WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Jul 17, 2024 – 04:07 pm BST

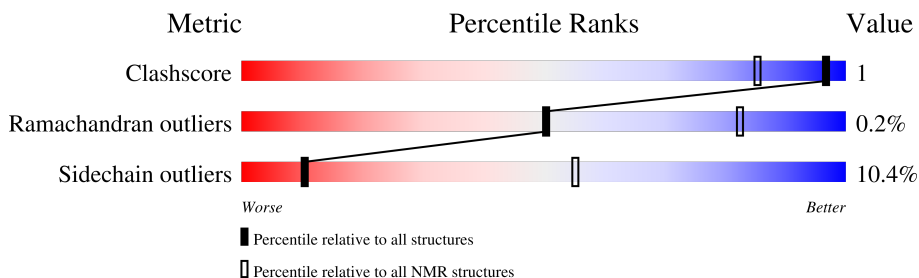|		
PDB ID	:	8PQU
BMRB ID	:	27852
Title	:	NMR structure of the Thermus thermophilus PilF-GSPIIB domain in the apo state
Authors	:	Neissner, K.; Woehnert, J.
Deposited on	:	2023-07-12

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 was not calculated.

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	Percentile Ranks	Value
Clashscore		1
Ramachandran outliers		0.2%
Sidechain outliers		10.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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

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

Mol	Chain	Length	Quality of chain
1	A	146	88% 6% 5%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy.*

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:165-A:302 (138)	0.65	12

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2319 atoms, of which 1171 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ATP-binding motif-containing protein pilF.

Mol	Chain	Residues	Atoms					Trace
1	A	146	Total	C	H	N	O	0
			2319	732	1171	201	215	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	PRO	engineered mutation	UNP Q72H73
A	158	SER	PRO	engineered mutation	UNP Q72H73

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
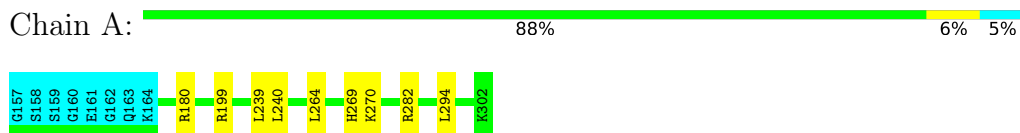
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
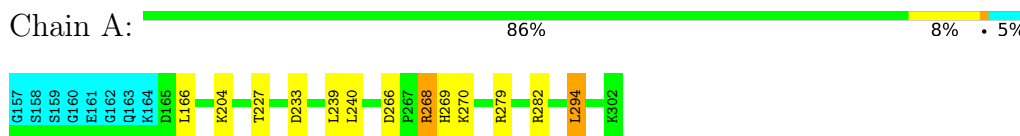
4.2.2 Score per residue for model 2

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
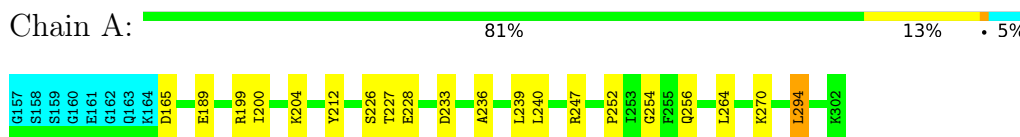
4.2.3 Score per residue for model 3

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
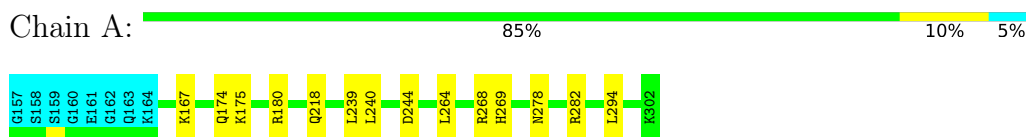
4.2.4 Score per residue for model 4

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
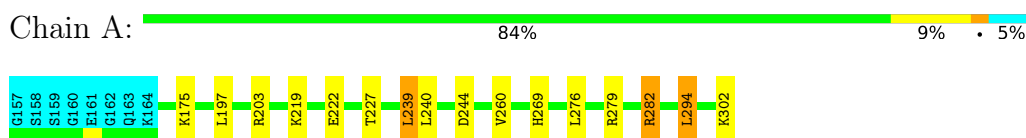
4.2.5 Score per residue for model 5

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
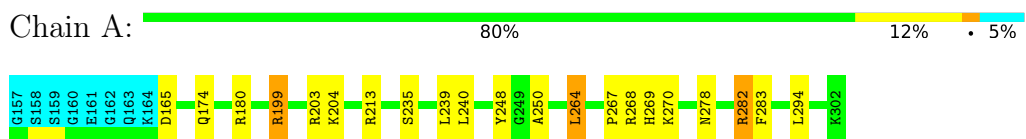
4.2.6 Score per residue for model 6

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
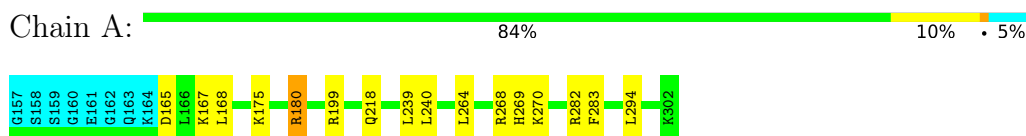
4.2.7 Score per residue for model 7

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
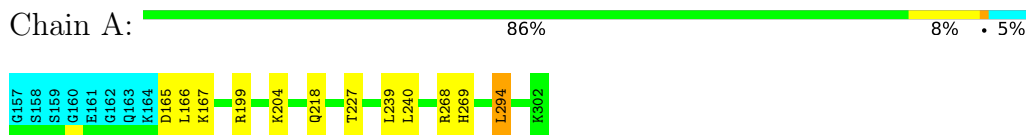
4.2.8 Score per residue for model 8

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
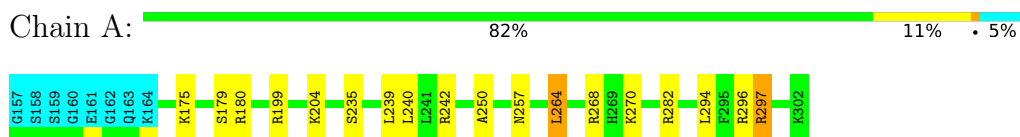
4.2.9 Score per residue for model 9

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
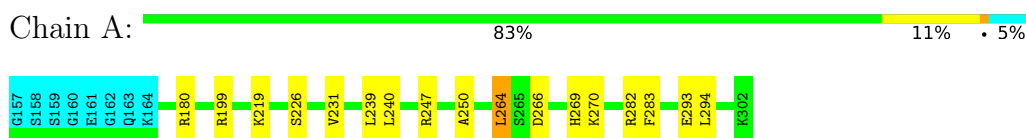
4.2.10 Score per residue for model 10

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
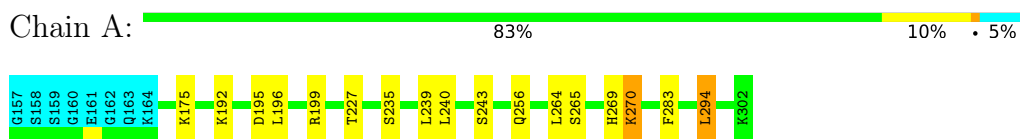
4.2.11 Score per residue for model 11

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
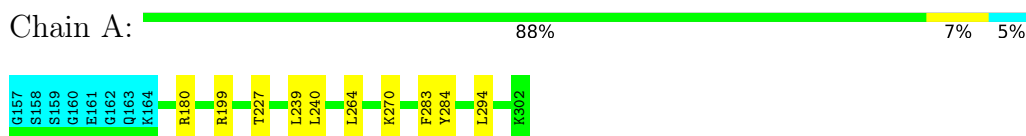
4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:
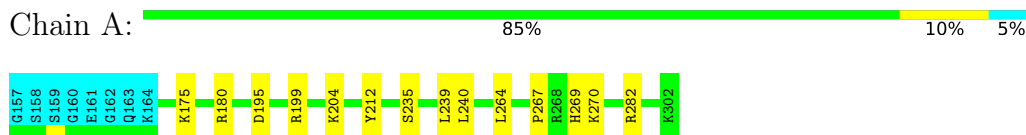
4.2.13 Score per residue for model 13

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:

85% 10% 5%

G157 S158 S159 G160 E161 G162 Q163 K164 L171 E181 L197 G198 R199 D233 L239 L240 D244 R247 K270 L276 R282 L294 F295 R296 K302
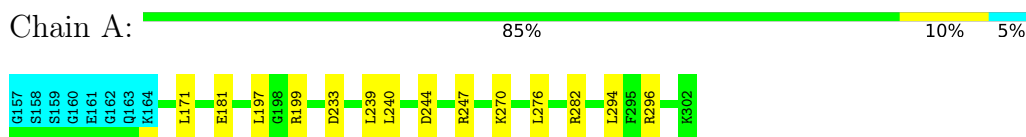
4.2.14 Score per residue for model 14

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:

86% 8% 5%

G157 S158 S159 G160 E161 G162 Q163 K164 K175 R180 D195 R199 E222 D233 L239 L240 L241 R242 L264 K270 R282 L294 K302
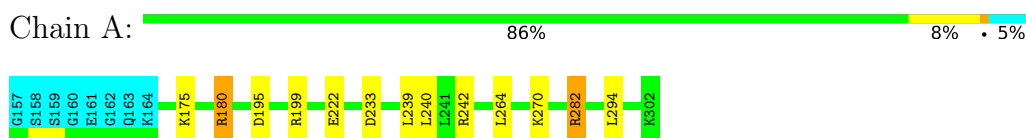
4.2.15 Score per residue for model 15

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:

84% 11% 5%

G157 S158 S159 G160 E161 G162 Q163 K164 K175 L183 K192 D195 R199 Y212 L215 L239 L240 L264 H269 K270 R282 L294 F295 R296 Y299 K302
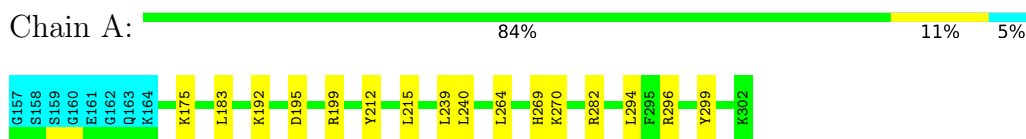
4.2.16 Score per residue for model 16

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:

86% 8% 5%

G157 S158 S159 G160 E161 G162 Q163 K164 D233 L239 L240 V263 L264 R268 H269 K270 R282 F283 Y284 L294 R297 K302
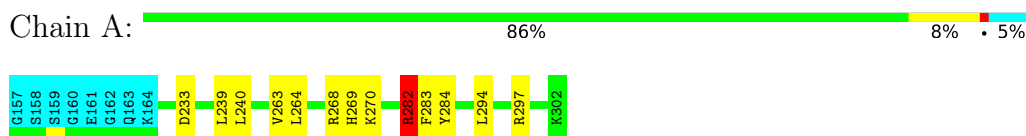
4.2.17 Score per residue for model 17

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:

84% 10% 5%

G157 S158 S159 G160 E161 G162 Q163 K164 E184 E185 D195 R199 Y212 Q218 D233 L239 L240 N257 V260 H269 K270 R282 F283 K302
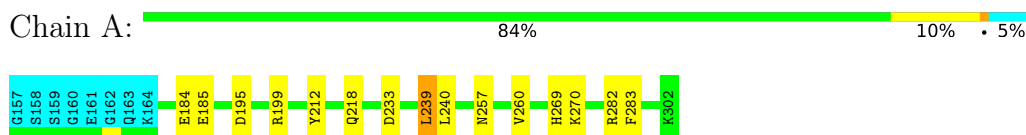
4.2.18 Score per residue for model 18

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:

84%　　　9%　　5%

G157 S158 S159 G160 E161 G162 Q163 K164 D165 A186 K204 V231 P232 D233 L239 L240 A250 L264 R268 H269 R279 R282 L294 F295 R296 K302
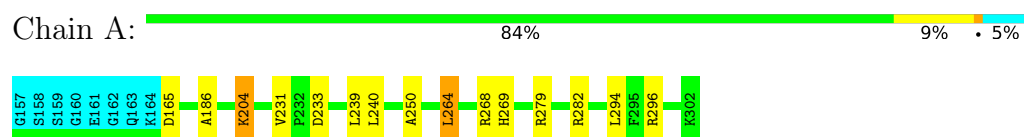
4.2.19 Score per residue for model 19

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:

80%　　　12%　　5%

G157 S158 S159 G160 E161 G162 Q163 K164 D165 L166 R180 E189 K192 R213 T227 E228 D233 P234 S235 L239 L240 A250 V260 L264 S265 D266 P267 R268 H269 K270 N278 R282 E293 L294 K302
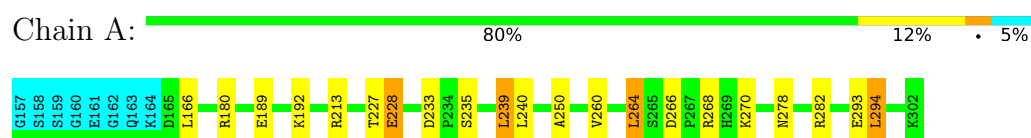
4.2.20 Score per residue for model 20

• Molecule 1: ATP-binding motif-containing protein pilF

Chain A:

84%　　　8%　　5%

G157 S158 S159 G160 E161 G162 Q163 K164 R180 R199 Q218 S235 L239 L240 S243 D244 A250 V260 L264 H269 N278 R282 L294 K302
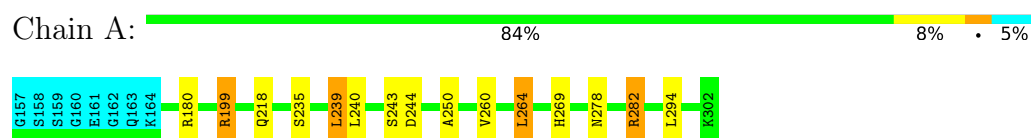
5 Refinement protocol and experimental data overview ⓘ

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	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	1861
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1861
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.57±0.01	0±0/1117 (0.0± 0.0%)	0.97±0.02	1±1/1511 (0.1± 0.1%)
All	All	0.57	0/22340 (0.0%)	0.97	16/30220 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.3±1.0
All	All	0	26

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
1	A	180	ARG	NE-CZ-NH2	-6.66	116.97	120.30	5	2
1	A	282	ARG	NE-CZ-NH2	-6.41	117.10	120.30	8	4
1	A	296	ARG	NE-CZ-NH2	-6.26	117.17	120.30	18	2
1	A	268	ARG	NE-CZ-NH2	-5.58	117.51	120.30	19	1
1	A	284	TYR	CB-CG-CD1	-5.24	117.86	121.00	11	1
1	A	199	ARG	NE-CZ-NH2	-5.16	117.72	120.30	11	1
1	A	279	ARG	NE-CZ-NH1	5.14	122.87	120.30	4	1
1	A	268	ARG	NE-CZ-NH1	5.10	122.85	120.30	7	1
1	A	213	ARG	NE-CZ-NH2	-5.09	117.76	120.30	19	2
1	A	199	ARG	NE-CZ-NH1	5.06	122.83	120.30	5	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	199	ARG	Sidechain	5
1	A	282	ARG	Sidechain	4
1	A	212	TYR	Sidechain	4
1	A	247	ARG	Sidechain	3
1	A	180	ARG	Sidechain	2
1	A	297	ARG	Sidechain	2
1	A	268	ARG	Sidechain	1
1	A	279	ARG	Sidechain	1
1	A	203	ARG	Sidechain	1
1	A	248	TYR	Sidechain	1
1	A	296	ARG	Sidechain	1
1	A	299	TYR	Sidechain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1097	1125	1125	2±1
All	All	21940	22500	22500	30

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:227:THR:HB	1:A:294:LEU:HD23	0.63	1.69	2	7
1:A:270:LYS:HE2	1:A:283:PHE:CD1	0.60	2.31	5	3
1:A:239:LEU:HD11	1:A:260:VAL:HG11	0.56	1.77	20	4
1:A:270:LYS:HE3	1:A:283:PHE:CD1	0.54	2.38	11	3
1:A:250:ALA:HB2	1:A:264:LEU:HD23	0.53	1.79	18	6
1:A:236:ALA:HB2	1:A:254:GLY:HA2	0.50	1.82	2	1
1:A:189:GLU:HB3	1:A:200:ILE:HD13	0.46	1.87	2	1
1:A:264:LEU:CD1	1:A:270:LYS:HE3	0.46	2.40	15	1
1:A:263:VAL:HG22	1:A:284:TYR:HB2	0.45	1.88	16	1
1:A:270:LYS:HE2	1:A:283:PHE:CG	0.42	2.49	16	1
1:A:186:ALA:HB2	1:A:204:LYS:HE2	0.42	1.91	18	1
1:A:236:ALA:HB1	1:A:252:PRO:HB2	0.40	1.94	2	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	137/146 (94%)	133±2 (97±1%)	4±2 (3±1%)	0±0 (0±0%)	50	82
All	All	2740/2920 (94%)	2661 (97%)	73 (3%)	6 (0%)	50	82

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	228	GLU	2
1	A	267	PRO	2
1	A	195	ASP	2

6.3.2 Protein sidechains ⓘ

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	113/118 (96%)	101±3 (90±2%)	12±3 (10±2%)	10	55
All	All	2260/2360 (96%)	2026 (90%)	234 (10%)	10	55

All 52 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	239	LEU	20
1	A	240	LEU	20
1	A	294	LEU	17
1	A	269	HIS	14
1	A	264	LEU	14
1	A	282	ARG	14
1	A	199	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	233	ASP	8
1	A	270	LYS	8
1	A	175	LYS	8
1	A	180	ARG	8
1	A	204	LYS	7
1	A	268	ARG	7
1	A	235	SER	6
1	A	165	ASP	5
1	A	218	GLN	5
1	A	244	ASP	4
1	A	278	ASN	4
1	A	166	LEU	3
1	A	266	ASP	3
1	A	167	LYS	3
1	A	192	LYS	3
1	A	195	ASP	3
1	A	226	SER	2
1	A	256	GLN	2
1	A	174	GLN	2
1	A	197	LEU	2
1	A	219	LYS	2
1	A	222	GLU	2
1	A	276	LEU	2
1	A	242	ARG	2
1	A	257	ASN	2
1	A	231	VAL	2
1	A	293	GLU	2
1	A	243	SER	2
1	A	302	LYS	1
1	A	203	ARG	1
1	A	168	LEU	1
1	A	179	SER	1
1	A	297	ARG	1
1	A	196	LEU	1
1	A	265	SER	1
1	A	171	LEU	1
1	A	181	GLU	1
1	A	183	LEU	1
1	A	215	LEU	1
1	A	296	ARG	1
1	A	184	GLU	1
1	A	185	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	279	ARG	1
1	A	189	GLU	1
1	A	228	GLU	1

6.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6   Ligand geometry ⓘ

There are no ligands in this entry.

6.7   Other polymers ⓘ

There are no such molecules in this entry.

6.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping ⓘ

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

Total number of shifts	1861
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1861
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. All 1861 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	GLY	C	174.458	0.3	1
1	A	4	GLY	CA	45.306	0.3	1
1	A	4	GLY	H	8.354	0.020	1
1	A	4	GLY	HA2	3.988	0.020	1
1	A	4	GLY	HA3	3.988	0.020	1
1	A	4	GLY	N	110.59	0.3	1
1	A	5	GLU	C	177.282	0.3	1
1	A	5	GLU	CA	56.943	0.3	1
1	A	5	GLU	CB	30.215	0.3	1
1	A	5	GLU	CG	36.126	0.3	1
1	A	5	GLU	H	8.255	0.020	1
1	A	5	GLU	HA	4.291	0.020	1
1	A	5	GLU	HB2	2.078	0.020	2
1	A	5	GLU	HB3	1.948	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	GLU	HG2	2.269	0.020	1
1	A	5	GLU	HG3	2.269	0.020	1
1	A	5	GLU	N	120.696	0.3	1
1	A	6	GLY	C	174.435	0.3	1
1	A	6	GLY	CA	45.673	0.3	1
1	A	6	GLY	H	8.404	0.020	1
1	A	6	GLY	HA2	3.953	0.020	1
1	A	6	GLY	HA3	3.953	0.020	1
1	A	6	GLY	N	109.485	0.3	1
1	A	7	GLN	C	176.427	0.3	1
1	A	7	GLN	CA	56.161	0.3	1
1	A	7	GLN	CB	29.096	0.3	1
1	A	7	GLN	CG	33.981	0.3	1
1	A	7	GLN	H	8.13	0.020	1
1	A	7	GLN	HA	4.33	0.020	1
1	A	7	GLN	HB2	2.123	0.020	2
1	A	7	GLN	HB3	1.996	0.020	2
1	A	7	GLN	HG2	2.365	0.020	1
1	A	7	GLN	HG3	2.365	0.020	1
1	A	7	GLN	HE21	7.364	0.020	1
1	A	7	GLN	HE22	6.706	0.020	1
1	A	7	GLN	N	119.766	0.3	1
1	A	7	GLN	NE2	111.265	0.3	1
1	A	8	LYS	C	176.84	0.3	1
1	A	8	LYS	CA	57.215	0.3	1
1	A	8	LYS	CB	32.813	0.3	1
1	A	8	LYS	CG	24.9	0.3	1
1	A	8	LYS	CD	29.063	0.3	1
1	A	8	LYS	CE	42.144	0.3	1
1	A	8	LYS	H	8.168	0.020	1
1	A	8	LYS	HA	4.218	0.020	1
1	A	8	LYS	HB2	1.812	0.020	1
1	A	8	LYS	HB3	1.812	0.020	1
1	A	8	LYS	HG2	1.393	0.020	1
1	A	8	LYS	HG3	1.393	0.020	1
1	A	8	LYS	HD2	1.681	0.020	1
1	A	8	LYS	HD3	1.681	0.020	1
1	A	8	LYS	HE2	2.959	0.020	1
1	A	8	LYS	HE3	2.959	0.020	1
1	A	8	LYS	N	121.445	0.3	1
1	A	9	ASP	C	176.372	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	ASP	CA	54.98	0.3	1
1	A	9	ASP	CB	40.784	0.3	1
1	A	9	ASP	H	8.294	0.020	1
1	A	9	ASP	HA	4.636	0.020	1
1	A	9	ASP	HB2	2.746	0.020	2
1	A	9	ASP	HB3	2.656	0.020	2
1	A	9	ASP	N	120.579	0.3	1
1	A	10	LEU	C	178.948	0.3	1
1	A	10	LEU	CA	56.691	0.3	1
1	A	10	LEU	CB	42.225	0.3	1
1	A	10	LEU	CG	27.048	0.3	1
1	A	10	LEU	CD1	24.815	0.3	1
1	A	10	LEU	CD2	24.067	0.3	1
1	A	10	LEU	H	7.846	0.020	1
1	A	10	LEU	HA	4.143	0.020	1
1	A	10	LEU	HB2	1.643	0.020	1
1	A	10	LEU	HB3	1.643	0.020	1
1	A	10	LEU	HG	1.637	0.020	1
1	A	10	LEU	HD11	0.901	0.020	2
1	A	10	LEU	HD12	0.901	0.020	2
1	A	10	LEU	HD13	0.901	0.020	2
1	A	10	LEU	HD21	0.84	0.020	2
1	A	10	LEU	HD22	0.84	0.020	2
1	A	10	LEU	HD23	0.84	0.020	2
1	A	10	LEU	N	121.574	0.3	1
1	A	11	LYS	C	178.468	0.3	1
1	A	11	LYS	CA	57.706	0.3	1
1	A	11	LYS	CB	32.088	0.3	1
1	A	11	LYS	CG	24.955	0.3	1
1	A	11	LYS	CD	29.016	0.3	1
1	A	11	LYS	CE	42.292	0.3	1
1	A	11	LYS	H	8.254	0.020	1
1	A	11	LYS	HA	4.142	0.020	1
1	A	11	LYS	HB2	1.817	0.020	1
1	A	11	LYS	HB3	1.817	0.020	1
1	A	11	LYS	HG2	1.527	0.020	1
1	A	11	LYS	HG3	1.527	0.020	1
1	A	11	LYS	HD2	1.682	0.020	1
1	A	11	LYS	HD3	1.682	0.020	1
1	A	11	LYS	HE2	3.004	0.020	1
1	A	11	LYS	HE3	3.004	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	LYS	N	119.223	0.3	1
1	A	12	LEU	C	178.368	0.3	1
1	A	12	LEU	CA	58.217	0.3	1
1	A	12	LEU	CB	41.545	0.3	1
1	A	12	LEU	CG	26.983	0.3	1
1	A	12	LEU	CD1	22.693	0.3	1
1	A	12	LEU	CD2	25.291	0.3	1
1	A	12	LEU	H	7.85	0.020	1
1	A	12	LEU	HA	3.897	0.020	1
1	A	12	LEU	HB2	1.799	0.020	2
1	A	12	LEU	HB3	1.644	0.020	2
1	A	12	LEU	HG	1.361	0.020	1
1	A	12	LEU	HD11	0.776	0.020	2
1	A	12	LEU	HD12	0.776	0.020	2
1	A	12	LEU	HD13	0.776	0.020	2
1	A	12	LEU	HD21	0.778	0.020	2
1	A	12	LEU	HD22	0.778	0.020	2
1	A	12	LEU	HD23	0.778	0.020	2
1	A	12	LEU	N	121.941	0.3	1
1	A	13	GLY	C	174.462	0.3	1
1	A	13	GLY	CA	48.084	0.3	1
1	A	13	GLY	H	8.081	0.020	1
1	A	13	GLY	HA2	3.704	0.020	2
1	A	13	GLY	HA3	3.428	0.020	2
1	A	13	GLY	N	104.181	0.3	1
1	A	14	GLU	C	178.82	0.3	1
1	A	14	GLU	CA	59.298	0.3	1
1	A	14	GLU	CB	29.588	0.3	1
1	A	14	GLU	CG	36.654	0.3	1
1	A	14	GLU	H	7.774	0.020	1
1	A	14	GLU	HA	3.894	0.020	1
1	A	14	GLU	HB2	2.098	0.020	1
1	A	14	GLU	HB3	2.098	0.020	1
1	A	14	GLU	HG2	2.363	0.020	2
1	A	14	GLU	HG3	2.192	0.020	2
1	A	14	GLU	N	119.106	0.3	1
1	A	15	LEU	C	178.695	0.3	1
1	A	15	LEU	CA	57.993	0.3	1
1	A	15	LEU	CB	42.076	0.3	1
1	A	15	LEU	CG	27.255	0.3	1
1	A	15	LEU	CD1	24.268	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	LEU	CD2	25.298	0.3	1
1	A	15	LEU	H	7.874	0.020	1
1	A	15	LEU	HA	4.072	0.020	1
1	A	15	LEU	HB2	1.752	0.020	2
1	A	15	LEU	HB3	1.707	0.020	2
1	A	15	LEU	HG	1.452	0.020	1
1	A	15	LEU	HD11	0.861	0.020	2
1	A	15	LEU	HD12	0.861	0.020	2
1	A	15	LEU	HD13	0.861	0.020	2
1	A	15	LEU	HD21	0.839	0.020	2
1	A	15	LEU	HD22	0.839	0.020	2
1	A	15	LEU	HD23	0.839	0.020	2
1	A	15	LEU	N	121.676	0.3	1
1	A	16	LEU	C	179.079	0.3	1
1	A	16	LEU	CA	58.177	0.3	1
1	A	16	LEU	CB	42.559	0.3	1
1	A	16	LEU	CG	26.843	0.3	1
1	A	16	LEU	CD1	27.478	0.3	1
1	A	16	LEU	CD2	24.61	0.3	1
1	A	16	LEU	H	7.948	0.020	1
1	A	16	LEU	HA	3.815	0.020	1
1	A	16	LEU	HB2	2.077	0.020	2
1	A	16	LEU	HB3	1.23	0.020	2
1	A	16	LEU	HG	1.832	0.020	1
1	A	16	LEU	HD11	0.728	0.020	2
1	A	16	LEU	HD12	0.728	0.020	2
1	A	16	LEU	HD13	0.728	0.020	2
1	A	16	LEU	HD21	0.916	0.020	2
1	A	16	LEU	HD22	0.916	0.020	2
1	A	16	LEU	HD23	0.916	0.020	2
1	A	16	LEU	N	117.538	0.3	1
1	A	17	LEU	C	180.862	0.3	1
1	A	17	LEU	CA	57.975	0.3	1
1	A	17	LEU	CB	42.429	0.3	1
1	A	17	LEU	CG	26.578	0.3	1
1	A	17	LEU	CD1	25.028	0.3	1
1	A	17	LEU	CD2	24.776	0.3	1
1	A	17	LEU	H	8.048	0.020	1
1	A	17	LEU	HA	4.217	0.020	1
1	A	17	LEU	HB2	1.803	0.020	2
1	A	17	LEU	HB3	1.597	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	LEU	HG	1.605	0.020	1
1	A	17	LEU	HD11	0.841	0.020	2
1	A	17	LEU	HD12	0.841	0.020	2
1	A	17	LEU	HD13	0.841	0.020	2
1	A	17	LEU	HD21	0.838	0.020	2
1	A	17	LEU	HD22	0.838	0.020	2
1	A	17	LEU	HD23	0.838	0.020	2
1	A	17	LEU	N	120.234	0.3	1
1	A	18	GLN	C	178.575	0.3	1
1	A	18	GLN	CA	58.898	0.3	1
1	A	18	GLN	CB	28.263	0.3	1
1	A	18	GLN	CG	33.82	0.3	1
1	A	18	GLN	H	8.405	0.020	1
1	A	18	GLN	HA	3.972	0.020	1
1	A	18	GLN	HB2	2.221	0.020	2
1	A	18	GLN	HB3	2.146	0.020	2
1	A	18	GLN	HG2	2.517	0.020	2
1	A	18	GLN	HG3	2.385	0.020	2
1	A	18	GLN	HE21	7.304	0.020	1
1	A	18	GLN	HE22	6.621	0.020	1
1	A	18	GLN	N	121.647	0.3	1
1	A	18	GLN	NE2	110.464	0.3	1
1	A	19	LYS	C	176.708	0.3	1
1	A	19	LYS	CA	56.329	0.3	1
1	A	19	LYS	CB	32.519	0.3	1
1	A	19	LYS	CG	24.698	0.3	1
1	A	19	LYS	CD	28.096	0.3	1
1	A	19	LYS	CE	41.821	0.3	1
1	A	19	LYS	H	7.621	0.020	1
1	A	19	LYS	HA	3.91	0.020	1
1	A	19	LYS	HB2	1.023	0.020	2
1	A	19	LYS	HB3	0.693	0.020	2
1	A	19	LYS	HG2	1.174	0.020	1
1	A	19	LYS	HG3	1.174	0.020	1
1	A	19	LYS	HD2	0.897	0.020	1
1	A	19	LYS	HD3	0.897	0.020	1
1	A	19	LYS	HE2	2.545	0.020	1
1	A	19	LYS	HE3	2.545	0.020	1
1	A	19	LYS	N	115.352	0.3	1
1	A	20	GLY	C	175.523	0.3	1
1	A	20	GLY	CA	45.173	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	GLY	H	7.778	0.020	1
1	A	20	GLY	HA2	4.115	0.020	2
1	A	20	GLY	HA3	3.945	0.020	2
1	A	20	GLY	N	105.656	0.3	1
1	A	21	TRP	C	175.092	0.3	1
1	A	21	TRP	CA	56.618	0.3	1
1	A	21	TRP	CB	30.771	0.3	1
1	A	21	TRP	CD1	125.34	0.3	1
1	A	21	TRP	CE3	120.457	0.3	1
1	A	21	TRP	CZ2	114.938	0.3	1
1	A	21	TRP	CZ3	122.225	0.3	1
1	A	21	TRP	CH2	124.457	0.3	1
1	A	21	TRP	H	7.84	0.020	1
1	A	21	TRP	HA	4.781	0.020	1
1	A	21	TRP	HB2	2.971	0.020	2
1	A	21	TRP	HB3	3.257	0.020	2
1	A	21	TRP	HD1	6.91	0.020	1
1	A	21	TRP	HE1	10.141	0.020	1
1	A	21	TRP	HE3	7.395	0.020	1
1	A	21	TRP	HZ2	7.522	0.020	1
1	A	21	TRP	HZ3	7.154	0.020	1
1	A	21	TRP	HH2	7.15	0.020	1
1	A	21	TRP	N	118.812	0.3	1
1	A	21	TRP	NE1	128.431	0.3	1
1	A	22	ILE	C	173.038	0.3	1
1	A	22	ILE	CA	58.454	0.3	1
1	A	22	ILE	CB	42.595	0.3	1
1	A	22	ILE	CG1	26.144	0.3	1
1	A	22	ILE	CG2	18.243	0.3	1
1	A	22	ILE	CD1	15.365	0.3	1
1	A	22	ILE	H	7.279	0.020	1
1	A	22	ILE	HA	4.71	0.020	1
1	A	22	ILE	HB	1.805	0.020	1
1	A	22	ILE	HG12	1.063	0.020	1
1	A	22	ILE	HG13	1.063	0.020	1
1	A	22	ILE	HG21	0.844	0.020	1
1	A	22	ILE	HG22	0.844	0.020	1
1	A	22	ILE	HG23	0.844	0.020	1
1	A	22	ILE	HD11	0.857	0.020	1
1	A	22	ILE	HD12	0.857	0.020	1
1	A	22	ILE	HD13	0.857	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	ILE	N	110.77	0.3	1
1	A	23	SER	C	174.964	0.3	1
1	A	23	SER	CA	56.311	0.3	1
1	A	23	SER	CB	65.922	0.3	1
1	A	23	SER	H	7.895	0.020	1
1	A	23	SER	HA	4.688	0.020	1
1	A	23	SER	HB2	4.422	0.020	2
1	A	23	SER	HB3	4.003	0.020	2
1	A	23	SER	N	117.06	0.3	1
1	A	24	ARG	C	178.247	0.3	1
1	A	24	ARG	CA	59.758	0.3	1
1	A	24	ARG	CB	29.344	0.3	1
1	A	24	ARG	CG	27.243	0.3	1
1	A	24	ARG	CD	43.0	0.3	1
1	A	24	ARG	H	8.943	0.020	1
1	A	24	ARG	HA	3.868	0.020	1
1	A	24	ARG	HB2	1.908	0.020	2
1	A	24	ARG	HB3	1.826	0.020	2
1	A	24	ARG	HG2	1.797	0.020	2
1	A	24	ARG	HG3	1.685	0.020	2
1	A	24	ARG	HD2	3.323	0.020	2
1	A	24	ARG	HD3	3.234	0.020	2
1	A	24	ARG	N	121.77	0.3	1
1	A	25	GLU	C	178.713	0.3	1
1	A	25	GLU	CA	60.275	0.3	1
1	A	25	GLU	CB	28.724	0.3	1
1	A	25	GLU	CG	36.867	0.3	1
1	A	25	GLU	H	8.942	0.020	1
1	A	25	GLU	HA	4.013	0.020	1
1	A	25	GLU	HB2	2.061	0.020	2
1	A	25	GLU	HB3	1.966	0.020	2
1	A	25	GLU	HG2	2.446	0.020	2
1	A	25	GLU	HG3	2.282	0.020	2
1	A	25	GLU	N	118.441	0.3	1
1	A	26	ALA	C	180.689	0.3	1
1	A	26	ALA	CA	54.711	0.3	1
1	A	26	ALA	CB	18.36	0.3	1
1	A	26	ALA	H	7.822	0.020	1
1	A	26	ALA	HA	4.157	0.020	1
1	A	26	ALA	HB1	1.485	0.020	1
1	A	26	ALA	HB2	1.485	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	ALA	HB3	1.485	0.020	1
1	A	26	ALA	N	122.509	0.3	1
1	A	27	LEU	C	177.874	0.3	1
1	A	27	LEU	CA	58.026	0.3	1
1	A	27	LEU	CB	40.968	0.3	1
1	A	27	LEU	CG	27.07	0.3	1
1	A	27	LEU	CD1	23.018	0.3	1
1	A	27	LEU	CD2	26.006	0.3	1
1	A	27	LEU	H	7.985	0.020	1
1	A	27	LEU	HA	3.992	0.020	1
1	A	27	LEU	HB2	2.112	0.020	2
1	A	27	LEU	HB3	1.437	0.020	2
1	A	27	LEU	HG	1.594	0.020	1
1	A	27	LEU	HD11	0.887	0.020	2
1	A	27	LEU	HD12	0.887	0.020	2
1	A	27	LEU	HD13	0.887	0.020	2
1	A	27	LEU	HD21	0.865	0.020	2
1	A	27	LEU	HD22	0.865	0.020	2
1	A	27	LEU	HD23	0.865	0.020	2
1	A	27	LEU	N	119.482	0.3	1
1	A	28	GLU	C	179.533	0.3	1
1	A	28	GLU	CA	60.003	0.3	1
1	A	28	GLU	CB	28.949	0.3	1
1	A	28	GLU	CG	36.111	0.3	1
1	A	28	GLU	H	8.407	0.020	1
1	A	28	GLU	HA	3.938	0.020	1
1	A	28	GLU	HB2	2.107	0.020	1
1	A	28	GLU	HB3	2.107	0.020	1
1	A	28	GLU	HG2	2.464	0.020	2
1	A	28	GLU	HG3	2.268	0.020	2
1	A	28	GLU	N	117.784	0.3	1
1	A	29	GLU	C	179.581	0.3	1
1	A	29	GLU	CA	59.227	0.3	1
1	A	29	GLU	CB	29.822	0.3	1
1	A	29	GLU	CG	36.357	0.3	1
1	A	29	GLU	H	7.997	0.020	1
1	A	29	GLU	HA	4.032	0.020	1
1	A	29	GLU	HB2	2.179	0.020	2
1	A	29	GLU	HB3	2.01	0.020	2
1	A	29	GLU	HG2	2.535	0.020	1
1	A	29	GLU	HG3	2.535	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	GLU	N	117.648	0.3	1
1	A	30	ALA	C	178.929	0.3	1
1	A	30	ALA	CA	54.885	0.3	1
1	A	30	ALA	CB	18.86	0.3	1
1	A	30	ALA	H	8.13	0.020	1
1	A	30	ALA	HA	4.035	0.020	1
1	A	30	ALA	HB1	1.451	0.020	1
1	A	30	ALA	HB2	1.451	0.020	1
1	A	30	ALA	HB3	1.451	0.020	1
1	A	30	ALA	N	122.857	0.3	1
1	A	31	LEU	C	180.55	0.3	1
1	A	31	LEU	CA	57.959	0.3	1
1	A	31	LEU	CB	41.427	0.3	1
1	A	31	LEU	CG	26.746	0.3	1
1	A	31	LEU	CD1	25.811	0.3	1
1	A	31	LEU	CD2	23.121	0.3	1
1	A	31	LEU	H	8.473	0.020	1
1	A	31	LEU	HA	4.036	0.020	1
1	A	31	LEU	HB2	2.003	0.020	2
1	A	31	LEU	HB3	1.499	0.020	2
1	A	31	LEU	HG	1.826	0.020	1
1	A	31	LEU	HD11	0.854	0.020	2
1	A	31	LEU	HD12	0.854	0.020	2
1	A	31	LEU	HD13	0.854	0.020	2
1	A	31	LEU	HD21	0.907	0.020	2
1	A	31	LEU	HD22	0.907	0.020	2
1	A	31	LEU	HD23	0.907	0.020	2
1	A	31	LEU	N	119.072	0.3	1
1	A	32	VAL	C	178.62	0.3	1
1	A	32	VAL	CA	66.448	0.3	1
1	A	32	VAL	CB	31.682	0.3	1
1	A	32	VAL	CG1	21.228	0.3	1
1	A	32	VAL	CG2	22.893	0.3	1
1	A	32	VAL	H	7.791	0.020	1
1	A	32	VAL	HA	3.798	0.020	1
1	A	32	VAL	HB	2.194	0.020	1
1	A	32	VAL	HG11	0.988	0.020	2
1	A	32	VAL	HG12	0.988	0.020	2
1	A	32	VAL	HG13	0.988	0.020	2
1	A	32	VAL	HG21	1.104	0.020	2
1	A	32	VAL	HG22	1.104	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	VAL	HG23	1.104	0.020	2
1	A	32	VAL	N	121.061	0.3	1
1	A	33	GLU	C	179.573	0.3	1
1	A	33	GLU	CA	59.752	0.3	1
1	A	33	GLU	CB	29.051	0.3	1
1	A	33	GLU	CG	36.326	0.3	1
1	A	33	GLU	H	7.813	0.020	1
1	A	33	GLU	HA	4.103	0.020	1
1	A	33	GLU	HB2	2.1	0.020	2
1	A	33	GLU	HB3	2.194	0.020	2
1	A	33	GLU	HG2	2.349	0.020	1
1	A	33	GLU	HG3	2.349	0.020	1
1	A	33	GLU	N	121.052	0.3	1
1	A	34	GLN	C	178.367	0.3	1
1	A	34	GLN	CA	60.016	0.3	1
1	A	34	GLN	CB	28.432	0.3	1
1	A	34	GLN	CG	33.712	0.3	1
1	A	34	GLN	H	8.859	0.020	1
1	A	34	GLN	HA	3.746	0.020	1
1	A	34	GLN	HB2	2.406	0.020	2
1	A	34	GLN	HB3	1.874	0.020	2
1	A	34	GLN	HG2	2.582	0.020	2
1	A	34	GLN	HG3	2.25	0.020	2
1	A	34	GLN	HE21	7.61	0.020	1
1	A	34	GLN	HE22	6.762	0.020	1
1	A	34	GLN	N	122.944	0.3	1
1	A	34	GLN	NE2	110.847	0.3	1
1	A	35	GLU	C	178.285	0.3	1
1	A	35	GLU	CA	59.39	0.3	1
1	A	35	GLU	CB	29.333	0.3	1
1	A	35	GLU	CG	36.09	0.3	1
1	A	35	GLU	H	7.857	0.020	1
1	A	35	GLU	HA	3.997	0.020	1
1	A	35	GLU	HB2	2.214	0.020	1
1	A	35	GLU	HB3	2.214	0.020	1
1	A	35	GLU	HG2	2.476	0.020	2
1	A	35	GLU	HG3	2.303	0.020	2
1	A	35	GLU	N	119.966	0.3	1
1	A	36	LYS	C	178.631	0.3	1
1	A	36	LYS	CA	58.545	0.3	1
1	A	36	LYS	CB	33.572	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	36	LYS	CG	25.041	0.3	1
1	A	36	LYS	CD	29.038	0.3	1
1	A	36	LYS	CE	42.149	0.3	1
1	A	36	LYS	H	7.727	0.020	1
1	A	36	LYS	HA	4.233	0.020	1
1	A	36	LYS	HB2	1.985	0.020	1
1	A	36	LYS	HB3	1.985	0.020	1
1	A	36	LYS	HG2	1.625	0.020	2
1	A	36	LYS	HG3	1.478	0.020	2
1	A	36	LYS	HD2	1.678	0.020	1
1	A	36	LYS	HD3	1.678	0.020	1
1	A	36	LYS	HE2	2.989	0.020	1
1	A	36	LYS	HE3	2.989	0.020	1
1	A	36	LYS	N	115.97	0.3	1
1	A	37	THR	C	176.72	0.3	1
1	A	37	THR	CA	62.476	0.3	1
1	A	37	THR	CB	72.023	0.3	1
1	A	37	THR	CG2	21.53	0.3	1
1	A	37	THR	H	8.256	0.020	1
1	A	37	THR	HA	4.488	0.020	1
1	A	37	THR	HB	4.286	0.020	1
1	A	37	THR	HG21	1.322	0.020	1
1	A	37	THR	HG22	1.322	0.020	1
1	A	37	THR	HG23	1.322	0.020	1
1	A	37	THR	N	106.463	0.3	1
1	A	38	GLY	C	174.142	0.3	1
1	A	38	GLY	CA	45.684	0.3	1
1	A	38	GLY	H	8.762	0.020	1
1	A	38	GLY	HA2	4.155	0.020	2
1	A	38	GLY	HA3	3.855	0.020	2
1	A	38	GLY	N	112.23	0.3	1
1	A	39	ASP	C	174.951	0.3	1
1	A	39	ASP	CA	53.404	0.3	1
1	A	39	ASP	CB	41.724	0.3	1
1	A	39	ASP	H	7.565	0.020	1
1	A	39	ASP	HA	4.628	0.020	1
1	A	39	ASP	HB2	2.523	0.020	1
1	A	39	ASP	HB3	2.523	0.020	1
1	A	39	ASP	N	119.668	0.3	1
1	A	40	LEU	C	178.812	0.3	1
1	A	40	LEU	CA	54.764	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	40	LEU	CB	42.5	0.3	1
1	A	40	LEU	CG	27.264	0.3	1
1	A	40	LEU	CD1	25.266	0.3	1
1	A	40	LEU	CD2	23.235	0.3	1
1	A	40	LEU	H	8.58	0.020	1
1	A	40	LEU	HA	4.218	0.020	1
1	A	40	LEU	HB2	1.79	0.020	2
1	A	40	LEU	HB3	1.47	0.020	2
1	A	40	LEU	HG	1.836	0.020	1
1	A	40	LEU	HD11	0.957	0.020	2
1	A	40	LEU	HD12	0.957	0.020	2
1	A	40	LEU	HD13	0.957	0.020	2
1	A	40	LEU	HD21	0.933	0.020	2
1	A	40	LEU	HD22	0.933	0.020	2
1	A	40	LEU	HD23	0.933	0.020	2
1	A	40	LEU	N	119.731	0.3	1
1	A	41	LEU	C	178.822	0.3	1
1	A	41	LEU	CA	58.265	0.3	1
1	A	41	LEU	CB	41.897	0.3	1
1	A	41	LEU	CG	26.918	0.3	1
1	A	41	LEU	CD1	23.537	0.3	1
1	A	41	LEU	CD2	25.69	0.3	1
1	A	41	LEU	H	8.838	0.020	1
1	A	41	LEU	HA	3.8	0.020	1
1	A	41	LEU	HB2	1.654	0.020	1
1	A	41	LEU	HB3	1.654	0.020	1
1	A	41	LEU	HG	1.425	0.020	1
1	A	41	LEU	HD11	0.78	0.020	2
1	A	41	LEU	HD12	0.78	0.020	2
1	A	41	LEU	HD13	0.78	0.020	2
1	A	41	LEU	HD21	0.801	0.020	2
1	A	41	LEU	HD22	0.801	0.020	2
1	A	41	LEU	HD23	0.801	0.020	2
1	A	41	LEU	N	124.917	0.3	1
1	A	42	GLY	C	174.852	0.3	1
1	A	42	GLY	CA	47.92	0.3	1
1	A	42	GLY	H	9.149	0.020	1
1	A	42	GLY	HA2	3.796	0.020	2
1	A	42	GLY	HA3	3.423	0.020	2
1	A	42	GLY	N	103.443	0.3	1
1	A	43	ARG	C	179.169	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	43	ARG	CA	58.749	0.3	1
1	A	43	ARG	CB	30.001	0.3	1
1	A	43	ARG	CG	27.255	0.3	1
1	A	43	ARG	CD	43.367	0.3	1
1	A	43	ARG	H	6.651	0.020	1
1	A	43	ARG	HA	4.04	0.020	1
1	A	43	ARG	HB2	1.935	0.020	1
1	A	43	ARG	HB3	1.935	0.020	1
1	A	43	ARG	HG2	1.69	0.020	1
1	A	43	ARG	HG3	1.69	0.020	1
1	A	43	ARG	HD2	3.324	0.020	1
1	A	43	ARG	HD3	3.324	0.020	1
1	A	43	ARG	N	117.449	0.3	1
1	A	44	ILE	C	177.967	0.3	1
1	A	44	ILE	CA	65.186	0.3	1
1	A	44	ILE	CB	38.437	0.3	1
1	A	44	ILE	CG1	28.421	0.3	1
1	A	44	ILE	CG2	17.685	0.3	1
1	A	44	ILE	CD1	14.005	0.3	1
1	A	44	ILE	H	7.664	0.020	1
1	A	44	ILE	HA	3.529	0.020	1
1	A	44	ILE	HB	1.887	0.020	1
1	A	44	ILE	HG12	0.969	0.020	1
1	A	44	ILE	HG13	0.969	0.020	1
1	A	44	ILE	HG21	0.898	0.020	1
1	A	44	ILE	HG22	0.898	0.020	1
1	A	44	ILE	HG23	0.898	0.020	1
1	A	44	ILE	HD11	0.716	0.020	1
1	A	44	ILE	HD12	0.716	0.020	1
1	A	44	ILE	HD13	0.716	0.020	1
1	A	44	ILE	N	120.696	0.3	1
1	A	45	LEU	C	179.825	0.3	1
1	A	45	LEU	CA	58.0	0.3	1
1	A	45	LEU	CB	41.404	0.3	1
1	A	45	LEU	CG	26.517	0.3	1
1	A	45	LEU	CD1	26.58	0.3	1
1	A	45	LEU	CD2	22.934	0.3	1
1	A	45	LEU	H	8.411	0.020	1
1	A	45	LEU	HA	3.87	0.020	1
1	A	45	LEU	HB2	1.871	0.020	2
1	A	45	LEU	HB3	1.295	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	LEU	HG	1.759	0.020	1
1	A	45	LEU	HD11	0.652	0.020	2
1	A	45	LEU	HD12	0.652	0.020	2
1	A	45	LEU	HD13	0.652	0.020	2
1	A	45	LEU	HD21	0.735	0.020	2
1	A	45	LEU	HD22	0.735	0.020	2
1	A	45	LEU	HD23	0.735	0.020	2
1	A	45	LEU	N	116.651	0.3	1
1	A	46	VAL	C	180.449	0.3	1
1	A	46	VAL	CA	64.949	0.3	1
1	A	46	VAL	CB	32.092	0.3	1
1	A	46	VAL	CG1	20.981	0.3	1
1	A	46	VAL	CG2	23.256	0.3	1
1	A	46	VAL	H	7.864	0.020	1
1	A	46	VAL	HA	4.674	0.020	1
1	A	46	VAL	HB	2.137	0.020	1
1	A	46	VAL	HG11	1.042	0.020	2
1	A	46	VAL	HG12	1.042	0.020	2
1	A	46	VAL	HG13	1.042	0.020	2
1	A	46	VAL	HG21	1.117	0.020	2
1	A	46	VAL	HG22	1.117	0.020	2
1	A	46	VAL	HG23	1.117	0.020	2
1	A	46	VAL	N	120.309	0.3	1
1	A	47	ARG	C	178.434	0.3	1
1	A	47	ARG	CA	59.496	0.3	1
1	A	47	ARG	CB	29.845	0.3	1
1	A	47	ARG	CG	28.106	0.3	1
1	A	47	ARG	CD	43.982	0.3	1
1	A	47	ARG	H	7.898	0.020	1
1	A	47	ARG	HA	4.155	0.020	1
1	A	47	ARG	HB2	2.092	0.020	2
1	A	47	ARG	HB3	1.976	0.020	2
1	A	47	ARG	HG2	1.839	0.020	2
1	A	47	ARG	HG3	1.703	0.020	2
1	A	47	ARG	HD2	3.264	0.020	1
1	A	47	ARG	HD3	3.264	0.020	1
1	A	47	ARG	N	122.342	0.3	1
1	A	48	LYS	C	176.491	0.3	1
1	A	48	LYS	CA	56.366	0.3	1
1	A	48	LYS	CB	32.274	0.3	1
1	A	48	LYS	CG	24.867	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	LYS	CD	28.669	0.3	1
1	A	48	LYS	CE	41.768	0.3	1
1	A	48	LYS	H	7.64	0.020	1
1	A	48	LYS	HA	4.32	0.020	1
1	A	48	LYS	HB2	1.805	0.020	2
1	A	48	LYS	HB3	2.221	0.020	2
1	A	48	LYS	HG2	1.526	0.020	1
1	A	48	LYS	HG3	1.526	0.020	1
1	A	48	LYS	HD2	1.622	0.020	1
1	A	48	LYS	HD3	1.622	0.020	1
1	A	48	LYS	HE2	2.923	0.020	1
1	A	48	LYS	HE3	2.923	0.020	1
1	A	48	LYS	N	116.454	0.3	1
1	A	49	GLY	C	174.466	0.3	1
1	A	49	GLY	CA	45.178	0.3	1
1	A	49	GLY	H	7.628	0.020	1
1	A	49	GLY	HA2	3.645	0.020	2
1	A	49	GLY	HA3	4.551	0.020	2
1	A	49	GLY	N	106.188	0.3	1
1	A	50	LEU	C	174.715	0.3	1
1	A	50	LEU	CA	53.175	0.3	1
1	A	50	LEU	CB	43.165	0.3	1
1	A	50	LEU	CG	25.915	0.3	1
1	A	50	LEU	CD1	25.185	0.3	1
1	A	50	LEU	CD2	28.838	0.3	1
1	A	50	LEU	H	8.16	0.020	1
1	A	50	LEU	HA	4.589	0.020	1
1	A	50	LEU	HB2	1.443	0.020	2
1	A	50	LEU	HB3	1.213	0.020	2
1	A	50	LEU	HG	1.745	0.020	1
1	A	50	LEU	HD11	0.929	0.020	2
1	A	50	LEU	HD12	0.929	0.020	2
1	A	50	LEU	HD13	0.929	0.020	2
1	A	50	LEU	HD21	0.769	0.020	2
1	A	50	LEU	HD22	0.769	0.020	2
1	A	50	LEU	HD23	0.769	0.020	2
1	A	50	LEU	N	126.621	0.3	1
1	A	51	PRO	C	178.305	0.3	1
1	A	51	PRO	CA	63.009	0.3	1
1	A	51	PRO	CB	32.344	0.3	1
1	A	51	PRO	CG	28.141	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	PRO	CD	51.116	0.3	1
1	A	51	PRO	HA	4.438	0.020	1
1	A	51	PRO	HB2	2.5	0.020	2
1	A	51	PRO	HB3	1.708	0.020	2
1	A	51	PRO	HG2	2.035	0.020	1
1	A	51	PRO	HG3	2.035	0.020	1
1	A	51	PRO	HD2	4.261	0.020	2
1	A	51	PRO	HD3	3.372	0.020	2
1	A	51	PRO	N	96.741	0.3	1
1	A	52	GLU	C	178.39	0.3	1
1	A	52	GLU	CA	60.283	0.3	1
1	A	52	GLU	CB	29.792	0.3	1
1	A	52	GLU	CG	37.482	0.3	1
1	A	52	GLU	H	9.037	0.020	1
1	A	52	GLU	HA	3.874	0.020	1
1	A	52	GLU	HB2	2.085	0.020	1
1	A	52	GLU	HB3	2.085	0.020	1
1	A	52	GLU	HG2	2.349	0.020	1
1	A	52	GLU	HG3	2.349	0.020	1
1	A	52	GLU	N	126.556	0.3	1
1	A	53	GLU	C	177.166	0.3	1
1	A	53	GLU	CA	60.314	0.3	1
1	A	53	GLU	CB	29.161	0.3	1
1	A	53	GLU	CG	36.541	0.3	1
1	A	53	GLU	H	9.289	0.020	1
1	A	53	GLU	HA	3.874	0.020	1
1	A	53	GLU	HB2	2.153	0.020	2
1	A	53	GLU	HB3	1.921	0.020	2
1	A	53	GLU	HG2	2.337	0.020	2
1	A	53	GLU	HG3	2.201	0.020	2
1	A	53	GLU	N	116.478	0.3	1
1	A	54	ALA	C	179.183	0.3	1
1	A	54	ALA	CA	54.466	0.3	1
1	A	54	ALA	CB	17.535	0.3	1
1	A	54	ALA	H	6.768	0.020	1
1	A	54	ALA	HA	3.551	0.020	1
1	A	54	ALA	HB1	0.824	0.020	1
1	A	54	ALA	HB2	0.824	0.020	1
1	A	54	ALA	HB3	0.824	0.020	1
1	A	54	ALA	N	119.833	0.3	1
1	A	55	LEU	C	178.044	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	55	LEU	CA	58.236	0.3	1
1	A	55	LEU	CB	40.876	0.3	1
1	A	55	LEU	CG	27.108	0.3	1
1	A	55	LEU	CD1	23.883	0.3	1
1	A	55	LEU	CD2	25.519	0.3	1
1	A	55	LEU	H	7.23	0.020	1
1	A	55	LEU	HA	3.863	0.020	1
1	A	55	LEU	HB2	2.183	0.020	2
1	A	55	LEU	HB3	1.344	0.020	2
1	A	55	LEU	HG	1.366	0.020	1
1	A	55	LEU	HD11	0.829	0.020	2
1	A	55	LEU	HD12	0.829	0.020	2
1	A	55	LEU	HD13	0.829	0.020	2
1	A	55	LEU	HD21	0.875	0.020	2
1	A	55	LEU	HD22	0.875	0.020	2
1	A	55	LEU	HD23	0.875	0.020	2
1	A	55	LEU	N	116.451	0.3	1
1	A	56	TYR	C	177.86	0.3	1
1	A	56	TYR	CA	62.894	0.3	1
1	A	56	TYR	CB	38.603	0.3	1
1	A	56	TYR	CD1	131.765	0.3	1
1	A	56	TYR	CD2	131.765	0.3	1
1	A	56	TYR	CE1	118.038	0.3	1
1	A	56	TYR	CE2	118.038	0.3	1
1	A	56	TYR	H	8.392	0.020	1
1	A	56	TYR	HA	3.843	0.020	1
1	A	56	TYR	HB2	2.916	0.020	2
1	A	56	TYR	HB3	2.637	0.020	2
1	A	56	TYR	HD1	7.107	0.020	1
1	A	56	TYR	HD2	7.107	0.020	1
1	A	56	TYR	HE1	6.973	0.020	1
1	A	56	TYR	HE2	6.973	0.020	1
1	A	56	TYR	N	117.43	0.3	1
1	A	57	ARG	C	179.701	0.3	1
1	A	57	ARG	CA	60.501	0.3	1
1	A	57	ARG	CB	29.98	0.3	1
1	A	57	ARG	CG	29.058	0.3	1
1	A	57	ARG	CD	43.389	0.3	1
1	A	57	ARG	H	8.048	0.020	1
1	A	57	ARG	HA	3.551	0.020	1
1	A	57	ARG	HB2	1.737	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	ARG	HB3	1.737	0.020	1
1	A	57	ARG	HG2	1.271	0.020	2
1	A	57	ARG	HG3	1.072	0.020	2
1	A	57	ARG	HD2	3.168	0.020	2
1	A	57	ARG	HD3	2.855	0.020	2
1	A	57	ARG	N	119.423	0.3	1
1	A	58	ALA	C	178.571	0.3	1
1	A	58	ALA	CA	55.333	0.3	1
1	A	58	ALA	CB	18.301	0.3	1
1	A	58	ALA	H	7.876	0.020	1
1	A	58	ALA	HA	4.102	0.020	1
1	A	58	ALA	HB1	1.451	0.020	1
1	A	58	ALA	HB2	1.451	0.020	1
1	A	58	ALA	HB3	1.451	0.020	1
1	A	58	ALA	N	122.39	0.3	1
1	A	59	LEU	C	179.147	0.3	1
1	A	59	LEU	CA	57.603	0.3	1
1	A	59	LEU	CB	42.888	0.3	1
1	A	59	LEU	CG	26.412	0.3	1
1	A	59	LEU	CD1	24.739	0.3	1
1	A	59	LEU	CD2	23.89	0.3	1
1	A	59	LEU	H	8.613	0.020	1
1	A	59	LEU	HA	3.894	0.020	1
1	A	59	LEU	HB2	1.62	0.020	2
1	A	59	LEU	HB3	1.095	0.020	2
1	A	59	LEU	HG	1.539	0.020	1
1	A	59	LEU	HD11	0.455	0.020	2
1	A	59	LEU	HD12	0.455	0.020	2
1	A	59	LEU	HD13	0.455	0.020	2
1	A	59	LEU	HD21	0.719	0.020	2
1	A	59	LEU	HD22	0.719	0.020	2
1	A	59	LEU	HD23	0.719	0.020	2
1	A	59	LEU	N	118.836	0.3	1
1	A	60	ALA	C	179.102	0.3	1
1	A	60	ALA	CA	55.785	0.3	1
1	A	60	ALA	CB	17.754	0.3	1
1	A	60	ALA	H	8.283	0.020	1
1	A	60	ALA	HA	3.802	0.020	1
1	A	60	ALA	HB1	1.615	0.020	1
1	A	60	ALA	HB2	1.615	0.020	1
1	A	60	ALA	HB3	1.615	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	ALA	N	119.623	0.3	1
1	A	61	GLU	C	179.763	0.3	1
1	A	61	GLU	CA	59.321	0.3	1
1	A	61	GLU	CB	29.555	0.3	1
1	A	61	GLU	CG	36.049	0.3	1
1	A	61	GLU	H	7.638	0.020	1
1	A	61	GLU	HA	4.096	0.020	1
1	A	61	GLU	HB2	2.214	0.020	2
1	A	61	GLU	HB3	2.098	0.020	2
1	A	61	GLU	HG2	2.465	0.020	1
1	A	61	GLU	HG3	2.465	0.020	1
1	A	61	GLU	N	118.162	0.3	1
1	A	62	GLN	C	177.731	0.3	1
1	A	62	GLN	CA	59.011	0.3	1
1	A	62	GLN	CB	29.327	0.3	1
1	A	62	GLN	CG	33.864	0.3	1
1	A	62	GLN	H	8.53	0.020	1
1	A	62	GLN	HA	3.948	0.020	1
1	A	62	GLN	HB2	2.207	0.020	2
1	A	62	GLN	HB3	2.043	0.020	2
1	A	62	GLN	HG2	2.37	0.020	1
1	A	62	GLN	HG3	2.37	0.020	1
1	A	62	GLN	HE21	7.293	0.020	1
1	A	62	GLN	HE22	6.982	0.020	1
1	A	62	GLN	N	118.886	0.3	1
1	A	62	GLN	NE2	112.692	0.3	1
1	A	63	LYS	C	176.196	0.3	1
1	A	63	LYS	CA	54.091	0.3	1
1	A	63	LYS	CB	32.519	0.3	1
1	A	63	LYS	CG	25.058	0.3	1
1	A	63	LYS	CD	29.071	0.3	1
1	A	63	LYS	CE	42.241	0.3	1
1	A	63	LYS	H	7.721	0.020	1
1	A	63	LYS	HA	4.45	0.020	1
1	A	63	LYS	HB2	1.649	0.020	2
1	A	63	LYS	HB3	1.955	0.020	2
1	A	63	LYS	HG2	1.524	0.020	1
1	A	63	LYS	HG3	1.524	0.020	1
1	A	63	LYS	HD2	1.677	0.020	1
1	A	63	LYS	HD3	1.677	0.020	1
1	A	63	LYS	HE2	2.994	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	63	LYS	HE3	2.994	0.020	1
1	A	63	LYS	N	113.515	0.3	1
1	A	64	GLY	C	174.528	0.3	1
1	A	64	GLY	CA	47.004	0.3	1
1	A	64	GLY	H	7.794	0.020	1
1	A	64	GLY	HA2	3.974	0.020	1
1	A	64	GLY	HA3	3.974	0.020	1
1	A	64	GLY	N	109.741	0.3	1
1	A	65	LEU	C	175.497	0.3	1
1	A	65	LEU	CA	52.992	0.3	1
1	A	65	LEU	CB	44.334	0.3	1
1	A	65	LEU	CG	27.444	0.3	1
1	A	65	LEU	CD1	27.056	0.3	1
1	A	65	LEU	CD2	25.124	0.3	1
1	A	65	LEU	H	8.593	0.020	1
1	A	65	LEU	HA	4.713	0.020	1
1	A	65	LEU	HB2	1.499	0.020	2
1	A	65	LEU	HB3	1.431	0.020	2
1	A	65	LEU	HG	1.602	0.020	1
1	A	65	LEU	HD11	0.784	0.020	2
1	A	65	LEU	HD12	0.784	0.020	2
1	A	65	LEU	HD13	0.784	0.020	2
1	A	65	LEU	HD21	0.803	0.020	2
1	A	65	LEU	HD22	0.803	0.020	2
1	A	65	LEU	HD23	0.803	0.020	2
1	A	65	LEU	N	119.47	0.3	1
1	A	66	GLU	C	175.709	0.3	1
1	A	66	GLU	CA	55.983	0.3	1
1	A	66	GLU	CB	31.1	0.3	1
1	A	66	GLU	CG	36.118	0.3	1
1	A	66	GLU	H	7.6	0.020	1
1	A	66	GLU	HA	4.505	0.020	1
1	A	66	GLU	HB2	1.955	0.020	2
1	A	66	GLU	HB3	1.746	0.020	2
1	A	66	GLU	HG2	2.214	0.020	1
1	A	66	GLU	HG3	2.214	0.020	1
1	A	66	GLU	N	120.319	0.3	1
1	A	67	PHE	C	174.351	0.3	1
1	A	67	PHE	CA	57.417	0.3	1
1	A	67	PHE	CB	40.565	0.3	1
1	A	67	PHE	CD1	131.042	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	67	PHE	CD2	131.042	0.3	1
1	A	67	PHE	CE1	131.352	0.3	1
1	A	67	PHE	CE2	131.352	0.3	1
1	A	67	PHE	H	8.967	0.020	1
1	A	67	PHE	HA	5.11	0.020	1
1	A	67	PHE	HB2	2.991	0.020	2
1	A	67	PHE	HB3	3.052	0.020	2
1	A	67	PHE	HD1	7.073	0.020	1
1	A	67	PHE	HD2	7.073	0.020	1
1	A	67	PHE	HE1	7.172	0.020	1
1	A	67	PHE	HE2	7.172	0.020	1
1	A	67	PHE	N	126.117	0.3	1
1	A	68	LEU	C	173.519	0.3	1
1	A	68	LEU	CA	53.017	0.3	1
1	A	68	LEU	CB	42.886	0.3	1
1	A	68	LEU	CG	26.361	0.3	1
1	A	68	LEU	CD1	24.804	0.3	1
1	A	68	LEU	CD2	24.614	0.3	1
1	A	68	LEU	H	8.409	0.020	1
1	A	68	LEU	HA	4.398	0.020	1
1	A	68	LEU	HB2	1.363	0.020	2
1	A	68	LEU	HB3	1.184	0.020	2
1	A	68	LEU	HG	1.333	0.020	1
1	A	68	LEU	HD11	0.479	0.020	2
1	A	68	LEU	HD12	0.479	0.020	2
1	A	68	LEU	HD13	0.479	0.020	2
1	A	68	LEU	HD21	0.544	0.020	2
1	A	68	LEU	HD22	0.544	0.020	2
1	A	68	LEU	HD23	0.544	0.020	2
1	A	68	LEU	N	130.952	0.3	1
1	A	69	GLU	C	176.304	0.3	1
1	A	69	GLU	CA	57.998	0.3	1
1	A	69	GLU	CB	30.089	0.3	1
1	A	69	GLU	CG	36.12	0.3	1
1	A	69	GLU	H	8.229	0.020	1
1	A	69	GLU	HA	3.761	0.020	1
1	A	69	GLU	HB2	2.039	0.020	2
1	A	69	GLU	HB3	1.922	0.020	1
1	A	69	GLU	HG2	2.344	0.020	1
1	A	69	GLU	HG3	2.344	0.020	1
1	A	69	GLU	N	122.724	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	70	SER	C	174.457	0.3	1
1	A	70	SER	CA	56.013	0.3	1
1	A	70	SER	CB	64.636	0.3	1
1	A	70	SER	H	7.409	0.020	1
1	A	70	SER	HA	4.663	0.020	1
1	A	70	SER	HB2	3.919	0.020	2
1	A	70	SER	HB3	3.597	0.020	2
1	A	70	SER	N	109.673	0.3	1
1	A	71	THR	C	175.33	0.3	1
1	A	71	THR	CA	60.852	0.3	1
1	A	71	THR	CB	68.811	0.3	1
1	A	71	THR	CG2	21.567	0.3	1
1	A	71	THR	H	8.703	0.020	1
1	A	71	THR	HA	4.319	0.020	1
1	A	71	THR	HB	4.404	0.020	1
1	A	71	THR	HG21	0.918	0.020	1
1	A	71	THR	HG22	0.918	0.020	1
1	A	71	THR	HG23	0.918	0.020	1
1	A	71	THR	N	112.594	0.3	1
1	A	72	GLU	C	177.315	0.3	1
1	A	72	GLU	CA	58.728	0.3	1
1	A	72	GLU	CB	29.36	0.3	1
1	A	72	GLU	CG	35.987	0.3	1
1	A	72	GLU	H	8.217	0.020	1
1	A	72	GLU	HA	4.008	0.020	1
1	A	72	GLU	HB2	1.921	0.020	1
1	A	72	GLU	HB3	1.921	0.020	1
1	A	72	GLU	HG2	2.235	0.020	1
1	A	72	GLU	HG3	2.235	0.020	1
1	A	72	GLU	N	124.323	0.3	1
1	A	73	GLY	C	174.079	0.3	1
1	A	73	GLY	CA	44.882	0.3	1
1	A	73	GLY	H	8.618	0.020	1
1	A	73	GLY	HA2	3.829	0.020	1
1	A	73	GLY	HA3	3.829	0.020	1
1	A	73	GLY	N	109.314	0.3	1
1	A	74	ILE	C	175.41	0.3	1
1	A	74	ILE	CA	61.251	0.3	1
1	A	74	ILE	CB	37.895	0.3	1
1	A	74	ILE	CG1	27.07	0.3	1
1	A	74	ILE	CG2	16.985	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	ILE	CD1	13.247	0.3	1
1	A	74	ILE	H	7.174	0.020	1
1	A	74	ILE	HA	3.863	0.020	1
1	A	74	ILE	HB	1.662	0.020	1
1	A	74	ILE	HG12	1.303	0.020	2
1	A	74	ILE	HG13	0.898	0.020	2
1	A	74	ILE	HG21	0.539	0.020	1
1	A	74	ILE	HG22	0.539	0.020	1
1	A	74	ILE	HG23	0.539	0.020	1
1	A	74	ILE	HD11	0.62	0.020	1
1	A	74	ILE	HD12	0.62	0.020	1
1	A	74	ILE	HD13	0.62	0.020	1
1	A	74	ILE	N	119.817	0.3	1
1	A	75	VAL	C	174.056	0.3	1
1	A	75	VAL	CA	59.249	0.3	1
1	A	75	VAL	CB	32.182	0.3	1
1	A	75	VAL	CG1	20.697	0.3	1
1	A	75	VAL	CG2	20.47	0.3	1
1	A	75	VAL	H	8.648	0.020	1
1	A	75	VAL	HA	4.32	0.020	1
1	A	75	VAL	HB	2.016	0.020	1
1	A	75	VAL	HG11	0.831	0.020	2
1	A	75	VAL	HG12	0.831	0.020	2
1	A	75	VAL	HG13	0.831	0.020	2
1	A	75	VAL	HG21	0.85	0.020	2
1	A	75	VAL	HG22	0.85	0.020	2
1	A	75	VAL	HG23	0.85	0.020	2
1	A	75	VAL	N	131.513	0.3	1
1	A	76	PRO	C	175.135	0.3	1
1	A	76	PRO	CA	62.645	0.3	1
1	A	76	PRO	CB	31.494	0.3	1
1	A	76	PRO	CG	27.285	0.3	1
1	A	76	PRO	CD	50.545	0.3	1
1	A	76	PRO	HA	4.291	0.020	1
1	A	76	PRO	HB2	2.044	0.020	2
1	A	76	PRO	HB3	1.867	0.020	2
1	A	76	PRO	HG2	1.435	0.020	1
1	A	76	PRO	HG3	1.435	0.020	1
1	A	76	PRO	HD2	3.728	0.020	2
1	A	76	PRO	HD3	3.631	0.020	2
1	A	76	PRO	N	137.173	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	ASP	C	176.441	0.3	1
1	A	77	ASP	CA	51.199	0.3	1
1	A	77	ASP	CB	42.533	0.3	1
1	A	77	ASP	H	8.018	0.020	1
1	A	77	ASP	HA	4.898	0.020	1
1	A	77	ASP	HB2	2.885	0.020	2
1	A	77	ASP	HB3	2.724	0.020	2
1	A	77	ASP	N	125.191	0.3	1
1	A	78	PRO	C	178.989	0.3	1
1	A	78	PRO	CA	64.81	0.3	1
1	A	78	PRO	CB	32.238	0.3	1
1	A	78	PRO	CG	27.316	0.3	1
1	A	78	PRO	CD	51.485	0.3	1
1	A	78	PRO	HA	4.38	0.020	1
1	A	78	PRO	HB2	2.393	0.020	2
1	A	78	PRO	HB3	1.989	0.020	2
1	A	78	PRO	HG2	2.114	0.020	2
1	A	78	PRO	HG3	2.03	0.020	2
1	A	78	PRO	HD2	4.201	0.020	2
1	A	78	PRO	HD3	4.001	0.020	2
1	A	78	PRO	N	99.66	0.3	1
1	A	79	SER	C	175.81	0.3	1
1	A	79	SER	CA	61.309	0.3	1
1	A	79	SER	CB	62.837	0.3	1
1	A	79	SER	H	8.595	0.020	1
1	A	79	SER	HA	4.272	0.020	1
1	A	79	SER	HB2	4.068	0.020	2
1	A	79	SER	HB3	3.965	0.020	2
1	A	79	SER	N	113.185	0.3	1
1	A	80	ALA	C	178.28	0.3	1
1	A	80	ALA	CA	53.089	0.3	1
1	A	80	ALA	CB	17.771	0.3	1
1	A	80	ALA	H	7.617	0.020	1
1	A	80	ALA	HA	4.181	0.020	1
1	A	80	ALA	HB1	0.728	0.020	1
1	A	80	ALA	HB2	0.728	0.020	1
1	A	80	ALA	HB3	0.728	0.020	1
1	A	80	ALA	N	123.105	0.3	1
1	A	81	ALA	C	178.851	0.3	1
1	A	81	ALA	CA	54.704	0.3	1
1	A	81	ALA	CB	17.253	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	ALA	H	7.177	0.020	1
1	A	81	ALA	HA	3.971	0.020	1
1	A	81	ALA	HB1	1.097	0.020	1
1	A	81	ALA	HB2	1.097	0.020	1
1	A	81	ALA	HB3	1.097	0.020	1
1	A	81	ALA	N	120.004	0.3	1
1	A	82	LEU	C	177.907	0.3	1
1	A	82	LEU	CA	55.971	0.3	1
1	A	82	LEU	CB	42.149	0.3	1
1	A	82	LEU	CG	26.58	0.3	1
1	A	82	LEU	CD1	24.991	0.3	1
1	A	82	LEU	CD2	23.811	0.3	1
1	A	82	LEU	H	6.981	0.020	1
1	A	82	LEU	HA	4.313	0.020	1
1	A	82	LEU	HB2	1.779	0.020	2
1	A	82	LEU	HB3	1.657	0.020	2
1	A	82	LEU	HG	1.894	0.020	1
1	A	82	LEU	HD11	0.943	0.020	2
1	A	82	LEU	HD12	0.943	0.020	2
1	A	82	LEU	HD13	0.943	0.020	2
1	A	82	LEU	HD21	0.951	0.020	2
1	A	82	LEU	HD22	0.951	0.020	2
1	A	82	LEU	HD23	0.951	0.020	2
1	A	82	LEU	N	112.466	0.3	1
1	A	83	LEU	C	176.817	0.3	1
1	A	83	LEU	CA	56.483	0.3	1
1	A	83	LEU	CB	42.15	0.3	1
1	A	83	LEU	CG	27.009	0.3	1
1	A	83	LEU	CD1	26.826	0.3	1
1	A	83	LEU	CD2	22.378	0.3	1
1	A	83	LEU	H	7.641	0.020	1
1	A	83	LEU	HA	4.126	0.020	1
1	A	83	LEU	HB2	1.839	0.020	2
1	A	83	LEU	HB3	1.533	0.020	2
1	A	83	LEU	HG	2.029	0.020	1
1	A	83	LEU	HD11	1.029	0.020	2
1	A	83	LEU	HD12	1.029	0.020	2
1	A	83	LEU	HD13	1.029	0.020	2
1	A	83	LEU	HD21	0.974	0.020	2
1	A	83	LEU	HD22	0.974	0.020	2
1	A	83	LEU	HD23	0.974	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	83	LEU	N	116.818	0.3	1
1	A	84	LEU	C	175.942	0.3	1
1	A	84	LEU	CA	53.278	0.3	1
1	A	84	LEU	CB	45.923	0.3	1
1	A	84	LEU	CG	27.132	0.3	1
1	A	84	LEU	CD1	26.003	0.3	1
1	A	84	LEU	CD2	25.596	0.3	1
1	A	84	LEU	H	7.454	0.020	1
1	A	84	LEU	HA	4.886	0.020	1
1	A	84	LEU	HB2	1.658	0.020	2
1	A	84	LEU	HB3	1.53	0.020	2
1	A	84	LEU	HG	1.604	0.020	1
1	A	84	LEU	HD11	0.902	0.020	2
1	A	84	LEU	HD12	0.902	0.020	2
1	A	84	LEU	HD13	0.902	0.020	2
1	A	84	LEU	HD21	0.952	0.020	2
1	A	84	LEU	HD22	0.952	0.020	2
1	A	84	LEU	HD23	0.952	0.020	2
1	A	84	LEU	N	116.583	0.3	1
1	A	85	LEU	C	179.002	0.3	1
1	A	85	LEU	CA	55.049	0.3	1
1	A	85	LEU	CB	42.649	0.3	1
1	A	85	LEU	CG	27.068	0.3	1
1	A	85	LEU	CD1	25.273	0.3	1
1	A	85	LEU	CD2	23.012	0.3	1
1	A	85	LEU	H	9.293	0.020	1
1	A	85	LEU	HA	4.381	0.020	1
1	A	85	LEU	HB2	1.727	0.020	2
1	A	85	LEU	HB3	1.727	0.020	1
1	A	85	LEU	HG	1.957	0.020	1
1	A	85	LEU	HD11	1.007	0.020	2
1	A	85	LEU	HD12	1.007	0.020	2
1	A	85	LEU	HD13	1.007	0.020	2
1	A	85	LEU	HD21	1.021	0.020	2
1	A	85	LEU	HD22	1.021	0.020	2
1	A	85	LEU	HD23	1.021	0.020	2
1	A	85	LEU	N	123.544	0.3	1
1	A	86	ARG	C	177.283	0.3	1
1	A	86	ARG	CA	59.808	0.3	1
1	A	86	ARG	CB	29.934	0.3	1
1	A	86	ARG	CG	27.517	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	ARG	CD	43.49	0.3	1
1	A	86	ARG	H	8.918	0.020	1
1	A	86	ARG	HA	3.11	0.020	1
1	A	86	ARG	HB2	1.737	0.020	1
1	A	86	ARG	HB3	1.737	0.020	2
1	A	86	ARG	HG2	1.306	0.020	1
1	A	86	ARG	HG3	1.306	0.020	1
1	A	86	ARG	N	124.378	0.3	1
1	A	87	SER	C	177.557	0.3	1
1	A	87	SER	CA	61.014	0.3	1
1	A	87	SER	CB	61.993	0.3	1
1	A	87	SER	H	8.089	0.020	1
1	A	87	SER	HA	4.061	0.020	1
1	A	87	SER	HB2	3.879	0.020	1
1	A	87	SER	HB3	3.879	0.020	1
1	A	87	SER	N	108.819	0.3	1
1	A	88	ASP	C	176.973	0.3	1
1	A	88	ASP	CA	57.455	0.3	1
1	A	88	ASP	CB	41.362	0.3	1
1	A	88	ASP	H	7.069	0.020	1
1	A	88	ASP	HA	4.689	0.020	1
1	A	88	ASP	HB2	2.896	0.020	2
1	A	88	ASP	HB3	2.589	0.020	2
1	A	88	ASP	N	123.9	0.3	1
1	A	89	ALA	C	180.386	0.3	1
1	A	89	ALA	CA	56.165	0.3	1
1	A	89	ALA	CB	18.76	0.3	1
1	A	89	ALA	H	8.513	0.020	1
1	A	89	ALA	HA	4.483	0.020	1
1	A	89	ALA	HB1	1.633	0.020	1
1	A	89	ALA	HB2	1.633	0.020	1
1	A	89	ALA	HB3	1.633	0.020	1
1	A	89	ALA	N	125.221	0.3	1
1	A	90	LEU	C	179.394	0.3	1
1	A	90	LEU	CA	57.459	0.3	1
1	A	90	LEU	CB	42.5	0.3	1
1	A	90	LEU	CG	26.788	0.3	1
1	A	90	LEU	CD1	23.697	0.3	1
1	A	90	LEU	CD2	24.607	0.3	1
1	A	90	LEU	H	7.969	0.020	1
1	A	90	LEU	HA	3.929	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	90	LEU	HB2	1.601	0.020	1
1	A	90	LEU	HB3	1.601	0.020	1
1	A	90	LEU	HG	1.451	0.020	1
1	A	90	LEU	HD11	0.711	0.020	2
1	A	90	LEU	HD12	0.711	0.020	2
1	A	90	LEU	HD13	0.711	0.020	2
1	A	90	LEU	HD21	0.681	0.020	2
1	A	90	LEU	HD22	0.681	0.020	2
1	A	90	LEU	HD23	0.681	0.020	2
1	A	90	LEU	N	114.275	0.3	1
1	A	91	ARG	C	177.692	0.3	1
1	A	91	ARG	CA	58.859	0.3	1
1	A	91	ARG	CB	29.884	0.3	1
1	A	91	ARG	CG	26.29	0.3	1
1	A	91	ARG	CD	43.393	0.3	1
1	A	91	ARG	H	7.664	0.020	1
1	A	91	ARG	HA	3.779	0.020	1
1	A	91	ARG	HB2	1.737	0.020	2
1	A	91	ARG	HB3	1.401	0.020	2
1	A	91	ARG	HG2	0.896	0.020	1
1	A	91	ARG	HG3	0.896	0.020	1
1	A	91	ARG	HD2	2.767	0.020	1
1	A	91	ARG	HD3	2.767	0.020	1
1	A	91	ARG	N	119.242	0.3	1
1	A	92	TYR	C	174.259	0.3	1
1	A	92	TYR	CA	56.732	0.3	1
1	A	92	TYR	CB	38.309	0.3	1
1	A	92	TYR	CD1	132.114	0.3	1
1	A	92	TYR	CD2	132.114	0.3	1
1	A	92	TYR	CE1	117.915	0.3	1
1	A	92	TYR	CE2	117.915	0.3	1
1	A	92	TYR	H	7.981	0.020	1
1	A	92	TYR	HA	4.006	0.020	1
1	A	92	TYR	HB2	2.425	0.020	2
1	A	92	TYR	HB3	3.093	0.020	2
1	A	92	TYR	HD1	6.735	0.020	1
1	A	92	TYR	HD2	6.735	0.020	1
1	A	92	TYR	HE1	6.632	0.020	1
1	A	92	TYR	HE2	6.632	0.020	1
1	A	92	TYR	N	114.266	0.3	1
1	A	93	GLY	C	173.468	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	GLY	CA	47.448	0.3	1
1	A	93	GLY	H	7.254	0.020	1
1	A	93	GLY	HA2	3.341	0.020	1
1	A	93	GLY	HA3	3.341	0.020	1
1	A	93	GLY	N	110.308	0.3	1
1	A	94	ALA	C	174.456	0.3	1
1	A	94	ALA	CA	50.33	0.3	1
1	A	94	ALA	CB	24.904	0.3	1
1	A	94	ALA	H	8.981	0.020	1
1	A	94	ALA	HA	5.633	0.020	1
1	A	94	ALA	HB1	1.199	0.020	1
1	A	94	ALA	HB2	1.199	0.020	1
1	A	94	ALA	HB3	1.199	0.020	1
1	A	94	ALA	N	120.937	0.3	1
1	A	95	VAL	C	174.133	0.3	1
1	A	95	VAL	CA	58.629	0.3	1
1	A	95	VAL	CB	35.527	0.3	1
1	A	95	VAL	CG1	21.94	0.3	1
1	A	95	VAL	CG2	21.94	0.3	1
1	A	95	VAL	H	8.989	0.020	1
1	A	95	VAL	HA	5.012	0.020	1
1	A	95	VAL	HB	1.919	0.020	1
1	A	95	VAL	HG11	0.619	0.020	2
1	A	95	VAL	HG12	0.619	0.020	2
1	A	95	VAL	HG13	0.619	0.020	2
1	A	95	VAL	HG21	0.768	0.020	2
1	A	95	VAL	HG22	0.768	0.020	2
1	A	95	VAL	HG23	0.768	0.020	2
1	A	95	VAL	N	116.975	0.3	1
1	A	96	PRO	C	176.565	0.3	1
1	A	96	PRO	CA	60.748	0.3	1
1	A	96	PRO	CB	31.764	0.3	1
1	A	96	PRO	CG	28.407	0.3	1
1	A	96	PRO	CD	52.194	0.3	1
1	A	96	PRO	HA	5.099	0.020	1
1	A	96	PRO	HB2	1.758	0.020	2
1	A	96	PRO	HB3	1.669	0.020	2
1	A	96	PRO	HG2	2.276	0.020	2
1	A	96	PRO	HG3	1.582	0.020	2
1	A	96	PRO	HD2	4.179	0.020	2
1	A	96	PRO	HD3	3.983	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	PRO	N	99.545	0.3	1
1	A	97	ILE	C	176.363	0.3	1
1	A	97	ILE	CA	61.506	0.3	1
1	A	97	ILE	CB	40.586	0.3	1
1	A	97	ILE	CG1	26.369	0.3	1
1	A	97	ILE	CG2	19.691	0.3	1
1	A	97	ILE	CD1	13.246	0.3	1
1	A	97	ILE	H	8.533	0.020	1
1	A	97	ILE	HA	4.524	0.020	1
1	A	97	ILE	HB	1.73	0.020	1
1	A	97	ILE	HG12	1.184	0.020	2
1	A	97	ILE	HG13	0.65	0.020	2
1	A	97	ILE	HG21	0.769	0.020	1
1	A	97	ILE	HG22	0.769	0.020	1
1	A	97	ILE	HG23	0.769	0.020	1
1	A	97	ILE	HD11	0.46	0.020	1
1	A	97	ILE	HD12	0.46	0.020	1
1	A	97	ILE	HD13	0.46	0.020	1
1	A	97	ILE	N	112.507	0.3	1
1	A	98	GLY	C	184.536	0.3	1
1	A	98	GLY	CA	45.345	0.3	1
1	A	98	GLY	H	7.081	0.020	1
1	A	98	GLY	HA2	4.411	0.020	2
1	A	98	GLY	HA3	3.715	0.020	2
1	A	98	GLY	N	109.214	0.3	1
1	A	99	PHE	C	175.701	0.3	1
1	A	99	PHE	CA	56.096	0.3	1
1	A	99	PHE	CB	42.637	0.3	1
1	A	99	PHE	CD1	132.294	0.3	1
1	A	99	PHE	CD2	132.294	0.3	1
1	A	99	PHE	H	8.838	0.020	1
1	A	99	PHE	HA	5.509	0.020	1
1	A	99	PHE	HB2	2.821	0.020	2
1	A	99	PHE	HB3	2.821	0.020	1
1	A	99	PHE	HD1	7.029	0.020	1
1	A	99	PHE	HD2	7.029	0.020	1
1	A	99	PHE	N	118.086	0.3	1
1	A	100	GLN	C	175.763	0.3	1
1	A	100	GLN	CA	55.116	0.3	1
1	A	100	GLN	CB	31.494	0.3	1
1	A	100	GLN	CG	33.958	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	GLN	H	9.054	0.020	1
1	A	100	GLN	HA	4.484	0.020	1
1	A	100	GLN	HB2	1.894	0.020	1
1	A	100	GLN	HB3	1.894	0.020	1
1	A	100	GLN	HG2	2.262	0.020	1
1	A	100	GLN	HG3	2.262	0.020	1
1	A	100	GLN	HE21	7.527	0.020	1
1	A	100	GLN	HE22	6.706	0.020	1
1	A	100	GLN	N	121.171	0.3	1
1	A	100	GLN	NE2	111.423	0.3	1
1	A	101	ASN	C	174.932	0.3	1
1	A	101	ASN	CA	54.443	0.3	1
1	A	101	ASN	CB	37.725	0.3	1
1	A	101	ASN	H	9.456	0.020	1
1	A	101	ASN	HA	4.37	0.020	1
1	A	101	ASN	HB2	3.093	0.020	2
1	A	101	ASN	HB3	2.773	0.020	2
1	A	101	ASN	HD21	7.598	0.020	1
1	A	101	ASN	HD22	6.815	0.020	1
1	A	101	ASN	N	125.634	0.3	1
1	A	101	ASN	ND2	112.93	0.3	1
1	A	102	GLY	C	174.079	0.3	1
1	A	102	GLY	CA	45.305	0.3	1
1	A	102	GLY	H	8.616	0.020	1
1	A	102	GLY	HA2	4.178	0.020	2
1	A	102	GLY	HA3	3.619	0.020	2
1	A	102	GLY	N	103.924	0.3	1
1	A	103	GLU	C	175.585	0.3	1
1	A	103	GLU	CA	54.562	0.3	1
1	A	103	GLU	CB	31.32	0.3	1
1	A	103	GLU	CG	36.233	0.3	1
1	A	103	GLU	H	7.981	0.020	1
1	A	103	GLU	HA	4.481	0.020	1
1	A	103	GLU	HB2	2.084	0.020	2
1	A	103	GLU	HB3	1.616	0.020	2
1	A	103	GLU	HG2	2.207	0.020	2
1	A	103	GLU	HG3	1.928	0.020	2
1	A	103	GLU	N	120.603	0.3	1
1	A	104	VAL	C	174.226	0.3	1
1	A	104	VAL	CA	60.731	0.3	1
1	A	104	VAL	CB	32.725	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	VAL	CG1	20.785	0.3	1
1	A	104	VAL	CG2	21.867	0.3	1
1	A	104	VAL	H	8.397	0.020	1
1	A	104	VAL	HA	4.281	0.020	1
1	A	104	VAL	HB	1.819	0.020	1
1	A	104	VAL	HG11	0.761	0.020	2
1	A	104	VAL	HG12	0.761	0.020	2
1	A	104	VAL	HG13	0.761	0.020	2
1	A	104	VAL	HG21	0.797	0.020	2
1	A	104	VAL	HG22	0.797	0.020	2
1	A	104	VAL	HG23	0.797	0.020	2
1	A	104	VAL	N	122.338	0.3	1
1	A	105	GLU	C	175.87	0.3	1
1	A	105	GLU	CA	55.447	0.3	1
1	A	105	GLU	CB	31.205	0.3	1
1	A	105	GLU	CG	37.023	0.3	1
1	A	105	GLU	H	8.79	0.020	1
1	A	105	GLU	HA	4.865	0.020	1
1	A	105	GLU	HB2	1.914	0.020	2
1	A	105	GLU	HB3	1.683	0.020	2
1	A	105	GLU	HG2	2.192	0.020	2
1	A	105	GLU	HG3	1.969	0.020	2
1	A	105	GLU	N	127.407	0.3	1
1	A	106	VAL	C	173.898	0.3	1
1	A	106	VAL	CA	60.626	0.3	1
1	A	106	VAL	CB	34.591	0.3	1
1	A	106	VAL	CG1	22.292	0.3	1
1	A	106	VAL	CG2	21.769	0.3	1
1	A	106	VAL	H	8.854	0.020	1
1	A	106	VAL	HA	4.685	0.020	1
1	A	106	VAL	HB	1.743	0.020	1
1	A	106	VAL	HG11	0.842	0.020	2
1	A	106	VAL	HG12	0.842	0.020	2
1	A	106	VAL	HG13	0.842	0.020	2
1	A	106	VAL	HG21	0.53	0.020	2
1	A	106	VAL	HG22	0.53	0.020	2
1	A	106	VAL	HG23	0.53	0.020	2
1	A	106	VAL	N	124.077	0.3	1
1	A	107	VAL	C	175.244	0.3	1
1	A	107	VAL	CA	61.735	0.3	1
1	A	107	VAL	CB	32.244	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	107	VAL	CG1	23.073	0.3	1
1	A	107	VAL	CG2	22.028	0.3	1
1	A	107	VAL	H	8.95	0.020	1
1	A	107	VAL	HA	4.66	0.020	1
1	A	107	VAL	HB	2.071	0.020	1
1	A	107	VAL	HG11	0.947	0.020	2
1	A	107	VAL	HG12	0.947	0.020	2
1	A	107	VAL	HG13	0.947	0.020	2
1	A	107	VAL	HG21	0.763	0.020	2
1	A	107	VAL	HG22	0.763	0.020	2
1	A	107	VAL	HG23	0.763	0.020	2
1	A	107	VAL	N	126.967	0.3	1
1	A	108	LEU	C	176.717	0.3	1
1	A	108	LEU	CA	53.326	0.3	1
1	A	108	LEU	CB	44.161	0.3	1
1	A	108	LEU	CG	27.295	0.3	1
1	A	108	LEU	CD1	25.656	0.3	1
1	A	108	LEU	CD2	23.135	0.3	1
1	A	108	LEU	H	9.57	0.020	1
1	A	108	LEU	HA	6.01	0.020	1
1	A	108	LEU	HB2	1.908	0.020	2
1	A	108	LEU	HB3	1.758	0.020	2
1	A	108	LEU	HG	2.092	0.020	1
1	A	108	LEU	HD11	0.76	0.020	2
1	A	108	LEU	HD12	0.76	0.020	2
1	A	108	LEU	HD13	0.76	0.020	2
1	A	108	LEU	HD21	1.045	0.020	2
1	A	108	LEU	HD22	1.045	0.020	2
1	A	108	LEU	HD23	1.045	0.020	2
1	A	108	LEU	N	129.294	0.3	1
1	A	109	SER	C	175.373	0.3	1
1	A	109	SER	CA	57.338	0.3	1
1	A	109	SER	CB	63.998	0.3	1
1	A	109	SER	H	8.478	0.020	1
1	A	109	SER	HA	4.912	0.020	1
1	A	109	SER	HB2	3.516	0.020	2
1	A	109	SER	HB3	2.562	0.020	2
1	A	109	SER	N	111.982	0.3	1
1	A	110	ASP	C	175.625	0.3	1
1	A	110	ASP	CA	51.087	0.3	1
1	A	110	ASP	CB	43.657	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	110	ASP	H	8.063	0.020	1
1	A	110	ASP	HA	4.899	0.020	1
1	A	110	ASP	HB2	2.715	0.020	2
1	A	110	ASP	HB3	2.522	0.020	2
1	A	110	ASP	N	121.898	0.3	1
1	A	111	PRO	C	177.056	0.3	1
1	A	111	PRO	CA	64.048	0.3	1
1	A	111	PRO	CB	32.219	0.3	1
1	A	111	PRO	CG	27.135	0.3	1
1	A	111	PRO	CD	50.53	0.3	1
1	A	111	PRO	HA	4.058	0.020	1
1	A	111	PRO	HB2	1.991	0.020	1
1	A	111	PRO	HB3	1.991	0.020	1
1	A	111	PRO	HG2	1.969	0.020	2
1	A	111	PRO	HG3	1.69	0.020	2
1	A	111	PRO	HD2	3.45	0.020	2
1	A	111	PRO	HD3	4.025	0.020	2
1	A	111	PRO	N	134.486	0.3	1
1	A	112	ARG	C	177.373	0.3	1
1	A	112	ARG	CA	58.343	0.3	1
1	A	112	ARG	CB	29.588	0.3	1
1	A	112	ARG	CG	26.256	0.3	1
1	A	112	ARG	CD	43.394	0.3	1
1	A	112	ARG	H	8.555	0.020	1
1	A	112	ARG	HA	4.053	0.020	1
1	A	112	ARG	HB2	1.514	0.020	1
1	A	112	ARG	HB3	1.514	0.020	1
1	A	112	ARG	HG2	1.259	0.020	2
1	A	112	ARG	HG3	1.121	0.020	2
1	A	112	ARG	HD2	3.039	0.020	1
1	A	112	ARG	HD3	3.039	0.020	1
1	A	112	ARG	N	118.204	0.3	1
1	A	113	HIS	C	174.468	0.3	1
1	A	113	HIS	CA	55.35	0.3	1
1	A	113	HIS	CB	31.67	0.3	1
1	A	113	HIS	CD2	119.446	0.3	1
1	A	113	HIS	CE1	138.34	0.3	1
1	A	113	HIS	H	6.973	0.020	1
1	A	113	HIS	HA	5.091	0.020	1
1	A	113	HIS	HB2	3.607	0.020	2
1	A	113	HIS	HB3	2.998	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	HIS	HD2	7.084	0.020	1
1	A	113	HIS	HE1	7.829	0.020	1
1	A	113	HIS	N	114.29	0.3	1
1	A	114	LYS	C	176.324	0.3	1
1	A	114	LYS	CA	60.976	0.3	1
1	A	114	LYS	CB	32.512	0.3	1
1	A	114	LYS	CG	22.973	0.3	1
1	A	114	LYS	CD	30.005	0.3	1
1	A	114	LYS	CE	41.882	0.3	1
1	A	114	LYS	H	7.183	0.020	1
1	A	114	LYS	HA	3.164	0.020	1
1	A	114	LYS	HB2	1.379	0.020	2
1	A	114	LYS	HB3	1.424	0.020	2
1	A	114	LYS	HG2	0.444	0.020	2
1	A	114	LYS	HG3	0.186	0.020	2
1	A	114	LYS	HD2	1.295	0.020	1
1	A	114	LYS	HD3	1.295	0.020	1
1	A	114	LYS	HE2	2.727	0.020	1
1	A	114	LYS	HE3	2.727	0.020	1
1	A	114	LYS	N	119.485	0.3	1
1	A	115	GLU	C	178.936	0.3	1
1	A	115	GLU	CA	60.403	0.3	1
1	A	115	GLU	CB	28.268	0.3	1
1	A	115	GLU	CG	37.113	0.3	1
1	A	115	GLU	H	8.549	0.020	1
1	A	115	GLU	HA	3.895	0.020	1
1	A	115	GLU	HB2	2.041	0.020	2
1	A	115	GLU	HB3	1.926	0.020	2
1	A	115	GLU	HG2	2.376	0.020	2
1	A	115	GLU	HG3	2.221	0.020	2
1	A	115	GLU	N	116.576	0.3	1
1	A	116	ALA	C	180.724	0.3	1
1	A	116	ALA	CA	54.69	0.3	1
1	A	116	ALA	CB	18.013	0.3	1
1	A	116	ALA	H	8.024	0.020	1
1	A	116	ALA	HA	3.962	0.020	1
1	A	116	ALA	HB1	1.122	0.020	1
1	A	116	ALA	HB2	1.122	0.020	1
1	A	116	ALA	HB3	1.122	0.020	1
1	A	116	ALA	N	122.337	0.3	1
1	A	117	VAL	C	177.522	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	117	VAL	CA	66.204	0.3	1
1	A	117	VAL	CB	31.139	0.3	1
1	A	117	VAL	CG1	22.029	0.3	1
1	A	117	VAL	CG2	24.824	0.3	1
1	A	117	VAL	H	7.846	0.020	1
1	A	117	VAL	HA	3.361	0.020	1
1	A	117	VAL	HB	2.126	0.020	1
1	A	117	VAL	HG11	0.997	0.020	2
1	A	117	VAL	HG12	0.997	0.020	2
1	A	117	VAL	HG13	0.997	0.020	2
1	A	117	VAL	HG21	0.896	0.020	2
1	A	117	VAL	HG22	0.896	0.020	2
1	A	117	VAL	HG23	0.896	0.020	2
1	A	117	VAL	N	117.661	0.3	1
1	A	118	ALA	C	181.024	0.3	1
1	A	118	ALA	CA	55.906	0.3	1
1	A	118	ALA	CB	18.007	0.3	1
1	A	118	ALA	H	8.653	0.020	1
1	A	118	ALA	HA	4.224	0.020	1
1	A	118	ALA	HB1	1.667	0.020	1
1	A	118	ALA	HB2	1.667	0.020	1
1	A	118	ALA	HB3	1.667	0.020	1
1	A	118	ALA	N	122.832	0.3	1
1	A	119	GLN	C	177.845	0.3	1
1	A	119	GLN	CA	58.248	0.3	1
1	A	119	GLN	CB	28.554	0.3	1
1	A	119	GLN	CG	34.081	0.3	1
1	A	119	GLN	H	7.839	0.020	1
1	A	119	GLN	HA	4.121	0.020	1
1	A	119	GLN	HB2	2.126	0.020	1
1	A	119	GLN	HB3	2.126	0.020	1
1	A	119	GLN	HG2	2.528	0.020	2
1	A	119	GLN	HG3	2.405	0.020	2
1	A	119	GLN	HE21	7.255	0.020	1
1	A	119	GLN	HE22	6.31	0.020	1
1	A	119	GLN	N	116.57	0.3	1
1	A	119	GLN	NE2	108.262	0.3	1
1	A	120	LEU	C	179.256	0.3	1
1	A	120	LEU	CA	57.215	0.3	1
1	A	120	LEU	CB	42.88	0.3	1
1	A	120	LEU	CG	26.824	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	LEU	CD1	24.938	0.3	1
1	A	120	LEU	CD2	24.042	0.3	1
1	A	120	LEU	H	7.529	0.020	1
1	A	120	LEU	HA	4.143	0.020	1
1	A	120	LEU	HB2	1.805	0.020	2
1	A	120	LEU	HB3	1.613	0.020	2
1	A	120	LEU	HG	1.717	0.020	1
1	A	120	LEU	HD11	0.848	0.020	2
1	A	120	LEU	HD12	0.848	0.020	2
1	A	120	LEU	HD13	0.848	0.020	2
1	A	120	LEU	HD21	0.884	0.020	2
1	A	120	LEU	HD22	0.884	0.020	2
1	A	120	LEU	HD23	0.884	0.020	2
1	A	120	LEU	N	119.915	0.3	1
1	A	121	LEU	C	177.887	0.3	1
1	A	121	LEU	CA	56.704	0.3	1
1	A	121	LEU	CB	43.043	0.3	1
1	A	121	LEU	CG	27.316	0.3	1
1	A	121	LEU	CD1	27.306	0.3	1
1	A	121	LEU	CD2	23.811	0.3	1
1	A	121	LEU	H	8.115	0.020	1
1	A	121	LEU	HA	4.123	0.020	1
1	A	121	LEU	HB2	2.0	0.020	2
1	A	121	LEU	HB3	1.315	0.020	2
1	A	121	LEU	HG	1.908	0.020	1
1	A	121	LEU	HD11	0.725	0.020	2
1	A	121	LEU	HD12	0.725	0.020	2
1	A	121	LEU	HD13	0.725	0.020	2
1	A	121	LEU	HD21	0.779	0.020	2
1	A	121	LEU	HD22	0.779	0.020	2
1	A	121	LEU	HD23	0.779	0.020	2
1	A	121	LEU	N	117.047	0.3	1
1	A	122	ASN	C	173.407	0.3	1
1	A	122	ASN	CA	53.802	0.3	1
1	A	122	ASN	CB	37.875	0.3	1
1	A	122	ASN	H	8.164	0.020	1
1	A	122	ASN	HA	4.436	0.020	1
1	A	122	ASN	HB2	3.213	0.020	2
1	A	122	ASN	HB3	2.527	0.020	2
1	A	122	ASN	HD21	7.474	0.020	1
1	A	122	ASN	HD22	6.743	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	ASN	N	113.79	0.3	1
1	A	122	ASN	ND2	110.941	0.3	1
1	A	123	ARG	C	172.532	0.3	1
1	A	123	ARG	CA	53.61	0.3	1
1	A	123	ARG	CB	30.537	0.3	1
1	A	123	ARG	CG	24.449	0.3	1
1	A	123	ARG	CD	44.157	0.3	1
1	A	123	ARG	H	7.289	0.020	1
1	A	123	ARG	HA	4.858	0.020	1
1	A	123	ARG	HB2	2.022	0.020	2
1	A	123	ARG	HB3	1.854	0.020	2
1	A	123	ARG	HG2	1.64	0.020	2
1	A	123	ARG	HG3	1.537	0.020	2
1	A	123	ARG	HD2	3.247	0.020	2
1	A	123	ARG	HD3	3.177	0.020	2
1	A	123	ARG	N	112.528	0.3	1
1	A	124	PRO	C	175.897	0.3	1
1	A	124	PRO	CA	64.389	0.3	1
1	A	124	PRO	CB	32.441	0.3	1
1	A	124	PRO	CG	27.844	0.3	1
1	A	124	PRO	CD	50.639	0.3	1
1	A	124	PRO	HA	4.393	0.020	1
1	A	124	PRO	HB2	2.453	0.020	2
1	A	124	PRO	HB3	1.955	0.020	2
1	A	124	PRO	HG2	2.21	0.020	1
1	A	124	PRO	HG3	2.21	0.020	1
1	A	124	PRO	HD2	3.852	0.020	2
1	A	124	PRO	HD3	3.739	0.020	2
1	A	124	PRO	N	134.789	0.3	1
1	A	125	ALA	C	174.645	0.3	1
1	A	125	ALA	CA	50.698	0.3	1
1	A	125	ALA	CB	23.031	0.3	1
1	A	125	ALA	H	8.139	0.020	1
1	A	125	ALA	HA	5.231	0.020	1
1	A	125	ALA	HB1	0.831	0.020	1
1	A	125	ALA	HB2	0.831	0.020	1
1	A	125	ALA	HB3	0.831	0.020	1
1	A	125	ALA	N	125.142	0.3	1
1	A	126	ARG	C	173.938	0.3	1
1	A	126	ARG	CA	54.45	0.3	1
1	A	126	ARG	CB	32.597	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	126	ARG	CG	26.561	0.3	1
1	A	126	ARG	CD	43.397	0.3	1
1	A	126	ARG	H	8.72	0.020	1
1	A	126	ARG	HA	4.474	0.020	1
1	A	126	ARG	HB2	1.657	0.020	2
1	A	126	ARG	HB3	1.587	0.020	2
1	A	126	ARG	HG2	1.437	0.020	2
1	A	126	ARG	HG3	1.285	0.020	2
1	A	126	ARG	HD2	3.153	0.020	1
1	A	126	ARG	HD3	3.153	0.020	1
1	A	126	ARG	N	122.384	0.3	1
1	A	127	PHE	C	174.967	0.3	1
1	A	127	PHE	CA	57.927	0.3	1
1	A	127	PHE	CB	42.733	0.3	1
1	A	127	PHE	CD1	132.17	0.3	1
1	A	127	PHE	CD2	132.17	0.3	1
1	A	127	PHE	H	8.457	0.020	1
1	A	127	PHE	HA	5.474	0.020	1
1	A	127	PHE	HB2	2.896	0.020	2
1	A	127	PHE	HB3	2.793	0.020	2
1	A	127	PHE	HD1	7.202	0.020	1
1	A	127	PHE	HD2	7.202	0.020	1
1	A	127	PHE	N	121.42	0.3	1
1	A	128	TYR	C	174.557	0.3	1
1	A	128	TYR	CA	55.384	0.3	1
1	A	128	TYR	CB	42.619	0.3	1
1	A	128	TYR	CD1	133.306	0.3	1
1	A	128	TYR	CD2	133.306	0.3	1
1	A	128	TYR	CE1	117.58	0.3	1
1	A	128	TYR	CE2	117.58	0.3	1
1	A	128	TYR	H	9.223	0.020	1
1	A	128	TYR	HA	5.458	0.020	1
1	A	128	TYR	HB2	2.991	0.020	2
1	A	128	TYR	HB3	2.734	0.020	2
1	A	128	TYR	HD1	6.871	0.020	1
1	A	128	TYR	HD2	6.871	0.020	1
1	A	128	TYR	HE1	6.588	0.020	1
1	A	128	TYR	HE2	6.588	0.020	1
1	A	128	TYR	N	120.935	0.3	1
1	A	129	LEU	C	173.153	0.3	1
1	A	129	LEU	CA	53.194	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	LEU	CB	46.416	0.3	1
1	A	129	LEU	CG	27.305	0.3	1
1	A	129	LEU	CD1	23.936	0.3	1
1	A	129	LEU	CD2	27.146	0.3	1
1	A	129	LEU	H	8.962	0.020	1
1	A	129	LEU	HA	5.382	0.020	1
1	A	129	LEU	HB2	1.894	0.020	2
1	A	129	LEU	HB3	1.279	0.020	2
1	A	129	LEU	HG	1.818	0.020	1
1	A	129	LEU	HD11	0.835	0.020	2
1	A	129	LEU	HD12	0.835	0.020	2
1	A	129	LEU	HD13	0.835	0.020	2
1	A	129	LEU	HD21	0.882	0.020	2
1	A	129	LEU	HD22	0.882	0.020	2
1	A	129	LEU	HD23	0.882	0.020	2
1	A	129	LEU	N	123.207	0.3	1
1	A	130	ALA	C	174.988	0.3	1
1	A	130	ALA	CA	49.521	0.3	1
1	A	130	ALA	CB	23.039	0.3	1
1	A	130	ALA	H	8.441	0.020	1
1	A	130	ALA	HA	4.878	0.020	1
1	A	130	ALA	HB1	1.213	0.020	1
1	A	130	ALA	HB2	1.213	0.020	1
1	A	130	ALA	HB3	1.213	0.020	1
1	A	130	ALA	N	126.168	0.3	1
1	A	131	LEU	C	176.493	0.3	1
1	A	131	LEU	CA	53.923	0.3	1
1	A	131	LEU	CB	40.723	0.3	1
1	A	131	LEU	CG	27.86	0.3	1
1	A	131	LEU	CD1	25.776	0.3	1
1	A	131	LEU	CD2	23.565	0.3	1
1	A	131	LEU	H	8.555	0.020	1
1	A	131	LEU	HA	3.905	0.020	1
1	A	131	LEU	HB2	1.604	0.020	1
1	A	131	LEU	HB3	1.604	0.020	1
1	A	131	LEU	HG	1.816	0.020	1
1	A	131	LEU	HD11	1.065	0.020	2
1	A	131	LEU	HD12	1.065	0.020	2
1	A	131	LEU	HD13	1.065	0.020	2
1	A	131	LEU	HD21	0.585	0.020	2
1	A	131	LEU	HD22	0.585	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	LEU	HD23	0.585	0.020	2
1	A	131	LEU	N	117.415	0.3	1
1	A	132	PRO	C	178.99	0.3	1
1	A	132	PRO	CA	67.015	0.3	1
1	A	132	PRO	CB	32.126	0.3	1
1	A	132	PRO	CG	27.87	0.3	1
1	A	132	PRO	CD	49.886	0.3	1
1	A	132	PRO	HA	4.241	0.020	1
1	A	132	PRO	HB2	2.458	0.020	2
1	A	132	PRO	HB3	2.026	0.020	2
1	A	132	PRO	HG2	2.245	0.020	2
1	A	132	PRO	HG3	2.119	0.020	2
1	A	132	PRO	HD2	3.467	0.020	1
1	A	132	PRO	HD3	3.467	0.020	1
1	A	132	PRO	N	134.99	0.3	1
1	A	133	GLN	C	178.179	0.3	1
1	A	133	GLN	CA	59.236	0.3	1
1	A	133	GLN	CB	27.813	0.3	1
1	A	133	GLN	CG	34.081	0.3	1
1	A	133	GLN	H	8.94	0.020	1
1	A	133	GLN	HA	4.196	0.020	1
1	A	133	GLN	HB2	2.032	0.020	2
1	A	133	GLN	HB3	2.104	0.020	2
1	A	133	GLN	HG2	2.507	0.020	2
1	A	133	GLN	HG3	2.46	0.020	2
1	A	133	GLN	HE21	7.558	0.020	1
1	A	133	GLN	HE22	6.892	0.020	1
1	A	133	GLN	N	116.087	0.3	1
1	A	133	GLN	NE2	112.395	0.3	1
1	A	134	ALA	C	180.455	0.3	1
1	A	134	ALA	CA	54.121	0.3	1
1	A	134	ALA	CB	18.96	0.3	1
1	A	134	ALA	H	6.943	0.020	1
1	A	134	ALA	HA	4.21	0.020	1
1	A	134	ALA	HB1	1.532	0.020	1
1	A	134	ALA	HB2	1.532	0.020	1
1	A	134	ALA	HB3	1.532	0.020	1
1	A	134	ALA	N	123.051	0.3	1
1	A	135	TRP	C	177.196	0.3	1
1	A	135	TRP	CA	63.521	0.3	1
1	A	135	TRP	CB	29.115	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	135	TRP	CD1	125.227	0.3	1
1	A	135	TRP	CE3	120.368	0.3	1
1	A	135	TRP	CZ2	114.745	0.3	1
1	A	135	TRP	CZ3	120.716	0.3	1
1	A	135	TRP	CH2	125.031	0.3	1
1	A	135	TRP	H	9.032	0.020	1
1	A	135	TRP	HA	3.55	0.020	1
1	A	135	TRP	HB2	2.862	0.020	1
1	A	135	TRP	HB3	2.862	0.020	1
1	A	135	TRP	HD1	6.693	0.020	1
1	A	135	TRP	HE1	8.693	0.020	1
1	A	135	TRP	HE3	7.377	0.020	1
1	A	135	TRP	HZ2	7.173	0.020	1
1	A	135	TRP	HZ3	6.706	0.020	1
1	A	135	TRP	HH2	6.329	0.020	1
1	A	135	TRP	N	120.807	0.3	1
1	A	135	TRP	NE1	128.694	0.3	1
1	A	136	GLU	C	178.428	0.3	1
1	A	136	GLU	CA	60.061	0.3	1
1	A	136	GLU	CB	29.329	0.3	1
1	A	136	GLU	CG	36.142	0.3	1
1	A	136	GLU	H	8.549	0.020	1
1	A	136	GLU	HA	3.761	0.020	1
1	A	136	GLU	HB2	2.322	0.020	2
1	A	136	GLU	HB3	2.194	0.020	2
1	A	136	GLU	HG2	2.582	0.020	2
1	A	136	GLU	HG3	2.5	0.020	2
1	A	136	GLU	N	118.385	0.3	1
1	A	137	GLU	C	178.588	0.3	1
1	A	137	GLU	CA	59.22	0.3	1
1	A	137	GLU	CB	29.475	0.3	1
1	A	137	GLU	CG	35.859	0.3	1
1	A	137	GLU	H	7.313	0.020	1
1	A	137	GLU	HA	3.96	0.020	1
1	A	137	GLU	HB2	2.071	0.020	2
1	A	137	GLU	HB3	2.01	0.020	2
1	A	137	GLU	HG2	2.419	0.020	2
1	A	137	GLU	HG3	2.276	0.020	2
1	A	137	GLU	N	117.533	0.3	1
1	A	138	LEU	C	177.908	0.3	1
1	A	138	LEU	CA	57.467	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	LEU	CB	41.671	0.3	1
1	A	138	LEU	CG	26.7	0.3	1
1	A	138	LEU	CD1	24.185	0.3	1
1	A	138	LEU	CD2	23.858	0.3	1
1	A	138	LEU	H	7.18	0.020	1
1	A	138	LEU	HA	3.83	0.020	1
1	A	138	LEU	HB2	1.431	0.020	1
1	A	138	LEU	HB3	1.431	0.020	1
1	A	138	LEU	HG	1.451	0.020	1
1	A	138	LEU	HD11	0.685	0.020	2
1	A	138	LEU	HD12	0.685	0.020	2
1	A	138	LEU	HD13	0.685	0.020	2
1	A	138	LEU	HD21	0.717	0.020	2
1	A	138	LEU	HD22	0.717	0.020	2
1	A	138	LEU	HD23	0.717	0.020	2
1	A	138	LEU	N	118.882	0.3	1
1	A	139	PHE	C	176.518	0.3	1
1	A	139	PHE	CA	62.059	0.3	1
1	A	139	PHE	CB	38.264	0.3	1
1	A	139	PHE	CD1	132.078	0.3	1
1	A	139	PHE	CD2	132.078	0.3	1
1	A	139	PHE	H	8.527	0.020	1
1	A	139	PHE	HA	3.589	0.020	1
1	A	139	PHE	HB2	2.46	0.020	2
1	A	139	PHE	HB3	1.317	0.020	2
1	A	139	PHE	HD1	6.899	0.020	1
1	A	139	PHE	HD2	6.899	0.020	1
1	A	139	PHE	N	120.761	0.3	1
1	A	140	ARG	C	177.915	0.3	1
1	A	140	ARG	CA	58.708	0.3	1
1	A	140	ARG	CB	30.317	0.3	1
1	A	140	ARG	CG	28.255	0.3	1
1	A	140	ARG	CD	43.882	0.3	1
1	A	140	ARG	H	7.829	0.020	1
1	A	140	ARG	HA	3.773	0.020	1
1	A	140	ARG	HB2	1.88	0.020	2
1	A	140	ARG	HB3	1.812	0.020	2
1	A	140	ARG	HG2	1.945	0.020	2
1	A	140	ARG	HG3	1.709	0.020	2
1	A	140	ARG	HD2	3.255	0.020	2
1	A	140	ARG	HD3	3.189	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	140	ARG	N	115.796	0.3	1
1	A	141	ARG	C	177.292	0.3	1
1	A	141	ARG	CA	57.865	0.3	1
1	A	141	ARG	CB	31.003	0.3	1
1	A	141	ARG	CG	28.048	0.3	1
1	A	141	ARG	CD	44.105	0.3	1
1	A	141	ARG	H	7.164	0.020	1
1	A	141	ARG	HA	4.074	0.020	1
1	A	141	ARG	HB2	1.778	0.020	2
1	A	141	ARG	HB3	1.71	0.020	2
1	A	141	ARG	HG2	1.843	0.020	2
1	A	141	ARG	HG3	1.57	0.020	2
1	A	141	ARG	HD2	3.243	0.020	2
1	A	141	ARG	HD3	3.107	0.020	2
1	A	141	ARG	N	115.242	0.3	1
1	A	142	ALA	C	176.426	0.3	1
1	A	142	ALA	CA	53.263	0.3	1
1	A	142	ALA	CB	20.528	0.3	1
1	A	142	ALA	H	7.953	0.020	1
1	A	142	ALA	HA	3.807	0.020	1
1	A	142	ALA	HB1	0.871	0.020	1
1	A	142	ALA	HB2	0.871	0.020	1
1	A	142	ALA	HB3	0.871	0.020	1
1	A	142	ALA	N	121.132	0.3	1
1	A	143	TYR	C	172.776	0.3	1
1	A	143	TYR	CA	55.106	0.3	1
1	A	143	TYR	CB	38.056	0.3	1
1	A	143	TYR	CD1	133.357	0.3	1
1	A	143	TYR	CD2	133.357	0.3	1
1	A	143	TYR	CE1	117.364	0.3	1
1	A	143	TYR	CE2	117.364	0.3	1
1	A	143	TYR	H	7.653	0.020	1
1	A	143	TYR	HA	4.639	0.020	1
1	A	143	TYR	HB2	2.463	0.020	2
1	A	143	TYR	HB3	1.88	0.020	2
1	A	143	TYR	HD1	6.806	0.020	1
1	A	143	TYR	HD2	6.806	0.020	1
1	A	143	TYR	HE1	6.803	0.020	1
1	A	143	TYR	HE2	6.803	0.020	1
1	A	143	TYR	N	113.866	0.3	1
1	A	144	PRO	C	177.314	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	144	PRO	CA	63.403	0.3	1
1	A	144	PRO	CB	32.1	0.3	1
1	A	144	PRO	CG	27.009	0.3	1
1	A	144	PRO	CD	50.009	0.3	1
1	A	144	PRO	HA	4.466	0.020	1
1	A	144	PRO	HB2	2.246	0.020	2
1	A	144	PRO	HB3	1.887	0.020	2
1	A	144	PRO	HG2	1.902	0.020	1
1	A	144	PRO	HG3	1.902	0.020	1
1	A	144	PRO	HD2	3.397	0.020	2
1	A	144	PRO	HD3	3.211	0.020	2
1	A	144	PRO	N	137.462	0.3	1
1	A	145	GLN	C	174.818	0.3	1
1	A	145	GLN	CA	56.501	0.3	1
1	A	145	GLN	CB	30.069	0.3	1
1	A	145	GLN	CG	34.118	0.3	1
1	A	145	GLN	H	8.398	0.020	1
1	A	145	GLN	HA	4.312	0.020	1
1	A	145	GLN	HB2	2.087	0.020	2
1	A	145	GLN	HB3	1.989	0.020	2
1	A	145	GLN	HG2	2.371	0.020	1
1	A	145	GLN	HG3	2.371	0.020	1
1	A	145	GLN	HE21	7.527	0.020	1
1	A	145	GLN	HE22	6.746	0.020	1
1	A	145	GLN	N	121.008	0.3	1
1	A	145	GLN	NE2	111.948	0.3	1
1	A	146	LYS	C	181.007	0.3	1
1	A	146	LYS	CA	57.725	0.3	1
1	A	146	LYS	CB	33.818	0.3	1
1	A	146	LYS	CG	24.682	0.3	1
1	A	146	LYS	CD	29.124	0.3	1
1	A	146	LYS	CE	42.199	0.3	1
1	A	146	LYS	H	7.864	0.020	1
1	A	146	LYS	HA	4.156	0.020	1
1	A	146	LYS	HB2	1.818	0.020	1
1	A	146	LYS	HB3	1.818	0.020	1
1	A	146	LYS	HG2	1.388	0.020	1
1	A	146	LYS	HG3	1.388	0.020	1
1	A	146	LYS	HD2	1.676	0.020	1
1	A	146	LYS	HD3	1.676	0.020	1
1	A	146	LYS	HE2	2.99	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	LYS	HE3	2.99	0.020	1
1	A	146	LYS	N	128.285	0.3	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	143	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_\beta$	131	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	143	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	143	0.00 ± 0.00	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1965. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/684 (0%)	0/278 (0%)	0/276 (0%)	0/130 (0%)
Sidechain	0/1174 (0%)	0/764 (0%)	0/361 (0%)	0/49 (0%)
Aromatic	0/107 (0%)	0/52 (0%)	0/52 (0%)	0/3 (0%)
Overall	0/1965 (0%)	0/1094 (0%)	0/689 (0%)	0/182 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2044. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/727 (0%)	0/297 (0%)	0/292 (0%)	0/138 (0%)
Sidechain	0/1210 (0%)	0/786 (0%)	0/373 (0%)	0/51 (0%)
Aromatic	0/107 (0%)	0/52 (0%)	0/52 (0%)	0/3 (0%)
Overall	0/2044 (0%)	0/1135 (0%)	0/717 (0%)	0/192 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules con-

taining 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	51	PRO	N	96.74	108.67 – 162.11	-7.2
1	A	96	PRO	N	99.55	108.67 – 162.11	-6.7
1	A	78	PRO	N	99.66	108.67 – 162.11	-6.7
1	A	98	GLY	C	184.54	164.92 – 182.89	5.9

7.1.5   Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:
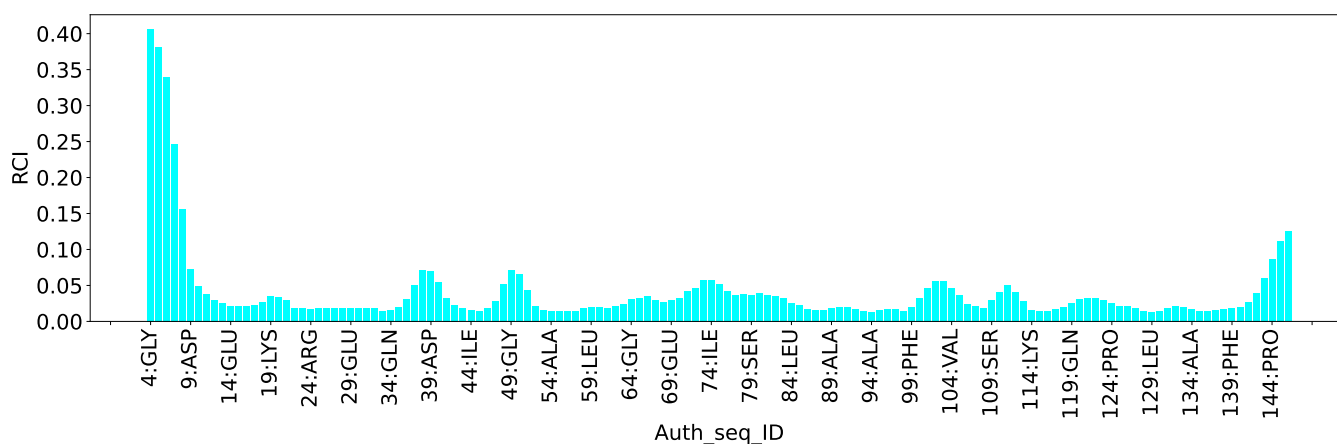
8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

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	2587
Intra-residue ($\|i-j\|=0$)	542
Sequential ($\|i-j\|=1$)	658
Medium range ($\|i-j\|>1$ and $\|i-j\|<5$)	607
Long range ($\|i-j\|\geq5$)	776
Inter-chain	0
Hydrogen bond restraints	4
Disulfide bond restraints	0
Total dihedral-angle restraints	232
Number of unmapped restraints	2819
Number of restraints per residue	19.3
Number of long range restraints per residue[1]	5.3

[1]Long 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 ⓘ

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 ⓘ

Distance violations less than 0.1 Å
are not included in the calculation.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations
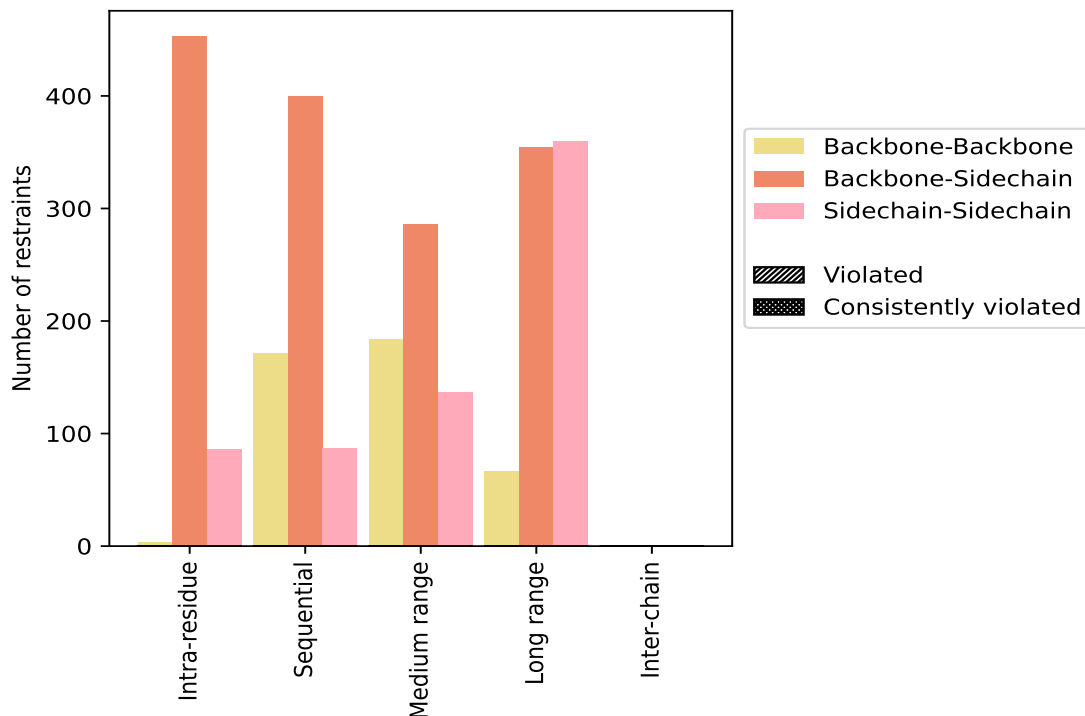
9 Distance violation analysis ⓘ

9.1 Summary of distance violations ⓘ

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)	542	21.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	453	17.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	86	3.3	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	658	25.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	171	6.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	400	15.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	87	3.4	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	607	23.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	184	7.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	286	11.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	137	5.3	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	776	30.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	66	2.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	350	13.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	360	13.9	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	4	0.2	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	2587	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	424	16.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1493	57.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	670	25.9	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 ⓘ

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 ⓘ

No violations found

9.3 Distance violation statistics for the ensemble ⓘ

No violations found

9.4 Most violated distance restraints in the ensemble ⓘ

No violations found

9.5 All violated distance restraints ⓘ

No violations found

10 Dihedral-angle violation analysis ⓘ

10.1 Summary of dihedral-angle violations ⓘ

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	$\%^2$	$\%^1$
PSI	116	50.0	0	0.0	0.0	0	0.0	0.0
PHI	116	50.0	0	0.0	0.0	0	0.0	0.0
Total	232	100.0	0	0.0	0.0	0	0.0	0.0

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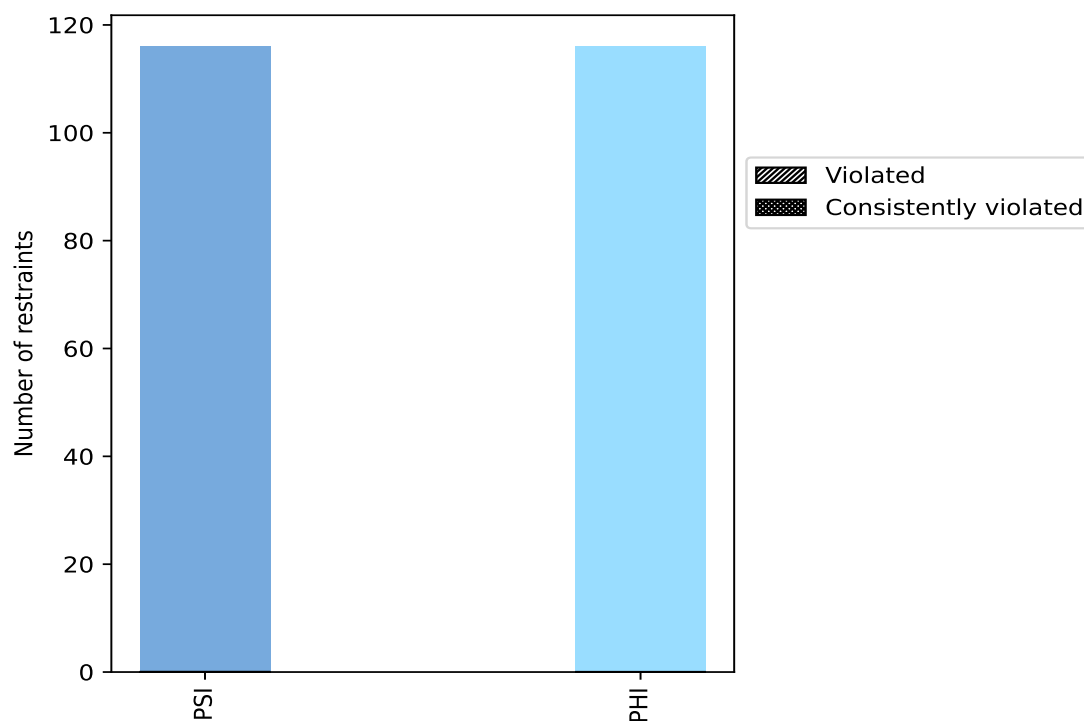
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

No violations found

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

No violations found

10.5 All violated dihedral-angle restraints ⓘ

No violations found