



wwPDB NMR Structure Validation Summary Report i

Mar 25, 2024 – 06:07 PM EDT

PDB ID : 8EO9
BMRB ID : 31044
Title : The solution structure of abxF, an enzyme catalyzing the formation of chiral spiroketal of an antibiotics, (-)-ABX
Authors : Jia, X.; Yan, X.; Mobli, M.; Qu, X.
Deposited on : 2022-10-02

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

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

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

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

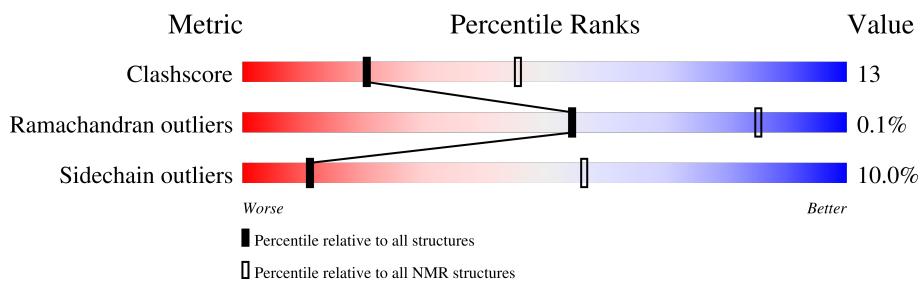
MolProbitiy : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

1 Overall quality at a glance

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

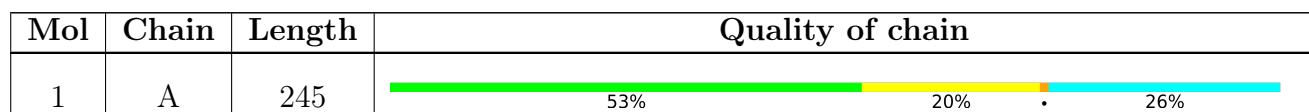
The overall completeness of chemical shifts assignment is 4%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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%



2 Ensemble composition and analysis [\(i\)](#)

This entry contains 20 models. Model 6 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:14-A:39, A:48-A:63, A:74-A:102, A:111-A:126, A:138-A:167, A:179-A:242 (181)	0.88	6

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. No single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 3460 atoms, of which 1688 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	3460	1110	1688	307	347	8	0

There are 3 discrepancies between the modelled and reference sequences:

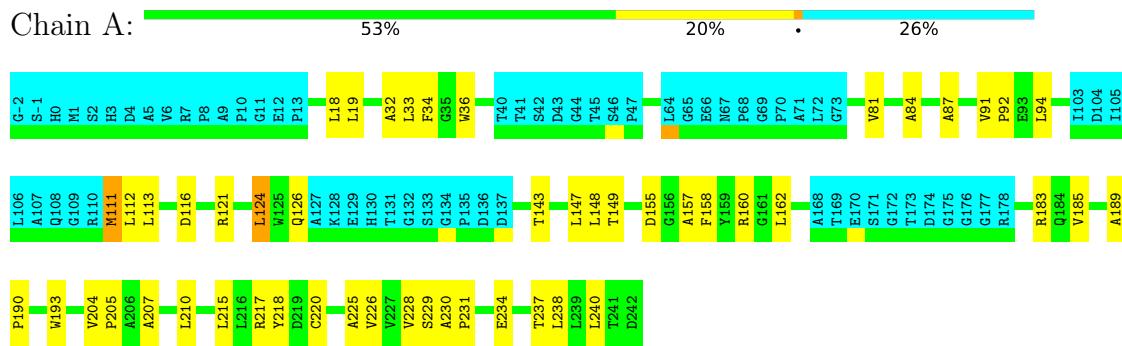
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A2I6B3F9
A	-1	SER	-	expression tag	UNP A0A2I6B3F9
A	0	HIS	-	expression tag	UNP A0A2I6B3F9

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



5 Refinement protocol and experimental data overview i

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

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

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

Software name	Classification	Version
CYANA	refinement	3.98.13
CYANA	structure calculation	3.98.13

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	2702
Number of shifts mapped to atoms	135
Number of unparsed shifts	0
Number of shifts with mapping errors	2567
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

6 Model quality [\(i\)](#)

6.1 Standard geometry [\(i\)](#)

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	1335	1290	1290	35±5
All	All	26700	25800	25800	708

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 13.

5 of 158 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:VAL:HG21	1:A:238:LEU:HD12	0.92	1.40	10	13
1:A:33:LEU:HD11	1:A:207:ALA:HB2	0.88	1.40	14	17
1:A:32:ALA:HB3	1:A:210:LEU:HD11	0.80	1.52	7	19
1:A:84:ALA:HB1	1:A:112:LEU:HD23	0.77	1.53	18	5
1:A:215:LEU:HD23	1:A:227:VAL:HG12	0.76	1.54	18	8

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	180/245 (73%)	167±2 (93±1%)	12±2 (7±1%)	0±0 (0±0%)	54 85
All	All	3600/4900 (73%)	3347 (93%)	250 (7%)	3 (0%)	54 85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	74	GLY	3

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	131/176 (74%)	118±2 (90±2%)	13±2 (10±2%)	11 56
All	All	2620/3520 (74%)	2357 (90%)	263 (10%)	11 56

5 of 45 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	111	MET	20
1	A	220	CYS	20
1	A	124	LEU	19
1	A	34	PHE	17
1	A	160	ARG	16

6.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

6.7 Other polymers [\(i\)](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 4% 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	2702
Number of shifts mapped to atoms	135
Number of unparsed shifts	0
Number of shifts with mapping errors	2567
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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 2567) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	MET	N	121.802	0.000	1
1	A	4	MET	H	8.377	0.000	1
1	A	4	MET	CA	55.448	0.000	1
1	A	4	MET	HA	4.46	0.000	1
1	A	4	MET	CB	32.986	0.000	1
1	A	4	MET	HB2	1.924	0.000	2
1	A	4	MET	HB3	2.037	0.004	2
1	A	4	MET	CG	31.867	0.001	1
1	A	4	MET	HG2	2.496	0.000	2
1	A	4	MET	HG3	2.429	0.000	2
1	A	4	MET	C	176.012	0.000	1
1	A	5	SER	N	117.042	0.000	1
1	A	5	SER	H	8.354	0.000	1
1	A	5	SER	CA	58.289	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	SER	HA	4.406	0.003	1
1	A	5	SER	CB	63.867	0.000	1
1	A	5	SER	HB2	3.845	0.000	2
1	A	5	SER	HB3	3.845	0.000	2
1	A	5	SER	C	174.488	0.000	1
1	A	6	HIS	N	120.939	0.001	1
1	A	6	HIS	H	8.479	0.000	1
1	A	6	HIS	CA	56.044	0.000	1
1	A	6	HIS	HA	4.673	0.000	1
1	A	6	HIS	CB	29.926	0.005	1
1	A	6	HIS	HB2	3.124	0.006	2
1	A	6	HIS	HB3	3.249	0.009	2
1	A	6	HIS	CD2	120.079	0.000	1
1	A	6	HIS	HD2	7.165	0.000	1
1	A	7	ASP	N	121.055	0.001	1
1	A	7	ASP	H	8.285	0.000	1
1	A	7	ASP	CA	54.363	0.002	1
1	A	7	ASP	HA	4.568	0.000	1
1	A	7	ASP	CB	41.253	0.001	1
1	A	7	ASP	HB2	2.571	0.002	2
1	A	7	ASP	HB3	2.684	0.002	2
1	A	7	ASP	C	175.706	0.005	1
1	A	8	ALA	N	124.042	0.001	1
1	A	8	ALA	H	8.151	0.000	1
1	A	8	ALA	CA	52.427	0.001	1
1	A	8	ALA	HA	4.336	0.000	1
1	A	8	ALA	HB1	1.359	0.000	1
1	A	8	ALA	HB2	1.359	0.000	1
1	A	8	ALA	HB3	1.359	0.000	1
1	A	8	ALA	CB	19.463	0.000	1
1	A	8	ALA	C	177.409	0.004	1
1	A	9	VAL	N	119.664	0.000	1
1	A	9	VAL	H	8.142	0.000	1
1	A	9	VAL	CA	62.233	0.001	1
1	A	9	VAL	HA	4.104	0.000	1
1	A	9	VAL	CB	32.783	0.003	1
1	A	9	VAL	HB	2.035	0.000	1
1	A	9	VAL	HG11	0.914	0.000	2
1	A	9	VAL	HG12	0.914	0.000	2
1	A	9	VAL	HG13	0.914	0.000	2
1	A	9	VAL	HG21	0.914	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	VAL	HG22	0.914	0.000	2
1	A	9	VAL	HG23	0.914	0.000	2
1	A	9	VAL	CG1	20.443	0.000	1
1	A	9	VAL	CG2	21.244	0.000	1
1	A	9	VAL	C	175.615	0.004	1
1	A	10	ARG	N	125.495	0.001	1
1	A	10	ARG	H	8.297	0.000	1
1	A	10	ARG	CA	53.757	0.000	1
1	A	10	ARG	HA	4.608	0.000	1
1	A	10	ARG	CB	30.586	0.003	1
1	A	10	ARG	HB2	1.7	0.003	2
1	A	10	ARG	HB3	1.833	0.001	2
1	A	10	ARG	CG	26.922	0.000	1
1	A	10	ARG	HG2	1.65	0.000	2
1	A	10	ARG	HG3	1.65	0.000	2
1	A	10	ARG	CD	43.378	0.001	1
1	A	10	ARG	HD2	3.219	0.001	2
1	A	10	ARG	HD3	3.219	0.001	2
1	A	10	ARG	C	173.772	0.000	1
1	A	11	PRO	CA	62.736	0.000	1
1	A	11	PRO	HA	4.453	0.000	1
1	A	11	PRO	CB	31.978	0.000	1
1	A	11	PRO	HB2	2.208	0.000	2
1	A	11	PRO	HB3	2.208	0.000	2
1	A	11	PRO	CG	27.48	0.000	1
1	A	11	PRO	HG2	1.952	0.000	2
1	A	11	PRO	HG3	1.952	0.000	2
1	A	11	PRO	CD	50.761	0.000	1
1	A	11	PRO	HD2	3.688	0.000	2
1	A	11	PRO	HD3	3.688	0.000	2
1	A	11	PRO	C	176.382	0.000	1
1	A	12	ALA	N	128.054	0.000	1
1	A	12	ALA	H	8.449	0.000	1
1	A	12	ALA	CA	50.327	0.002	1
1	A	12	ALA	HA	4.593	0.004	1
1	A	12	ALA	HB1	1.44	0.000	1
1	A	12	ALA	HB2	1.44	0.000	1
1	A	12	ALA	HB3	1.44	0.000	1
1	A	12	ALA	CB	17.983	0.003	1
1	A	12	ALA	C	174.781	0.000	1
1	A	14	GLY	N	116.224	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	GLY	H	9.601	0.001	1
1	A	14	GLY	CA	43.836	0.000	1
1	A	14	GLY	HA2	3.321	0.000	2
1	A	14	GLY	HA3	3.321	0.000	2
1	A	14	GLY	C	173.927	0.000	1
1	A	15	GLU	N	123.523	0.000	1
1	A	15	GLU	H	8.228	0.000	1
1	A	15	GLU	CA	55.098	0.003	1
1	A	15	GLU	HA	4.457	0.001	1
1	A	15	GLU	CB	31.652	0.000	1
1	A	15	GLU	HB2	2.091	0.000	2
1	A	15	GLU	HB3	2.249	0.000	2
1	A	15	GLU	CG	35.947	0.000	1
1	A	15	GLU	HG2	2.574	0.000	2
1	A	15	GLU	HG3	2.574	0.000	2
1	A	15	GLU	C	176.125	0.000	1
1	A	16	PRO	CA	63.91	0.001	1
1	A	16	PRO	HA	4.78	0.000	1
1	A	16	PRO	C	175.976	0.000	1
1	A	17	THR	N	119.156	0.003	1
1	A	17	THR	H	8.929	0.000	1
1	A	17	THR	CA	62.791	0.002	1
1	A	17	THR	HA	4.773	0.000	1
1	A	17	THR	CB	71.52	0.000	1
1	A	17	THR	HB	3.969	0.000	1
1	A	17	THR	HG21	1.145	0.000	1
1	A	17	THR	HG22	1.145	0.000	1
1	A	17	THR	HG23	1.145	0.000	1
1	A	17	THR	CG2	22.424	0.000	1
1	A	17	THR	C	172.64	0.000	1
1	A	18	TRP	N	121.501	0.000	1
1	A	18	TRP	H	7.848	0.000	1
1	A	18	TRP	CA	55.605	0.000	1
1	A	18	TRP	CB	32.327	0.000	1
1	A	18	TRP	CD1	127.797	0.000	1
1	A	18	TRP	NE1	130.322	0.000	1
1	A	18	TRP	HD1	5.932	0.000	1
1	A	18	TRP	CZ2	114.298	0.000	1
1	A	18	TRP	HE1	9.741	0.000	1
1	A	18	TRP	HZ2	6.97	0.000	1
1	A	18	TRP	C	171.639	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	VAL	N	116.677	0.000	1
1	A	19	VAL	H	8.443	0.000	1
1	A	19	VAL	CA	58.356	0.001	1
1	A	19	VAL	HA	5.224	0.000	1
1	A	19	VAL	CB	35.602	0.003	1
1	A	19	VAL	HB	1.849	0.000	1
1	A	19	VAL	HG11	0.076	0.000	2
1	A	19	VAL	HG12	0.076	0.000	2
1	A	19	VAL	HG13	0.076	0.000	2
1	A	19	VAL	HG21	0.443	0.000	2
1	A	19	VAL	HG22	0.443	0.000	2
1	A	19	VAL	HG23	0.443	0.000	2
1	A	19	VAL	CG1	18.227	0.001	1
1	A	19	VAL	CG2	23.555	0.000	1
1	A	21	LEU	CA	53.082	0.005	1
1	A	21	LEU	HA	4.308	0.002	1
1	A	21	LEU	CB	42.893	0.001	1
1	A	21	LEU	HB2	-1.285	0.000	2
1	A	21	LEU	HB3	-1.285	0.000	2
1	A	21	LEU	CG	26.872	0.002	1
1	A	21	LEU	HG	0.635	0.001	1
1	A	21	LEU	HD11	-0.075	0.000	2
1	A	21	LEU	HD12	-0.075	0.000	2
1	A	21	LEU	HD13	-0.075	0.000	2
1	A	21	LEU	HD21	0.346	0.000	2
1	A	21	LEU	HD22	0.346	0.000	2
1	A	21	LEU	HD23	0.346	0.000	2
1	A	21	LEU	CD1	22.221	0.000	1
1	A	21	LEU	CD2	25.631	0.000	1
1	A	21	LEU	C	174.367	0.000	1
1	A	22	LEU	N	125.348	0.000	1
1	A	22	LEU	H	7.447	0.000	1
1	A	22	LEU	CA	52.851	0.000	1
1	A	22	LEU	HA	4.858	0.000	1
1	A	22	LEU	CB	43.273	0.005	1
1	A	22	LEU	HB2	0.88	0.001	2
1	A	22	LEU	HB3	1.801	0.001	2
1	A	22	LEU	CG	26.129	0.000	1
1	A	22	LEU	HG	1.66	0.000	1
1	A	22	LEU	HD11	0.669	0.002	2
1	A	22	LEU	HD12	0.669	0.002	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	LEU	HD13	0.669	0.002	2
1	A	22	LEU	HD21	0.88	0.001	2
1	A	22	LEU	HD22	0.88	0.001	2
1	A	22	LEU	HD23	0.88	0.001	2
1	A	22	LEU	CD1	22.926	0.004	1
1	A	22	LEU	CD2	25.653	0.000	1
1	A	22	LEU	C	175.687	0.001	1
1	A	23	THR	N	117.617	0.000	1
1	A	23	THR	H	8.496	0.000	1
1	A	23	THR	CA	55.787	0.000	1
1	A	23	THR	HA	5.228	0.000	1
1	A	23	THR	CB	70.036	0.000	1
1	A	23	THR	HB	3.781	0.000	1
1	A	23	THR	HG21	0.974	0.000	1
1	A	23	THR	HG22	0.974	0.000	1
1	A	23	THR	HG23	0.974	0.000	1
1	A	23	THR	CG2	19.176	0.003	1
1	A	23	THR	C	172.273	0.000	1
1	A	24	PRO	CA	64.062	0.000	1
1	A	24	PRO	HA	4.804	0.000	1
1	A	24	PRO	CB	32.306	0.001	1
1	A	24	PRO	HB2	2.362	0.000	1
1	A	24	PRO	HB3	2.088	0.002	1
1	A	24	PRO	CG	26.973	0.007	1
1	A	24	PRO	HG2	2.056	0.005	2
1	A	24	PRO	HG3	2.056	0.005	2
1	A	24	PRO	CD	52.401	0.004	1
1	A	24	PRO	HD2	4.112	0.000	2
1	A	24	PRO	HD3	3.695	0.002	2
1	A	24	PRO	C	175.67	0.002	1
1	A	25	ASP	N	118.504	0.000	1
1	A	25	ASP	H	7.967	0.001	1
1	A	25	ASP	CA	52.405	0.000	1
1	A	25	ASP	HA	4.858	0.000	1
1	A	25	ASP	CB	40.881	0.001	1
1	A	25	ASP	HB2	2.337	0.001	2
1	A	25	ASP	HB3	2.864	0.000	2
1	A	25	ASP	C	175.161	0.000	1
1	A	26	ARG	N	127.949	0.001	1
1	A	26	ARG	H	9.06	0.001	1
1	A	26	ARG	CA	59.985	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	ARG	HA	3.634	0.001	1
1	A	26	ARG	CB	30.936	0.000	1
1	A	26	ARG	HB2	1.827	0.001	2
1	A	26	ARG	HB3	1.827	0.001	2
1	A	26	ARG	CG	26.509	0.003	1
1	A	26	ARG	HG2	1.293	0.000	2
1	A	26	ARG	HG3	1.449	0.000	2
1	A	26	ARG	CD	44.357	0.006	1
1	A	26	ARG	HD2	2.964	0.002	2
1	A	26	ARG	HD3	3.167	0.002	2
1	A	26	ARG	NE	81.684	0.002	1
1	A	26	ARG	HE	7.442	0.001	1
1	A	26	ARG	CZ	173.631	0.000	1
1	A	26	ARG	C	177.473	0.009	1
1	A	27	GLY	N	106.398	0.000	1
1	A	27	GLY	H	8.861	0.000	1
1	A	27	GLY	CA	47.565	0.001	1
1	A	27	GLY	HA2	3.656	0.000	1
1	A	27	GLY	HA3	3.939	0.000	1
1	A	27	GLY	C	176.698	0.002	1
1	A	28	ALA	N	124.026	0.001	1
1	A	28	ALA	H	7.798	0.000	1
1	A	28	ALA	CA	54.373	0.001	1
1	A	28	ALA	HA	4.164	0.000	1
1	A	28	ALA	HB1	1.34	0.000	1
1	A	28	ALA	HB2	1.34	0.000	1
1	A	28	ALA	HB3	1.34	0.000	1
1	A	28	ALA	CB	18.576	0.007	1
1	A	28	ALA	C	181.163	0.008	1
1	A	29	ALA	N	122.818	0.000	1
1	A	29	ALA	H	7.909	0.000	1
1	A	29	ALA	CA	55.43	0.008	1
1	A	29	ALA	HA	4.312	0.000	1
1	A	29	ALA	HB1	1.657	0.000	1
1	A	29	ALA	HB2	1.657	0.000	1
1	A	29	ALA	HB3	1.657	0.000	1
1	A	29	ALA	CB	18.399	0.000	1
1	A	29	ALA	C	179.154	0.000	1
1	A	30	LEU	N	117.931	0.000	1
1	A	30	LEU	H	8.732	0.000	1
1	A	30	LEU	CA	58.492	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	LEU	HA	3.785	0.000	1
1	A	30	LEU	CB	40.183	0.000	1
1	A	30	LEU	HB2	0.727	0.000	2
1	A	30	LEU	HB3	1.626	0.000	2
1	A	30	LEU	CG	26.592	0.002	1
1	A	30	LEU	HG	1.525	0.002	1
1	A	30	LEU	HD11	0.189	0.000	2
1	A	30	LEU	HD12	0.189	0.000	2
1	A	30	LEU	HD13	0.189	0.000	2
1	A	30	LEU	HD21	0.502	0.001	2
1	A	30	LEU	HD22	0.502	0.001	2
1	A	30	LEU	HD23	0.502	0.001	2
1	A	30	LEU	CD1	23.041	0.001	1
1	A	30	LEU	CD2	25.298	0.003	1
1	A	30	LEU	C	179.824	0.001	1
1	A	31	GLN	N	116.54	0.000	1
1	A	31	GLN	H	7.491	0.001	1
1	A	31	GLN	CA	59.235	0.002	1
1	A	31	GLN	HA	4.03	0.000	1
1	A	31	GLN	CB	28.61	0.003	1
1	A	31	GLN	HB2	2.205	0.000	2
1	A	31	GLN	HB3	2.205	0.000	2
1	A	31	GLN	CG	33.845	0.000	1
1	A	31	GLN	HG2	2.562	0.000	1
1	A	31	GLN	HG3	2.486	0.000	1
1	A	31	GLN	NE2	111.988	0.002	1
1	A	31	GLN	HE21	6.878	0.000	2
1	A	31	GLN	HE22	7.51	0.000	2
1	A	31	GLN	C	177.852	0.003	1
1	A	32	PHE	N	121.08	0.000	1
1	A	32	PHE	H	7.753	0.000	1
1	A	32	PHE	CA	61.589	0.002	1
1	A	32	PHE	HA	4.15	0.000	1
1	A	32	PHE	CB	39.067	0.001	1
1	A	32	PHE	HB2	3.176	0.000	1
1	A	32	PHE	HB3	2.914	0.001	1
1	A	32	PHE	CD1	132.519	0.000	1
1	A	32	PHE	HD1	6.307	0.002	1
1	A	32	PHE	CE1	130.957	0.000	1
1	A	32	PHE	HE1	7.022	0.001	1
1	A	32	PHE	CZ	131.684	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	PHE	HZ	7.412	0.000	1
1	A	32	PHE	CE2	130.957	0.002	1
1	A	32	PHE	HE2	7.022	0.001	1
1	A	32	PHE	CD2	132.519	0.000	1
1	A	32	PHE	HD2	6.307	0.002	1
1	A	32	PHE	C	175.608	0.002	1
1	A	33	TYR	N	115.537	0.001	1
1	A	33	TYR	H	8.659	0.000	1
1	A	33	TYR	CA	63.345	0.001	1
1	A	33	TYR	HA	3.238	0.001	1
1	A	33	TYR	CB	39.307	0.001	1
1	A	33	TYR	HB2	2.541	0.001	1
1	A	33	TYR	HB3	2.7	0.000	1
1	A	33	TYR	CD1	132.794	0.000	1
1	A	33	TYR	HD1	6.755	0.000	1
1	A	33	TYR	CE1	118.382	0.002	1
1	A	33	TYR	HE1	6.755	0.000	1
1	A	33	TYR	CE2	118.382	0.000	1
1	A	33	TYR	HE2	6.755	0.000	1
1	A	33	TYR	CD2	132.794	0.000	1
1	A	33	TYR	HD2	6.755	0.000	1
1	A	33	TYR	HH	12.211	0.001	1
1	A	33	TYR	C	179.157	0.000	1
1	A	34	SER	N	113.044	0.000	1
1	A	34	SER	H	8.333	0.000	1
1	A	34	SER	CA	61.765	0.001	1
1	A	34	SER	HA	4.164	0.001	1
1	A	34	SER	CB	63.35	0.000	1
1	A	34	SER	HB2	4.293	0.000	1
1	A	34	SER	HB3	4.226	0.000	1
1	A	34	SER	C	177.581	0.000	1
1	A	35	ALA	N	124.317	0.000	1
1	A	35	ALA	H	7.44	0.000	1
1	A	35	ALA	CA	54.804	0.003	1
1	A	35	ALA	HA	4.007	0.001	1
1	A	35	ALA	HB1	1.386	0.003	1
1	A	35	ALA	HB2	1.386	0.003	1
1	A	35	ALA	HB3	1.386	0.003	1
1	A	35	ALA	CB	18.507	0.005	1
1	A	35	ALA	C	179.505	0.002	1
1	A	36	LEU	N	116.809	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	36	LEU	H	7.433	0.000	1
1	A	36	LEU	CA	56.767	0.003	1
1	A	36	LEU	HA	3.594	0.000	1
1	A	36	LEU	CB	42.418	0.004	1
1	A	36	LEU	HB2	0.232	0.000	1
1	A	36	LEU	HB3	0.142	0.000	1
1	A	36	LEU	CG	25.84	0.000	1
1	A	36	LEU	HG	0.236	0.000	1
1	A	36	LEU	HD11	0.367	0.000	2
1	A	36	LEU	HD12	0.367	0.000	2
1	A	36	LEU	HD13	0.367	0.000	2
1	A	36	LEU	HD21	0.095	0.000	2
1	A	36	LEU	HD22	0.095	0.000	2
1	A	36	LEU	HD23	0.095	0.000	2
1	A	36	LEU	CD1	23.608	0.000	1
1	A	36	LEU	CD2	26.027	0.003	1
1	A	36	LEU	C	177.754	0.003	1
1	A	37	PHE	N	111.786	0.004	1
1	A	37	PHE	H	7.546	0.000	1
1	A	37	PHE	CA	55.879	0.000	1
1	A	37	PHE	HA	4.792	0.000	1
1	A	37	PHE	CB	41.355	0.001	1
1	A	37	PHE	HB2	1.226	0.004	1
1	A	37	PHE	HB3	2.849	0.001	1
1	A	37	PHE	CD1	130.786	0.000	1
1	A	37	PHE	HD1	6.211	0.003	1
1	A	37	PHE	CE1	129.659	0.000	1
1	A	37	PHE	HE1	6.514	0.002	1
1	A	37	PHE	CZ	129.66	0.000	1
1	A	37	PHE	HZ	6.94	0.004	1
1	A	37	PHE	CE2	129.659	0.000	1
1	A	37	PHE	HE2	6.514	0.002	1
1	A	37	PHE	CD2	130.786	0.002	1
1	A	37	PHE	HD2	6.211	0.003	1
1	A	37	PHE	C	176.848	0.000	1
1	A	38	GLY	N	107.445	0.000	1
1	A	38	GLY	H	7.987	0.000	1
1	A	38	GLY	CA	45.825	0.000	1
1	A	38	GLY	HA2	4.106	0.000	1
1	A	38	GLY	HA3	3.946	0.002	1
1	A	38	GLY	C	174.504	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	39	TRP	N	116.929	0.002	1
1	A	39	TRP	H	6.361	0.001	1
1	A	39	TRP	CA	55.455	0.000	1
1	A	39	TRP	HA	4.915	0.000	1
1	A	39	TRP	CB	30.593	0.000	1
1	A	39	TRP	HB2	2.908	0.000	1
1	A	39	TRP	HB3	2.99	0.000	1
1	A	39	TRP	CD1	122.928	0.000	1
1	A	39	TRP	NE1	129.327	0.000	1
1	A	39	TRP	HD1	6.805	0.001	1
1	A	39	TRP	CZ3	122.735	0.000	1
1	A	39	TRP	CZ2	115.868	0.002	1
1	A	39	TRP	HE1	10.473	0.000	1
1	A	39	TRP	HZ3	6.437	0.000	1
1	A	39	TRP	CH2	125.037	0.000	1
1	A	39	TRP	HZ2	6.081	0.000	1
1	A	39	TRP	HH2	5.966	0.000	1
1	A	39	TRP	C	174.67	0.000	1
1	A	40	GLU	N	120.581	0.000	1
1	A	40	GLU	H	9.472	0.000	1
1	A	40	GLU	CA	54.623	0.001	1
1	A	40	GLU	HA	4.516	0.000	1
1	A	40	GLU	CB	32.463	0.008	1
1	A	40	GLU	HB2	1.915	0.000	2
1	A	40	GLU	HB3	2.006	0.000	2
1	A	40	GLU	CG	36.505	0.004	1
1	A	40	GLU	HG2	2.221	0.003	2
1	A	40	GLU	HG3	2.421	0.000	2
1	A	40	GLU	C	175.916	0.001	1
1	A	41	PHE	N	118.759	0.000	1
1	A	41	PHE	H	8.218	0.000	1
1	A	41	PHE	CA	55.914	0.001	1
1	A	41	PHE	HA	5.42	0.000	1
1	A	41	PHE	CB	41.791	0.000	1
1	A	41	PHE	HB2	2.959	0.000	2
1	A	41	PHE	HB3	3.336	0.000	2
1	A	41	PHE	CD1	132.483	0.003	1
1	A	41	PHE	HD1	7.164	0.000	1
1	A	41	PHE	CE1	129.456	0.000	1
1	A	41	PHE	HE1	7.13	0.000	1
1	A	41	PHE	CZ	130.619	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	PHE	HZ	7.055	0.000	1
1	A	41	PHE	CE2	129.456	0.000	1
1	A	41	PHE	HE2	7.13	0.000	1
1	A	41	PHE	CD2	132.483	0.000	1
1	A	41	PHE	HD2	7.164	0.000	1
1	A	41	PHE	C	175.066	0.003	1
1	A	43	THR	N	118.142	0.000	1
1	A	43	THR	H	8.744	0.000	1
1	A	43	THR	CA	62.255	0.000	1
1	A	43	THR	HA	4.657	0.000	1
1	A	43	THR	CB	69.723	0.001	1
1	A	43	THR	HB	4.337	0.000	1
1	A	43	THR	HG21	1.286	0.000	1
1	A	43	THR	HG22	1.286	0.000	1
1	A	43	THR	HG23	1.286	0.000	1
1	A	43	THR	CG2	21.873	0.000	1
1	A	43	THR	C	174.903	0.000	1
1	A	44	THR	N	117.195	0.007	1
1	A	44	THR	H	8.388	0.001	1
1	A	44	THR	CA	61.4	0.002	1
1	A	44	THR	HA	4.492	0.002	1
1	A	44	THR	CB	69.756	0.000	1
1	A	44	THR	HB	4.181	0.000	1
1	A	44	THR	HG21	1.157	0.000	1
1	A	44	THR	HG22	1.157	0.000	1
1	A	44	THR	HG23	1.157	0.000	1
1	A	44	THR	CG2	21.45	0.000	1
1	A	44	THR	C	174.542	0.000	1
1	A	45	SER	N	117.844	0.000	1
1	A	45	SER	H	8.509	0.000	1
1	A	45	SER	CA	58.427	0.002	1
1	A	45	SER	HA	4.575	0.000	1
1	A	45	SER	CB	63.929	0.000	1
1	A	45	SER	HB2	3.856	0.000	2
1	A	45	SER	HB3	3.95	0.000	2
1	A	45	SER	C	174.418	0.000	1
1	A	46	ASP	N	121.995	0.000	1
1	A	46	ASP	H	8.31	0.000	1
1	A	46	ASP	CA	54.136	0.000	1
1	A	46	ASP	HA	4.685	0.000	1
1	A	46	ASP	CB	41.109	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	46	ASP	HB2	2.831	0.000	2
1	A	46	ASP	HB3	2.735	0.000	2
1	A	46	ASP	C	176.811	0.000	1
1	A	47	GLY	N	109.282	0.000	1
1	A	47	GLY	H	8.377	0.000	1
1	A	47	GLY	CA	45.686	0.000	1
1	A	47	GLY	HA2	3.924	0.000	2
1	A	47	GLY	HA3	4.118	0.000	2
1	A	47	GLY	C	174.904	0.007	1
1	A	48	THR	N	112.898	0.001	1
1	A	48	THR	H	8.29	0.000	1
1	A	48	THR	CA	62.66	0.002	1
1	A	48	THR	HA	4.336	0.000	1
1	A	48	THR	CB	69.772	0.000	1
1	A	48	THR	HB	4.296	0.001	1
1	A	48	THR	HG21	1.187	0.000	1
1	A	48	THR	HG22	1.187	0.000	1
1	A	48	THR	HG23	1.187	0.000	1
1	A	48	THR	CG2	21.546	0.000	1
1	A	48	THR	C	174.854	0.003	1
1	A	49	SER	N	118.015	0.002	1
1	A	49	SER	H	8.23	0.001	1
1	A	49	SER	CA	55.875	0.006	1
1	A	49	SER	HA	4.875	0.000	1
1	A	49	SER	CB	64.126	0.000	1
1	A	49	SER	HB2	3.862	0.000	2
1	A	49	SER	HB3	3.862	0.000	2
1	A	49	SER	C	173.72	0.000	1
1	A	50	PRO	CA	63.556	0.002	1
1	A	50	PRO	HA	4.625	0.001	1
1	A	50	PRO	CB	31.736	0.001	1
1	A	50	PRO	HB2	1.967	0.003	2
1	A	50	PRO	HB3	2.176	0.000	2
1	A	50	PRO	CG	26.911	0.000	1
1	A	50	PRO	HG2	2.008	0.001	2
1	A	50	PRO	HG3	2.008	0.001	2
1	A	50	PRO	CD	50.756	0.003	1
1	A	50	PRO	HD2	3.745	0.001	2
1	A	50	PRO	HD3	3.745	0.001	2
1	A	50	PRO	C	175.004	0.000	1
1	A	51	TYR	N	115.379	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	TYR	H	7.651	0.000	1
1	A	51	TYR	CA	56.442	0.001	1
1	A	51	TYR	HA	4.914	0.000	1
1	A	51	TYR	CB	41.015	0.000	1
1	A	51	TYR	HB2	2.937	0.001	2
1	A	51	TYR	HB3	2.806	0.002	2
1	A	51	TYR	CD1	133.261	0.000	1
1	A	51	TYR	HD1	6.913	0.001	1
1	A	51	TYR	CE1	118.233	0.000	1
1	A	51	TYR	HE1	6.744	0.002	1
1	A	51	TYR	CE2	118.233	0.003	1
1	A	51	TYR	HE2	6.744	0.002	1
1	A	51	TYR	CD2	133.261	0.001	1
1	A	51	TYR	HD2	6.913	0.001	1
1	A	51	TYR	C	174.617	0.000	1
1	A	52	THR	N	119.65	0.000	1
1	A	52	THR	H	9.478	0.000	1
1	A	52	THR	CA	62.751	0.002	1
1	A	52	THR	HA	4.599	0.002	1
1	A	52	THR	CB	71.486	0.005	1
1	A	52	THR	HB	3.945	0.000	1
1	A	52	THR	HG21	1.387	0.000	1
1	A	52	THR	HG22	1.387	0.000	1
1	A	52	THR	HG23	1.387	0.000	1
1	A	52	THR	CG2	23.398	0.004	1
1	A	52	THR	C	173.745	0.001	1
1	A	53	MET	N	127.214	0.001	1
1	A	53	MET	H	9.043	0.000	1
1	A	53	MET	CA	54.532	0.000	1
1	A	53	MET	HA	4.97	0.000	1
1	A	53	MET	CB	32.303	0.006	1
1	A	53	MET	HB2	2.091	0.000	2
1	A	53	MET	HB3	2.173	0.000	2
1	A	53	MET	CG	32.38	0.004	1
1	A	53	MET	HG2	2.57	0.000	2
1	A	53	MET	HG3	2.756	0.006	2
1	A	53	MET	C	175.654	0.005	1
1	A	54	CYS	N	123.924	0.000	1
1	A	54	CYS	H	8.763	0.000	1
1	A	54	CYS	CA	57.771	0.000	1
1	A	54	CYS	HA	5.273	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	CYS	CB	29.613	0.001	1
1	A	54	CYS	HB2	2.094	0.000	2
1	A	54	CYS	HB3	2.768	0.001	2
1	A	54	CYS	C	174.316	0.000	1
1	A	55	ARG	N	123.351	0.000	1
1	A	55	ARG	H	9.464	0.000	1
1	A	55	ARG	CA	54.706	0.003	1
1	A	55	ARG	HA	5.18	0.002	1
1	A	55	ARG	CB	35.186	0.004	1
1	A	55	ARG	HB2	1.562	0.000	1
1	A	55	ARG	HB3	1.46	0.000	1
1	A	55	ARG	CG	28.478	0.001	1
1	A	55	ARG	HG2	1.242	0.000	2
1	A	55	ARG	HG3	1.461	0.000	2
1	A	55	ARG	CD	43.245	0.005	1
1	A	55	ARG	HD2	3.005	0.001	1
1	A	55	ARG	HD3	3.063	0.000	1
1	A	55	ARG	NE	84.497	0.001	1
1	A	55	ARG	HE	7.566	0.000	1
1	A	55	ARG	C	174.07	0.000	1
1	A	56	LEU	N	120.564	0.000	1
1	A	56	LEU	H	8.819	0.000	1
1	A	56	LEU	CA	54.564	0.000	1
1	A	56	LEU	HA	4.698	0.000	1
1	A	56	LEU	CB	45.824	0.001	1
1	A	56	LEU	HB2	1.406	0.001	1
1	A	56	LEU	HB3	1.638	0.000	1
1	A	56	LEU	CG	27.592	0.003	1
1	A	56	LEU	HG	1.365	0.000	1
1	A	56	LEU	HD11	1.18	0.001	2
1	A	56	LEU	HD12	1.18	0.001	2
1	A	56	LEU	HD13	1.18	0.001	2
1	A	56	LEU	HD21	1.073	0.000	2
1	A	56	LEU	HD22	1.073	0.000	2
1	A	56	LEU	HD23	1.073	0.000	2
1	A	56	LEU	CD1	23.049	0.000	1
1	A	56	LEU	CD2	26.182	0.007	1
1	A	56	LEU	C	176.328	0.000	1
1	A	57	ARG	N	126.961	0.001	1
1	A	57	ARG	H	9.802	0.001	1
1	A	57	ARG	CA	57.674	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	ARG	HA	3.899	0.000	1
1	A	57	ARG	CB	28.496	0.000	1
1	A	57	ARG	HB2	1.923	0.000	2
1	A	57	ARG	HB3	1.923	0.000	2
1	A	57	ARG	C	176.573	0.000	1
1	A	58	GLY	N	103.29	0.000	1
1	A	58	GLY	H	8.892	0.000	1
1	A	58	GLY	CA	45.429	0.001	1
1	A	58	GLY	HA2	3.601	0.001	2
1	A	58	GLY	HA3	4.175	0.000	2
1	A	58	GLY	C	174.075	0.003	1
1	A	59	ARG	N	120.006	0.000	1
1	A	59	ARG	H	7.79	0.000	1
1	A	59	ARG	CA	54.041	0.001	1
1	A	59	ARG	HA	4.726	0.000	1
1	A	59	ARG	CB	32.631	0.000	1
1	A	59	ARG	HB2	1.889	0.000	1
1	A	59	ARG	HB3	1.621	0.000	1
1	A	59	ARG	CG	27.067	0.000	1
1	A	59	ARG	HG2	1.695	0.000	1
1	A	59	ARG	HG3	1.567	0.000	1
1	A	59	ARG	CD	43.32	0.000	1
1	A	59	ARG	HD2	3.253	0.000	2
1	A	59	ARG	HD3	3.253	0.000	2
1	A	59	ARG	NE	85.005	0.000	1
1	A	59	ARG	HE	7.307	0.000	1
1	A	59	ARG	C	175.552	0.009	1
1	A	60	GLU	N	121.994	0.001	1
1	A	60	GLU	H	9.005	0.000	1
1	A	60	GLU	CA	58.289	0.001	1
1	A	60	GLU	HA	4.284	0.000	1
1	A	60	GLU	CB	29.929	0.003	1
1	A	60	GLU	HB2	2.204	0.000	2
1	A	60	GLU	HB3	2.204	0.000	2
1	A	60	GLU	CG	37.208	0.008	1
1	A	60	GLU	HG2	2.383	0.001	2
1	A	60	GLU	HG3	2.383	0.001	2
1	A	60	GLU	C	176.18	0.000	1
1	A	61	VAL	N	123.148	0.002	1
1	A	61	VAL	H	9.022	0.000	1
1	A	61	VAL	CA	63.308	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	VAL	HA	4.111	0.002	1
1	A	61	VAL	CB	34.287	0.000	1
1	A	61	VAL	HB	1.007	0.000	1
1	A	61	VAL	HG11	0.334	0.001	2
1	A	61	VAL	HG12	0.334	0.001	2
1	A	61	VAL	HG13	0.334	0.001	2
1	A	61	VAL	HG21	0.578	0.000	2
1	A	61	VAL	HG22	0.578	0.000	2
1	A	61	VAL	HG23	0.578	0.000	2
1	A	61	VAL	CG1	20.309	0.001	1
1	A	61	VAL	CG2	21.555	0.006	1
1	A	61	VAL	C	173.726	0.007	1
1	A	62	CYS	N	108.935	0.002	1
1	A	62	CYS	H	7.067	0.000	1
1	A	62	CYS	CA	56.116	0.001	1
1	A	62	CYS	HA	3.389	0.000	1
1	A	62	CYS	CB	29.763	0.000	1
1	A	62	CYS	HB2	2.61	0.000	2
1	A	62	CYS	HB3	2.61	0.000	2
1	A	62	CYS	C	171.556	0.000	1
1	A	63	SER	N	109.875	0.005	1
1	A	63	SER	H	6.932	0.000	1
1	A	63	SER	CA	56.696	0.000	1
1	A	63	SER	HA	5.521	0.000	1
1	A	63	SER	CB	66.844	0.000	1
1	A	63	SER	HB2	3.917	0.000	2
1	A	63	SER	HB3	4.031	0.001	2
1	A	63	SER	C	172.719	0.000	1
1	A	64	ILE	N	119.868	0.001	1
1	A	64	ILE	H	8.679	0.000	1
1	A	64	ILE	CA	60.831	0.002	1
1	A	64	ILE	HA	4.885	0.000	1
1	A	64	ILE	CB	41.057	0.001	1
1	A	64	ILE	HB	1.406	0.000	1
1	A	64	ILE	HG21	0.712	0.001	1
1	A	64	ILE	HG22	0.712	0.001	1
1	A	64	ILE	HG23	0.712	0.001	1
1	A	64	ILE	CG2	17.523	0.004	1
1	A	64	ILE	CG1	27.297	0.000	1
1	A	64	ILE	HG12	1.612	0.000	2
1	A	64	ILE	HG13	1.612	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	ILE	HD11	0.805	0.000	1
1	A	64	ILE	HD12	0.805	0.000	1
1	A	64	ILE	HD13	0.805	0.000	1
1	A	64	ILE	CD1	13.624	0.002	1
1	A	64	ILE	C	174.993	0.000	1
1	A	66	ASP	N	117.987	0.001	1
1	A	66	ASP	H	8.204	0.000	1
1	A	66	ASP	CA	54.113	0.000	1
1	A	66	ASP	HA	4.975	0.000	1
1	A	66	ASP	CB	41.822	0.003	1
1	A	66	ASP	HB2	2.513	0.001	2
1	A	66	ASP	HB3	2.746	0.000	2
1	A	66	ASP	C	175.714	0.000	1
1	A	67	LEU	N	124.388	0.000	1
1	A	67	LEU	H	7.652	0.000	1
1	A	67	LEU	CA	55.806	0.006	1
1	A	67	LEU	HA	4.102	0.001	1
1	A	67	LEU	CB	43.461	0.000	1
1	A	67	LEU	HB2	0.887	0.000	1
1	A	67	LEU	HB3	1.496	0.000	1
1	A	67	LEU	CG	26.126	0.002	1
1	A	67	LEU	HG	0.83	0.000	1
1	A	67	LEU	HD11	0.761	0.000	2
1	A	67	LEU	HD12	0.761	0.000	2
1	A	67	LEU	HD13	0.761	0.000	2
1	A	67	LEU	HD21	0.826	0.000	2
1	A	67	LEU	HD22	0.826	0.000	2
1	A	67	LEU	HD23	0.826	0.000	2
1	A	67	LEU	CD1	24.139	0.003	1
1	A	67	LEU	CD2	25.945	0.000	1
1	A	67	LEU	C	176.919	0.001	1
1	A	68	GLY	N	109.275	0.000	1
1	A	68	GLY	H	8.513	0.000	1
1	A	68	GLY	CA	44.738	0.000	1
1	A	68	GLY	HA2	3.937	0.000	2
1	A	68	GLY	HA3	3.937	0.000	2
1	A	68	GLY	C	173.585	0.000	1
1	A	69	GLU	N	118.926	0.000	1
1	A	69	GLU	H	8.267	0.000	1
1	A	69	GLU	CA	56.589	0.004	1
1	A	69	GLU	HA	4.249	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	GLU	CB	30.438	0.004	1
1	A	69	GLU	HB2	1.886	0.000	2
1	A	69	GLU	HB3	2.078	0.000	2
1	A	69	GLU	CG	36.304	0.002	1
1	A	69	GLU	HG2	2.219	0.000	2
1	A	69	GLU	HG3	2.283	0.000	2
1	A	69	GLU	C	176.396	0.005	1
1	A	70	ASN	N	118.361	0.000	1
1	A	70	ASN	H	8.444	0.001	1
1	A	70	ASN	CA	51.947	0.004	1
1	A	70	ASN	HA	4.903	0.000	1
1	A	70	ASN	CB	39.219	0.000	1
1	A	70	ASN	HB2	2.651	0.000	2
1	A	70	ASN	HB3	2.756	0.000	2
1	A	70	ASN	ND2	114.001	0.001	1
1	A	70	ASN	HD21	7.617	0.000	1
1	A	70	ASN	HD22	6.924	0.001	1
1	A	70	ASN	C	172.592	0.000	1
1	A	71	PRO	CA	63.502	0.000	1
1	A	71	PRO	HA	4.431	0.000	1
1	A	71	PRO	CB	32.232	0.000	1
1	A	71	PRO	HB2	2.012	0.000	2
1	A	71	PRO	HB3	2.193	0.000	2
1	A	71	PRO	CG	27.147	0.000	1
1	A	71	PRO	HG2	1.963	0.000	2
1	A	71	PRO	HG3	2.036	0.000	2
1	A	71	PRO	CD	50.328	0.000	1
1	A	71	PRO	HD2	3.668	0.002	2
1	A	71	PRO	HD3	3.668	0.002	2
1	A	71	PRO	C	177.364	0.000	1
1	A	72	GLY	N	109.788	0.000	1
1	A	72	GLY	H	8.311	0.000	1
1	A	72	GLY	CA	44.95	0.008	1
1	A	72	GLY	HA2	4.146	0.000	2
1	A	72	GLY	HA3	3.963	0.000	2
1	A	72	GLY	C	172.49	0.000	1
1	A	73	PRO	CA	63.705	0.001	1
1	A	73	PRO	HA	4.413	0.000	1
1	A	73	PRO	CB	32.058	0.000	1
1	A	73	PRO	HB2	1.895	0.000	2
1	A	73	PRO	HB3	2.303	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	73	PRO	CG	27.115	0.007	1
1	A	73	PRO	HG2	2.007	0.002	2
1	A	73	PRO	HG3	2.007	0.002	2
1	A	73	PRO	CD	49.878	0.001	1
1	A	73	PRO	HD2	3.626	0.000	2
1	A	73	PRO	HD3	3.626	0.000	2
1	A	73	PRO	C	176.836	0.000	1
1	A	74	ALA	N	121.775	0.010	1
1	A	74	ALA	H	8.125	0.000	1
1	A	74	ALA	CA	52.765	0.002	1
1	A	74	ALA	HA	4.248	0.000	1
1	A	74	ALA	HB1	1.353	0.000	1
1	A	74	ALA	HB2	1.353	0.000	1
1	A	74	ALA	HB3	1.353	0.000	1
1	A	74	ALA	CB	19.243	0.000	1
1	A	74	ALA	C	176.562	0.002	1
1	A	75	LEU	N	118.701	0.000	1
1	A	75	LEU	H	7.667	0.000	1
1	A	75	LEU	CA	54.205	0.005	1
1	A	75	LEU	HA	4.421	0.000	1
1	A	75	LEU	CB	43.778	0.002	1
1	A	75	LEU	HB2	1.505	0.000	2
1	A	75	LEU	HB3	1.6	0.000	2
1	A	75	LEU	CG	26.872	0.000	1
1	A	75	LEU	HG	1.568	0.000	1
1	A	75	LEU	HD11	0.796	0.000	2
1	A	75	LEU	HD12	0.796	0.000	2
1	A	75	LEU	HD13	0.796	0.000	2
1	A	75	LEU	HD21	0.892	0.000	2
1	A	75	LEU	HD22	0.892	0.000	2
1	A	75	LEU	HD23	0.892	0.000	2
1	A	75	LEU	CD1	22.956	0.000	1
1	A	75	LEU	CD2	25.328	0.000	1
1	A	75	LEU	C	176.836	0.001	1
1	A	76	GLY	N	107.704	0.000	1
1	A	76	GLY	H	8.404	0.000	1
1	A	76	GLY	CA	45.204	0.000	1
1	A	76	GLY	HA2	3.928	0.000	2
1	A	76	GLY	HA3	4.165	0.000	2
1	A	76	GLY	C	174.588	0.001	1
1	A	77	GLY	N	108.756	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	GLY	H	8.481	0.000	1
1	A	77	GLY	CA	44.452	0.002	1
1	A	77	GLY	HA2	3.701	0.002	2
1	A	77	GLY	HA3	4.631	0.000	2
1	A	77	GLY	C	174.456	0.000	1
1	A	78	TRP	N	122.197	0.000	1
1	A	78	TRP	H	9.414	0.000	1
1	A	78	TRP	CA	58.331	0.006	1
1	A	78	TRP	HA	5.113	0.000	1
1	A	78	TRP	CB	30.571	0.001	1
1	A	78	TRP	HB2	3.037	0.000	2
1	A	78	TRP	HB3	3.595	0.000	2
1	A	78	TRP	CD1	126.348	0.000	1
1	A	78	TRP	NE1	127.803	0.000	1
1	A	78	TRP	HD1	7.543	0.002	1
1	A	78	TRP	CZ2	114.407	0.002	1
1	A	78	TRP	HE1	9.853	0.001	1
1	A	78	TRP	CH2	126.07	0.000	1
1	A	78	TRP	HZ2	6.314	0.001	1
1	A	78	TRP	HH2	7.24	0.001	1
1	A	78	TRP	C	178.659	0.002	1
1	A	79	SER	N	125.248	0.000	1
1	A	79	SER	H	10.303	0.000	1
1	A	79	SER	CA	58.482	0.000	1
1	A	79	SER	HA	4.814	0.000	1
1	A	79	SER	CB	64.627	0.000	1
1	A	79	SER	HB2	3.318	0.000	2
1	A	79	SER	HB3	4.054	0.002	2
1	A	79	SER	C	172.503	0.000	1
1	A	81	TYR	N	119.645	0.003	1
1	A	81	TYR	H	8.46	0.000	1
1	A	81	TYR	CA	56.111	0.000	1
1	A	81	TYR	HA	4.796	0.000	1
1	A	81	TYR	CB	39.256	0.000	1
1	A	81	TYR	HB2	2.749	0.000	2
1	A	81	TYR	HB3	2.497	0.001	2
1	A	81	TYR	CD1	132.864	0.001	1
1	A	81	TYR	HD1	6.756	0.000	1
1	A	81	TYR	CE1	118.234	0.000	1
1	A	81	TYR	HE1	6.743	0.000	1
1	A	81	TYR	CE2	118.234	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	TYR	HE2	6.743	0.000	1
1	A	81	TYR	CD2	132.864	0.000	1
1	A	81	TYR	HD2	6.756	0.000	1
1	A	81	TYR	C	174.506	0.000	1
1	A	82	LEU	N	125.236	0.000	1
1	A	82	LEU	H	8.896	0.000	1
1	A	82	LEU	CA	52.469	0.000	1
1	A	82	LEU	HA	4.848	0.000	1
1	A	82	LEU	CB	42.609	0.002	1
1	A	82	LEU	HB2	1.665	0.000	2
1	A	82	LEU	HB3	1.722	0.000	2
1	A	82	LEU	CG	27.521	0.002	1
1	A	82	LEU	HG	1.217	0.001	1
1	A	82	LEU	HD11	0.296	0.000	2
1	A	82	LEU	HD12	0.296	0.000	2
1	A	82	LEU	HD13	0.296	0.000	2
1	A	82	LEU	HD21	0.392	0.000	2
1	A	82	LEU	HD22	0.392	0.000	2
1	A	82	LEU	HD23	0.392	0.000	2
1	A	82	LEU	CD1	21.56	0.005	1
1	A	82	LEU	CD2	25.34	0.002	1
1	A	82	LEU	C	176.98	0.000	1
1	A	83	SER	N	116.74	0.000	1
1	A	83	SER	H	8.443	0.000	1
1	A	83	SER	CA	59.415	0.005	1
1	A	83	SER	HA	5.094	0.000	1
1	A	83	SER	CB	63.758	0.001	1
1	A	83	SER	HB2	3.92	0.000	2
1	A	83	SER	HB3	4.124	0.000	2
1	A	83	SER	C	175.169	0.000	1
1	A	84	VAL	N	116.318	0.000	1
1	A	84	VAL	H	8.271	0.003	1
1	A	84	VAL	CA	59.225	0.001	1
1	A	84	VAL	HA	4.849	0.000	1
1	A	84	VAL	CB	35.884	0.000	1
1	A	84	VAL	HB	2.123	0.000	1
1	A	84	VAL	HG11	0.669	0.001	1
1	A	84	VAL	HG12	0.669	0.001	1
1	A	84	VAL	HG13	0.669	0.001	1
1	A	84	VAL	HG21	1.099	0.001	1
1	A	84	VAL	HG22	1.099	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	VAL	HG23	1.099	0.001	1
1	A	84	VAL	CG1	18.432	0.002	1
1	A	84	VAL	CG2	24.126	0.004	1
1	A	84	VAL	C	175.172	0.000	1
1	A	86	ASP	N	116.213	0.000	1
1	A	86	ASP	H	7.288	0.000	1
1	A	86	ASP	CA	53.061	0.001	1
1	A	86	ASP	HA	4.573	0.000	1
1	A	86	ASP	CB	42.751	0.000	1
1	A	86	ASP	HB2	2.438	0.000	1
1	A	86	ASP	HB3	2.725	0.000	1
1	A	86	ASP	C	176.214	0.003	1
1	A	88	ASP	N	118.838	0.000	1
1	A	88	ASP	H	8.256	0.000	1
1	A	88	ASP	CA	57.944	0.003	1
1	A	88	ASP	HA	4.325	0.000	1
1	A	88	ASP	CB	39.826	0.005	1
1	A	88	ASP	HB2	2.805	0.000	1
1	A	88	ASP	HB3	2.539	0.000	1
1	A	88	ASP	C	179.282	0.001	1
1	A	91	ALA	N	118.511	0.000	1
1	A	91	ALA	H	8.237	0.000	1
1	A	91	ALA	CA	55.001	0.000	1
1	A	91	ALA	HA	3.716	0.002	1
1	A	91	ALA	HB1	1.528	0.000	1
1	A	91	ALA	HB2	1.528	0.000	1
1	A	91	ALA	HB3	1.528	0.000	1
1	A	91	ALA	CB	18.166	0.000	1
1	A	91	ALA	C	179.055	0.003	1
1	A	92	ALA	N	117.432	0.000	1
1	A	92	ALA	H	7.374	0.001	1
1	A	92	ALA	CA	53.819	0.003	1
1	A	92	ALA	HA	4.132	0.001	1
1	A	92	ALA	HB1	1.437	0.000	1
1	A	92	ALA	HB2	1.437	0.000	1
1	A	92	ALA	HB3	1.437	0.000	1
1	A	92	ALA	CB	18.26	0.001	1
1	A	92	ALA	C	179.058	0.000	1
1	A	93	ALA	N	120.222	0.000	1
1	A	93	ALA	H	7.494	0.001	1
1	A	93	ALA	CA	53.932	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	ALA	HA	4.172	0.000	1
1	A	93	ALA	HB1	1.279	0.000	1
1	A	93	ALA	HB2	1.279	0.000	1
1	A	93	ALA	HB3	1.279	0.000	1
1	A	93	ALA	CB	18.929	0.003	1
1	A	93	ALA	C	179.17	0.000	1
1	A	94	VAL	N	115.394	0.000	1
1	A	94	VAL	H	7.788	0.000	1
1	A	94	VAL	CA	69.3	0.001	1
1	A	94	VAL	HA	3.523	0.000	1
1	A	94	VAL	CB	30.297	0.000	1
1	A	94	VAL	HB	2.082	0.000	1
1	A	94	VAL	HG11	0.793	0.000	1
1	A	94	VAL	HG12	0.793	0.000	1
1	A	94	VAL	HG13	0.793	0.000	1
1	A	94	VAL	HG21	0.926	0.001	1
1	A	94	VAL	HG22	0.926	0.001	1
1	A	94	VAL	HG23	0.926	0.001	1
1	A	94	VAL	CG1	22.172	0.001	1
1	A	94	VAL	CG2	24.428	0.000	1
1	A	94	VAL	C	175.743	0.000	1
1	A	95	PRO	CA	64.86	0.000	1
1	A	95	PRO	HA	4.669	0.000	1
1	A	95	PRO	CB	30.943	0.002	1
1	A	95	PRO	HB2	2.396	0.001	1
1	A	95	PRO	HB3	1.943	0.001	1
1	A	95	PRO	CG	28.557	0.006	1
1	A	95	PRO	HG2	1.921	0.000	2
1	A	95	PRO	HG3	2.158	0.000	2
1	A	95	PRO	CD	50.393	0.000	1
1	A	95	PRO	HD2	3.764	0.000	1
1	A	95	PRO	HD3	3.469	0.000	1
1	A	95	PRO	C	181.038	0.000	1
1	A	96	GLU	N	118.803	0.000	1
1	A	96	GLU	H	6.96	0.000	1
1	A	96	GLU	CA	58.392	0.003	1
1	A	96	GLU	HA	4.133	0.000	1
1	A	96	GLU	CB	29.15	0.001	1
1	A	96	GLU	HB2	2.186	0.000	1
1	A	96	GLU	HB3	2.152	0.000	1
1	A	96	GLU	CG	35.975	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	GLU	HG2	2.428	0.000	1
1	A	96	GLU	HG3	2.286	0.000	1
1	A	96	GLU	C	178.264	0.005	1
1	A	97	LEU	N	117.747	0.000	1
1	A	97	LEU	H	7.577	0.000	1
1	A	97	LEU	CA	54.417	0.000	1
1	A	97	LEU	HA	4.405	0.000	1
1	A	97	LEU	CB	44.039	0.000	1
1	A	97	LEU	HB2	1.798	0.001	2
1	A	97	LEU	HB3	1.798	0.001	2
1	A	97	LEU	CG	25.737	0.000	1
1	A	97	LEU	HG	1.623	0.000	1
1	A	97	LEU	HD11	0.364	0.000	1
1	A	97	LEU	HD12	0.364	0.000	1
1	A	97	LEU	HD13	0.364	0.000	1
1	A	97	LEU	HD21	0.801	0.000	1
1	A	97	LEU	HD22	0.801	0.000	1
1	A	97	LEU	HD23	0.801	0.000	1
1	A	97	LEU	CD1	25.521	0.000	1
1	A	97	LEU	CD2	22.626	0.000	1
1	A	97	LEU	C	176.933	0.005	1
1	A	98	GLY	N	105.108	0.001	1
1	A	98	GLY	H	7.616	0.000	1
1	A	98	GLY	CA	45.145	0.001	1
1	A	98	GLY	HA2	3.824	0.003	2
1	A	98	GLY	HA3	4.395	0.002	2
1	A	98	GLY	C	175.172	0.000	1
1	A	99	GLY	N	108.038	0.000	1
1	A	99	GLY	H	8.007	0.000	1
1	A	99	GLY	CA	43.302	0.000	1
1	A	99	GLY	HA2	3.437	0.002	2
1	A	99	GLY	HA3	4.039	0.000	2
1	A	99	GLY	C	171.412	0.000	1
1	A	100	ALA	N	120.583	0.001	1
1	A	100	ALA	H	8.525	0.001	1
1	A	100	ALA	CA	50.798	0.005	1
1	A	100	ALA	HA	4.599	0.002	1
1	A	100	ALA	HB1	1.172	0.002	1
1	A	100	ALA	HB2	1.172	0.002	1
1	A	100	ALA	HB3	1.172	0.002	1
1	A	100	ALA	CB	22.287	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	ALA	C	176.384	0.010	1
1	A	101	VAL	N	123.043	0.002	1
1	A	101	VAL	H	9.186	0.001	1
1	A	101	VAL	CA	64.123	0.000	1
1	A	101	VAL	HA	3.975	0.004	1
1	A	101	VAL	CB	31.58	0.001	1
1	A	101	VAL	HB	2.099	0.000	1
1	A	101	VAL	HG11	0.869	0.000	2
1	A	101	VAL	HG12	0.869	0.000	2
1	A	101	VAL	HG13	0.869	0.000	2
1	A	101	VAL	HG21	0.985	0.000	2
1	A	101	VAL	HG22	0.985	0.000	2
1	A	101	VAL	HG23	0.985	0.000	2
1	A	101	VAL	CG1	21.755	0.003	1
1	A	101	VAL	CG2	22.829	0.001	1
1	A	101	VAL	C	175.815	0.008	1
1	A	102	LEU	N	128.71	0.001	1
1	A	102	LEU	H	9.022	0.001	1
1	A	102	LEU	CA	55.591	0.001	1
1	A	102	LEU	HA	4.37	0.000	1
1	A	102	LEU	CB	42.706	0.002	1
1	A	102	LEU	HB2	1.395	0.000	2
1	A	102	LEU	HB3	1.395	0.000	2
1	A	102	LEU	CG	27.37	0.006	1
1	A	102	LEU	HG	1.503	0.001	1
1	A	102	LEU	HD11	0.726	0.000	2
1	A	102	LEU	HD12	0.726	0.000	2
1	A	102	LEU	HD13	0.726	0.000	2
1	A	102	LEU	HD21	0.723	0.000	2
1	A	102	LEU	HD22	0.723	0.000	2
1	A	102	LEU	HD23	0.723	0.000	2
1	A	102	LEU	CD1	21.928	0.000	1
1	A	102	LEU	CD2	25.237	0.000	1
1	A	102	LEU	C	177.009	0.003	1
1	A	103	LEU	N	118.857	0.001	1
1	A	103	LEU	H	7.641	0.000	1
1	A	103	LEU	CA	55.889	0.004	1
1	A	103	LEU	HA	4.473	0.000	1
1	A	103	LEU	CB	45.957	0.001	1
1	A	103	LEU	HB2	1.49	0.000	2
1	A	103	LEU	HB3	1.654	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	LEU	CG	27.527	0.005	1
1	A	103	LEU	HG	1.506	0.000	1
1	A	103	LEU	HD11	0.851	0.000	2
1	A	103	LEU	HD12	0.851	0.000	2
1	A	103	LEU	HD13	0.851	0.000	2
1	A	103	LEU	HD21	0.96	0.001	2
1	A	103	LEU	HD22	0.96	0.001	2
1	A	103	LEU	HD23	0.96	0.001	2
1	A	103	LEU	CD1	25.715	0.005	1
1	A	103	LEU	CD2	24.258	0.002	1
1	A	103	LEU	C	175.425	0.000	1
1	A	104	GLY	N	112.002	0.001	1
1	A	104	GLY	H	8.843	0.000	1
1	A	104	GLY	CA	44.121	0.001	1
1	A	104	GLY	HA2	4.473	0.001	2
1	A	104	GLY	HA3	3.473	0.000	2
1	A	104	GLY	C	170.681	0.000	1
1	A	105	PRO	CA	61.979	0.004	1
1	A	105	PRO	HA	5.157	0.002	1
1	A	105	PRO	CB	34.564	0.000	1
1	A	105	PRO	HB2	1.918	0.000	2
1	A	105	PRO	HB3	1.918	0.000	2
1	A	105	PRO	CG	26.23	0.000	1
1	A	105	PRO	HG2	1.641	0.000	2
1	A	105	PRO	HG3	1.641	0.000	2
1	A	105	PRO	CD	50.358	0.000	1
1	A	105	PRO	HD2	3.478	0.000	2
1	A	105	PRO	HD3	3.478	0.000	2
1	A	105	PRO	C	175.779	0.000	1
1	A	106	ILE	N	120.903	0.000	1
1	A	106	ILE	H	9.351	0.000	1
1	A	106	ILE	CA	59.522	0.000	1
1	A	106	ILE	HA	4.649	0.000	1
1	A	106	ILE	CB	42.592	0.008	1
1	A	106	ILE	HB	1.842	0.000	1
1	A	106	ILE	HG21	0.939	0.002	1
1	A	106	ILE	HG22	0.939	0.002	1
1	A	106	ILE	HG23	0.939	0.002	1
1	A	106	ILE	CG2	17.913	0.000	1
1	A	106	ILE	CG1	26.826	0.001	1
1	A	106	ILE	HG12	1.483	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	ILE	HG13	1.095	0.001	2
1	A	106	ILE	HD11	0.849	0.000	1
1	A	106	ILE	HD12	0.849	0.000	1
1	A	106	ILE	HD13	0.849	0.000	1
1	A	106	ILE	CD1	13.65	0.006	1
1	A	106	ILE	C	173.932	0.001	1
1	A	107	ASP	N	124.072	0.000	1
1	A	107	ASP	H	8.551	0.001	1
1	A	107	ASP	CA	54.684	0.000	1
1	A	107	ASP	HA	4.909	0.000	1
1	A	107	ASP	CB	41.559	0.003	1
1	A	107	ASP	HB2	2.532	0.000	2
1	A	107	ASP	HB3	2.532	0.000	2
1	A	107	ASP	C	175.503	0.000	1
1	A	108	ILE	N	124.131	0.000	1
1	A	108	ILE	H	8.511	0.000	1
1	A	108	ILE	CA	58.778	0.003	1
1	A	108	ILE	HA	4.252	0.004	1
1	A	108	ILE	CB	37.169	0.002	1
1	A	108	ILE	HB	1.764	0.001	1
1	A	108	ILE	HG21	0.766	0.001	1
1	A	108	ILE	HG22	0.766	0.001	1
1	A	108	ILE	HG23	0.766	0.001	1
1	A	108	ILE	CG2	17.272	0.008	1
1	A	108	ILE	CG1	26.542	0.000	1
1	A	108	ILE	HG12	1.267	0.000	2
1	A	108	ILE	HG13	1.124	0.000	2
1	A	108	ILE	HD11	0.604	0.000	1
1	A	108	ILE	HD12	0.604	0.000	1
1	A	108	ILE	HD13	0.604	0.000	1
1	A	108	ILE	CD1	11.43	0.001	1
1	A	109	LEU	N	126.687	0.000	1
1	A	109	LEU	H	8.632	0.001	1
1	A	109	LEU	CA	56.859	0.002	1
1	A	109	LEU	HA	3.914	0.000	1
1	A	109	LEU	CB	40.996	0.003	1
1	A	109	LEU	HB2	1.592	0.000	2
1	A	109	LEU	HB3	1.724	0.001	2
1	A	109	LEU	CG	27.166	0.003	1
1	A	109	LEU	HG	1.606	0.000	1
1	A	109	LEU	HD11	0.891	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	LEU	HD12	0.891	0.000	2
1	A	109	LEU	HD13	0.891	0.000	2
1	A	109	LEU	HD21	0.877	0.000	2
1	A	109	LEU	HD22	0.877	0.000	2
1	A	109	LEU	HD23	0.877	0.000	2
1	A	109	LEU	CD1	23.59	0.000	1
1	A	109	LEU	CD2	24.953	0.000	1
1	A	110	ALA	CA	52.792	0.002	1
1	A	110	ALA	HA	4.289	0.000	1
1	A	110	ALA	HB1	1.418	0.000	1
1	A	110	ALA	HB2	1.418	0.000	1
1	A	110	ALA	HB3	1.418	0.000	1
1	A	110	ALA	CB	18.136	0.002	1
1	A	111	GLN	N	116.726	0.002	1
1	A	111	GLN	H	8.503	0.000	1
1	A	111	GLN	CA	57.064	0.002	1
1	A	111	GLN	HA	4.405	0.001	1
1	A	111	GLN	CB	30.733	0.000	1
1	A	111	GLN	HB2	1.913	0.001	2
1	A	111	GLN	HB3	1.913	0.001	2
1	A	111	GLN	CG	33.751	0.005	1
1	A	111	GLN	HG2	2.238	0.003	2
1	A	111	GLN	HG3	2.327	0.002	2
1	A	111	GLN	NE2	110.167	0.000	1
1	A	111	GLN	HE21	6.364	0.000	2
1	A	111	GLN	HE22	7.12	0.002	2
1	A	111	GLN	C	176.452	0.000	1
1	A	112	GLY	N	106.359	0.002	1
1	A	112	GLY	H	7.693	0.000	1
1	A	112	GLY	CA	45.358	0.001	1
1	A	112	GLY	HA2	3.622	0.000	2
1	A	112	GLY	HA3	3.72	0.002	2
1	A	112	GLY	C	170.786	0.000	1
1	A	113	ARG	N	122.158	0.000	1
1	A	113	ARG	H	8.216	0.000	1
1	A	113	ARG	CA	54.886	0.003	1
1	A	113	ARG	HA	5.039	0.000	1
1	A	113	ARG	CB	33.362	0.004	1
1	A	113	ARG	HB2	1.407	0.001	2
1	A	113	ARG	HB3	1.407	0.001	2
1	A	113	ARG	CG	27.106	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	ARG	HG2	1.095	0.003	2
1	A	113	ARG	HG3	1.483	0.002	2
1	A	113	ARG	CD	43.44	0.000	1
1	A	113	ARG	HD2	2.942	0.000	2
1	A	113	ARG	HD3	3.185	0.000	2
1	A	113	ARG	NE	83.262	0.007	1
1	A	113	ARG	HE	7.507	0.001	1
1	A	113	ARG	C	173.477	0.001	1
1	A	114	MET	N	122.909	0.000	1
1	A	114	MET	H	9.017	0.000	1
1	A	114	MET	CA	53.47	0.000	1
1	A	114	MET	HA	5.667	0.001	1
1	A	114	MET	CB	37.093	0.006	1
1	A	114	MET	HB2	1.798	0.000	2
1	A	114	MET	HB3	1.992	0.000	2
1	A	114	MET	CG	31.724	0.000	1
1	A	114	MET	HG2	2.419	0.000	2
1	A	114	MET	HG3	2.419	0.000	2
1	A	114	MET	HE1	1.882	0.000	1
1	A	114	MET	HE2	1.882	0.000	1
1	A	114	MET	HE3	1.882	0.000	1
1	A	114	MET	CE	17.733	0.003	1
1	A	114	MET	C	174.074	0.001	1
1	A	115	LEU	N	119.336	0.000	1
1	A	115	LEU	H	9.063	0.000	1
1	A	115	LEU	CA	55.513	0.001	1
1	A	115	LEU	HA	5.018	0.000	1
1	A	115	LEU	CB	45.397	0.004	1
1	A	115	LEU	HB2	1.509	0.000	1
1	A	115	LEU	HB3	2.038	0.000	1
1	A	115	LEU	CG	26.23	0.000	1
1	A	115	LEU	HG	1.779	0.000	1
1	A	115	LEU	HD11	0.855	0.000	2
1	A	115	LEU	HD12	0.855	0.000	2
1	A	115	LEU	HD13	0.855	0.000	2
1	A	115	LEU	HD21	1.005	0.000	2
1	A	115	LEU	HD22	1.005	0.000	2
1	A	115	LEU	HD23	1.005	0.000	2
1	A	115	LEU	CD1	27.542	0.000	1
1	A	115	LEU	CD2	27.744	0.005	1
1	A	115	LEU	C	174.116	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	LEU	N	120.7	0.000	1
1	A	116	LEU	H	8.814	0.000	1
1	A	116	LEU	CA	53.699	0.006	1
1	A	116	LEU	HA	5.261	0.001	1
1	A	116	LEU	CB	45.355	0.002	1
1	A	116	LEU	HB2	1.386	0.001	2
1	A	116	LEU	HB3	1.657	0.000	2
1	A	116	LEU	CG	27.076	0.006	1
1	A	116	LEU	HG	1.67	0.001	1
1	A	116	LEU	HD11	0.889	0.000	2
1	A	116	LEU	HD12	0.889	0.000	2
1	A	116	LEU	HD13	0.889	0.000	2
1	A	116	LEU	HD21	0.885	0.000	2
1	A	116	LEU	HD22	0.885	0.000	2
1	A	116	LEU	HD23	0.885	0.000	2
1	A	116	LEU	CD1	23.833	0.001	1
1	A	116	LEU	CD2	25.129	0.001	1
1	A	116	LEU	C	175.218	0.007	1
1	A	117	ALA	N	127.31	0.001	1
1	A	117	ALA	H	9.579	0.000	1
1	A	117	ALA	CA	49.84	0.001	1
1	A	117	ALA	HA	5.365	0.001	1
1	A	117	ALA	HB1	1.363	0.000	1
1	A	117	ALA	HB2	1.363	0.000	1
1	A	117	ALA	HB3	1.363	0.000	1
1	A	117	ALA	CB	22.843	0.000	1
1	A	117	ALA	C	174.298	0.008	1
1	A	118	GLY	N	107.111	0.000	1
1	A	118	GLY	H	9.438	0.000	1
1	A	118	GLY	CA	43.269	0.007	1
1	A	118	GLY	HA2	3.997	0.000	2
1	A	118	GLY	HA3	3.298	0.000	2
1	A	118	GLY	C	173.053	0.000	1
1	A	119	ASP	N	122.511	0.000	1
1	A	119	ASP	H	8.058	0.000	1
1	A	119	ASP	CA	51.592	0.000	1
1	A	119	ASP	HA	3.158	0.002	1
1	A	119	ASP	CB	39.258	0.001	1
1	A	119	ASP	HB2	2.458	0.002	2
1	A	119	ASP	HB3	2.633	0.000	2
1	A	119	ASP	C	175.344	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	PRO	CA	65.76	0.000	1
1	A	120	PRO	HA	4.112	0.000	1
1	A	120	PRO	CB	31.682	0.000	1
1	A	120	PRO	HB2	2.384	0.000	2
1	A	120	PRO	HB3	2.384	0.000	2
1	A	120	PRO	CG	28.31	0.000	1
1	A	120	PRO	HG2	1.478	0.000	2
1	A	120	PRO	HG3	1.478	0.000	2
1	A	120	PRO	CD	50.358	0.002	1
1	A	120	PRO	HD2	3.142	0.001	2
1	A	120	PRO	HD3	2.153	0.001	2
1	A	120	PRO	C	177.782	0.000	1
1	A	121	SER	N	111.956	0.000	1
1	A	121	SER	H	7.48	0.000	1
1	A	121	SER	CA	58.916	0.000	1
1	A	121	SER	HA	4.301	0.000	1
1	A	121	SER	CB	63.034	0.001	1
1	A	121	SER	HB2	3.46	0.000	2
1	A	121	SER	HB3	3.673	0.000	2
1	A	121	SER	C	173.701	0.000	1
1	A	122	GLY	N	109.107	0.002	1
1	A	122	GLY	H	8.261	0.000	1
1	A	122	GLY	CA	44.759	0.006	1
1	A	122	GLY	HA2	4.044	0.000	2
1	A	122	GLY	HA3	3.418	0.000	2
1	A	122	GLY	C	175.197	0.000	1
1	A	123	HIS	N	120.927	0.000	1
1	A	123	HIS	H	8.164	0.001	1
1	A	123	HIS	CA	55.657	0.000	1
1	A	123	HIS	HA	4.792	0.000	1
1	A	123	HIS	CB	27.039	0.001	1
1	A	123	HIS	HB2	3.406	0.000	2
1	A	123	HIS	HB3	3.617	0.000	2
1	A	123	HIS	CD2	120.571	0.000	1
1	A	123	HIS	HD2	7.386	0.000	1
1	A	124	ARG	N	123.574	0.000	1
1	A	124	ARG	H	8.571	0.000	1
1	A	124	ARG	CA	55.888	0.001	1
1	A	124	ARG	HA	5.219	0.000	1
1	A	124	ARG	CB	31.885	0.000	1
1	A	124	ARG	HB2	1.854	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	124	ARG	HB3	1.9	0.000	2
1	A	124	ARG	CG	27.615	0.003	1
1	A	124	ARG	HG2	1.517	0.000	2
1	A	124	ARG	HG3	1.684	0.000	2
1	A	124	ARG	CD	43.951	0.000	1
1	A	124	ARG	HD2	3.212	0.000	2
1	A	124	ARG	HD3	3.297	0.000	2
1	A	124	ARG	NE	84.04	0.000	1
1	A	124	ARG	HE	7.174	0.000	1
1	A	124	ARG	C	176.305	0.007	1
1	A	125	VAL	N	127.014	0.000	1
1	A	125	VAL	H	9.851	0.000	1
1	A	125	VAL	CA	60.904	0.000	1
1	A	125	VAL	HA	4.258	0.000	1
1	A	125	VAL	CB	35.831	0.000	1
1	A	125	VAL	HB	2.112	0.000	1
1	A	125	VAL	HG11	0.471	0.000	1
1	A	125	VAL	HG12	0.471	0.000	1
1	A	125	VAL	HG13	0.471	0.000	1
1	A	125	VAL	HG21	1.055	0.000	1
1	A	125	VAL	HG22	1.055	0.000	1
1	A	125	VAL	HG23	1.055	0.000	1
1	A	125	VAL	CG1	20.923	0.001	1
1	A	125	VAL	CG2	17.928	0.000	1
1	A	125	VAL	C	171.528	0.000	1
1	A	126	GLY	N	114.519	0.000	1
1	A	126	GLY	H	8.269	0.001	1
1	A	126	GLY	CA	44.717	0.001	1
1	A	126	GLY	HA2	3.256	0.000	1
1	A	126	GLY	HA3	5.005	0.000	1
1	A	126	GLY	C	172.478	0.000	1
1	A	127	LEU	N	124.56	0.000	1
1	A	127	LEU	H	9.379	0.000	1
1	A	127	LEU	CA	53.616	0.003	1
1	A	127	LEU	HA	5.781	0.000	1
1	A	127	LEU	CB	42.893	0.001	1
1	A	127	LEU	HB2	1.394	0.000	2
1	A	127	LEU	HB3	1.898	0.000	2
1	A	127	LEU	CG	27.415	0.005	1
1	A	127	LEU	HG	1.7	0.003	1
1	A	127	LEU	HD11	0.769	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	LEU	HD12	0.769	0.000	1
1	A	127	LEU	HD13	0.769	0.000	1
1	A	127	LEU	HD21	1.05	0.000	1
1	A	127	LEU	HD22	1.05	0.000	1
1	A	127	LEU	HD23	1.05	0.000	1
1	A	127	LEU	CD1	26.182	0.000	1
1	A	127	LEU	CD2	24.63	0.000	1
1	A	127	LEU	C	175.325	0.005	1
1	A	128	TRP	N	124.436	0.000	1
1	A	128	TRP	H	9.041	0.000	1
1	A	128	TRP	CA	55.711	0.000	1
1	A	128	TRP	HA	5.238	0.000	1
1	A	128	TRP	CB	33.923	0.002	1
1	A	128	TRP	HB2	2.875	0.000	2
1	A	128	TRP	HB3	3.066	0.000	2
1	A	128	TRP	CD1	126.278	0.002	1
1	A	128	TRP	CE3	119.493	0.000	1
1	A	128	TRP	NE1	128.253	0.002	1
1	A	128	TRP	HD1	6.989	0.000	1
1	A	128	TRP	HE3	7.302	0.000	1
1	A	128	TRP	CZ3	121.975	0.009	1
1	A	128	TRP	CZ2	113.619	0.002	1
1	A	128	TRP	HE1	9.963	0.002	1
1	A	128	TRP	HZ3	6.521	0.001	1
1	A	128	TRP	CH2	123.409	0.001	1
1	A	128	TRP	HZ2	6.855	0.001	1
1	A	128	TRP	HH2	6.49	0.000	1
1	A	128	TRP	C	174.008	0.000	1
1	A	129	GLN	N	131.383	0.000	1
1	A	129	GLN	H	9.171	0.000	1
1	A	129	GLN	CA	53.405	0.002	1
1	A	129	GLN	HA	5.035	0.001	1
1	A	129	GLN	CB	30.245	0.005	1
1	A	129	GLN	HB2	1.562	0.000	2
1	A	129	GLN	HB3	2.02	0.000	2
1	A	129	GLN	CG	32.632	0.000	1
1	A	129	GLN	HG2	2.382	0.000	2
1	A	129	GLN	HG3	1.956	0.000	2
1	A	129	GLN	NE2	112.421	0.000	1
1	A	129	GLN	HE21	7.155	0.000	2
1	A	129	GLN	HE22	7.615	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	GLN	C	174.178	0.000	1
1	A	130	ALA	N	130.163	0.000	1
1	A	130	ALA	H	8.761	0.000	1
1	A	130	ALA	CA	53.141	0.002	1
1	A	130	ALA	HA	3.985	0.000	1
1	A	130	ALA	HB1	1.352	0.000	1
1	A	130	ALA	HB2	1.352	0.000	1
1	A	130	ALA	HB3	1.352	0.000	1
1	A	130	ALA	CB	19.694	0.003	1
1	A	130	ALA	C	177.657	0.006	1
1	A	131	LYS	N	122.377	0.000	1
1	A	131	LYS	H	8.066	0.000	1
1	A	131	LYS	CA	57.08	0.000	1
1	A	131	LYS	HA	4.233	0.000	1
1	A	131	LYS	CB	32.437	0.000	1
1	A	131	LYS	HB2	1.257	0.000	2
1	A	131	LYS	HB3	1.682	0.000	2
1	A	131	LYS	CG	25.047	0.002	1
1	A	131	LYS	HG2	1.227	0.000	2
1	A	131	LYS	HG3	1.103	0.000	2
1	A	131	LYS	CD	28.824	0.000	1
1	A	131	LYS	HD2	1.309	0.005	2
1	A	131	LYS	HD3	1.309	0.005	2
1	A	131	LYS	CE	41.937	0.001	1
1	A	131	LYS	HE2	2.554	0.000	2
1	A	131	LYS	HE3	2.633	0.000	2
1	A	131	LYS	C	175.912	0.002	1
1	A	132	GLU	N	119.685	0.004	1
1	A	132	GLU	H	8.187	0.000	1
1	A	132	GLU	CA	56.654	0.000	1
1	A	132	GLU	HA	4.271	0.000	1
1	A	132	GLU	CB	30.58	0.000	1
1	A	132	GLU	HB2	1.886	0.000	2
1	A	132	GLU	HB3	2.075	0.000	2
1	A	132	GLU	CG	36.304	0.000	1
1	A	132	GLU	HG2	2.179	0.000	2
1	A	132	GLU	HG3	2.265	0.000	2
1	A	132	GLU	C	175.777	0.001	1
1	A	133	HIS	N	120.224	0.000	1
1	A	133	HIS	H	8.645	0.000	1
1	A	133	HIS	CA	55.761	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	HIS	HA	4.8	0.000	1
1	A	133	HIS	CB	30.943	0.000	1
1	A	133	HIS	HB2	3.057	0.000	2
1	A	133	HIS	HB3	3.196	0.002	2
1	A	133	HIS	CD2	119.023	0.002	1
1	A	133	HIS	HD2	6.854	0.000	1
1	A	134	THR	N	116.228	0.000	1
1	A	134	THR	H	8.297	0.000	1
1	A	134	THR	CA	61.789	0.000	1
1	A	134	THR	HA	4.819	0.000	1
1	A	134	THR	CB	69.731	0.000	1
1	A	134	THR	HB	4.307	0.000	1
1	A	134	THR	HG21	1.153	0.000	1
1	A	134	THR	HG22	1.153	0.000	1
1	A	134	THR	HG23	1.153	0.000	1
1	A	134	THR	CG2	21.214	0.000	1
1	A	135	GLY	CA	44.995	0.000	1
1	A	135	GLY	HA2	3.719	0.000	2
1	A	135	GLY	HA3	4.256	0.000	2
1	A	135	GLY	C	173.663	0.000	1
1	A	136	SER	N	116.477	0.000	1
1	A	136	SER	H	8.599	0.000	1
1	A	136	SER	CA	58.959	0.001	1
1	A	136	SER	HA	4.585	0.002	1
1	A	136	SER	CB	64.338	0.001	1
1	A	136	SER	HB2	3.924	0.000	2
1	A	136	SER	HB3	4.005	0.001	2
1	A	136	SER	C	175.376	0.003	1
1	A	137	GLY	N	111.673	0.001	1
1	A	137	GLY	H	8.713	0.001	1
1	A	137	GLY	CA	44.916	0.005	1
1	A	137	GLY	HA2	4.274	0.000	2
1	A	137	GLY	HA3	4.019	0.000	2
1	A	137	GLY	C	171.411	0.000	1
1	A	138	PRO	CA	63.137	0.001	1
1	A	138	PRO	HA	4.428	0.001	1
1	A	138	PRO	CB	32.357	0.000	1
1	A	138	PRO	HB2	1.914	0.000	2
1	A	138	PRO	HB3	2.279	0.000	2
1	A	138	PRO	CG	27.116	0.000	1
1	A	138	PRO	HG2	1.995	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	PRO	HG3	1.995	0.000	2
1	A	138	PRO	CD	49.928	0.000	1
1	A	138	PRO	HD2	3.633	0.000	2
1	A	138	PRO	HD3	3.633	0.000	2
1	A	138	PRO	C	176.413	0.000	1
1	A	139	ASP	N	120.811	0.000	1
1	A	139	ASP	H	8.487	0.000	1
1	A	139	ASP	CA	53.643	0.000	1
1	A	139	ASP	HA	4.543	0.000	1
1	A	139	ASP	CB	41.135	0.000	1
1	A	139	ASP	HB2	2.629	0.000	2
1	A	139	ASP	HB3	2.732	0.001	2
1	A	139	ASP	C	175.628	0.000	1
1	A	140	ASP	N	123.149	0.000	1
1	A	140	ASP	H	8.101	0.001	1
1	A	140	ASP	CA	53.477	0.000	1
1	A	140	ASP	HA	4.646	0.000	1
1	A	140	ASP	CB	41.229	0.000	1
1	A	140	ASP	HB2	2.546	0.000	2
1	A	140	ASP	HB3	2.731	0.002	2
1	A	140	ASP	C	176.269	0.001	1
1	A	141	GLY	N	107.309	0.001	1
1	A	141	GLY	H	8.039	0.000	1
1	A	141	GLY	CA	44.28	0.000	1
1	A	141	GLY	HA2	3.974	0.000	2
1	A	141	GLY	HA3	3.974	0.000	2
1	A	141	GLY	C	173.273	0.002	1
1	A	142	ILE	N	118.362	0.005	1
1	A	142	ILE	H	8.368	0.000	1
1	A	142	ILE	CA	62.485	0.001	1
1	A	142	ILE	HA	3.467	0.001	1
1	A	142	ILE	CB	37.101	0.001	1
1	A	142	ILE	HB	1.887	0.000	1
1	A	142	ILE	HG21	1.082	0.000	1
1	A	142	ILE	HG22	1.082	0.000	1
1	A	142	ILE	HG23	1.082	0.000	1
1	A	142	ILE	CG2	18.204	0.000	1
1	A	142	ILE	CG1	27.805	0.006	1
1	A	142	ILE	HG12	1.589	0.000	1
1	A	142	ILE	HG13	1.289	0.002	1
1	A	142	ILE	HD11	0.814	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	142	ILE	HD12	0.814	0.000	1
1	A	142	ILE	HD13	0.814	0.000	1
1	A	142	ILE	CD1	12.188	0.003	1
1	A	142	ILE	C	178.029	0.002	1
1	A	143	GLY	N	116.829	0.000	1
1	A	143	GLY	H	9.622	0.000	1
1	A	143	GLY	CA	45.131	0.002	1
1	A	143	GLY	HA2	3.305	0.001	2
1	A	143	GLY	HA3	4.439	0.001	2
1	A	143	GLY	C	172.009	0.000	1
1	A	144	ALA	N	118.932	0.000	1
1	A	144	ALA	H	7.468	0.001	1
1	A	144	ALA	CA	51.269	0.004	1
1	A	144	ALA	HA	4.34	0.001	1
1	A	144	ALA	HB1	1.416	0.000	1
1	A	144	ALA	HB2	1.416	0.000	1
1	A	144	ALA	HB3	1.416	0.000	1
1	A	144	ALA	CB	20.159	0.003	1
1	A	144	ALA	C	177.106	0.003	1
1	A	145	TYR	N	119.756	0.000	1
1	A	145	TYR	H	8.394	0.000	1
1	A	145	TYR	CA	57.067	0.000	1
1	A	145	TYR	HA	4.48	0.000	1
1	A	145	TYR	HB2	2.724	0.000	1
1	A	145	TYR	HB3	2.849	0.000	1
1	A	146	THR	N	126.333	0.000	1
1	A	146	THR	H	8.372	0.002	1
1	A	146	THR	CA	64.965	0.000	1
1	A	146	THR	HA	4.088	0.000	1
1	A	146	THR	CB	69.786	0.000	1
1	A	146	THR	HB	3.428	0.001	1
1	A	146	THR	HG21	0.97	0.000	1
1	A	146	THR	HG22	0.97	0.000	1
1	A	146	THR	HG23	0.97	0.000	1
1	A	146	THR	CG2	22.03	0.000	1
1	A	146	THR	C	173.143	0.000	1
1	A	147	ARG	N	109.298	0.001	1
1	A	147	ARG	H	6.705	0.000	1
1	A	147	ARG	CA	55.316	0.004	1
1	A	147	ARG	HA	3.773	0.000	1
1	A	147	ARG	CB	30.347	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	ARG	CG	25.986	0.000	1
1	A	147	ARG	C	173.649	0.001	1
1	A	148	SER	N	110.2	0.000	1
1	A	148	SER	H	6.384	0.000	1
1	A	148	SER	CA	58.038	0.002	1
1	A	148	SER	HA	5.773	0.000	1
1	A	148	SER	CB	66.59	0.002	1
1	A	148	SER	HB2	3.464	0.000	2
1	A	148	SER	HB3	4.131	0.002	2
1	A	148	SER	C	171.562	0.002	1
1	A	149	GLU	N	119.137	0.000	1
1	A	149	GLU	H	8.599	0.000	1
1	A	149	GLU	CA	55.035	0.001	1
1	A	149	GLU	HA	5.069	0.000	1
1	A	149	GLU	CB	33.335	0.001	1
1	A	149	GLU	HB2	1.675	0.000	2
1	A	149	GLU	HB3	1.675	0.000	2
1	A	149	GLU	CG	37.836	0.002	1
1	A	149	GLU	HG2	2.683	0.000	2
1	A	149	GLU	HG3	1.926	0.000	2
1	A	149	GLU	C	173.137	0.000	1
1	A	150	LEU	N	125.099	0.001	1
1	A	150	LEU	H	8.014	0.000	1
1	A	150	LEU	CA	52.413	0.003	1
1	A	150	LEU	HA	3.582	0.001	1
1	A	150	LEU	CB	40.219	0.000	1
1	A	150	LEU	HB2	-1.825	0.000	2
1	A	150	LEU	HB3	-1.825	0.000	2
1	A	150	LEU	CG	26.211	0.000	1
1	A	150	LEU	HG	0.499	0.000	1
1	A	150	LEU	HD11	-0.598	0.002	2
1	A	150	LEU	HD12	-0.598	0.002	2
1	A	150	LEU	HD13	-0.598	0.002	2
1	A	150	LEU	HD21	0.584	0.001	2
1	A	150	LEU	HD22	0.584	0.001	2
1	A	150	LEU	HD23	0.584	0.001	2
1	A	150	LEU	CD1	19.957	0.002	1
1	A	150	LEU	CD2	26.163	0.002	1
1	A	150	LEU	C	173.334	0.000	1
1	A	151	LEU	N	130.193	0.000	1
1	A	151	LEU	H	8.3	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	LEU	CA	53.633	0.000	1
1	A	151	LEU	HA	4.703	0.000	1
1	A	151	LEU	CB	40.243	0.003	1
1	A	151	LEU	HB2	1.528	0.000	1
1	A	151	LEU	HB3	1.798	0.000	1
1	A	151	LEU	CG	28.767	0.000	1
1	A	151	LEU	HG	1.537	0.000	1
1	A	151	LEU	HD11	0.461	0.001	2
1	A	151	LEU	HD12	0.461	0.001	2
1	A	151	LEU	HD13	0.461	0.001	2
1	A	151	LEU	HD21	0.695	0.001	2
1	A	151	LEU	HD22	0.695	0.001	2
1	A	151	LEU	HD23	0.695	0.001	2
1	A	151	LEU	CD1	22.95	0.002	1
1	A	151	LEU	CD2	24.294	0.007	1
1	A	151	LEU	C	175.398	0.000	1
1	A	152	THR	N	116.84	0.001	1
1	A	152	THR	H	8.578	0.000	1
1	A	152	THR	CA	57.314	0.000	1
1	A	152	THR	HA	4.871	0.000	1
1	A	152	THR	CB	68.496	0.000	1
1	A	152	THR	HB	3.635	0.000	1
1	A	152	THR	HG21	0.852	0.000	1
1	A	152	THR	HG22	0.852	0.000	1
1	A	152	THR	HG23	0.852	0.000	1
1	A	152	THR	CG2	21.902	0.000	1
1	A	152	THR	C	172.063	0.000	1
1	A	153	GLY	N	115.202	0.000	1
1	A	153	GLY	H	8.666	0.000	1
1	A	153	GLY	CA	45.488	0.000	1
1	A	153	GLY	HA2	4.771	0.001	1
1	A	153	GLY	HA3	3.682	0.000	1
1	A	153	GLY	C	174.882	0.000	1
1	A	154	ALA	N	130.159	0.000	1
1	A	154	ALA	H	9.143	0.000	1
1	A	154	ALA	CA	50.109	0.001	1
1	A	154	ALA	HA	4.927	0.000	1
1	A	154	ALA	HB1	1.234	0.000	1
1	A	154	ALA	HB2	1.234	0.000	1
1	A	154	ALA	HB3	1.234	0.000	1
1	A	154	ALA	CB	18.593	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	154	ALA	C	176.474	0.001	1
1	A	155	SER	N	115.992	0.000	1
1	A	155	SER	H	8.411	0.001	1
1	A	155	SER	CA	63.228	0.001	1
1	A	155	SER	HA	3.765	0.000	1
1	A	155	SER	CB	62.317	0.004	1
1	A	155	SER	HB2	3.725	0.000	2
1	A	155	SER	HB3	3.8	0.001	2
1	A	155	SER	C	177.816	0.000	1
1	A	156	ALA	N	126.187	0.000	1
1	A	156	ALA	H	8.637	0.000	1
1	A	156	ALA	CA	55.522	0.001	1
1	A	156	ALA	HA	4.348	0.000	1
1	A	156	ALA	HB1	1.516	0.000	1
1	A	156	ALA	HB2	1.516	0.000	1
1	A	156	ALA	HB3	1.516	0.000	1
1	A	156	ALA	CB	18.154	0.000	1
1	A	156	ALA	C	180.558	0.000	1
1	A	157	THR	N	115.083	0.001	1
1	A	157	THR	H	7.879	0.000	1
1	A	157	THR	CA	65.42	0.000	1
1	A	157	THR	HA	4.116	0.000	1
1	A	157	THR	CB	68.655	0.001	1
1	A	157	THR	HB	4.147	0.000	1
1	A	157	THR	HG21	1.24	0.000	1
1	A	157	THR	HG22	1.24	0.000	1
1	A	157	THR	HG23	1.24	0.000	1
1	A	157	THR	CG2	22.05	0.000	1
1	A	157	THR	C	177.619	0.001	1
1	A	158	ASP	N	124.324	0.000	1
1	A	158	ASP	H	8.934	0.000	1
1	A	158	ASP	CA	58.31	0.002	1
1	A	158	ASP	HA	4.536	0.006	1
1	A	158	ASP	CB	39.963	0.000	1
1	A	158	ASP	HB2	2.616	0.001	1
1	A	158	ASP	HB3	2.746	0.001	1
1	A	158	ASP	C	179.127	0.006	1
1	A	159	GLY	N	106.849	0.000	1
1	A	159	GLY	H	8.466	0.001	1
1	A	159	GLY	CA	48.059	0.000	1
1	A	159	GLY	HA2	3.923	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	159	GLY	HA3	4.146	0.000	1
1	A	159	GLY	C	174.993	0.004	1
1	A	160	ALA	N	121.604	0.000	1
1	A	160	ALA	H	7.512	0.000	1
1	A	160	ALA	CA	55.316	0.001	1
1	A	160	ALA	HA	4.204	0.000	1
1	A	160	ALA	HB1	1.585	0.000	1
1	A	160	ALA	HB2	1.585	0.000	1
1	A	160	ALA	HB3	1.585	0.000	1
1	A	160	ALA	CB	17.995	0.004	1
1	A	160	ALA	C	180.329	0.007	1
1	A	161	PHE	N	120.296	0.000	1
1	A	161	PHE	H	7.412	0.000	1
1	A	161	PHE	CA	61.069	0.003	1
1	A	161	PHE	HA	4.343	0.000	1
1	A	161	PHE	CB	38.515	0.004	1
1	A	161	PHE	HB2	2.998	0.002	2
1	A	161	PHE	HB3	3.305	0.001	2
1	A	161	PHE	C	175.721	0.002	1
1	A	162	TYR	N	116.081	0.000	1
1	A	162	TYR	H	7.827	0.000	1
1	A	162	TYR	CA	62.938	0.000	1
1	A	162	TYR	HA	3.495	0.000	1
1	A	162	TYR	CB	39.657	0.000	1
1	A	162	TYR	HB2	2.802	0.000	1
1	A	162	TYR	HB3	3.026	0.000	1
1	A	162	TYR	HH	12.412	0.000	1
1	A	162	TYR	C	178.471	0.001	1
1	A	163	ARG	N	118.577	0.000	1
1	A	163	ARG	H	8.846	0.000	1
1	A	163	ARG	CA	58.649	0.000	1
1	A	163	ARG	HA	4.397	0.000	1
1	A	163	ARG	CB	30.095	0.004	1
1	A	163	ARG	HB2	1.761	0.000	2
1	A	163	ARG	HB3	1.85	0.000	2
1	A	163	ARG	CG	31.098	0.000	1
1	A	163	ARG	HG2	1.992	0.000	2
1	A	163	ARG	HG3	2.134	0.000	2
1	A	163	ARG	CD	43.895	0.002	1
1	A	163	ARG	HD2	3.398	0.000	2
1	A	163	ARG	HD3	3.202	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	163	ARG	NE	86.322	0.003	1
1	A	163	ARG	HE	7.207	0.000	1
1	A	163	ARG	CZ	173.461	0.000	1
1	A	163	ARG	C	179.9	0.006	1
1	A	165	LEU	N	120.225	0.000	1
1	A	165	LEU	H	6.853	0.000	1
1	A	165	LEU	CA	56.424	0.002	1
1	A	165	LEU	HA	3.721	0.000	1
1	A	165	LEU	CB	42.322	0.001	1
1	A	165	LEU	HB2	0.127	0.001	1
1	A	165	LEU	HB3	0.457	0.000	1
1	A	165	LEU	CG	25.404	0.000	1
1	A	165	LEU	HG	0.55	0.000	1
1	A	165	LEU	HD11	0.046	0.000	1
1	A	165	LEU	HD12	0.046	0.000	1
1	A	165	LEU	HD13	0.046	0.000	1
1	A	165	LEU	HD21	0.155	0.000	1
1	A	165	LEU	HD22	0.155	0.000	1
1	A	165	LEU	HD23	0.155	0.000	1
1	A	165	LEU	CD1	24.872	0.003	1
1	A	165	LEU	CD2	23.819	0.001	1
1	A	165	LEU	C	178.68	0.000	1
1	A	166	PHE	N	113.958	0.000	1
1	A	166	PHE	H	8.055	0.000	1
1	A	166	PHE	CA	56.747	0.000	1
1	A	166	PHE	HA	4.878	0.000	1
1	A	166	PHE	CB	41.497	0.001	1
1	A	166	PHE	HB2	2.451	0.001	2
1	A	166	PHE	HB3	3.306	0.001	2
1	A	166	PHE	HD1	6.451	0.000	1
1	A	166	PHE	HD2	6.451	0.000	1
1	A	166	PHE	C	176.266	0.000	1
1	A	167	GLY	N	110.611	0.001	1
1	A	167	GLY	H	8.004	0.000	1
1	A	167	GLY	CA	44.173	0.002	1
1	A	167	GLY	HA2	3.856	0.000	2
1	A	167	GLY	HA3	4.751	0.000	2
1	A	167	GLY	C	174.295	0.001	1
1	A	169	ASP	N	112.907	0.000	1
1	A	169	ASP	H	8.37	0.000	1
1	A	169	ASP	CA	53.959	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	169	ASP	HA	4.64	0.000	1
1	A	169	ASP	CB	40.509	0.001	1
1	A	169	ASP	HB2	2.667	0.001	2
1	A	169	ASP	HB3	2.729	0.000	2
1	A	169	ASP	C	177.11	0.009	1
1	A	170	PHE	N	123.951	0.000	1
1	A	170	PHE	H	7.947	0.001	1
1	A	170	PHE	CA	60.164	0.000	1
1	A	170	PHE	HA	4.231	0.000	1
1	A	170	PHE	CB	39.928	0.000	1
1	A	170	PHE	HB2	3.304	0.000	2
1	A	170	PHE	HB3	3.067	0.001	2
1	A	170	PHE	CD1	132.729	0.000	1
1	A	170	PHE	HD1	7.255	0.001	1
1	A	170	PHE	CD2	132.729	0.001	1
1	A	170	PHE	HD2	7.255	0.001	1
1	A	170	PHE	C	175.325	0.001	1
1	A	171	ALA	N	126.104	0.002	1
1	A	171	ALA	H	8.716	0.002	1
1	A	171	ALA	CA	52.5	0.000	1
1	A	171	ALA	HA	3.777	0.002	1
1	A	171	ALA	HB1	0.975	0.000	1
1	A	171	ALA	HB2	0.975	0.000	1
1	A	171	ALA	HB3	0.975	0.000	1
1	A	171	ALA	CB	16.881	0.001	1
1	A	171	ALA	C	176.429	0.002	1
1	A	172	THR	N	109.751	0.000	1
1	A	172	THR	H	7.61	0.000	1
1	A	172	THR	CA	61.556	0.002	1
1	A	172	THR	HA	4.492	0.001	1
1	A	172	THR	CB	70.872	0.001	1
1	A	172	THR	HB	4.275	0.000	1
1	A	172	THR	HG21	1.238	0.000	1
1	A	172	THR	HG22	1.238	0.000	1
1	A	172	THR	HG23	1.238	0.000	1
1	A	172	THR	CG2	21.763	0.000	1
1	A	172	THR	C	175.183	0.004	1
1	A	173	GLU	N	122.828	0.003	1
1	A	173	GLU	H	8.752	0.001	1
1	A	173	GLU	CA	56.918	0.001	1
1	A	173	GLU	HA	4.32	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	173	GLU	CB	29.907	0.000	1
1	A	173	GLU	HB2	2.098	0.000	2
1	A	173	GLU	HB3	1.959	0.001	2
1	A	173	GLU	CG	36.497	0.001	1
1	A	173	GLU	HG2	2.245	0.001	2
1	A	173	GLU	HG3	2.245	0.001	2
1	A	173	GLU	C	176.553	0.001	1
1	A	174	SER	N	116.467	0.000	1
1	A	174	SER	H	8.327	0.001	1
1	A	174	SER	CA	58.312	0.006	1
1	A	174	SER	HA	4.488	0.001	1
1	A	174	SER	CB	64.041	0.002	1
1	A	174	SER	HB2	3.814	0.000	2
1	A	174	SER	HB3	3.888	0.000	2
1	A	174	SER	C	175.115	0.009	1
1	A	176	THR	N	112.752	0.000	1
1	A	176	THR	H	8.098	0.000	1
1	A	176	THR	CA	61.772	0.002	1
1	A	176	THR	HA	4.359	0.001	1
1	A	176	THR	CB	69.809	0.000	1
1	A	176	THR	HB	4.281	0.000	1
1	A	176	THR	HG21	1.161	0.000	1
1	A	176	THR	HG22	1.161	0.000	1
1	A	176	THR	HG23	1.161	0.000	1
1	A	176	THR	CG2	21.54	0.000	1
1	A	176	THR	C	174.675	0.000	1
1	A	177	ASP	N	122.46	0.001	1
1	A	177	ASP	H	8.368	0.000	1
1	A	177	ASP	CA	54.624	0.003	1
1	A	177	ASP	HA	4.618	0.000	1
1	A	177	ASP	CB	41.223	0.000	1
1	A	177	ASP	HB2	2.691	0.000	2
1	A	177	ASP	HB3	2.691	0.000	2
1	A	177	ASP	C	176.713	0.000	1
1	A	178	GLY	N	109.385	0.000	1
1	A	178	GLY	H	8.403	0.000	1
1	A	178	GLY	CA	45.439	0.000	1
1	A	178	GLY	HA2	3.959	0.000	2
1	A	178	GLY	HA3	3.959	0.000	2
1	A	178	GLY	C	175.002	0.000	1
1	A	179	GLY	N	108.906	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	179	GLY	H	8.387	0.001	1
1	A	179	GLY	CA	45.42	0.000	1
1	A	179	GLY	HA2	3.936	0.006	2
1	A	179	GLY	HA3	3.936	0.006	2
1	A	179	GLY	C	174.687	0.000	1
1	A	180	GLY	N	108.865	0.000	1
1	A	180	GLY	H	8.23	0.000	1
1	A	180	GLY	CA	45.134	0.000	1
1	A	180	GLY	HA2	3.906	0.000	2
1	A	180	GLY	HA3	3.906	0.000	2
1	A	180	GLY	C	174.019	0.000	1
1	A	181	ARG	N	120.473	0.003	1
1	A	181	ARG	H	8.278	0.000	1
1	A	181	ARG	CA	56.085	0.000	1
1	A	181	ARG	HA	4.507	0.000	1
1	A	181	ARG	CB	31.097	0.000	1
1	A	181	ARG	HB2	1.795	0.000	2
1	A	181	ARG	HB3	1.795	0.000	2
1	A	181	ARG	CG	28.207	0.000	1
1	A	181	ARG	HG2	1.648	0.000	2
1	A	181	ARG	C	175.89	0.000	1
1	A	182	ARG	N	119.764	0.000	1
1	A	182	ARG	H	7.777	0.000	1
1	A	182	ARG	CA	54.607	0.000	1
1	A	182	ARG	HA	4.517	0.000	1
1	A	182	ARG	CB	32.397	0.000	1
1	A	182	ARG	HB2	1.604	0.000	2
1	A	182	ARG	HB3	1.773	0.000	2
1	A	182	ARG	CG	27.218	0.000	1
1	A	182	ARG	HG2	1.571	0.000	2
1	A	182	ARG	HG3	1.571	0.000	2
1	A	182	ARG	CD	43.359	0.000	1
1	A	182	ARG	HD2	3.165	0.000	2
1	A	182	ARG	HD3	3.165	0.000	2
1	A	182	ARG	NE	85.198	0.005	1
1	A	182	ARG	HE	7.222	0.000	1
1	A	182	ARG	C	175.099	0.000	1
1	A	183	ALA	N	122.495	0.001	1
1	A	183	ALA	H	8.594	0.000	1
1	A	183	ALA	CA	51.833	0.000	1
1	A	183	ALA	HA	4.627	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	183	ALA	HB1	1.388	0.000	1
1	A	183	ALA	HB2	1.388	0.000	1
1	A	183	ALA	HB3	1.388	0.000	1
1	A	183	ALA	CB	20.625	0.000	1
1	A	183	ALA	C	175.635	0.000	1
1	A	184	ALA	N	117.658	0.000	1
1	A	184	ALA	H	6.877	0.000	1
1	A	184	ALA	CA	50.633	0.000	1
1	A	184	ALA	HA	4.53	0.000	1
1	A	184	ALA	HB1	1.131	0.000	1
1	A	184	ALA	HB2	1.131	0.000	1
1	A	184	ALA	HB3	1.131	0.000	1
1	A	184	ALA	CB	23.284	0.001	1
1	A	184	ALA	C	174.48	0.005	1
1	A	185	ILE	N	119.761	0.000	1
1	A	185	ILE	H	8.585	0.000	1
1	A	185	ILE	CA	60.843	0.006	1
1	A	185	ILE	HA	4.423	0.003	1
1	A	185	ILE	CB	40.214	0.003	1
1	A	185	ILE	HB	1.611	0.000	1
1	A	185	ILE	HG21	0.672	0.001	1
1	A	185	ILE	HG22	0.672	0.001	1
1	A	185	ILE	HG23	0.672	0.001	1
1	A	185	ILE	CG2	17.275	0.004	1
1	A	185	ILE	CG1	26.676	0.001	1
1	A	185	ILE	HG12	1.379	0.000	2
1	A	185	ILE	HG13	1.379	0.000	2
1	A	185	ILE	HD11	0.985	0.002	1
1	A	185	ILE	HD12	0.985	0.002	1
1	A	185	ILE	HD13	0.985	0.002	1
1	A	185	ILE	CD1	13.733	0.001	1
1	A	185	ILE	C	174.696	0.000	1
1	A	186	ARG	N	126.563	0.000	1
1	A	186	ARG	H	9.503	0.001	1
1	A	186	ARG	CA	52.49	0.002	1
1	A	186	ARG	HA	4.567	0.001	1
1	A	186	ARG	CB	30.729	0.000	1
1	A	186	ARG	HB2	1.339	0.000	2
1	A	186	ARG	HB3	1.51	0.001	2
1	A	186	ARG	CG	25.664	0.000	1
1	A	186	ARG	HG2	1.299	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	186	ARG	HG3	1.161	0.000	2
1	A	186	ARG	CD	42.746	0.001	1
1	A	186	ARG	HD2	2.982	0.000	2
1	A	186	ARG	HD3	2.75	0.000	2
1	A	186	ARG	NE	88.699	0.003	1
1	A	186	ARG	HE	8.348	0.001	1
1	A	186	ARG	C	173.899	0.008	1
1	A	187	GLN	N	124.139	0.000	1
1	A	187	GLN	H	8.352	0.000	1
1	A	187	GLN	CA	54.731	0.001	1
1	A	187	GLN	HA	5.009	0.000	1
1	A	187	GLN	CB	28.13	0.000	1
1	A	187	GLN	HB2	1.915	0.000	1
1	A	187	GLN	HB3	2.013	0.000	1
1	A	187	GLN	CG	32.886	0.001	1
1	A	187	GLN	HG2	2.192	0.000	2
1	A	187	GLN	HG3	2.49	0.000	2
1	A	187	GLN	NE2	113.726	0.000	1
1	A	187	GLN	HE21	7.425	0.000	1
1	A	187	GLN	HE22	6.926	0.000	1
1	A	187	GLN	C	176.247	0.001	1
1	A	188	VAL	N	121.492	0.000	1
1	A	188	VAL	H	8.151	0.000	1
1	A	188	VAL	CA	59.402	0.008	1
1	A	188	VAL	HA	4.651	0.000	1
1	A	188	VAL	CB	35.217	0.005	1
1	A	188	VAL	HB	2.075	0.001	1
1	A	188	VAL	HG11	0.565	0.000	1
1	A	188	VAL	HG12	0.565	0.000	1
1	A	188	VAL	HG13	0.565	0.000	1
1	A	188	VAL	HG21	0.572	0.000	1
1	A	188	VAL	HG22	0.572	0.000	1
1	A	188	VAL	HG23	0.572	0.000	1
1	A	188	VAL	CG1	21.641	0.004	1
1	A	188	VAL	CG2	17.586	0.001	1
1	A	188	VAL	C	175.719	0.000	1
1	A	189	GLY	N	106.76	0.000	1
1	A	189	GLY	H	8.282	0.000	1
1	A	189	GLY	CA	44.478	0.003	1
1	A	189	GLY	HA2	3.967	0.000	2
1	A	189	GLY	HA3	4.336	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	189	GLY	C	173.321	0.000	1
1	A	191	ALA	N	120.398	0.000	1
1	A	191	ALA	H	8.397	0.001	1
1	A	191	ALA	CA	51.986	0.001	1
1	A	191	ALA	HA	4.427	0.001	1
1	A	191	ALA	HB1	1.405	0.000	1
1	A	191	ALA	HB2	1.405	0.000	1
1	A	191	ALA	HB3	1.405	0.000	1
1	A	191	ALA	CB	18.896	0.000	1
1	A	191	ALA	C	177.075	0.004	1
1	A	192	ALA	N	122.316	0.000	1
1	A	192	ALA	H	7.197	0.000	1
1	A	192	ALA	CA	50.271	0.000	1
1	A	192	ALA	HA	4.522	0.000	1
1	A	192	ALA	HB1	1.347	0.000	1
1	A	192	ALA	HB2	1.347	0.000	1
1	A	192	ALA	HB3	1.347	0.000	1
1	A	192	ALA	CB	18.853	0.000	1
1	A	192	ALA	C	174.734	0.000	1
1	A	193	PRO	CA	62.988	0.001	1
1	A	193	PRO	HA	4.445	0.000	1
1	A	193	PRO	CB	30.9	0.000	1
1	A	193	PRO	HB2	1.809	0.000	2
1	A	193	PRO	HB3	2.176	0.000	2
1	A	193	PRO	CG	27.858	0.000	1
1	A	193	PRO	HG2	1.754	0.000	2
1	A	193	PRO	HG3	1.754	0.000	2
1	A	193	PRO	CD	49.761	0.005	1
1	A	193	PRO	HD2	3.734	0.000	1
1	A	193	PRO	HD3	3.371	0.000	1
1	A	193	PRO	C	173.321	0.000	1
1	A	194	SER	N	111.037	0.002	1
1	A	194	SER	H	8.075	0.000	1
1	A	194	SER	CA	56.408	0.000	1
1	A	194	SER	HA	4.979	0.002	1
1	A	194	SER	CB	66.466	0.002	1
1	A	194	SER	HB2	3.786	0.000	2
1	A	194	SER	HB3	3.889	0.002	2
1	A	194	SER	C	175.929	0.000	1
1	A	195	GLY	N	112.622	0.005	1
1	A	195	GLY	H	9.146	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	195	GLY	CA	43.554	0.001	1
1	A	195	GLY	HA2	2.836	0.000	1
1	A	195	GLY	HA3	4.348	0.001	1
1	A	195	GLY	C	171.719	0.000	1
1	A	196	TRP	N	118.503	0.000	1
1	A	196	TRP	H	8.917	0.000	1
1	A	196	TRP	CA	57.104	0.000	1
1	A	196	TRP	HA	4.765	0.000	1
1	A	196	TRP	CB	30.27	0.000	1
1	A	196	TRP	HB2	2.797	0.000	2
1	A	196	TRP	HB3	3.205	0.000	2
1	A	196	TRP	CD1	126.395	0.001	1
1	A	196	TRP	CE3	119.385	0.000	1
1	A	196	TRP	NE1	128.931	0.000	1
1	A	196	TRP	HD1	7.137	0.007	1
1	A	196	TRP	HE3	6.951	0.000	1
1	A	196	TRP	CZ3	121.289	0.000	1
1	A	196	TRP	CZ2	114.246	0.000	1
1	A	196	TRP	HE1	10.359	0.002	1
1	A	196	TRP	HZ3	6.806	0.001	1
1	A	196	TRP	CH2	122.932	0.003	1
1	A	196	TRP	HZ2	6.154	0.003	1
1	A	196	TRP	HH2	6.692	0.003	1
1	A	196	TRP	C	178.337	0.001	1
1	A	197	TYR	N	123.748	0.000	1
1	A	197	TYR	H	9.462	0.000	1
1	A	197	TYR	CA	55.763	0.000	1
1	A	197	TYR	HA	5.41	0.000	1
1	A	197	TYR	CB	40.554	0.000	1
1	A	197	TYR	HB2	3.047	0.000	1
1	A	197	TYR	HB3	2.68	0.000	1
1	A	197	TYR	CD1	133.798	0.001	1
1	A	197	TYR	HD1	7.087	0.002	1
1	A	197	TYR	CE1	118.231	0.001	1
1	A	197	TYR	HE1	6.512	0.001	1
1	A	197	TYR	CE2	118.231	0.000	1
1	A	197	TYR	HE2	6.512	0.001	1
1	A	197	TYR	CD2	133.798	0.000	1
1	A	197	TYR	HD2	7.087	0.002	1
1	A	197	TYR	C	173.165	0.000	1
1	A	198	PRO	CA	61.991	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	198	PRO	HA	4.976	0.000	1
1	A	198	PRO	CB	32.853	0.000	1
1	A	198	PRO	HB2	1.162	0.001	1
1	A	198	PRO	HB3	1.689	0.000	1
1	A	198	PRO	CG	26.491	0.000	1
1	A	198	PRO	HG2	1.859	0.000	1
1	A	198	PRO	HG3	1.455	0.000	1
1	A	198	PRO	CD	51.001	0.004	1
1	A	198	PRO	HD2	4.207	0.000	2
1	A	198	PRO	HD3	4.207	0.000	2
1	A	198	PRO	C	174.077	0.000	1
1	A	199	CYS	N	116.798	0.000	1
1	A	199	CYS	H	8.467	0.000	1
1	A	199	CYS	CA	56.052	0.000	1
1	A	199	CYS	HA	5.368	0.000	1
1	A	199	CYS	CB	28.82	0.001	1
1	A	199	CYS	HB2	2.208	0.000	2
1	A	199	CYS	HB3	2.711	0.000	2
1	A	199	CYS	C	173.559	0.002	1
1	A	200	PHE	N	123.824	0.000	1
1	A	200	PHE	H	8.961	0.000	1
1	A	200	PHE	CA	55.691	0.000	1
1	A	200	PHE	HA	5.387	0.000	1
1	A	200	PHE	CB	42.734	0.004	1
1	A	200	PHE	HB2	2.301	0.000	2
1	A	200	PHE	HB3	2.563	0.000	2
1	A	200	PHE	CD1	132.062	0.001	1
1	A	200	PHE	HD1	7.009	0.000	1
1	A	200	PHE	CE1	129.918	0.000	1
1	A	200	PHE	HE1	6.414	0.002	1
1	A	200	PHE	CZ	129.0	0.001	1
1	A	200	PHE	HZ	5.769	0.004	1
1	A	200	PHE	CE2	129.918	0.001	1
1	A	200	PHE	HE2	6.414	0.002	1
1	A	200	PHE	CD2	132.062	0.000	1
1	A	200	PHE	HD2	7.009	0.000	1
1	A	200	PHE	C	175.343	0.000	1
1	A	201	ARG	N	124.161	0.000	1
1	A	201	ARG	H	8.216	0.000	1
1	A	201	ARG	CA	56.95	0.000	1
1	A	201	ARG	HA	4.687	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	201	ARG	CB	30.267	0.003	1
1	A	201	ARG	HB2	1.887	0.000	2
1	A	201	ARG	HB3	1.887	0.000	2
1	A	201	ARG	CG	27.834	0.000	1
1	A	201	ARG	HG2	1.473	0.000	2
1	A	201	ARG	HG3	1.728	0.000	2
1	A	201	ARG	CD	42.743	0.002	1
1	A	201	ARG	HD2	2.968	0.000	2
1	A	201	ARG	HD3	3.149	0.000	2
1	A	201	ARG	C	176.19	0.000	1
1	A	202	ALA	N	127.36	0.000	1
1	A	202	ALA	H	8.945	0.000	1
1	A	202	ALA	CA	51.351	0.000	1
1	A	202	ALA	HA	4.927	0.000	1
1	A	202	ALA	HB1	1.52	0.000	1
1	A	202	ALA	HB2	1.52	0.000	1
1	A	202	ALA	HB3	1.52	0.000	1
1	A	202	ALA	CB	23.914	0.002	1
1	A	202	ALA	C	175.005	0.010	1
1	A	203	GLN	N	116.756	0.000	1
1	A	203	GLN	H	8.487	0.000	1
1	A	203	GLN	CA	54.863	0.002	1
1	A	203	GLN	HA	4.913	0.000	1
1	A	203	GLN	CB	31.03	0.000	1
1	A	203	GLN	HB2	2.38	0.000	1
1	A	203	GLN	HB3	2.054	0.003	1
1	A	203	GLN	CG	34.896	0.000	1
1	A	203	GLN	HG2	2.492	0.000	2
1	A	203	GLN	HG3	2.359	0.001	2
1	A	203	GLN	NE2	113.113	0.002	1
1	A	203	GLN	HE21	7.851	0.000	2
1	A	203	GLN	HE22	6.894	0.001	2
1	A	203	GLN	C	177.625	0.008	1
1	A	204	GLU	N	121.608	0.002	1
1	A	204	GLU	H	9.304	0.001	1
1	A	204	GLU	CA	60.502	0.001	1
1	A	204	GLU	HA	4.014	0.000	1
1	A	204	GLU	CB	29.156	0.001	1
1	A	204	GLU	HB2	2.137	0.000	2
1	A	204	GLU	HB3	2.137	0.000	2
1	A	204	GLU	CG	36.03	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	204	GLU	HG2	2.335	0.004	2
1	A	204	GLU	HG3	2.389	0.000	2
1	A	204	GLU	C	178.404	0.003	1
1	A	205	SER	N	112.13	0.000	1
1	A	205	SER	H	8.076	0.000	1
1	A	205	SER	CA	59.836	0.002	1
1	A	205	SER	HA	4.155	0.000	1
1	A	205	SER	CB	62.453	0.001	1
1	A	205	SER	HB2	3.899	0.000	2
1	A	205	SER	HB3	4.046	0.000	2
1	A	205	SER	C	175.217	0.000	1
1	A	207	VAL	N	114.558	0.000	1
1	A	207	VAL	H	7.628	0.000	1
1	A	207	VAL	CA	68.553	0.001	1
1	A	207	VAL	HA	3.616	0.002	1
1	A	207	VAL	CB	28.711	0.001	1
1	A	207	VAL	HB	2.461	0.001	1
1	A	207	VAL	HG11	0.848	0.000	1
1	A	207	VAL	HG12	0.848	0.000	1
1	A	207	VAL	HG13	0.848	0.000	1
1	A	207	VAL	HG21	1.017	0.000	1
1	A	207	VAL	HG22	1.017	0.000	1
1	A	207	VAL	HG23	1.017	0.000	1
1	A	207	VAL	CG1	21.658	0.002	1
1	A	207	VAL	CG2	23.597	0.001	1
1	A	208	PRO	CA	65.187	0.003	1
1	A	208	PRO	HA	4.266	0.003	1
1	A	208	PRO	CB	30.137	0.001	1
1	A	208	PRO	HB2	1.893	0.000	1
1	A	208	PRO	HB3	2.222	0.004	1
1	A	208	PRO	CG	27.77	0.004	1
1	A	208	PRO	HG2	2.136	0.000	1
1	A	208	PRO	HG3	1.988	0.000	1
1	A	208	PRO	CD	49.377	0.004	1
1	A	208	PRO	HD2	4.08	0.000	1
1	A	208	PRO	HD3	3.503	0.000	1
1	A	208	PRO	C	179.83	0.000	1
1	A	209	ALA	N	119.854	0.000	1
1	A	209	ALA	H	7.06	0.000	1
1	A	209	ALA	CA	55.29	0.000	1
1	A	209	ALA	HA	4.043	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	209	ALA	HB1	1.326	0.000	1
1	A	209	ALA	HB2	1.326	0.000	1
1	A	209	ALA	HB3	1.326	0.000	1
1	A	209	ALA	CB	17.988	0.002	1
1	A	209	ALA	C	179.226	0.007	1
1	A	210	ALA	N	120.733	0.001	1
1	A	210	ALA	H	8.442	0.000	1
1	A	210	ALA	CA	55.228	0.000	1
1	A	210	ALA	HA	3.88	0.001	1
1	A	210	ALA	HB1	1.476	0.000	1
1	A	210	ALA	HB2	1.476	0.000	1
1	A	210	ALA	HB3	1.476	0.000	1
1	A	210	ALA	CB	16.235	0.001	1
1	A	210	ALA	C	180.225	0.000	1
1	A	211	VAL	N	120.04	0.000	1
1	A	211	VAL	H	8.156	0.000	1
1	A	211	VAL	CA	65.542	0.001	1
1	A	211	VAL	HA	4.091	0.000	1
1	A	211	VAL	CB	31.952	0.003	1
1	A	211	VAL	HB	2.062	0.001	1
1	A	211	VAL	HG11	0.985	0.000	1
1	A	211	VAL	HG12	0.985	0.000	1
1	A	211	VAL	HG13	0.985	0.000	1
1	A	211	VAL	HG21	0.932	0.000	1
1	A	211	VAL	HG22	0.932	0.000	1
1	A	211	VAL	HG23	0.932	0.000	1
1	A	211	VAL	CG1	20.872	0.001	1
1	A	211	VAL	CG2	22.073	0.007	1
1	A	211	VAL	C	181.034	0.000	1
1	A	212	MET	N	122.436	0.009	1
1	A	212	MET	H	8.321	0.000	1
1	A	212	MET	CA	58.583	0.003	1
1	A	212	MET	HA	4.235	0.001	1
1	A	212	MET	CB	32.021	0.002	1
1	A	212	MET	HB2	2.22	0.000	2
1	A	212	MET	HB3	2.22	0.000	2
1	A	212	MET	CG	32.08	0.001	1
1	A	212	MET	HG2	2.635	0.000	1
1	A	212	MET	HG3	2.694	0.001	1
1	A	212	MET	C	178.12	0.002	1
1	A	213	LEU	N	118.279	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	213	LEU	H	7.473	0.000	1
1	A	213	LEU	CA	55.157	0.008	1
1	A	213	LEU	HA	4.369	0.000	1
1	A	213	LEU	CB	42.63	0.005	1
1	A	213	LEU	HB2	2.144	0.001	1
1	A	213	LEU	HB3	1.994	0.002	1
1	A	213	LEU	CG	26.689	0.005	1
1	A	213	LEU	HG	1.778	0.002	1
1	A	213	LEU	HD11	0.543	0.000	1
1	A	213	LEU	HD12	0.543	0.000	1
1	A	213	LEU	HD13	0.543	0.000	1
1	A	213	LEU	HD21	0.84	0.000	1
1	A	213	LEU	HD22	0.84	0.000	1
1	A	213	LEU	HD23	0.84	0.000	1
1	A	213	LEU	CD1	25.749	0.009	1
1	A	213	LEU	CD2	22.229	0.001	1
1	A	213	LEU	C	176.509	0.000	1
1	A	214	GLY	N	105.322	0.000	1
1	A	214	GLY	H	7.925	0.001	1
1	A	214	GLY	CA	44.974	0.003	1
1	A	214	GLY	HA2	3.906	0.000	2
1	A	214	GLY	HA3	3.753	0.000	2
1	A	214	GLY	C	174.81	0.001	1
1	A	215	ALA	N	124.091	0.000	1
1	A	215	ALA	H	8.52	0.000	1
1	A	215	ALA	CA	51.262	0.000	1
1	A	215	ALA	HA	4.699	0.000	1
1	A	215	ALA	HB1	1.221	0.000	1
1	A	215	ALA	HB2	1.221	0.000	1
1	A	215	ALA	HB3	1.221	0.000	1
1	A	215	ALA	CB	21.494	0.004	1
1	A	215	ALA	C	175.819	0.005	1
1	A	216	SER	N	111.747	0.000	1
1	A	216	SER	H	8.5	0.000	1
1	A	216	SER	CA	57.137	0.000	1
1	A	216	SER	HA	4.837	0.000	1
1	A	216	SER	CB	65.73	0.004	1
1	A	216	SER	HB2	3.631	0.000	2
1	A	216	SER	HB3	3.698	0.000	2
1	A	216	SER	C	173.057	0.007	1
1	A	217	VAL	N	123.927	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	217	VAL	H	8.803	0.000	1
1	A	217	VAL	CA	63.876	0.001	1
1	A	217	VAL	HA	3.894	0.001	1
1	A	217	VAL	CB	31.962	0.004	1
1	A	217	VAL	HB	1.895	0.000	1
1	A	217	VAL	HG11	0.748	0.000	1
1	A	217	VAL	HG12	0.748	0.000	1
1	A	217	VAL	HG13	0.748	0.000	1
1	A	217	VAL	HG21	0.714	0.001	1
1	A	217	VAL	HG22	0.714	0.001	1
1	A	217	VAL	HG23	0.714	0.001	1
1	A	217	VAL	CG1	21.24	0.002	1
1	A	217	VAL	CG2	21.258	0.009	1
1	A	217	VAL	C	176.396	0.000	1
1	A	218	LEU	N	127.568	0.000	1
1	A	218	LEU	H	9.421	0.000	1
1	A	218	LEU	CA	55.582	0.003	1
1	A	218	LEU	HA	4.452	0.003	1
1	A	218	LEU	CB	43.778	0.004	1
1	A	218	LEU	HB2	1.293	0.002	2
1	A	218	LEU	HB3	1.363	0.006	2
1	A	218	LEU	CG	26.447	0.005	1
1	A	218	LEU	HG	1.557	0.000	1
1	A	218	LEU	HD11	0.742	0.000	2
1	A	218	LEU	HD12	0.742	0.000	2
1	A	218	LEU	HD13	0.742	0.000	2
1	A	218	LEU	HD21	0.775	0.000	2
1	A	218	LEU	HD22	0.775	0.000	2
1	A	218	LEU	HD23	0.775	0.000	2
1	A	218	LEU	CD1	21.814	0.000	1
1	A	218	LEU	CD2	26.403	0.002	1
1	A	218	LEU	C	176.977	0.000	1
1	A	219	LEU	N	118.029	0.000	1
1	A	219	LEU	H	7.491	0.000	1
1	A	219	LEU	CA	55.112	0.000	1
1	A	219	LEU	HA	4.523	0.000	1
1	A	219	LEU	CB	45.69	0.002	1
1	A	219	LEU	HB2	1.51	0.002	1
1	A	219	LEU	HB3	1.455	0.002	1
1	A	219	LEU	CG	27.329	0.002	1
1	A	219	LEU	HG	1.581	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	219	LEU	HD11	1.065	0.000	1
1	A	219	LEU	HD12	1.065	0.000	1
1	A	219	LEU	HD13	1.065	0.000	1
1	A	219	LEU	HD21	0.821	0.000	1
1	A	219	LEU	HD22	0.821	0.000	1
1	A	219	LEU	HD23	0.821	0.000	1
1	A	219	LEU	CD1	23.676	0.006	1
1	A	219	LEU	CD2	26.613	0.005	1
1	A	219	LEU	C	173.025	0.001	1
1	A	220	ARG	N	124.849	0.001	1
1	A	220	ARG	H	8.388	0.000	1
1	A	220	ARG	CA	55.006	0.006	1
1	A	220	ARG	HA	5.405	0.000	1
1	A	220	ARG	CB	32.589	0.002	1
1	A	220	ARG	HB2	1.613	0.001	2
1	A	220	ARG	HB3	1.94	0.000	2
1	A	220	ARG	CG	28.647	0.003	1
1	A	220	ARG	HG2	1.547	0.001	2
1	A	220	ARG	HG3	1.547	0.001	2
1	A	220	ARG	CD	43.385	0.000	1
1	A	220	ARG	HD2	3.134	0.000	2
1	A	220	ARG	HD3	3.134	0.000	2
1	A	220	ARG	NE	85.49	0.006	1
1	A	220	ARG	HE	7.287	0.001	1
1	A	220	ARG	C	174.92	0.007	1
1	A	221	TYR	N	121.661	0.000	1
1	A	221	TYR	H	9.002	0.000	1
1	A	221	TYR	CA	56.48	0.001	1
1	A	221	TYR	HA	4.893	0.000	1
1	A	221	TYR	CB	39.656	0.001	1
1	A	221	TYR	HB2	3.086	0.000	1
1	A	221	TYR	HB3	2.826	0.001	1
1	A	221	TYR	CD1	132.939	0.000	1
1	A	221	TYR	HD1	6.629	0.001	1
1	A	221	TYR	CE1	118.231	0.000	1
1	A	221	TYR	HE1	6.513	0.004	1
1	A	221	TYR	CE2	118.231	0.000	1
1	A	221	TYR	HE2	6.513	0.004	1
1	A	221	TYR	CD2	132.939	0.002	1
1	A	221	TYR	HD2	6.629	0.001	1
1	A	221	TYR	C	171.809	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	223	CYS	N	120.231	0.002	1
1	A	223	CYS	H	8.095	0.002	1
1	A	223	CYS	CA	56.774	0.000	1
1	A	223	CYS	HA	4.819	0.000	1
1	A	223	CYS	CB	27.856	0.004	1
1	A	223	CYS	HB2	2.758	0.003	1
1	A	223	CYS	HB3	3.331	0.002	1
1	A	223	CYS	C	174.131	0.000	1
1	A	225	ASP	N	109.313	0.001	1
1	A	225	ASP	H	8.7	0.000	1
1	A	225	ASP	CA	52.115	0.000	1
1	A	225	ASP	HA	4.55	0.000	1
1	A	225	ASP	CB	39.015	0.003	1
1	A	225	ASP	HB2	2.536	0.002	2
1	A	225	ASP	HB3	2.87	0.000	2
1	A	225	ASP	C	175.235	0.001	1
1	A	226	GLY	N	109.188	0.000	1
1	A	226	GLY	H	7.316	0.000	1
1	A	226	GLY	CA	45.089	0.001	1
1	A	226	GLY	HA2	3.856	0.002	2
1	A	226	GLY	HA3	3.856	0.002	2
1	A	226	GLY	C	169.638	0.000	1
1	A	227	PRO	CA	63.282	0.000	1
1	A	227	PRO	HA	4.635	0.000	1
1	A	227	PRO	CB	32.593	0.001	1
1	A	227	PRO	HB2	1.693	0.002	1
1	A	227	PRO	HB3	2.359	0.000	1
1	A	227	PRO	CG	27.321	0.000	1
1	A	227	PRO	HG2	1.983	0.000	2
1	A	227	PRO	HG3	2.08	0.000	2
1	A	227	PRO	CD	50.76	0.000	1
1	A	227	PRO	HD2	3.673	0.000	2
1	A	227	PRO	HD3	3.673	0.000	2
1	A	227	PRO	C	174.462	0.000	1
1	A	228	ALA	N	124.141	0.001	1
1	A	228	ALA	H	8.816	0.001	1
1	A	228	ALA	CA	49.843	0.004	1
1	A	228	ALA	HA	5.231	0.000	1
1	A	228	ALA	HB1	0.192	0.000	1
1	A	228	ALA	HB2	0.192	0.000	1
1	A	228	ALA	HB3	0.192	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	228	ALA	CB	20.94	0.003	1
1	A	228	ALA	C	177.08	0.000	1
1	A	229	VAL	N	121.399	0.001	1
1	A	229	VAL	H	9.008	0.000	1
1	A	229	VAL	CA	61.146	0.000	1
1	A	229	VAL	HA	4.601	0.000	1
1	A	229	VAL	CB	34.456	0.001	1
1	A	229	VAL	HB	1.926	0.000	1
1	A	229	VAL	HG11	0.85	0.000	1
1	A	229	VAL	HG12	0.85	0.000	1
1	A	229	VAL	HG13	0.85	0.000	1
1	A	229	VAL	HG21	0.864	0.000	1
1	A	229	VAL	HG22	0.864	0.000	1
1	A	229	VAL	HG23	0.864	0.000	1
1	A	229	VAL	CG1	22.589	0.001	1
1	A	229	VAL	CG2	21.347	0.000	1
1	A	229	VAL	C	174.085	0.001	1
1	A	230	VAL	N	129.491	0.000	1
1	A	230	VAL	H	9.332	0.000	1
1	A	230	VAL	CA	62.19	0.000	1
1	A	230	VAL	HA	4.356	0.000	1
1	A	230	VAL	CB	31.713	0.000	1
1	A	230	VAL	HB	1.889	0.000	1
1	A	230	VAL	HG11	0.466	0.001	1
1	A	230	VAL	HG12	0.466	0.001	1
1	A	230	VAL	HG13	0.466	0.001	1
1	A	230	VAL	HG21	0.982	0.000	1
1	A	230	VAL	HG22	0.982	0.000	1
1	A	230	VAL	HG23	0.982	0.000	1
1	A	230	VAL	CG1	21.906	0.003	1
1	A	230	VAL	CG2	21.746	0.000	1
1	A	230	VAL	C	175.818	0.001	1
1	A	231	VAL	N	126.162	0.000	1
1	A	231	VAL	H	9.409	0.000	1
1	A	231	VAL	CA	59.633	0.000	1
1	A	231	VAL	HA	4.826	0.000	1
1	A	231	VAL	CB	34.814	0.004	1
1	A	231	VAL	HB	1.211	0.000	1
1	A	231	VAL	HG11	0.298	0.000	2
1	A	231	VAL	HG12	0.298	0.000	2
1	A	231	VAL	HG13	0.298	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	231	VAL	HG21	0.598	0.000	2
1	A	231	VAL	HG22	0.598	0.000	2
1	A	231	VAL	HG23	0.598	0.000	2
1	A	231	VAL	CG1	20.331	0.000	1
1	A	231	VAL	CG2	22.875	0.000	1
1	A	231	VAL	C	173.341	0.000	1
1	A	232	SER	N	115.301	0.000	1
1	A	232	SER	H	8.925	0.000	1
1	A	232	SER	CA	55.441	0.010	1
1	A	232	SER	HA	5.023	0.000	1
1	A	232	SER	CB	64.345	0.004	1
1	A	232	SER	HB2	3.651	0.001	1
1	A	232	SER	HB3	3.793	0.001	1
1	A	232	SER	C	174.912	0.000	1
1	A	233	ALA	N	128.124	0.000	1
1	A	233	ALA	H	9.268	0.000	1
1	A	233	ALA	CA	50.588	0.005	1
1	A	233	ALA	HA	3.914	0.002	1
1	A	233	ALA	HB1	1.361	0.000	1
1	A	233	ALA	HB2	1.361	0.000	1
1	A	233	ALA	HB3	1.361	0.000	1
1	A	233	ALA	CB	18.723	0.001	1
1	A	233	ALA	C	176.115	0.000	1
1	A	234	PRO	CA	65.547	0.001	1
1	A	234	PRO	HA	4.022	0.000	1
1	A	234	PRO	CB	30.795	0.002	1
1	A	234	PRO	HB2	1.787	0.000	2
1	A	234	PRO	HB3	2.183	0.000	2
1	A	234	PRO	CG	27.796	0.000	1
1	A	234	PRO	HG2	1.754	0.000	2
1	A	234	PRO	HG3	1.754	0.000	2
1	A	234	PRO	CD	49.864	0.000	1
1	A	234	PRO	HD2	3.735	0.001	2
1	A	234	PRO	HD3	3.735	0.001	2
1	A	234	PRO	C	178.198	0.000	1
1	A	235	GLY	N	103.88	0.003	1
1	A	235	GLY	H	8.404	0.001	1
1	A	235	GLY	CA	45.761	0.001	1
1	A	235	GLY	HA2	3.927	0.000	2
1	A	235	GLY	HA3	4.056	0.002	2
1	A	235	GLY	C	175.288	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	236	GLY	N	108.776	0.001	1
1	A	236	GLY	H	7.975	0.001	1
1	A	236	GLY	CA	44.761	0.005	1
1	A	236	GLY	HA2	3.496	0.001	2
1	A	236	GLY	HA3	4.485	0.002	2
1	A	236	GLY	C	174.372	0.001	1
1	A	237	GLU	N	123.732	0.000	1
1	A	237	GLU	H	9.758	0.001	1
1	A	237	GLU	CA	56.722	0.000	1
1	A	237	GLU	HA	4.806	0.000	1
1	A	237	GLU	CB	27.758	0.000	1
1	A	237	GLU	HB2	2.325	0.000	2
1	A	237	GLU	HB3	2.325	0.000	2
1	A	237	GLU	CG	35.336	0.000	1
1	A	237	GLU	HG2	2.703	0.002	2
1	A	237	GLU	HG3	2.703	0.002	2
1	A	237	GLU	C	173.379	0.000	1
1	A	238	VAL	N	121.937	0.000	1
1	A	238	VAL	H	8.391	0.000	1
1	A	238	VAL	CA	61.393	0.003	1
1	A	238	VAL	HA	5.503	0.001	1
1	A	238	VAL	CB	34.92	0.002	1
1	A	238	VAL	HB	2.045	0.000	1
1	A	238	VAL	HG11	0.255	0.000	1
1	A	238	VAL	HG12	0.255	0.000	1
1	A	238	VAL	HG13	0.255	0.000	1
1	A	238	VAL	HG21	0.983	0.000	1
1	A	238	VAL	HG22	0.983	0.000	1
1	A	238	VAL	HG23	0.983	0.000	1
1	A	238	VAL	CG1	22.408	0.007	1
1	A	238	VAL	CG2	22.169	0.000	1
1	A	238	VAL	C	175.613	0.000	1
1	A	239	PHE	N	121.706	0.000	1
1	A	239	PHE	H	8.957	0.000	1
1	A	239	PHE	CA	56.4	0.007	1
1	A	239	PHE	HA	5.051	0.000	1
1	A	239	PHE	CB	41.639	0.001	1
1	A	239	PHE	HB2	3.156	0.001	2
1	A	239	PHE	HB3	3.348	0.000	2
1	A	239	PHE	CD1	133.116	0.005	1
1	A	239	PHE	HD1	7.551	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	239	PHE	CE1	130.782	0.000	1
1	A	239	PHE	HE1	7.403	0.003	1
1	A	239	PHE	CZ	128.326	0.000	1
1	A	239	PHE	HZ	7.064	0.001	1
1	A	239	PHE	CE2	130.782	0.005	1
1	A	239	PHE	HE2	7.403	0.003	1
1	A	239	PHE	CD2	133.116	0.000	1
1	A	239	PHE	HD2	7.551	0.001	1
1	A	239	PHE	C	170.416	0.003	1
1	A	240	THR	N	116.945	0.002	1
1	A	240	THR	H	9.048	0.000	1
1	A	240	THR	CA	61.454	0.000	1
1	A	240	THR	HA	5.26	0.000	1
1	A	240	THR	CB	70.221	0.003	1
1	A	240	THR	HB	4.291	0.000	1
1	A	240	THR	HG21	0.908	0.000	1
1	A	240	THR	HG22	0.908	0.000	1
1	A	240	THR	HG23	0.908	0.000	1
1	A	240	THR	CG2	21.429	0.000	1
1	A	240	THR	C	173.954	0.001	1
1	A	241	LEU	N	126.782	0.000	1
1	A	241	LEU	H	9.426	0.001	1
1	A	241	LEU	CA	52.911	0.006	1
1	A	241	LEU	HA	5.239	0.000	1
1	A	241	LEU	CB	44.299	0.000	1
1	A	241	LEU	HB2	1.2	0.000	2
1	A	241	LEU	HB3	1.931	0.001	2
1	A	241	LEU	CG	26.453	0.003	1
1	A	241	LEU	HG	1.912	0.000	1
1	A	241	LEU	HD11	0.764	0.000	1
1	A	241	LEU	HD12	0.764	0.000	1
1	A	241	LEU	HD13	0.764	0.000	1
1	A	241	LEU	HD21	1.234	0.002	1
1	A	241	LEU	HD22	1.234	0.002	1
1	A	241	LEU	HD23	1.234	0.002	1
1	A	241	LEU	CD1	26.586	0.000	1
1	A	241	LEU	CD2	25.64	0.004	1
1	A	241	LEU	C	174.679	0.000	1
1	A	242	LEU	N	125.469	0.001	1
1	A	242	LEU	H	8.632	0.000	1
1	A	242	LEU	CA	52.903	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	242	LEU	HA	4.861	0.000	1
1	A	242	LEU	CB	43.514	0.001	1
1	A	242	LEU	HB2	1.023	0.000	2
1	A	242	LEU	HB3	1.505	0.000	2
1	A	242	LEU	CG	27.277	0.000	1
1	A	242	LEU	HG	1.221	0.000	1
1	A	242	LEU	HD11	0.563	0.001	2
1	A	242	LEU	HD12	0.563	0.001	2
1	A	242	LEU	HD13	0.563	0.001	2
1	A	242	LEU	HD21	0.641	0.000	2
1	A	242	LEU	HD22	0.641	0.000	2
1	A	242	LEU	HD23	0.641	0.000	2
1	A	242	LEU	CD1	23.905	0.001	1
1	A	242	LEU	CD2	24.925	0.001	1
1	A	242	LEU	C	176.197	0.009	1
1	A	243	LEU	N	125.682	0.000	1
1	A	243	LEU	H	8.666	0.000	1
1	A	243	LEU	CA	54.23	0.001	1
1	A	243	LEU	HA	4.949	0.001	1
1	A	243	LEU	CB	40.53	0.006	1
1	A	243	LEU	HB2	1.233	0.000	2
1	A	243	LEU	HB3	1.877	0.002	2
1	A	243	LEU	CG	26.434	0.000	1
1	A	243	LEU	HG	1.591	0.000	1
1	A	243	LEU	HD11	0.828	0.000	1
1	A	243	LEU	HD12	0.828	0.000	1
1	A	243	LEU	HD13	0.828	0.000	1
1	A	243	LEU	HD21	0.594	0.000	1
1	A	243	LEU	HD22	0.594	0.000	1
1	A	243	LEU	HD23	0.594	0.000	1
1	A	243	LEU	CD1	25.714	0.000	1
1	A	243	LEU	CD2	23.13	0.000	1
1	A	243	LEU	C	177.6	0.001	1
1	A	244	THR	N	115.203	0.001	1
1	A	244	THR	H	8.376	0.000	1
1	A	244	THR	CA	61.258	0.001	1
1	A	244	THR	HA	4.49	0.005	1
1	A	244	THR	CB	70.641	0.002	1
1	A	244	THR	HB	4.171	0.000	1
1	A	244	THR	HG21	1.13	0.000	1
1	A	244	THR	HG22	1.13	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	244	THR	HG23	1.13	0.000	1
1	A	244	THR	CG2	20.757	0.007	1
1	A	244	THR	C	173.756	0.000	1
1	A	245	ASP	N	128.186	0.001	1
1	A	245	ASP	H	8.129	0.000	1
1	A	245	ASP	CA	56.242	0.000	1
1	A	245	ASP	HA	4.478	0.003	1
1	A	245	ASP	CB	42.513	0.000	1
1	A	245	ASP	HB2	2.72	0.000	2
1	A	245	ASP	HB3	2.531	0.000	2
1	A	245	ASP	C	180.688	0.000	1

7.1.2 Chemical shift referencing [\(i\)](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	242	-0.91 \pm 0.23	Should be checked
$^{13}\text{C}_\beta$	205	0.23 \pm 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	231	-0.21 \pm 0.28	None needed (< 0.5 ppm)
^{15}N	220	-2.16 \pm 0.72	Should be applied

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 90 atoms were assigned a chemical shift out of a possible 2295. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	47/906 (5%)	19/374 (5%)	20/362 (6%)	8/170 (5%)
Sidechain	43/1179 (4%)	30/783 (4%)	13/359 (4%)	0/37 (0%)
Aromatic	0/210 (0%)	0/102 (0%)	0/102 (0%)	0/6 (0%)
Overall	90/2295 (4%)	49/1259 (4%)	33/823 (4%)	8/213 (4%)

7.1.4 Statistically unusual chemical shifts [\(i\)](#)

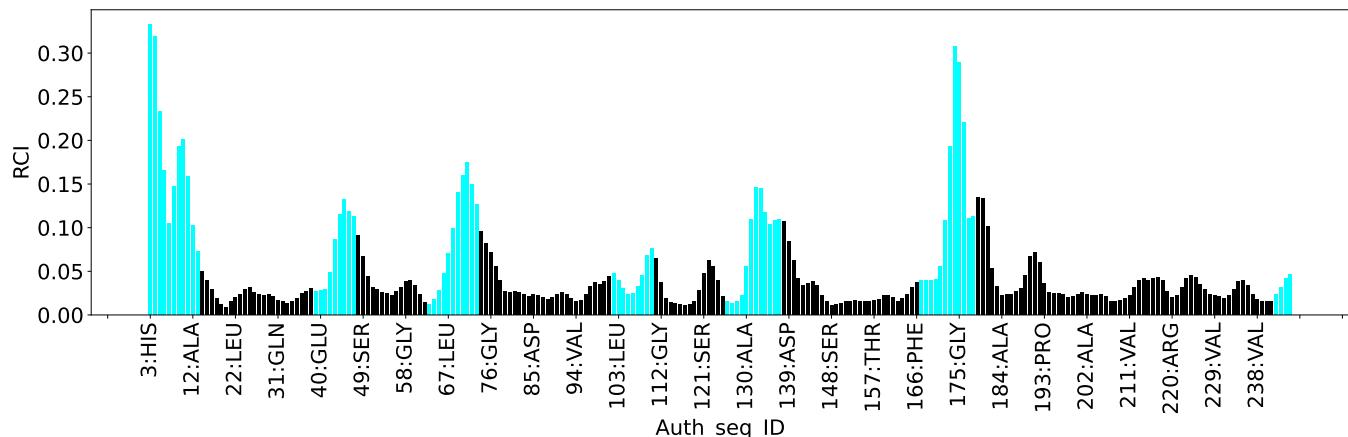
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	150	LEU	HB2	-1.82	-0.07 – 3.30	-10.2
1	A	150	LEU	HB3	-1.82	-0.26 – 3.31	-9.4
1	A	21	LEU	HB2	-1.28	-0.07 – 3.30	-8.6
1	A	21	LEU	HB3	-1.28	-0.26 – 3.31	-7.9

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:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	3255
Intra-residue ($ i-j =0$)	780
Sequential ($ i-j =1$)	997
Medium range ($ i-j >1$ and $ i-j <5$)	465
Long range ($ i-j \geq 5$)	1013
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	2202
Number of unmapped restraints	5407
Number of restraints per residue	22.3
Number of long range restraints per residue ¹	4.1

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.1	0.12
0.2-0.5 (Medium)	0.1	0.26
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model [\(i\)](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.5	4.82
10.0-20.0 (Medium)	0.1	17.2
>20.0 (Large)	3.5	135.65

9 Distance violation analysis (i)

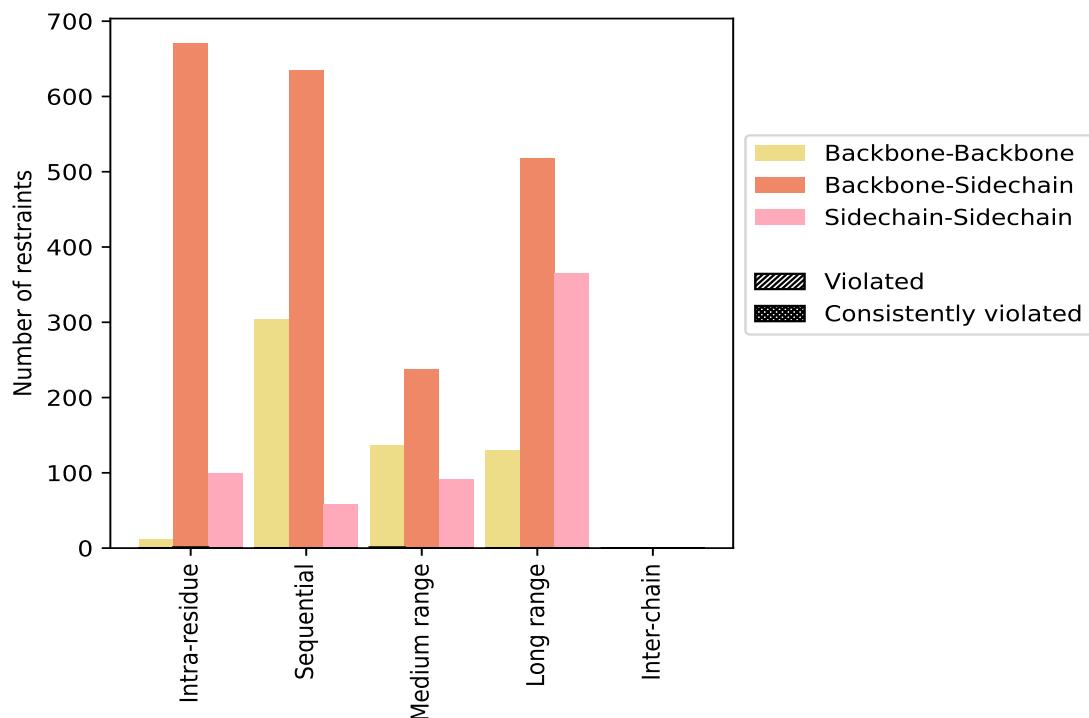
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	780	24.0	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	11	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	670	20.6	1	0.1	0.0	0	0.0	0.0
Sidechain-Sidechain	99	3.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	997	30.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	304	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	635	19.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	58	1.8	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1 \text{ & } i-j <5$)	465	14.3	1	0.2	0.0	0	0.0	0.0
Backbone-Backbone	136	4.2	1	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	238	7.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	91	2.8	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	1013	31.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	130	4.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	518	15.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	365	11.2	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3255	100.0	2	0.1	0.1	0	0.0	0.0
Backbone-Backbone	581	17.8	1	0.2	0.0	0	0.0	0.0
Backbone-Sidechain	2061	63.3	1	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	613	18.8	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [\(i\)](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [\(i\)](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	1	0	0	0	0	1	0.12	0.12	0.0	0.12
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	1	0	0	1	0.26	0.26	0.0	0.26
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0

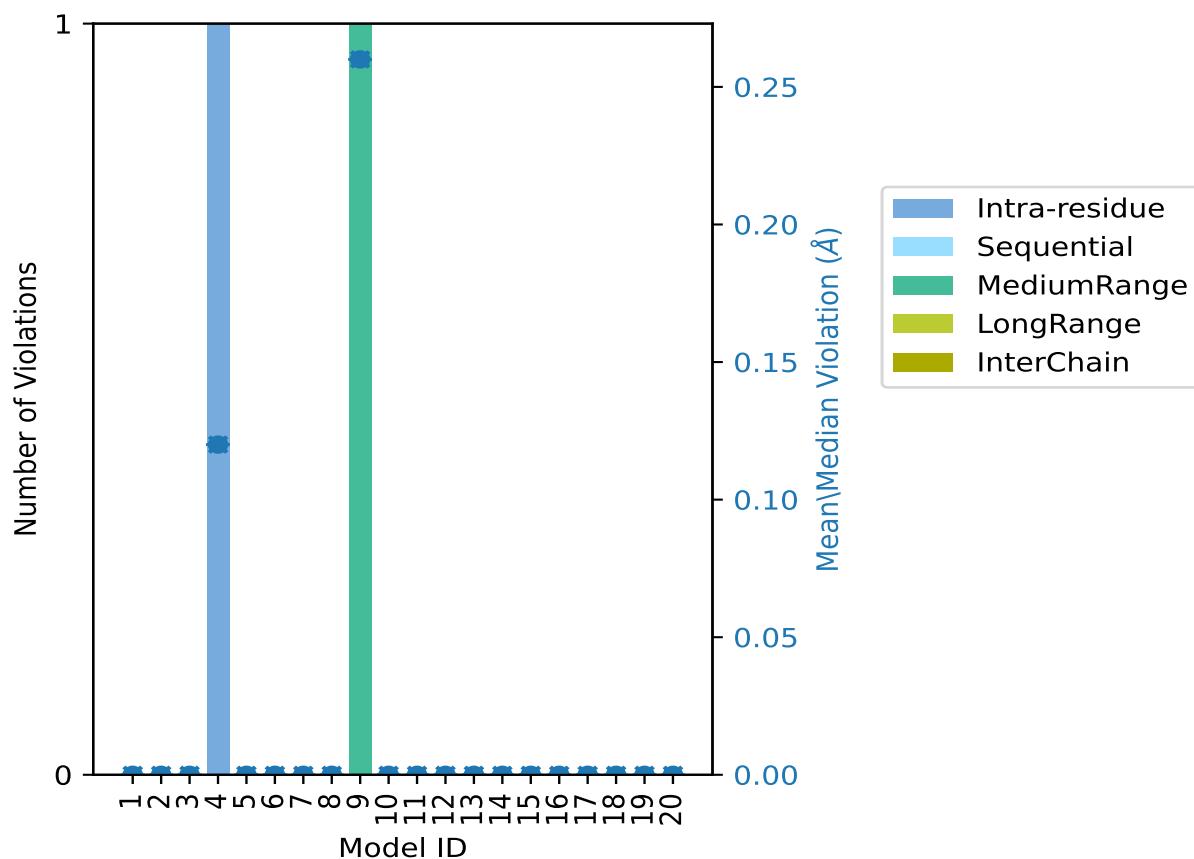
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,
⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [\(i\)](#)

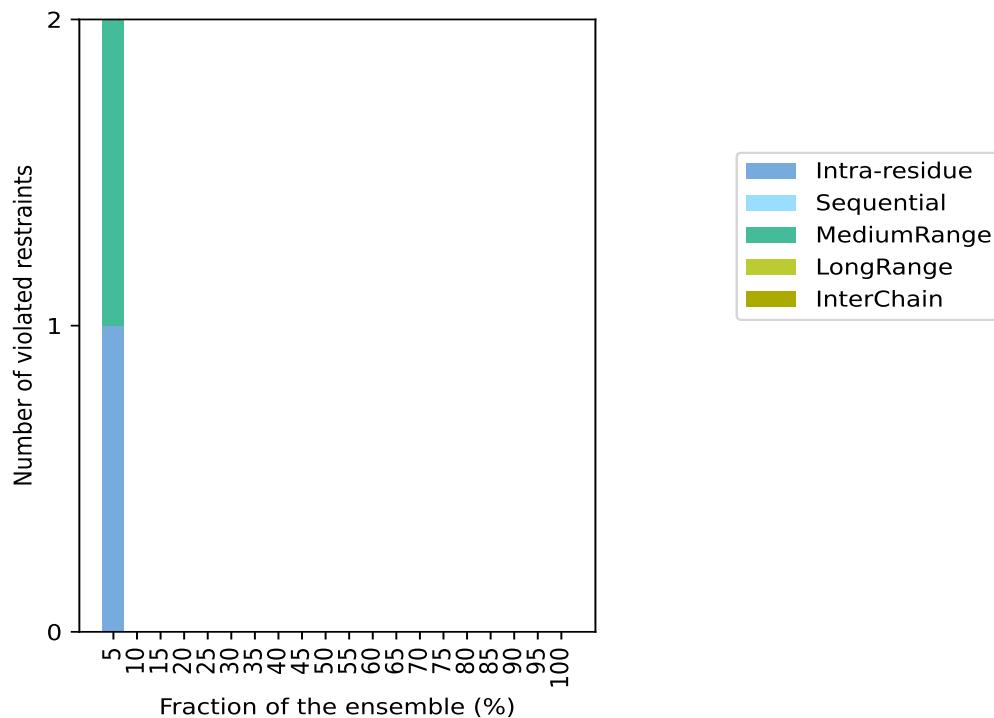
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3253(IR:779, SQ:997, MR:464, LR:1013, IC:0) restraints are not violated in the ensemble.

IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Fraction of the ensemble	
						Count ⁶	%
1	0	1	0	0	2	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble [\(i\)](#)



9.4 Most violated distance restraints in the ensemble [\(i\)](#)

No violations found

9.5 All violated distance restraints [\(i\)](#)

9.5.1 Histogram : Distribution of distance violations [\(i\)](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.

Data insufficient to plot histogram

9.5.2 Table : All distance violations [\(i\)](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:87:A:ALA:HA	1:89:A:ALA:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	1:42:A:SER:H	1:42:A:SER:HB2	4	0.12
(1,1771)	1:42:A:SER:H	1:42:A:SER:HB3	4	0.12

10 Dihedral-angle violation analysis [\(i\)](#)

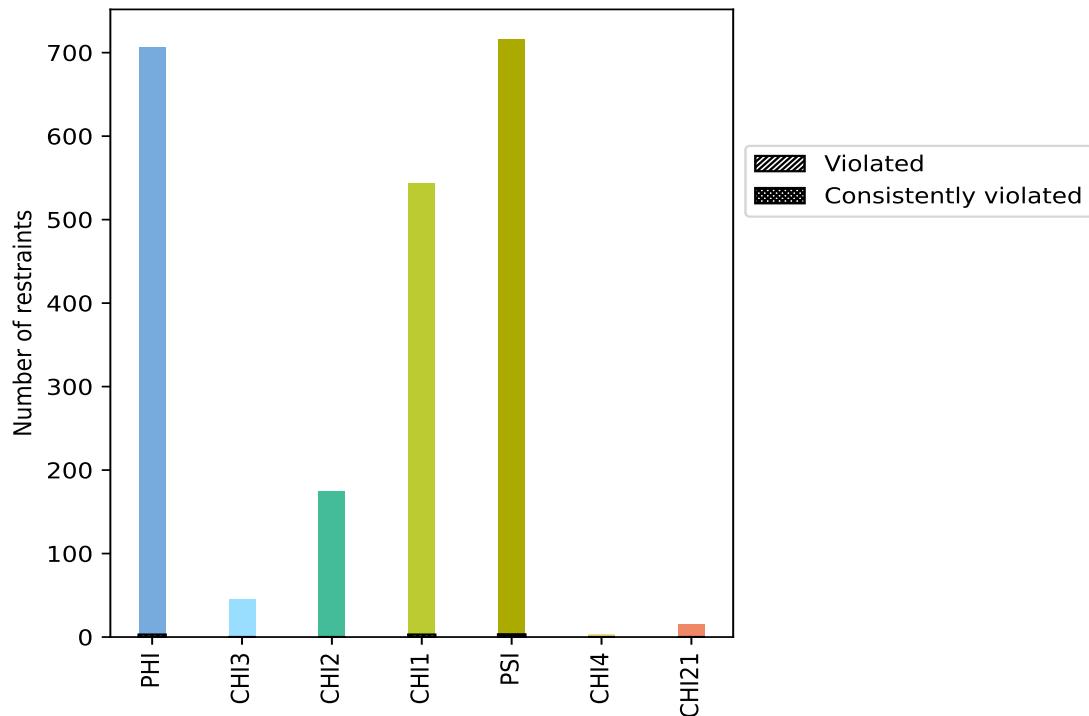
10.1 Summary of dihedral-angle violations [\(i\)](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	706	32.1	3	0.4	0.1	0	0.0	0.0
CHI3	45	2.0	0	0.0	0.0	0	0.0	0.0
CHI2	174	7.9	0	0.0	0.0	0	0.0	0.0
CHI1	543	24.7	3	0.6	0.1	0	0.0	0.0
PSI	716	32.5	3	0.4	0.1	3	0.4	0.1
CHI4	3	0.1	0	0.0	0.0	0	0.0	0.0
CHI21	15	0.7	0	0.0	0.0	0	0.0	0.0
Total	2202	100.0	9	0.4	0.4	3	0.1	0.1

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [\(i\)](#)



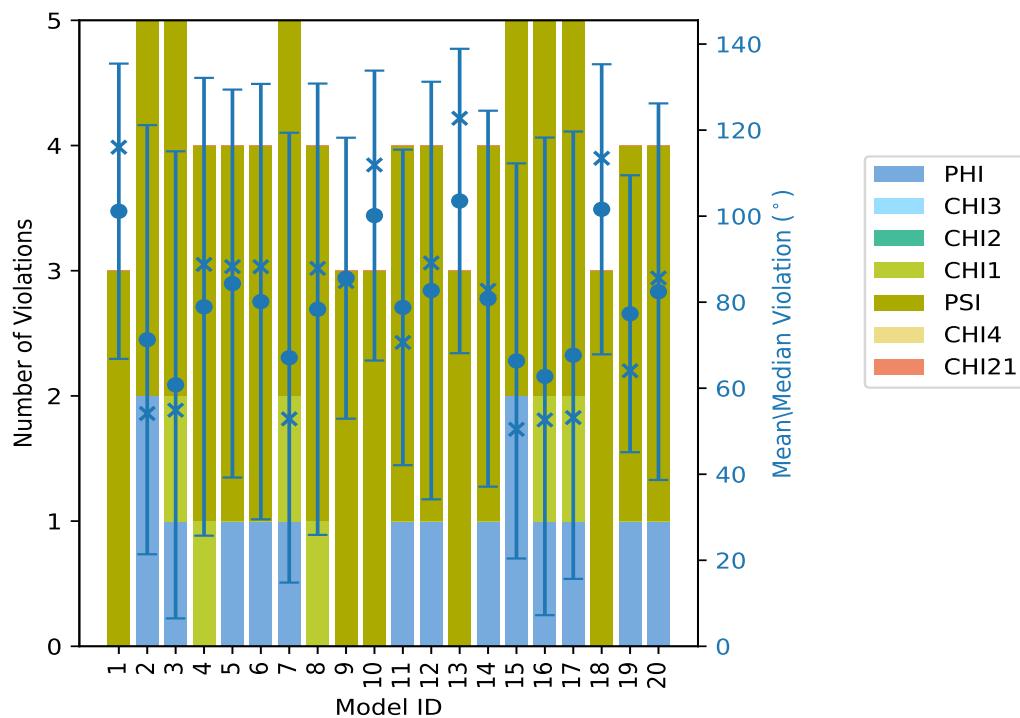
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [\(i\)](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations								Mean ($^\circ$)	Max ($^\circ$)	SD ($^\circ$)	Median ($^\circ$)
	PHI	CHI3	CHI2	CHI1	PSI	CHI4	CHI21	Total				
1	0	0	0	0	3	0	0	3	101.14	133.69	34.32	116.03
2	2	0	0	0	0	3	0	5	71.28	134.12	49.88	54.12
3	1	0	0	1	3	0	0	5	60.78	134.89	54.29	54.89
4	0	0	0	1	3	0	0	4	78.93	134.73	53.21	88.78
5	1	0	0	0	3	0	0	4	84.33	133.64	45.09	88.27
6	1	0	0	0	3	0	0	4	80.13	133.58	50.61	88.24
7	1	0	0	1	3	0	0	5	67.1	132.87	52.29	52.87
8	0	0	0	1	3	0	0	4	78.36	132.9	52.46	87.86
9	0	0	0	0	3	0	0	3	85.57	125.96	32.66	84.78
10	0	0	0	0	3	0	0	3	100.13	134.24	33.7	111.9
11	1	0	0	0	3	0	0	4	78.78	135.04	36.68	70.64
12	1	0	0	0	3	0	0	4	82.7	135.37	48.54	89.12
13	0	0	0	0	3	0	0	3	103.52	133.91	35.38	122.75
14	1	0	0	0	3	0	0	4	80.81	132.82	43.7	82.78
15	2	0	0	0	3	0	0	5	66.34	130.44	45.93	50.44
16	1	0	0	1	3	0	0	5	62.75	132.63	55.52	52.63
17	1	0	0	1	3	0	0	5	67.67	133.17	52.0	53.17
18	0	0	0	0	3	0	0	3	101.59	135.65	33.72	113.46
19	1	0	0	0	3	0	0	4	77.31	130.55	32.19	64.06
20	1	0	0	0	3	0	0	4	82.44	128.79	43.77	85.62

10.2.1 Bar graph : Dihedral violation statistics for each model [\(i\)](#)



The mean(dot), median(x) and the standard deviation are shown in blue with respect to the y axis on the right

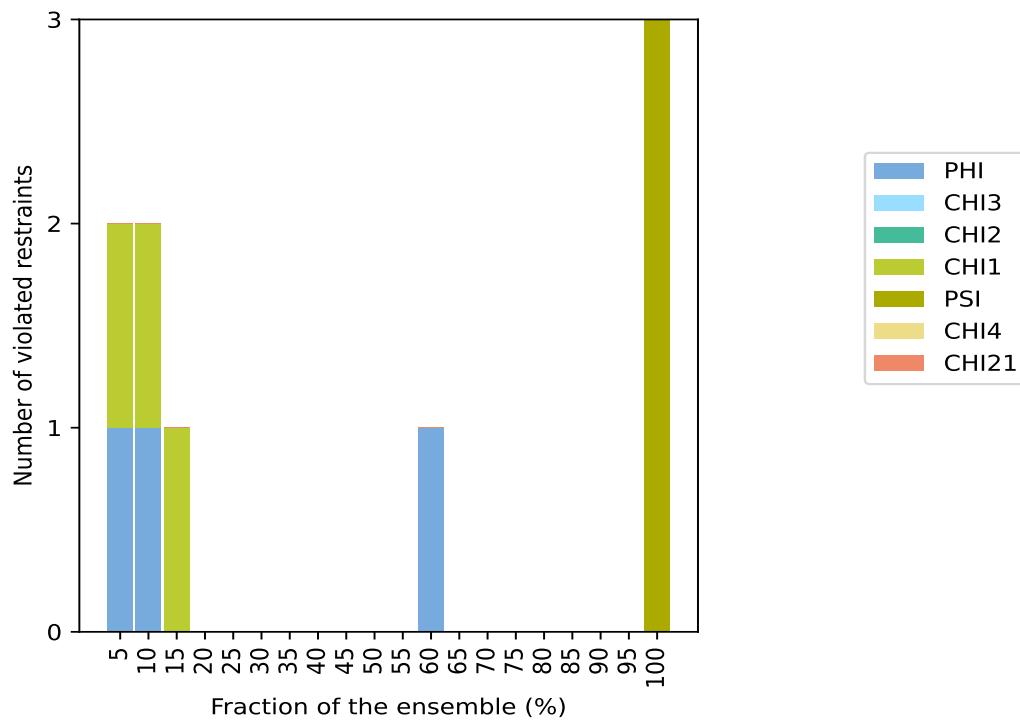
10.3 Dihedral-angle violation statistics for the ensemble [\(i\)](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

PHI	Number of violated restraints							Fraction of the ensemble	
	CHI3	CHI2	CHI1	PSI	CHI4	CHI21	Total	Count ¹	%
1	0	0	1	0	0	0	2	1	5.0
1	0	0	1	0	0	0	2	2	10.0
0	0	0	1	0	0	0	1	3	15.0
0	0	0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	0	0	11	55.0
1	0	0	0	0	0	0	1	12	60.0
0	0	0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	0	0	19	95.0
0	0	0	0	3	0	0	3	20	100.0

¹ Number of models with violations

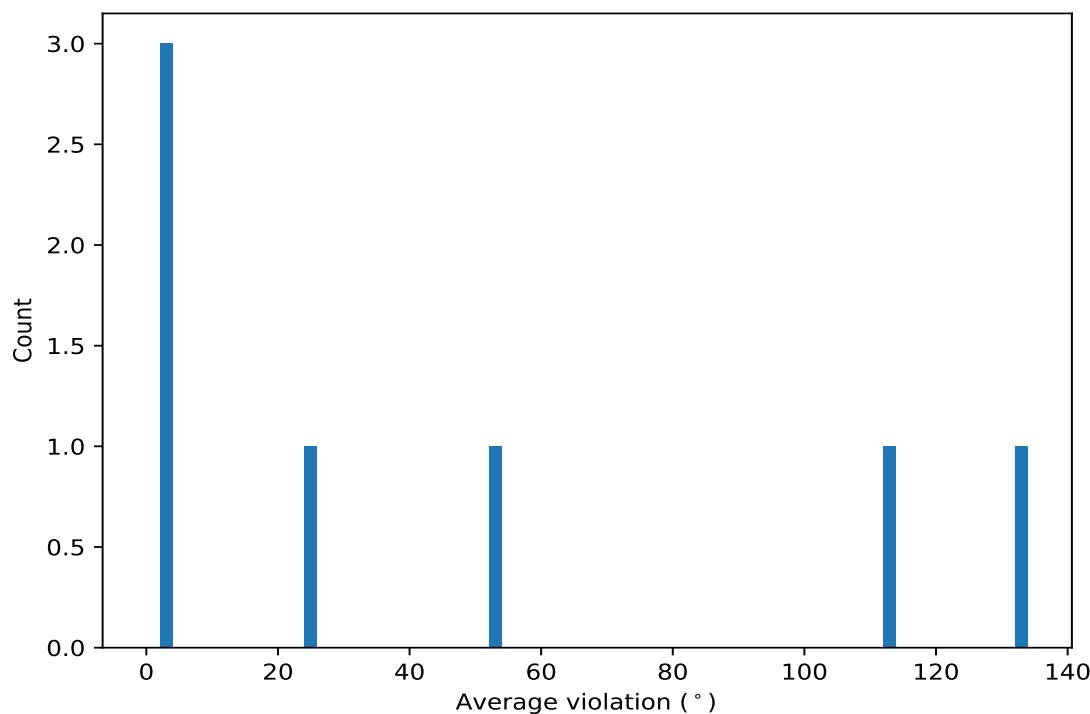
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [\(i\)](#)



10.4 Most violated dihedral-angle restraints in the ensemble [\(i\)](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [\(i\)](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble.



10.4.2 Table: Most violated dihedral-angle restraints [\(i\)](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

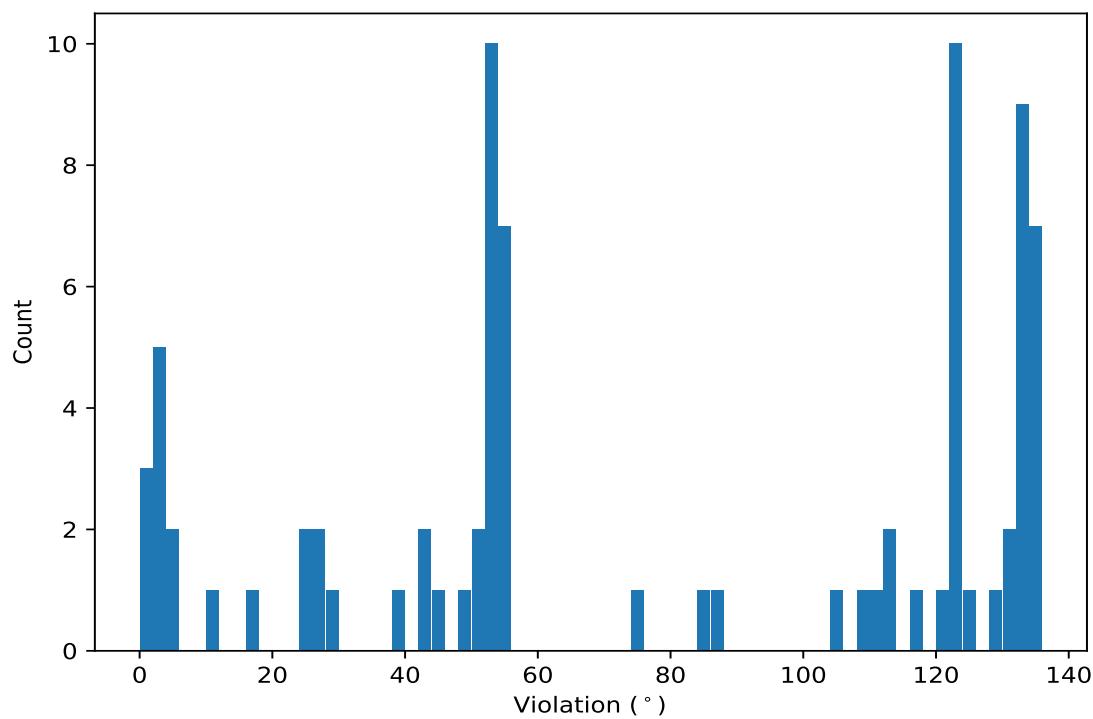
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	20	132.95	2.33	133.61
(1,4)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:HIS:N	20	113.24	14.24	121.87
(1,388)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	20	52.95	2.33	53.61
(1,11)	1:2:A:SER:C	1:3:A:HIS:N	1:3:A:HIS:CA	1:3:A:HIS:C	12	24.47	12.96	26.08
(1,1067)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:CB	1:2:A:SER:OG	3	2.05	0.98	1.45
(1,1069)	1:3:A:HIS:N	1:3:A:HIS:CA	1:3:A:HIS:CB	1:3:A:HIS:CG	2	3.92	0.9	3.92
(1,7)	1:2:A:SER:C	1:3:A:HIS:N	1:3:A:HIS:CA	1:3:A:HIS:C	2	2.59	0.04	2.59

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [\(i\)](#)

10.5.1 Histogram : Distribution of violations [\(i\)](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [\(i\)](#)

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	18	135.65
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	12	135.37
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	11	135.04
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	3	134.89
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	4	134.73
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	10	134.24
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	2	134.12
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	13	133.91
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	1	133.69
(1,390)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:ALA:N	5	133.64