Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2KUG
BMRB ID	:	16764
Title	:	Halothane binds to druggable sites in calcium-calmodulin: Solution Structure of halothane-CaM N-terminal domain
Authors	:	Juranic, N.; Macura, S.; Simeonov, M.V.; Jones, K.A.; Penheiter, A.R.; Hock, T.J.; Streiff, J.H.
Deposited on	:	2010-02-17

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

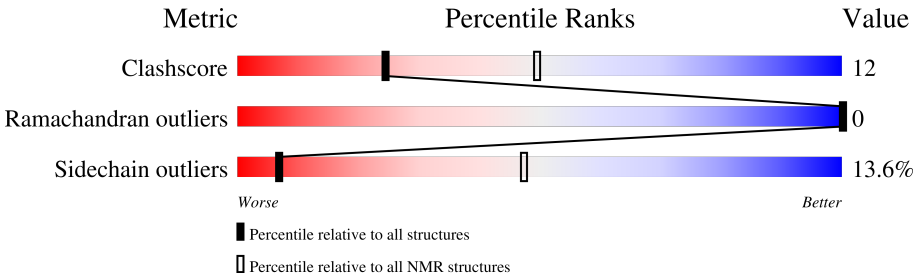
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 94%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	148	35% 12% • 49%

2 Ensemble composition and analysis (i)

This entry contains 5 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:73 (70)	0.46	5

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1160 atoms, of which 563 are hydrogens and 0 are deuteriums.

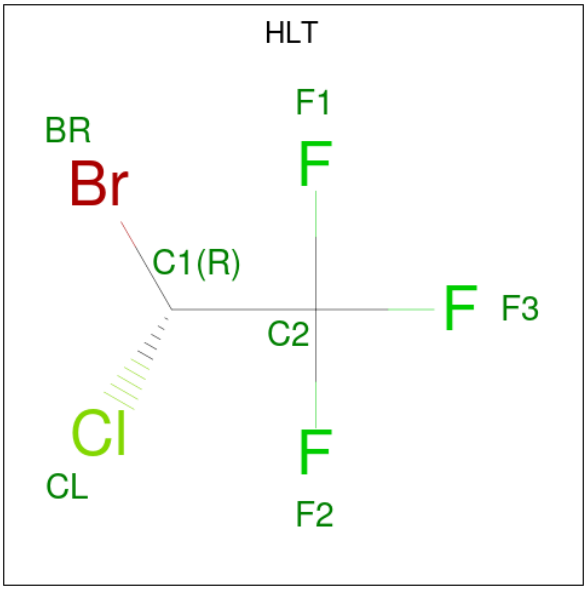
- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1150	363	562	93	127	5	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

- Molecule 3 is 2-BROMO-2-CHLORO-1,1,1-TRIFLUOROETHANE (three-letter code: HLT) (formula: $C_2HBrClF_3$).



Mol	Chain	Residues	Atoms					
			Total	Br	C	Cl	F	H
3	A	1	8	1	2	1	3	1

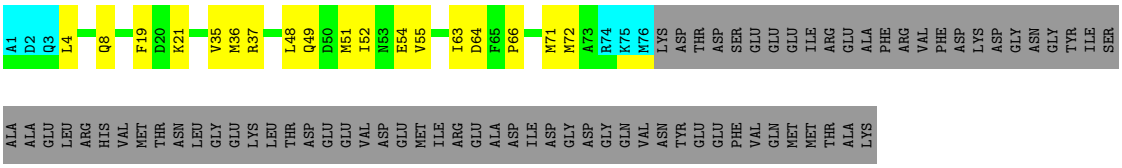
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Calmodulin-1

Chain A: 35% 12% • 49%



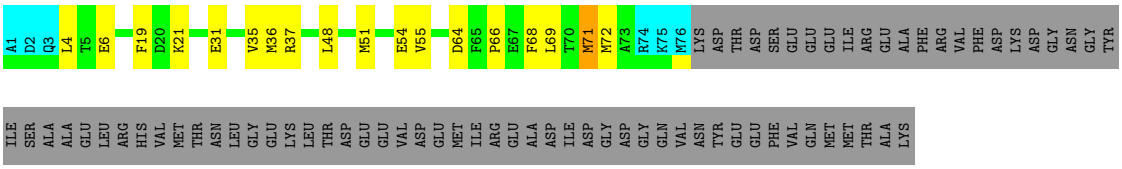
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Calmodulin-1

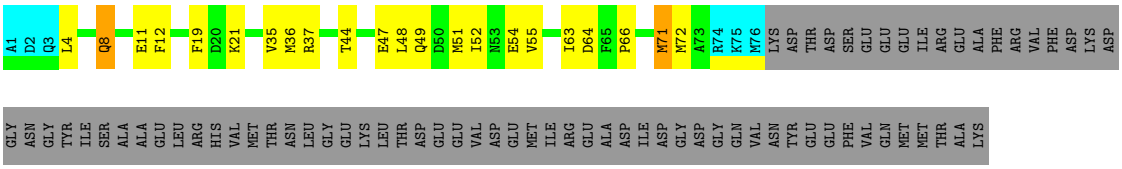
Chain A: 35% 11% • • 49%



4.2.2 Score per residue for model 2

• Molecule 1: Calmodulin-1

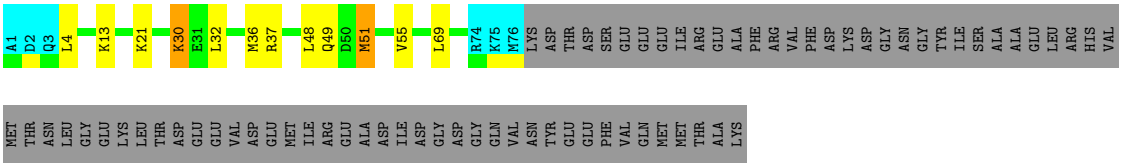
Chain A: 32% 14% • • 49%



4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin-1

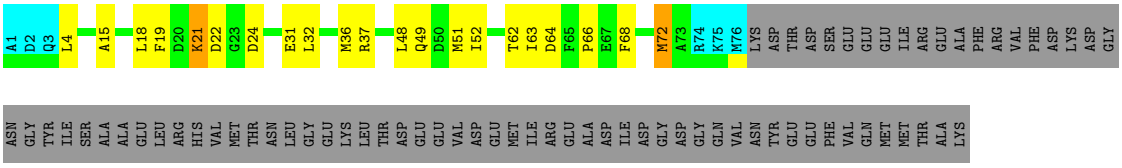
Chain A: 39% 7% • • 49%



4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin-1

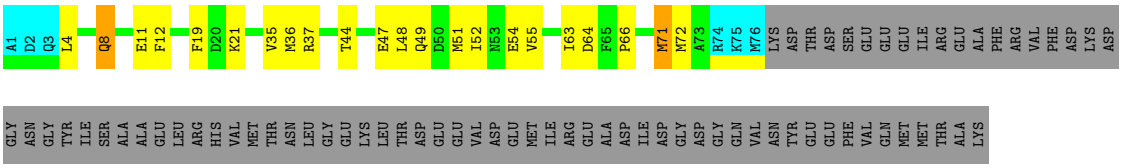
Chain A: 33% 13% • • 49%



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Calmodulin-1

Chain A: 32% 14% • • 49%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, CHARMm22 energy minimization.*

Of the 50 calculated structures, 5 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	**Classification**	**Version**
X-PLOR	geometry optimization	MSI XPLOR 3.843
X-PLOR	refinement	MSI XPLOR 3.843

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	1801
Number of shifts mapped to atoms	923
Number of unparsed shifts	0
Number of shifts with mapping errors	878
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality (i)

6.1 Standard geometry (i)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	538	508	508	12±3
3	A	7	1	0	6±2
All	All	2735	2545	2540	62

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:MET:CE	3:A:149:HLT:BR	1.25	2.40	1	3
1:A:71:MET:SD	3:A:149:HLT:BR	1.13	2.60	1	1
1:A:36:MET:CE	3:A:149:HLT:BR	1.10	2.54	5	4
1:A:71:MET:HE1	3:A:149:HLT:BR	1.07	2.04	1	3
1:A:36:MET:SD	3:A:149:HLT:CL	1.00	2.57	1	1
1:A:36:MET:HE1	3:A:149:HLT:BR	0.98	2.13	5	3
1:A:71:MET:HE2	3:A:149:HLT:BR	0.93	2.16	2	2
1:A:36:MET:SD	3:A:149:HLT:BR	0.82	2.92	5	4
1:A:51:MET:SD	3:A:149:HLT:CL	0.72	2.84	1	1
1:A:71:MET:HE3	3:A:149:HLT:BR	0.60	2.45	1	1
1:A:36:MET:HE1	3:A:149:HLT:F2	0.60	1.86	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:MET:SD	3:A:149:HLT:F2	0.58	2.51	1	1
1:A:36:MET:HE3	3:A:149:HLT:BR	0.58	2.53	2	4
1:A:32:LEU:HD21	3:A:149:HLT:BR	0.57	2.54	3	1
1:A:19:PHE:CD1	1:A:35:VAL:HG22	0.56	2.36	5	3
1:A:54:GLU:HG3	1:A:55:VAL:HG13	0.53	1.81	1	3
1:A:68:PHE:CE1	1:A:72:MET:SD	0.52	3.02	4	1
1:A:36:MET:CE	3:A:149:HLT:F2	0.50	2.49	1	1
1:A:12:PHE:CE1	1:A:72:MET:SD	0.49	3.05	2	2
1:A:64:ASP:CG	1:A:66:PRO:HD2	0.49	2.28	5	4
1:A:15:ALA:HA	1:A:18:LEU:HD12	0.48	1.84	4	1
1:A:51:MET:HB3	3:A:149:HLT:CL	0.47	2.46	3	1
1:A:31:GLU:O	1:A:35:VAL:HG23	0.47	2.10	1	1
1:A:30:LYS:HA	1:A:48:LEU:HD23	0.47	1.85	3	1
1:A:51:MET:O	1:A:55:VAL:HG22	0.46	2.11	1	2
1:A:71:MET:SD	1:A:72:MET:SD	0.44	3.16	1	1
1:A:8:GLN:HA	1:A:11:GLU:OE1	0.43	2.13	2	2
1:A:21:LYS:HE3	1:A:31:GLU:OE2	0.43	2.13	4	1
1:A:44:THR:HB	1:A:47:GLU:OE1	0.42	2.14	2	2
1:A:52:ILE:HG23	1:A:63:ILE:HG12	0.42	1.90	4	3
1:A:22:ASP:OD1	1:A:24:ASP:CG	0.41	2.59	4	1
1:A:19:PHE:CE2	1:A:68:PHE:CE1	0.41	3.08	4	1
1:A:19:PHE:HE2	1:A:68:PHE:CE1	0.40	2.35	1	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/148 (47%)	67±0 (95±1%)	3±0 (5±1%)	0±0 (0±0%)	100	100
All	All	350/740 (47%)	333 (95%)	17 (5%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	59/126 (47%)	51±1 (86±1%)	8±1 (14±1%)	7 47
All	All	295/630 (47%)	255 (86%)	40 (14%)	7 47

All 15 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	4	LEU	5
1	A	21	LYS	5
1	A	37	ARG	5
1	A	48	LEU	4
1	A	49	GLN	4
1	A	51	MET	4
1	A	71	MET	3
1	A	69	LEU	2
1	A	8	GLN	2
1	A	6	GLU	1
1	A	13	LYS	1
1	A	30	LYS	1
1	A	32	LEU	1
1	A	62	THR	1
1	A	72	MET	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
3	HLT	A	149	-	4,6,6	3.06±0.02	1±0 (25±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
3	HLT	A	149	-	3,9,9	1.16±0.00	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HLT	A	149	-	-	0±0,3,6,6	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	149	HLT	BR-C1	5.53	1.78	1.96	3	5

There are no bond-angle outliers.

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 (i)

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1801
Number of shifts mapped to atoms	923
Number of unparsed shifts	0
Number of shifts with mapping errors	878
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- Chemical shift has been reported more than once. All 2 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	UNMAPPED	1	HAL	CA	53.60	0.10	1
1	UNMAPPED	1	HAL	HA	6.30	0.05	1

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

- No matching atom found in the structure. All 878 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	ALA	H	7.77	0.05	1
1	A	77	LYS	H	7.76	0.05	1
1	A	77	LYS	HA	4.2	0.05	1
1	A	77	LYS	HB2	1.74	0.05	2
1	A	77	LYS	HB3	1.74	0.05	2
1	A	77	LYS	HD3	1.55	0.05	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	LYS	HE2	2.9	0.05	1
1	A	77	LYS	HE3	2.9	0.05	1
1	A	77	LYS	HG2	1.38	0.05	2
1	A	77	LYS	HG3	1.38	0.05	2
1	A	77	LYS	CA	57.0	0.10	1
1	A	77	LYS	CB	32.9	0.10	1
1	A	77	LYS	CD	29.0	0.10	1
1	A	77	LYS	CE	42.0	0.10	1
1	A	77	LYS	CG	24.6	0.10	1
1	A	77	LYS	N	120.68	0.10	1
1	A	78	ASP	H	8.22	0.05	1
1	A	78	ASP	HA	4.56	0.05	1
1	A	78	ASP	HB2	2.67	0.05	2
1	A	78	ASP	HB3	2.56	0.05	2
1	A	78	ASP	C	176.68	0.10	1
1	A	78	ASP	CA	55.0	0.10	1
1	A	78	ASP	CB	41.0	0.10	1
1	A	78	ASP	N	121.8	0.10	1
1	A	79	THR	H	8.05	0.05	1
1	A	79	THR	HA	4.19	0.05	1
1	A	79	THR	HB	4.17	0.05	1
1	A	79	THR	HG21	1.11	0.05	1
1	A	79	THR	HG22	1.11	0.05	1
1	A	79	THR	HG23	1.11	0.05	1
1	A	79	THR	CA	62.5	0.10	1
1	A	79	THR	CB	69.9	0.10	1
1	A	79	THR	CG2	21.6	0.10	1
1	A	79	THR	N	114.79	0.10	1
1	A	80	ASP	H	8.36	0.05	1
1	A	80	ASP	HA	4.56	0.05	1
1	A	80	ASP	HB2	2.46	0.05	2
1	A	80	ASP	HB3	2.58	0.05	2
1	A	80	ASP	C	176.76	0.10	1
1	A	80	ASP	CA	55.2	0.10	1
1	A	80	ASP	CB	41.3	0.10	1
1	A	80	ASP	N	123.22	0.10	1
1	A	81	SER	H	8.36	0.05	1
1	A	81	SER	HA	4.33	0.05	1
1	A	81	SER	HB2	3.86	0.05	2
1	A	81	SER	HB3	3.97	0.05	2
1	A	81	SER	C	174.7	0.10	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	SER	CA	59.3	0.10	1
1	A	81	SER	CB	63.8	0.10	1
1	A	81	SER	N	117.15	0.10	1
1	A	82	GLU	H	8.4	0.05	1
1	A	82	GLU	HA	4.06	0.05	1
1	A	82	GLU	HB2	2.02	0.05	2
1	A	82	GLU	HB3	2.26	0.05	2
1	A	82	GLU	HG2	2.3	0.05	2
1	A	82	GLU	HG3	2.3	0.05	2
1	A	82	GLU	C	176.84	0.10	1
1	A	82	GLU	CA	58.6	0.10	1
1	A	82	GLU	CB	29.5	0.10	1
1	A	82	GLU	CG	36.2	0.10	1
1	A	82	GLU	N	122.46	0.10	1
1	A	83	GLU	H	8.23	0.05	1
1	A	83	GLU	HA	3.96	0.05	1
1	A	83	GLU	HB2	1.83	0.05	2
1	A	83	GLU	HB3	1.99	0.05	2
1	A	83	GLU	HG2	2.2	0.05	2
1	A	83	GLU	HG3	2.27	0.05	2
1	A	83	GLU	C	175.47	0.10	1
1	A	83	GLU	CA	59.7	0.10	1
1	A	83	GLU	CB	29.4	0.10	1
1	A	83	GLU	CG	37.0	0.10	1
1	A	83	GLU	N	119.5	0.10	1
1	A	84	GLU	H	8.05	0.05	1
1	A	84	GLU	HA	4.04	0.05	1
1	A	84	GLU	HB2	2.23	0.05	2
1	A	84	GLU	HB3	1.84	0.05	2
1	A	84	GLU	HG2	2.2	0.05	2
1	A	84	GLU	HG3	2.24	0.05	2
1	A	84	GLU	C	175.12	0.10	1
1	A	84	GLU	CA	59.4	0.10	1
1	A	84	GLU	CB	30.3	0.10	1
1	A	84	GLU	CG	36.8	0.10	1
1	A	84	GLU	N	118.9	0.10	1
1	A	85	ILE	H	7.94	0.05	1
1	A	85	ILE	HA	3.96	0.05	1
1	A	85	ILE	HB	2.09	0.05	1
1	A	85	ILE	HD11	0.7	0.05	1
1	A	85	ILE	HD12	0.7	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	ILE	HD13	0.7	0.05	1
1	A	85	ILE	HG12	1.01	0.05	1
1	A	85	ILE	HG13	1.71	0.05	1
1	A	85	ILE	HG21	1.03	0.05	1
1	A	85	ILE	HG22	1.03	0.05	1
1	A	85	ILE	HG23	1.03	0.05	1
1	A	85	ILE	C	178.68	0.10	1
1	A	85	ILE	CA	64.7	0.10	1
1	A	85	ILE	CB	37.3	0.10	1
1	A	85	ILE	CD1	13.2	0.10	1
1	A	85	ILE	CG1	29.2	0.10	1
1	A	85	ILE	CG2	19.2	0.10	1
1	A	85	ILE	N	122.02	0.10	1
1	A	86	ARG	H	8.33	0.05	1
1	A	86	ARG	HA	4.03	0.05	1
1	A	86	ARG	HB2	1.75	0.05	2
1	A	86	ARG	HB3	1.76	0.05	2
1	A	86	ARG	HD2	2.87	0.05	2
1	A	86	ARG	HD3	2.86	0.05	2
1	A	86	ARG	HG2	1.63	0.05	2
1	A	86	ARG	HG3	1.47	0.05	2
1	A	86	ARG	C	179.65	0.10	1
1	A	86	ARG	CA	60.0	0.10	1
1	A	86	ARG	CB	29.8	0.10	1
1	A	86	ARG	CD	43.1	0.10	1
1	A	86	ARG	CG	27.6	0.10	1
1	A	86	ARG	N	121.7	0.10	1
1	A	87	GLU	H	8.06	0.05	1
1	A	87	GLU	HA	4.04	0.05	1
1	A	87	GLU	HB2	1.97	0.05	2
1	A	87	GLU	HB3	2.01	0.05	2
1	A	87	GLU	HG2	2.24	0.05	2
1	A	87	GLU	HG3	2.24	0.05	2
1	A	87	GLU	C	177.93	0.10	1
1	A	87	GLU	CA	59.06	0.10	1
1	A	87	GLU	CB	29.5	0.10	1
1	A	87	GLU	CG	36.5	0.10	1
1	A	87	GLU	N	118.5	0.10	1
1	A	88	ALA	H	7.86	0.05	1
1	A	88	ALA	HA	4.11	0.05	1
1	A	88	ALA	HB1	1.7	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	ALA	HB2	1.7	0.05	1
1	A	88	ALA	HB3	1.7	0.05	1
1	A	88	ALA	C	179.34	0.10	1
1	A	88	ALA	CA	55.1	0.10	1
1	A	88	ALA	CB	17.63	0.10	1
1	A	88	ALA	N	121.84	0.10	1
1	A	89	PHE	H	8.44	0.05	1
1	A	89	PHE	HA	3.04	0.05	1
1	A	89	PHE	HB2	3.13	0.05	2
1	A	89	PHE	HB3	2.9	0.05	2
1	A	89	PHE	HD1	7.16	0.05	1
1	A	89	PHE	HD2	7.16	0.05	1
1	A	89	PHE	HE1	6.5	0.05	1
1	A	89	PHE	HE2	6.5	0.05	1
1	A	89	PHE	HZ	6.9	0.05	1
1	A	89	PHE	C	178.64	0.10	1
1	A	89	PHE	CA	62.09	0.10	1
1	A	89	PHE	CB	39.25	0.10	1
1	A	89	PHE	CD1	131.4	0.10	1
1	A	89	PHE	CD2	131.4	0.10	1
1	A	89	PHE	CE1	131.3	0.10	1
1	A	89	PHE	CE2	131.3	0.10	1
1	A	89	PHE	CZ	131.5	0.10	1
1	A	89	PHE	N	119.0	0.10	1
1	A	90	ARG	H	7.63	0.05	1
1	A	90	ARG	HA	3.77	0.05	1
1	A	90	ARG	HB2	1.84	0.05	2
1	A	90	ARG	HB3	1.84	0.05	2
1	A	90	ARG	HD2	3.12	0.05	2
1	A	90	ARG	HD3	3.12	0.05	2
1	A	90	ARG	HG2	1.56	0.05	2
1	A	90	ARG	HG3	1.56	0.05	2
1	A	90	ARG	C	179.31	0.10	1
1	A	90	ARG	CA	58.9	0.10	1
1	A	90	ARG	CB	30.3	0.10	1
1	A	90	ARG	CD	43.53	0.10	1
1	A	90	ARG	CG	27.9	0.10	1
1	A	90	ARG	N	115.76	0.10	1
1	A	91	VAL	H	7.38	0.05	1
1	A	91	VAL	HA	3.37	0.05	1
1	A	91	VAL	HB	2.04	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	VAL	HG11	0.91	0.05	1
1	A	91	VAL	HG12	0.91	0.05	1
1	A	91	VAL	HG13	0.91	0.05	1
1	A	91	VAL	HG21	0.53	0.05	1
1	A	91	VAL	HG22	0.53	0.05	1
1	A	91	VAL	HG23	0.53	0.05	1
1	A	91	VAL	C	176.6	0.10	1
1	A	91	VAL	CA	65.7	0.10	1
1	A	91	VAL	CB	31.5	0.10	1
1	A	91	VAL	CG1	22.8	0.10	1
1	A	91	VAL	CG2	21.0	0.10	1
1	A	91	VAL	N	118.21	0.10	1
1	A	92	PHE	H	7.28	0.05	1
1	A	92	PHE	HA	4.12	0.05	1
1	A	92	PHE	HB2	2.58	0.05	2
1	A	92	PHE	HB3	3.3	0.05	2
1	A	92	PHE	HD1	7.12	0.05	1
1	A	92	PHE	HD2	7.12	0.05	1
1	A	92	PHE	HE1	6.95	0.05	1
1	A	92	PHE	HE2	6.95	0.05	1
1	A	92	PHE	HZ	7.09	0.05	1
1	A	92	PHE	C	178.12	0.10	1
1	A	92	PHE	CA	60.06	0.10	1
1	A	92	PHE	CB	40.5	0.10	1
1	A	92	PHE	CD1	130.3	0.10	1
1	A	92	PHE	CD2	130.3	0.10	1
1	A	92	PHE	CE1	129.5	0.10	1
1	A	92	PHE	CE2	129.5	0.10	1
1	A	92	PHE	CZ	130.1	0.10	1
1	A	92	PHE	N	116.0	0.10	1
1	A	93	ASP	H	7.75	0.05	1
1	A	93	ASP	HA	4.44	0.05	1
1	A	93	ASP	HB2	2.2	0.05	2
1	A	93	ASP	HB3	1.28	0.05	2
1	A	93	ASP	C	177.27	0.10	1
1	A	93	ASP	CA	52.33	0.10	1
1	A	93	ASP	CB	38.4	0.10	1
1	A	93	ASP	N	116.8	0.10	1
1	A	94	LYS	H	7.64	0.05	1
1	A	94	LYS	HA	3.81	0.05	1
1	A	94	LYS	HB2	1.75	0.05	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	LYS	HB3	1.75	0.05	2
1	A	94	LYS	HD2	1.53	0.05	2
1	A	94	LYS	HD3	1.54	0.05	2
1	A	94	LYS	HE2	2.76	0.05	1
1	A	94	LYS	HE3	2.72	0.05	1
1	A	94	LYS	HG2	1.43	0.05	2
1	A	94	LYS	HG3	1.34	0.05	2
1	A	94	LYS	C	177.03	0.10	1
1	A	94	LYS	CA	59.09	0.10	1
1	A	94	LYS	CB	32.6	0.10	1
1	A	94	LYS	CD	28.6	0.10	1
1	A	94	LYS	CE	41.8	0.10	1
1	A	94	LYS	CG	24.25	0.10	1
1	A	94	LYS	N	125.83	0.10	1
1	A	95	ASP	H	8.09	0.05	1
1	A	95	ASP	HA	4.46	0.05	1
1	A	95	ASP	HB2	2.56	0.05	2
1	A	95	ASP	HB3	2.98	0.05	2
1	A	95	ASP	C	177.55	0.10	1
1	A	95	ASP	CA	52.7	0.10	1
1	A	95	ASP	CB	39.65	0.10	1
1	A	95	ASP	N	114.02	0.10	1
1	A	96	GLY	H	7.69	0.05	1
1	A	96	GLY	HA2	3.72	0.05	1
1	A	96	GLY	HA3	3.75	0.05	1
1	A	96	GLY	C	178.32	0.10	1
1	A	96	GLY	CA	47.2	0.10	1
1	A	96	GLY	N	109.3	0.10	1
1	A	97	ASN	H	8.23	0.05	1
1	A	97	ASN	HA	4.54	0.05	1
1	A	97	ASN	HB2	2.57	0.05	2
1	A	97	ASN	HB3	3.31	0.05	2
1	A	97	ASN	HD21	7.99	0.05	2
1	A	97	ASN	HD22	7.3	0.05	2
1	A	97	ASN	CA	52.7	0.10	1
1	A	97	ASN	CB	38.1	0.10	1
1	A	97	ASN	N	119.6	0.10	1
1	A	97	ASN	ND2	116.4	0.10	1
1	A	98	GLY	H	10.55	0.05	1
1	A	98	GLY	HA2	3.32	0.05	1
1	A	98	GLY	HA3	3.93	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	GLY	C	177.94	0.10	1
1	A	98	GLY	CA	45.2	0.10	1
1	A	98	GLY	N	112.9	0.10	1
1	A	99	TYR	H	7.53	0.05	1
1	A	99	TYR	HA	4.96	0.05	1
1	A	99	TYR	HB2	2.4	0.05	2
1	A	99	TYR	HB3	2.4	0.05	2
1	A	99	TYR	HD1	6.64	0.05	1
1	A	99	TYR	HD2	6.64	0.05	1
1	A	99	TYR	HE1	6.8	0.05	1
1	A	99	TYR	HE2	6.8	0.05	1
1	A	99	TYR	C	176.13	0.10	1
1	A	99	TYR	CA	56.0	0.10	1
1	A	99	TYR	CB	43.0	0.10	1
1	A	99	TYR	CD1	133.4	0.10	1
1	A	99	TYR	CD2	133.4	0.10	1
1	A	99	TYR	CE1	118.3	0.10	1
1	A	99	TYR	CE2	118.3	0.10	1
1	A	99	TYR	N	115.89	0.10	1
1	A	100	ILE	H	10.04	0.05	1
1	A	100	ILE	HA	4.68	0.05	1
1	A	100	ILE	HB	1.76	0.05	1
1	A	100	ILE	HD11	0.23	0.05	1
1	A	100	ILE	HD12	0.23	0.05	1
1	A	100	ILE	HD13	0.23	0.05	1
1	A	100	ILE	HG12	0.22	0.05	1
1	A	100	ILE	HG13	1.12	0.05	1
1	A	100	ILE	HG21	0.83	0.05	1
1	A	100	ILE	HG22	0.83	0.05	1
1	A	100	ILE	HG23	0.83	0.05	1
1	A	100	ILE	C	172.47	0.10	1
1	A	100	ILE	CA	60.5	0.10	1
1	A	100	ILE	CB	38.8	0.10	1
1	A	100	ILE	CD1	15.4	0.10	1
1	A	100	ILE	CG1	27.0	0.10	1
1	A	100	ILE	CG2	17.6	0.10	1
1	A	100	ILE	N	127.36	0.10	1
1	A	101	SER	H	8.85	0.05	1
1	A	101	SER	HA	4.73	0.05	1
1	A	101	SER	HB2	4.33	0.05	2
1	A	101	SER	HB3	3.85	0.05	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	SER	C	174.58	0.10	1
1	A	101	SER	CA	56.0	0.10	1
1	A	101	SER	CB	66.7	0.10	1
1	A	101	SER	N	123.7	0.10	1
1	A	102	ALA	H	9.12	0.05	1
1	A	102	ALA	HA	3.83	0.05	1
1	A	102	ALA	HB1	1.37	0.05	1
1	A	102	ALA	HB2	1.37	0.05	1
1	A	102	ALA	HB3	1.37	0.05	1
1	A	102	ALA	C	175.55	0.10	1
1	A	102	ALA	CA	55.97	0.10	1
1	A	102	ALA	CB	18.0	0.10	1
1	A	102	ALA	N	122.87	0.10	1
1	A	103	ALA	H	8.17	0.05	1
1	A	103	ALA	HA	3.97	0.05	1
1	A	103	ALA	HB1	1.33	0.05	1
1	A	103	ALA	HB2	1.33	0.05	1
1	A	103	ALA	HB3	1.33	0.05	1
1	A	103	ALA	C	175.24	0.10	1
1	A	103	ALA	CA	55.28	0.10	1
1	A	103	ALA	CB	18.5	0.10	1
1	A	103	ALA	N	118.45	0.10	1
1	A	104	GLU	H	7.8	0.05	1
1	A	104	GLU	HA	3.94	0.05	1
1	A	104	GLU	HB2	1.98	0.05	2
1	A	104	GLU	HB3	2.23	0.05	2
1	A	104	GLU	HG2	2.2	0.05	2
1	A	104	GLU	HG3	2.2	0.05	2
1	A	104	GLU	C	179.34	0.10	1
1	A	104	GLU	CA	59.3	0.10	1
1	A	104	GLU	CB	29.18	0.10	1
1	A	104	GLU	CG	36.3	0.10	1
1	A	104	GLU	N	120.0	0.10	1
1	A	105	LEU	H	8.5	0.05	1
1	A	105	LEU	HA	4.05	0.05	1
1	A	105	LEU	HB2	1.83	0.05	2
1	A	105	LEU	HB3	1.43	0.05	2
1	A	105	LEU	HD11	0.85	0.05	1
1	A	105	LEU	HD12	0.85	0.05	1
1	A	105	LEU	HD13	0.85	0.05	1
1	A	105	LEU	HD21	0.87	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	105	LEU	HD22	0.87	0.05	1
1	A	105	LEU	HD23	0.87	0.05	1
1	A	105	LEU	HG	1.53	0.05	1
1	A	105	LEU	C	181.48	0.10	1
1	A	105	LEU	CA	58.3	0.10	1
1	A	105	LEU	CB	42.0	0.10	1
1	A	105	LEU	CD1	26.3	0.10	1
1	A	105	LEU	CD2	24.4	0.10	1
1	A	105	LEU	CG	26.0	0.10	1
1	A	105	LEU	N	121.07	0.10	1
1	A	106	ARG	H	8.54	0.05	1
1	A	106	ARG	HA	3.71	0.05	1
1	A	106	ARG	HB2	1.86	0.05	2
1	A	106	ARG	HB3	1.86	0.05	2
1	A	106	ARG	HD2	3.13	0.05	2
1	A	106	ARG	HD3	3.04	0.05	2
1	A	106	ARG	HG2	1.53	0.05	2
1	A	106	ARG	HG3	1.53	0.05	2
1	A	106	ARG	C	179.3	0.10	1
1	A	106	ARG	CA	59.99	0.10	1
1	A	106	ARG	CB	30.2	0.10	1
1	A	106	ARG	CD	44.0	0.10	1
1	A	106	ARG	CG	27.7	0.10	1
1	A	106	ARG	N	117.73	0.10	1
1	A	107	HIS	H	7.83	0.05	1
1	A	107	HIS	HA	4.22	0.05	1
1	A	107	HIS	HB2	3.25	0.05	2
1	A	107	HIS	HB3	3.16	0.05	2
1	A	107	HIS	HD1	6.38	0.05	1
1	A	107	HIS	HD2	6.96	0.05	1
1	A	107	HIS	HE1	7.69	0.05	1
1	A	107	HIS	C	177.97	0.10	1
1	A	107	HIS	CA	59.7	0.10	1
1	A	107	HIS	CB	30.8	0.10	1
1	A	107	HIS	CD2	120.4	0.10	1
1	A	107	HIS	CE1	120.0	0.10	1
1	A	107	HIS	N	118.4	0.10	1
1	A	108	VAL	H	7.88	0.05	1
1	A	108	VAL	HA	3.4	0.05	1
1	A	108	VAL	HB	1.92	0.05	1
1	A	108	VAL	HG11	0.35	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	VAL	HG12	0.35	0.05	1
1	A	108	VAL	HG13	0.35	0.05	1
1	A	108	VAL	HG21	0.78	0.05	1
1	A	108	VAL	HG22	0.78	0.05	1
1	A	108	VAL	HG23	0.78	0.05	1
1	A	108	VAL	CA	66.3	0.10	1
1	A	108	VAL	CB	31.9	0.10	1
1	A	108	VAL	CG1	20.8	0.10	1
1	A	108	VAL	CG2	23.3	0.10	1
1	A	108	VAL	N	118.87	0.10	1
1	A	109	MET	H	8.21	0.05	1
1	A	109	MET	HA	4.22	0.05	1
1	A	109	MET	HB2	2.1	0.05	2
1	A	109	MET	HB3	2.01	0.05	2
1	A	109	MET	HE1	1.95	0.05	1
1	A	109	MET	HE2	1.95	0.05	1
1	A	109	MET	HE3	1.95	0.05	1
1	A	109	MET	HG2	2.68	0.05	2
1	A	109	MET	HG3	2.52	0.05	2
1	A	109	MET	CA	57.7	0.10	1
1	A	109	MET	CB	31.1	0.10	1
1	A	109	MET	CE	17.5	0.10	1
1	A	109	MET	CG	33.1	0.10	1
1	A	109	MET	N	116.22	0.10	1
1	A	110	THR	H	8.11	0.05	1
1	A	110	THR	HA	4.05	0.05	1
1	A	110	THR	HB	4.2	0.05	1
1	A	110	THR	HG21	1.14	0.05	1
1	A	110	THR	HG22	1.14	0.05	1
1	A	110	THR	HG23	1.14	0.05	1
1	A	110	THR	C	178.18	0.10	1
1	A	110	THR	CA	66.02	0.10	1
1	A	110	THR	CB	68.8	0.10	1
1	A	110	THR	CG2	21.5	0.10	1
1	A	110	THR	N	115.32	0.10	1
1	A	111	ASN	H	7.78	0.05	1
1	A	111	ASN	HA	4.39	0.05	1
1	A	111	ASN	HB2	2.69	0.05	2
1	A	111	ASN	HB3	2.7	0.05	2
1	A	111	ASN	HD21	6.4	0.05	2
1	A	111	ASN	HD22	7.3	0.05	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	ASN	CA	55.5	0.10	1
1	A	111	ASN	CB	38.1	0.10	1
1	A	111	ASN	N	122.24	0.10	1
1	A	111	ASN	ND2	111.4	0.10	1
1	A	112	LEU	H	7.83	0.05	1
1	A	112	LEU	HA	4.25	0.05	1
1	A	112	LEU	HB2	1.79	0.05	2
1	A	112	LEU	HB3	1.61	0.05	2
1	A	112	LEU	HD11	0.72	0.05	1
1	A	112	LEU	HD12	0.72	0.05	1
1	A	112	LEU	HD13	0.72	0.05	1
1	A	112	LEU	HD21	0.76	0.05	1
1	A	112	LEU	HD22	0.76	0.05	1
1	A	112	LEU	HD23	0.76	0.05	1
1	A	112	LEU	HG	1.7	0.05	1
1	A	112	LEU	C	177.74	0.10	1
1	A	112	LEU	CA	55.36	0.10	1
1	A	112	LEU	CB	42.1	0.10	1
1	A	112	LEU	CD1	22.7	0.10	1
1	A	112	LEU	CD2	25.8	0.10	1
1	A	112	LEU	CG	26.6	0.10	1
1	A	112	LEU	N	119.16	0.10	1
1	A	113	GLY	H	7.74	0.05	1
1	A	113	GLY	HA2	3.64	0.05	1
1	A	113	GLY	HA3	4.13	0.05	1
1	A	113	GLY	C	178.72	0.10	1
1	A	113	GLY	CA	45.5	0.10	1
1	A	113	GLY	N	106.48	0.10	1
1	A	114	GLU	H	7.86	0.05	1
1	A	114	GLU	HA	4.33	0.05	1
1	A	114	GLU	HB2	1.63	0.05	2
1	A	114	GLU	HB3	1.85	0.05	2
1	A	114	GLU	HG2	2.0	0.05	2
1	A	114	GLU	HG3	2.12	0.05	2
1	A	114	GLU	C	177.23	0.10	1
1	A	114	GLU	CA	55.28	0.10	1
1	A	114	GLU	CB	30.62	0.10	1
1	A	114	GLU	CG	35.5	0.10	1
1	A	114	GLU	N	120.54	0.10	1
1	A	115	LYS	H	8.48	0.05	1
1	A	115	LYS	HA	4.28	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	115	LYS	HB2	1.6	0.05	2
1	A	115	LYS	HB3	1.68	0.05	2
1	A	115	LYS	HD2	1.39	0.05	2
1	A	115	LYS	HD3	1.56	0.05	2
1	A	115	LYS	HE2	2.84	0.05	1
1	A	115	LYS	HE3	2.88	0.05	1
1	A	115	LYS	HG2	1.22	0.05	2
1	A	115	LYS	HG3	1.3	0.05	2
1	A	115	LYS	C	174.38	0.10	1
1	A	115	LYS	CA	55.7	0.10	1
1	A	115	LYS	CB	32.1	0.10	1
1	A	115	LYS	CD	29.2	0.10	1
1	A	115	LYS	CE	42.2	0.10	1
1	A	115	LYS	CG	24.6	0.10	1
1	A	115	LYS	N	124.13	0.10	1
1	A	116	LEU	H	8.07	0.05	1
1	A	116	LEU	HA	4.68	0.05	1
1	A	116	LEU	HB2	1.49	0.05	2
1	A	116	LEU	HB3	1.38	0.05	2
1	A	116	LEU	HD11	0.7	0.05	1
1	A	116	LEU	HD12	0.7	0.05	1
1	A	116	LEU	HD13	0.7	0.05	1
1	A	116	LEU	HD21	0.72	0.05	1
1	A	116	LEU	HD22	0.72	0.05	1
1	A	116	LEU	HD23	0.72	0.05	1
1	A	116	LEU	HG	1.47	0.05	1
1	A	116	LEU	C	175.43	0.10	1
1	A	116	LEU	CA	54.0	0.10	1
1	A	116	LEU	CB	44.8	0.10	1
1	A	116	LEU	CD1	24.0	0.10	1
1	A	116	LEU	CD2	27.0	0.10	1
1	A	116	LEU	CG	27.6	0.10	1
1	A	116	LEU	N	125.02	0.10	1
1	A	117	THR	H	9.14	0.05	1
1	A	117	THR	HA	4.35	0.05	1
1	A	117	THR	HB	4.66	0.05	1
1	A	117	THR	HG21	1.24	0.05	1
1	A	117	THR	HG22	1.24	0.05	1
1	A	117	THR	HG23	1.24	0.05	1
1	A	117	THR	C	175.7	0.10	1
1	A	117	THR	CA	60.74	0.10	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	117	THR	CB	71.2	0.10	1
1	A	117	THR	CG2	21.8	0.10	1
1	A	117	THR	N	114.59	0.10	1
1	A	118	ASP	H	8.83	0.05	1
1	A	118	ASP	HA	4.11	0.05	1
1	A	118	ASP	HB2	2.66	0.05	2
1	A	118	ASP	HB3	2.49	0.05	2
1	A	118	ASP	C	178.09	0.10	1
1	A	118	ASP	CA	58.1	0.10	1
1	A	118	ASP	CB	39.8	0.10	1
1	A	118	ASP	N	120.99	0.10	1
1	A	119	GLU	H	8.57	0.05	1
1	A	119	GLU	HA	3.96	0.05	1
1	A	119	GLU	HB2	1.83	0.05	2
1	A	119	GLU	HB3	1.96	0.05	2
1	A	119	GLU	HG2	2.2	0.05	2
1	A	119	GLU	HG3	2.2	0.05	2
1	A	119	GLU	C	175.51	0.10	1
1	A	119	GLU	CA	59.8	0.10	1
1	A	119	GLU	CB	29.0	0.10	1
1	A	119	GLU	CG	36.3	0.10	1
1	A	119	GLU	N	119.1	0.10	1
1	A	120	GLU	H	7.68	0.05	1
1	A	120	GLU	HA	4.0	0.05	1
1	A	120	GLU	HB2	2.33	0.05	2
1	A	120	GLU	HB3	1.82	0.05	2
1	A	120	GLU	HG2	2.2	0.05	2
1	A	120	GLU	HG3	2.31	0.05	2
1	A	120	GLU	C	178.63	0.10	1
1	A	120	GLU	CA	59.35	0.10	1
1	A	120	GLU	CB	30.55	0.10	1
1	A	120	GLU	CG	36.3	0.10	1
1	A	120	GLU	N	120.52	0.10	1
1	A	121	VAL	H	8.01	0.05	1
1	A	121	VAL	HA	3.5	0.05	1
1	A	121	VAL	HB	2.13	0.05	1
1	A	121	VAL	HG11	0.93	0.05	1
1	A	121	VAL	HG12	0.93	0.05	1
1	A	121	VAL	HG13	0.93	0.05	1
1	A	121	VAL	HG21	0.87	0.05	1
1	A	121	VAL	HG22	0.87	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	121	VAL	HG23	0.87	0.05	1
1	A	121	VAL	CA	67.0	0.10	1
1	A	121	VAL	CB	31.5	0.10	1
1	A	121	VAL	CG1	22.3	0.10	1
1	A	121	VAL	CG2	23.9	0.10	1
1	A	121	VAL	N	121.2	0.10	1
1	A	122	ASP	H	7.96	0.05	1
1	A	122	ASP	HA	4.23	0.05	1
1	A	122	ASP	HB2	2.53	0.05	2
1	A	122	ASP	HB3	2.67	0.05	2
1	A	122	ASP	C	180.16	0.10	1
1	A	122	ASP	CA	57.6	0.10	1
1	A	122	ASP	CB	40.3	0.10	1
1	A	122	ASP	N	119.53	0.10	1
1	A	123	GLU	H	7.92	0.05	1
1	A	123	GLU	HA	3.88	0.05	1
1	A	123	GLU	HB2	1.93	0.05	2
1	A	123	GLU	HB3	2.2	0.05	2
1	A	123	GLU	HG2	2.2	0.05	2
1	A	123	GLU	HG3	2.2	0.05	2
1	A	123	GLU	C	177.3	0.10	1
1	A	123	GLU	CA	59.29	0.10	1
1	A	123	GLU	CB	29.4	0.10	1
1	A	123	GLU	CG	36.2	0.10	1
1	A	123	GLU	N	119.47	0.10	1
1	A	124	MET	H	7.69	0.05	1
1	A	124	MET	HA	3.96	0.05	1
1	A	124	MET	HB2	2.19	0.05	2
1	A	124	MET	HB3	1.96	0.05	2
1	A	124	MET	HE1	1.96	0.05	1
1	A	124	MET	HE2	1.96	0.05	1
1	A	124	MET	HE3	1.96	0.05	1
1	A	124	MET	HG2	2.39	0.05	2
1	A	124	MET	HG3	2.68	0.05	2
1	A	124	MET	C	179.26	0.10	1
1	A	124	MET	CA	59.3	0.10	1
1	A	124	MET	CB	33.1	0.10	1
1	A	124	MET	CE	17.33	0.10	1
1	A	124	MET	CG	31.6	0.10	1
1	A	124	MET	N	119.5	0.10	1
1	A	125	ILE	H	7.83	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	ILE	HA	3.4	0.05	1
1	A	125	ILE	HB	2.02	0.05	1
1	A	125	ILE	HD11	0.61	0.05	1
1	A	125	ILE	HD12	0.61	0.05	1
1	A	125	ILE	HD13	0.61	0.05	1
1	A	125	ILE	HG12	1.22	0.05	1
1	A	125	ILE	HG13	1.43	0.05	1
1	A	125	ILE	HG21	0.61	0.05	1
1	A	125	ILE	HG22	0.61	0.05	1
1	A	125	ILE	HG23	0.61	0.05	1
1	A	125	ILE	C	178.09	0.10	1
1	A	125	ILE	CA	63.78	0.10	1
1	A	125	ILE	CB	36.4	0.10	1
1	A	125	ILE	CD1	10.7	0.10	1
1	A	125	ILE	CG1	28.3	0.10	1
1	A	125	ILE	CG2	16.1	0.10	1
1	A	125	ILE	N	118.29	0.10	1
1	A	126	ARG	H	8.13	0.05	1
1	A	126	ARG	HA	3.89	0.05	1
1	A	126	ARG	HB2	1.83	0.05	2
1	A	126	ARG	HB3	1.75	0.05	2
1	A	126	ARG	HD2	3.12	0.05	2
1	A	126	ARG	HD3	3.12	0.05	2
1	A	126	ARG	HG2	1.53	0.05	2
1	A	126	ARG	HG3	1.67	0.05	2
1	A	126	ARG	C	179.3	0.10	1
1	A	126	ARG	CA	59.7	0.10	1
1	A	126	ARG	CB	30.1	0.10	1
1	A	126	ARG	CD	43.43	0.10	1
1	A	126	ARG	CG	27.75	0.10	1
1	A	126	ARG	N	118.27	0.10	1
1	A	127	GLU	H	7.78	0.05	1
1	A	127	GLU	HA	3.88	0.05	1
1	A	127	GLU	HB2	1.61	0.05	2
1	A	127	GLU	HB3	1.94	0.05	2
1	A	127	GLU	HG2	2.26	0.05	2
1	A	127	GLU	HG3	2.26	0.05	2
1	A	127	GLU	C	177.23	0.10	1
1	A	127	GLU	CA	58.63	0.10	1
1	A	127	GLU	CB	29.5	0.10	1
1	A	127	GLU	CG	36.4	0.10	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	GLU	N	116.13	0.10	1
1	A	128	ALA	H	7.19	0.05	1
1	A	128	ALA	HA	4.34	0.05	1
1	A	128	ALA	HB1	1.33	0.05	1
1	A	128	ALA	HB2	1.33	0.05	1
1	A	128	ALA	HB3	1.33	0.05	1
1	A	128	ALA	C	179.34	0.10	1
1	A	128	ALA	CA	52.1	0.10	1
1	A	128	ALA	CB	21.45	0.10	1
1	A	128	ALA	N	118.71	0.10	1
1	A	129	ASP	H	7.8	0.05	1
1	A	129	ASP	HA	4.38	0.05	1
1	A	129	ASP	HB2	2.39	0.05	2
1	A	129	ASP	HB3	2.7	0.05	2
1	A	129	ASP	C	177.31	0.10	1
1	A	129	ASP	CA	54.12	0.10	1
1	A	129	ASP	CB	40.4	0.10	1
1	A	129	ASP	N	117.54	0.10	1
1	A	130	ILE	H	8.22	0.05	1
1	A	130	ILE	HA	3.79	0.05	1
1	A	130	ILE	HB	1.9	0.05	1
1	A	130	ILE	HD11	0.79	0.05	1
1	A	130	ILE	HD12	0.79	0.05	1
1	A	130	ILE	HD13	0.79	0.05	1
1	A	130	ILE	HG12	1.22	0.05	1
1	A	130	ILE	HG13	1.59	0.05	1
1	A	130	ILE	HG21	0.84	0.05	1
1	A	130	ILE	HG22	0.84	0.05	1
1	A	130	ILE	HG23	0.84	0.05	1
1	A	130	ILE	C	177.9	0.10	1
1	A	130	ILE	CA	63.4	0.10	1
1	A	130	ILE	CB	38.6	0.10	1
1	A	130	ILE	CD1	12.3	0.10	1
1	A	130	ILE	CG1	28.0	0.10	1
1	A	130	ILE	CG2	17.4	0.10	1
1	A	130	ILE	N	127.84	0.10	1
1	A	131	ASP	H	8.22	0.05	1
1	A	131	ASP	HA	4.44	0.05	1
1	A	131	ASP	HB2	2.98	0.05	2
1	A	131	ASP	HB3	2.55	0.05	2
1	A	131	ASP	C	176.06	0.10	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	ASP	CA	53.9	0.10	1
1	A	131	ASP	CB	39.7	0.10	1
1	A	131	ASP	N	116.53	0.10	1
1	A	132	GLY	H	7.51	0.05	1
1	A	132	GLY	HA2	3.88	0.05	1
1	A	132	GLY	HA3	3.72	0.05	1
1	A	132	GLY	C	177.97	0.10	1
1	A	132	GLY	CA	47.55	0.10	1
1	A	132	GLY	N	108.56	0.10	1
1	A	133	ASP	H	8.24	0.05	1
1	A	133	ASP	HA	4.37	0.05	1
1	A	133	ASP	HB2	2.4	0.05	2
1	A	133	ASP	HB3	2.88	0.05	2
1	A	133	ASP	C	178.32	0.10	1
1	A	133	ASP	CA	53.8	0.10	1
1	A	133	ASP	CB	40.25	0.10	1
1	A	133	ASP	N	120.81	0.10	1
1	A	134	GLY	H	10.27	0.05	1
1	A	134	GLY	HA2	3.94	0.05	1
1	A	134	GLY	HA3	3.32	0.05	1
1	A	134	GLY	C	175.32	0.10	1
1	A	134	GLY	CA	45.7	0.10	1
1	A	134	GLY	N	112.85	0.10	1
1	A	135	GLN	H	7.86	0.05	1
1	A	135	GLN	HA	4.77	0.05	1
1	A	135	GLN	HB2	1.59	0.05	2
1	A	135	GLN	HB3	1.87	0.05	2
1	A	135	GLN	HE21	5.82	0.05	1
1	A	135	GLN	HE22	6.38	0.05	1
1	A	135	GLN	HG2	1.88	0.05	2
1	A	135	GLN	HG3	1.82	0.05	2
1	A	135	GLN	C	177.62	0.10	1
1	A	135	GLN	CA	53.1	0.10	1
1	A	135	GLN	CB	32.6	0.10	1
1	A	135	GLN	CG	32.8	0.10	1
1	A	135	GLN	N	115.39	0.10	1
1	A	135	GLN	NE2	108.7	0.10	1
1	A	136	VAL	H	9.02	0.05	1
1	A	136	VAL	HA	5.11	0.05	1
1	A	136	VAL	HB	2.19	0.05	1
1	A	136	VAL	HG11	0.82	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	VAL	HG12	0.82	0.05	1
1	A	136	VAL	HG13	0.82	0.05	1
1	A	136	VAL	HG21	1.18	0.05	1
1	A	136	VAL	HG22	1.18	0.05	1
1	A	136	VAL	HG23	1.18	0.05	1
1	A	136	VAL	C	172.85	0.10	1
1	A	136	VAL	CA	61.8	0.10	1
1	A	136	VAL	CB	33.9	0.10	1
1	A	136	VAL	CG1	22.4	0.10	1
1	A	136	VAL	CG2	21.8	0.10	1
1	A	136	VAL	N	125.41	0.10	1
1	A	137	ASN	H	9.39	0.05	1
1	A	137	ASN	HA	5.16	0.05	1
1	A	137	ASN	HB2	3.15	0.05	2
1	A	137	ASN	HB3	3.15	0.05	2
1	A	137	ASN	HD21	6.77	0.05	2
1	A	137	ASN	HD22	7.14	0.05	2
1	A	137	ASN	CA	51.2	0.10	1
1	A	137	ASN	CB	38.3	0.10	1
1	A	137	ASN	N	128.9	0.10	1
1	A	137	ASN	ND2	108.1	0.10	1
1	A	138	TYR	H	8.34	0.05	1
1	A	138	TYR	HA	3.32	0.05	1
1	A	138	TYR	HB2	1.99	0.05	2
1	A	138	TYR	HB3	2.29	0.05	2
1	A	138	TYR	HD1	6.17	0.05	1
1	A	138	TYR	HD2	6.17	0.05	1
1	A	138	TYR	HE1	6.39	0.05	1
1	A	138	TYR	HE2	6.39	0.05	1
1	A	138	TYR	C	175.9	0.10	1
1	A	138	TYR	CA	62.7	0.10	1
1	A	138	TYR	CB	37.5	0.10	1
1	A	138	TYR	CD1	132.4	0.10	1
1	A	138	TYR	CD2	132.4	0.10	1
1	A	138	TYR	CE1	118.2	0.10	1
1	A	138	TYR	CE2	118.2	0.10	1
1	A	138	TYR	N	118.47	0.10	1
1	A	139	GLU	H	8.03	0.05	1
1	A	139	GLU	HA	3.54	0.05	1
1	A	139	GLU	HB2	1.96	0.05	2
1	A	139	GLU	HB3	1.84	0.05	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	139	GLU	HG2	2.22	0.05	2
1	A	139	GLU	HG3	2.16	0.05	2
1	A	139	GLU	C	174.92	0.10	1
1	A	139	GLU	CA	60.37	0.10	1
1	A	139	GLU	CB	28.8	0.10	1
1	A	139	GLU	CG	37.1	0.10	1
1	A	139	GLU	N	118.4	0.10	1
1	A	140	GLU	H	8.68	0.05	1
1	A	140	GLU	HA	3.91	0.05	1
1	A	140	GLU	HB2	1.87	0.05	2
1	A	140	GLU	HB3	1.97	0.05	2
1	A	140	GLU	HG2	2.3	0.05	2
1	A	140	GLU	HG3	2.3	0.05	2
1	A	140	GLU	C	176.14	0.10	1
1	A	140	GLU	CA	58.6	0.10	1
1	A	140	GLU	CB	29.4	0.10	1
1	A	140	GLU	CG	36.8	0.10	1
1	A	140	GLU	N	119.87	0.10	1
1	A	141	PHE	H	8.81	0.05	1
1	A	141	PHE	HA	3.85	0.05	1
1	A	141	PHE	HB2	3.32	0.05	2
1	A	141	PHE	HB3	3.07	0.05	2
1	A	141	PHE	HD1	6.85	0.05	1
1	A	141	PHE	HD2	6.87	0.05	1
1	A	141	PHE	HE1	6.91	0.05	1
1	A	141	PHE	HE2	6.91	0.05	1
1	A	141	PHE	HZ	7.05	0.05	1
1	A	141	PHE	C	180.63	0.10	1
1	A	141	PHE	CA	61.84	0.10	1
1	A	141	PHE	CB	39.9	0.10	1
1	A	141	PHE	CD1	131.9	0.10	1
1	A	141	PHE	CD2	131.9	0.10	1
1	A	141	PHE	CE1	131.4	0.10	1
1	A	141	PHE	CE2	131.4	0.10	1
1	A	141	PHE	CZ	131.1	0.10	1
1	A	141	PHE	N	124.67	0.10	1
1	A	142	VAL	H	8.53	0.05	1
1	A	142	VAL	HA	3.03	0.05	1
1	A	142	VAL	HB	1.76	0.05	1
1	A	142	VAL	HG11	0.4	0.05	1
1	A	142	VAL	HG12	0.4	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	142	VAL	HG13	0.4	0.05	1
1	A	142	VAL	HG21	0.64	0.05	1
1	A	142	VAL	HG22	0.64	0.05	1
1	A	142	VAL	HG23	0.64	0.05	1
1	A	142	VAL	C	179.49	0.10	1
1	A	142	VAL	CA	67.1	0.10	1
1	A	142	VAL	CB	31.7	0.10	1
1	A	142	VAL	CG1	23.05	0.10	1
1	A	142	VAL	CG2	21.4	0.10	1
1	A	142	VAL	N	119.45	0.10	1
1	A	143	GLN	H	7.38	0.05	1
1	A	143	GLN	HA	3.78	0.05	1
1	A	143	GLN	HB2	2.04	0.05	2
1	A	143	GLN	HB3	2.04	0.05	2
1	A	143	GLN	HE21	7.4	0.05	1
1	A	143	GLN	HE22	6.67	0.05	1
1	A	143	GLN	HG2	2.31	0.05	2
1	A	143	GLN	HG3	2.31	0.05	2
1	A	143	GLN	C	176.84	0.10	1
1	A	143	GLN	CA	58.8	0.10	1
1	A	143	GLN	CB	28.2	0.10	1
1	A	143	GLN	CG	33.9	0.10	1
1	A	143	GLN	N	118.2	0.10	1
1	A	143	GLN	NE2	111.3	0.10	1
1	A	144	MET	H	7.73	0.05	1
1	A	144	MET	HA	4.08	0.05	1
1	A	144	MET	HB2	1.97	0.05	2
1	A	144	MET	HB3	1.97	0.05	2
1	A	144	MET	HE1	1.81	0.05	1
1	A	144	MET	HE2	1.81	0.05	1
1	A	144	MET	HE3	1.81	0.05	1
1	A	144	MET	HG2	2.44	0.05	2
1	A	144	MET	HG3	2.32	0.05	2
1	A	144	MET	C	179.61	0.10	1
1	A	144	MET	CA	58.2	0.10	1
1	A	144	MET	CB	32.8	0.10	1
1	A	144	MET	CE	17.15	0.10	1
1	A	144	MET	CG	31.6	0.10	1
1	A	144	MET	N	119.0	0.10	1
1	A	145	MET	H	7.79	0.05	1
1	A	145	MET	HA	4.2	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	145	MET	HB2	1.58	0.05	2
1	A	145	MET	HB3	1.73	0.05	2
1	A	145	MET	HE1	1.72	0.05	1
1	A	145	MET	HE2	1.72	0.05	1
1	A	145	MET	HE3	1.72	0.05	1
1	A	145	MET	HG2	1.76	0.05	2
1	A	145	MET	HG3	1.76	0.05	2
1	A	145	MET	C	177.97	0.10	1
1	A	145	MET	CA	55.27	0.10	1
1	A	145	MET	CB	32.82	0.10	1
1	A	145	MET	CE	17.18	0.10	1
1	A	145	MET	CG	32.2	0.10	1
1	A	145	MET	N	115.0	0.10	1
1	A	146	THR	H	7.51	0.05	1
1	A	146	THR	HA	4.2	0.05	1
1	A	146	THR	HB	4.17	0.05	1
1	A	146	THR	HG21	1.11	0.05	1
1	A	146	THR	HG22	1.11	0.05	1
1	A	146	THR	HG23	1.11	0.05	1
1	A	146	THR	C	178.13	0.10	1
1	A	146	THR	CA	62.6	0.10	1
1	A	146	THR	CB	70.2	0.10	1
1	A	146	THR	CG2	21.6	0.10	1
1	A	146	THR	N	111.42	0.10	1
1	A	147	ALA	H	7.67	0.05	1
1	A	147	ALA	HA	4.21	0.05	1
1	A	147	ALA	HB1	1.32	0.05	1
1	A	147	ALA	HB2	1.32	0.05	1
1	A	147	ALA	HB3	1.32	0.05	1
1	A	147	ALA	C	177.62	0.10	1
1	A	147	ALA	CA	52.9	0.10	1
1	A	147	ALA	CB	18.9	0.10	1
1	A	147	ALA	N	126.53	0.10	1
1	A	148	LYS	H	7.68	0.05	1
1	A	148	LYS	HA	4.04	0.05	1
1	A	148	LYS	HB2	1.72	0.05	2
1	A	148	LYS	HB3	1.59	0.05	2
1	A	148	LYS	HD2	1.4	0.05	2
1	A	148	LYS	HD3	1.56	0.05	2
1	A	148	LYS	HE2	2.88	0.05	1
1	A	148	LYS	HE3	2.88	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	148	LYS	HG2	1.3	0.05	2
1	A	148	LYS	HG3	1.3	0.05	2
1	A	148	LYS	C	174.23	0.10	1
1	A	148	LYS	CA	57.7	0.10	1
1	A	148	LYS	CB	33.6	0.10	1
1	A	148	LYS	CD	29.1	0.10	1
1	A	148	LYS	CE	42.1	0.10	1
1	A	148	LYS	CG	24.6	0.10	1
1	A	148	LYS	N	125.65	0.10	1
1	UNMAPPED	1	HAL	CA	53.6	0.10	1
1	UNMAPPED	1	HAL	HA	6.3	0.05	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	148	-0.20 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	137	0.14 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	123	-0.67 ± 0.25	Should be applied
^{15}N	146	0.28 ± 0.24	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 847 atoms were assigned a chemical shift out of a possible 898. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	337/352 (96%)	144/144 (100%)	125/140 (89%)	68/68 (100%)
Sidechain	462/496 (93%)	315/320 (98%)	141/164 (86%)	6/12 (50%)
Aromatic	48/50 (96%)	24/25 (96%)	24/25 (96%)	0/0 (—%)
Overall	847/898 (94%)	483/489 (99%)	290/329 (88%)	74/80 (92%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 922 atoms were assigned a chemical shift out of a possible 987. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

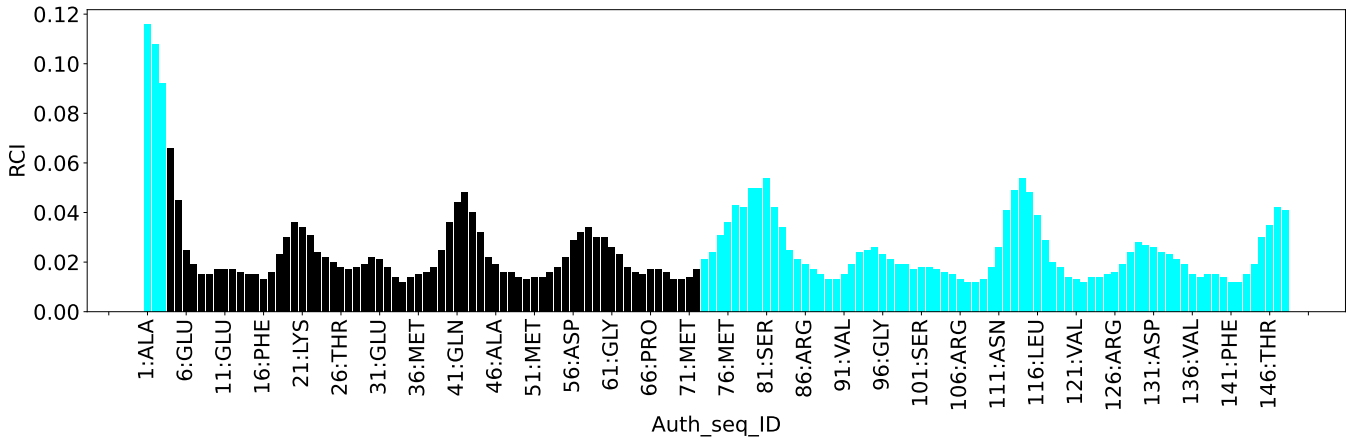
	Total	^{1}H	^{13}C	^{15}N
Backbone	365/382 (96%)	156/156 (100%)	135/152 (89%)	74/74 (100%)
Sidechain	509/555 (92%)	347/357 (97%)	155/181 (86%)	7/17 (41%)
Aromatic	48/50 (96%)	24/25 (96%)	24/25 (96%)	0/0 (—%)
Overall	922/987 (93%)	527/538 (98%)	314/358 (88%)	81/91 (89%)

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	107	HIS	CE1	120.00	126.08 – 149.12	-7.6
1	A	93	ASP	HB3	1.28	1.32 – 4.00	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A: