



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:59 AM BST

PDB ID : 2LCQ
Title : Solution structure of the endonuclease Nob1 from P.horikoshii
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Deposited on : 2011-05-05

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

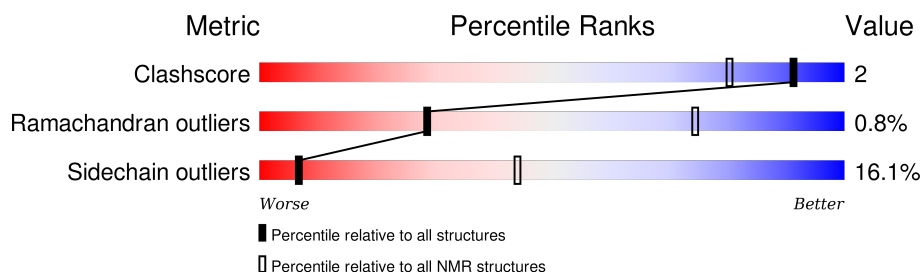
1 Overall quality at a glance

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	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	165	 75% 11% 12%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:7-A:116 (110)	0.25	8
2	A:127-A:157 (31)	0.23	3

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 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2600 atoms, of which 1338 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative toxin VapC6.

Mol	Chain	Residues	Atoms						Trace
1	A	161	Total	C	H	N	O	S	0
			2599	806	1338	217	233	5	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP O58440
A	-2	SER	-	EXPRESSION TAG	UNP O58440
A	-1	MET	-	EXPRESSION TAG	UNP O58440
A	0	GLY	-	EXPRESSION TAG	UNP O58440

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Putative toxin VapC6

Chain A: 



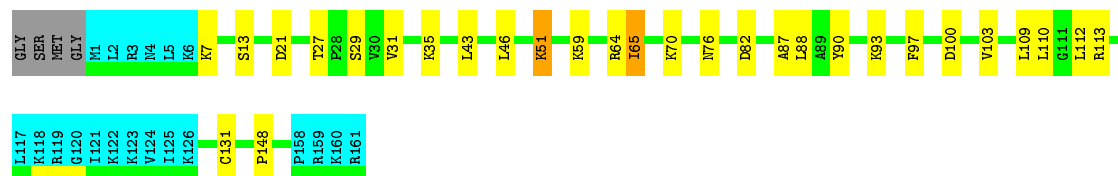
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Putative toxin VapC6

Chain A: 



4.2.2 Score per residue for model 2

- Molecule 1: Putative toxin VapC6

Chain A: 

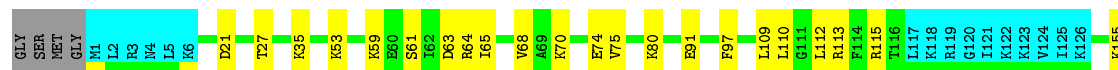




4.2.3 Score per residue for model 3

- Molecule 1: Putative toxin VapC6

Chain A: 72% 13% 12%



4.2.4 Score per residue for model 4

- Molecule 1: Putative toxin VapC6

Chain A: 71% 14% 12%



4.2.5 Score per residue for model 5

- Molecule 1: Putative toxin VapC6

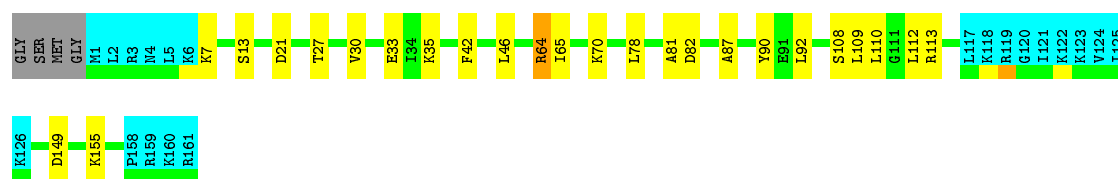
Chain A: 65% 19% 12%



4.2.6 Score per residue for model 6

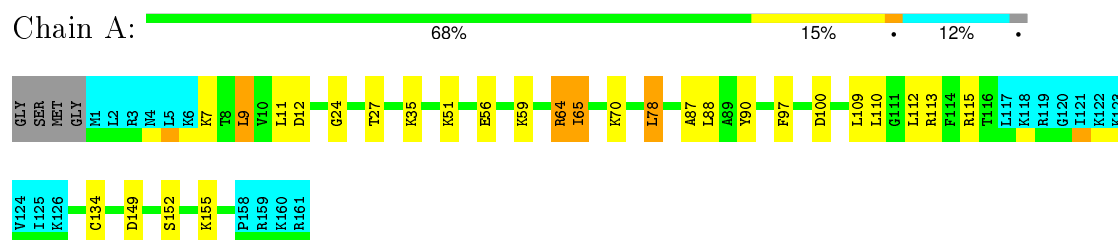
- Molecule 1: Putative toxin VapC6

Chain A: 70% 15% 12%



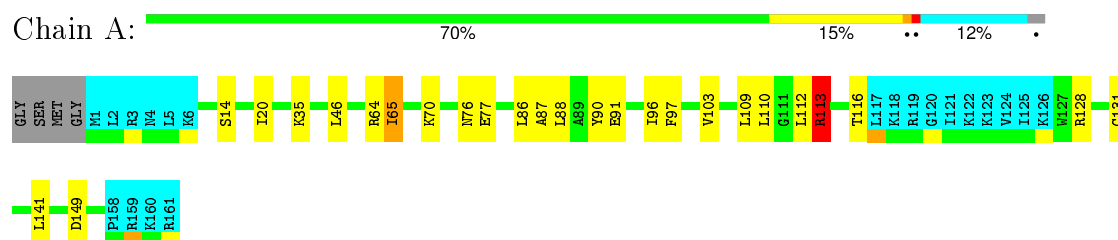
4.2.7 Score per residue for model 7

- Molecule 1: Putative toxin VapC6



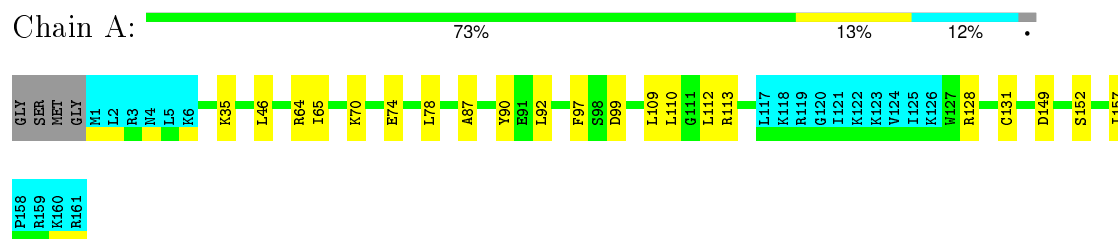
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Putative toxin VapC6



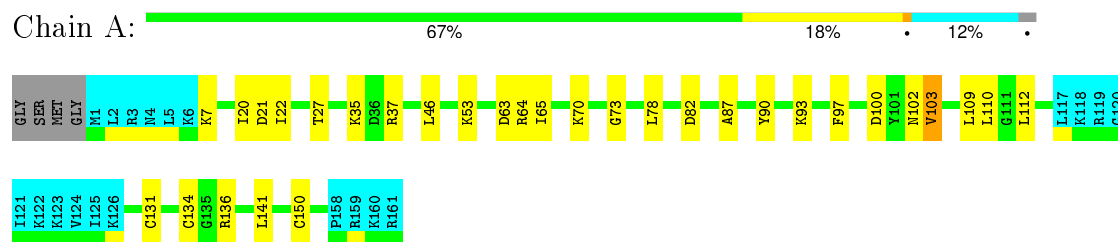
4.2.9 Score per residue for model 9

- Molecule 1: Putative toxin VapC6



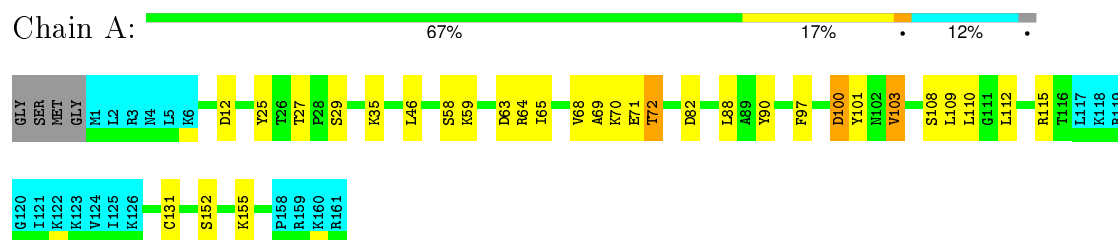
4.2.10 Score per residue for model 10

- Molecule 1: Putative toxin VapC6



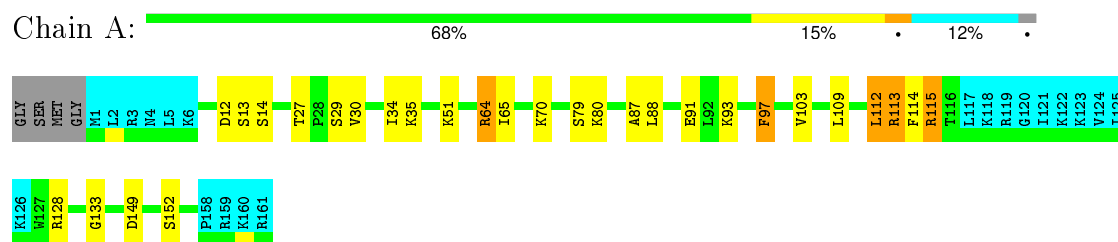
4.2.11 Score per residue for model 11

- Molecule 1: Putative toxin VapC6



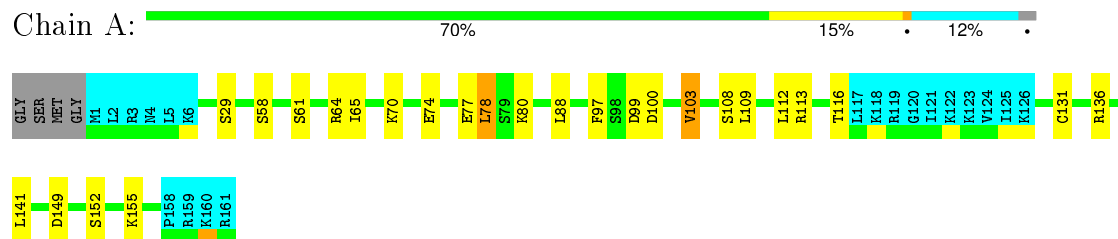
4.2.12 Score per residue for model 12

- Molecule 1: Putative toxin VapC6



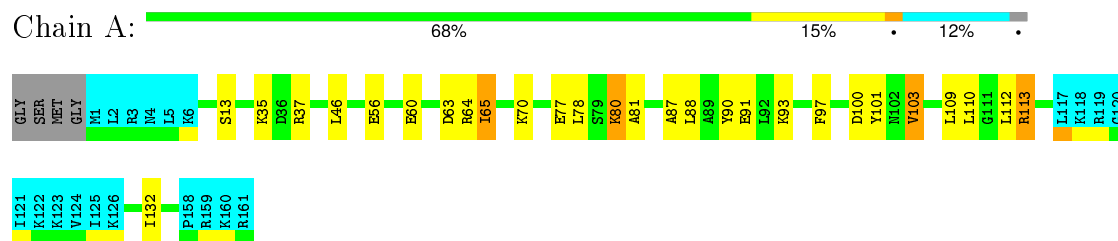
4.2.13 Score per residue for model 13

- Molecule 1: Putative toxin VapC6



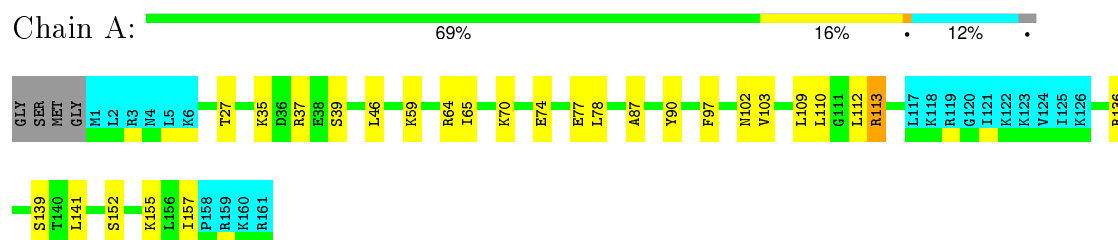
4.2.14 Score per residue for model 14

- Molecule 1: Putative toxin VapC6



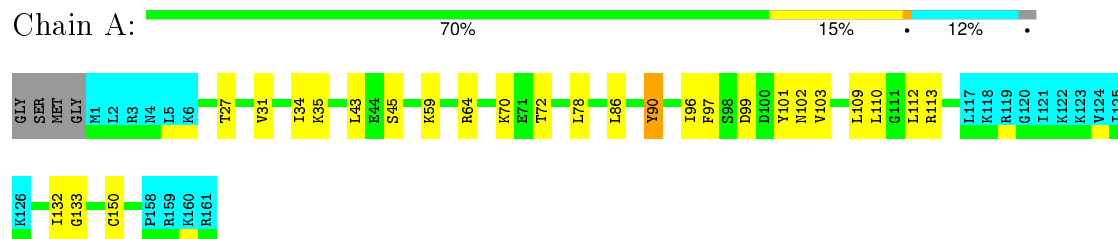
4.2.15 Score per residue for model 15

- Molecule 1: Putative toxin VapC6



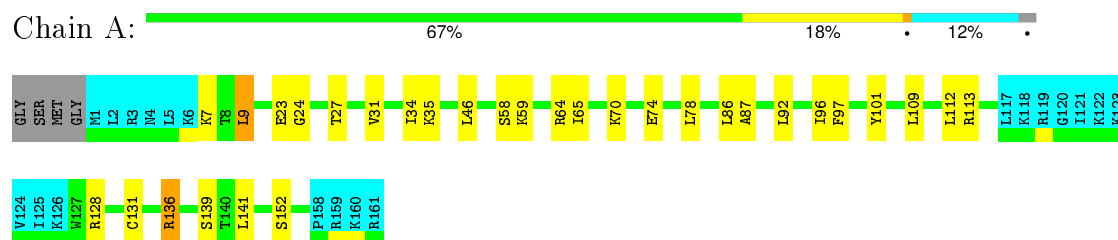
4.2.16 Score per residue for model 16

- Molecule 1: Putative toxin VapC6



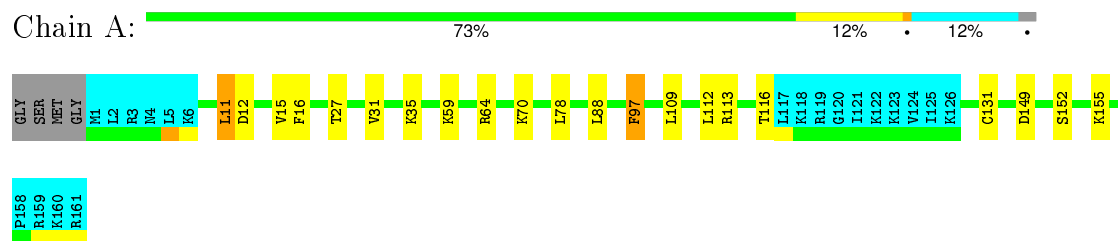
4.2.17 Score per residue for model 17

- Molecule 1: Putative toxin VapC6



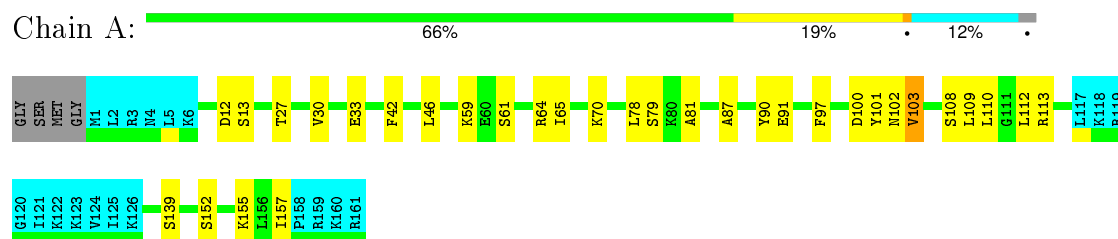
4.2.18 Score per residue for model 18

- Molecule 1: Putative toxin VapC6



4.2.19 Score per residue for model 19

- Molecule 1: Putative toxin VapC6



4.2.20 Score per residue for model 20

- Molecule 1: Putative toxin VapC6



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
OPALp	refinement	
CYANA	structure solution	3.0
TALOS+	structure solution	
CANDID	structure solution	
ATNOS	refinement	
CANDID	refinement	
CYANA	refinement	3.0

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)	2lcq_cs.str
Number of chemical shift lists	1
Total number of shifts	1961
Number of shifts mapped to atoms	0
Number of unparsed shifts	1961
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

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

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	0.55±0.01	0±0/1105 (0.0±0.0%)	1.02±0.02	1±1/1493 (0.1±0.1%)
All	All	0.55	0/22100 (0.0%)	1.02	23/29860 (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	0.9±0.9
All	All	0	19

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	115	ARG	NE-CZ-NH2	-6.29	117.15	120.30	20	3
1	A	64	ARG	NE-CZ-NH1	6.26	123.43	120.30	6	1
1	A	114	PHE	CB-CG-CD2	-5.95	116.63	120.80	12	1
1	A	113	ARG	NE-CZ-NH2	-5.66	117.47	120.30	8	2
1	A	31	VAL	CA-CB-CG1	5.66	119.39	110.90	18	2
1	A	37	ARG	NE-CZ-NH2	-5.64	117.48	120.30	10	2
1	A	136	ARG	NE-CZ-NH1	5.63	123.11	120.30	17	1
1	A	64	ARG	NE-CZ-NH2	-5.60	117.50	120.30	4	2
1	A	128	ARG	NE-CZ-NH2	-5.59	117.50	120.30	17	1
1	A	97	PHE	CB-CG-CD2	-5.49	116.95	120.80	12	2
1	A	90	TYR	CB-CG-CD2	-5.21	117.87	121.00	16	2
1	A	136	ARG	NE-CZ-NH2	-5.17	117.71	120.30	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	99	ASP	CB-CG-OD1	5.10	122.89	118.30	4	1
1	A	115	ARG	NE-CZ-NH1	5.09	122.85	120.30	3	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	101	TYR	Sidechain	7
1	A	64	ARG	Sidechain	3
1	A	113	ARG	Sidechain	3
1	A	115	ARG	Sidechain	2
1	A	136	ARG	Sidechain	2
1	A	37	ARG	Sidechain	1
1	A	25	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	1089	1119	1119	4±2
All	All	21800	22380	22380	88

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:VAL:HG11	1:A:110:LEU:HD21	0.82	1.50	11	3
1:A:11:LEU:HB3	1:A:15:VAL:HG11	0.74	1.59	18	1
1:A:65:ILE:HD11	1:A:87:ALA:HA	0.62	1.70	6	15
1:A:78:LEU:H	1:A:78:LEU:HD12	0.53	1.64	7	2
1:A:9:LEU:HD23	1:A:24:GLY:HA3	0.52	1.79	17	3
1:A:12:ASP:O	1:A:15:VAL:HG12	0.51	2.05	18	1
1:A:90:TYR:CE2	1:A:110:LEU:HG	0.50	2.41	8	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:PHE:CZ	1:A:46:LEU:HD11	0.50	2.42	6	3
1:A:9:LEU:HD22	1:A:23:GLU:O	0.49	2.07	20	1
1:A:9:LEU:CD2	1:A:24:GLY:HA3	0.49	2.38	20	1
1:A:9:LEU:HD21	1:A:11:LEU:HD11	0.47	1.85	7	2
1:A:65:ILE:HD12	1:A:90:TYR:CE2	0.47	2.45	10	7
1:A:112:LEU:HD13	1:A:113:ARG:N	0.46	2.25	12	1
1:A:100:ASP:H	1:A:103:VAL:HG12	0.46	1.71	10	4
1:A:42:PHE:CE2	1:A:46:LEU:HD11	0.46	2.45	6	2
1:A:51:LYS:HA	1:A:51:LYS:HE3	0.45	1.89	1	1
1:A:86:LEU:HD23	1:A:96:ILE:HD13	0.44	1.88	4	4
1:A:31:VAL:HG23	1:A:43:LEU:HD21	0.44	1.88	1	1
1:A:100:ASP:H	1:A:103:VAL:CG1	0.44	2.25	14	3
1:A:65:ILE:HD11	1:A:87:ALA:CA	0.43	2.44	14	3
1:A:13:SER:HB2	1:A:30:VAL:HG21	0.43	1.90	2	1
1:A:31:VAL:HG23	1:A:43:LEU:HD13	0.43	1.89	16	1
1:A:134:CYS:SG	1:A:150:CYS:SG	0.43	3.17	10	1
1:A:30:VAL:HG22	1:A:81:ALA:CB	0.42	2.45	20	2
1:A:86:LEU:CD1	1:A:96:ILE:HD13	0.42	2.45	17	1
1:A:78:LEU:HD12	1:A:78:LEU:H	0.41	1.75	13	2
1:A:15:VAL:HG13	1:A:16:PHE:CD1	0.41	2.50	18	1
1:A:30:VAL:HG22	1:A:81:ALA:HB1	0.41	1.92	6	1
1:A:69:ALA:HA	1:A:72:THR:HG22	0.41	1.91	11	1
1:A:31:VAL:HG23	1:A:43:LEU:CD2	0.41	2.46	1	1
1:A:80:LYS:HE3	1:A:81:ALA:N	0.41	2.31	14	1
1:A:78:LEU:N	1:A:78:LEU:HD12	0.40	2.31	19	1
1:A:127:TRP:CH2	1:A:157:ILE:HD13	0.40	2.52	20	1
1:A:78:LEU:HD12	1:A:78:LEU:N	0.40	2.31	10	1
1:A:15:VAL:HG13	1:A:16:PHE:CE1	0.40	2.52	18	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	141/165 (85%)	129±2 (92±1%)	11±2 (7±1%)	1±1 (1±1%)	29	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2820/3300 (85%)	2587 (92%)	210 (7%)	23 (1%)	29	74

All 10 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	74	GLU	6
1	A	34	ILE	4
1	A	133	GLY	3
1	A	132	ILE	2
1	A	7	LYS	2
1	A	148	PRO	2
1	A	22	ILE	1
1	A	73	GLY	1
1	A	128	ARG	1
1	A	75	VAL	1

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	123/144 (85%)	103±3 (84±3%)	20±3 (16±3%)	7	44
All	All	2460/2880 (85%)	2063 (84%)	397 (16%)	7	44

All 69 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	109	LEU	20
1	A	112	LEU	20
1	A	70	LYS	20
1	A	64	ARG	20
1	A	97	PHE	19
1	A	35	LYS	18
1	A	113	ARG	16
1	A	27	THR	14
1	A	103	VAL	13

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Mol	Chain	Res	Type	Models (Total)
1	A	131	CYS	12
1	A	78	LEU	11
1	A	152	SER	11
1	A	59	LYS	10
1	A	155	LYS	10
1	A	46	LEU	9
1	A	65	ILE	9
1	A	149	ASP	9
1	A	88	LEU	9
1	A	141	LEU	7
1	A	82	ASP	6
1	A	93	LYS	6
1	A	91	GLU	6
1	A	13	SER	5
1	A	100	ASP	5
1	A	29	SER	5
1	A	63	ASP	5
1	A	108	SER	5
1	A	77	GLU	5
1	A	80	LYS	5
1	A	102	ASN	5
1	A	9	LEU	4
1	A	21	ASP	4
1	A	116	THR	4
1	A	139	SER	4
1	A	58	SER	4
1	A	51	LYS	4
1	A	157	ILE	4
1	A	12	ASP	4
1	A	92	LEU	3
1	A	33	GLU	3
1	A	99	ASP	3
1	A	7	LYS	3
1	A	61	SER	3
1	A	76	ASN	3
1	A	79	SER	2
1	A	14	SER	2
1	A	136	ARG	2
1	A	128	ARG	2
1	A	56	GLU	2
1	A	72	THR	2
1	A	53	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	39	SER	1
1	A	37	ARG	1
1	A	140	THR	1
1	A	132	ILE	1
1	A	74	GLU	1
1	A	71	GLU	1
1	A	23	GLU	1
1	A	30	VAL	1
1	A	45	SER	1
1	A	134	CYS	1
1	A	36	ASP	1
1	A	44	GLU	1
1	A	48	SER	1
1	A	60	GLU	1
1	A	11	LEU	1
1	A	22	ILE	1
1	A	32	GLU	1
1	A	150	CYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

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: 2lcq_cs.str

Chemical shift list name: *assigned_chem_shift_list_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	1961
Number of shifts mapped to atoms	0
Number of unparsed shifts	1961
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Entity instance (chain) must be specified. All 1961 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	.	3	ARG	H	8.384	0.020	1
2	.	3	ARG	HA	4.341	0.020	1
3	.	3	ARG	HB2	1.798	0.020	1
4	.	3	ARG	HB3	1.798	0.020	1
5	.	3	ARG	C	175.508	0.3	1
6	.	3	ARG	CA	55.834	0.3	1
7	.	3	ARG	CB	30.948	0.3	1
8	.	3	ARG	N	122.107	0.3	1
9	.	4	ASN	H	8.411	0.020	1
10	.	4	ASN	HA	4.673	0.020	1
11	.	4	ASN	HB2	2.840	0.020	2
12	.	4	ASN	HB3	2.737	0.020	2
13	.	4	ASN	HD21	7.544	0.020	1
14	.	4	ASN	HD22	6.842	0.020	1
15	.	4	ASN	C	174.798	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	.	4	ASN	CA	52.978	0.3	1
17	.	4	ASN	CB	38.445	0.3	1
18	.	4	ASN	N	119.629	0.3	1
19	.	4	ASN	ND2	112.284	0.3	1
20	.	5	LEU	H	8.157	0.020	1
21	.	5	LEU	HA	4.335	0.020	1
22	.	5	LEU	HB2	1.605	0.020	2
23	.	5	LEU	HB3	1.583	0.020	2
24	.	5	LEU	C	177.074	0.3	1
25	.	5	LEU	CA	55.120	0.3	1
26	.	5	LEU	CB	42.271	0.3	1
27	.	5	LEU	CG	26.869	0.3	1
28	.	5	LEU	CD1	24.739	0.3	1
29	.	5	LEU	CD2	23.474	0.3	1
30	.	5	LEU	N	122.833	0.3	1
31	.	6	LYS	H	8.208	0.020	1
32	.	6	LYS	HA	4.317	0.020	1
33	.	6	LYS	HB2	1.761	0.020	2
34	.	6	LYS	HB3	1.829	0.020	2
35	.	6	LYS	HG2	1.458	0.020	2
36	.	6	LYS	HG3	1.407	0.020	2
37	.	6	LYS	HD2	1.301	0.020	1
38	.	6	LYS	HE2	3.001	0.020	2
39	.	6	LYS	HE3	3.034	0.020	2
40	.	6	LYS	C	176.257	0.3	1
41	.	6	LYS	CA	56.177	0.3	1
42	.	6	LYS	CB	33.094	0.3	1
43	.	6	LYS	CG	24.727	0.3	1
44	.	6	LYS	CD	28.834	0.3	1
45	.	6	LYS	CE	42.244	0.3	1
46	.	6	LYS	N	121.843	0.3	1
47	.	7	LYS	H	8.211	0.020	1
48	.	7	LYS	HA	4.428	0.020	1
49	.	7	LYS	HB2	1.807	0.020	2
50	.	7	LYS	HB3	1.742	0.020	2
51	.	7	LYS	C	176.315	0.3	1
52	.	7	LYS	CA	55.791	0.3	1
53	.	7	LYS	CB	33.082	0.3	1
54	.	7	LYS	CG	24.560	0.3	1
55	.	7	LYS	CD	28.832	0.3	1
56	.	7	LYS	CE	42.067	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	.	7	LYS	N	122.500	0.3	1
58	.	8	THR	H	8.402	0.020	1
59	.	8	THR	HA	4.257	0.020	1
60	.	8	THR	HB	3.965	0.020	1
61	.	8	THR	HG2	1.081	0.020	1
62	.	8	THR	HG2	1.081	0.020	1
63	.	8	THR	HG2	1.081	0.020	1
64	.	8	THR	C	172.367	0.3	1
65	.	8	THR	CA	62.856	0.3	1
66	.	8	THR	CB	69.470	0.3	1
67	.	8	THR	CG2	22.558	0.3	1
68	.	8	THR	N	119.414	0.3	1
69	.	9	LEU	H	8.322	0.020	1
70	.	9	LEU	HA	5.114	0.020	1
71	.	9	LEU	HB2	1.744	0.020	2
72	.	9	LEU	HB3	1.630	0.020	2
73	.	9	LEU	HG	1.631	0.020	1
74	.	9	LEU	HD1	0.863	0.020	1
75	.	9	LEU	HD1	0.863	0.020	1
76	.	9	LEU	HD1	0.863	0.020	1
77	.	9	LEU	C	175.069	0.3	1
78	.	9	LEU	CA	53.799	0.3	1
79	.	9	LEU	CB	44.586	0.3	1
80	.	9	LEU	CG	27.189	0.3	1
81	.	9	LEU	CD1	25.251	0.3	1
82	.	9	LEU	N	128.282	0.3	1
83	.	10	VAL	H	9.179	0.020	1
84	.	10	VAL	HA	4.903	0.020	1
85	.	10	VAL	HB	1.876	0.020	1
86	.	10	VAL	HG1	1.214	0.020	1
87	.	10	VAL	HG1	1.214	0.020	1
88	.	10	VAL	HG1	1.214	0.020	1
89	.	10	VAL	HG2	0.768	0.020	1
90	.	10	VAL	HG2	0.768	0.020	1
91	.	10	VAL	HG2	0.768	0.020	1
92	.	10	VAL	C	174.080	0.3	1
93	.	10	VAL	CA	61.651	0.3	1
94	.	10	VAL	CB	32.924	0.3	1
95	.	10	VAL	CG1	22.689	0.3	1
96	.	10	VAL	CG2	21.205	0.3	1
97	.	10	VAL	N	124.869	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	.	11	LEU	H	9.212	0.020	1
99	.	11	LEU	HA	4.692	0.020	1
100	.	11	LEU	HB2	1.914	0.020	2
101	.	11	LEU	HB3	1.217	0.020	2
102	.	11	LEU	HG	0.808	0.020	1
103	.	11	LEU	HD1	0.812	0.020	1
104	.	11	LEU	HD1	0.812	0.020	1
105	.	11	LEU	HD1	0.812	0.020	1
106	.	11	LEU	HD2	0.633	0.020	1
107	.	11	LEU	HD2	0.633	0.020	1
108	.	11	LEU	HD2	0.633	0.020	1
109	.	11	LEU	C	175.111	0.3	1
110	.	11	LEU	CA	54.105	0.3	1
111	.	11	LEU	CB	43.734	0.3	1
112	.	11	LEU	CG	26.598	0.3	1
113	.	11	LEU	CD1	24.427	0.3	1
114	.	11	LEU	CD2	22.864	0.3	1
115	.	11	LEU	N	126.916	0.3	1
116	.	12	ASP	H	7.588	0.020	1
117	.	12	ASP	HA	5.076	0.020	1
118	.	12	ASP	HB2	3.415	0.020	2
119	.	12	ASP	HB3	2.828	0.020	2
120	.	12	ASP	C	175.793	0.3	1
121	.	12	ASP	CA	51.604	0.3	1
122	.	12	ASP	CB	41.963	0.3	1
123	.	12	ASP	N	122.119	0.3	1
124	.	13	SER	H	8.745	0.020	1
125	.	13	SER	HA	4.082	0.020	1
126	.	13	SER	HB2	3.957	0.020	1
127	.	13	SER	HB3	3.957	0.020	1
128	.	13	SER	C	176.361	0.3	1
129	.	13	SER	CA	61.824	0.3	1
130	.	13	SER	CB	62.834	0.3	1
131	.	13	SER	N	110.901	0.3	1
132	.	14	SER	H	7.954	0.020	1
133	.	14	SER	HA	4.072	0.020	1
134	.	14	SER	HB2	3.829	0.020	1
135	.	14	SER	HB3	3.829	0.020	1
136	.	14	SER	C	175.744	0.3	1
137	.	14	SER	CA	61.501	0.3	1
138	.	14	SER	CB	62.791	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	.	14	SER	N	116.918	0.3	1
140	.	15	VAL	H	7.119	0.020	1
141	.	15	VAL	HA	3.210	0.020	1
142	.	15	VAL	HB	1.314	0.020	1
143	.	15	VAL	HG1	0.371	0.020	1
144	.	15	VAL	HG1	0.371	0.020	1
145	.	15	VAL	HG1	0.371	0.020	1
146	.	15	VAL	HG2	0.268	0.020	1
147	.	15	VAL	HG2	0.268	0.020	1
148	.	15	VAL	HG2	0.268	0.020	1
149	.	15	VAL	C	176.183	0.3	1
150	.	15	VAL	CA	65.279	0.3	1
151	.	15	VAL	CB	31.317	0.3	1
152	.	15	VAL	CG1	22.310	0.3	1
153	.	15	VAL	CG2	21.516	0.3	1
154	.	15	VAL	N	120.289	0.3	1
155	.	16	PHE	H	6.530	0.020	1
156	.	16	PHE	HA	4.604	0.020	1
157	.	16	PHE	HB2	3.384	0.020	2
158	.	16	PHE	HB3	2.892	0.020	2
159	.	16	PHE	HD1	7.101	0.020	1
160	.	16	PHE	HD2	7.101	0.020	1
161	.	16	PHE	HE1	7.149	0.020	1
162	.	16	PHE	HE2	7.149	0.020	1
163	.	16	PHE	HZ	6.944	0.020	1
164	.	16	PHE	C	178.054	0.3	1
165	.	16	PHE	CA	59.362	0.3	1
166	.	16	PHE	CB	38.515	0.3	1
167	.	16	PHE	CD1	130.883	0.3	1
168	.	16	PHE	CE1	132.039	0.3	1
169	.	16	PHE	CZ	130.039	0.3	1
170	.	16	PHE	N	116.759	0.3	1
171	.	17	ILE	H	8.048	0.020	1
172	.	17	ILE	HA	4.142	0.020	1
173	.	17	ILE	HB	1.804	0.020	1
174	.	17	ILE	HG12	1.621	0.020	2
175	.	17	ILE	HG13	1.322	0.020	2
176	.	17	ILE	HG2	0.914	0.020	1
177	.	17	ILE	HG2	0.914	0.020	1
178	.	17	ILE	HG2	0.914	0.020	1
179	.	17	ILE	HD1	0.614	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	.	17	ILE	HD1	0.614	0.020	1
181	.	17	ILE	HD1	0.614	0.020	1
182	.	17	ILE	C	177.365	0.3	1
183	.	17	ILE	CA	63.006	0.3	1
184	.	17	ILE	CB	38.467	0.3	1
185	.	17	ILE	CG1	28.510	0.3	1
186	.	17	ILE	CG2	17.432	0.3	1
187	.	17	ILE	CD1	12.674	0.3	1
188	.	17	ILE	N	119.975	0.3	1
189	.	18	GLN	H	7.532	0.020	1
190	.	18	GLN	HA	4.045	0.020	1
191	.	18	GLN	HB2	2.138	0.020	2
192	.	18	GLN	HB3	1.992	0.020	2
193	.	18	GLN	HG2	2.425	0.020	2
194	.	18	GLN	HG3	2.281	0.020	2
195	.	18	GLN	HE21	7.275	0.020	1
196	.	18	GLN	HE22	6.951	0.020	1
197	.	18	GLN	C	176.283	0.3	1
198	.	18	GLN	CA	56.142	0.3	1
199	.	18	GLN	CB	28.910	0.3	1
200	.	18	GLN	CG	34.681	0.3	1
201	.	18	GLN	N	115.636	0.3	1
202	.	18	GLN	NE2	111.377	0.3	1
203	.	19	GLY	H	7.281	0.020	1
204	.	19	GLY	HA2	2.583	0.020	2
205	.	19	GLY	HA3	3.317	0.020	2
206	.	19	GLY	C	173.840	0.3	1
207	.	19	GLY	CA	46.342	0.3	1
208	.	19	GLY	N	107.893	0.3	1
209	.	20	ILE	H	7.503	0.020	1
210	.	20	ILE	HA	3.865	0.020	1
211	.	20	ILE	HB	1.743	0.020	1
212	.	20	ILE	HG12	1.282	0.020	2
213	.	20	ILE	HG13	1.032	0.020	2
214	.	20	ILE	HG2	0.741	0.020	1
215	.	20	ILE	HG2	0.741	0.020	1
216	.	20	ILE	HG2	0.741	0.020	1
217	.	20	ILE	HD1	0.710	0.020	1
218	.	20	ILE	HD1	0.710	0.020	1
219	.	20	ILE	HD1	0.710	0.020	1
220	.	20	ILE	C	173.299	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	.	20	ILE	CA	60.577	0.3	1
222	.	20	ILE	CB	37.635	0.3	1
223	.	20	ILE	CG1	27.182	0.3	1
224	.	20	ILE	CG2	17.180	0.3	1
225	.	20	ILE	CD1	12.853	0.3	1
226	.	20	ILE	N	120.508	0.3	1
227	.	21	ASP	H	8.054	0.020	1
228	.	21	ASP	HA	4.538	0.020	1
229	.	21	ASP	HB2	2.836	0.020	1
230	.	21	ASP	HB3	2.836	0.020	2
231	.	21	ASP	C	174.456	0.3	1
232	.	21	ASP	CA	54.166	0.3	1
233	.	21	ASP	CB	40.834	0.3	1
234	.	21	ASP	N	124.953	0.3	1
235	.	22	ILE	H	7.275	0.020	1
236	.	22	ILE	HA	4.362	0.020	1
237	.	22	ILE	HB	1.536	0.020	1
238	.	22	ILE	HG12	1.507	0.020	2
239	.	22	ILE	HG13	1.187	0.020	2
240	.	22	ILE	HG2	0.578	0.020	1
241	.	22	ILE	HG2	0.578	0.020	1
242	.	22	ILE	HG2	0.578	0.020	1
243	.	22	ILE	HD1	0.726	0.020	1
244	.	22	ILE	HD1	0.726	0.020	1
245	.	22	ILE	HD1	0.726	0.020	1
246	.	22	ILE	C	170.755	0.3	1
247	.	22	ILE	CA	59.233	0.3	1
248	.	22	ILE	CB	41.728	0.3	1
249	.	22	ILE	CG1	28.774	0.3	1
250	.	22	ILE	CG2	16.899	0.3	1
251	.	22	ILE	CD1	15.007	0.3	1
252	.	22	ILE	N	125.491	0.3	1
253	.	23	GLU	H	7.014	0.020	1
254	.	23	GLU	HA	4.702	0.020	1
255	.	23	GLU	HB2	2.038	0.020	1
256	.	23	GLU	HB3	2.038	0.020	2
257	.	23	GLU	C	176.511	0.3	1
258	.	23	GLU	CA	54.291	0.3	1
259	.	23	GLU	CB	32.242	0.3	1
260	.	23	GLU	N	118.789	0.3	1
261	.	24	GLY	H	8.100	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	.	24	GLY	HA2	4.379	0.020	2
263	.	24	GLY	HA3	4.152	0.020	2
264	.	24	GLY	C	171.469	0.3	1
265	.	24	GLY	CA	46.012	0.3	1
266	.	24	GLY	N	106.688	0.3	1
267	.	25	TYR	H	9.242	0.020	1
268	.	25	TYR	HA	5.735	0.020	1
269	.	25	TYR	HB2	2.865	0.020	2
270	.	25	TYR	HB3	2.754	0.020	2
271	.	25	TYR	HD1	6.994	0.020	1
272	.	25	TYR	HD2	6.994	0.020	1
273	.	25	TYR	HE1	6.796	0.020	1
274	.	25	TYR	HE2	6.796	0.020	1
275	.	25	TYR	C	175.862	0.3	1
276	.	25	TYR	CA	56.587	0.3	1
277	.	25	TYR	CB	42.879	0.3	1
278	.	25	TYR	CD1	132.724	0.3	1
279	.	25	TYR	CE1	117.963	0.3	1
280	.	25	TYR	N	119.724	0.3	1
281	.	26	THR	H	9.138	0.020	1
282	.	26	THR	HA	4.782	0.020	1
283	.	26	THR	HB	4.258	0.020	1
284	.	26	THR	HG2	0.932	0.020	1
285	.	26	THR	HG2	0.932	0.020	1
286	.	26	THR	HG2	0.932	0.020	1
287	.	26	THR	C	171.533	0.3	1
288	.	26	THR	CA	61.853	0.3	1
289	.	26	THR	CB	70.576	0.3	1
290	.	26	THR	CG2	17.683	0.3	1
291	.	26	THR	N	115.135	0.3	1
292	.	27	THR	H	7.917	0.020	1
293	.	27	THR	HA	5.956	0.020	1
294	.	27	THR	HB	4.730	0.020	1
295	.	27	THR	HG2	1.263	0.020	1
296	.	27	THR	HG2	1.263	0.020	1
297	.	27	THR	HG2	1.263	0.020	1
298	.	27	THR	C	174.337	0.3	1
299	.	27	THR	CA	59.229	0.3	1
300	.	27	THR	CB	67.746	0.3	1
301	.	27	THR	CG2	22.312	0.3	1
302	.	27	THR	N	109.590	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	.	28	PRO	HA	4.206	0.020	1
304	.	28	PRO	HB2	2.423	0.020	2
305	.	28	PRO	HB3	2.107	0.020	2
306	.	28	PRO	HG2	2.206	0.020	2
307	.	28	PRO	HG3	1.855	0.020	2
308	.	28	PRO	HD2	3.913	0.020	1
309	.	28	PRO	HD3	3.913	0.020	1
310	.	28	PRO	C	179.697	0.3	1
311	.	28	PRO	CA	65.472	0.3	1
312	.	28	PRO	CB	32.043	0.3	1
313	.	28	PRO	CG	28.003	0.3	1
314	.	28	PRO	CD	50.650	0.3	1
315	.	29	SER	H	8.868	0.020	1
316	.	29	SER	HA	4.288	0.020	1
317	.	29	SER	HB2	3.776	0.020	1
318	.	29	SER	HB3	3.776	0.020	1
319	.	29	SER	C	177.170	0.3	1
320	.	29	SER	CA	61.384	0.3	1
321	.	29	SER	CB	61.384	0.3	1
322	.	29	SER	N	110.505	0.3	1
323	.	30	VAL	H	7.547	0.020	1
324	.	30	VAL	HA	3.689	0.020	1
325	.	30	VAL	HB	2.576	0.020	1
326	.	30	VAL	HG1	1.243	0.020	1
327	.	30	VAL	HG1	1.243	0.020	1
328	.	30	VAL	HG1	1.243	0.020	1
329	.	30	VAL	HG2	0.986	0.020	1
330	.	30	VAL	HG2	0.986	0.020	1
331	.	30	VAL	HG2	0.986	0.020	1
332	.	30	VAL	C	177.422	0.3	1
333	.	30	VAL	CA	66.801	0.3	1
334	.	30	VAL	CB	31.366	0.3	1
335	.	30	VAL	CG1	23.703	0.3	1
336	.	30	VAL	CG2	21.544	0.3	1
337	.	30	VAL	N	124.754	0.3	1
338	.	31	VAL	H	7.126	0.020	1
339	.	31	VAL	HA	3.262	0.020	1
340	.	31	VAL	HB	2.253	0.020	1
341	.	31	VAL	HG1	0.951	0.020	1
342	.	31	VAL	HG1	0.951	0.020	1
343	.	31	VAL	HG1	0.951	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	.	31	VAL	HG2	0.871	0.020	1
345	.	31	VAL	HG2	0.871	0.020	1
346	.	31	VAL	HG2	0.871	0.020	1
347	.	31	VAL	C	178.847	0.3	1
348	.	31	VAL	CA	66.478	0.3	1
349	.	31	VAL	CB	30.973	0.3	1
350	.	31	VAL	CG1	21.915	0.3	1
351	.	31	VAL	CG2	20.830	0.3	1
352	.	31	VAL	N	117.035	0.3	1
353	.	32	GLU	H	7.564	0.020	1
354	.	32	GLU	HA	3.970	0.020	1
355	.	32	GLU	HB2	2.072	0.020	2
356	.	32	GLU	HB3	2.005	0.020	2
357	.	32	GLU	HG2	2.352	0.020	2
358	.	32	GLU	HG3	2.279	0.020	2
359	.	32	GLU	C	177.359	0.3	1
360	.	32	GLU	CA	58.172	0.3	1
361	.	32	GLU	CB	30.166	0.3	1
362	.	32	GLU	CG	36.347	0.3	1
363	.	32	GLU	N	115.499	0.3	1
364	.	33	GLU	H	7.537	0.020	1
365	.	33	GLU	HA	4.205	0.020	1
366	.	33	GLU	HB2	2.328	0.020	1
367	.	33	GLU	HB3	2.328	0.020	2
368	.	33	GLU	C	176.932	0.3	1
369	.	33	GLU	CA	57.475	0.3	1
370	.	33	GLU	CB	29.857	0.3	1
371	.	33	GLU	CG	36.398	0.3	1
372	.	33	GLU	N	116.652	0.3	1
373	.	34	ILE	H	7.291	0.020	1
374	.	34	ILE	HA	4.024	0.020	1
375	.	34	ILE	HB	2.038	0.020	1
376	.	34	ILE	HG12	1.657	0.020	2
377	.	34	ILE	HG13	1.477	0.020	2
378	.	34	ILE	HG2	0.822	0.020	1
379	.	34	ILE	HG2	0.822	0.020	1
380	.	34	ILE	HG2	0.822	0.020	1
381	.	34	ILE	HD1	0.885	0.020	1
382	.	34	ILE	HD1	0.885	0.020	1
383	.	34	ILE	HD1	0.885	0.020	1
384	.	34	ILE	C	175.043	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	.	34	ILE	CA	61.116	0.3	1
386	.	34	ILE	CB	35.981	0.3	1
387	.	34	ILE	CG1	27.165	0.3	1
388	.	34	ILE	CG2	18.276	0.3	1
389	.	34	ILE	CD1	13.403	0.3	1
390	.	34	ILE	N	120.124	0.3	1
391	.	35	LYS	H	8.174	0.020	1
392	.	35	LYS	HA	4.404	0.020	1
393	.	35	LYS	HB2	1.931	0.020	2
394	.	35	LYS	HB3	1.757	0.020	2
395	.	35	LYS	HG2	1.491	0.020	2
396	.	35	LYS	HG3	1.455	0.020	2
397	.	35	LYS	HD2	1.676	0.020	2
398	.	35	LYS	HD3	1.502	0.020	2
399	.	35	LYS	C	176.879	0.3	1
400	.	35	LYS	CA	56.043	0.3	1
401	.	35	LYS	CB	34.130	0.3	1
402	.	35	LYS	CG	24.727	0.3	1
403	.	35	LYS	CD	29.047	0.3	1
404	.	35	LYS	CE	42.426	0.3	1
405	.	35	LYS	N	125.475	0.3	1
406	.	36	ASP	H	7.945	0.020	1
407	.	36	ASP	HA	4.649	0.020	1
408	.	36	ASP	HB2	2.807	0.020	2
409	.	36	ASP	HB3	2.635	0.020	2
410	.	36	ASP	C	175.864	0.3	1
411	.	36	ASP	CA	54.043	0.3	1
412	.	36	ASP	CB	42.511	0.3	1
413	.	36	ASP	N	120.342	0.3	1
414	.	37	ARG	H	8.641	0.020	1
415	.	37	ARG	HA	3.930	0.020	1
416	.	37	ARG	HB2	1.963	0.020	2
417	.	37	ARG	HB3	1.868	0.020	2
418	.	37	ARG	C	177.823	0.3	1
419	.	37	ARG	CA	59.510	0.3	1
420	.	37	ARG	CB	30.420	0.3	1
421	.	37	ARG	CG	26.997	0.3	1
422	.	37	ARG	CD	43.200	0.3	1
423	.	37	ARG	N	124.586	0.3	1
424	.	38	GLU	H	8.659	0.020	1
425	.	38	GLU	HA	4.014	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	.	38	GLU	HB2	2.136	0.020	2
427	.	38	GLU	HB3	2.062	0.020	2
428	.	38	GLU	HG2	2.444	0.020	2
429	.	38	GLU	HG3	2.353	0.020	2
430	.	38	GLU	C	179.748	0.3	1
431	.	38	GLU	CA	59.966	0.3	1
432	.	38	GLU	CB	29.038	0.3	1
433	.	38	GLU	CG	36.925	0.3	1
434	.	38	GLU	N	117.285	0.3	1
435	.	39	SER	H	8.089	0.020	1
436	.	39	SER	HA	4.484	0.020	1
437	.	39	SER	HB2	3.888	0.020	1
438	.	39	SER	HB3	3.705	0.020	1
439	.	39	SER	C	175.528	0.3	1
440	.	39	SER	CA	61.491	0.3	1
441	.	39	SER	CB	62.739	0.3	1
442	.	39	SER	N	116.786	0.3	1
443	.	40	LYS	H	8.258	0.020	1
444	.	40	LYS	HA	3.842	0.020	1
445	.	40	LYS	HB2	1.913	0.020	2
446	.	40	LYS	HB3	1.747	0.020	2
447	.	40	LYS	HG2	1.690	0.020	2
448	.	40	LYS	HG3	1.394	0.020	2
449	.	40	LYS	C	178.359	0.3	1
450	.	40	LYS	CA	59.871	0.3	1
451	.	40	LYS	CB	32.141	0.3	1
452	.	40	LYS	CG	24.443	0.3	1
453	.	40	LYS	CD	28.918	0.3	1
454	.	40	LYS	CE	41.532	0.3	1
455	.	40	LYS	N	123.024	0.3	1
456	.	41	ILE	H	8.121	0.020	1
457	.	41	ILE	HA	3.799	0.020	1
458	.	41	ILE	HB	1.956	0.020	1
459	.	41	ILE	HG12	1.713	0.020	2
460	.	41	ILE	HG13	1.226	0.020	2
461	.	41	ILE	HG2	0.972	0.020	1
462	.	41	ILE	HG2	0.972	0.020	1
463	.	41	ILE	HG2	0.972	0.020	1
464	.	41	ILE	HD1	0.853	0.020	1
465	.	41	ILE	HD1	0.853	0.020	1
466	.	41	ILE	HD1	0.853	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	.	41	ILE	C	178.857	0.3	1
468	.	41	ILE	CA	64.750	0.3	1
469	.	41	ILE	CB	37.928	0.3	1
470	.	41	ILE	CG1	29.093	0.3	1
471	.	41	ILE	CG2	17.135	0.3	1
472	.	41	ILE	CD1	13.193	0.3	1
473	.	41	ILE	N	119.303	0.3	1
474	.	42	PHE	H	7.888	0.020	1
475	.	42	PHE	HA	4.367	0.020	1
476	.	42	PHE	HB2	3.406	0.020	2
477	.	42	PHE	HB3	3.307	0.020	2
478	.	42	PHE	HD1	7.386	0.020	1
479	.	42	PHE	HD2	7.386	0.020	1
480	.	42	PHE	HE1	7.347	0.020	1
481	.	42	PHE	HE2	7.347	0.020	1
482	.	42	PHE	HZ	7.112	0.020	1
483	.	42	PHE	C	177.960	0.3	1
484	.	42	PHE	CA	61.306	0.3	1
485	.	42	PHE	CB	39.266	0.3	1
486	.	42	PHE	CD1	131.388	0.3	1
487	.	42	PHE	CE1	131.370	0.3	1
488	.	42	PHE	CZ	130.857	0.3	1
489	.	42	PHE	N	122.429	0.3	1
490	.	43	LEU	H	8.437	0.020	1
491	.	43	LEU	HA	3.637	0.020	1
492	.	43	LEU	HB2	1.949	0.020	2
493	.	43	LEU	HB3	1.094	0.020	2
494	.	43	LEU	HG	1.168	0.020	1
495	.	43	LEU	HD1	-0.162	0.020	1
496	.	43	LEU	HD1	-0.162	0.020	1
497	.	43	LEU	HD1	-0.162	0.020	1
498	.	43	LEU	HD2	0.580	0.020	1
499	.	43	LEU	HD2	0.580	0.020	1
500	.	43	LEU	HD2	0.580	0.020	1
501	.	43	LEU	C	177.990	0.3	1
502	.	43	LEU	CA	58.653	0.3	1
503	.	43	LEU	CB	41.187	0.3	1
504	.	43	LEU	CG	26.746	0.3	1
505	.	43	LEU	CD1	22.058	0.3	1
506	.	43	LEU	CD2	27.182	0.3	1
507	.	43	LEU	N	121.513	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	.	44	GLU	H	8.621	0.020	1
509	.	44	GLU	HA	3.780	0.020	1
510	.	44	GLU	HB2	2.123	0.020	2
511	.	44	GLU	HB3	1.995	0.020	2
512	.	44	GLU	HG2	2.446	0.020	2
513	.	44	GLU	HG3	2.345	0.020	2
514	.	44	GLU	C	179.546	0.3	1
515	.	44	GLU	CA	59.771	0.3	1
516	.	44	GLU	CB	28.664	0.3	1
517	.	44	GLU	CG	36.596	0.3	1
518	.	44	GLU	N	117.470	0.3	1
519	.	45	SER	H	8.299	0.020	1
520	.	45	SER	HA	4.305	0.020	1
521	.	45	SER	HB2	4.005	0.020	1
522	.	45	SER	HB3	4.005	0.020	1
523	.	45	SER	C	176.745	0.3	1
524	.	45	SER	CA	61.343	0.3	1
525	.	45	SER	CB	62.293	0.3	1
526	.	45	SER	N	117.566	0.3	1
527	.	46	LEU	H	7.613	0.020	1
528	.	46	LEU	HA	4.032	0.020	1
529	.	46	LEU	HB2	1.881	0.020	2
530	.	46	LEU	HB3	1.252	0.020	2
531	.	46	LEU	HG	1.263	0.020	1
532	.	46	LEU	HD1	0.807	0.020	1
533	.	46	LEU	HD1	0.807	0.020	1
534	.	46	LEU	HD1	0.807	0.020	1
535	.	46	LEU	HD2	0.700	0.020	1
536	.	46	LEU	HD2	0.700	0.020	1
537	.	46	LEU	HD2	0.700	0.020	1
538	.	46	LEU	C	180.383	0.3	1
539	.	46	LEU	CA	58.321	0.3	1
540	.	46	LEU	CB	41.945	0.3	1
541	.	46	LEU	CG	26.330	0.3	1
542	.	46	LEU	CD1	24.201	0.3	1
543	.	46	LEU	CD2	22.560	0.3	1
544	.	46	LEU	N	124.196	0.3	1
545	.	47	ILE	H	8.256	0.020	1
546	.	47	ILE	HA	4.239	0.020	1
547	.	47	ILE	HB	1.768	0.020	1
548	.	47	ILE	HG12	1.524	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	.	47	ILE	HG13	0.726	0.020	2
550	.	47	ILE	HG2	0.898	0.020	1
551	.	47	ILE	HG2	0.898	0.020	1
552	.	47	ILE	HG2	0.898	0.020	1
553	.	47	ILE	HD1	0.602	0.020	1
554	.	47	ILE	HD1	0.602	0.020	1
555	.	47	ILE	HD1	0.602	0.020	1
556	.	47	ILE	C	181.474	0.3	1
557	.	47	ILE	CA	64.354	0.3	1
558	.	47	ILE	CB	38.459	0.3	1
559	.	47	ILE	CG1	28.739	0.3	1
560	.	47	ILE	CG2	16.904	0.3	1
561	.	47	ILE	CD1	13.956	0.3	1
562	.	47	ILE	N	122.104	0.3	1
563	.	48	SER	H	8.770	0.020	1
564	.	48	SER	HA	4.186	0.020	1
565	.	48	SER	HB2	3.961	0.020	1
566	.	48	SER	HB3	3.961	0.020	1
567	.	48	SER	C	175.868	0.3	1
568	.	48	SER	CA	61.603	0.3	1
569	.	48	SER	CB	62.539	0.3	1
570	.	48	SER	N	118.493	0.3	1
571	.	49	ALA	H	7.489	0.020	1
572	.	49	ALA	HA	4.391	0.020	1
573	.	49	ALA	HB	1.529	0.020	1
574	.	49	ALA	HB	1.529	0.020	1
575	.	49	ALA	HB	1.529	0.020	1
576	.	49	ALA	C	177.680	0.3	1
577	.	49	ALA	CA	52.377	0.3	1
578	.	49	ALA	CB	19.390	0.3	1
579	.	49	ALA	N	119.479	0.3	1
580	.	50	GLY	H	7.875	0.020	1
581	.	50	GLY	HA2	4.148	0.020	2
582	.	50	GLY	HA3	3.814	0.020	2
583	.	50	GLY	C	174.081	0.3	1
584	.	50	GLY	CA	45.030	0.3	1
585	.	50	GLY	N	106.323	0.3	1
586	.	51	LYS	H	7.772	0.020	1
587	.	51	LYS	HA	4.088	0.020	1
588	.	51	LYS	HB2	2.053	0.020	2
589	.	51	LYS	HB3	1.735	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	.	51	LYS	HG2	1.644	0.020	2
591	.	51	LYS	HG3	1.414	0.020	2
592	.	51	LYS	HD2	1.712	0.020	2
593	.	51	LYS	HD3	1.579	0.020	2
594	.	51	LYS	HE2	2.882	0.020	1
595	.	51	LYS	HE3	2.882	0.020	1
596	.	51	LYS	C	175.977	0.3	1
597	.	51	LYS	CA	58.527	0.3	1
598	.	51	LYS	CB	33.889	0.3	1
599	.	51	LYS	CG	26.043	0.3	1
600	.	51	LYS	CD	29.734	0.3	1
601	.	51	LYS	CE	41.534	0.3	1
602	.	51	LYS	N	118.430	0.3	1
603	.	52	VAL	H	6.671	0.020	1
604	.	52	VAL	HA	4.976	0.020	1
605	.	52	VAL	HB	1.251	0.020	1
606	.	52	VAL	HG1	0.944	0.020	1
607	.	52	VAL	HG1	0.944	0.020	1
608	.	52	VAL	HG1	0.944	0.020	1
609	.	52	VAL	HG2	0.681	0.020	1
610	.	52	VAL	HG2	0.681	0.020	1
611	.	52	VAL	HG2	0.681	0.020	1
612	.	52	VAL	C	174.131	0.3	1
613	.	52	VAL	CA	59.418	0.3	1
614	.	52	VAL	CB	34.169	0.3	1
615	.	52	VAL	CG1	23.719	0.3	1
616	.	52	VAL	CG2	21.469	0.3	1
617	.	52	VAL	N	116.639	0.3	1
618	.	53	LYS	H	7.948	0.020	1
619	.	53	LYS	HA	4.436	0.020	1
620	.	53	LYS	HB2	1.548	0.020	2
621	.	53	LYS	HB3	0.985	0.020	2
622	.	53	LYS	HG2	1.199	0.020	2
623	.	53	LYS	HG3	1.138	0.020	2
624	.	53	LYS	HD2	1.412	0.020	1
625	.	53	LYS	HD3	1.412	0.020	1
626	.	53	LYS	HE2	2.900	0.020	2
627	.	53	LYS	HE3	2.791	0.020	2
628	.	53	LYS	C	174.364	0.3	1
629	.	53	LYS	CA	53.896	0.3	1
630	.	53	LYS	CB	34.921	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	.	53	LYS	CG	24.998	0.3	1
632	.	53	LYS	CD	28.816	0.3	1
633	.	53	LYS	CE	41.996	0.3	1
634	.	53	LYS	N	126.272	0.3	1
635	.	54	ILE	H	8.433	0.020	1
636	.	54	ILE	HA	4.581	0.020	1
637	.	54	ILE	HB	1.757	0.020	1
638	.	54	ILE	HG12	1.379	0.020	2
639	.	54	ILE	HG13	0.950	0.020	2
640	.	54	ILE	HG2	0.733	0.020	1
641	.	54	ILE	HG2	0.733	0.020	1
642	.	54	ILE	HG2	0.733	0.020	1
643	.	54	ILE	HD1	0.622	0.020	1
644	.	54	ILE	HD1	0.622	0.020	1
645	.	54	ILE	HD1	0.622	0.020	1
646	.	54	ILE	C	175.988	0.3	1
647	.	54	ILE	CA	59.245	0.3	1
648	.	54	ILE	CB	37.389	0.3	1
649	.	54	ILE	CG1	27.167	0.3	1
650	.	54	ILE	CG2	17.183	0.3	1
651	.	54	ILE	CD1	12.587	0.3	1
652	.	54	ILE	N	122.204	0.3	1
653	.	55	ALA	H	9.197	0.020	1
654	.	55	ALA	HA	4.747	0.020	1
655	.	55	ALA	HB	1.369	0.020	1
656	.	55	ALA	HB	1.369	0.020	1
657	.	55	ALA	HB	1.369	0.020	1
658	.	55	ALA	C	173.904	0.3	1
659	.	55	ALA	CA	50.853	0.3	1
660	.	55	ALA	CB	23.098	0.3	1
661	.	55	ALA	N	131.213	0.3	1
662	.	56	GLU	H	8.250	0.020	1
663	.	56	GLU	HA	4.960	0.020	1
664	.	56	GLU	HB2	2.032	0.020	2
665	.	56	GLU	HB3	1.861	0.020	2
666	.	56	GLU	C	174.706	0.3	1
667	.	56	GLU	CA	52.131	0.3	1
668	.	56	GLU	CB	32.022	0.3	1
669	.	56	GLU	N	117.419	0.3	1
670	.	57	PRO	HA	4.674	0.020	1
671	.	57	PRO	HB2	2.207	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	.	57	PRO	HB3	1.836	0.020	2
673	.	57	PRO	HG2	2.480	0.020	2
674	.	57	PRO	HG3	2.096	0.020	2
675	.	57	PRO	HD2	4.054	0.020	2
676	.	57	PRO	HD3	3.676	0.020	2
677	.	57	PRO	C	175.124	0.3	1
678	.	57	PRO	CA	61.482	0.3	1
679	.	57	PRO	CB	32.613	0.3	1
680	.	57	PRO	CG	26.263	0.3	1
681	.	57	PRO	CD	49.933	0.3	1
682	.	58	SER	H	10.041	0.020	1
683	.	58	SER	HA	4.421	0.020	1
684	.	58	SER	HB2	4.649	0.020	1
685	.	58	SER	HB3	4.222	0.020	1
686	.	58	SER	C	175.137	0.3	1
687	.	58	SER	CA	58.151	0.3	1
688	.	58	SER	CB	65.174	0.3	1
689	.	58	SER	N	117.943	0.3	1
690	.	59	LYS	H	8.756	0.020	1
691	.	59	LYS	HA	3.920	0.020	1
692	.	59	LYS	HB2	1.937	0.020	2
693	.	59	LYS	HB3	1.821	0.020	2
694	.	59	LYS	HE2	2.340	0.020	1
695	.	59	LYS	HE3	2.340	0.020	1
696	.	59	LYS	C	178.138	0.3	1
697	.	59	LYS	CA	59.534	0.3	1
698	.	59	LYS	CB	32.305	0.3	1
699	.	59	LYS	CG	24.528	0.3	1
700	.	59	LYS	CD	28.554	0.3	1
701	.	59	LYS	N	122.229	0.3	1
702	.	60	GLU	H	8.676	0.020	1
703	.	60	GLU	HA	4.094	0.020	1
704	.	60	GLU	HB2	2.113	0.020	1
705	.	60	GLU	HB3	2.113	0.020	2
706	.	60	GLU	C	179.668	0.3	1
707	.	60	GLU	CA	60.215	0.3	1
708	.	60	GLU	CB	28.793	0.3	1
709	.	60	GLU	N	117.491	0.3	1
710	.	61	SER	H	7.836	0.020	1
711	.	61	SER	HA	4.254	0.020	1
712	.	61	SER	HB2	4.200	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	.	61	SER	HB3	4.200	0.020	1
714	.	61	SER	C	175.515	0.3	1
715	.	61	SER	CA	61.572	0.3	1
716	.	61	SER	N	118.226	0.3	1
717	.	62	ILE	H	7.811	0.020	1
718	.	62	ILE	HA	3.342	0.020	1
719	.	62	ILE	HB	1.976	0.020	1
720	.	62	ILE	HG12	1.609	0.020	2
721	.	62	ILE	HG13	0.773	0.020	2
722	.	62	ILE	HG2	0.878	0.020	1
723	.	62	ILE	HG2	0.878	0.020	1
724	.	62	ILE	HG2	0.878	0.020	1
725	.	62	ILE	HD1	0.844	0.020	1
726	.	62	ILE	HD1	0.844	0.020	1
727	.	62	ILE	HD1	0.844	0.020	1
728	.	62	ILE	C	177.316	0.3	1
729	.	62	ILE	CA	65.968	0.3	1
730	.	62	ILE	CB	37.688	0.3	1
731	.	62	ILE	CG1	29.307	0.3	1
732	.	62	ILE	CG2	16.902	0.3	1
733	.	62	ILE	CD1	13.491	0.3	1
734	.	62	ILE	N	123.056	0.3	1
735	.	63	ASP	H	8.547	0.020	1
736	.	63	ASP	HA	4.322	0.020	1
737	.	63	ASP	HB2	2.732	0.020	1
738	.	63	ASP	HB3	2.732	0.020	2
739	.	63	ASP	C	179.055	0.3	1
740	.	63	ASP	CA	57.482	0.3	1
741	.	63	ASP	CB	40.051	0.3	1
742	.	63	ASP	N	118.355	0.3	1
743	.	64	ARG	H	7.537	0.020	1
744	.	64	ARG	HA	4.025	0.020	1
745	.	64	ARG	HB2	1.805	0.020	1
746	.	64	ARG	HB3	1.805	0.020	1
747	.	64	ARG	HG2	1.300	0.020	1
748	.	64	ARG	HG3	1.300	0.020	1
749	.	64	ARG	HD2	3.026	0.020	1
750	.	64	ARG	HD3	3.026	0.020	1
751	.	64	ARG	C	177.687	0.3	1
752	.	64	ARG	CA	58.182	0.3	1
753	.	64	ARG	CB	29.070	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	.	64	ARG	CG	26.347	0.3	1
755	.	64	ARG	CD	42.578	0.3	1
756	.	64	ARG	N	119.966	0.3	1
757	.	65	ILE	H	7.580	0.020	1
758	.	65	ILE	HA	3.495	0.020	1
759	.	65	ILE	HB	2.276	0.020	1
760	.	65	ILE	HG12	1.963	0.020	2
761	.	65	ILE	HG13	1.136	0.020	2
762	.	65	ILE	HG2	0.903	0.020	1
763	.	65	ILE	HG2	0.903	0.020	1
764	.	65	ILE	HG2	0.903	0.020	1
765	.	65	ILE	HD1	0.413	0.020	1
766	.	65	ILE	HD1	0.413	0.020	1
767	.	65	ILE	HD1	0.413	0.020	1
768	.	65	ILE	C	177.952	0.3	1
769	.	65	ILE	CA	62.197	0.3	1
770	.	65	ILE	CB	34.696	0.3	1
771	.	65	ILE	CG1	27.427	0.3	1
772	.	65	ILE	CG2	19.595	0.3	1
773	.	65	ILE	CD1	10.169	0.3	1
774	.	65	ILE	N	118.440	0.3	1
775	.	66	ILE	H	8.413	0.020	1
776	.	66	ILE	HA	3.460	0.020	1
777	.	66	ILE	HB	1.949	0.020	1
778	.	66	ILE	HG12	1.099	0.020	2
779	.	66	ILE	HG13	0.836	0.020	2
780	.	66	ILE	HG2	0.887	0.020	1
781	.	66	ILE	HG2	0.887	0.020	1
782	.	66	ILE	HG2	0.887	0.020	1
783	.	66	ILE	HD1	0.841	0.020	1
784	.	66	ILE	HD1	0.841	0.020	1
785	.	66	ILE	HD1	0.841	0.020	1
786	.	66	ILE	C	177.687	0.3	1
787	.	66	ILE	CA	65.413	0.3	1
788	.	66	ILE	CB	37.369	0.3	1
789	.	66	ILE	CG1	29.356	0.3	1
790	.	66	ILE	CG2	17.176	0.3	1
791	.	66	ILE	CD1	12.635	0.3	1
792	.	66	ILE	N	120.222	0.3	1
793	.	67	GLN	H	7.929	0.020	1
794	.	67	GLN	HA	3.961	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	.	67	GLN	HB2	2.391	0.020	2
796	.	67	GLN	HB3	2.213	0.020	2
797	.	67	GLN	HG2	2.451	0.020	2
798	.	67	GLN	HG3	2.387	0.020	2
799	.	67	GLN	HE21	7.617	0.020	1
800	.	67	GLN	HE22	6.759	0.020	1
801	.	67	GLN	C	178.849	0.3	1
802	.	67	GLN	CA	59.395	0.3	1
803	.	67	GLN	CB	27.968	0.3	1
804	.	67	GLN	CG	33.350	0.3	1
805	.	67	GLN	N	118.249	0.3	1
806	.	67	GLN	NE2	112.285	0.3	1
807	.	68	VAL	H	7.811	0.020	1
808	.	68	VAL	HA	3.820	0.020	1
809	.	68	VAL	HB	2.058	0.020	1
810	.	68	VAL	HG1	1.022	0.020	1
811	.	68	VAL	HG1	1.022	0.020	1
812	.	68	VAL	HG1	1.022	0.020	1
813	.	68	VAL	HG2	0.935	0.020	1
814	.	68	VAL	HG2	0.935	0.020	1
815	.	68	VAL	HG2	0.935	0.020	1
816	.	68	VAL	C	178.442	0.3	1
817	.	68	VAL	CA	65.745	0.3	1
818	.	68	VAL	CB	31.757	0.3	1
819	.	68	VAL	CG1	22.595	0.3	1
820	.	68	VAL	CG2	22.036	0.3	1
821	.	68	VAL	N	119.041	0.3	1
822	.	69	ALA	H	8.824	0.020	1
823	.	69	ALA	HA	3.939	0.020	1
824	.	69	ALA	HB	1.246	0.020	1
825	.	69	ALA	HB	1.246	0.020	1
826	.	69	ALA	HB	1.246	0.020	1
827	.	69	ALA	C	179.998	0.3	1
828	.	69	ALA	CA	54.796	0.3	1
829	.	69	ALA	CB	17.835	0.3	1
830	.	69	ALA	N	122.910	0.3	1
831	.	70	LYS	H	8.641	0.020	1
832	.	70	LYS	HA	4.019	0.020	1
833	.	70	LYS	HB2	1.977	0.020	2
834	.	70	LYS	HB3	1.939	0.020	2
835	.	70	LYS	HG2	1.657	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	.	70	LYS	HG3	1.423	0.020	2
837	.	70	LYS	HE2	2.910	0.020	2
838	.	70	LYS	HE3	2.857	0.020	2
839	.	70	LYS	C	179.505	0.3	1
840	.	70	LYS	CA	59.802	0.3	1
841	.	70	LYS	CB	32.580	0.3	1
842	.	70	LYS	CG	25.813	0.3	1
843	.	70	LYS	CD	29.573	0.3	1
844	.	70	LYS	CE	41.737	0.3	1
845	.	70	LYS	N	119.460	0.3	1
846	.	71	GLU	H	7.965	0.020	1
847	.	71	GLU	HA	4.126	0.020	1
848	.	71	GLU	HB2	2.188	0.020	1
849	.	71	GLU	HB3	2.188	0.020	1
850	.	71	GLU	C	178.341	0.3	1
851	.	71	GLU	CA	58.836	0.3	1
852	.	71	GLU	CB	29.393	0.3	1
853	.	71	GLU	CG	36.259	0.3	1
854	.	71	GLU	N	119.872	0.3	1
855	.	72	THR	H	7.799	0.020	1
856	.	72	THR	HA	4.352	0.020	1
857	.	72	THR	HB	4.313	0.020	1
858	.	72	THR	HG2	1.226	0.020	1
859	.	72	THR	HG2	1.226	0.020	1
860	.	72	THR	HG2	1.226	0.020	1
861	.	72	THR	C	175.772	0.3	1
862	.	72	THR	CA	62.332	0.3	1
863	.	72	THR	CB	70.369	0.3	1
864	.	72	THR	CG2	22.073	0.3	1
865	.	72	THR	N	107.140	0.3	1
866	.	73	GLY	H	7.668	0.020	1
867	.	73	GLY	HA2	4.203	0.020	2
868	.	73	GLY	HA3	3.948	0.020	2
869	.	73	GLY	C	174.856	0.3	1
870	.	73	GLY	CA	45.930	0.3	1
871	.	73	GLY	N	109.329	0.3	1
872	.	74	GLU	H	8.169	0.020	1
873	.	74	GLU	HA	4.516	0.020	1
874	.	74	GLU	HB2	2.177	0.020	1
875	.	74	GLU	HB3	2.177	0.020	2
876	.	74	GLU	C	177.003	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	.	74	GLU	CA	56.183	0.3	1
878	.	74	GLU	CB	30.392	0.3	1
879	.	74	GLU	CG	35.356	0.3	1
880	.	74	GLU	N	118.619	0.3	1
881	.	75	VAL	H	7.431	0.020	1
882	.	75	VAL	HA	3.697	0.020	1
883	.	75	VAL	HB	1.747	0.020	1
884	.	75	VAL	HG1	0.986	0.020	1
885	.	75	VAL	HG1	0.986	0.020	1
886	.	75	VAL	HG1	0.986	0.020	1
887	.	75	VAL	HG2	0.949	0.020	1
888	.	75	VAL	HG2	0.949	0.020	1
889	.	75	VAL	HG2	0.949	0.020	1
890	.	75	VAL	C	175.152	0.3	1
891	.	75	VAL	CA	64.682	0.3	1
892	.	75	VAL	CB	31.757	0.3	1
893	.	75	VAL	CG1	21.595	0.3	1
894	.	75	VAL	CG2	19.615	0.3	1
895	.	75	VAL	N	119.348	0.3	1
896	.	76	ASN	H	8.277	0.020	1
897	.	76	ASN	HA	4.647	0.020	1
898	.	76	ASN	HB2	2.841	0.020	2
899	.	76	ASN	HB3	2.736	0.020	2
900	.	76	ASN	HD21	7.585	0.020	1
901	.	76	ASN	HD22	6.849	0.020	1
902	.	76	ASN	C	175.344	0.3	1
903	.	76	ASN	CA	54.448	0.3	1
904	.	76	ASN	CB	38.272	0.3	1
905	.	76	ASN	N	117.648	0.3	1
906	.	76	ASN	ND2	112.690	0.3	1
907	.	77	GLU	H	7.864	0.020	1
908	.	77	GLU	HA	4.358	0.020	1
909	.	77	GLU	HB2	2.252	0.020	2
910	.	77	GLU	HB3	1.849	0.020	2
911	.	77	GLU	C	175.909	0.3	1
912	.	77	GLU	CA	56.027	0.3	1
913	.	77	GLU	CB	30.197	0.3	1
914	.	77	GLU	CG	36.813	0.3	1
915	.	77	GLU	N	117.521	0.3	1
916	.	78	LEU	H	7.178	0.020	1
917	.	78	LEU	HA	4.673	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	.	78	LEU	HB2	1.716	0.020	2
919	.	78	LEU	HB3	1.470	0.020	2
920	.	78	LEU	HG	0.635	0.020	1
921	.	78	LEU	HD1	1.222	0.020	1
922	.	78	LEU	HD1	1.222	0.020	1
923	.	78	LEU	HD1	1.222	0.020	1
924	.	78	LEU	HD2	0.644	0.020	1
925	.	78	LEU	HD2	0.644	0.020	1
926	.	78	LEU	HD2	0.644	0.020	1
927	.	78	LEU	C	176.581	0.3	1
928	.	78	LEU	CA	53.821	0.3	1
929	.	78	LEU	CB	43.331	0.3	1
930	.	78	LEU	CG	26.337	0.3	1
931	.	78	LEU	CD1	23.761	0.3	1
932	.	78	LEU	CD2	21.716	0.3	1
933	.	78	LEU	N	119.109	0.3	1
934	.	79	SER	H	9.273	0.020	1
935	.	79	SER	HA	4.560	0.020	1
936	.	79	SER	HB2	3.967	0.020	1
937	.	79	SER	HB3	4.363	0.020	1
938	.	79	SER	C	174.172	0.3	1
939	.	79	SER	CA	56.361	0.3	1
940	.	79	SER	CB	65.728	0.3	1
941	.	79	SER	N	120.457	0.3	1
942	.	80	LYS	H	8.583	0.020	1
943	.	80	LYS	HA	3.948	0.020	1
944	.	80	LYS	HB2	1.886	0.020	2
945	.	80	LYS	HB3	1.778	0.020	2
946	.	80	LYS	HG2	1.505	0.020	2
947	.	80	LYS	HG3	1.343	0.020	2
948	.	80	LYS	HD2	1.681	0.020	1
949	.	80	LYS	HD3	1.681	0.020	1
950	.	80	LYS	HE2	2.877	0.020	2
951	.	80	LYS	HE3	3.087	0.020	2
952	.	80	LYS	C	178.557	0.3	1
953	.	80	LYS	CA	60.776	0.3	1
954	.	80	LYS	CB	32.544	0.3	1
955	.	80	LYS	CG	24.733	0.3	1
956	.	80	LYS	CD	29.568	0.3	1
957	.	80	LYS	CE	43.654	0.3	1
958	.	80	LYS	N	120.724	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
959	.	81	ALA	H	8.162	0.020	1
960	.	81	ALA	HA	3.972	0.020	1
961	.	81	ALA	HB	1.202	0.020	1
962	.	81	ALA	HB	1.202	0.020	1
963	.	81	ALA	HB	1.202	0.020	1
964	.	81	ALA	C	177.837	0.3	1
965	.	81	ALA	CA	55.245	0.3	1
966	.	81	ALA	CB	18.348	0.3	1
967	.	81	ALA	N	119.810	0.3	1
968	.	82	ASP	H	7.793	0.020	1
969	.	82	ASP	HA	4.160	0.020	1
970	.	82	ASP	HB2	3.024	0.020	2
971	.	82	ASP	HB3	2.365	0.020	2
972	.	82	ASP	C	177.948	0.3	1
973	.	82	ASP	CA	57.100	0.3	1
974	.	82	ASP	CB	41.201	0.3	1
975	.	82	ASP	N	117.428	0.3	1
976	.	83	ILE	H	7.855	0.020	1
977	.	83	ILE	HA	3.502	0.020	1
978	.	83	ILE	HB	1.988	0.020	1
979	.	83	ILE	HG12	1.667	0.020	2
980	.	83	ILE	HG13	0.909	0.020	2
981	.	83	ILE	HG2	1.259	0.020	1
982	.	83	ILE	HG2	1.259	0.020	1
983	.	83	ILE	HG2	1.259	0.020	1
984	.	83	ILE	HD1	0.716	0.020	1
985	.	83	ILE	HD1	0.716	0.020	1
986	.	83	ILE	HD1	0.716	0.020	1
987	.	83	ILE	C	177.509	0.3	1
988	.	83	ILE	CA	64.876	0.3	1
989	.	83	ILE	CB	37.663	0.3	1
990	.	83	ILE	CG1	30.127	0.3	1
991	.	83	ILE	CG2	17.973	0.3	1
992	.	83	ILE	CD1	12.595	0.3	1
993	.	83	ILE	N	117.303	0.3	1
994	.	84	GLU	H	8.160	0.020	1
995	.	84	GLU	HA	3.823	0.020	1
996	.	84	GLU	HB2	2.283	0.020	2
997	.	84	GLU	HB3	2.016	0.020	2
998	.	84	GLU	HG2	2.728	0.020	2
999	.	84	GLU	HG3	2.093	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1000	.	84	GLU	C	178.524	0.3	1
1001	.	84	GLU	CA	60.579	0.3	1
1002	.	84	GLU	CB	30.150	0.3	1
1003	.	84	GLU	CG	37.933	0.3	1
1004	.	84	GLU	N	118.547	0.3	1
1005	.	85	VAL	H	8.848	0.020	1
1006	.	85	VAL	HA	3.623	0.020	1
1007	.	85	VAL	HB	2.269	0.020	1
1008	.	85	VAL	HG1	1.189	0.020	1
1009	.	85	VAL	HG1	1.189	0.020	1
1010	.	85	VAL	HG1	1.189	0.020	1
1011	.	85	VAL	HG2	0.965	0.020	1
1012	.	85	VAL	HG2	0.965	0.020	1
1013	.	85	VAL	HG2	0.965	0.020	1
1014	.	85	VAL	C	178.074	0.3	1
1015	.	85	VAL	CA	66.766	0.3	1
1016	.	85	VAL	CB	31.445	0.3	1
1017	.	85	VAL	CG1	23.745	0.3	1
1018	.	85	VAL	CG2	21.400	0.3	1
1019	.	85	VAL	N	120.337	0.3	1
1020	.	86	LEU	H	7.850	0.020	1
1021	.	86	LEU	HA	3.789	0.020	1
1022	.	86	LEU	HB2	2.171	0.020	2
1023	.	86	LEU	HB3	1.122	0.020	2
1024	.	86	LEU	HG	1.730	0.020	1
1025	.	86	LEU	HD1	0.930	0.020	1
1026	.	86	LEU	HD1	0.930	0.020	1
1027	.	86	LEU	HD1	0.930	0.020	1
1028	.	86	LEU	HD2	0.921	0.020	1
1029	.	86	LEU	HD2	0.921	0.020	1
1030	.	86	LEU	HD2	0.921	0.020	1
1031	.	86	LEU	C	178.045	0.3	1
1032	.	86	LEU	CA	58.411	0.3	1
1033	.	86	LEU	CB	43.282	0.3	1
1034	.	86	LEU	CG	27.948	0.3	1
1035	.	86	LEU	CD1	26.333	0.3	1
1036	.	86	LEU	CD2	23.328	0.3	1
1037	.	86	LEU	N	120.523	0.3	1
1038	.	87	ALA	H	8.704	0.020	1
1039	.	87	ALA	HA	3.867	0.020	1
1040	.	87	ALA	HB	1.360	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1041	.	87	ALA	HB	1.360	0.020	1
1042	.	87	ALA	HB	1.360	0.020	1
1043	.	87	ALA	C	179.013	0.3	1
1044	.	87	ALA	CA	54.973	0.3	1
1045	.	87	ALA	CB	18.791	0.3	1
1046	.	87	ALA	N	120.596	0.3	1
1047	.	88	LEU	H	8.831	0.020	1
1048	.	88	LEU	HA	4.067	0.020	1
1049	.	88	LEU	HB2	1.918	0.020	2
1050	.	88	LEU	HB3	1.293	0.020	2
1051	.	88	LEU	HG	0.705	0.020	1
1052	.	88	LEU	HD1	0.823	0.020	1
1053	.	88	LEU	HD1	0.823	0.020	1
1054	.	88	LEU	HD1	0.823	0.020	1
1055	.	88	LEU	HD2	0.639	0.020	1
1056	.	88	LEU	HD2	0.639	0.020	1
1057	.	88	LEU	HD2	0.639	0.020	1
1058	.	88	LEU	C	178.211	0.3	1
1059	.	88	LEU	CA	57.610	0.3	1
1060	.	88	LEU	CB	41.811	0.3	1
1061	.	88	LEU	CG	27.117	0.3	1
1062	.	88	LEU	CD1	25.549	0.3	1
1063	.	88	LEU	CD2	22.857	0.3	1
1064	.	88	LEU	N	119.230	0.3	1
1065	.	89	ALA	H	8.423	0.020	1
1066	.	89	ALA	HA	3.686	0.020	1
1067	.	89	ALA	HB	1.389	0.020	1
1068	.	89	ALA	HB	1.389	0.020	1
1069	.	89	ALA	HB	1.389	0.020	1
1070	.	89	ALA	C	179.191	0.3	1
1071	.	89	ALA	CA	56.200	0.3	1
1072	.	89	ALA	CB	18.177	0.3	1
1073	.	89	ALA	N	120.223	0.3	1
1074	.	90	TYR	H	8.688	0.020	1
1075	.	90	TYR	HA	4.150	0.020	1
1076	.	90	TYR	HB2	3.349	0.020	2
1077	.	90	TYR	HB3	3.109	0.020	2
1078	.	90	TYR	HD1	7.076	0.020	1
1079	.	90	TYR	HD2	7.076	0.020	1
1080	.	90	TYR	HE1	6.922	0.020	1
1081	.	90	TYR	HE2	6.922	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1082	.	90	TYR	C	177.663	0.3	1
1083	.	90	TYR	CA	61.672	0.3	1
1084	.	90	TYR	CB	38.676	0.3	1
1085	.	90	TYR	CD1	132.594	0.3	1
1086	.	90	TYR	CE1	118.284	0.3	1
1087	.	90	TYR	N	117.864	0.3	1
1088	.	91	GLU	H	8.557	0.020	1
1089	.	91	GLU	HA	3.798	0.020	1
1090	.	91	GLU	HB2	2.540	0.020	2
1091	.	91	GLU	HB3	2.183	0.020	2
1092	.	91	GLU	C	178.380	0.3	1
1093	.	91	GLU	CA	59.603	0.3	1
1094	.	91	GLU	CB	30.958	0.3	1
1095	.	91	GLU	CG	36.420	0.3	1
1096	.	91	GLU	N	121.649	0.3	1
1097	.	92	LEU	H	8.143	0.020	1
1098	.	92	LEU	HA	4.148	0.020	1
1099	.	92	LEU	HB2	1.362	0.020	2
1100	.	92	LEU	HB3	1.331	0.020	2
1101	.	92	LEU	HG	1.623	0.020	1
1102	.	92	LEU	HD1	0.191	0.020	1
1103	.	92	LEU	HD1	0.191	0.020	1
1104	.	92	LEU	HD1	0.191	0.020	1
1105	.	92	LEU	HD2	0.587	0.020	1
1106	.	92	LEU	HD2	0.587	0.020	1
1107	.	92	LEU	HD2	0.587	0.020	1
1108	.	92	LEU	C	176.466	0.3	1
1109	.	92	LEU	CA	54.622	0.3	1
1110	.	92	LEU	CB	41.972	0.3	1
1111	.	92	LEU	CG	26.269	0.3	1
1112	.	92	LEU	CD1	25.001	0.3	1
1113	.	92	LEU	CD2	21.482	0.3	1
1114	.	92	LEU	N	115.162	0.3	1
1115	.	93	LYS	H	7.769	0.020	1
1116	.	93	LYS	HA	3.748	0.020	1
1117	.	93	LYS	HB2	2.104	0.020	2
1118	.	93	LYS	HB3	1.797	0.020	2
1119	.	93	LYS	HG2	1.308	0.020	1
1120	.	93	LYS	HG3	1.308	0.020	1
1121	.	93	LYS	HE2	2.919	0.020	1
1122	.	93	LYS	HE3	2.919	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1123	.	93	LYS	C	176.872	0.3	1
1124	.	93	LYS	CA	56.707	0.3	1
1125	.	93	LYS	CB	28.529	0.3	1
1126	.	93	LYS	CG	24.688	0.3	1
1127	.	93	LYS	CE	42.332	0.3	1
1128	.	93	LYS	N	118.438	0.3	1
1129	.	94	GLY	H	8.611	0.020	1
1130	.	94	GLY	HA2	4.554	0.020	2
1131	.	94	GLY	HA3	3.232	0.020	2
1132	.	94	GLY	C	172.121	0.3	1
1133	.	94	GLY	CA	44.071	0.3	1
1134	.	94	GLY	N	104.932	0.3	1
1135	.	95	GLU	H	8.204	0.020	1
1136	.	95	GLU	HA	4.864	0.020	1
1137	.	95	GLU	HB2	1.827	0.020	2
1138	.	95	GLU	HB3	1.774	0.020	2
1139	.	95	GLU	HG2	1.950	0.020	1
1140	.	95	GLU	HG3	1.950	0.020	1
1141	.	95	GLU	C	176.897	0.3	1
1142	.	95	GLU	CA	54.038	0.3	1
1143	.	95	GLU	CB	32.547	0.3	1
1144	.	95	GLU	CG	36.379	0.3	1
1145	.	95	GLU	N	119.896	0.3	1
1146	.	96	ILE	H	8.321	0.020	1
1147	.	96	ILE	HA	4.892	0.020	1
1148	.	96	ILE	HB	1.523	0.020	1
1149	.	96	ILE	HG12	1.189	0.020	2
1150	.	96	ILE	HG13	0.807	0.020	2
1151	.	96	ILE	HG2	0.773	0.020	1
1152	.	96	ILE	HG2	0.773	0.020	1
1153	.	96	ILE	HG2	0.773	0.020	1
1154	.	96	ILE	HD1	0.816	0.020	1
1155	.	96	ILE	HD1	0.816	0.020	1
1156	.	96	ILE	HD1	0.816	0.020	1
1157	.	96	ILE	C	173.475	0.3	1
1158	.	96	ILE	CA	59.773	0.3	1
1159	.	96	ILE	CB	41.720	0.3	1
1160	.	96	ILE	CG1	29.027	0.3	1
1161	.	96	ILE	CG2	17.714	0.3	1
1162	.	96	ILE	CD1	15.827	0.3	1
1163	.	96	ILE	N	122.806	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1164	.	97	PHE	H	9.104	0.020	1
1165	.	97	PHE	HA	5.358	0.020	1
1166	.	97	PHE	HB2	3.417	0.020	2
1167	.	97	PHE	HB3	2.605	0.020	2
1168	.	97	PHE	HD1	6.978	0.020	1
1169	.	97	PHE	HD2	6.978	0.020	1
1170	.	97	PHE	HE1	6.941	0.020	1
1171	.	97	PHE	HE2	6.941	0.020	1
1172	.	97	PHE	HZ	7.114	0.020	1
1173	.	97	PHE	C	173.420	0.3	1
1174	.	97	PHE	CA	53.955	0.3	1
1175	.	97	PHE	CB	40.077	0.3	1
1176	.	97	PHE	CD1	130.039	0.3	1
1177	.	97	PHE	CE1	129.747	0.3	1
1178	.	97	PHE	CZ	129.037	0.3	1
1179	.	97	PHE	N	130.540	0.3	1
1180	.	98	SER	H	7.925	0.020	1
1181	.	98	SER	HA	4.481	0.020	1
1182	.	98	SER	HB2	3.825	0.020	1
1183	.	98	SER	HB3	3.079	0.020	1
1184	.	98	SER	C	173.708	0.3	1
1185	.	98	SER	CA	58.036	0.3	1
1186	.	98	SER	CB	65.697	0.3	1
1187	.	98	SER	N	114.132	0.3	1
1188	.	99	ASP	H	8.369	0.020	1
1189	.	99	ASP	HA	4.843	0.020	1
1190	.	99	ASP	HB2	2.734	0.020	1
1191	.	99	ASP	HB3	2.734	0.020	2
1192	.	99	ASP	C	175.490	0.3	1
1193	.	99	ASP	CA	53.337	0.3	1
1194	.	99	ASP	CB	42.095	0.3	1
1195	.	99	ASP	N	126.303	0.3	1
1196	.	100	ASP	H	8.753	0.020	1
1197	.	100	ASP	HA	4.523	0.020	1
1198	.	100	ASP	HB2	2.755	0.020	1
1199	.	100	ASP	HB3	2.755	0.020	2
1200	.	100	ASP	C	176.058	0.3	1
1201	.	100	ASP	CA	54.296	0.3	1
1202	.	100	ASP	CB	43.231	0.3	1
1203	.	100	ASP	N	122.952	0.3	1
1204	.	101	TYR	H	8.489	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1205	.	101	TYR	HA	3.918	0.020	1
1206	.	101	TYR	HB2	3.046	0.020	2
1207	.	101	TYR	HB3	2.870	0.020	2
1208	.	101	TYR	HD1	7.051	0.020	1
1209	.	101	TYR	HD2	7.051	0.020	1
1210	.	101	TYR	HE1	6.825	0.020	1
1211	.	101	TYR	HE2	6.825	0.020	1
1212	.	101	TYR	C	177.013	0.3	1
1213	.	101	TYR	CA	60.760	0.3	1
1214	.	101	TYR	CB	38.486	0.3	1
1215	.	101	TYR	CD1	133.084	0.3	1
1216	.	101	TYR	CE1	117.962	0.3	1
1217	.	101	TYR	N	126.865	0.3	1
1218	.	102	ASN	H	8.178	0.020	1
1219	.	102	ASN	HA	4.334	0.020	1
1220	.	102	ASN	HB2	2.968	0.020	2
1221	.	102	ASN	HB3	2.416	0.020	2
1222	.	102	ASN	HD21	8.331	0.020	1
1223	.	102	ASN	HD22	7.109	0.020	1
1224	.	102	ASN	C	177.809	0.3	1
1225	.	102	ASN	CA	56.444	0.3	1
1226	.	102	ASN	CB	37.936	0.3	1
1227	.	102	ASN	N	117.785	0.3	1
1228	.	102	ASN	ND2	114.687	0.3	1
1229	.	103	VAL	H	8.138	0.020	1
1230	.	103	VAL	HA	3.424	0.020	1
1231	.	103	VAL	HB	2.235	0.020	1
1232	.	103	VAL	HG1	0.955	0.020	1
1233	.	103	VAL	HG1	0.955	0.020	1
1234	.	103	VAL	HG1	0.955	0.020	1
1235	.	103	VAL	HG2	0.860	0.020	1
1236	.	103	VAL	HG2	0.860	0.020	1
1237	.	103	VAL	HG2	0.860	0.020	1
1238	.	103	VAL	C	177.454	0.3	1
1239	.	103	VAL	CA	66.513	0.3	1
1240	.	103	VAL	CB	31.485	0.3	1
1241	.	103	VAL	CG1	22.311	0.3	1
1242	.	103	VAL	CG2	21.342	0.3	1
1243	.	103	VAL	N	121.355	0.3	1
1244	.	104	GLN	H	7.802	0.020	1
1245	.	104	GLN	HA	2.909	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1246	.	104	GLN	HB2	1.461	0.020	2
1247	.	104	GLN	HB3	0.951	0.020	2
1248	.	104	GLN	HG2	1.953	0.020	2
1249	.	104	GLN	HG3	1.158	0.020	2
1250	.	104	GLN	HE21	7.295	0.020	1
1251	.	104	GLN	HE22	6.555	0.020	1
1252	.	104	GLN	C	177.755	0.3	1
1253	.	104	GLN	CA	58.961	0.3	1
1254	.	104	GLN	CB	27.154	0.3	1
1255	.	104	GLN	CG	32.533	0.3	1
1256	.	104	GLN	N	117.281	0.3	1
1257	.	104	GLN	NE2	108.243	0.3	1
1258	.	105	ASN	H	7.967	0.020	1
1259	.	105	ASN	HA	4.260	0.020	1
1260	.	105	ASN	HB2	2.750	0.020	2
1261	.	105	ASN	HB3	2.642	0.020	2
1262	.	105	ASN	HD21	7.834	0.020	1
1263	.	105	ASN	HD22	6.514	0.020	1
1264	.	105	ASN	C	177.765	0.3	1
1265	.	105	ASN	CA	56.523	0.3	1
1266	.	105	ASN	CB	38.732	0.3	1
1267	.	105	ASN	N	116.878	0.3	1
1268	.	105	ASN	ND2	112.652	0.3	1
1269	.	106	ILE	H	7.771	0.020	1
1270	.	106	ILE	HA	3.683	0.020	1
1271	.	106	ILE	HB	1.925	0.020	1
1272	.	106	ILE	HG12	1.570	0.020	2
1273	.	106	ILE	HG13	1.400	0.020	2
1274	.	106	ILE	HG2	0.855	0.020	1
1275	.	106	ILE	HG2	0.855	0.020	1
1276	.	106	ILE	HG2	0.855	0.020	1
1277	.	106	ILE	HD1	0.652	0.020	1
1278	.	106	ILE	HD1	0.652	0.020	1
1279	.	106	ILE	HD1	0.652	0.020	1
1280	.	106	ILE	C	177.349	0.3	1
1281	.	106	ILE	CA	63.558	0.3	1
1282	.	106	ILE	CB	35.532	0.3	1
1283	.	106	ILE	CG1	28.496	0.3	1
1284	.	106	ILE	CG2	18.696	0.3	1
1285	.	106	ILE	CD1	11.505	0.3	1
1286	.	106	ILE	N	118.502	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1287	.	107	ALA	H	8.507	0.020	1
1288	.	107	ALA	HA	3.824	0.020	1
1289	.	107	ALA	HB	1.448	0.020	1
1290	.	107	ALA	HB	1.448	0.020	1
1291	.	107	ALA	HB	1.448	0.020	1
1292	.	107	ALA	C	179.509	0.3	1
1293	.	107	ALA	CA	56.202	0.3	1
1294	.	107	ALA	CB	17.457	0.3	1
1295	.	107	ALA	N	121.756	0.3	1
1296	.	108	SER	H	8.189	0.020	1
1297	.	108	SER	HA	4.404	0.020	1
1298	.	108	SER	HB2	4.109	0.020	1
1299	.	108	SER	HB3	4.109	0.020	1
1300	.	108	SER	C	178.192	0.3	1
1301	.	108	SER	CA	61.746	0.3	1
1302	.	108	SER	CB	62.859	0.3	1
1303	.	108	SER	N	112.032	0.3	1
1304	.	109	LEU	H	7.764	0.020	1
1305	.	109	LEU	HA	4.143	0.020	1
1306	.	109	LEU	HB2	1.915	0.020	2
1307	.	109	LEU	HB3	1.591	0.020	2
1308	.	109	LEU	HG	1.780	0.020	1
1309	.	109	LEU	HD1	1.272	0.020	1
1310	.	109	LEU	HD1	1.272	0.020	1
1311	.	109	LEU	HD1	1.272	0.020	1
1312	.	109	LEU	HD2	0.852	0.020	1
1313	.	109	LEU	HD2	0.852	0.020	1
1314	.	109	LEU	HD2	0.852	0.020	1
1315	.	109	LEU	C	179.088	0.3	1
1316	.	109	LEU	CA	57.863	0.3	1
1317	.	109	LEU	CB	41.999	0.3	1
1318	.	109	LEU	CG	26.699	0.3	1
1319	.	109	LEU	CD1	24.712	0.3	1
1320	.	109	LEU	CD2	23.602	0.3	1
1321	.	109	LEU	N	123.998	0.3	1
1322	.	110	LEU	H	7.807	0.020	1
1323	.	110	LEU	HA	4.352	0.020	1
1324	.	110	LEU	HB2	1.915	0.020	2
1325	.	110	LEU	HB3	1.762	0.020	2
1326	.	110	LEU	HG	0.705	0.020	1
1327	.	110	LEU	HD1	0.746	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1328	.	110	LEU	HD1	0.746	0.020	1
1329	.	110	LEU	HD1	0.746	0.020	1
1330	.	110	LEU	HD2	0.668	0.020	1
1331	.	110	LEU	HD2	0.668	0.020	1
1332	.	110	LEU	HD2	0.668	0.020	1
1333	.	110	LEU	C	176.822	0.3	1
1334	.	110	LEU	CA	54.948	0.3	1
1335	.	110	LEU	CB	43.615	0.3	1
1336	.	110	LEU	CG	27.192	0.3	1
1337	.	110	LEU	CD1	22.388	0.3	1
1338	.	110	LEU	CD2	23.676	0.3	1
1339	.	110	LEU	N	117.407	0.3	1
1340	.	111	GLY	H	7.943	0.020	1
1341	.	111	GLY	HA2	4.142	0.020	2
1342	.	111	GLY	HA3	3.869	0.020	2
1343	.	111	GLY	C	174.657	0.3	1
1344	.	111	GLY	CA	45.942	0.3	1
1345	.	111	GLY	N	108.110	0.3	1
1346	.	112	LEU	H	8.320	0.020	1
1347	.	112	LEU	HA	4.600	0.020	1
1348	.	112	LEU	HB2	1.693	0.020	2
1349	.	112	LEU	HB3	1.541	0.020	2
1350	.	112	LEU	HG	0.933	0.020	1
1351	.	112	LEU	HD1	0.938	0.020	1
1352	.	112	LEU	HD1	0.938	0.020	1
1353	.	112	LEU	HD1	0.938	0.020	1
1354	.	112	LEU	HD2	0.665	0.020	1
1355	.	112	LEU	HD2	0.665	0.020	1
1356	.	112	LEU	HD2	0.665	0.020	1
1357	.	112	LEU	C	176.147	0.3	1
1358	.	112	LEU	CA	53.099	0.3	1
1359	.	112	LEU	CB	42.546	0.3	1
1360	.	112	LEU	CG	26.248	0.3	1
1361	.	112	LEU	CD1	22.314	0.3	1
1362	.	112	LEU	CD2	23.745	0.3	1
1363	.	112	LEU	N	120.494	0.3	1
1364	.	113	ARG	H	8.615	0.020	1
1365	.	113	ARG	HA	4.258	0.020	1
1366	.	113	ARG	HB2	1.677	0.020	1
1367	.	113	ARG	HB3	1.677	0.020	1
1368	.	113	ARG	HG2	1.698	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1369	.	113	ARG	HG3	1.554	0.020	2
1370	.	113	ARG	HD2	3.141	0.020	1
1371	.	113	ARG	HD3	3.141	0.020	1
1372	.	113	ARG	C	174.712	0.3	1
1373	.	113	ARG	CA	55.650	0.3	1
1374	.	113	ARG	CB	31.326	0.3	1
1375	.	113	ARG	CG	27.483	0.3	1
1376	.	113	ARG	CD	43.104	0.3	1
1377	.	113	ARG	N	121.878	0.3	1
1378	.	114	PHE	H	7.721	0.020	1
1379	.	114	PHE	HA	5.765	0.020	1
1380	.	114	PHE	HB2	3.020	0.020	2
1381	.	114	PHE	HB3	2.721	0.020	2
1382	.	114	PHE	HD1	6.946	0.020	1
1383	.	114	PHE	HD2	6.946	0.020	1
1384	.	114	PHE	HE1	7.212	0.020	1
1385	.	114	PHE	HE2	7.212	0.020	1
1386	.	114	PHE	HZ	7.213	0.020	1
1387	.	114	PHE	C	173.527	0.3	1
1388	.	114	PHE	CA	54.997	0.3	1
1389	.	114	PHE	CB	42.561	0.3	1
1390	.	114	PHE	CD1	131.877	0.3	1
1391	.	114	PHE	CE1	131.384	0.3	1
1392	.	114	PHE	CZ	130.163	0.3	1
1393	.	114	PHE	N	117.113	0.3	1
1394	.	115	ARG	H	9.256	0.020	1
1395	.	115	ARG	HA	4.519	0.020	1
1396	.	115	ARG	HB2	1.403	0.020	2
1397	.	115	ARG	HB3	1.298	0.020	2
1398	.	115	ARG	HG2	0.929	0.020	1
1399	.	115	ARG	HG3	0.929	0.020	1
1400	.	115	ARG	HD2	2.645	0.020	2
1401	.	115	ARG	HD3	2.507	0.020	2
1402	.	115	ARG	C	173.291	0.3	1
1403	.	115	ARG	CA	54.141	0.3	1
1404	.	115	ARG	CB	33.103	0.3	1
1405	.	115	ARG	CG	26.108	0.3	1
1406	.	115	ARG	CD	43.196	0.3	1
1407	.	115	ARG	N	123.939	0.3	1
1408	.	116	THR	H	7.893	0.020	1
1409	.	116	THR	HA	4.619	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1410	.	116	THR	HB	4.352	0.020	1
1411	.	116	THR	HG2	0.868	0.020	1
1412	.	116	THR	HG2	0.868	0.020	1
1413	.	116	THR	HG2	0.868	0.020	1
1414	.	116	THR	C	173.937	0.3	1
1415	.	116	THR	CA	60.118	0.3	1
1416	.	116	THR	CB	70.246	0.3	1
1417	.	116	THR	CG2	20.710	0.3	1
1418	.	116	THR	N	113.217	0.3	1
1419	.	117	LEU	H	8.749	0.020	1
1420	.	117	LEU	HA	4.406	0.020	1
1421	.	117	LEU	HB2	1.640	0.020	2
1422	.	117	LEU	HB3	1.596	0.020	2
1423	.	117	LEU	HG	0.953	0.020	1
1424	.	117	LEU	HD1	0.732	0.020	1
1425	.	117	LEU	HD1	0.732	0.020	1
1426	.	117	LEU	HD1	0.732	0.020	1
1427	.	117	LEU	HD2	0.668	0.020	1
1428	.	117	LEU	HD2	0.668	0.020	1
1429	.	117	LEU	HD2	0.668	0.020	1
1430	.	117	LEU	C	177.073	0.3	1
1431	.	117	LEU	CA	55.383	0.3	1
1432	.	117	LEU	CB	42.489	0.3	1
1433	.	117	LEU	CG	27.215	0.3	1
1434	.	117	LEU	CD1	24.346	0.3	1
1435	.	117	LEU	CD2	23.602	0.3	1
1436	.	117	LEU	N	125.186	0.3	1
1437	.	118	LYS	H	8.520	0.020	1
1438	.	118	LYS	HA	4.283	0.020	1
1439	.	118	LYS	HB2	1.807	0.020	1
1440	.	118	LYS	HB3	1.807	0.020	1
1441	.	118	LYS	C	176.168	0.3	1
1442	.	118	LYS	CA	56.307	0.3	1
1443	.	118	LYS	CB	32.700	0.3	1
1444	.	118	LYS	N	122.291	0.3	1
1445	.	119	ARG	H	8.256	0.020	1
1446	.	119	ARG	HA	4.356	0.020	1
1447	.	119	ARG	HB2	1.820	0.020	1
1448	.	119	ARG	HB3	1.820	0.020	1
1449	.	119	ARG	C	176.559	0.3	1
1450	.	119	ARG	CA	56.106	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1451	.	119	ARG	CB	30.925	0.3	1
1452	.	119	ARG	CG	26.999	0.3	1
1453	.	119	ARG	CD	43.345	0.3	1
1454	.	119	ARG	N	121.676	0.3	1
1455	.	120	GLY	H	8.388	0.020	1
1456	.	120	GLY	HA2	3.962	0.020	2
1457	.	120	GLY	HA3	3.947	0.020	2
1458	.	120	GLY	C	173.894	0.3	1
1459	.	120	GLY	CA	45.267	0.3	1
1460	.	120	GLY	N	110.081	0.3	1
1461	.	121	ILE	H	7.946	0.020	1
1462	.	121	ILE	HA	4.172	0.020	1
1463	.	121	ILE	HB	1.861	0.020	1
1464	.	121	ILE	HG12	1.421	0.020	2
1465	.	121	ILE	HG13	1.179	0.020	2
1466	.	121	ILE	HG2	0.931	0.020	1
1467	.	121	ILE	HG2	0.931	0.020	1
1468	.	121	ILE	HG2	0.931	0.020	1
1469	.	121	ILE	HD1	0.849	0.020	1
1470	.	121	ILE	HD1	0.849	0.020	1
1471	.	121	ILE	HD1	0.849	0.020	1
1472	.	121	ILE	C	176.064	0.3	1
1473	.	121	ILE	CA	61.101	0.3	1
1474	.	121	ILE	CB	38.727	0.3	1
1475	.	121	ILE	CG1	27.155	0.3	1
1476	.	121	ILE	CG2	17.444	0.3	1
1477	.	121	ILE	CD1	13.164	0.3	1
1478	.	121	ILE	N	119.542	0.3	1
1479	.	122	LYS	H	8.275	0.020	1
1480	.	122	LYS	HA	4.307	0.020	1
1481	.	122	LYS	HB2	1.760	0.020	1
1482	.	122	LYS	HB3	1.760	0.020	1
1483	.	122	LYS	HG2	1.466	0.020	2
1484	.	122	LYS	HG3	1.395	0.020	2
1485	.	122	LYS	HD2	2.124	0.020	2
1486	.	122	LYS	HD3	1.992	0.020	2
1487	.	122	LYS	C	175.973	0.3	1
1488	.	122	LYS	CA	56.288	0.3	1
1489	.	122	LYS	CB	33.022	0.3	1
1490	.	122	LYS	CG	24.716	0.3	1
1491	.	122	LYS	CD	29.039	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1492	.	122	LYS	CE	42.000	0.3	1
1493	.	122	LYS	N	124.783	0.3	1
1494	.	123	LYS	H	8.188	0.020	1
1495	.	123	LYS	HA	4.295	0.020	1
1496	.	123	LYS	HB2	1.688	0.020	2
1497	.	123	LYS	HB3	1.588	0.020	2
1498	.	123	LYS	C	175.901	0.3	1
1499	.	123	LYS	CA	56.069	0.3	1
1500	.	123	LYS	CB	33.104	0.3	1
1501	.	123	LYS	CG	24.528	0.3	1
1502	.	123	LYS	CE	42.053	0.3	1
1503	.	123	LYS	N	123.081	0.3	1
1504	.	124	VAL	H	8.087	0.020	1
1505	.	124	VAL	HA	4.024	0.020	1
1506	.	124	VAL	HB	1.922	0.020	1
1507	.	124	VAL	HG1	1.201	0.020	1
1508	.	124	VAL	HG1	1.201	0.020	1
1509	.	124	VAL	HG1	1.201	0.020	1
1510	.	124	VAL	HG2	0.787	0.020	1
1511	.	124	VAL	HG2	0.787	0.020	1
1512	.	124	VAL	HG2	0.787	0.020	1
1513	.	124	VAL	C	175.553	0.3	1
1514	.	124	VAL	CA	62.063	0.3	1
1515	.	124	VAL	CB	32.877	0.3	1
1516	.	124	VAL	CG1	22.643	0.3	1
1517	.	124	VAL	CG2	21.110	0.3	1
1518	.	124	VAL	N	122.522	0.3	1
1519	.	125	ILE	H	8.125	0.020	1
1520	.	125	ILE	HA	3.930	0.020	1
1521	.	125	ILE	HB	1.521	0.020	1
1522	.	125	ILE	HG12	1.328	0.020	2
1523	.	125	ILE	HG13	1.000	0.020	2
1524	.	125	ILE	HG2	0.400	0.020	1
1525	.	125	ILE	HG2	0.400	0.020	1
1526	.	125	ILE	HG2	0.400	0.020	1
1527	.	125	ILE	HD1	0.741	0.020	1
1528	.	125	ILE	HD1	0.741	0.020	1
1529	.	125	ILE	HD1	0.741	0.020	1
1530	.	125	ILE	C	175.210	0.3	1
1531	.	125	ILE	CA	60.601	0.3	1
1532	.	125	ILE	CB	38.467	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1533	.	125	ILE	CG1	27.195	0.3	1
1534	.	125	ILE	CG2	17.180	0.3	1
1535	.	125	ILE	CD1	12.603	0.3	1
1536	.	125	ILE	N	126.170	0.3	1
1537	.	126	LYS	H	8.076	0.020	1
1538	.	126	LYS	HA	4.122	0.020	1
1539	.	126	LYS	HB2	1.424	0.020	1
1540	.	126	LYS	HB3	1.424	0.020	1
1541	.	126	LYS	HG2	1.063	0.020	2
1542	.	126	LYS	HG3	0.920	0.020	2
1543	.	126	LYS	HD2	2.140	0.020	2
1544	.	126	LYS	HD3	1.992	0.020	2
1545	.	126	LYS	HE2	2.790	0.020	1
1546	.	126	LYS	HE3	2.790	0.020	1
1547	.	126	LYS	C	175.529	0.3	1
1548	.	126	LYS	CA	55.777	0.3	1
1549	.	126	LYS	CB	33.108	0.3	1
1550	.	126	LYS	CG	24.484	0.3	1
1551	.	126	LYS	CD	29.083	0.3	1
1552	.	126	LYS	CE	42.017	0.3	1
1553	.	126	LYS	N	125.925	0.3	1
1554	.	127	TRP	H	7.747	0.020	1
1555	.	127	TRP	HA	4.730	0.020	1
1556	.	127	TRP	HB2	3.085	0.020	2
1557	.	127	TRP	HB3	3.061	0.020	2
1558	.	127	TRP	HD1	7.217	0.020	1
1559	.	127	TRP	HE1	10.126	0.020	1
1560	.	127	TRP	HE3	7.235	0.020	1
1561	.	127	TRP	HZ2	7.440	0.020	1
1562	.	127	TRP	HZ3	7.042	0.020	1
1563	.	127	TRP	HH2	7.182	0.020	1
1564	.	127	TRP	C	175.627	0.3	1
1565	.	127	TRP	CA	55.759	0.3	1
1566	.	127	TRP	CB	30.654	0.3	1
1567	.	127	TRP	CD1	127.935	0.3	1
1568	.	127	TRP	CE3	120.198	0.3	1
1569	.	127	TRP	CZ2	114.532	0.3	1
1570	.	127	TRP	CZ3	121.752	0.3	1
1571	.	127	TRP	CH2	124.323	0.3	1
1572	.	127	TRP	N	121.230	0.3	1
1573	.	127	TRP	NE1	129.084	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1574	.	128	ARG	H	8.441	0.020	1
1575	.	128	ARG	HA	4.535	0.020	1
1576	.	128	ARG	HB2	1.508	0.020	1
1577	.	128	ARG	HB3	1.508	0.020	1
1578	.	128	ARG	C	174.484	0.3	1
1579	.	128	ARG	CA	56.200	0.3	1
1580	.	128	ARG	CB	34.362	0.3	1
1581	.	128	ARG	N	120.438	0.3	1
1582	.	129	TYR	H	8.441	0.020	1
1583	.	129	TYR	HA	5.495	0.020	1
1584	.	129	TYR	HB2	2.887	0.020	2
1585	.	129	TYR	HB3	2.627	0.020	2
1586	.	129	TYR	HD1	6.597	0.020	1
1587	.	129	TYR	HD2	6.597	0.020	1
1588	.	129	TYR	HE1	6.743	0.020	1
1589	.	129	TYR	HE2	6.743	0.020	1
1590	.	129	TYR	C	174.031	0.3	1
1591	.	129	TYR	CA	56.460	0.3	1
1592	.	129	TYR	CB	42.887	0.3	1
1593	.	129	TYR	CD1	132.572	0.3	1
1594	.	129	TYR	CE1	118.659	0.3	1
1595	.	129	TYR	N	116.750	0.3	1
1596	.	130	VAL	H	9.708	0.020	1
1597	.	130	VAL	HA	5.397	0.020	1
1598	.	130	VAL	HB	1.830	0.020	1
1599	.	130	VAL	HG1	0.893	0.020	1
1600	.	130	VAL	HG1	0.893	0.020	1
1601	.	130	VAL	HG1	0.893	0.020	1
1602	.	130	VAL	HG2	0.856	0.020	1
1603	.	130	VAL	HG2	0.856	0.020	1
1604	.	130	VAL	HG2	0.856	0.020	1
1605	.	130	VAL	C	172.414	0.3	1
1606	.	130	VAL	CA	58.912	0.3	1
1607	.	130	VAL	CB	35.769	0.3	1
1608	.	130	VAL	CG1	21.187	0.3	1
1609	.	130	VAL	CG2	18.970	0.3	1
1610	.	130	VAL	N	119.980	0.3	1
1611	.	131	CYS	H	9.291	0.020	1
1612	.	131	CYS	HA	4.674	0.020	1
1613	.	131	CYS	HB2	3.262	0.020	2
1614	.	131	CYS	HB3	2.929	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1615	.	131	CYS	C	178.397	0.3	1
1616	.	131	CYS	CA	59.993	0.3	1
1617	.	131	CYS	CB	30.925	0.3	1
1618	.	131	CYS	N	129.161	0.3	1
1619	.	132	ILE	H	8.594	0.020	1
1620	.	132	ILE	HA	4.162	0.020	1
1621	.	132	ILE	HB	2.158	0.020	1
1622	.	132	ILE	HG12	1.594	0.020	2
1623	.	132	ILE	HG13	1.419	0.020	2
1624	.	132	ILE	HG2	1.003	0.020	1
1625	.	132	ILE	HG2	1.003	0.020	1
1626	.	132	ILE	HG2	1.003	0.020	1
1627	.	132	ILE	HD1	0.901	0.020	1
1628	.	132	ILE	HD1	0.901	0.020	1
1629	.	132	ILE	HD1	0.901	0.020	1
1630	.	132	ILE	C	175.676	0.3	1
1631	.	132	ILE	CA	63.547	0.3	1
1632	.	132	ILE	CB	37.880	0.3	1
1633	.	132	ILE	CG1	26.059	0.3	1
1634	.	132	ILE	CG2	17.994	0.3	1
1635	.	132	ILE	CD1	14.223	0.3	1
1636	.	132	ILE	N	127.133	0.3	1
1637	.	133	GLY	H	9.913	0.020	1
1638	.	133	GLY	HA2	4.193	0.020	2
1639	.	133	GLY	HA3	3.861	0.020	2
1640	.	133	GLY	C	174.497	0.3	1
1641	.	133	GLY	CA	46.157	0.3	1
1642	.	133	GLY	N	115.957	0.3	1
1643	.	134	CYS	H	9.300	0.020	1
1644	.	134	CYS	HA	4.896	0.020	1
1645	.	134	CYS	HB2	3.199	0.020	2
1646	.	134	CYS	HB3	2.876	0.020	2
1647	.	134	CYS	C	177.307	0.3	1
1648	.	134	CYS	CA	59.227	0.3	1
1649	.	134	CYS	CB	32.265	0.3	1
1650	.	134	CYS	N	123.821	0.3	1
1651	.	135	GLY	H	7.524	0.020	1
1652	.	135	GLY	HA2	4.110	0.020	2
1653	.	135	GLY	HA3	3.784	0.020	2
1654	.	135	GLY	C	173.291	0.3	1
1655	.	135	GLY	CA	46.015	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1656	.	135	GLY	N	111.507	0.3	1
1657	.	136	ARG	H	8.422	0.020	1
1658	.	136	ARG	HA	3.791	0.020	1
1659	.	136	ARG	HB2	1.822	0.020	2
1660	.	136	ARG	HB3	1.495	0.020	2
1661	.	136	ARG	HG2	1.336	0.020	2
1662	.	136	ARG	HG3	0.583	0.020	2
1663	.	136	ARG	HD2	3.086	0.020	2
1664	.	136	ARG	HD3	2.874	0.020	2
1665	.	136	ARG	C	173.588	0.3	1
1666	.	136	ARG	CA	58.182	0.3	1
1667	.	136	ARG	CB	30.420	0.3	1
1668	.	136	ARG	CG	27.455	0.3	1
1669	.	136	ARG	CD	43.605	0.3	1
1670	.	136	ARG	N	124.636	0.3	1
1671	.	137	LYS	H	7.546	0.020	1
1672	.	137	LYS	HA	5.094	0.020	1
1673	.	137	LYS	HB2	1.201	0.020	2
1674	.	137	LYS	HB3	0.465	0.020	2
1675	.	137	LYS	HG2	1.073	0.020	1
1676	.	137	LYS	HG3	1.073	0.020	1
1677	.	137	LYS	HD2	1.284	0.020	2
1678	.	137	LYS	HD3	1.006	0.020	2
1679	.	137	LYS	HE2	2.533	0.020	2
1680	.	137	LYS	HE3	2.485	0.020	2
1681	.	137	LYS	C	175.322	0.3	1
1682	.	137	LYS	CA	54.673	0.3	1
1683	.	137	LYS	CB	34.467	0.3	1
1684	.	137	LYS	CG	25.293	0.3	1
1685	.	137	LYS	CD	28.803	0.3	1
1686	.	137	LYS	CE	41.737	0.3	1
1687	.	137	LYS	N	122.179	0.3	1
1688	.	138	PHE	H	8.875	0.020	1
1689	.	138	PHE	HA	5.225	0.020	1
1690	.	138	PHE	HB2	3.809	0.020	2
1691	.	138	PHE	HB3	2.735	0.020	2
1692	.	138	PHE	HD1	7.178	0.020	1
1693	.	138	PHE	HD2	7.178	0.020	1
1694	.	138	PHE	HE1	7.137	0.020	1
1695	.	138	PHE	HE2	7.137	0.020	1
1696	.	138	PHE	HZ	7.801	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1697	.	138	PHE	C	177.263	0.3	1
1698	.	138	PHE	CA	56.555	0.3	1
1699	.	138	PHE	CB	43.896	0.3	1
1700	.	138	PHE	CD1	132.394	0.3	1
1701	.	138	PHE	CE1	131.195	0.3	1
1702	.	138	PHE	CZ	128.957	0.3	1
1703	.	138	PHE	N	114.631	0.3	1
1704	.	139	SER	HA	4.909	0.020	1
1705	.	139	SER	HB2	4.037	0.020	1
1706	.	139	SER	HB3	3.840	0.020	1
1707	.	139	SER	C	173.564	0.3	1
1708	.	139	SER	CA	60.323	0.3	1
1709	.	139	SER	CB	64.058	0.3	1
1710	.	140	THR	H	7.616	0.020	1
1711	.	140	THR	HA	4.671	0.020	1
1712	.	140	THR	HB	4.150	0.020	1
1713	.	140	THR	HG2	1.192	0.020	1
1714	.	140	THR	HG2	1.192	0.020	1
1715	.	140	THR	HG2	1.192	0.020	1
1716	.	140	THR	C	172.560	0.3	1
1717	.	140	THR	CA	59.750	0.3	1
1718	.	140	THR	CB	71.369	0.3	1
1719	.	140	THR	CG2	21.537	0.3	1
1720	.	140	THR	N	112.426	0.3	1
1721	.	141	LEU	H	8.202	0.020	1
1722	.	141	LEU	HA	3.271	0.020	1
1723	.	141	LEU	HB2	1.448	0.020	2
1724	.	141	LEU	HB3	0.838	0.020	2
1725	.	141	LEU	HG	1.200	0.020	1
1726	.	141	LEU	HD1	0.607	0.020	1
1727	.	141	LEU	HD1	0.607	0.020	1
1728	.	141	LEU	HD1	0.607	0.020	1
1729	.	141	LEU	HD2	0.314	0.020	1
1730	.	141	LEU	HD2	0.314	0.020	1
1731	.	141	LEU	HD2	0.314	0.020	1
1732	.	141	LEU	C	174.566	0.3	1
1733	.	141	LEU	CA	53.238	0.3	1
1734	.	141	LEU	CB	42.103	0.3	1
1735	.	141	LEU	CG	25.281	0.3	1
1736	.	141	LEU	CD1	25.571	0.3	1
1737	.	141	LEU	CD2	24.054	0.3	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1738	.	141	LEU	N	126.119	0.3	1
1739	.	142	PRO	HA	4.561	0.020	1
1740	.	142	PRO	HB2	1.971	0.020	2
1741	.	142	PRO	HB3	1.845	0.020	2
1742	.	142	PRO	HG2	0.876	0.020	2
1743	.	142	PRO	HG3	0.705	0.020	2
1744	.	142	PRO	HD2	3.158	0.020	2
1745	.	142	PRO	HD3	2.681	0.020	2
1746	.	142	PRO	CA	61.400	0.3	1
1747	.	142	PRO	CB	29.789	0.3	1
1748	.	142	PRO	CG	26.898	0.3	1
1749	.	142	PRO	CD	50.268	0.3	1
1750	.	143	PRO	HA	4.223	0.020	1
1751	.	143	PRO	HB2	2.287	0.020	2
1752	.	143	PRO	HB3	1.853	0.020	2
1753	.	143	PRO	HG2	2.161	0.020	2
1754	.	143	PRO	HG3	2.023	0.020	2
1755	.	143	PRO	HD2	3.816	0.020	2
1756	.	143	PRO	HD3	3.578	0.020	2
1757	.	143	PRO	C	178.755	0.3	1
1758	.	143	PRO	CA	64.151	0.3	1
1759	.	143	PRO	CB	31.449	0.3	1
1760	.	143	PRO	CG	27.611	0.3	1
1761	.	143	PRO	CD	50.282	0.3	1
1762	.	144	GLY	H	8.848	0.020	1
1763	.	144	GLY	HA2	4.034	0.020	2
1764	.	144	GLY	HA3	3.717	0.020	2
1765	.	144	GLY	C	174.826	0.3	1
1766	.	144	GLY	CA	45.533	0.3	1
1767	.	144	GLY	N	113.453	0.3	1
1768	.	145	GLY	H	8.838	0.020	1
1769	.	145	GLY	HA2	3.086	0.020	2
1770	.	145	GLY	HA3	3.990	0.020	2
1771	.	145	GLY	C	172.606	0.3	1
1772	.	145	GLY	CA	46.134	0.3	1
1773	.	145	GLY	N	107.906	0.3	1
1774	.	146	VAL	H	6.562	0.020	1
1775	.	146	VAL	HA	4.647	0.020	1
1776	.	146	VAL	HB	1.700	0.020	1
1777	.	146	VAL	HG1	0.860	0.020	1
1778	.	146	VAL	HG1	0.860	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1779	.	146	VAL	HG1	0.860	0.020	1
1780	.	146	VAL	HG2	0.678	0.020	1
1781	.	146	VAL	HG2	0.678	0.020	1
1782	.	146	VAL	HG2	0.678	0.020	1
1783	.	146	VAL	C	174.086	0.3	1
1784	.	146	VAL	CA	58.675	0.3	1
1785	.	146	VAL	CB	34.826	0.3	1
1786	.	146	VAL	CG1	21.057	0.3	1
1787	.	146	VAL	CG2	18.814	0.3	1
1788	.	146	VAL	N	112.550	0.3	1
1789	.	147	CYS	H	9.212	0.020	1
1790	.	147	CYS	HA	4.170	0.020	1
1791	.	147	CYS	HB2	3.293	0.020	2
1792	.	147	CYS	HB3	3.131	0.020	2
1793	.	147	CYS	C	176.676	0.3	1
1794	.	147	CYS	CA	57.062	0.3	1
1795	.	147	CYS	CB	33.363	0.3	1
1796	.	147	CYS	N	128.043	0.3	1
1797	.	148	PRO	HA	4.389	0.020	1
1798	.	148	PRO	HB2	2.511	0.020	2
1799	.	148	PRO	HB3	2.098	0.020	2
1800	.	148	PRO	HG2	2.215	0.020	2
1801	.	148	PRO	HG3	2.195	0.020	2
1802	.	148	PRO	HD2	4.279	0.020	2
1803	.	148	PRO	HD3	3.917	0.020	2
1804	.	148	PRO	C	176.186	0.3	1
1805	.	148	PRO	CA	64.009	0.3	1
1806	.	148	PRO	CB	32.620	0.3	1
1807	.	148	PRO	CG	26.733	0.3	1
1808	.	148	PRO	CD	51.941	0.3	1
1809	.	149	ASP	H	9.131	0.020	1
1810	.	149	ASP	HA	4.773	0.020	1
1811	.	149	ASP	HB2	2.676	0.020	2
1812	.	149	ASP	HB3	2.765	0.020	2
1813	.	149	ASP	C	177.307	0.3	1
1814	.	149	ASP	CA	56.523	0.3	1
1815	.	149	ASP	CB	41.739	0.3	1
1816	.	149	ASP	N	120.310	0.3	1
1817	.	150	CYS	H	8.532	0.020	1
1818	.	150	CYS	HA	5.067	0.020	1
1819	.	150	CYS	HB2	3.257	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1820	.	150	CYS	HB3	2.618	0.020	2
1821	.	150	CYS	C	176.983	0.3	1
1822	.	150	CYS	CA	58.417	0.3	1
1823	.	150	CYS	CB	32.547	0.3	1
1824	.	150	CYS	N	118.498	0.3	1
1825	.	151	GLY	H	8.065	0.020	1
1826	.	151	GLY	HA2	3.799	0.020	2
1827	.	151	GLY	HA3	4.189	0.020	2
1828	.	151	GLY	C	173.990	0.3	1
1829	.	151	GLY	CA	46.204	0.3	1
1830	.	151	GLY	N	112.768	0.3	1
1831	.	152	SER	H	8.426	0.020	1
1832	.	152	SER	HA	4.533	0.020	1
1833	.	152	SER	HB2	4.279	0.020	1
1834	.	152	SER	HB3	3.860	0.020	1
1835	.	152	SER	C	171.555	0.3	1
1836	.	152	SER	CA	59.217	0.3	1
1837	.	152	SER	CB	63.299	0.3	1
1838	.	152	SER	N	118.493	0.3	1
1839	.	153	LYS	H	8.218	0.020	1
1840	.	153	LYS	HA	4.383	0.020	1
1841	.	153	LYS	HB2	1.855	0.020	2
1842	.	153	LYS	HB3	1.817	0.020	2
1843	.	153	LYS	HG2	1.616	0.020	2
1844	.	153	LYS	HG3	1.522	0.020	2
1845	.	153	LYS	HD2	1.741	0.020	2
1846	.	153	LYS	HD3	1.505	0.020	2
1847	.	153	LYS	HE2	3.048	0.020	1
1848	.	153	LYS	HE3	3.048	0.020	1
1849	.	153	LYS	C	174.634	0.3	1
1850	.	153	LYS	CA	57.202	0.3	1
1851	.	153	LYS	CB	33.340	0.3	1
1852	.	153	LYS	CG	25.398	0.3	1
1853	.	153	LYS	CD	28.780	0.3	1
1854	.	153	LYS	CE	42.110	0.3	1
1855	.	153	LYS	N	120.008	0.3	1
1856	.	154	VAL	H	7.347	0.020	1
1857	.	154	VAL	HA	4.911	0.020	1
1858	.	154	VAL	HB	1.494	0.020	1
1859	.	154	VAL	HG1	0.545	0.020	1
1860	.	154	VAL	HG1	0.545	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1861	.	154	VAL	HG1	0.545	0.020	1
1862	.	154	VAL	HG2	0.437	0.020	1
1863	.	154	VAL	HG2	0.437	0.020	1
1864	.	154	VAL	HG2	0.437	0.020	1
1865	.	154	VAL	C	174.895	0.3	1
1866	.	154	VAL	CA	59.905	0.3	1
1867	.	154	VAL	CB	32.838	0.3	1
1868	.	154	VAL	CG1	22.853	0.3	1
1869	.	154	VAL	CG2	20.434	0.3	1
1870	.	154	VAL	N	116.314	0.3	1
1871	.	155	LYS	H	9.040	0.020	1
1872	.	155	LYS	HA	4.972	0.020	1
1873	.	155	LYS	HB2	1.824	0.020	1
1874	.	155	LYS	HB3	1.824	0.020	1
1875	.	155	LYS	HG2	1.440	0.020	2
1876	.	155	LYS	HG3	1.344	0.020	2
1877	.	155	LYS	HD2	1.677	0.020	1
1878	.	155	LYS	HD3	1.677	0.020	1
1879	.	155	LYS	HE2	2.994	0.020	1
1880	.	155	LYS	HE3	2.994	0.020	1
1881	.	155	LYS	C	175.344	0.3	1
1882	.	155	LYS	CA	53.849	0.3	1
1883	.	155	LYS	CB	36.887	0.3	1
1884	.	155	LYS	CG	24.042	0.3	1
1885	.	155	LYS	CD	29.408	0.3	1
1886	.	155	LYS	CE	42.265	0.3	1
1887	.	155	LYS	N	122.916	0.3	1
1888	.	156	LEU	H	8.533	0.020	1
1889	.	156	LEU	HA	4.225	0.020	1
1890	.	156	LEU	HB2	1.543	0.020	2
1891	.	156	LEU	HB3	1.488	0.020	2
1892	.	156	LEU	HG	0.766	0.020	1
1893	.	156	LEU	C	177.485	0.3	1
1894	.	156	LEU	CA	55.602	0.3	1
1895	.	156	LEU	CB	43.045	0.3	1
1896	.	156	LEU	CG	24.740	0.3	1
1897	.	156	LEU	CD1	27.434	0.3	1
1898	.	156	LEU	N	123.382	0.3	1
1899	.	157	ILE	H	8.072	0.020	1
1900	.	157	ILE	HA	4.095	0.020	1
1901	.	157	ILE	HB	1.478	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1902	.	157	ILE	HG12	1.337	0.020	2
1903	.	157	ILE	HG13	0.912	0.020	2
1904	.	157	ILE	HG2	0.902	0.020	1
1905	.	157	ILE	HG2	0.902	0.020	1
1906	.	157	ILE	HG2	0.902	0.020	1
1907	.	157	ILE	HD1	0.721	0.020	1
1908	.	157	ILE	HD1	0.721	0.020	1
1909	.	157	ILE	HD1	0.721	0.020	1
1910	.	157	ILE	C	174.456	0.3	1
1911	.	157	ILE	CA	60.026	0.3	1
1912	.	157	ILE	CB	39.263	0.3	1
1913	.	157	ILE	CG1	29.028	0.3	1
1914	.	157	ILE	CG2	16.640	0.3	1
1915	.	157	ILE	CD1	13.947	0.3	1
1916	.	157	ILE	N	126.495	0.3	1
1917	.	158	PRO	HA	4.375	0.020	1
1918	.	158	PRO	HB2	2.237	0.020	2
1919	.	158	PRO	HB3	2.067	0.020	2
1920	.	158	PRO	HG2	2.072	0.020	2
1921	.	158	PRO	HG3	1.993	0.020	2
1922	.	158	PRO	HD2	3.956	0.020	2
1923	.	158	PRO	HD3	3.668	0.020	2
1924	.	158	PRO	C	176.403	0.3	1
1925	.	158	PRO	CA	62.954	0.3	1
1926	.	158	PRO	CB	32.052	0.3	1
1927	.	158	PRO	CG	27.308	0.3	1
1928	.	158	PRO	CD	51.105	0.3	1
1929	.	159	ARG	H	8.283	0.020	1
1930	.	159	ARG	HA	4.319	0.020	1
1931	.	159	ARG	HB2	1.799	0.020	1
1932	.	159	ARG	HB3	1.799	0.020	1
1933	.	159	ARG	C	176.005	0.3	1
1934	.	159	ARG	CA	55.871	0.3	1
1935	.	159	ARG	CB	31.192	0.3	1
1936	.	159	ARG	CG	26.999	0.3	1
1937	.	159	ARG	CD	43.408	0.3	1
1938	.	159	ARG	N	121.967	0.3	1
1939	.	160	LYS	H	8.315	0.020	1
1940	.	160	LYS	HA	4.342	0.020	1
1941	.	160	LYS	HB2	1.823	0.020	2
1942	.	160	LYS	HB3	1.789	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1943	.	160	LYS	HG2	1.466	0.020	2
1944	.	160	LYS	HG3	1.433	0.020	2
1945	.	160	LYS	HD2	1.711	0.020	1
1946	.	160	LYS	HD3	1.711	0.020	1
1947	.	160	LYS	HE2	2.986	0.020	1
1948	.	160	LYS	HE3	2.986	0.020	1
1949	.	160	LYS	C	175.350	0.3	1
1950	.	160	LYS	CA	56.182	0.3	1
1951	.	160	LYS	CB	33.099	0.3	1
1952	.	160	LYS	CG	24.772	0.3	1
1953	.	160	LYS	CD	29.056	0.3	1
1954	.	160	LYS	CE	41.846	0.3	1
1955	.	160	LYS	N	123.417	0.3	1
1956	.	161	ARG	H	7.953	0.020	1
1957	.	161	ARG	HA	4.155	0.020	1
1958	.	161	ARG	C	180.700	0.3	1
1959	.	161	ARG	CA	57.479	0.3	1
1960	.	161	ARG	CB	31.456	0.3	1
1961	.	161	ARG	N	127.830	0.3	1

7.1.2 Chemical shift referencing ⓘ

No chemical shift referencing corrections were calculated (not enough data).

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 1710. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/695 (0%)	0/277 (0%)	0/282 (0%)	0/136 (0%)
Sidechain	0/926 (0%)	0/539 (0%)	0/351 (0%)	0/36 (0%)
Aromatic	0/89 (0%)	0/47 (0%)	0/41 (0%)	0/1 (0%)
Overall	0/1710 (0%)	0/863 (0%)	0/674 (0%)	0/173 (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 2033. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/793 (0%)	0/316 (0%)	0/322 (0%)	0/155 (0%)
Sidechain	0/1151 (0%)	0/674 (0%)	0/422 (0%)	0/55 (0%)
Aromatic	0/89 (0%)	0/47 (0%)	0/41 (0%)	0/1 (0%)
Overall	0/2033 (0%)	0/1037 (0%)	0/785 (0%)	0/211 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.