



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 19, 2026 – 12:02 PM UTC

PDB ID : 8EPY / pdb_00008epy
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

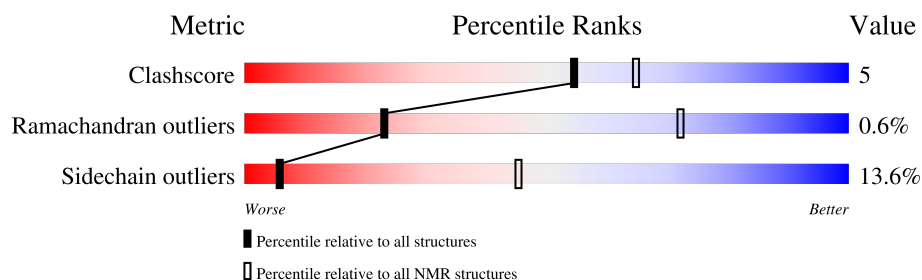
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 60%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	245	 68% 11% • 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.

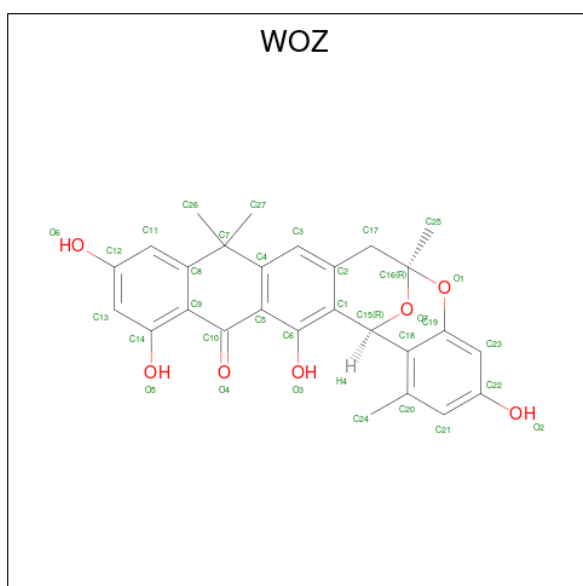
- Molecule 1 is a protein called Glyoxalase.

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 (CCD ID: WOZ) (formula: C₂₇H₂₄O₇) (labeled as "Ligand of Interest" by depositor).



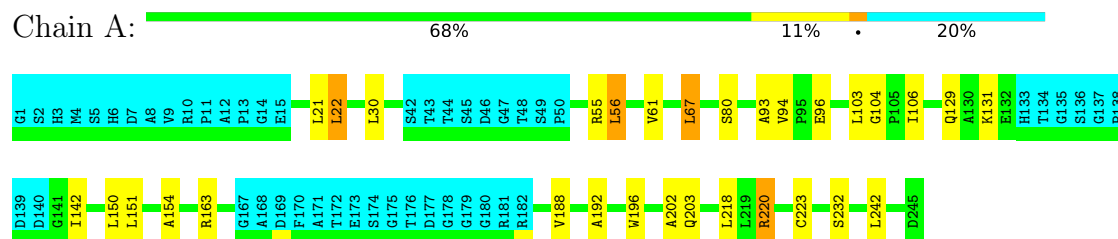
Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	A	1	58	27	24	7

4 Residue-property plots [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.

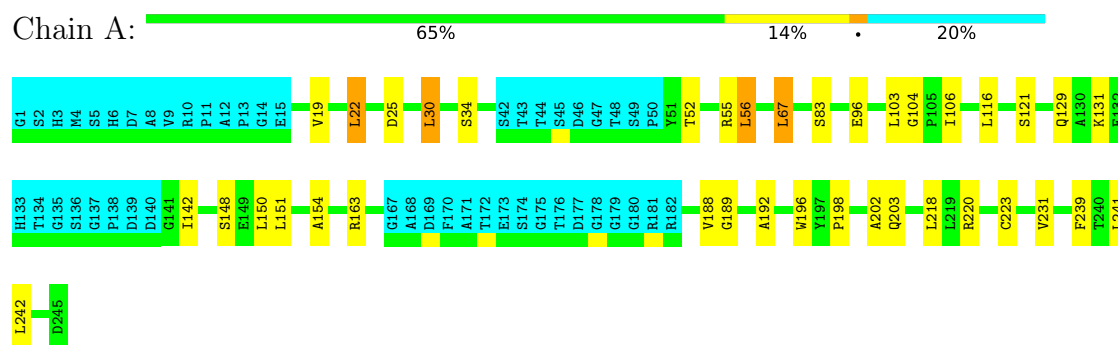
- Molecule 1: Glyoxalase



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	2789
Number of shifts mapped to atoms	1845
Number of unparsed shifts	0
Number of shifts with mapping errors	944
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%

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: WOZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.01	0±0/1484 (0.0± 0.0%)	0.80±0.01	0±1/2026 (0.0± 0.0%)
All	All	0.73	0/29680 (0.0%)	0.80	9/40520 (0.0%)

There are no bond-length outliers.

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
1	A	25	ASP	CA-CB-CG	-6.74	105.86	112.60	10	6
1	A	88	ASP	CA-CB-CG	-5.36	107.24	112.60	16	1
1	A	119	ASP	CA-CB-CG	-5.28	107.32	112.60	13	1
1	A	107	ASP	CA-CB-CG	-5.23	107.37	112.60	14	1

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	1446	1410	1410	15±2
All	All	29600	28680	28200	296

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 49 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:HD22	1:A:22:LEU:C	0.62	2.19	15	20
1:A:22:LEU:HD23	1:A:67:LEU:HD22	0.62	1.72	15	1
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%)	23	72
All	All	3920/4900 (80%)	3581 (91%)	316 (8%)	23 (1%)	23	72

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

Mol	Chain	Res	Type	Models (Total)
1	A	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±1%)	19±2 (14±1%)	6	45
All	All	2840/3520 (81%)	2454 (86%)	386 (14%)	6	45

5 of 50 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	96	GLU	20
1	A	131	LYS	20
1	A	218	LEU	20

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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 60% for the well-defined parts and 60% 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	2789
Number of shifts mapped to atoms	1845
Number of unparsed shifts	0
Number of shifts with mapping errors	944
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	340

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 944) 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
1	A	0	HIS	CB	30.083	0.000	1
1	A	0	HIS	CD2	119.954	0.000	1
1	A	0	HIS	HD2	7.128	0.000	1
1	A	0	HIS	C	174.962	0.000	1
1	A	1	GLY	H	8.382	0.000	1
1	A	1	GLY	CB	32.985	0.001	.
1	A	1	GLY	HB2	1.941	0.000	.
1	A	1	GLY	HB3	2.042	0.000	.
1	A	1	GLY	CG	31.873	0.000	.
1	A	1	GLY	HG2	2.443	0.000	.
1	A	1	GLY	HG3	2.512	0.000	.
1	A	6	HIS	HG11	0.937	0.005	.
1	A	6	HIS	HG12	0.937	0.005	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	HIS	HG13	0.937	0.005	.
1	A	6	HIS	HG21	0.935	0.000	.
1	A	6	HIS	HG22	0.935	0.000	.
1	A	6	HIS	HG23	0.935	0.000	.
1	A	6	HIS	CG1	20.654	0.000	.
1	A	6	HIS	CG2	21.284	0.000	.
1	A	7	ASP	HG2	1.683	0.000	.
1	A	7	ASP	HG3	1.683	0.000	.
1	A	7	ASP	CD	43.35	0.000	.
1	A	7	ASP	HD2	3.247	0.000	1
1	A	7	ASP	HD3	3.247	0.000	.
1	A	8	ALA	CD	50.761	0.000	.
1	A	8	ALA	CG	27.482	0.000	.
1	A	8	ALA	HG2	2.017	0.000	.
1	A	8	ALA	HG3	2.017	0.000	.
1	A	8	ALA	HD2	3.688	0.000	.
1	A	8	ALA	HD3	3.688	0.000	.
1	A	9	VAL	HB1	1.481	0.000	.
1	A	9	VAL	HB2	1.481	0.000	.
1	A	9	VAL	HB3	1.481	0.000	.
1	A	11	PRO	H	9.682	0.000	1
1	A	11	PRO	HA2	3.451	0.000	.
1	A	11	PRO	HA3	3.451	0.000	.
1	A	12	ALA	CG	35.817	0.000	.
1	A	12	ALA	HG2	2.65	0.000	.
1	A	12	ALA	HG3	2.65	0.000	.
1	A	14	GLY	CB	72.28	0.004	.
1	A	14	GLY	HB	4.05	0.001	.
1	A	14	GLY	HG21	1.476	0.000	.
1	A	14	GLY	HG22	1.476	0.000	.
1	A	14	GLY	HG23	1.476	0.000	.
1	A	14	GLY	CG2	21.34	0.001	.
1	A	16	PRO	H	8.409	0.000	1
1	A	16	PRO	HG11	-0.077	0.000	.
1	A	16	PRO	HG12	-0.077	0.000	.
1	A	16	PRO	HG13	-0.077	0.000	.
1	A	16	PRO	HG21	0.556	0.000	.
1	A	16	PRO	HG22	0.556	0.000	.
1	A	16	PRO	HG23	0.556	0.000	.
1	A	16	PRO	CG1	17.85	0.000	.
1	A	16	PRO	CG2	24.136	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	TRP	HG	0.649	0.000	.
1	A	18	TRP	HD11	-0.1	0.000	.
1	A	18	TRP	HD12	-0.1	0.000	.
1	A	18	TRP	HD13	-0.1	0.000	.
1	A	18	TRP	HD21	0.371	0.001	.
1	A	18	TRP	HD22	0.371	0.001	.
1	A	18	TRP	HD23	0.371	0.001	.
1	A	19	VAL	HB2	0.813	0.000	.
1	A	19	VAL	HB3	1.897	0.000	.
1	A	19	VAL	HD11	0.659	0.000	.
1	A	19	VAL	HD12	0.659	0.000	.
1	A	19	VAL	HD13	0.659	0.000	.
1	A	19	VAL	HD21	0.845	0.000	.
1	A	19	VAL	HD22	0.845	0.000	.
1	A	19	VAL	HD23	0.845	0.000	.
1	A	19	VAL	CD1	23.84	0.003	.
1	A	19	VAL	CD2	26.169	0.000	.
1	A	20	ASP	HG21	0.981	0.000	.
1	A	20	ASP	HG22	0.981	0.000	.
1	A	20	ASP	HG23	0.981	0.000	.
1	A	20	ASP	CG2	19.055	0.000	.
1	A	21	LEU	HG2	2.064	0.000	.
1	A	21	LEU	HG3	2.064	0.000	.
1	A	21	LEU	HD3	4.157	0.001	.
1	A	23	THR	HB2	1.925	0.000	.
1	A	23	THR	HB3	1.627	0.000	.
1	A	23	THR	HG3	1.421	0.001	.
1	A	23	THR	CD	44.39	0.001	.
1	A	23	THR	HD2	2.639	0.000	.
1	A	23	THR	HD3	3.219	0.001	.
1	A	24	PRO	H	8.928	0.000	1
1	A	24	PRO	HA2	3.605	0.003	.
1	A	24	PRO	HA3	3.924	0.000	.
1	A	27	GLY	CB	39.284	0.000	.
1	A	27	GLY	HB2	1.105	0.000	.
1	A	27	GLY	HB3	1.643	0.000	.
1	A	27	GLY	CG	25.807	0.000	.
1	A	27	GLY	HG	1.486	0.000	.
1	A	27	GLY	HD11	0.043	0.000	.
1	A	27	GLY	HD12	0.043	0.000	.
1	A	27	GLY	HD13	0.043	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	GLY	HD21	0.483	0.000	.
1	A	27	GLY	HD22	0.483	0.000	.
1	A	27	GLY	HD23	0.483	0.000	.
1	A	27	GLY	CD1	22.051	0.000	.
1	A	27	GLY	CD2	24.415	0.000	.
1	A	28	ALA	CG	33.918	0.002	.
1	A	28	ALA	HG2	2.442	0.000	.
1	A	28	ALA	HG3	2.553	0.000	.
1	A	28	ALA	HE21	6.842	0.000	.
1	A	28	ALA	HE22	7.469	0.000	.
1	A	29	ALA	HD1	6.298	0.000	.
1	A	29	ALA	HD2	6.298	0.000	.
1	A	29	ALA	HE1	7.021	0.000	.
1	A	29	ALA	HE2	7.021	0.000	.
1	A	29	ALA	CD1	132.466	0.000	.
1	A	29	ALA	CE1	130.932	0.000	.
1	A	29	ALA	CZ	129.466	0.001	.
1	A	29	ALA	HZ	7.423	0.000	.
1	A	29	ALA	CE2	130.932	0.000	.
1	A	29	ALA	CD2	132.466	0.000	.
1	A	30	LEU	HH	12.3	0.000	.
1	A	33	TYR	HG	0.191	0.000	.
1	A	33	TYR	HD11	0.362	0.000	.
1	A	33	TYR	HD12	0.362	0.000	.
1	A	33	TYR	HD13	0.362	0.000	.
1	A	33	TYR	HD21	0.106	0.000	.
1	A	33	TYR	HD22	0.106	0.000	.
1	A	33	TYR	HD23	0.106	0.000	.
1	A	34	SER	HD1	6.129	0.000	.
1	A	34	SER	HD2	6.129	0.000	.
1	A	34	SER	HE1	6.476	0.000	.
1	A	34	SER	HE2	6.476	0.000	.
1	A	34	SER	CD1	130.824	0.000	.
1	A	34	SER	CE1	129.585	0.000	.
1	A	34	SER	CZ	129.397	0.006	.
1	A	34	SER	HZ	6.897	0.003	.
1	A	34	SER	CE2	129.585	0.000	.
1	A	34	SER	CD2	130.824	0.000	.
1	A	35	ALA	HA2	3.944	0.000	.
1	A	35	ALA	HA3	4.095	0.000	.
1	A	36	LEU	CE3	119.7	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	36	LEU	HE3	7.312	0.000	.
1	A	36	LEU	CZ3	121.81	0.005	.
1	A	36	LEU	CZ2	115.722	0.000	.
1	A	36	LEU	HE1	10.46	0.000	.
1	A	36	LEU	HZ3	6.341	0.002	.
1	A	36	LEU	CH2	125.482	0.001	.
1	A	36	LEU	HZ2	5.912	0.000	.
1	A	36	LEU	HH2	5.856	0.003	.
1	A	37	PHE	HG2	2.139	0.000	.
1	A	37	PHE	HG3	2.31	0.000	.
1	A	38	GLY	CB	41.996	0.001	.
1	A	38	GLY	HB2	2.891	0.000	.
1	A	38	GLY	HB3	3.241	0.000	.
1	A	38	GLY	HD1	7.27	0.000	.
1	A	38	GLY	HD2	7.27	0.000	.
1	A	38	GLY	CD1	131.912	0.000	.
1	A	38	GLY	CD2	131.912	0.002	.
1	A	40	GLU	HG21	1.239	0.000	.
1	A	40	GLU	HG22	1.239	0.000	.
1	A	40	GLU	HG23	1.239	0.000	.
1	A	40	GLU	CG2	21.873	0.000	.
1	A	41	PHE	HG21	0.733	0.000	.
1	A	41	PHE	HG22	0.733	0.000	.
1	A	41	PHE	HG23	0.733	0.000	.
1	A	41	PHE	CG2	21.619	0.000	.
1	A	43	THR	HB2	2.904	0.000	.
1	A	43	THR	HB3	2.737	0.001	.
1	A	44	THR	HA2	3.835	0.000	.
1	A	44	THR	HA3	4.369	0.000	.
1	A	45	SER	HG21	1.263	0.000	.
1	A	45	SER	HG22	1.263	0.000	.
1	A	45	SER	HG23	1.263	0.000	.
1	A	45	SER	CG2	21.675	0.000	.
1	A	48	THR	HB2	3.159	0.000	.
1	A	48	THR	HB3	3.159	0.000	.
1	A	48	THR	HD1	7.062	0.001	.
1	A	48	THR	HD2	7.062	0.001	.
1	A	48	THR	HE1	6.692	0.004	.
1	A	48	THR	HE2	6.692	0.004	.
1	A	48	THR	CD1	134.56	0.005	.
1	A	48	THR	CE1	118.176	0.007	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	THR	CE2	118.176	0.000	.
1	A	48	THR	CD2	134.56	0.000	.
1	A	49	SER	HG21	1.305	0.000	.
1	A	49	SER	HG22	1.305	0.000	.
1	A	49	SER	HG23	1.305	0.000	.
1	A	49	SER	CG2	23.706	0.008	.
1	A	50	PRO	H	9.006	0.000	1
1	A	50	PRO	HE1	2.05	0.000	.
1	A	50	PRO	HE2	2.05	0.000	.
1	A	50	PRO	HE3	2.05	0.000	.
1	A	50	PRO	CE	16.962	0.000	.
1	A	52	THR	HB2	1.451	0.000	.
1	A	52	THR	HB3	1.511	0.000	.
1	A	52	THR	HG3	1.407	0.000	.
1	A	52	THR	CD	43.422	0.001	.
1	A	52	THR	HD2	2.951	0.000	.
1	A	52	THR	HD3	3.129	0.000	.
1	A	52	THR	HE	7.338	0.000	.
1	A	53	MET	HD11	1.122	0.000	.
1	A	53	MET	HD12	1.122	0.000	.
1	A	53	MET	HD13	1.122	0.000	.
1	A	53	MET	HD21	1.085	0.000	.
1	A	53	MET	HD22	1.085	0.000	.
1	A	53	MET	HD23	1.085	0.000	.
1	A	53	MET	CD1	22.928	0.000	.
1	A	53	MET	CD2	26.406	0.000	.
1	A	55	ARG	HA2	3.601	0.001	.
1	A	55	ARG	HA3	4.174	0.000	.
1	A	56	LEU	HG2	1.701	0.001	.
1	A	56	LEU	HG3	1.701	0.001	.
1	A	56	LEU	HD3	3.21	0.001	.
1	A	56	LEU	HE	7.341	0.000	.
1	A	58	GLY	CB	34.455	0.000	.
1	A	58	GLY	HB	0.832	0.000	.
1	A	58	GLY	HG11	0.492	0.000	.
1	A	58	GLY	HG12	0.492	0.000	.
1	A	58	GLY	HG13	0.492	0.000	.
1	A	58	GLY	HG21	0.586	0.000	.
1	A	58	GLY	HG22	0.586	0.000	.
1	A	58	GLY	HG23	0.586	0.000	.
1	A	58	GLY	CG1	20.593	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	GLY	CG2	21.54	0.000	.
1	A	61	VAL	HD11	0.725	0.000	.
1	A	61	VAL	HD12	0.725	0.000	.
1	A	61	VAL	HD13	0.725	0.000	.
1	A	61	VAL	CD1	14.265	0.005	.
1	A	62	CYS	HA2	3.982	0.000	.
1	A	62	CYS	HA3	3.982	0.000	.
1	A	64	ILE	HB2	0.827	0.002	.
1	A	64	ILE	HB3	1.484	0.000	.
1	A	64	ILE	HD21	0.826	0.000	.
1	A	64	ILE	HD22	0.826	0.000	.
1	A	64	ILE	HD23	0.826	0.000	.
1	A	64	ILE	CD2	25.945	0.000	.
1	A	66	ASP	HG2	2.275	0.000	.
1	A	66	ASP	HG3	2.213	0.000	.
1	A	68	GLY	CD	50.406	0.000	.
1	A	68	GLY	CB	32.232	0.000	.
1	A	68	GLY	HB2	2.012	0.000	.
1	A	68	GLY	HB3	2.193	0.000	.
1	A	68	GLY	CG	27.152	0.003	.
1	A	68	GLY	HG2	1.963	0.000	.
1	A	68	GLY	HG3	2.036	0.000	.
1	A	68	GLY	HD2	3.676	0.000	.
1	A	68	GLY	HD3	3.676	0.000	.
1	A	69	GLU	HA2	4.167	0.000	.
1	A	69	GLU	HA3	3.963	0.000	.
1	A	70	ASN	CD	49.879	0.000	.
1	A	70	ASN	HG2	2.008	0.000	.
1	A	70	ASN	HG3	2.008	0.000	.
1	A	70	ASN	HD3	3.626	0.000	.
1	A	71	PRO	H	7.979	0.000	1
1	A	72	GLY	CB	44.351	0.000	.
1	A	72	GLY	HB2	1.511	0.000	.
1	A	72	GLY	HB3	1.555	0.000	.
1	A	72	GLY	CG	26.873	0.000	.
1	A	72	GLY	HG	1.568	0.000	.
1	A	72	GLY	HD11	0.809	0.001	.
1	A	72	GLY	HD12	0.809	0.001	.
1	A	72	GLY	HD13	0.809	0.001	.
1	A	72	GLY	HD21	0.855	0.000	.
1	A	72	GLY	HD22	0.855	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	GLY	HD23	0.855	0.000	.
1	A	72	GLY	CD1	23.268	0.001	.
1	A	72	GLY	CD2	25.451	0.002	.
1	A	73	PRO	H	8.453	0.000	1
1	A	73	PRO	HA2	4.015	0.000	.
1	A	73	PRO	HA3	4.015	0.000	.
1	A	74	ALA	HA2	3.624	0.000	.
1	A	74	ALA	HA3	4.631	0.000	.
1	A	75	LEU	CE3	119.583	0.001	.
1	A	75	LEU	HE3	7.209	0.001	.
1	A	75	LEU	CZ2	114.468	0.001	.
1	A	75	LEU	HE1	9.884	0.000	.
1	A	75	LEU	CH2	126.008	0.000	.
1	A	75	LEU	HZ2	6.446	0.000	.
1	A	75	LEU	HH2	7.044	0.000	.
1	A	76	GLY	CB	64.837	0.000	.
1	A	76	GLY	HB2	3.419	0.000	.
1	A	76	GLY	HB3	4.208	0.000	.
1	A	77	GLY	CB	64.913	0.000	.
1	A	77	GLY	HB2	3.404	0.000	.
1	A	77	GLY	HB3	3.404	0.000	.
1	A	78	TRP	HD2	6.855	0.001	.
1	A	78	TRP	HE2	6.868	0.000	.
1	A	78	TRP	CE1	118.298	0.000	.
1	A	79	SER	CG	27.791	0.000	.
1	A	79	SER	HD11	0.338	0.000	.
1	A	79	SER	HD12	0.338	0.000	.
1	A	79	SER	HD13	0.338	0.000	.
1	A	79	SER	HD21	0.471	0.000	.
1	A	79	SER	HD22	0.471	0.000	.
1	A	79	SER	HD23	0.471	0.000	.
1	A	79	SER	CD1	21.824	0.000	.
1	A	79	SER	CD2	25.322	0.000	.
1	A	81	TYR	HG11	0.661	0.000	.
1	A	81	TYR	HG12	0.661	0.000	.
1	A	81	TYR	HG13	0.661	0.000	.
1	A	81	TYR	HG21	1.083	0.000	.
1	A	81	TYR	HG22	1.083	0.000	.
1	A	81	TYR	HG23	1.083	0.000	.
1	A	81	TYR	CG1	18.683	0.000	.
1	A	81	TYR	CG2	23.869	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	VAL	HB1	1.113	0.000	.
1	A	84	VAL	HB2	1.113	0.000	.
1	A	84	VAL	HB3	1.113	0.000	.
1	A	91	ALA	HG11	0.795	0.000	.
1	A	91	ALA	HG12	0.795	0.000	.
1	A	91	ALA	HG13	0.795	0.000	.
1	A	91	ALA	HG21	0.927	0.000	.
1	A	91	ALA	HG22	0.927	0.000	.
1	A	91	ALA	HG23	0.927	0.000	.
1	A	91	ALA	CG1	22.189	0.000	.
1	A	91	ALA	CG2	24.321	0.000	.
1	A	92	ALA	CD	50.422	0.000	.
1	A	92	ALA	CG	28.567	0.000	.
1	A	92	ALA	HG2	1.921	0.000	.
1	A	92	ALA	HG3	2.154	0.000	.
1	A	92	ALA	HD2	3.46	0.000	.
1	A	92	ALA	HD3	3.768	0.000	.
1	A	93	ALA	CG	35.909	0.000	.
1	A	93	ALA	HG2	2.293	0.000	.
1	A	93	ALA	HG3	2.431	0.000	.
1	A	94	VAL	HB2	1.767	0.000	.
1	A	94	VAL	HB3	1.806	0.000	.
1	A	94	VAL	HD11	0.801	0.000	.
1	A	94	VAL	HD12	0.801	0.000	.
1	A	94	VAL	HD13	0.801	0.000	.
1	A	94	VAL	HD21	0.362	0.000	.
1	A	94	VAL	HD22	0.362	0.000	.
1	A	94	VAL	HD23	0.362	0.000	.
1	A	94	VAL	CD1	22.627	0.000	.
1	A	94	VAL	CD2	25.452	0.000	.
1	A	95	PRO	H	7.617	0.000	1
1	A	95	PRO	HA2	3.822	0.000	.
1	A	95	PRO	HA3	4.393	0.000	.
1	A	96	GLU	HA2	3.435	0.000	.
1	A	96	GLU	HA3	4.044	0.000	.
1	A	98	GLY	CB	31.575	0.001	.
1	A	98	GLY	HB	2.091	0.000	.
1	A	98	GLY	HG11	0.891	0.000	.
1	A	98	GLY	HG12	0.891	0.000	.
1	A	98	GLY	HG13	0.891	0.000	.
1	A	98	GLY	HG21	0.995	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	GLY	HG22	0.995	0.000	.
1	A	98	GLY	HG23	0.995	0.000	.
1	A	98	GLY	CG1	21.759	0.001	.
1	A	98	GLY	CG2	22.839	0.000	.
1	A	99	GLY	CB	42.813	0.000	.
1	A	99	GLY	HB2	1.398	0.000	.
1	A	99	GLY	HB3	1.398	0.000	.
1	A	99	GLY	CG	27.377	0.000	.
1	A	99	GLY	HG	1.504	0.000	.
1	A	99	GLY	HD11	0.739	0.000	.
1	A	99	GLY	HD12	0.739	0.000	.
1	A	99	GLY	HD13	0.739	0.000	.
1	A	99	GLY	HD21	0.747	0.000	.
1	A	99	GLY	HD22	0.747	0.000	.
1	A	99	GLY	HD23	0.747	0.000	.
1	A	99	GLY	CD1	21.93	0.000	.
1	A	99	GLY	CD2	25.183	0.000	.
1	A	100	ALA	CG	27.532	0.000	.
1	A	100	ALA	HG	1.59	0.000	.
1	A	100	ALA	HD11	0.996	0.000	.
1	A	100	ALA	HD12	0.996	0.000	.
1	A	100	ALA	HD13	0.996	0.000	.
1	A	100	ALA	HD21	1.055	0.000	.
1	A	100	ALA	HD22	1.055	0.000	.
1	A	100	ALA	HD23	1.055	0.000	.
1	A	100	ALA	CD1	26.054	0.004	.
1	A	100	ALA	CD2	24.403	0.000	.
1	A	101	VAL	HA2	3.474	0.000	.
1	A	101	VAL	HA3	4.567	0.000	.
1	A	102	LEU	HG2	1.611	0.000	.
1	A	102	LEU	HG3	1.611	0.000	.
1	A	102	LEU	HD3	3.618	0.000	.
1	A	103	LEU	HG21	0.904	0.000	.
1	A	103	LEU	HG22	0.904	0.000	.
1	A	103	LEU	HG23	0.904	0.000	.
1	A	103	LEU	CG2	17.807	0.000	.
1	A	103	LEU	CG1	27.152	0.000	.
1	A	103	LEU	HG12	1.44	0.000	.
1	A	103	LEU	HG13	1.084	0.000	.
1	A	104	GLY	CB	41.725	0.000	.
1	A	104	GLY	HB2	2.497	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	GLY	HB3	2.497	0.000	.
1	A	105	PRO	H	8.022	0.000	1
1	A	105	PRO	HG21	0.357	0.002	.
1	A	105	PRO	HG22	0.357	0.002	.
1	A	105	PRO	HG23	0.357	0.002	.
1	A	105	PRO	CG2	16.459	0.007	.
1	A	105	PRO	CG1	26.547	0.000	.
1	A	105	PRO	HG12	0.829	0.000	.
1	A	105	PRO	HG13	0.507	0.000	.
1	A	105	PRO	HD11	-0.473	0.003	.
1	A	105	PRO	HD12	-0.473	0.003	.
1	A	105	PRO	HD13	-0.473	0.003	.
1	A	105	PRO	CD1	10.553	0.003	.
1	A	106	ILE	HB2	1.605	0.000	.
1	A	106	ILE	HB3	1.872	0.000	.
1	A	106	ILE	HD21	0.985	0.000	.
1	A	106	ILE	HD22	0.985	0.000	.
1	A	106	ILE	HD23	0.985	0.000	.
1	A	106	ILE	CD2	25.894	0.000	.
1	A	108	ILE	HB2	1.915	0.000	.
1	A	108	ILE	HB3	1.915	0.000	.
1	A	108	ILE	HG3	2.447	0.000	.
1	A	108	ILE	HE21	6.656	0.008	.
1	A	108	ILE	HE22	7.22	0.003	.
1	A	109	LEU	HA2	2.959	0.000	.
1	A	109	LEU	HA3	3.083	0.000	.
1	A	110	ALA	CG	26.905	0.000	.
1	A	110	ALA	HG2	1.558	0.000	.
1	A	110	ALA	HG3	1.558	0.000	.
1	A	110	ALA	CD	43.239	0.000	.
1	A	110	ALA	HD2	2.812	0.000	.
1	A	110	ALA	HD3	3.098	0.000	.
1	A	110	ALA	HE	7.577	0.000	.
1	A	111	GLN	HE1	1.754	0.005	.
1	A	111	GLN	HE3	1.754	0.005	.
1	A	111	GLN	CE	17.974	0.000	.
1	A	112	GLY	CB	45.949	0.000	.
1	A	112	GLY	HB2	1.622	0.000	.
1	A	112	GLY	HB3	1.9	0.000	.
1	A	112	GLY	CG	26.421	0.000	.
1	A	112	GLY	HG	1.757	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	112	GLY	HD11	0.87	0.000	.
1	A	112	GLY	HD12	0.87	0.000	.
1	A	112	GLY	HD13	0.87	0.000	.
1	A	112	GLY	HD21	0.965	0.000	.
1	A	112	GLY	HD22	0.965	0.000	.
1	A	112	GLY	HD23	0.965	0.000	.
1	A	112	GLY	CD1	27.013	0.000	.
1	A	112	GLY	CD2	27.558	0.000	.
1	A	113	ARG	HD11	0.964	0.001	.
1	A	113	ARG	HD12	0.964	0.001	.
1	A	113	ARG	HD13	0.964	0.001	.
1	A	113	ARG	HD21	1.006	0.005	.
1	A	113	ARG	HD22	1.006	0.005	.
1	A	113	ARG	HD23	1.006	0.005	.
1	A	113	ARG	CD1	24.138	0.000	.
1	A	113	ARG	CD2	25.334	0.000	.
1	A	115	LEU	HA2	3.319	0.000	.
1	A	115	LEU	HA3	5.095	0.001	.
1	A	117	ALA	CD	50.391	0.000	.
1	A	117	ALA	CG	28.429	0.000	.
1	A	117	ALA	HG2	1.498	0.000	.
1	A	117	ALA	HG3	1.498	0.000	.
1	A	117	ALA	HD2	3.114	0.000	.
1	A	117	ALA	HD3	2.17	0.000	.
1	A	118	GLY	CB	62.924	0.000	.
1	A	118	GLY	HB2	3.455	0.000	.
1	A	118	GLY	HB3	3.664	0.000	.
1	A	119	ASP	HA2	3.426	0.008	.
1	A	119	ASP	HA3	4.05	0.000	.
1	A	120	PRO	H	8.155	0.000	1
1	A	120	PRO	CD2	120.461	0.000	.
1	A	121	SER	CG	27.272	0.000	.
1	A	121	SER	HG2	1.517	0.000	.
1	A	121	SER	HG3	1.698	0.000	.
1	A	121	SER	CD	43.925	0.000	.
1	A	121	SER	HD2	3.226	0.000	.
1	A	121	SER	HD3	3.38	0.000	.
1	A	121	SER	HE	7.18	0.000	.
1	A	122	GLY	CB	35.842	0.000	.
1	A	122	GLY	HB	2.2	0.000	.
1	A	122	GLY	HG11	1.106	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	GLY	HG12	1.106	0.000	.
1	A	122	GLY	HG13	1.106	0.000	.
1	A	122	GLY	HG21	0.552	0.000	.
1	A	122	GLY	HG22	0.552	0.000	.
1	A	122	GLY	HG23	0.552	0.000	.
1	A	122	GLY	CG1	17.732	0.003	.
1	A	122	GLY	CG2	20.96	0.000	.
1	A	123	HIS	HA2	3.06	0.000	.
1	A	123	HIS	HA3	4.987	0.000	.
1	A	124	ARG	HD11	1.074	0.000	.
1	A	124	ARG	HD12	1.074	0.000	.
1	A	124	ARG	HD13	1.074	0.000	.
1	A	124	ARG	HD21	0.795	0.000	.
1	A	124	ARG	HD22	0.795	0.000	.
1	A	124	ARG	HD23	0.795	0.000	.
1	A	124	ARG	CD1	24.634	0.000	.
1	A	124	ARG	CD2	25.83	0.000	.
1	A	125	VAL	HB2	2.953	0.005	.
1	A	125	VAL	HB3	3.16	0.000	.
1	A	125	VAL	CD1	126.321	0.000	.
1	A	125	VAL	HD1	7.001	0.000	.
1	A	125	VAL	CZ2	113.163	0.000	.
1	A	125	VAL	HE1	9.141	0.000	.
1	A	125	VAL	CH2	121.943	0.001	.
1	A	125	VAL	HZ2	6.515	0.000	.
1	A	125	VAL	HH2	5.745	0.000	.
1	A	126	GLY	CB	29.882	0.000	.
1	A	126	GLY	HB2	1.738	0.000	.
1	A	126	GLY	HB3	1.738	0.000	.
1	A	126	GLY	CG	32.328	0.000	.
1	A	126	GLY	HG2	2.3	0.000	.
1	A	126	GLY	HG3	2.3	0.000	.
1	A	126	GLY	HE21	7.091	0.000	.
1	A	126	GLY	HE22	7.61	0.000	.
1	A	128	TRP	HG2	1.027	0.000	.
1	A	128	TRP	HG3	1.285	0.000	.
1	A	128	TRP	HD2	1.342	0.000	.
1	A	128	TRP	HD3	1.436	0.000	.
1	A	128	TRP	HE2	2.571	0.000	.
1	A	131	LYS	HG21	1.102	0.000	.
1	A	131	LYS	HG22	1.102	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	LYS	HG23	1.102	0.000	.
1	A	131	LYS	CG2	21.633	0.000	.
1	A	132	GLU	HA2	3.92	0.000	.
1	A	132	GLU	HA3	4.927	0.000	.
1	A	134	THR	HA2	3.845	0.000	.
1	A	134	THR	HA3	4.381	0.000	.
1	A	135	GLY	CD	49.565	0.000	.
1	A	135	GLY	CB	32.039	0.000	.
1	A	135	GLY	HB2	1.777	0.000	.
1	A	135	GLY	HB3	2.27	0.000	.
1	A	135	GLY	CG	27.116	0.000	.
1	A	135	GLY	HG2	1.995	0.000	.
1	A	135	GLY	HG3	1.995	0.000	.
1	A	135	GLY	HD2	3.669	0.000	.
1	A	135	GLY	HD3	3.669	0.000	.
1	A	137	GLY	CB	41.229	0.001	.
1	A	137	GLY	HB2	2.334	0.001	.
1	A	137	GLY	HB3	2.891	0.000	.
1	A	138	PRO	H	7.732	0.000	1
1	A	138	PRO	HA2	3.688	0.001	.
1	A	138	PRO	HA3	4.325	0.001	.
1	A	139	ASP	HG21	1.062	0.001	.
1	A	139	ASP	HG22	1.062	0.001	.
1	A	139	ASP	HG23	1.062	0.001	.
1	A	139	ASP	CG2	18.229	0.000	.
1	A	139	ASP	CG1	27.46	0.000	.
1	A	139	ASP	HG12	1.219	0.000	.
1	A	139	ASP	HG13	1.576	0.000	.
1	A	139	ASP	HD11	0.816	0.000	.
1	A	139	ASP	HD12	0.816	0.000	.
1	A	139	ASP	HD13	0.816	0.000	.
1	A	139	ASP	CD1	12.733	0.000	.
1	A	140	ASP	HA2	3.227	0.001	.
1	A	140	ASP	HA3	4.381	0.000	.
1	A	141	GLY	HB1	1.559	0.000	.
1	A	141	GLY	HB2	1.559	0.000	.
1	A	141	GLY	HB3	1.559	0.000	.
1	A	141	GLY	CB	19.958	0.000	.
1	A	142	ILE	HB2	2.868	0.000	.
1	A	142	ILE	HB3	2.582	0.000	.
1	A	142	ILE	HE1	7.053	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	142	ILE	HE2	7.053	0.000	.
1	A	142	ILE	CE1	118.169	0.000	.
1	A	142	ILE	CE2	118.169	0.000	.
1	A	142	ILE	CD2	130.631	0.000	.
1	A	143	GLY	CB	69.488	0.001	.
1	A	143	GLY	HB	3.363	0.000	.
1	A	143	GLY	HG21	0.98	0.000	.
1	A	143	GLY	HG22	0.98	0.000	.
1	A	143	GLY	HG23	0.98	0.000	.
1	A	143	GLY	CG2	22.471	0.002	.
1	A	146	THR	HB2	1.7	0.000	.
1	A	146	THR	HB3	1.7	0.000	.
1	A	146	THR	HG3	2.683	0.000	.
1	A	147	ARG	HD11	-0.554	0.000	.
1	A	147	ARG	HD12	-0.554	0.000	.
1	A	147	ARG	HD13	-0.554	0.000	.
1	A	147	ARG	HD21	0.598	0.000	.
1	A	147	ARG	HD22	0.598	0.000	.
1	A	147	ARG	HD23	0.598	0.000	.
1	A	147	ARG	CD1	19.992	0.000	.
1	A	147	ARG	CD2	26.07	0.000	.
1	A	148	SER	CG	28.864	0.000	.
1	A	148	SER	HD11	0.414	0.000	.
1	A	148	SER	HD12	0.414	0.000	.
1	A	148	SER	HD13	0.414	0.000	.
1	A	148	SER	HD21	0.637	0.000	.
1	A	148	SER	HD22	0.637	0.000	.
1	A	148	SER	HD23	0.637	0.000	.
1	A	148	SER	CD1	22.959	0.000	.
1	A	148	SER	CD2	24.122	0.000	.
1	A	149	GLU	HG21	0.567	0.001	.
1	A	149	GLU	HG22	0.567	0.001	.
1	A	149	GLU	HG23	0.567	0.001	.
1	A	149	GLU	CG2	21.482	0.000	.
1	A	150	LEU	HA2	3.692	0.000	.
1	A	150	LEU	HA3	4.769	0.001	.
1	A	152	THR	HB2	3.737	0.000	.
1	A	152	THR	HB3	3.813	0.000	.
1	A	153	GLY	HB1	1.524	0.000	.
1	A	153	GLY	HB2	1.524	0.000	.
1	A	153	GLY	HB3	1.524	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	153	GLY	CB	18.163	0.001	.
1	A	154	ALA	HG21	1.238	0.000	.
1	A	154	ALA	HG22	1.238	0.000	.
1	A	154	ALA	HG23	1.238	0.000	.
1	A	154	ALA	CG2	22.157	0.000	.
1	A	156	ALA	HA2	3.925	0.000	.
1	A	156	ALA	HA3	4.168	0.000	.
1	A	157	THR	HB1	1.596	0.000	.
1	A	157	THR	HB2	1.596	0.000	.
1	A	157	THR	HB3	1.596	0.000	.
1	A	158	ASP	HD1	7.117	0.000	.
1	A	158	ASP	HD2	7.117	0.000	1
1	A	158	ASP	HE1	6.778	0.000	.
1	A	158	ASP	HE2	6.778	0.000	.
1	A	158	ASP	CD1	129.229	0.000	.
1	A	158	ASP	CE1	128.714	0.001	.
1	A	158	ASP	CE2	128.714	0.000	.
1	A	158	ASP	CD2	129.229	0.000	.
1	A	159	GLY	CB	39.879	0.000	.
1	A	159	GLY	HB2	2.791	0.000	.
1	A	159	GLY	HB3	2.924	0.000	.
1	A	159	GLY	HD1	7.147	0.000	.
1	A	159	GLY	HD2	7.147	0.000	.
1	A	159	GLY	HE1	7.147	0.000	.
1	A	159	GLY	HE2	7.147	0.000	.
1	A	159	GLY	HH	12.372	0.000	.
1	A	160	ALA	CG	30.784	0.001	.
1	A	160	ALA	HG2	1.992	0.000	.
1	A	160	ALA	HG3	2.134	0.000	.
1	A	160	ALA	CD	43.899	0.000	.
1	A	160	ALA	HD2	3.227	0.000	.
1	A	160	ALA	HD3	3.404	0.000	.
1	A	160	ALA	HE	7.216	0.000	.
1	A	161	PHE	HA2	3.547	0.000	.
1	A	161	PHE	HA3	3.788	0.000	.
1	A	162	TYR	HG	0.536	0.000	.
1	A	162	TYR	HD11	0.148	0.000	.
1	A	162	TYR	HD12	0.148	0.000	.
1	A	162	TYR	HD13	0.148	0.000	.
1	A	162	TYR	HD21	0.06	0.000	.
1	A	162	TYR	HD22	0.06	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	162	TYR	HD23	0.06	0.000	.
1	A	167	GLY	CB	39.855	0.001	.
1	A	167	GLY	HB2	3.082	0.000	.
1	A	167	GLY	HB3	3.33	0.000	.
1	A	167	GLY	HD1	7.262	0.000	.
1	A	167	GLY	HD2	7.262	0.000	.
1	A	167	GLY	CD1	133.043	0.002	.
1	A	167	GLY	CD2	133.043	0.000	.
1	A	169	ASP	HG21	1.255	0.000	.
1	A	169	ASP	HG22	1.255	0.000	.
1	A	169	ASP	HG23	1.255	0.000	.
1	A	169	ASP	CG2	21.6	0.000	.
1	A	170	PHE	HG2	2.248	0.000	.
1	A	170	PHE	HG3	2.248	0.000	.
1	A	172	THR	HA2	4.016	0.000	.
1	A	172	THR	HA3	4.016	0.000	.
1	A	173	GLU	HG21	1.161	0.000	.
1	A	173	GLU	HG22	1.161	0.000	.
1	A	173	GLU	HG23	1.161	0.000	.
1	A	173	GLU	CG2	21.54	0.000	.
1	A	176	THR	HA2	3.975	0.000	.
1	A	176	THR	HA3	3.975	0.000	.
1	A	177	ASP	HA2	3.999	0.000	.
1	A	177	ASP	HA3	3.999	0.000	.
1	A	178	GLY	CB	31.097	0.000	.
1	A	178	GLY	HB2	1.795	0.000	.
1	A	178	GLY	HB3	1.795	0.000	.
1	A	179	GLY	CB	32.38	0.000	.
1	A	179	GLY	HB2	1.604	0.000	.
1	A	179	GLY	HB3	1.936	0.000	.
1	A	179	GLY	CG	26.968	0.001	.
1	A	179	GLY	HG2	1.575	0.000	.
1	A	179	GLY	HG3	1.575	0.000	.
1	A	179	GLY	CD	43.353	0.000	.
1	A	179	GLY	HD2	3.14	0.000	.
1	A	179	GLY	HD3	3.22	0.000	.
1	A	179	GLY	HE	7.192	0.000	.
1	A	180	GLY	HB1	1.358	0.000	.
1	A	180	GLY	HB2	1.358	0.000	.
1	A	180	GLY	HB3	1.358	0.000	.
1	A	180	GLY	CB	20.694	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	182	ARG	HG21	0.669	0.000	.
1	A	182	ARG	HG22	0.669	0.000	.
1	A	182	ARG	HG23	0.669	0.000	.
1	A	182	ARG	CG2	17.231	0.000	.
1	A	182	ARG	CG1	26.711	0.000	.
1	A	182	ARG	HG12	1.386	0.000	.
1	A	182	ARG	HG13	1.386	0.000	.
1	A	182	ARG	HD11	0.992	0.000	.
1	A	182	ARG	HD12	0.992	0.000	.
1	A	182	ARG	HD13	0.992	0.000	.
1	A	182	ARG	CD1	13.608	0.000	.
1	A	183	ALA	CG	25.904	0.000	.
1	A	183	ALA	HG2	1.3	0.000	.
1	A	183	ALA	HG3	1.193	0.000	.
1	A	183	ALA	CD	42.716	0.001	.
1	A	183	ALA	HD2	3.013	0.000	.
1	A	183	ALA	HD3	2.773	0.000	.
1	A	183	ALA	HE	8.366	0.000	.
1	A	184	ALA	CG	33.115	0.000	.
1	A	184	ALA	HG2	2.204	0.000	.
1	A	184	ALA	HG3	2.49	0.000	.
1	A	184	ALA	HE21	6.925	0.000	.
1	A	184	ALA	HE22	7.435	0.000	.
1	A	186	ARG	HA2	3.964	0.000	.
1	A	186	ARG	HA3	4.348	0.000	.
1	A	187	GLN	HD2	3.676	0.000	.
1	A	187	GLN	HD3	3.676	0.000	.
1	A	188	VAL	HB1	1.408	0.000	.
1	A	188	VAL	HB2	1.408	0.000	.
1	A	188	VAL	HB3	1.408	0.000	.
1	A	189	GLY	HB1	1.338	0.000	.
1	A	189	GLY	HB2	1.338	0.000	.
1	A	189	GLY	HB3	1.338	0.000	.
1	A	189	GLY	CB	18.74	0.000	.
1	A	192	ALA	HA2	2.844	0.000	.
1	A	192	ALA	HA3	4.397	0.000	.
1	A	193	PRO	H	9.063	0.000	1
1	A	193	PRO	CD1	126.594	0.000	.
1	A	193	PRO	CE3	119.18	0.000	.
1	A	193	PRO	HE3	6.96	0.000	.
1	A	193	PRO	CZ3	120.926	0.004	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	193	PRO	CZ2	114.125	0.002	.
1	A	193	PRO	HE1	10.386	0.000	.
1	A	193	PRO	HZ3	6.78	0.001	.
1	A	193	PRO	CH2	122.776	0.006	.
1	A	193	PRO	HZ2	6.191	0.000	.
1	A	193	PRO	HH2	6.709	0.000	.
1	A	194	SER	HD1	7.043	0.000	.
1	A	194	SER	HD2	7.043	0.000	.
1	A	194	SER	HE1	6.463	0.000	.
1	A	194	SER	HE2	6.463	0.000	.
1	A	194	SER	CD1	133.511	0.000	.
1	A	194	SER	CE1	118.215	0.000	.
1	A	194	SER	CE2	118.215	0.000	.
1	A	194	SER	CD2	133.511	0.000	.
1	A	195	GLY	CD	51.081	0.000	.
1	A	195	GLY	CB	33.092	0.006	.
1	A	195	GLY	HB2	1.131	0.000	.
1	A	195	GLY	HB3	1.606	0.000	.
1	A	195	GLY	CG	26.762	0.007	.
1	A	195	GLY	HG2	1.468	0.000	.
1	A	195	GLY	HG3	1.728	0.000	.
1	A	195	GLY	HD2	4.077	0.000	.
1	A	195	GLY	HD3	4.077	0.000	.
1	A	197	TYR	HZ	5.747	0.001	.
1	A	198	PRO	H	8.333	0.000	1
1	A	200	PHE	HG2	2.357	0.000	.
1	A	200	PHE	HG3	2.461	0.000	.
1	A	200	PHE	HE21	6.885	0.000	.
1	A	200	PHE	HE22	7.793	0.000	.
1	A	204	GLU	HG11	0.843	0.000	.
1	A	204	GLU	HG12	0.843	0.000	.
1	A	204	GLU	HG13	0.843	0.000	.
1	A	204	GLU	HG21	1.016	0.000	.
1	A	204	GLU	HG22	1.016	0.000	.
1	A	204	GLU	HG23	1.016	0.000	.
1	A	204	GLU	CG1	21.654	0.000	.
1	A	204	GLU	CG2	23.679	0.000	.
1	A	205	SER	CD	49.304	0.000	.
1	A	205	SER	CG	27.632	0.000	.
1	A	205	SER	HG2	1.988	0.000	.
1	A	205	SER	HG3	2.14	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	205	SER	HD2	3.495	0.000	.
1	A	205	SER	HD3	4.076	0.000	.
1	A	207	VAL	HB1	1.467	0.000	.
1	A	207	VAL	HB2	1.467	0.000	.
1	A	207	VAL	HB3	1.467	0.000	.
1	A	208	PRO	H	8.207	0.000	1
1	A	208	PRO	HG11	0.985	0.000	.
1	A	208	PRO	HG12	0.985	0.000	.
1	A	208	PRO	HG13	0.985	0.000	.
1	A	208	PRO	HG21	0.92	0.000	.
1	A	208	PRO	HG22	0.92	0.000	.
1	A	208	PRO	HG23	0.92	0.000	.
1	A	208	PRO	CG1	20.871	0.000	.
1	A	208	PRO	CG2	22.02	0.000	.
1	A	209	ALA	CG	32.293	0.002	.
1	A	209	ALA	HG2	2.632	0.000	.
1	A	209	ALA	HG3	2.689	0.000	.
1	A	210	ALA	CG	26.696	0.000	.
1	A	210	ALA	HG	1.775	0.000	.
1	A	210	ALA	HD11	0.845	0.000	.
1	A	210	ALA	HD12	0.845	0.000	.
1	A	210	ALA	HD13	0.845	0.000	.
1	A	210	ALA	HD21	0.523	0.000	.
1	A	210	ALA	HD22	0.523	0.000	.
1	A	210	ALA	HD23	0.523	0.000	.
1	A	210	ALA	CD1	22.255	0.000	.
1	A	210	ALA	CD2	25.804	0.000	.
1	A	211	VAL	HA2	3.754	0.000	.
1	A	211	VAL	HA3	4.421	0.000	.
1	A	214	GLY	CB	31.953	0.000	.
1	A	214	GLY	HB	1.894	0.000	.
1	A	214	GLY	HG11	0.707	0.000	.
1	A	214	GLY	HG12	0.707	0.000	.
1	A	214	GLY	HG13	0.707	0.000	.
1	A	214	GLY	HG21	0.748	0.000	.
1	A	214	GLY	HG22	0.748	0.000	.
1	A	214	GLY	HG23	0.748	0.000	.
1	A	214	GLY	CG1	21.196	0.000	.
1	A	214	GLY	CG2	21.237	0.000	.
1	A	215	ALA	CG	26.425	0.000	.
1	A	215	ALA	HG	1.551	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	215	ALA	HD11	0.742	0.000	.
1	A	215	ALA	HD12	0.742	0.000	.
1	A	215	ALA	HD13	0.742	0.000	.
1	A	215	ALA	HD21	0.793	0.000	.
1	A	215	ALA	HD22	0.793	0.000	.
1	A	215	ALA	HD23	0.793	0.000	.
1	A	215	ALA	CD1	21.842	0.000	.
1	A	215	ALA	CD2	26.399	0.000	.
1	A	216	SER	CG	27.388	0.003	.
1	A	216	SER	HD11	1.07	0.000	.
1	A	216	SER	HD12	1.07	0.000	.
1	A	216	SER	HD13	1.07	0.000	.
1	A	216	SER	HD21	0.794	0.000	.
1	A	216	SER	HD22	0.794	0.000	.
1	A	216	SER	HD23	0.794	0.000	.
1	A	216	SER	CD1	23.304	0.002	.
1	A	216	SER	CD2	26.471	0.000	.
1	A	217	VAL	HB2	1.615	0.000	.
1	A	217	VAL	HB3	1.94	0.000	.
1	A	217	VAL	HG3	1.55	0.000	.
1	A	217	VAL	CD	43.385	0.000	.
1	A	217	VAL	HD2	3.134	0.000	.
1	A	217	VAL	HD3	3.134	0.000	.
1	A	217	VAL	HE	7.287	0.000	.
1	A	218	LEU	HE1	6.468	0.003	.
1	A	218	LEU	HE2	6.468	0.003	.
1	A	218	LEU	CE1	118.252	0.000	.
1	A	218	LEU	CE2	118.252	0.002	.
1	A	221	TYR	HG2	2.15	0.001	.
1	A	221	TYR	HG3	2.15	0.001	.
1	A	223	CYS	HA2	4.375	0.001	.
1	A	223	CYS	HA3	3.854	0.000	.
1	A	226	GLY	CB	34.647	0.000	.
1	A	226	GLY	HB	1.917	0.000	.
1	A	226	GLY	HG11	0.874	0.000	.
1	A	226	GLY	HG12	0.874	0.000	.
1	A	226	GLY	HG13	0.874	0.000	.
1	A	226	GLY	HG21	0.856	0.000	.
1	A	226	GLY	HG22	0.856	0.000	.
1	A	226	GLY	HG23	0.856	0.000	.
1	A	226	GLY	CG1	21.276	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	226	GLY	CG2	22.604	0.000	.
1	A	227	PRO	H	9.32	0.000	1
1	A	227	PRO	HG11	0.432	0.000	.
1	A	227	PRO	HG12	0.432	0.000	.
1	A	227	PRO	HG13	0.432	0.000	.
1	A	227	PRO	HG21	0.937	0.000	.
1	A	227	PRO	HG22	0.937	0.000	.
1	A	227	PRO	HG23	0.937	0.000	.
1	A	227	PRO	CG1	21.769	0.000	.
1	A	227	PRO	CG2	21.388	0.000	.
1	A	228	ALA	HG11	0.277	0.000	.
1	A	228	ALA	HG12	0.277	0.000	.
1	A	228	ALA	HG13	0.277	0.000	.
1	A	228	ALA	HG21	0.593	0.000	.
1	A	228	ALA	HG22	0.593	0.000	.
1	A	228	ALA	HG23	0.593	0.000	.
1	A	228	ALA	CG1	19.97	0.000	.
1	A	228	ALA	CG2	22.626	0.000	.
1	A	229	VAL	HB2	3.651	0.001	.
1	A	229	VAL	HB3	3.796	0.000	.
1	A	230	VAL	HB1	1.32	0.000	.
1	A	230	VAL	HB2	1.32	0.000	.
1	A	230	VAL	HB3	1.32	0.000	.
1	A	231	VAL	CD	49.864	0.001	.
1	A	231	VAL	HB2	1.805	0.000	.
1	A	231	VAL	HB3	2.183	0.000	.
1	A	231	VAL	HG3	1.74	0.000	.
1	A	231	VAL	HD2	3.735	0.000	.
1	A	231	VAL	HD3	3.735	0.000	.
1	A	232	SER	HA2	3.927	0.000	.
1	A	232	SER	HA3	4.06	0.000	.
1	A	233	ALA	HA2	3.495	0.000	.
1	A	233	ALA	HA3	4.483	0.000	.
1	A	234	PRO	H	9.852	0.000	1
1	A	235	GLY	CB	35.461	0.000	.
1	A	235	GLY	HB	2.124	0.000	.
1	A	235	GLY	HG11	0.419	0.000	.
1	A	235	GLY	HG12	0.419	0.000	.
1	A	235	GLY	HG13	0.419	0.000	.
1	A	235	GLY	HG21	1.029	0.000	.
1	A	235	GLY	HG22	1.029	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	235	GLY	HG23	1.029	0.000	.
1	A	235	GLY	CG1	22.968	0.000	.
1	A	235	GLY	CG2	21.895	0.000	.
1	A	236	GLY	CB	41.634	0.000	.
1	A	236	GLY	HB2	3.171	0.000	.
1	A	236	GLY	HB3	3.348	0.000	.
1	A	236	GLY	HD1	7.524	0.000	.
1	A	236	GLY	HD2	7.524	0.000	.
1	A	236	GLY	HE1	7.424	0.000	.
1	A	236	GLY	HE2	7.424	0.000	.
1	A	236	GLY	CD1	132.919	0.001	.
1	A	236	GLY	CE1	130.755	0.000	.
1	A	236	GLY	CZ	128.323	0.000	.
1	A	236	GLY	HZ	7.079	0.000	.
1	A	236	GLY	CE2	130.755	0.000	.
1	A	236	GLY	CD2	132.919	0.000	.
1	A	237	GLU	HG21	0.894	0.000	.
1	A	237	GLU	HG22	0.894	0.000	.
1	A	237	GLU	HG23	0.894	0.000	.
1	A	237	GLU	CG2	24.15	0.005	.
1	A	238	VAL	HB2	1.187	0.000	.
1	A	238	VAL	HB3	1.93	0.000	.
1	A	238	VAL	HD11	1.24	0.000	.
1	A	238	VAL	HD12	1.24	0.000	.
1	A	238	VAL	HD13	1.24	0.000	.
1	A	238	VAL	HD21	0.762	0.000	.
1	A	238	VAL	HD22	0.762	0.000	.
1	A	238	VAL	HD23	0.762	0.000	.
1	A	238	VAL	CD1	25.564	0.000	.
1	A	238	VAL	CD2	26.61	0.000	.
1	A	239	PHE	HG	1.213	0.000	.
1	A	239	PHE	HD11	0.551	0.000	.
1	A	239	PHE	HD12	0.551	0.000	.
1	A	239	PHE	HD13	0.551	0.000	.
1	A	239	PHE	HD21	0.638	0.000	.
1	A	239	PHE	HD22	0.638	0.000	.
1	A	239	PHE	HD23	0.638	0.000	.
1	A	240	THR	HB2	1.168	0.000	.
1	A	240	THR	HB3	1.918	0.000	.
1	A	240	THR	HD11	0.58	0.000	.
1	A	240	THR	HD12	0.58	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	240	THR	HD13	0.58	0.000	.
1	A	240	THR	HD21	0.827	0.000	.
1	A	240	THR	HD22	0.827	0.000	.
1	A	240	THR	HD23	0.827	0.000	.
1	A	240	THR	CD1	23.362	0.000	.
1	A	240	THR	CD2	25.714	0.000	.
1	A	241	LEU	HG21	1.093	0.000	.
1	A	241	LEU	HG22	1.093	0.000	.
1	A	241	LEU	HG23	1.093	0.000	.
1	A	241	LEU	CG2	20.804	0.000	.
1	A	301	WOZ	H1	3.722	0.000	1
1	A	301	WOZ	H2	6.735	0.000	1
1	A	301	WOZ	H3	6.197	0.000	1
1	A	301	WOZ	H4	6.016	0.000	1
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
1	A	301	WOZ	H10	2.435	0.000	1
1	A	301	WOZ	H11	2.435	0.000	1
1	A	301	WOZ	H9	2.435	0.000	1
1	A	301	WOZ	H19	0.737	0.000	.
1	A	301	WOZ	H20	0.737	0.000	.
1	A	301	WOZ	H21	0.737	0.000	.
1	A	301	WOZ	H22	0.573	0.000	.
1	A	301	WOZ	H23	0.573	0.000	.
1	A	301	WOZ	H24	0.573	0.000	.
1	A	301	WOZ	H13	12.835	0.000	1
1	A	301	WOZ	H14	10.192	0.000	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	241	0.25 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	173	-2.55 ± 0.63	Should be checked
$^{13}\text{C}'$	220	-0.03 ± 0.14	None needed (< 0.5 ppm)
^{15}N	217	-0.38 ± 0.73	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 60%, i.e. 1507 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	¹ H	¹³ C	¹⁵ N
Backbone	894/983 (91%)	359/406 (88%)	371/394 (94%)	164/183 (90%)
Sidechain	587/1317 (45%)	385/874 (44%)	202/403 (50%)	0/40 (0%)
Aromatic	26/200 (13%)	9/97 (9%)	17/97 (18%)	0/6 (0%)
Overall	1507/2500 (60%)	753/1377 (55%)	590/894 (66%)	164/229 (72%)

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	187	GLN	CD	49.76	173.59 – 185.85	-106.0
1	A	239	PHE	CD2	25.19	125.53 – 137.61	-88.1
1	A	239	PHE	CD1	23.81	125.33 – 137.83	-86.2
1	A	33	TYR	CD1	23.51	125.84 – 139.60	-79.4
1	A	162	TYR	CD1	23.78	125.84 – 139.60	-79.2
1	A	162	TYR	CD2	24.68	125.28 – 140.14	-72.7
1	A	33	TYR	CD2	26.21	125.28 – 140.14	-71.7
1	A	142	ILE	CD1	130.63	5.18 – 21.60	71.4
1	A	218	LEU	CD1	132.93	16.71 – 32.55	68.4
1	A	218	LEU	CD2	132.93	15.73 – 32.47	65.0
1	A	75	LEU	CD1	126.64	16.71 – 32.55	64.4
1	A	36	LEU	CD1	122.77	16.71 – 32.55	62.0
1	A	70	ASN	CG	27.12	164.52 – 188.90	-61.4
1	A	221	TYR	CD1	50.49	125.84 – 139.60	-59.8
1	A	18	TRP	CD1	22.32	117.34 – 135.80	-56.5
1	A	221	TYR	CD2	50.49	125.28 – 140.14	-55.3
1	A	18	TRP	CD2	25.60	118.40 – 137.65	-53.2
1	A	128	TRP	CD1	29.07	117.34 – 135.80	-52.8
1	A	128	TRP	CD2	29.07	118.40 – 137.65	-51.4
1	A	128	TRP	CG	25.30	101.31 – 120.62	-44.4
1	A	128	TRP	CE3	41.94	111.58 – 129.41	-44.1
1	A	18	TRP	CG	26.79	101.31 – 120.62	-43.6
1	A	239	PHE	CG	27.28	123.09 – 153.41	-36.6
1	A	200	PHE	CG	34.81	123.09 – 153.41	-34.1

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	170	PHE	CG	36.56	123.09 – 153.41	-33.5
1	A	37	PHE	CG	36.62	123.09 – 153.41	-33.5
1	A	162	TYR	CG	25.27	112.42 – 146.96	-30.2
1	A	157	THR	CB	18.00	61.12 – 78.27	-30.1
1	A	33	TYR	CG	25.90	112.42 – 146.96	-30.1
1	A	5	SER	CB	19.40	56.28 – 71.32	-29.5
1	A	221	TYR	CG	28.36	112.42 – 146.96	-29.3
1	A	154	ALA	CB	68.60	10.19 – 27.75	28.3
1	A	191	ALA	CB	66.63	10.19 – 27.75	27.1
1	A	171	ALA	CB	64.04	10.19 – 27.75	25.7
1	A	7	ASP	CG	27.18	149.18 – 208.82	-25.4
1	A	202	ALA	CB	62.46	10.19 – 27.75	24.8
1	A	75	LEU	HD11	7.49	-0.61 – 2.12	24.7
1	A	75	LEU	HD12	7.49	-0.61 – 2.12	24.7
1	A	75	LEU	HD13	7.49	-0.61 – 2.12	24.7
1	A	67	LEU	HD22	7.59	-0.65 – 2.13	24.7
1	A	66	ASP	CG	36.31	149.18 – 208.82	-23.9
1	A	237	GLU	CB	70.04	21.56 – 38.37	23.8
1	A	173	GLU	CB	69.86	21.56 – 38.37	23.7
1	A	40	GLU	CB	69.36	21.56 – 38.37	23.4
1	A	149	GLU	CB	68.65	21.56 – 38.37	23.0
1	A	23	THR	CB	30.82	61.12 – 78.27	-22.7
1	A	205	SER	CB	30.01	56.28 – 71.32	-22.5
1	A	67	LEU	HD21	6.88	-0.65 – 2.13	22.1
1	A	36	LEU	HD11	6.71	-0.61 – 2.12	21.8
1	A	36	LEU	HD12	6.71	-0.61 – 2.12	21.8
1	A	36	LEU	HD13	6.71	-0.61 – 2.12	21.8
1	A	60	GLU	CB	66.29	21.56 – 38.37	21.6
1	A	218	LEU	HD11	6.61	-0.61 – 2.12	21.4
1	A	218	LEU	HD12	6.61	-0.61 – 2.12	21.4
1	A	218	LEU	HD13	6.61	-0.61 – 2.12	21.4
1	A	121	SER	CB	31.89	56.28 – 71.32	-21.2
1	A	146	THR	CB	33.34	61.12 – 78.27	-21.2
1	A	218	LEU	HD21	6.61	-0.65 – 2.13	21.1
1	A	218	LEU	HD22	6.61	-0.65 – 2.13	21.1
1	A	218	LEU	HD23	6.61	-0.65 – 2.13	21.1
1	A	131	LYS	CB	68.67	24.03 – 41.47	20.6
1	A	52	THR	CB	35.04	61.12 – 78.27	-20.2
1	A	142	ILE	HD11	6.31	-0.72 – 2.09	20.0
1	A	142	ILE	HD12	6.31	-0.72 – 2.09	20.0
1	A	142	ILE	HD13	6.31	-0.72 – 2.09	20.0
1	A	30	LEU	HD11	6.19	-0.61 – 2.12	19.9

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	30	LEU	HD12	6.19	-0.61 – 2.12	19.9
1	A	30	LEU	HD13	6.19	-0.61 – 2.12	19.9
1	A	30	LEU	HD21	6.19	-0.65 – 2.13	19.6
1	A	30	LEU	HD22	6.19	-0.65 – 2.13	19.6
1	A	30	LEU	HD23	6.19	-0.65 – 2.13	19.6
1	A	31	GLN	CB	63.02	20.34 – 37.98	19.2
1	A	169	ASP	CB	70.91	32.98 – 48.76	19.0
1	A	20	ASP	CB	69.83	32.98 – 48.76	18.4
1	A	39	TRP	CB	65.14	20.06 – 39.75	17.9
1	A	229	VAL	CB	64.24	23.86 – 41.50	17.9
1	A	48	THR	CB	39.36	61.12 – 78.27	-17.7
1	A	21	LEU	CD1	52.42	16.71 – 32.55	17.6
1	A	240	THR	CB	39.78	61.12 – 78.27	-17.4
1	A	21	LEU	CD2	52.42	15.73 – 32.47	16.9
1	A	43	THR	CB	41.33	61.12 – 78.27	-16.5
1	A	102	LEU	CD1	50.35	16.71 – 32.55	16.2
1	A	133	HIS	CB	64.23	19.76 – 40.75	16.2
1	A	136	SER	CB	39.84	56.28 – 71.32	-15.9
1	A	155	SER	CB	39.99	56.28 – 71.32	-15.8
1	A	102	LEU	CD2	50.35	15.73 – 32.47	15.7
1	A	143	GLY	CA	65.49	38.93 – 51.79	15.7
1	A	148	SER	CB	40.33	56.28 – 71.32	-15.6
1	A	241	LEU	CB	70.54	33.11 – 51.34	15.5
1	A	100	ALA	CB	46.09	10.19 – 27.75	15.4
1	A	194	SER	CB	40.88	56.28 – 71.32	-15.2
1	A	174	SER	CB	41.23	56.28 – 71.32	-15.0
1	A	34	SER	CB	41.30	56.28 – 71.32	-15.0
1	A	163	ARG	HD2	6.53	1.97 – 4.26	14.9
1	A	63	SER	CB	41.51	56.28 – 71.32	-14.8
1	A	46	ASP	CB	64.20	32.98 – 48.76	14.8
1	A	98	GLY	CA	64.26	38.93 – 51.79	14.7
1	A	128	TRP	CE2	41.94	105.29 – 170.61	-14.7
1	A	146	THR	CG2	37.66	16.06 – 27.03	14.7
1	A	14	GLY	CA	64.24	38.93 – 51.79	14.7
1	A	41	PHE	CB	69.72	29.72 – 50.07	14.7
1	A	86	ASP	CB	17.79	32.98 – 48.76	-14.6
1	A	88	ASP	CB	18.02	32.98 – 48.76	-14.5
1	A	68	GLY	CA	63.91	38.93 – 51.79	14.4
1	A	18	TRP	HB2	-1.65	1.51 – 4.87	-14.4
1	A	214	GLY	CA	63.80	38.93 – 51.79	14.3
1	A	58	GLY	CA	63.67	38.93 – 51.79	14.2
1	A	215	ALA	CB	43.92	10.19 – 27.75	14.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	25	ASP	CB	18.56	32.98 – 48.76	-14.1
1	A	83	SER	CB	42.72	56.28 – 71.32	-14.0
1	A	147	ARG	HB2	-1.79	0.52 – 3.08	-14.0
1	A	135	GLY	CA	63.28	38.93 – 51.79	13.9
1	A	107	ASP	CB	19.22	32.98 – 48.76	-13.7
1	A	159	GLY	CA	62.94	38.93 – 51.79	13.7
1	A	79	SER	CB	43.30	56.28 – 71.32	-13.6
1	A	210	ALA	CB	42.59	10.19 – 27.75	13.4
1	A	163	ARG	HD3	6.53	1.81 – 4.39	13.3
1	A	147	ARG	HB3	-1.79	0.43 – 3.11	-13.3
1	A	11	PRO	CA	43.89	55.85 – 70.84	-13.0
1	A	145	TYR	CB	66.66	28.67 – 49.81	13.0
1	A	151	LEU	CB	18.59	33.11 – 51.34	-13.0
1	A	213	LEU	CB	65.73	33.11 – 51.34	12.9
1	A	195	GLY	CA	61.90	38.93 – 51.79	12.9
1	A	138	PRO	CA	44.28	55.85 – 70.84	-12.7
1	A	108	ILE	CG2	34.22	10.93 – 24.12	12.7
1	A	225	ASP	CB	20.98	32.98 – 48.76	-12.6
1	A	165	LEU	CB	19.32	33.11 – 51.34	-12.6
1	A	111	GLN	HE21	1.75	5.02 – 9.43	-12.4
1	A	235	GLY	CA	61.30	38.93 – 51.79	12.4
1	A	111	GLN	HE22	1.75	4.88 – 9.19	-12.2
1	A	226	GLY	CA	61.01	38.93 – 51.79	12.2
1	A	122	GLY	CA	60.97	38.93 – 51.79	12.1
1	A	127	LEU	CB	20.13	33.11 – 51.34	-12.1
1	A	95	PRO	CA	45.25	55.85 – 70.84	-12.1
1	A	216	SER	CB	45.70	56.28 – 71.32	-12.0
1	A	131	LYS	HB2	4.61	0.58 – 2.97	11.8
1	A	79	SER	HB2	0.89	2.61 – 5.13	-11.8
1	A	73	PRO	CA	45.77	55.85 – 70.84	-11.7
1	A	56	LEU	CD1	43.00	16.71 – 32.55	11.6
1	A	29	ALA	CB	39.25	10.19 – 27.75	11.6
1	A	167	GLY	CA	60.14	38.93 – 51.79	11.5
1	A	154	ALA	HB1	4.16	0.14 – 2.58	11.5
1	A	154	ALA	HB2	4.16	0.14 – 2.58	11.5
1	A	154	ALA	HB3	4.16	0.14 – 2.58	11.5
1	A	237	GLU	HB2	4.36	1.00 – 3.05	11.4
1	A	221	TYR	HD1	3.65	5.49 – 8.39	-11.4
1	A	221	TYR	HD2	3.65	5.48 – 8.39	-11.3
1	A	56	LEU	CD2	43.00	15.73 – 32.47	11.3
1	A	18	TRP	HB3	-0.96	1.31 – 4.93	-11.3
1	A	237	GLU	HB3	4.36	0.95 – 3.05	11.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	128	TRP	HE3	2.73	5.27 – 9.37	-11.2
1	A	131	LYS	HB3	4.61	0.46 – 3.04	11.1
1	A	71	PRO	CB	19.09	26.06 – 37.61	-11.0
1	A	202	ALA	HB3	4.05	0.14 – 2.58	11.0
1	A	173	GLU	HB2	4.26	1.00 – 3.05	10.9
1	A	97	LEU	CB	22.37	33.11 – 51.34	-10.9
1	A	120	PRO	HD2	7.40	1.93 – 5.38	10.9
1	A	34	SER	HB2	1.15	2.61 – 5.13	-10.8
1	A	173	GLU	HB3	4.26	0.95 – 3.05	10.8
1	A	21	LEU	HD21	3.69	-0.65 – 2.13	10.6
1	A	21	LEU	HD22	3.69	-0.65 – 2.13	10.6
1	A	21	LEU	HD23	3.69	-0.65 – 2.13	10.6
1	A	118	GLY	CA	58.90	38.93 – 51.79	10.5
1	A	191	ALA	HB3	3.93	0.14 – 2.58	10.5
1	A	32	PHE	CB	18.51	29.72 – 50.07	-10.5
1	A	24	PRO	CA	47.63	55.85 – 70.84	-10.5
1	A	76	GLY	CA	58.80	38.93 – 51.79	10.4
1	A	77	GLY	CA	58.80	38.93 – 51.79	10.4
1	A	197	TYR	CZ	128.95	143.41 – 170.10	-10.4
1	A	171	ALA	HB3	3.89	0.14 – 2.58	10.4
1	A	202	ALA	HB2	3.88	0.14 – 2.58	10.3
1	A	27	GLY	CA	58.37	38.93 – 51.79	10.1
1	A	171	ALA	HB2	3.81	0.14 – 2.58	10.1
1	A	40	GLU	HB2	4.08	1.00 – 3.05	10.1
1	A	191	ALA	HB2	3.79	0.14 – 2.58	10.0
1	A	60	GLU	HB3	4.09	0.95 – 3.05	10.0
1	A	40	GLU	HB3	4.08	0.95 – 3.05	9.9
1	A	5	SER	HB2	1.38	2.61 – 5.13	-9.9
1	A	60	GLU	HB2	4.03	1.00 – 3.05	9.8
1	A	102	LEU	HD21	3.46	-0.65 – 2.13	9.8
1	A	102	LEU	HD22	3.46	-0.65 – 2.13	9.8
1	A	102	LEU	HD23	3.46	-0.65 – 2.13	9.8
1	A	216	SER	HB2	1.43	2.61 – 5.13	-9.7
1	A	225	ASP	HB2	0.20	1.41 – 4.01	-9.7
1	A	193	PRO	HD3	7.21	1.76 – 5.48	9.7
1	A	207	VAL	CB	16.23	23.86 – 41.50	-9.3
1	A	148	SER	HB2	1.53	2.61 – 5.13	-9.3
1	A	225	ASP	HB3	0.20	1.32 – 4.00	-9.2
1	A	5	SER	HB3	1.38	2.49 – 5.20	-9.1
1	A	197	TYR	CE2	129.20	111.68 – 124.17	9.0
1	A	228	ALA	CB	34.75	10.19 – 27.75	9.0
1	A	56	LEU	HD21	3.21	-0.65 – 2.13	8.9

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	56	LEU	HD22	3.21	-0.65 – 2.13	8.9
1	A	56	LEU	HD23	3.21	-0.65 – 2.13	8.9
1	A	178	GLY	CA	56.77	38.93 – 51.79	8.9
1	A	216	SER	HB3	1.46	2.49 – 5.20	-8.8
1	A	31	GLN	HB2	4.23	0.80 – 3.29	8.8
1	A	31	GLN	HB3	4.30	0.71 – 3.33	8.7
1	A	113	ARG	CB	46.06	21.74 – 39.52	8.7
1	A	236	GLY	CA	56.38	38.93 – 51.79	8.6
1	A	84	VAL	CB	17.84	23.86 – 41.50	-8.4
1	A	91	ALA	CA	69.34	43.52 – 62.81	8.4
1	A	197	TYR	CE1	129.20	111.24 – 124.66	8.4
1	A	130	ALA	CB	33.53	10.19 – 27.75	8.3
1	A	38	GLY	CA	55.99	38.93 – 51.79	8.3
1	A	9	VAL	CB	18.18	23.86 – 41.50	-8.2
1	A	110	ALA	CB	33.21	10.19 – 27.75	8.1
1	A	121	SER	HB2	1.87	2.61 – 5.13	-7.9
1	A	99	GLY	CA	55.56	38.93 – 51.79	7.9
1	A	112	GLY	CA	55.55	38.93 – 51.79	7.9
1	A	149	GLU	HB2	3.65	1.00 – 3.05	7.9
1	A	230	VAL	CB	18.72	23.86 – 41.50	-7.9
1	A	79	SER	HB3	1.71	2.49 – 5.20	-7.9
1	A	153	GLY	CA	55.52	38.93 – 51.79	7.9
1	A	205	SER	HB2	1.88	2.61 – 5.13	-7.9
1	A	1	GLY	CA	55.45	38.93 – 51.79	7.8
1	A	149	GLU	HB3	3.65	0.95 – 3.05	7.8
1	A	188	VAL	CB	18.88	23.86 – 41.50	-7.8
1	A	70	ASN	HD21	3.63	4.94 – 9.72	-7.8
1	A	162	TYR	HB2	0.11	1.09 – 4.72	-7.7
1	A	33	TYR	HB2	0.11	1.09 – 4.72	-7.7
1	A	241	LEU	HB2	4.19	-0.07 – 3.30	7.7
1	A	10	ARG	CD	50.18	38.57 – 47.75	7.7
1	A	148	SER	HB3	1.78	2.49 – 5.20	-7.6
1	A	130	ALA	HB3	3.21	0.14 – 2.58	7.6
1	A	29	ALA	HB3	3.19	0.14 – 2.58	7.5
1	A	241	LEU	HB3	4.19	-0.26 – 3.31	7.5
1	A	209	ALA	CB	32.02	10.19 – 27.75	7.4
1	A	8	ALA	CB	31.99	10.19 – 27.75	7.4
1	A	201	ARG	CG	36.03	21.24 – 33.19	7.4
1	A	234	PRO	CG	35.34	21.69 – 32.72	7.4
1	A	106	ILE	CG2	27.17	10.93 – 24.12	7.3
1	A	146	THR	HG21	2.68	0.08 – 2.19	7.3
1	A	146	THR	HG22	2.68	0.08 – 2.19	7.3

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	146	THR	HG23	2.68	0.08 – 2.19	7.3
1	A	146	THR	HG3	2.68	0.08 – 2.19	7.3
1	A	130	ALA	HB2	3.14	0.14 – 2.58	7.3
1	A	198	PRO	CD	42.73	45.11 – 55.58	-7.3
1	A	117	ALA	CB	31.60	10.19 – 27.75	7.2
1	A	26	ARG	CB	17.91	21.74 – 39.52	-7.2
1	A	70	ASN	HD22	3.63	4.69 – 9.61	-7.2
1	A	124	ARG	CB	43.34	21.74 – 39.52	7.2
1	A	12	ALA	CB	31.49	10.19 – 27.75	7.1
1	A	104	GLY	CA	54.38	38.93 – 51.79	7.0
1	A	33	TYR	HB3	0.20	0.93 – 4.76	-6.9
1	A	71	PRO	CA	53.00	55.85 – 70.84	-6.9
1	A	66	ASP	CB	30.03	32.98 – 48.76	-6.9
1	A	103	LEU	CD1	13.79	16.71 – 32.55	-6.8
1	A	121	SER	HB3	1.99	2.49 – 5.20	-6.8
1	A	179	GLY	CA	54.16	38.93 – 51.79	6.8
1	A	92	ALA	CB	30.95	10.19 – 27.75	6.8
1	A	72	GLY	CA	54.13	38.93 – 51.79	6.8
1	A	96	GLU	CA	43.29	47.03 – 67.62	-6.8
1	A	183	ALA	CB	30.80	10.19 – 27.75	6.7
1	A	64	ILE	CG2	26.30	10.93 – 24.12	6.7
1	A	176	THR	CA	45.16	49.41 – 75.05	-6.7
1	A	238	VAL	CB	44.33	23.86 – 41.50	6.6
1	A	134	THR	CA	45.33	49.41 – 75.05	-6.6
1	A	44	THR	CA	45.35	49.41 – 75.05	-6.6
1	A	7	ASP	CB	30.58	32.98 – 48.76	-6.5
1	A	117	ALA	CA	65.75	43.52 – 62.81	6.5
1	A	101	VAL	CA	44.12	48.38 – 76.73	-6.5
1	A	50	PRO	CA	53.62	55.85 – 70.84	-6.5
1	A	172	THR	CA	45.58	49.41 – 75.05	-6.5
1	A	91	ALA	CB	30.30	10.19 – 27.75	6.5
1	A	94	VAL	CB	44.03	23.86 – 41.50	6.4
1	A	144	ALA	CB	30.23	10.19 – 27.75	6.4
1	A	64	ILE	CD1	23.91	5.18 – 21.60	6.4
1	A	154	ALA	CA	65.50	43.52 – 62.81	6.4
1	A	75	LEU	CB	30.64	33.11 – 51.34	-6.4
1	A	232	SER	CA	45.76	48.46 – 68.96	-6.3
1	A	29	ALA	HB2	2.90	0.14 – 2.58	6.3
1	A	108	ILE	HG3	2.45	-0.56 – 2.11	6.2
1	A	160	ALA	CB	29.95	10.19 – 27.75	6.2
1	A	211	VAL	CA	44.97	48.38 – 76.73	-6.2
1	A	36	LEU	CB	30.98	33.11 – 51.34	-6.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	162	TYR	HB3	0.48	0.93 – 4.76	-6.2
1	A	163	ARG	CB	41.55	21.74 – 39.52	6.1
1	A	213	LEU	HB3	3.71	-0.26 – 3.31	6.1
1	A	53	MET	CB	45.93	22.22 – 43.61	6.1
1	A	92	ALA	CA	64.87	43.52 – 62.81	6.1
1	A	169	ASP	HB3	4.29	1.32 – 4.00	6.1
1	A	187	GLN	CG	27.20	28.36 – 39.21	-6.1
1	A	52	THR	CG2	28.19	16.06 – 27.03	6.1
1	A	169	ASP	HB2	4.29	1.41 – 4.01	6.1
1	A	205	SER	HB3	2.21	2.49 – 5.20	-6.1
1	A	128	TRP	HB2	1.16	1.51 – 4.87	-6.0
1	A	185	ILE	CG1	17.53	19.24 – 36.26	-6.0
1	A	213	LEU	HB2	3.63	-0.07 – 3.30	6.0
1	A	19	VAL	CB	43.23	23.86 – 41.50	6.0
1	A	75	LEU	HB3	3.66	-0.26 – 3.31	6.0
1	A	163	ARG	HB3	3.36	0.43 – 3.11	6.0
1	A	115	LEU	CA	43.26	45.17 – 66.21	-5.9
1	A	83	SER	HB2	2.40	2.61 – 5.13	-5.8
1	A	132	GLU	CA	45.32	47.03 – 67.62	-5.8
1	A	106	ILE	CD1	22.95	5.18 – 21.60	5.8
1	A	220	ARG	HB3	3.33	0.43 – 3.11	5.8
1	A	69	GLU	CA	45.38	47.03 – 67.62	-5.8
1	A	93	ALA	CB	29.14	10.19 – 27.75	5.8
1	A	108	ILE	HG21	2.33	-0.56 – 2.11	5.8
1	A	108	ILE	HG22	2.33	-0.56 – 2.11	5.8
1	A	108	ILE	HG23	2.33	-0.56 – 2.11	5.8
1	A	126	GLY	N	130.33	91.59 – 127.52	5.8
1	A	137	GLY	CA	52.79	38.93 – 51.79	5.8
1	A	95	PRO	N	105.09	108.67 – 162.11	-5.7
1	A	18	TRP	CB	40.95	20.06 – 39.75	5.6
1	A	126	GLY	CA	52.53	38.93 – 51.79	5.6
1	A	28	ALA	CB	28.70	10.19 – 27.75	5.5
1	A	239	PHE	HB2	1.01	1.20 – 4.80	-5.5
1	A	21	LEU	CB	32.20	33.11 – 51.34	-5.5
1	A	61	VAL	CB	42.34	23.86 – 41.50	5.5
1	A	70	ASN	CA	63.65	44.28 – 62.79	5.5
1	A	147	ARG	CB	40.32	21.74 – 39.52	5.5
1	A	186	ARG	CA	44.48	45.44 – 68.13	-5.4
1	A	204	GLU	CA	68.47	47.03 – 67.62	5.4
1	A	212	MET	CB	21.40	22.22 – 43.61	-5.4
1	A	24	PRO	N	106.76	108.67 – 162.11	-5.4
1	A	122	GLY	N	128.72	91.59 – 127.52	5.3

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	56	LEU	CB	32.53	33.11 – 51.34	-5.3
1	A	182	ARG	CB	40.09	21.74 – 39.52	5.3
1	A	138	PRO	N	107.16	108.67 – 162.11	-5.3
1	A	25	ASP	HB2	1.34	1.41 – 4.01	-5.3
1	A	99	GLY	N	128.50	91.59 – 127.52	5.3
1	A	73	PRO	N	107.48	108.67 – 162.11	-5.2
1	A	203	GLN	CB	19.96	20.34 – 37.98	-5.2
1	A	184	ALA	CB	28.12	10.19 – 27.75	5.2
1	A	49	SER	CB	71.62	56.28 – 71.32	5.2
1	A	51	TYR	CB	28.27	28.67 – 49.81	-5.2
1	A	217	VAL	CG1	28.54	14.71 – 28.29	5.2
1	A	86	ASP	HB2	1.36	1.41 – 4.01	-5.2
1	A	63	SER	HB2	2.57	2.61 – 5.13	-5.2
1	A	107	ASP	HB2	1.37	1.41 – 4.01	-5.2
1	A	8	ALA	CA	63.05	43.52 – 62.81	5.1
1	A	120	PRO	CA	55.66	55.85 – 70.84	-5.1
1	A	143	GLY	N	127.83	91.59 – 127.52	5.1
1	A	123	HIS	CA	44.85	45.04 – 67.94	-5.1
1	A	109	LEU	CA	45.05	45.17 – 66.21	-5.1
1	A	78	TRP	HE1	6.87	6.88 – 13.28	-5.0
1	A	38	GLY	HA3	5.71	2.08 – 5.71	5.0
1	A	55	ARG	CA	45.43	45.44 – 68.13	-5.0

7.1.5 Random Coil Index (RCI) plots

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:

