0.000	.
1	A	149	THR	N	116.934	0.000	.
1	A	149	THR	H	8.619	0.000	.
1	A	149	THR	CA	57.314	0.000	.
1	A	149	THR	HA	4.895	0.000	.
1	A	149	THR	CB	68.652	0.000	.
1	A	149	THR	HB	3.645	0.000	.
1	A	149	THR	HG21	0.567	0.001	.
1	A	149	THR	HG22	0.567	0.001	.
1	A	149	THR	HG23	0.567	0.001	.
1	A	149	THR	CG2	21.482	0.000	.
1	A	149	THR	C	172.075	0.006	.
1	A	150	GLY	N	115.314	0.000	.
1	A	150	GLY	H	8.683	0.000	.
1	A	150	GLY	CA	45.474	0.001	.
1	A	150	GLY	HA2	3.692	0.000	.
1	A	150	GLY	HA3	4.769	0.001	.
1	A	150	GLY	C	174.888	0.002	.
1	A	151	ALA	N	130.202	0.000	.
1	A	151	ALA	H	9.164	0.000	.
1	A	151	ALA	CA	50.063	0.000	.
1	A	151	ALA	HA	4.94	0.000	.
1	A	151	ALA	HB1	1.24	0.000	.
1	A	151	ALA	HB2	1.24	0.000	.
1	A	151	ALA	HB3	1.24	0.000	.
1	A	151	ALA	CB	18.59	0.000	.
1	A	151	ALA	C	176.447	0.000	.
1	A	152	SER	N	116.014	0.000	.
1	A	152	SER	H	8.411	0.000	.
1	A	152	SER	CA	63.345	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	152	SER	HA	3.776	0.000	.
1	A	152	SER	CB	62.321	0.000	.
1	A	152	SER	HB2	3.737	0.000	.
1	A	152	SER	HB3	3.813	0.000	.
1	A	152	SER	C	177.801	0.000	.
1	A	153	ALA	N	126.079	0.000	.
1	A	153	ALA	H	8.642	0.000	.
1	A	153	ALA	CA	55.523	0.000	.
1	A	153	ALA	HA	4.348	0.000	.
1	A	153	ALA	HB1	1.524	0.000	.
1	A	153	ALA	HB2	1.524	0.000	.
1	A	153	ALA	HB3	1.524	0.000	.
1	A	153	ALA	CB	18.163	0.001	.
1	A	153	ALA	C	180.574	0.000	.
1	A	154	THR	N	115.016	0.000	.
1	A	154	THR	H	7.876	0.000	.
1	A	154	THR	CA	65.504	0.000	.
1	A	154	THR	HA	4.092	0.000	.
1	A	154	THR	CB	68.601	0.000	.
1	A	154	THR	HB	4.159	0.000	.
1	A	154	THR	HG21	1.238	0.000	.
1	A	154	THR	HG22	1.238	0.000	.
1	A	154	THR	HG23	1.238	0.000	.
1	A	154	THR	CG2	22.157	0.000	.
1	A	154	THR	C	177.646	0.001	.
1	A	155	ASP	N	124.309	0.000	.
1	A	155	ASP	H	8.94	0.000	.
1	A	155	ASP	CA	58.312	0.000	.
1	A	155	ASP	HA	4.54	0.000	.
1	A	155	ASP	CB	39.988	0.000	.
1	A	155	ASP	HB2	2.628	0.000	.
1	A	155	ASP	HB3	2.753	0.000	.
1	A	155	ASP	C	179.23	0.000	.
1	A	156	GLY	N	106.804	0.000	.
1	A	156	GLY	H	8.468	0.000	.
1	A	156	GLY	CA	48.068	0.001	.
1	A	156	GLY	HA2	3.925	0.000	.
1	A	156	GLY	HA3	4.168	0.000	.
1	A	156	GLY	C	174.993	0.001	.
1	A	157	ALA	N	121.554	0.000	.
1	A	157	ALA	H	7.494	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	157	ALA	CA	55.349	0.000	.
1	A	157	ALA	HA	4.208	0.000	.
1	A	157	ALA	HB1	1.596	0.000	.
1	A	157	ALA	HB2	1.596	0.000	.
1	A	157	ALA	HB3	1.596	0.000	.
1	A	157	ALA	CB	18.001	0.000	.
1	A	157	ALA	C	180.332	0.000	.
1	A	158	PHE	N	120.341	0.000	.
1	A	158	PHE	H	7.421	0.000	.
1	A	158	PHE	CA	61.074	0.001	.
1	A	158	PHE	HA	4.357	0.000	.
1	A	158	PHE	CB	38.521	0.001	.
1	A	158	PHE	HB2	3.011	0.000	.
1	A	158	PHE	HB3	3.319	0.000	.
1	A	158	PHE	HD1	7.117	0.000	.
1	A	158	PHE	HD2	7.117	0.000	.
1	A	158	PHE	HE1	6.778	0.000	.
1	A	158	PHE	HE2	6.778	0.000	.
1	A	158	PHE	CD1	129.229	0.000	.
1	A	158	PHE	CE1	128.714	0.001	.
1	A	158	PHE	CE2	128.714	0.000	.
1	A	158	PHE	CD2	129.229	0.000	.
1	A	158	PHE	C	175.707	0.002	.
1	A	159	TYR	N	116.19	0.000	.
1	A	159	TYR	H	7.79	0.000	.
1	A	159	TYR	CA	62.938	0.000	.
1	A	159	TYR	HA	3.512	0.000	.
1	A	159	TYR	CB	39.879	0.000	.
1	A	159	TYR	HB2	2.791	0.000	.
1	A	159	TYR	HB3	2.924	0.000	.
1	A	159	TYR	HD1	7.147	0.000	.
1	A	159	TYR	HD2	7.147	0.000	.
1	A	159	TYR	HE1	7.147	0.000	.
1	A	159	TYR	HE2	7.147	0.000	.
1	A	159	TYR	HH	12.372	0.000	.
1	A	159	TYR	C	178.481	0.000	.
1	A	160	ARG	N	118.486	0.000	.
1	A	160	ARG	H	8.839	0.000	.
1	A	160	ARG	CA	58.641	0.000	.
1	A	160	ARG	HA	4.404	0.000	.
1	A	160	ARG	CB	29.948	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	160	ARG	HB2	1.761	0.000	.
1	A	160	ARG	HB3	1.85	0.000	.
1	A	160	ARG	CG	30.784	0.001	.
1	A	160	ARG	HG2	1.992	0.000	.
1	A	160	ARG	HG3	2.134	0.000	.
1	A	160	ARG	CD	43.899	0.000	.
1	A	160	ARG	HD2	3.227	0.000	.
1	A	160	ARG	HD3	3.404	0.000	.
1	A	160	ARG	NE	86.283	0.000	.
1	A	160	ARG	HE	7.216	0.000	.
1	A	160	ARG	C	179.885	0.000	.
1	A	161	GLY	N	109.979	0.000	.
1	A	161	GLY	H	7.814	0.000	.
1	A	161	GLY	CA	46.605	0.000	.
1	A	161	GLY	HA2	3.547	0.000	.
1	A	161	GLY	HA3	3.788	0.000	.
1	A	161	GLY	C	174.805	0.000	.
1	A	162	LEU	N	120.227	0.000	.
1	A	162	LEU	H	6.868	0.000	.
1	A	162	LEU	CA	56.404	0.000	.
1	A	162	LEU	HA	3.717	0.000	.
1	A	162	LEU	CB	42.284	0.000	.
1	A	162	LEU	HB2	0.106	0.000	.
1	A	162	LEU	HB3	0.481	0.000	.
1	A	162	LEU	CG	25.271	0.001	.
1	A	162	LEU	HG	0.536	0.000	.
1	A	162	LEU	HD11	0.148	0.000	.
1	A	162	LEU	HD12	0.148	0.000	.
1	A	162	LEU	HD13	0.148	0.000	.
1	A	162	LEU	HD21	0.06	0.000	.
1	A	162	LEU	HD22	0.06	0.000	.
1	A	162	LEU	HD23	0.06	0.000	.
1	A	162	LEU	CD1	23.776	0.000	.
1	A	162	LEU	CD2	24.685	0.000	.
1	A	162	LEU	C	178.59	0.000	.
1	A	163	PHE	N	113.675	0.001	.
1	A	163	PHE	H	8.031	0.000	.
1	A	163	PHE	CA	57.084	0.000	.
1	A	163	PHE	HA	4.879	0.000	.
1	A	163	PHE	CB	41.548	0.002	.
1	A	163	PHE	HB2	2.504	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	163	PHE	HB3	3.362	0.006	.
1	A	163	PHE	HD1	6.528	0.000	.
1	A	163	PHE	HD2	6.528	0.000	.
1	A	163	PHE	C	176.271	0.000	.
1	A	165	ALA	N	119.824	0.000	.
1	A	165	ALA	H	8.332	0.001	.
1	A	165	ALA	CA	55.023	0.000	.
1	A	165	ALA	HA	3.981	0.000	.
1	A	165	ALA	HB1	1.463	0.000	.
1	A	165	ALA	HB2	1.463	0.000	.
1	A	165	ALA	HB3	1.463	0.000	.
1	A	165	ALA	CB	19.318	0.000	.
1	A	165	ALA	C	177.803	0.002	.
1	A	166	ASP	N	113.029	0.000	.
1	A	166	ASP	H	8.38	0.000	.
1	A	166	ASP	CA	53.959	0.000	.
1	A	166	ASP	HA	4.64	0.001	.
1	A	166	ASP	CB	40.495	0.000	.
1	A	166	ASP	HB2	2.683	0.000	.
1	A	166	ASP	HB3	2.75	0.000	.
1	A	166	ASP	C	177.091	0.005	.
1	A	167	PHE	N	123.84	0.000	.
1	A	167	PHE	H	7.93	0.000	.
1	A	167	PHE	CA	60.141	0.000	.
1	A	167	PHE	HA	4.257	0.000	.
1	A	167	PHE	CB	39.855	0.001	.
1	A	167	PHE	HB2	3.082	0.000	.
1	A	167	PHE	HB3	3.33	0.000	.
1	A	167	PHE	HD1	7.262	0.000	.
1	A	167	PHE	HD2	7.262	0.000	.
1	A	167	PHE	CD1	133.043	0.002	.
1	A	167	PHE	CD2	133.043	0.000	.
1	A	167	PHE	C	175.402	0.000	.
1	A	169	THR	N	109.619	0.000	.
1	A	169	THR	H	7.613	0.000	.
1	A	169	THR	CA	61.577	0.000	.
1	A	169	THR	HA	4.506	0.000	.
1	A	169	THR	CB	70.911	0.000	.
1	A	169	THR	HB	4.287	0.000	.
1	A	169	THR	HG21	1.255	0.000	.
1	A	169	THR	HG22	1.255	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	169	THR	HG23	1.255	0.000	.
1	A	169	THR	CG2	21.6	0.000	.
1	A	169	THR	C	175.18	0.000	.
1	A	170	GLU	N	122.606	0.000	.
1	A	170	GLU	H	8.726	0.000	.
1	A	170	GLU	CA	56.926	0.000	.
1	A	170	GLU	HA	4.319	0.000	.
1	A	170	GLU	CB	29.9	0.003	.
1	A	170	GLU	HB2	1.955	0.000	.
1	A	170	GLU	HB3	2.11	0.000	.
1	A	170	GLU	CG	36.562	0.000	.
1	A	170	GLU	HG2	2.248	0.000	.
1	A	170	GLU	HG3	2.248	0.000	.
1	A	170	GLU	C	176.574	0.000	.
1	A	171	SER	N	116.348	0.000	.
1	A	171	SER	H	8.304	0.000	.
1	A	171	SER	CA	58.316	0.000	.
1	A	171	SER	HA	4.489	0.000	.
1	A	171	SER	CB	64.038	0.000	.
1	A	171	SER	HB2	3.814	0.000	.
1	A	171	SER	HB3	3.888	0.000	.
1	A	171	SER	C	175.071	0.000	.
1	A	172	GLY	N	110.804	0.000	.
1	A	172	GLY	H	8.442	0.000	.
1	A	172	GLY	CA	45.58	0.000	.
1	A	172	GLY	HA2	4.016	0.000	.
1	A	172	GLY	HA3	4.016	0.000	.
1	A	172	GLY	C	174.48	0.000	.
1	A	173	THR	N	112.852	0.001	.
1	A	173	THR	H	8.091	0.000	.
1	A	173	THR	CA	61.647	0.000	.
1	A	173	THR	HA	4.374	0.000	.
1	A	173	THR	CB	69.859	0.000	.
1	A	173	THR	HB	4.264	0.000	.
1	A	173	THR	HG21	1.161	0.000	.
1	A	173	THR	HG22	1.161	0.000	.
1	A	173	THR	HG23	1.161	0.000	.
1	A	173	THR	CG2	21.54	0.000	.
1	A	173	THR	C	174.561	0.000	.
1	A	174	ASP	N	122.678	0.000	.
1	A	174	ASP	H	8.41	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	174	ASP	CA	54.558	0.000	.
1	A	174	ASP	HA	4.628	0.000	.
1	A	174	ASP	CB	41.226	0.000	.
1	A	174	ASP	HB2	2.692	0.000	.
1	A	174	ASP	HB3	2.692	0.000	.
1	A	174	ASP	C	176.68	0.000	.
1	A	176	GLY	N	108.87	0.000	.
1	A	176	GLY	H	8.373	0.000	.
1	A	176	GLY	CA	45.16	0.000	.
1	A	176	GLY	HA2	3.975	0.000	.
1	A	176	GLY	HA3	3.975	0.000	.
1	A	176	GLY	C	174.495	0.000	.
1	A	177	GLY	N	108.905	0.000	.
1	A	177	GLY	H	8.204	0.000	.
1	A	177	GLY	CA	44.722	0.000	.
1	A	177	GLY	HA2	3.999	0.000	.
1	A	177	GLY	HA3	3.999	0.000	.
1	A	177	GLY	C	174.063	0.000	.
1	A	178	ARG	N	121.089	0.000	.
1	A	178	ARG	H	8.48	0.000	.
1	A	178	ARG	CA	56.769	0.000	.
1	A	178	ARG	HA	4.507	0.000	.
1	A	178	ARG	CB	31.097	0.000	.
1	A	178	ARG	HB2	1.795	0.000	.
1	A	178	ARG	HB3	1.795	0.000	.
1	A	178	ARG	C	176.051	0.005	.
1	A	179	ARG	N	120.077	0.000	.
1	A	179	ARG	H	7.991	0.000	.
1	A	179	ARG	CA	54.157	0.000	.
1	A	179	ARG	HA	4.648	0.000	.
1	A	179	ARG	CB	32.38	0.000	.
1	A	179	ARG	HB2	1.604	0.000	.
1	A	179	ARG	HB3	1.936	0.000	.
1	A	179	ARG	CG	26.968	0.001	.
1	A	179	ARG	HG2	1.575	0.000	.
1	A	179	ARG	HG3	1.575	0.000	.
1	A	179	ARG	CD	43.353	0.000	.
1	A	179	ARG	HD2	3.14	0.000	.
1	A	179	ARG	HD3	3.22	0.000	.
1	A	179	ARG	NE	85.239	0.000	.
1	A	179	ARG	HE	7.192	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	179	ARG	C	174.905	0.000	.
1	A	180	ALA	N	123.062	0.000	.
1	A	180	ALA	H	8.603	0.000	.
1	A	180	ALA	CA	51.375	0.000	.
1	A	180	ALA	HA	4.623	0.000	.
1	A	180	ALA	HB1	1.358	0.000	.
1	A	180	ALA	HB2	1.358	0.000	.
1	A	180	ALA	HB3	1.358	0.000	.
1	A	180	ALA	CB	20.694	0.000	.
1	A	180	ALA	C	175.474	0.000	.
1	A	181	ALA	N	117.031	0.000	.
1	A	181	ALA	H	6.827	0.000	.
1	A	181	ALA	CA	50.805	0.000	.
1	A	181	ALA	HA	4.552	0.000	.
1	A	181	ALA	HB1	1.129	0.000	.
1	A	181	ALA	HB2	1.129	0.000	.
1	A	181	ALA	HB3	1.129	0.000	.
1	A	181	ALA	CB	23.205	0.000	.
1	A	181	ALA	C	174.519	0.000	.
1	A	182	ILE	N	119.999	0.001	.
1	A	182	ILE	H	8.611	0.000	.
1	A	182	ILE	CA	60.902	0.000	.
1	A	182	ILE	HA	4.454	0.000	.
1	A	182	ILE	CB	40.094	0.000	.
1	A	182	ILE	HB	1.623	0.000	.
1	A	182	ILE	HG21	0.669	0.000	.
1	A	182	ILE	HG22	0.669	0.000	.
1	A	182	ILE	HG23	0.669	0.000	.
1	A	182	ILE	CG2	17.231	0.000	.
1	A	182	ILE	CG1	26.711	0.000	.
1	A	182	ILE	HG12	1.386	0.000	.
1	A	182	ILE	HG13	1.386	0.000	.
1	A	182	ILE	HD11	0.992	0.000	.
1	A	182	ILE	HD12	0.992	0.000	.
1	A	182	ILE	HD13	0.992	0.000	.
1	A	182	ILE	CD1	13.608	0.000	.
1	A	182	ILE	C	174.733	0.000	.
1	A	183	ARG	N	126.472	0.000	.
1	A	183	ARG	H	9.519	0.000	.
1	A	183	ARG	CA	52.478	0.000	.
1	A	183	ARG	HA	4.588	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	183	ARG	CB	30.8	0.000	.
1	A	183	ARG	HB2	1.368	0.000	.
1	A	183	ARG	HB3	1.51	0.000	.
1	A	183	ARG	CG	25.904	0.000	.
1	A	183	ARG	HG2	1.3	0.000	.
1	A	183	ARG	HG3	1.193	0.000	.
1	A	183	ARG	CD	42.716	0.001	.
1	A	183	ARG	HD2	3.013	0.000	.
1	A	183	ARG	HD3	2.773	0.000	.
1	A	183	ARG	NE	88.73	0.000	.
1	A	183	ARG	HE	8.366	0.000	.
1	A	183	ARG	C	173.917	0.000	.
1	A	184	GLN	N	124.191	0.001	.
1	A	184	GLN	H	8.363	0.000	.
1	A	184	GLN	CA	54.76	0.000	.
1	A	184	GLN	HA	5.037	0.000	.
1	A	184	GLN	CB	28.12	0.005	.
1	A	184	GLN	HB2	1.921	0.000	.
1	A	184	GLN	HB3	2.021	0.000	.
1	A	184	GLN	CG	33.115	0.000	.
1	A	184	GLN	HG2	2.204	0.000	.
1	A	184	GLN	HG3	2.49	0.000	.
1	A	184	GLN	NE2	113.62	0.006	.
1	A	184	GLN	HE21	6.925	0.000	.
1	A	184	GLN	HE22	7.435	0.000	.
1	A	184	GLN	C	176.22	0.000	.
1	A	185	VAL	N	121.317	0.000	.
1	A	185	VAL	H	8.129	0.000	.
1	A	185	VAL	CA	59.32	0.000	.
1	A	185	VAL	HA	4.653	0.000	.
1	A	185	VAL	CB	35.31	0.000	.
1	A	185	VAL	HB	2.074	0.000	.
1	A	185	VAL	HG11	0.564	0.000	.
1	A	185	VAL	HG12	0.564	0.000	.
1	A	185	VAL	HG13	0.564	0.000	.
1	A	185	VAL	HG21	0.552	0.000	.
1	A	185	VAL	HG22	0.552	0.000	.
1	A	185	VAL	HG23	0.552	0.000	.
1	A	185	VAL	CG1	17.532	0.000	.
1	A	185	VAL	CG2	21.665	0.000	.
1	A	185	VAL	C	175.72	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	186	GLY	N	106.792	0.000	.
1	A	186	GLY	H	8.272	0.000	.
1	A	186	GLY	CA	44.48	0.000	.
1	A	186	GLY	HA2	3.964	0.000	.
1	A	186	GLY	HA3	4.348	0.000	.
1	A	186	GLY	C	173.225	0.000	.
1	A	187	PRO	CD	49.756	0.000	.
1	A	187	PRO	CA	64.587	0.000	.
1	A	187	PRO	HA	4.392	0.000	.
1	A	187	PRO	CB	31.985	0.000	.
1	A	187	PRO	HB2	2.002	0.000	.
1	A	187	PRO	HB3	2.331	0.000	.
1	A	187	PRO	CG	27.202	0.000	.
1	A	187	PRO	HG2	2.002	0.000	.
1	A	187	PRO	HG3	2.002	0.000	.
1	A	187	PRO	HD2	3.676	0.000	.
1	A	187	PRO	HD3	3.676	0.000	.
1	A	187	PRO	C	177.272	0.000	.
1	A	188	ALA	N	120.342	0.000	.
1	A	188	ALA	H	8.396	0.000	.
1	A	188	ALA	CA	51.987	0.000	.
1	A	188	ALA	HA	4.426	0.000	.
1	A	188	ALA	HB1	1.408	0.000	.
1	A	188	ALA	HB2	1.408	0.000	.
1	A	188	ALA	HB3	1.408	0.000	.
1	A	188	ALA	CB	18.877	0.000	.
1	A	188	ALA	C	177.037	0.003	.
1	A	189	ALA	N	122.349	0.000	.
1	A	189	ALA	H	7.193	0.000	.
1	A	189	ALA	CA	50.235	0.000	.
1	A	189	ALA	HA	4.522	0.000	.
1	A	189	ALA	HB1	1.338	0.000	.
1	A	189	ALA	HB2	1.338	0.000	.
1	A	189	ALA	HB3	1.338	0.000	.
1	A	189	ALA	CB	18.74	0.000	.
1	A	189	ALA	C	174.753	0.000	.
1	A	191	SER	N	111.133	0.000	.
1	A	191	SER	H	8.091	0.000	.
1	A	191	SER	CA	56.539	0.000	.
1	A	191	SER	HA	4.989	0.000	.
1	A	191	SER	CB	66.627	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	191	SER	HB2	3.789	0.000	.
1	A	191	SER	HB3	3.927	0.000	.
1	A	191	SER	C	176.096	0.000	.
1	A	192	GLY	N	112.333	0.000	.
1	A	192	GLY	H	9.246	0.000	.
1	A	192	GLY	CA	43.54	0.000	.
1	A	192	GLY	HA2	2.844	0.000	.
1	A	192	GLY	HA3	4.397	0.000	.
1	A	192	GLY	C	171.9	0.000	.
1	A	193	TRP	N	118.721	0.000	.
1	A	193	TRP	H	9.063	0.000	.
1	A	193	TRP	CA	57.105	0.000	.
1	A	193	TRP	HA	4.9	0.000	.
1	A	193	TRP	CB	30.156	0.000	.
1	A	193	TRP	HB2	2.842	0.000	.
1	A	193	TRP	HB3	3.255	0.003	.
1	A	193	TRP	CD1	126.594	0.000	.
1	A	193	TRP	CE3	119.18	0.000	.
1	A	193	TRP	NE1	129.214	0.000	.
1	A	193	TRP	HD1	7.209	0.000	.
1	A	193	TRP	HE3	6.96	0.000	.
1	A	193	TRP	CZ3	120.926	0.004	.
1	A	193	TRP	CZ2	114.125	0.002	.
1	A	193	TRP	HE1	10.386	0.000	.
1	A	193	TRP	HZ3	6.78	0.001	.
1	A	193	TRP	CH2	122.776	0.006	.
1	A	193	TRP	HZ2	6.191	0.000	.
1	A	193	TRP	HH2	6.709	0.000	.
1	A	193	TRP	C	178.667	0.000	.
1	A	194	TYR	N	123.184	0.000	.
1	A	194	TYR	H	9.478	0.000	.
1	A	194	TYR	CA	56.022	0.000	.
1	A	194	TYR	HA	5.339	0.000	.
1	A	194	TYR	CB	40.878	0.000	.
1	A	194	TYR	HB2	2.696	0.000	.
1	A	194	TYR	HB3	3.043	0.000	.
1	A	194	TYR	HD1	7.043	0.000	.
1	A	194	TYR	HD2	7.043	0.000	.
1	A	194	TYR	HE1	6.463	0.000	.
1	A	194	TYR	HE2	6.463	0.000	.
1	A	194	TYR	CD1	133.511	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	194	TYR	CE1	118.215	0.000	.
1	A	194	TYR	CE2	118.215	0.000	.
1	A	194	TYR	CD2	133.511	0.000	.
1	A	194	TYR	C	173.356	0.000	.
1	A	195	PRO	CD	51.081	0.000	.
1	A	195	PRO	CA	61.899	0.000	.
1	A	195	PRO	HA	4.841	0.000	.
1	A	195	PRO	CB	33.092	0.006	.
1	A	195	PRO	HB2	1.131	0.000	.
1	A	195	PRO	HB3	1.606	0.000	.
1	A	195	PRO	CG	26.762	0.007	.
1	A	195	PRO	HG2	1.468	0.000	.
1	A	195	PRO	HG3	1.728	0.000	.
1	A	195	PRO	HD2	4.077	0.000	.
1	A	195	PRO	HD3	4.077	0.000	.
1	A	195	PRO	C	174.534	0.000	.
1	A	196	CYS	N	117.655	0.000	.
1	A	196	CYS	H	8.481	0.000	.
1	A	196	CYS	CA	56.125	0.000	.
1	A	196	CYS	HA	5.37	0.000	.
1	A	196	CYS	CB	28.587	0.002	.
1	A	196	CYS	HB2	2.2	0.001	.
1	A	196	CYS	HB3	2.757	0.000	.
1	A	196	CYS	C	173.595	0.000	.
1	A	197	PHE	N	123.996	0.000	.
1	A	197	PHE	H	8.949	0.000	.
1	A	197	PHE	CA	56.151	0.008	.
1	A	197	PHE	HA	5.354	0.000	.
1	A	197	PHE	CB	42.742	0.001	.
1	A	197	PHE	HB2	2.422	0.000	.
1	A	197	PHE	HB3	2.578	0.000	.
1	A	197	PHE	HD1	6.971	0.000	.
1	A	197	PHE	HD2	6.971	0.000	.
1	A	197	PHE	HE1	6.307	0.000	.
1	A	197	PHE	HE2	6.307	0.000	.
1	A	197	PHE	CD1	131.873	0.006	.
1	A	197	PHE	CE1	129.201	0.000	.
1	A	197	PHE	CZ	128.95	0.001	.
1	A	197	PHE	HZ	5.747	0.001	.
1	A	197	PHE	CE2	129.201	0.000	.
1	A	197	PHE	CD2	131.873	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	197	PHE	C	174.962	0.000	.
1	A	198	ARG	N	124.83	0.000	.
1	A	198	ARG	H	8.333	0.000	.
1	A	198	ARG	CA	57.465	0.000	.
1	A	198	ARG	HA	4.492	0.000	.
1	A	198	ARG	CB	30.263	0.000	.
1	A	198	ARG	HB2	1.887	0.000	.
1	A	198	ARG	HB3	1.887	0.000	.
1	A	198	ARG	CG	27.86	0.007	.
1	A	198	ARG	HG2	1.485	0.000	.
1	A	198	ARG	HG3	1.741	0.000	.
1	A	198	ARG	CD	42.735	0.008	.
1	A	198	ARG	HD2	2.968	0.000	.
1	A	198	ARG	HD3	3.148	0.000	.
1	A	198	ARG	C	176.261	0.000	.
1	A	199	ALA	N	128.106	0.000	.
1	A	199	ALA	H	8.991	0.000	.
1	A	199	ALA	CA	51.503	0.002	.
1	A	199	ALA	HA	4.955	0.000	.
1	A	199	ALA	HB1	1.511	0.000	.
1	A	199	ALA	HB2	1.511	0.000	.
1	A	199	ALA	HB3	1.511	0.000	.
1	A	199	ALA	CB	23.859	0.000	.
1	A	199	ALA	C	174.799	0.001	.
1	A	200	GLN	N	116.193	0.000	.
1	A	200	GLN	H	8.33	0.000	.
1	A	200	GLN	CA	54.537	0.000	.
1	A	200	GLN	HA	4.914	0.000	.
1	A	200	GLN	CB	31.218	0.000	.
1	A	200	GLN	HB2	2.07	0.000	.
1	A	200	GLN	HB3	2.296	0.000	.
1	A	200	GLN	CG	34.806	0.000	.
1	A	200	GLN	HG2	2.357	0.000	.
1	A	200	GLN	HG3	2.461	0.000	.
1	A	200	GLN	NE2	112.968	0.000	.
1	A	200	GLN	HE21	6.885	0.000	.
1	A	200	GLN	HE22	7.793	0.000	.
1	A	200	GLN	C	177.527	0.000	.
1	A	201	GLU	N	121.86	0.000	.
1	A	201	GLU	H	9.291	0.000	.
1	A	201	GLU	CA	60.587	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	201	GLU	HA	4.014	0.000	.
1	A	201	GLU	CB	29.148	0.000	.
1	A	201	GLU	HB2	2.135	0.000	.
1	A	201	GLU	HB3	2.135	0.000	.
1	A	201	GLU	CG	36.026	0.001	.
1	A	201	GLU	HG2	2.316	0.000	.
1	A	201	GLU	HG3	2.388	0.000	.
1	A	201	GLU	C	178.457	0.000	.
1	A	202	SER	N	112.055	0.000	.
1	A	202	SER	H	8.135	0.000	.
1	A	202	SER	CA	59.872	0.000	.
1	A	202	SER	HA	4.158	0.003	.
1	A	202	SER	CB	62.457	0.005	.
1	A	202	SER	HB2	3.882	0.000	.
1	A	202	SER	HB3	4.046	0.000	.
1	A	202	SER	C	175.178	0.000	.
1	A	203	ALA	N	125.841	0.000	.
1	A	203	ALA	H	8.448	0.000	.
1	A	203	ALA	CA	54.387	0.000	.
1	A	203	ALA	HA	4.219	0.000	.
1	A	203	ALA	HB1	1.559	0.000	.
1	A	203	ALA	HB2	1.559	0.000	.
1	A	203	ALA	HB3	1.559	0.000	.
1	A	203	ALA	CB	19.958	0.000	.
1	A	203	ALA	C	178.413	0.003	.
1	A	204	VAL	N	114.394	0.000	.
1	A	204	VAL	H	7.596	0.000	.
1	A	204	VAL	CA	68.475	0.000	.
1	A	204	VAL	HA	3.621	0.000	.
1	A	204	VAL	CB	28.71	0.000	.
1	A	204	VAL	HB	2.451	0.000	.
1	A	204	VAL	HG11	0.843	0.000	.
1	A	204	VAL	HG12	0.843	0.000	.
1	A	204	VAL	HG13	0.843	0.000	.
1	A	204	VAL	HG21	1.016	0.000	.
1	A	204	VAL	HG22	1.016	0.000	.
1	A	204	VAL	HG23	1.016	0.000	.
1	A	204	VAL	CG1	21.654	0.000	.
1	A	204	VAL	CG2	23.679	0.000	.
1	A	204	VAL	C	174.462	0.000	.
1	A	205	PRO	CD	49.304	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	205	PRO	CA	65.188	0.001	.
1	A	205	PRO	HA	4.261	0.000	.
1	A	205	PRO	CB	30.006	0.000	.
1	A	205	PRO	HB2	1.881	0.000	.
1	A	205	PRO	HB3	2.205	0.000	.
1	A	205	PRO	CG	27.632	0.000	.
1	A	205	PRO	HG2	1.988	0.000	.
1	A	205	PRO	HG3	2.14	0.000	.
1	A	205	PRO	HD2	3.495	0.000	.
1	A	205	PRO	HD3	4.076	0.000	.
1	A	205	PRO	C	179.755	0.000	.
1	A	207	ALA	N	120.649	0.000	.
1	A	207	ALA	H	8.42	0.000	.
1	A	207	ALA	CA	55.237	0.000	.
1	A	207	ALA	HA	3.884	0.000	.
1	A	207	ALA	HB1	1.467	0.000	.
1	A	207	ALA	HB2	1.467	0.000	.
1	A	207	ALA	HB3	1.467	0.000	.
1	A	207	ALA	CB	16.225	0.000	.
1	A	207	ALA	C	180.23	0.000	.
1	A	208	VAL	N	120.05	0.000	.
1	A	208	VAL	H	8.207	0.000	.
1	A	208	VAL	CA	65.533	0.000	.
1	A	208	VAL	HA	4.103	0.000	.
1	A	208	VAL	CB	31.94	0.006	.
1	A	208	VAL	HB	2.072	0.000	.
1	A	208	VAL	HG11	0.985	0.000	.
1	A	208	VAL	HG12	0.985	0.000	.
1	A	208	VAL	HG13	0.985	0.000	.
1	A	208	VAL	HG21	0.92	0.000	.
1	A	208	VAL	HG22	0.92	0.000	.
1	A	208	VAL	HG23	0.92	0.000	.
1	A	208	VAL	CG1	20.871	0.000	.
1	A	208	VAL	CG2	22.02	0.000	.
1	A	208	VAL	C	181.017	0.000	.
1	A	209	MET	N	122.465	0.001	.
1	A	209	MET	H	8.324	0.000	.
1	A	209	MET	CA	58.466	0.000	.
1	A	209	MET	HA	4.233	0.000	.
1	A	209	MET	CB	32.02	0.000	.
1	A	209	MET	HB2	2.226	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	209	MET	HB3	2.226	0.000	.
1	A	209	MET	CG	32.293	0.002	.
1	A	209	MET	HG2	2.632	0.000	.
1	A	209	MET	HG3	2.689	0.000	.
1	A	209	MET	C	178.138	0.000	.
1	A	210	LEU	N	118.186	0.000	.
1	A	210	LEU	H	7.454	0.000	.
1	A	210	LEU	CA	55.145	0.001	.
1	A	210	LEU	HA	4.358	0.000	.
1	A	210	LEU	CB	42.588	0.002	.
1	A	210	LEU	HB2	1.982	0.000	.
1	A	210	LEU	HB3	2.136	0.000	.
1	A	210	LEU	CG	26.696	0.000	.
1	A	210	LEU	HG	1.775	0.000	.
1	A	210	LEU	HD11	0.845	0.000	.
1	A	210	LEU	HD12	0.845	0.000	.
1	A	210	LEU	HD13	0.845	0.000	.
1	A	210	LEU	HD21	0.523	0.000	.
1	A	210	LEU	HD22	0.523	0.000	.
1	A	210	LEU	HD23	0.523	0.000	.
1	A	210	LEU	CD1	22.255	0.000	.
1	A	210	LEU	CD2	25.804	0.000	.
1	A	210	LEU	C	176.496	0.000	.
1	A	211	GLY	N	105.306	0.000	.
1	A	211	GLY	H	7.934	0.000	.
1	A	211	GLY	CA	44.971	0.000	.
1	A	211	GLY	HA2	3.754	0.000	.
1	A	211	GLY	HA3	4.421	0.000	.
1	A	211	GLY	C	174.824	0.000	.
1	A	212	ALA	N	123.929	0.000	.
1	A	212	ALA	H	8.52	0.000	.
1	A	212	ALA	CA	51.272	0.000	.
1	A	212	ALA	HA	4.727	0.000	.
1	A	212	ALA	HB1	1.199	0.000	.
1	A	212	ALA	HB2	1.199	0.000	.
1	A	212	ALA	HB3	1.199	0.000	.
1	A	212	ALA	CB	21.398	0.000	.
1	A	212	ALA	C	175.781	0.000	.
1	A	213	SER	N	111.856	0.000	.
1	A	213	SER	H	8.519	0.000	.
1	A	213	SER	CA	57.137	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	213	SER	HA	4.845	0.000	.
1	A	213	SER	CB	65.735	0.000	.
1	A	213	SER	HB2	3.631	0.000	.
1	A	213	SER	HB3	3.705	0.000	.
1	A	213	SER	C	173.076	0.000	.
1	A	214	VAL	N	123.846	0.000	.
1	A	214	VAL	H	8.796	0.000	.
1	A	214	VAL	CA	63.8	0.001	.
1	A	214	VAL	HA	3.921	0.000	.
1	A	214	VAL	CB	31.953	0.000	.
1	A	214	VAL	HB	1.894	0.000	.
1	A	214	VAL	HG11	0.707	0.000	.
1	A	214	VAL	HG12	0.707	0.000	.
1	A	214	VAL	HG13	0.707	0.000	.
1	A	214	VAL	HG21	0.748	0.000	.
1	A	214	VAL	HG22	0.748	0.000	.
1	A	214	VAL	HG23	0.748	0.000	.
1	A	214	VAL	CG1	21.196	0.000	.
1	A	214	VAL	CG2	21.237	0.000	.
1	A	214	VAL	C	176.385	0.001	.
1	A	215	LEU	N	127.468	0.000	.
1	A	215	LEU	H	9.414	0.000	.
1	A	215	LEU	CA	55.578	0.000	.
1	A	215	LEU	HA	4.448	0.000	.
1	A	215	LEU	CB	43.921	0.000	.
1	A	215	LEU	HB2	1.29	0.000	.
1	A	215	LEU	HB3	1.369	0.000	.
1	A	215	LEU	CG	26.425	0.000	.
1	A	215	LEU	HG	1.551	0.000	.
1	A	215	LEU	HD11	0.742	0.000	.
1	A	215	LEU	HD12	0.742	0.000	.
1	A	215	LEU	HD13	0.742	0.000	.
1	A	215	LEU	HD21	0.793	0.000	.
1	A	215	LEU	HD22	0.793	0.000	.
1	A	215	LEU	HD23	0.793	0.000	.
1	A	215	LEU	CD1	21.842	0.000	.
1	A	215	LEU	CD2	26.399	0.000	.
1	A	215	LEU	C	176.922	0.005	.
1	A	216	LEU	N	118.114	0.000	.
1	A	216	LEU	H	7.436	0.000	.
1	A	216	LEU	CA	55.173	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	216	LEU	HA	4.514	0.000	.
1	A	216	LEU	CB	45.698	0.008	.
1	A	216	LEU	HB2	1.427	0.000	.
1	A	216	LEU	HB3	1.461	0.000	.
1	A	216	LEU	CG	27.388	0.003	.
1	A	216	LEU	HG	1.581	0.000	.
1	A	216	LEU	HD11	1.07	0.000	.
1	A	216	LEU	HD12	1.07	0.000	.
1	A	216	LEU	HD13	1.07	0.000	.
1	A	216	LEU	HD21	0.794	0.000	.
1	A	216	LEU	HD22	0.794	0.000	.
1	A	216	LEU	HD23	0.794	0.000	.
1	A	216	LEU	CD1	23.304	0.002	.
1	A	216	LEU	CD2	26.471	0.000	.
1	A	216	LEU	C	173.002	0.003	.
1	A	217	ARG	N	125.403	0.001	.
1	A	217	ARG	H	8.408	0.000	.
1	A	217	ARG	CA	54.962	0.000	.
1	A	217	ARG	HA	5.421	0.000	.
1	A	217	ARG	CB	32.478	0.000	.
1	A	217	ARG	HB2	1.615	0.000	.
1	A	217	ARG	HB3	1.94	0.000	.
1	A	217	ARG	CG	28.543	0.000	.
1	A	217	ARG	HG2	1.55	0.000	.
1	A	217	ARG	HG3	1.55	0.000	.
1	A	217	ARG	CD	43.385	0.000	.
1	A	217	ARG	HD2	3.134	0.000	.
1	A	217	ARG	HD3	3.134	0.000	.
1	A	217	ARG	NE	85.449	0.001	.
1	A	217	ARG	HE	7.287	0.000	.
1	A	217	ARG	C	174.892	0.000	.
1	A	218	TYR	N	122.089	0.000	.
1	A	218	TYR	H	9.067	0.000	.
1	A	218	TYR	CA	56.306	0.000	.
1	A	218	TYR	HA	4.915	0.000	.
1	A	218	TYR	CB	39.749	0.008	.
1	A	218	TYR	HB2	2.836	0.000	.
1	A	218	TYR	HB3	3.085	0.000	.
1	A	218	TYR	HD1	6.61	0.000	.
1	A	218	TYR	HD2	6.61	0.000	.
1	A	218	TYR	HE1	6.468	0.003	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	218	TYR	HE2	6.468	0.003	.
1	A	218	TYR	CD1	132.93	0.000	.
1	A	218	TYR	CE1	118.252	0.000	.
1	A	218	TYR	CE2	118.252	0.002	.
1	A	218	TYR	CD2	132.93	0.000	.
1	A	218	TYR	C	171.774	0.004	.
1	A	219	ASP	N	118.737	0.001	.
1	A	219	ASP	H	8.557	0.000	.
1	A	219	ASP	CA	54.956	0.001	.
1	A	219	ASP	HA	4.992	0.000	.
1	A	219	ASP	CB	43.354	0.000	.
1	A	219	ASP	HB2	2.465	0.000	.
1	A	219	ASP	HB3	2.465	0.000	.
1	A	219	ASP	C	175.623	0.005	.
1	A	220	CYS	N	120.237	0.000	.
1	A	220	CYS	H	8.089	0.000	.
1	A	220	CYS	CA	56.956	0.000	.
1	A	220	CYS	HA	4.826	0.000	.
1	A	220	CYS	CB	27.85	0.001	.
1	A	220	CYS	HB2	2.762	0.001	.
1	A	220	CYS	HB3	3.327	0.000	.
1	A	220	CYS	C	174.069	0.000	.
1	A	221	PRO	CD	50.492	0.000	.
1	A	221	PRO	CA	65.45	0.000	.
1	A	221	PRO	HA	4.267	0.000	.
1	A	221	PRO	CB	31.817	0.000	.
1	A	221	PRO	HB2	1.854	0.000	.
1	A	221	PRO	HB3	2.402	0.000	.
1	A	221	PRO	CG	28.361	0.000	.
1	A	221	PRO	HG2	2.15	0.001	.
1	A	221	PRO	HG3	2.15	0.001	.
1	A	221	PRO	HD2	3.647	0.000	.
1	A	221	PRO	HD3	3.647	0.000	.
1	A	221	PRO	C	176.694	0.000	.
1	A	223	GLY	N	108.932	0.000	.
1	A	223	GLY	H	7.304	0.000	.
1	A	223	GLY	CA	45.09	0.000	.
1	A	223	GLY	HA2	4.375	0.001	.
1	A	223	GLY	HA3	3.854	0.000	.
1	A	223	GLY	C	169.416	0.000	.
1	A	225	ALA	N	124.14	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	225	ALA	H	8.807	0.000	.
1	A	225	ALA	CA	49.776	0.000	.
1	A	225	ALA	HA	5.198	0.000	.
1	A	225	ALA	HB1	0.195	0.000	.
1	A	225	ALA	HB2	0.195	0.000	.
1	A	225	ALA	HB3	0.195	0.000	.
1	A	225	ALA	CB	20.985	0.003	.
1	A	225	ALA	C	176.961	0.000	.
1	A	226	VAL	N	121.141	0.000	.
1	A	226	VAL	H	8.944	0.000	.
1	A	226	VAL	CA	61.008	0.000	.
1	A	226	VAL	HA	4.652	0.000	.
1	A	226	VAL	CB	34.647	0.000	.
1	A	226	VAL	HB	1.917	0.000	.
1	A	226	VAL	HG11	0.874	0.000	.
1	A	226	VAL	HG12	0.874	0.000	.
1	A	226	VAL	HG13	0.874	0.000	.
1	A	226	VAL	HG21	0.856	0.000	.
1	A	226	VAL	HG22	0.856	0.000	.
1	A	226	VAL	HG23	0.856	0.000	.
1	A	226	VAL	CG1	21.276	0.001	.
1	A	226	VAL	CG2	22.604	0.000	.
1	A	226	VAL	C	174.135	0.000	.
1	A	227	VAL	N	129.402	0.000	.
1	A	227	VAL	H	9.32	0.000	.
1	A	227	VAL	CA	62.21	0.000	.
1	A	227	VAL	HA	4.358	0.000	.
1	A	227	VAL	CB	31.937	0.000	.
1	A	227	VAL	HB	1.864	0.000	.
1	A	227	VAL	HG11	0.432	0.000	.
1	A	227	VAL	HG12	0.432	0.000	.
1	A	227	VAL	HG13	0.432	0.000	.
1	A	227	VAL	HG21	0.937	0.000	.
1	A	227	VAL	HG22	0.937	0.000	.
1	A	227	VAL	HG23	0.937	0.000	.
1	A	227	VAL	CG1	21.769	0.000	.
1	A	227	VAL	CG2	21.388	0.000	.
1	A	227	VAL	C	175.854	0.000	.
1	A	228	VAL	N	125.583	0.000	.
1	A	228	VAL	H	9.477	0.000	.
1	A	228	VAL	CA	59.499	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	228	VAL	HA	4.856	0.000	.
1	A	228	VAL	CB	34.749	0.000	.
1	A	228	VAL	HB	1.292	0.000	.
1	A	228	VAL	HG11	0.277	0.000	.
1	A	228	VAL	HG12	0.277	0.000	.
1	A	228	VAL	HG13	0.277	0.000	.
1	A	228	VAL	HG21	0.593	0.000	.
1	A	228	VAL	HG22	0.593	0.000	.
1	A	228	VAL	HG23	0.593	0.000	.
1	A	228	VAL	CG1	19.97	0.000	.
1	A	228	VAL	CG2	22.626	0.000	.
1	A	228	VAL	C	173.309	0.000	.
1	A	229	SER	N	115.241	0.001	.
1	A	229	SER	H	8.911	0.000	.
1	A	229	SER	CA	55.444	0.000	.
1	A	229	SER	HA	5.037	0.000	.
1	A	229	SER	CB	64.237	0.001	.
1	A	229	SER	HB2	3.651	0.001	.
1	A	229	SER	HB3	3.796	0.000	.
1	A	229	SER	C	173.303	0.000	.
1	A	230	ALA	N	128.38	0.000	.
1	A	230	ALA	H	9.272	0.000	.
1	A	230	ALA	CA	50.74	0.000	.
1	A	230	ALA	HA	3.906	0.000	.
1	A	230	ALA	HB1	1.32	0.000	.
1	A	230	ALA	HB2	1.32	0.000	.
1	A	230	ALA	HB3	1.32	0.000	.
1	A	230	ALA	CB	18.719	0.000	.
1	A	230	ALA	C	176.113	0.000	.
1	A	231	PRO	CD	49.864	0.001	.
1	A	231	PRO	CA	65.546	0.001	.
1	A	231	PRO	HA	4.039	0.000	.
1	A	231	PRO	CB	30.795	0.000	.
1	A	231	PRO	HB2	1.805	0.000	.
1	A	231	PRO	HB3	2.183	0.000	.
1	A	231	PRO	CG	27.796	0.001	.
1	A	231	PRO	HG2	1.74	0.000	.
1	A	231	PRO	HG3	1.74	0.000	.
1	A	231	PRO	HD2	3.735	0.000	.
1	A	231	PRO	HD3	3.735	0.000	.
1	A	231	PRO	C	178.14	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	232	GLY	N	103.872	0.000	.
1	A	232	GLY	H	8.357	0.000	.
1	A	232	GLY	CA	45.76	0.000	.
1	A	232	GLY	HA2	3.927	0.000	.
1	A	232	GLY	HA3	4.06	0.000	.
1	A	232	GLY	C	175.326	0.000	.
1	A	233	GLY	N	108.712	0.000	.
1	A	233	GLY	H	7.952	0.000	.
1	A	233	GLY	CA	44.755	0.000	.
1	A	233	GLY	HA2	3.495	0.000	.
1	A	233	GLY	HA3	4.483	0.000	.
1	A	233	GLY	C	174.359	0.000	.
1	A	234	GLU	N	124.033	0.000	.
1	A	234	GLU	H	9.852	0.000	.
1	A	234	GLU	CA	56.605	0.000	.
1	A	234	GLU	HA	4.78	0.000	.
1	A	234	GLU	CB	27.713	0.000	.
1	A	234	GLU	HB2	2.186	0.001	.
1	A	234	GLU	HB3	2.304	0.000	.
1	A	234	GLU	CG	35.335	0.000	.
1	A	234	GLU	HG2	2.645	0.001	.
1	A	234	GLU	HG3	2.645	0.001	.
1	A	234	GLU	C	173.219	0.002	.
1	A	235	VAL	N	121.051	0.000	.
1	A	235	VAL	H	8.552	0.000	.
1	A	235	VAL	CA	61.295	0.000	.
1	A	235	VAL	HA	5.566	0.000	.
1	A	235	VAL	CB	35.461	0.000	.
1	A	235	VAL	HB	2.124	0.000	.
1	A	235	VAL	HG11	0.419	0.000	.
1	A	235	VAL	HG12	0.419	0.000	.
1	A	235	VAL	HG13	0.419	0.000	.
1	A	235	VAL	HG21	1.029	0.000	.
1	A	235	VAL	HG22	1.029	0.000	.
1	A	235	VAL	HG23	1.029	0.000	.
1	A	235	VAL	CG1	22.968	0.000	.
1	A	235	VAL	CG2	21.895	0.000	.
1	A	235	VAL	C	175.611	0.001	.
1	A	236	PHE	N	121.141	0.000	.
1	A	236	PHE	H	8.893	0.000	.
1	A	236	PHE	CA	56.384	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	236	PHE	HA	5.096	0.000	.
1	A	236	PHE	CB	41.634	0.000	.
1	A	236	PHE	HB2	3.171	0.000	.
1	A	236	PHE	HB3	3.348	0.000	.
1	A	236	PHE	HD1	7.524	0.000	.
1	A	236	PHE	HD2	7.524	0.000	.
1	A	236	PHE	HE1	7.424	0.000	.
1	A	236	PHE	HE2	7.424	0.000	.
1	A	236	PHE	CD1	132.919	0.001	.
1	A	236	PHE	CE1	130.755	0.000	.
1	A	236	PHE	CZ	128.323	0.000	.
1	A	236	PHE	HZ	7.079	0.000	.
1	A	236	PHE	CE2	130.755	0.000	.
1	A	236	PHE	CD2	132.919	0.000	.
1	A	236	PHE	C	170.306	0.000	.
1	A	237	THR	N	117.174	0.000	.
1	A	237	THR	H	9.187	0.000	.
1	A	237	THR	CA	61.401	0.000	.
1	A	237	THR	HA	5.284	0.000	.
1	A	237	THR	CB	70.037	0.000	.
1	A	237	THR	HB	4.358	0.000	.
1	A	237	THR	HG21	0.894	0.000	.
1	A	237	THR	HG22	0.894	0.000	.
1	A	237	THR	HG23	0.894	0.000	.
1	A	237	THR	CG2	24.15	0.005	.
1	A	237	THR	C	173.97	0.002	.
1	A	238	LEU	N	126.937	0.000	.
1	A	238	LEU	H	9.396	0.000	.
1	A	238	LEU	CA	52.89	0.000	.
1	A	238	LEU	HA	5.202	0.000	.
1	A	238	LEU	CB	44.325	0.000	.
1	A	238	LEU	HB2	1.187	0.000	.
1	A	238	LEU	HB3	1.93	0.000	.
1	A	238	LEU	CG	26.368	0.001	.
1	A	238	LEU	HG	1.923	0.000	.
1	A	238	LEU	HD11	1.24	0.000	.
1	A	238	LEU	HD12	1.24	0.000	.
1	A	238	LEU	HD13	1.24	0.000	.
1	A	238	LEU	HD21	0.762	0.000	.
1	A	238	LEU	HD22	0.762	0.000	.
1	A	238	LEU	HD23	0.762	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	238	LEU	CD1	25.564	0.000	.
1	A	238	LEU	CD2	26.61	0.000	.
1	A	238	LEU	C	174.624	0.000	.
1	A	239	LEU	N	125.653	0.000	.
1	A	239	LEU	H	8.65	0.000	.
1	A	239	LEU	CA	53.058	0.000	.
1	A	239	LEU	HA	4.842	0.000	.
1	A	239	LEU	CB	43.662	0.000	.
1	A	239	LEU	HB2	1.011	0.000	.
1	A	239	LEU	HB3	1.517	0.000	.
1	A	239	LEU	CG	27.283	0.000	.
1	A	239	LEU	HG	1.213	0.000	.
1	A	239	LEU	HD11	0.551	0.000	.
1	A	239	LEU	HD12	0.551	0.000	.
1	A	239	LEU	HD13	0.551	0.000	.
1	A	239	LEU	HD21	0.638	0.000	.
1	A	239	LEU	HD22	0.638	0.000	.
1	A	239	LEU	HD23	0.638	0.000	.
1	A	239	LEU	CD1	23.813	0.000	.
1	A	239	LEU	CD2	25.194	0.000	.
1	A	239	LEU	C	176.05	0.000	.
1	A	240	LEU	N	126.147	0.000	.
1	A	240	LEU	H	8.772	0.000	.
1	A	240	LEU	CA	54.12	0.000	.
1	A	240	LEU	HA	4.86	0.000	.
1	A	240	LEU	CB	39.782	0.000	.
1	A	240	LEU	HB2	1.168	0.000	.
1	A	240	LEU	HB3	1.918	0.000	.
1	A	240	LEU	CG	26.434	0.000	.
1	A	240	LEU	HG	1.591	0.000	.
1	A	240	LEU	HD11	0.58	0.000	.
1	A	240	LEU	HD12	0.58	0.000	.
1	A	240	LEU	HD13	0.58	0.000	.
1	A	240	LEU	HD21	0.827	0.000	.
1	A	240	LEU	HD22	0.827	0.000	.
1	A	240	LEU	HD23	0.827	0.000	.
1	A	240	LEU	CD1	23.362	0.000	.
1	A	240	LEU	CD2	25.714	0.000	.
1	A	240	LEU	C	177.332	0.000	.
1	A	241	THR	N	114.683	0.000	.
1	A	241	THR	H	8.35	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	241	THR	CA	61.603	0.000	.
1	A	241	THR	HA	4.43	0.000	.
1	A	241	THR	CB	70.544	0.000	.
1	A	241	THR	HB	4.192	0.000	.
1	A	241	THR	HG21	1.093	0.000	.
1	A	241	THR	HG22	1.093	0.000	.
1	A	241	THR	HG23	1.093	0.000	.
1	A	241	THR	CG2	20.804	0.000	.
1	A	241	THR	C	174.119	0.000	.
1	A	242	ASP	N	128.315	0.000	.
1	A	242	ASP	H	8.125	0.000	.
1	A	242	ASP	CA	56.157	0.001	.
1	A	242	ASP	HA	4.484	0.000	.
1	A	242	ASP	CB	42.615	0.000	.
1	A	242	ASP	HB2	2.463	0.000	.
1	A	242	ASP	HB3	2.714	0.000	.
1	A	242	ASP	C	180.403	0.000	.
1	A	301	WOZ	H1	3.722	0.000	.
1	A	301	WOZ	H2	6.735	0.000	.
1	A	301	WOZ	H3	6.197	0.000	.
1	A	301	WOZ	H4	6.016	0.000	.
1	A	301	WOZ	H5	2.129	0.000	.
1	A	301	WOZ	H6	1.352	0.000	.
1	A	301	WOZ	H7	5.998	0.000	.
1	A	301	WOZ	Q24	2.435	0.000	.
1	A	301	WOZ	Q26	0.737	0.000	.
1	A	301	WOZ	Q27	0.573	0.000	.
1	A	301	WOZ	H13	12.835	0.000	.
1	A	301	WOZ	H14	10.192	0.000	.

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	241	$0.06 \pm 0.30$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	205	$0.61 \pm 0.65$	None needed (imprecise)
$^{13}\text{C}'$	220	$0.47 \pm 0.34$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	217	$0.65 \pm 0.89$	None needed (imprecise)

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 96 atoms were assigned a chemical shift out of a possible 2500. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	53/983 (5%)	22/406 (5%)	22/394 (6%)	9/183 (5%)
Sidechain	43/1317 (3%)	30/874 (3%)	13/403 (3%)	0/40 (0%)
Aromatic	0/200 (0%)	0/97 (0%)	0/97 (0%)	0/6 (0%)
Overall	96/2500 (4%)	52/1377 (4%)	35/894 (4%)	9/229 (4%)

### 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	147	LEU	HB2	-1.79	-0.07 – 3.30	-10.1
1	A	18	LEU	HB2	-1.65	-0.07 – 3.30	-9.7
1	A	147	LEU	HB3	-1.79	-0.26 – 3.31	-9.3
1	A	18	LEU	HB3	-0.96	-0.26 – 3.31	-7.0
1	A	34	PHE	HB2	1.15	1.20 – 4.80	-5.1

### 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:

