



Full wwPDB NMR Structure Validation Report ⓘ

Dec 6, 2016 – 10:07 PM EST

PDB ID : 2NB1
Title : P63/p73 hetero-tetramerisation domain
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Doetsch, V.
Deposited on : 2016-01-19

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-20028442
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

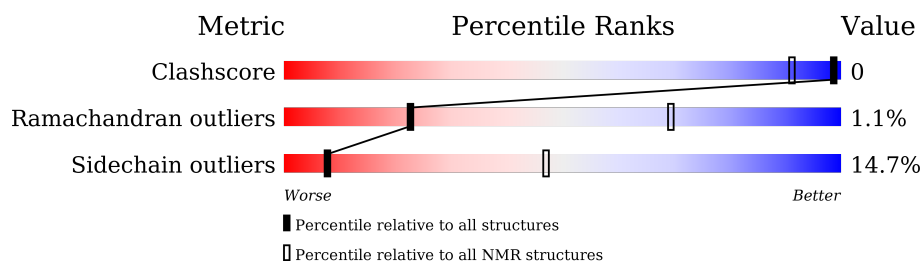
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 20%.

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	60	<div> <div style="width: 65%; background-color: green;"></div> <div style="width: 32%; background-color: cyan;"></div> <div style="width: 3%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>65% . 32%</div>
1	C	60	<div> <div style="width: 67%; background-color: green;"></div> <div style="width: 32%; background-color: cyan;"></div> <div style="width: 3%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>67% . 32%</div>
2	B	50	<div> <div style="width: 82%; background-color: green;"></div> <div style="width: 14%; background-color: cyan;"></div> <div style="width: 4%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>82% . 14%</div>
2	D	50	<div> <div style="width: 78%; background-color: green;"></div> <div style="width: 14%; background-color: cyan;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>78% 8% 14%</div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:32, B:98-B:140, C:1004-C:1032, D:1098- D:1140 (144)	0.48	3
2	A:35-A:46 (12)	0.17	17
3	C:1035-C:1046 (12)	0.18	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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3732 atoms, of which 1862 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor protein 63.

Mol	Chain	Residues	Atoms						Trace
1	A	60	Total	C	H	N	O	S	0
			1016	320	503	89	102	2	
1	C	60	Total	C	H	N	O	S	0
			1016	320	503	89	102	2	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9H3D4
A	21	GLU	LYS	ENGINEERED MUTATION	UNP Q9H3D4
C	1001	SER	-	EXPRESSION TAG	UNP Q9H3D4
C	1021	GLU	LYS	ENGINEERED MUTATION	UNP Q9H3D4

- Molecule 2 is a protein called Tumor protein p73.

Mol	Chain	Residues	Atoms						Trace
2	B	50	Total	C	H	N	O	S	0
			850	266	428	73	81	2	
2	D	50	Total	C	H	N	O	S	0
			850	266	428	73	81	2	

There are 6 discrepancies between the modelled and reference sequences:

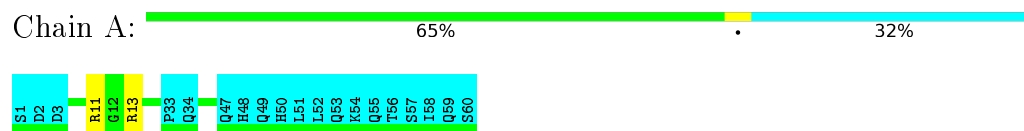
Chain	Residue	Modelled	Actual	Comment	Reference
B	93	GLY	-	EXPRESSION TAG	UNP O15350
B	94	SER	-	EXPRESSION TAG	UNP O15350
B	107	LYS	GLU	ENGINEERED MUTATION	UNP O15350
D	1093	GLY	-	EXPRESSION TAG	UNP O15350
D	1094	SER	-	EXPRESSION TAG	UNP O15350
D	1107	LYS	GLU	ENGINEERED MUTATION	UNP O15350

4 Residue-property plots [i](#)

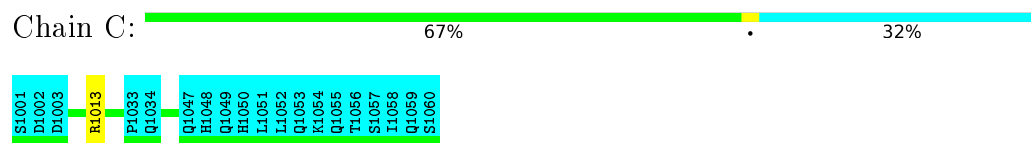
4.1 Average score per residue in the NMR ensemble

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.

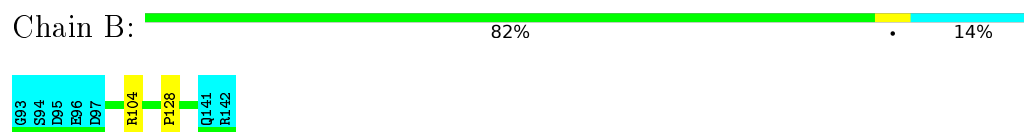
- Molecule 1: Tumor protein 63



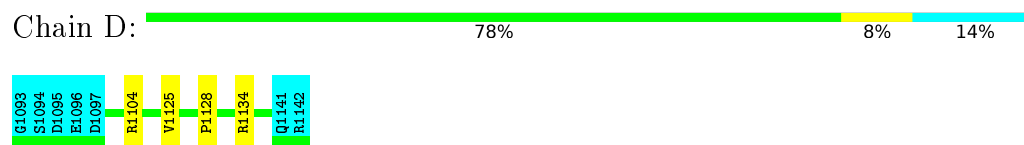
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73

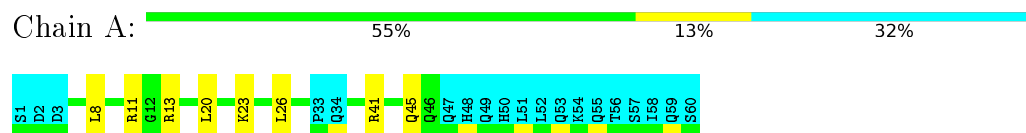


4.2 Scores per residue for each member of the ensemble

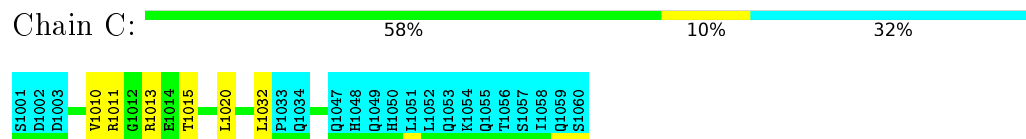
Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

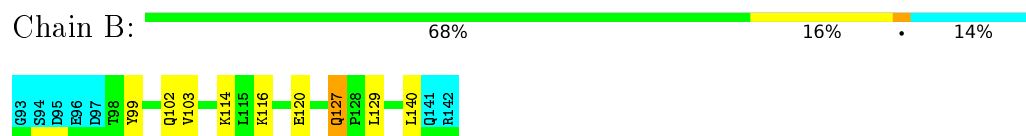
- Molecule 1: Tumor protein 63



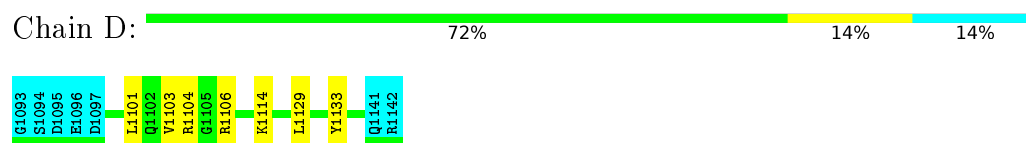
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

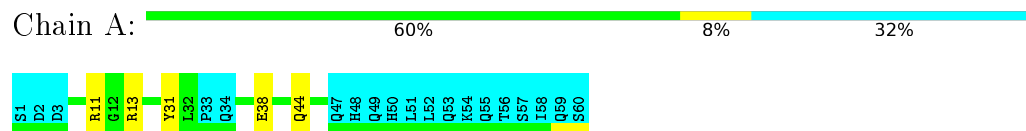


- Molecule 2: Tumor protein p73

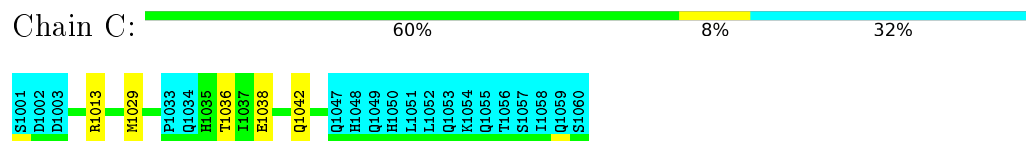


4.2.2 Score per residue for model 2

- Molecule 1: Tumor protein 63



- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73



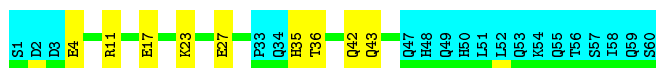


- Molecule 2: Tumor protein p73



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Tumor protein 63



- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73



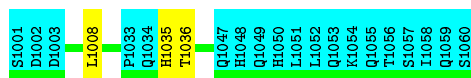
4.2.4 Score per residue for model 4

- Molecule 1: Tumor protein 63





- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73



4.2.5 Score per residue for model 5

- Molecule 1: Tumor protein 63



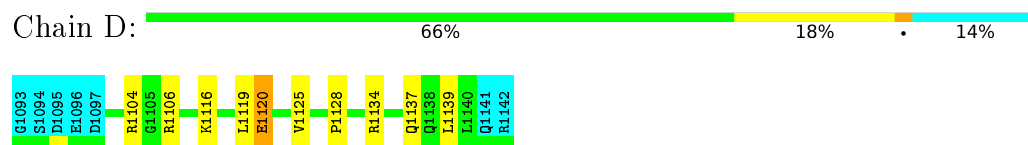
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

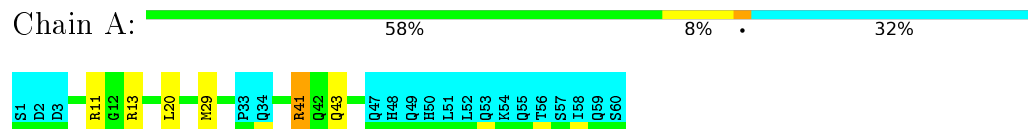


- Molecule 2: Tumor protein p73

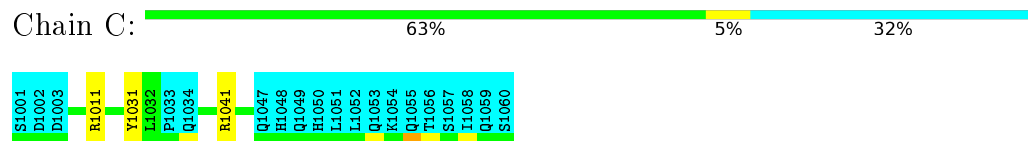


4.2.6 Score per residue for model 6

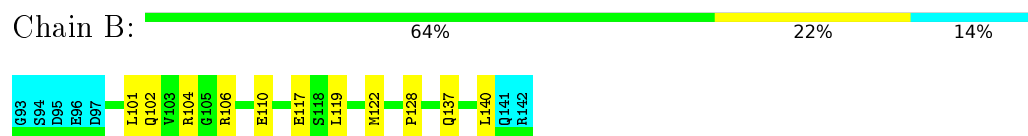
- Molecule 1: Tumor protein 63



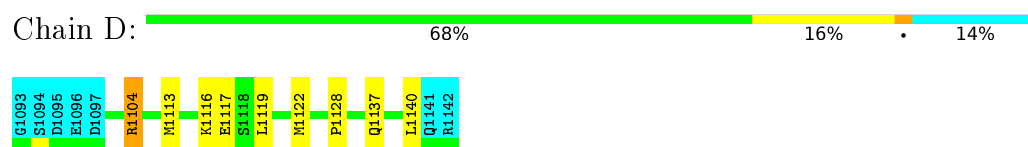
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

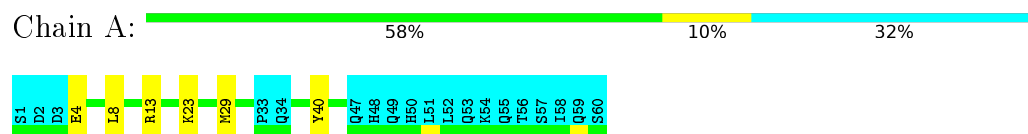


- Molecule 2: Tumor protein p73



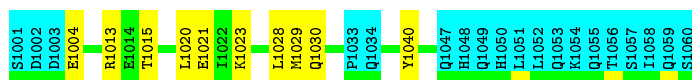
4.2.7 Score per residue for model 7

- Molecule 1: Tumor protein 63

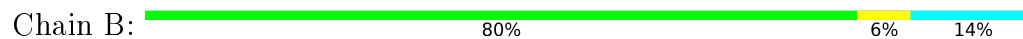


- Molecule 1: Tumor protein 63

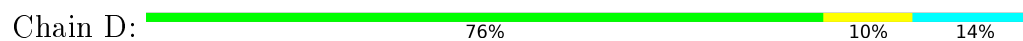




- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73

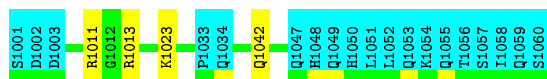


4.2.8 Score per residue for model 8

- Molecule 1: Tumor protein 63



- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

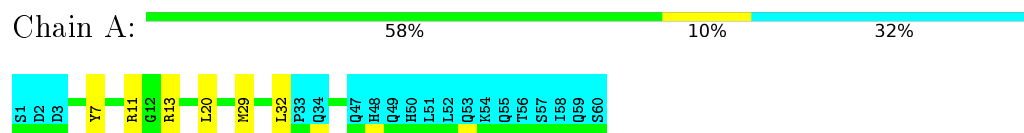


- Molecule 2: Tumor protein p73

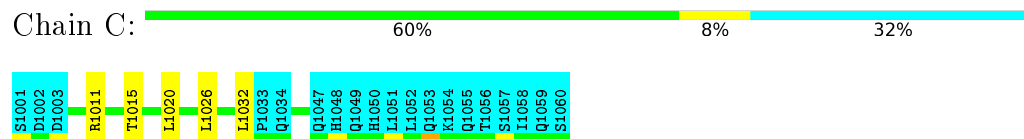


4.2.9 Score per residue for model 9

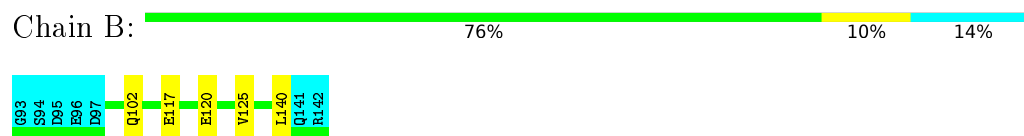
- Molecule 1: Tumor protein 63



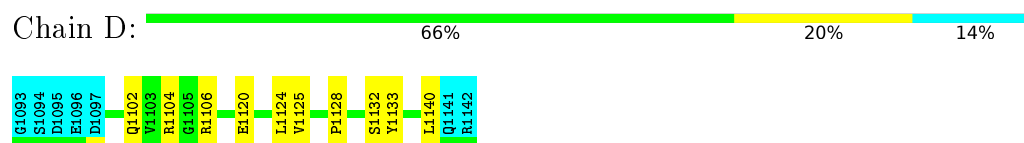
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

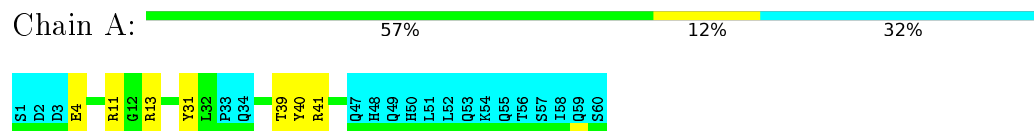


- Molecule 2: Tumor protein p73

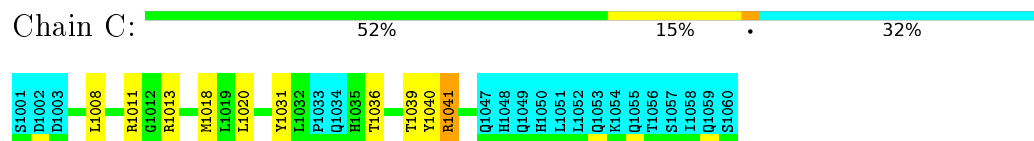


4.2.10 Score per residue for model 10

- Molecule 1: Tumor protein 63



- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73





- Molecule 2: Tumor protein p73

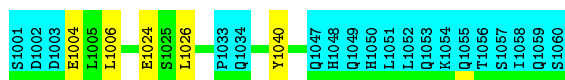


4.2.11 Score per residue for model 11

- Molecule 1: Tumor protein 63



- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73



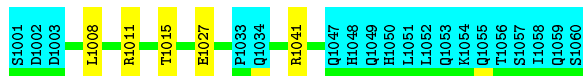
4.2.12 Score per residue for model 12

- Molecule 1: Tumor protein 63





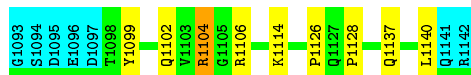
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73

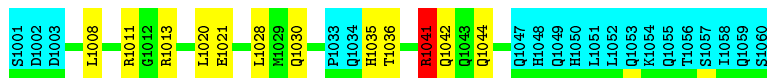


4.2.13 Score per residue for model 13

- Molecule 1: Tumor protein 63



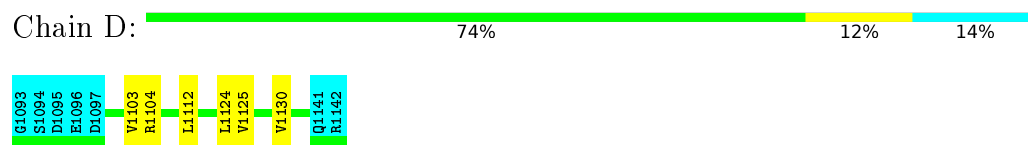
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

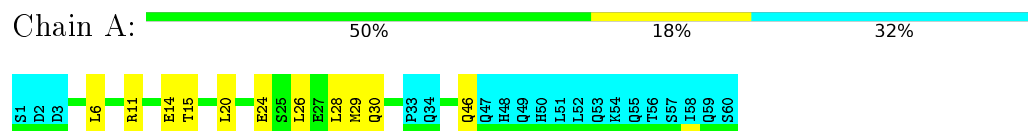


- Molecule 2: Tumor protein p73

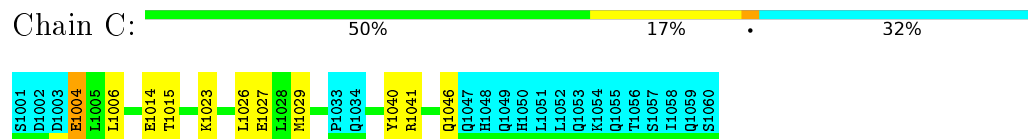


4.2.14 Score per residue for model 14

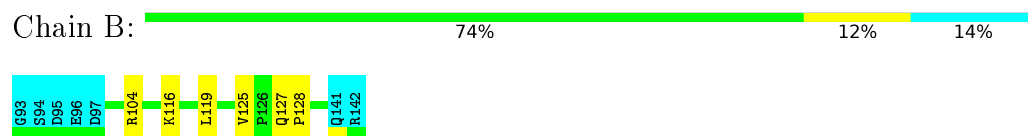
- Molecule 1: Tumor protein 63



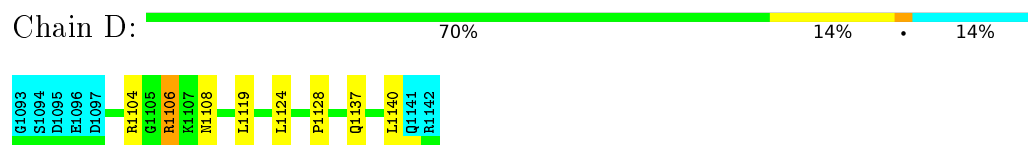
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

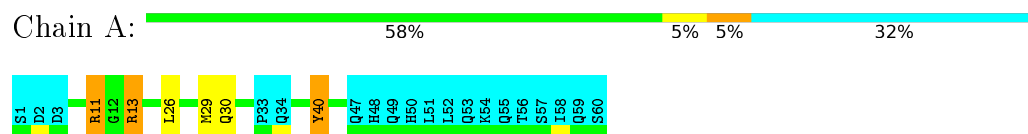


- Molecule 2: Tumor protein p73



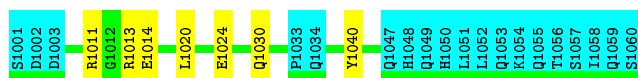
4.2.15 Score per residue for model 15

- Molecule 1: Tumor protein 63

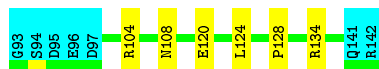


- Molecule 1: Tumor protein 63





- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73

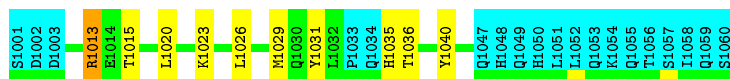


4.2.16 Score per residue for model 16

- Molecule 1: Tumor protein 63



- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

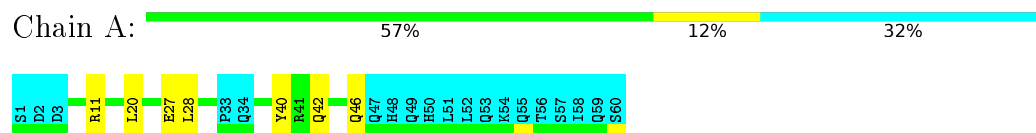


- Molecule 2: Tumor protein p73

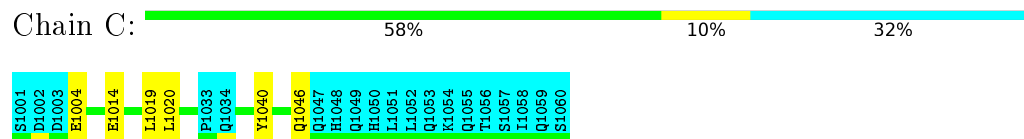


4.2.17 Score per residue for model 17

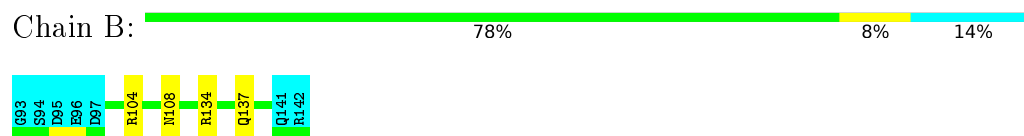
- Molecule 1: Tumor protein 63



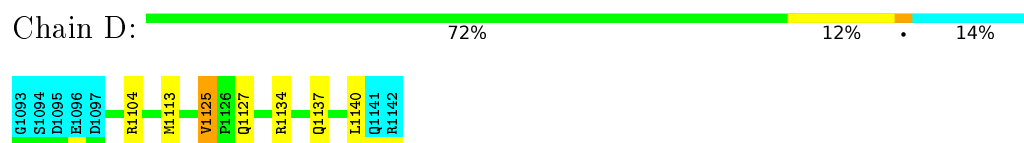
- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73

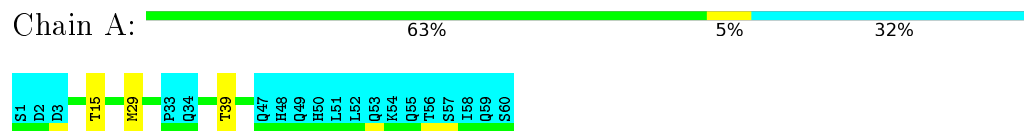


- Molecule 2: Tumor protein p73

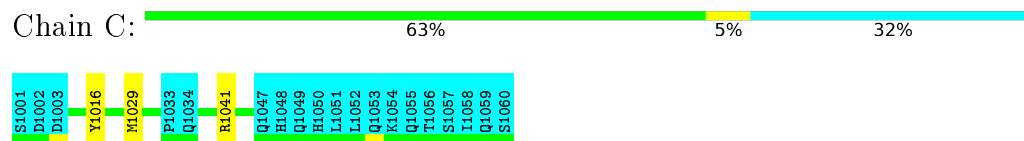


4.2.18 Score per residue for model 18

- Molecule 1: Tumor protein 63

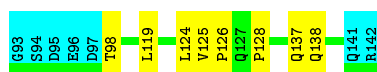


- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73





- Molecule 2: Tumor protein p73



4.2.19 Score per residue for model 19

- Molecule 1: Tumor protein 63



- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73



4.2.20 Score per residue for model 20

- Molecule 1: Tumor protein 63

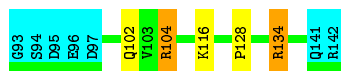
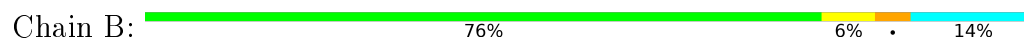




- Molecule 1: Tumor protein 63



- Molecule 2: Tumor protein p73



- Molecule 2: Tumor protein p73



5 Refinement protocol and experimental data overview

The models were refined using the following method: *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
CYANA	structure solution	3.97
OPALp	refinement	1.4

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)	2nb1_cs.cif
Number of chemical shift lists	1
Total number of shifts	2706
Number of shifts mapped to atoms	723
Number of unparsed shifts	1983
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	20%

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

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	0.64±0.01	0±0/364 (0.0±0.0%)	0.95±0.04	0±0/492 (0.0±0.1%)
1	C	0.64±0.01	0±0/364 (0.0±0.0%)	0.96±0.04	0±1/492 (0.1±0.1%)
2	B	0.63±0.01	0±0/373 (0.0±0.0%)	0.99±0.04	0±0/502 (0.1±0.1%)
2	D	0.63±0.01	0±0/373 (0.0±0.0%)	0.98±0.05	1±1/502 (0.1±0.1%)
All	All	0.64	0/29480 (0.0%)	0.97	26/39760 (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	0.7±0.7
1	C	0.0±0.0	0.5±0.6
2	B	0.0±0.0	0.5±0.6
2	D	0.0±0.0	0.6±0.7
All	All	0	45

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
2	B	104	ARG	NE-CZ-NH2	-7.33	116.63	120.30	12	3
2	D	1104	ARG	NE-CZ-NH2	-7.27	116.67	120.30	4	4
2	B	106	ARG	NE-CZ-NH2	-6.52	117.04	120.30	6	1
2	D	1125	VAL	CA-CB-CG1	6.03	119.95	110.90	13	2
1	C	1011	ARG	NE-CZ-NH2	-5.66	117.47	120.30	12	1
1	A	41	ARG	NE-CZ-NH2	-5.51	117.55	120.30	20	1
2	B	133	TYR	CB-CG-CD1	-5.49	117.71	121.00	8	1
1	C	1013	ARG	NE-CZ-NH2	-5.38	117.61	120.30	16	3
2	D	1106	ARG	NE-CZ-NH2	-5.36	117.62	120.30	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	1041	ARG	NE-CZ-NH1	5.36	122.98	120.30	13	1
2	D	1133	TYR	CB-CG-CD1	-5.21	117.87	121.00	1	2
2	B	100	TYR	CB-CG-CD1	-5.13	117.92	121.00	13	1
1	A	11	ARG	NE-CZ-NH2	-5.10	117.75	120.30	2	1
1	C	1011	ARG	NE-CZ-NH1	5.09	122.85	120.30	12	1
1	A	13	ARG	NE-CZ-NH2	-5.09	117.75	120.30	15	1
1	A	41	ARG	NE-CZ-NH1	5.01	122.81	120.30	4	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	11	ARG	Sidechain	5
2	B	99	TYR	Sidechain	4
2	D	1099	TYR	Sidechain	4
1	A	13	ARG	Sidechain	3
1	C	1013	ARG	Sidechain	3
1	A	40	TYR	Sidechain	3
2	D	1106	ARG	Sidechain	3
2	B	106	ARG	Sidechain	3
1	C	1041	ARG	Sidechain	3
1	C	1040	TYR	Sidechain	2
2	B	134	ARG	Sidechain	2
2	D	1104	ARG	Sidechain	2
1	A	41	ARG	Sidechain	2
1	C	1011	ARG	Sidechain	1
2	D	1133	TYR	Sidechain	1
1	C	1016	TYR	Sidechain	1
2	D	1134	ARG	Sidechain	1
1	A	7	TYR	Sidechain	1
2	B	100	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	358	358	358	0±0
1	C	358	358	358	0±0
2	D	367	385	385	0±0
2	B	367	385	385	0±0
All	All	29000	29720	29720	11

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:119:LEU:HD12	2:D:1108:ASN:HD21	0.49	1.67	14	1
1:C:1037:ILE:H	1:C:1037:ILE:HD12	0.47	1.70	5	1
2:B:101:LEU:HD22	2:D:1116:LYS:HE2	0.46	1.87	6	1
1:C:1028:LEU:HD22	2:D:1130:VAL:HG23	0.46	1.86	13	1
1:C:1036:THR:HG23	2:D:1125:VAL:HG21	0.46	1.87	10	1
2:D:1116:LYS:HZ1	2:D:1120:GLU:CG	0.44	2.26	5	1
2:B:103:VAL:HG11	2:D:1116:LYS:HE3	0.43	1.90	3	1
2:B:99:TYR:HB3	2:D:1109:PHE:CD2	0.42	2.49	8	1
1:A:23:LYS:HE2	1:C:1010:VAL:HG11	0.42	1.92	1	1
1:A:8:LEU:HD21	1:C:1023:LYS:HE2	0.41	1.93	7	1
2:B:116:LYS:HD2	2:D:1103:VAL:HG11	0.40	1.93	19	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	41/60 (68%)	39±1 (95±2%)	2±1 (5±2%)	0±0 (0±1%)	59	88
1	C	41/60 (68%)	39±1 (96±2%)	2±1 (4±2%)	0±0 (0±1%)	59	88
2	B	43/50 (86%)	40±1 (93±2%)	2±1 (5±2%)	1±1 (2±2%)	13	53
2	D	43/50 (86%)	40±1 (93±2%)	2±1 (5±2%)	1±1 (2±2%)	14	55
All	All	3360/4400 (76%)	3166 (94%)	157 (5%)	37 (1%)	23	69

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occur-

rence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	128	PRO	13
2	D	1128	PRO	12
2	B	126	PRO	4
2	D	1126	PRO	4
1	C	1004	GLU	1
1	A	4	GLU	1
2	B	127	GLN	1
2	D	1127	GLN	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	40/59 (68%)	34±2 (86±6%)	6±2 (14±6%)	8	49
1	C	40/59 (68%)	34±3 (86±6%)	6±3 (14±6%)	8	47
2	B	42/48 (88%)	36±2 (86±5%)	6±2 (14±5%)	8	48
2	D	42/48 (88%)	35±2 (84±5%)	7±2 (16±5%)	7	44
All	All	3280/4280 (77%)	2799 (85%)	481 (15%)	8	47

All 128 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)
2	D	1104	ARG	14
2	D	1134	ARG	11
2	D	1137	GLN	10
1	C	1020	LEU	10
2	B	102	GLN	10
1	A	20	LEU	9
2	D	1140	LEU	9
2	D	1125	VAL	8
1	A	29	MET	8
2	B	104	ARG	8
2	D	1119	LEU	8
1	C	1011	ARG	8
1	C	1036	THR	7

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Mol	Chain	Res	Type	Models (Total)
1	A	13	ARG	7
2	B	119	LEU	7
2	B	137	GLN	7
2	B	134	ARG	7
2	B	124	LEU	7
1	C	1026	LEU	7
1	C	1029	MET	7
2	B	125	VAL	6
1	A	26	LEU	6
2	D	1098	THR	6
1	A	11	ARG	6
1	C	1015	THR	6
1	C	1041	ARG	6
2	B	140	LEU	6
1	A	8	LEU	6
1	C	1004	GLU	5
1	C	1013	ARG	5
1	A	41	ARG	5
2	D	1113	MET	5
1	C	1008	LEU	5
2	B	98	THR	5
2	B	127	GLN	5
2	B	116	LYS	5
1	C	1040	TYR	5
2	D	1103	VAL	5
2	D	1122	MET	5
1	A	28	LEU	4
1	C	1042	GLN	4
2	B	103	VAL	4
2	D	1101	LEU	4
2	B	122	MET	4
2	D	1120	GLU	4
1	A	36	THR	4
1	A	23	LYS	4
2	D	1124	LEU	4
2	D	1102	GLN	4
1	A	15	THR	4
1	C	1014	GLU	4
1	A	40	TYR	4
2	B	101	LEU	4
1	C	1023	LYS	4
1	A	27	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	C	1035	HIS	4
2	D	1132	SER	3
1	A	31	TYR	3
2	D	1117	GLU	3
1	A	38	GLU	3
2	D	1129	LEU	3
2	B	110	GLU	3
1	A	4	GLU	3
2	B	136	GLN	3
1	A	46	GLN	3
1	A	24	GLU	3
2	D	1106	ARG	3
2	B	108	ASN	3
1	C	1030	GLN	3
2	B	120	GLU	3
2	D	1112	LEU	3
2	B	129	LEU	3
2	D	1127	GLN	3
1	C	1019	LEU	3
1	C	1024	GLU	3
2	B	117	GLU	3
1	C	1031	TYR	3
2	D	1116	LYS	3
1	C	1032	LEU	2
2	B	139	LEU	2
1	A	43	GLN	2
2	D	1110	GLU	2
1	A	44	GLN	2
1	C	1021	GLU	2
1	A	30	GLN	2
1	C	1027	GLU	2
1	A	14	GLU	2
2	B	132	SER	2
2	B	112	LEU	2
2	D	1136	GLN	2
2	D	1114	LYS	2
2	D	1121	LEU	2
1	C	1046	GLN	2
1	A	42	GLN	2
2	B	113	MET	2
2	D	1131	ASP	2
1	A	39	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	19	LEU	2
2	D	1139	LEU	2
1	A	32	LEU	2
1	C	1006	LEU	2
1	A	21	GLU	2
1	A	35	HIS	2
2	D	1118	SER	1
2	B	133	TYR	1
2	D	1138	GLN	1
1	C	1039	THR	1
1	A	6	LEU	1
1	A	25	SER	1
1	C	1018	MET	1
1	A	45	GLN	1
2	B	106	ARG	1
1	C	1038	GLU	1
2	B	114	LYS	1
1	C	1044	GLN	1
2	D	1123	GLU	1
1	A	5	LEU	1
2	D	1108	ASN	1
2	B	135	GLN	1
1	C	1028	LEU	1
1	C	1045	GLN	1
1	A	17	GLU	1
2	B	131	ASP	1
2	B	138	GLN	1
2	B	107	LYS	1
1	C	1005	LEU	1
2	D	1107	LYS	1
2	B	121	LEU	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 [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 20% for the well-defined parts and 22% for the entire structure.

7.1 Chemical shift list 1

File name: 2nb1_cs.cif

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	2706
Number of shifts mapped to atoms	723
Number of unparsed shifts	1983
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- Entity instance (chain) must be specified. All 1983 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
724	?	94	SER	CA	58.711	0.400	1
725	?	94	SER	CB	63.860	0.400	1
726	?	94	SER	HB2	3.928	0.020	2
727	?	94	SER	HB3	3.890	0.020	2
728	?	95	ASP	N	122.025	0.400	1
729	?	95	ASP	H	8.562	0.020	1
730	?	95	ASP	CA	54.810	0.400	1
731	?	95	ASP	HA	4.639	0.020	1
732	?	95	ASP	CB	41.016	0.400	1
733	?	95	ASP	HB2	2.764	0.020	2
734	?	95	ASP	HB3	2.665	0.020	2
735	?	95	ASP	C	176.278	0.400	1
736	?	96	GLU	N	120.066	0.400	1
737	?	96	GLU	H	8.250	0.020	1
738	?	96	GLU	CA	56.585	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
739	?	96	GLU	HA	4.298	0.020	1
740	?	96	GLU	CB	30.397	0.400	1
741	?	96	GLU	HB2	2.122	0.020	2
742	?	96	GLU	HB3	1.905	0.020	2
743	?	96	GLU	CG	36.418	0.400	1
744	?	96	GLU	HG2	2.250	0.020	2
745	?	96	GLU	HG3	2.250	0.020	2
746	?	96	GLU	C	176.192	0.400	1
747	?	97	ASP	N	121.351	0.400	1
748	?	97	ASP	H	8.201	0.020	1
749	?	97	ASP	CA	54.406	0.400	1
750	?	97	ASP	HA	4.573	0.020	1
751	?	97	ASP	CB	41.369	0.400	1
752	?	97	ASP	HB2	2.601	0.020	2
753	?	97	ASP	HB3	2.601	0.020	2
754	?	97	ASP	C	174.498	0.400	1
755	?	98	THR	N	114.380	0.400	1
756	?	98	THR	H	7.557	0.020	1
757	?	98	THR	CA	62.159	0.400	1
758	?	98	THR	HA	4.655	0.020	1
759	?	98	THR	CB	70.272	0.400	1
760	?	98	THR	HB	3.722	0.020	1
761	?	98	THR	CG2	21.804	0.400	1
762	?	98	THR	HG21	0.862	0.020	1
763	?	98	THR	HG22	0.862	0.020	1
764	?	98	THR	HG23	0.862	0.020	1
765	?	98	THR	C	172.624	0.400	1
766	?	99	TYR	N	124.760	0.400	1
767	?	99	TYR	H	8.926	0.020	1
768	?	99	TYR	CA	56.835	0.400	1
769	?	99	TYR	HA	4.350	0.020	1
770	?	99	TYR	CB	42.581	0.400	1
771	?	99	TYR	HB2	2.104	0.020	2
772	?	99	TYR	HB3	2.104	0.020	2
773	?	99	TYR	CD1	133.400	0.400	1
774	?	99	TYR	HD1	6.485	0.020	1
775	?	99	TYR	CE1	117.091	0.400	1
776	?	99	TYR	HE1	6.445	0.020	1
777	?	99	TYR	HE2	6.445	0.020	1
778	?	99	TYR	HD2	6.485	0.020	1
779	?	99	TYR	C	174.022	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
780	?	100	TYR	N	118.700	0.400	1
781	?	100	TYR	H	8.401	0.020	1
782	?	100	TYR	CA	57.289	0.400	1
783	?	100	TYR	HA	5.441	0.020	1
784	?	100	TYR	CB	41.584	0.400	1
785	?	100	TYR	HB2	2.920	0.020	2
786	?	100	TYR	HB3	2.821	0.020	2
787	?	100	TYR	CD1	133.033	0.400	1
788	?	100	TYR	HD1	6.984	0.020	1
789	?	100	TYR	CE1	118.034	0.400	1
790	?	100	TYR	HE1	6.663	0.020	1
791	?	100	TYR	HE2	6.663	0.020	1
792	?	100	TYR	HD2	6.984	0.020	1
793	?	100	TYR	C	174.891	0.400	1
794	?	101	LEU	N	121.632	0.400	1
795	?	101	LEU	H	9.204	0.020	1
796	?	101	LEU	CA	54.498	0.400	1
797	?	101	LEU	HA	4.992	0.020	1
798	?	101	LEU	CB	46.266	0.400	1
799	?	101	LEU	HB2	1.854	0.020	2
800	?	101	LEU	HB3	1.620	0.020	2
801	?	101	LEU	CG	26.939	0.400	1
802	?	101	LEU	HG	1.775	0.020	1
803	?	101	LEU	CD1	26.375	0.400	1
804	?	101	LEU	HD11	0.819	0.020	2
805	?	101	LEU	HD12	0.819	0.020	2
806	?	101	LEU	HD13	0.819	0.020	2
807	?	101	LEU	CD2	27.073	0.400	1
808	?	101	LEU	HD21	0.776	0.020	2
809	?	101	LEU	HD22	0.776	0.020	2
810	?	101	LEU	HD23	0.776	0.020	2
811	?	101	LEU	C	174.466	0.400	1
812	?	102	GLN	N	123.532	0.400	1
813	?	102	GLN	H	9.013	0.020	1
814	?	102	GLN	CA	54.374	0.400	1
815	?	102	GLN	HA	5.080	0.020	1
816	?	102	GLN	CB	31.382	0.400	1
817	?	102	GLN	HB2	1.817	0.020	2
818	?	102	GLN	HB3	1.936	0.020	2
819	?	102	GLN	CG	34.225	0.400	1
820	?	102	GLN	HG2	1.993	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
821	?	102	GLN	HG3	1.993	0.020	2
822	?	102	GLN	NE2	111.543	0.400	1
823	?	102	GLN	HE21	6.763	0.020	2
824	?	102	GLN	HE22	7.171	0.020	2
825	?	102	GLN	C	174.509	0.400	1
826	?	103	VAL	N	124.091	0.400	1
827	?	103	VAL	H	9.159	0.020	1
828	?	103	VAL	CA	60.198	0.400	1
829	?	103	VAL	HA	4.599	0.020	1
830	?	103	VAL	CB	35.603	0.400	1
831	?	103	VAL	HB	1.858	0.020	1
832	?	103	VAL	CG1	22.465	0.400	1
833	?	103	VAL	HG11	0.974	0.020	2
834	?	103	VAL	HG12	0.974	0.020	2
835	?	103	VAL	HG13	0.974	0.020	2
836	?	103	VAL	CG2	20.695	0.400	1
837	?	103	VAL	HG21	0.942	0.020	2
838	?	103	VAL	HG22	0.942	0.020	2
839	?	103	VAL	HG23	0.942	0.020	2
840	?	103	VAL	C	172.608	0.400	1
841	?	104	ARG	N	129.114	0.400	1
842	?	104	ARG	H	9.324	0.020	1
843	?	104	ARG	CA	55.820	0.400	1
844	?	104	ARG	HA	4.890	0.020	1
845	?	104	ARG	CB	31.257	0.400	1
846	?	104	ARG	HB2	1.824	0.020	2
847	?	104	ARG	HB3	1.699	0.020	2
848	?	104	ARG	CG	27.514	0.400	1
849	?	104	ARG	HG2	1.595	0.020	2
850	?	104	ARG	HG3	1.595	0.020	2
851	?	104	ARG	CD	43.493	0.400	1
852	?	104	ARG	HD2	3.221	0.020	2
853	?	104	ARG	HD3	3.221	0.020	2
854	?	104	ARG	NE	136.282	0.400	1
855	?	104	ARG	HE	8.184	0.020	1
856	?	104	ARG	C	176.488	0.400	1
857	?	105	GLY	N	114.585	0.400	1
858	?	105	GLY	H	8.813	0.020	1
859	?	105	GLY	CA	44.970	0.400	1
860	?	105	GLY	HA2	4.696	0.020	2
861	?	105	GLY	HA3	3.911	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
862	?	105	GLY	C	176.498	0.400	1
863	?	106	ARG	N	127.937	0.400	1
864	?	106	ARG	H	8.866	0.020	1
865	?	106	ARG	CA	59.637	0.400	1
866	?	106	ARG	HA	3.525	0.020	1
867	?	106	ARG	CB	29.841	0.400	1
868	?	106	ARG	HB2	2.044	0.020	2
869	?	106	ARG	HB3	1.862	0.020	2
870	?	106	ARG	CG	26.877	0.400	1
871	?	106	ARG	HG2	1.693	0.020	2
872	?	106	ARG	HG3	1.693	0.020	2
873	?	106	ARG	CD	42.924	0.400	1
874	?	106	ARG	HD2	3.112	0.020	2
875	?	106	ARG	HD3	3.112	0.020	2
876	?	106	ARG	C	177.603	0.400	1
877	?	107	LYS	N	119.095	0.400	1
878	?	107	LYS	H	8.556	0.020	1
879	?	107	LYS	CA	59.527	0.400	1
880	?	107	LYS	HA	4.024	0.020	1
881	?	107	LYS	CB	31.368	0.400	1
882	?	107	LYS	HB2	1.864	0.020	2
883	?	107	LYS	HB3	1.765	0.020	2
884	?	107	LYS	CG	24.515	0.400	1
885	?	107	LYS	HG2	1.478	0.020	2
886	?	107	LYS	HG3	1.355	0.020	2
887	?	107	LYS	CD	29.078	0.400	1
888	?	107	LYS	HD2	1.688	0.020	2
889	?	107	LYS	HD3	1.688	0.020	2
890	?	107	LYS	CE	42.151	0.400	1
891	?	107	LYS	HE2	2.947	0.020	2
892	?	107	LYS	HE3	2.947	0.020	2
893	?	107	LYS	C	178.726	0.400	1
894	?	108	ASN	N	116.769	0.400	1
895	?	108	ASN	H	7.617	0.020	1
896	?	108	ASN	CA	55.393	0.400	1
897	?	108	ASN	HA	4.402	0.020	1
898	?	108	ASN	CB	37.528	0.400	1
899	?	108	ASN	HB2	2.957	0.020	2
900	?	108	ASN	HB3	2.268	0.020	2
901	?	108	ASN	ND2	114.634	0.400	1
902	?	108	ASN	HD21	6.624	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
903	?	108	ASN	C	176.932	0.400	1
904	?	109	PHE	N	120.646	0.400	1
905	?	109	PHE	H	8.051	0.020	1
906	?	109	PHE	CA	61.430	0.400	1
907	?	109	PHE	HA	3.901	0.020	1
908	?	109	PHE	CB	39.099	0.400	1
909	?	109	PHE	HB2	2.594	0.020	2
910	?	109	PHE	HB3	2.724	0.020	2
911	?	109	PHE	CD1	131.521	0.400	1
912	?	109	PHE	HD1	6.635	0.020	1
913	?	109	PHE	CE1	131.117	0.400	1
914	?	109	PHE	HE1	7.213	0.020	1
915	?	109	PHE	HE2	7.213	0.020	1
916	?	109	PHE	HD2	6.635	0.020	1
917	?	109	PHE	C	175.757	0.400	1
918	?	110	GLU	N	117.509	0.400	1
919	?	110	GLU	H	8.364	0.020	1
920	?	110	GLU	CA	59.873	0.400	1
921	?	110	GLU	HA	3.505	0.020	1
922	?	110	GLU	CB	29.177	0.400	1
923	?	110	GLU	HB2	2.096	0.020	2
924	?	110	GLU	HB3	1.930	0.020	2
925	?	110	GLU	CG	37.152	0.400	1
926	?	110	GLU	HG2	2.176	0.020	2
927	?	110	GLU	HG3	2.534	0.020	2
928	?	110	GLU	C	180.017	0.400	1
929	?	111	ILE	N	119.260	0.400	1
930	?	111	ILE	H	7.670	0.020	1
931	?	111	ILE	CA	65.580	0.400	1
932	?	111	ILE	HA	3.644	0.020	1
933	?	111	ILE	CB	38.429	0.400	1
934	?	111	ILE	HB	1.833	0.020	1
935	?	111	ILE	CG2	17.073	0.400	1
936	?	111	ILE	HG21	0.806	0.020	1
937	?	111	ILE	HG22	0.806	0.020	1
938	?	111	ILE	HG23	0.806	0.020	1
939	?	111	ILE	CG1	29.459	0.400	1
940	?	111	ILE	HG12	1.833	0.020	2
941	?	111	ILE	HG13	0.984	0.020	2
942	?	111	ILE	CD1	13.733	0.400	1
943	?	111	ILE	HD11	0.840	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
944	?	111	ILE	HD12	0.840	0.020	1
945	?	111	ILE	HD13	0.840	0.020	1
946	?	111	ILE	C	177.344	0.400	1
947	?	112	LEU	N	117.913	0.400	1
948	?	112	LEU	H	7.937	0.020	1
949	?	112	LEU	CA	58.221	0.400	1
950	?	112	LEU	HA	3.804	0.020	1
951	?	112	LEU	CB	41.337	0.400	1
952	?	112	LEU	HB2	1.150	0.020	2
953	?	112	LEU	HB3	1.150	0.020	2
954	?	112	LEU	CG	26.751	0.400	1
955	?	112	LEU	HG	1.828	0.020	1
956	?	112	LEU	CD1	23.470	0.400	1
957	?	112	LEU	HD11	0.731	0.020	2
958	?	112	LEU	HD12	0.731	0.020	2
959	?	112	LEU	HD13	0.731	0.020	2
960	?	112	LEU	C	178.883	0.400	1
961	?	113	MET	N	118.279	0.400	1
962	?	113	MET	H	8.659	0.020	1
963	?	113	MET	CA	57.871	0.400	1
964	?	113	MET	HA	4.032	0.020	1
965	?	113	MET	CB	31.907	0.400	1
966	?	113	MET	HB2	1.904	0.020	2
967	?	113	MET	HB3	1.843	0.020	2
968	?	113	MET	CG	31.572	0.400	1
969	?	113	MET	HG2	1.821	0.020	2
970	?	113	MET	HG3	1.716	0.020	2
971	?	113	MET	CE	16.833	0.400	1
972	?	113	MET	HE1	1.883	0.020	1
973	?	113	MET	HE2	1.883	0.020	1
974	?	113	MET	HE3	1.883	0.020	1
975	?	113	MET	C	178.742	0.400	1
976	?	114	LYS	N	120.560	0.400	1
977	?	114	LYS	H	7.381	0.020	1
978	?	114	LYS	CA	59.346	0.400	1
979	?	114	LYS	HA	4.023	0.020	1
980	?	114	LYS	CB	32.224	0.400	1
981	?	114	LYS	HB2	1.911	0.020	2
982	?	114	LYS	HB3	1.817	0.020	2
983	?	114	LYS	CG	25.296	0.400	1
984	?	114	LYS	HG2	1.377	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
985	?	114	LYS	HG3	1.547	0.020	2
986	?	114	LYS	CD	29.305	0.400	1
987	?	114	LYS	HD2	1.633	0.020	2
988	?	114	LYS	HD3	1.633	0.020	2
989	?	114	LYS	CE	42.200	0.400	1
990	?	114	LYS	HE2	2.890	0.020	2
991	?	114	LYS	HE3	2.890	0.020	2
992	?	114	LYS	C	179.072	0.400	1
993	?	115	LEU	N	118.891	0.400	1
994	?	115	LEU	H	7.688	0.020	1
995	?	115	LEU	CA	56.462	0.400	1
996	?	115	LEU	HA	4.345	0.020	1
997	?	115	LEU	CB	41.718	0.400	1
998	?	115	LEU	HB2	1.644	0.020	2
999	?	115	LEU	HB3	1.234	0.020	2
1000	?	115	LEU	CG	26.351	0.400	1
1001	?	115	LEU	HG	0.721	0.020	1
1002	?	115	LEU	CD1	24.109	0.400	1
1003	?	115	LEU	HD11	0.695	0.020	2
1004	?	115	LEU	HD12	0.695	0.020	2
1005	?	115	LEU	HD13	0.695	0.020	2
1006	?	115	LEU	C	177.923	0.400	1
1007	?	116	LYS	N	121.250	0.400	1
1008	?	116	LYS	H	8.884	0.020	1
1009	?	116	LYS	CA	60.465	0.400	1
1010	?	116	LYS	HA	3.730	0.020	1
1011	?	116	LYS	CB	33.137	0.400	1
1012	?	116	LYS	HB2	2.102	0.020	2
1013	?	116	LYS	HB3	1.897	0.020	2
1014	?	116	LYS	CG	24.741	0.400	1
1015	?	116	LYS	HG2	1.413	0.020	2
1016	?	116	LYS	HG3	1.581	0.020	2
1017	?	116	LYS	CD	30.050	0.400	1
1018	?	116	LYS	HD2	1.682	0.020	2
1019	?	116	LYS	HD3	1.925	0.020	2
1020	?	116	LYS	CE	43.381	0.400	1
1021	?	116	LYS	C	177.059	0.400	1
1022	?	117	GLU	N	116.755	0.400	1
1023	?	117	GLU	H	7.660	0.020	1
1024	?	117	GLU	CA	58.898	0.400	1
1025	?	117	GLU	HA	4.276	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1026	?	117	GLU	CB	30.277	0.400	1
1027	?	117	GLU	HB2	2.250	0.020	2
1028	?	117	GLU	HB3	2.250	0.020	2
1029	?	117	GLU	CG	37.309	0.400	1
1030	?	117	GLU	HG2	2.037	0.020	2
1031	?	117	GLU	HG3	2.353	0.020	2
1032	?	117	GLU	C	177.169	0.400	1
1033	?	118	SER	N	114.369	0.400	1
1034	?	118	SER	H	7.659	0.020	1
1035	?	118	SER	CA	62.553	0.400	1
1036	?	118	SER	HA	4.169	0.020	1
1037	?	118	SER	CB	62.632	0.400	1
1038	?	118	SER	HB2	3.738	0.020	2
1039	?	118	SER	HB3	3.818	0.020	2
1040	?	118	SER	C	177.177	0.400	1
1041	?	119	LEU	N	123.247	0.400	1
1042	?	119	LEU	H	8.486	0.020	1
1043	?	119	LEU	CA	58.379	0.400	1
1044	?	119	LEU	HA	4.039	0.020	1
1045	?	119	LEU	CB	40.787	0.400	1
1046	?	119	LEU	HB2	1.787	0.020	2
1047	?	119	LEU	HB3	1.417	0.020	2
1048	?	119	LEU	CG	25.848	0.400	1
1049	?	119	LEU	HG	0.689	0.020	1
1050	?	119	LEU	CD1	21.773	0.400	1
1051	?	119	LEU	HD11	0.852	0.020	2
1052	?	119	LEU	HD12	0.852	0.020	2
1053	?	119	LEU	HD13	0.852	0.020	2
1054	?	119	LEU	C	180.394	0.400	1
1055	?	120	GLU	N	117.672	0.400	1
1056	?	120	GLU	H	8.410	0.020	1
1057	?	120	GLU	CA	59.795	0.400	1
1058	?	120	GLU	HA	4.069	0.020	1
1059	?	120	GLU	CB	29.567	0.400	1
1060	?	120	GLU	HB2	2.296	0.020	2
1061	?	120	GLU	HB3	2.026	0.020	2
1062	?	120	GLU	CG	38.477	0.400	1
1063	?	120	GLU	HG2	2.886	0.020	2
1064	?	120	GLU	HG3	2.341	0.020	2
1065	?	120	GLU	C	180.268	0.400	1
1066	?	121	LEU	N	119.445	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1067	?	121	LEU	H	8.323	0.020	1
1068	?	121	LEU	CA	57.093	0.400	1
1069	?	121	LEU	HA	3.865	0.020	1
1070	?	121	LEU	CB	41.526	0.400	1
1071	?	121	LEU	HB2	1.085	0.020	2
1072	?	121	LEU	HB3	1.741	0.020	2
1073	?	121	LEU	CG	27.031	0.400	1
1074	?	121	LEU	HG	1.749	0.020	1
1075	?	121	LEU	CD1	23.424	0.400	1
1076	?	121	LEU	HD11	0.447	0.020	2
1077	?	121	LEU	HD12	0.447	0.020	2
1078	?	121	LEU	HD13	0.447	0.020	2
1079	?	121	LEU	CD2	27.068	0.400	1
1080	?	121	LEU	HD21	0.496	0.020	2
1081	?	121	LEU	HD22	0.496	0.020	2
1082	?	121	LEU	HD23	0.496	0.020	2
1083	?	121	LEU	C	179.058	0.400	1
1084	?	122	MET	N	118.025	0.400	1
1085	?	122	MET	H	7.662	0.020	1
1086	?	122	MET	CA	58.894	0.400	1
1087	?	122	MET	HA	4.002	0.020	1
1088	?	122	MET	CB	31.981	0.400	1
1089	?	122	MET	HB2	2.705	0.020	2
1090	?	122	MET	HB3	2.515	0.020	2
1091	?	122	MET	CG	32.264	0.400	1
1092	?	122	MET	HG2	2.194	0.020	2
1093	?	122	MET	HG3	2.114	0.020	2
1094	?	122	MET	CE	17.346	0.400	1
1095	?	122	MET	HE1	2.024	0.020	1
1096	?	122	MET	HE2	2.024	0.020	1
1097	?	122	MET	HE3	2.024	0.020	1
1098	?	122	MET	C	178.224	0.400	1
1099	?	123	GLU	N	115.784	0.400	1
1100	?	123	GLU	H	7.235	0.020	1
1101	?	123	GLU	CA	57.957	0.400	1
1102	?	123	GLU	HA	4.157	0.020	1
1103	?	123	GLU	CB	29.809	0.400	1
1104	?	123	GLU	HB2	2.130	0.020	2
1105	?	123	GLU	HB3	2.130	0.020	2
1106	?	123	GLU	CG	36.187	0.400	1
1107	?	123	GLU	HG2	2.390	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1108	?	123	GLU	HG3	2.390	0.020	2
1109	?	123	GLU	C	176.954	0.400	1
1110	?	124	LEU	N	117.445	0.400	1
1111	?	124	LEU	H	7.964	0.020	1
1112	?	124	LEU	CA	54.748	0.400	1
1113	?	124	LEU	HA	4.308	0.020	1
1114	?	124	LEU	CB	42.099	0.400	1
1115	?	124	LEU	HB2	1.905	0.020	2
1116	?	124	LEU	HB3	1.905	0.020	2
1117	?	124	LEU	CG	27.458	0.400	1
1118	?	124	LEU	HG	1.667	0.020	1
1119	?	124	LEU	HD1	0.895	0.020	2
1120	?	124	LEU	HD1	0.895	0.020	2
1121	?	124	LEU	HD1	0.895	0.020	2
1122	?	124	LEU	HD2	0.895	0.020	2
1123	?	124	LEU	HD2	0.895	0.020	2
1124	?	124	LEU	HD2	0.895	0.020	2
1125	?	124	LEU	CD1	25.800	0.400	1
1126	?	124	LEU	CD2	22.551	0.400	1
1127	?	124	LEU	C	177.537	0.400	1
1128	?	125	VAL	N	122.935	0.400	1
1129	?	125	VAL	H	7.375	0.020	1
1130	?	125	VAL	CA	61.225	0.400	1
1131	?	125	VAL	HA	3.932	0.020	1
1132	?	125	VAL	CB	32.131	0.400	1
1133	?	125	VAL	HB	2.038	0.020	1
1134	?	125	VAL	HG1	0.958	0.020	2
1135	?	125	VAL	HG1	0.958	0.020	2
1136	?	125	VAL	HG1	0.958	0.020	2
1137	?	125	VAL	HG2	0.958	0.020	2
1138	?	125	VAL	HG2	0.958	0.020	2
1139	?	125	VAL	HG2	0.958	0.020	2
1140	?	125	VAL	C	174.154	0.400	1
1141	?	126	PRO	CD	51.276	0.400	1
1142	?	126	PRO	CA	63.358	0.400	1
1143	?	126	PRO	HA	4.393	0.020	1
1144	?	126	PRO	CB	33.330	0.400	1
1145	?	126	PRO	HB2	1.917	0.020	2
1146	?	126	PRO	HB3	2.490	0.020	2
1147	?	126	PRO	CG	27.975	0.400	1
1148	?	126	PRO	HG2	2.195	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1149	?	126	PRO	HG3	2.105	0.020	2
1150	?	126	PRO	HD2	4.219	0.020	2
1151	?	126	PRO	HD3	3.564	0.020	2
1152	?	126	PRO	C	177.633	0.400	1
1153	?	127	GLN	N	125.241	0.400	1
1154	?	127	GLN	H	8.993	0.020	1
1155	?	127	GLN	CA	60.076	0.400	1
1156	?	127	GLN	HA	3.959	0.020	1
1157	?	127	GLN	CB	26.139	0.400	1
1158	?	127	GLN	HB2	2.279	0.020	2
1159	?	127	GLN	HB3	2.141	0.020	2
1160	?	127	GLN	C	174.012	0.400	1
1161	?	128	PRO	CD	50.402	0.400	1
1162	?	128	PRO	CA	66.248	0.400	1
1163	?	128	PRO	HA	4.427	0.020	1
1164	?	128	PRO	CB	31.154	0.400	1
1165	?	128	PRO	HB2	2.415	0.020	2
1166	?	128	PRO	HB3	1.764	0.020	2
1167	?	128	PRO	CG	28.668	0.400	1
1168	?	128	PRO	HG2	2.016	0.020	2
1169	?	128	PRO	HG3	2.016	0.020	2
1170	?	128	PRO	HD2	3.821	0.020	2
1171	?	128	PRO	HD3	3.515	0.020	2
1172	?	128	PRO	C	179.719	0.400	1
1173	?	129	LEU	N	116.655	0.400	1
1174	?	129	LEU	H	7.220	0.020	1
1175	?	129	LEU	CA	57.174	0.400	1
1176	?	129	LEU	HA	4.162	0.020	1
1177	?	129	LEU	CB	41.264	0.400	1
1178	?	129	LEU	HB2	1.204	0.020	2
1179	?	129	LEU	HB3	1.732	0.020	2
1180	?	129	LEU	CG	27.511	0.400	1
1181	?	129	LEU	HG	1.571	0.020	1
1182	?	129	LEU	CD1	24.993	0.400	1
1183	?	129	LEU	HD11	0.871	0.020	2
1184	?	129	LEU	HD12	0.871	0.020	2
1185	?	129	LEU	HD13	0.871	0.020	2
1186	?	129	LEU	CD2	23.290	0.400	1
1187	?	129	LEU	HD21	0.761	0.020	2
1188	?	129	LEU	HD22	0.761	0.020	2
1189	?	129	LEU	HD23	0.761	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1190	?	129	LEU	C	178.871	0.400	1
1191	?	130	VAL	N	121.976	0.400	1
1192	?	130	VAL	H	7.465	0.020	1
1193	?	130	VAL	CA	67.124	0.400	1
1194	?	130	VAL	HA	3.471	0.020	1
1195	?	130	VAL	CB	31.438	0.400	1
1196	?	130	VAL	HB	2.220	0.020	1
1197	?	130	VAL	HG1	0.936	0.020	2
1198	?	130	VAL	HG1	0.936	0.020	2
1199	?	130	VAL	HG1	0.936	0.020	2
1200	?	130	VAL	HG2	0.936	0.020	2
1201	?	130	VAL	HG2	0.936	0.020	2
1202	?	130	VAL	HG2	0.936	0.020	2
1203	?	130	VAL	CG1	22.511	0.400	1
1204	?	130	VAL	CG2	21.028	0.400	1
1205	?	130	VAL	C	178.353	0.400	1
1206	?	131	ASP	N	118.845	0.400	1
1207	?	131	ASP	H	8.605	0.020	1
1208	?	131	ASP	CA	57.796	0.400	1
1209	?	131	ASP	HA	4.365	0.020	1
1210	?	131	ASP	CB	40.198	0.400	1
1211	?	131	ASP	HB2	2.672	0.020	2
1212	?	131	ASP	HB3	2.672	0.020	2
1213	?	131	ASP	C	179.398	0.400	1
1214	?	132	SER	N	115.275	0.400	1
1215	?	132	SER	H	7.817	0.020	1
1216	?	132	SER	CA	61.726	0.400	1
1217	?	132	SER	HA	4.239	0.020	1
1218	?	132	SER	CB	62.897	0.400	1
1219	?	132	SER	HB2	3.980	0.020	2
1220	?	132	SER	HB3	4.028	0.020	2
1221	?	132	SER	C	179.406	0.400	1
1222	?	133	TYR	N	124.425	0.400	1
1223	?	133	TYR	H	8.247	0.020	1
1224	?	133	TYR	CA	61.719	0.400	1
1225	?	133	TYR	HA	4.175	0.020	1
1226	?	133	TYR	CB	38.434	0.400	1
1227	?	133	TYR	HB2	3.291	0.020	2
1228	?	133	TYR	HB3	3.059	0.020	2
1229	?	133	TYR	CD1	133.170	0.400	1
1230	?	133	TYR	HD1	7.085	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1231	?	133	TYR	CE1	117.977	0.400	1
1232	?	133	TYR	HE1	6.801	0.020	1
1233	?	133	TYR	HE2	6.801	0.020	1
1234	?	133	TYR	HD2	7.085	0.020	1
1235	?	133	TYR	C	178.220	0.400	1
1236	?	134	ARG	N	119.750	0.400	1
1237	?	134	ARG	H	8.731	0.020	1
1238	?	134	ARG	CA	60.458	0.400	1
1239	?	134	ARG	HA	3.734	0.020	1
1240	?	134	ARG	CB	29.662	0.400	1
1241	?	134	ARG	HB2	1.791	0.020	2
1242	?	134	ARG	HB3	2.157	0.020	2
1243	?	134	ARG	CD	43.719	0.400	1
1244	?	134	ARG	HD2	3.185	0.020	2
1245	?	134	ARG	HD3	3.185	0.020	2
1246	?	134	ARG	NE	135.124	0.400	1
1247	?	134	ARG	HE	7.364	0.020	1
1248	?	134	ARG	C	179.611	0.400	1
1249	?	135	GLN	N	119.346	0.400	1
1250	?	135	GLN	H	8.063	0.020	1
1251	?	135	GLN	CA	58.813	0.400	1
1252	?	135	GLN	HA	4.078	0.020	1
1253	?	135	GLN	CB	28.394	0.400	1
1254	?	135	GLN	HB2	2.085	0.020	2
1255	?	135	GLN	HB3	1.918	0.020	2
1256	?	135	GLN	CG	34.014	0.400	1
1257	?	135	GLN	HG2	2.531	0.020	2
1258	?	135	GLN	HG3	2.410	0.020	2
1259	?	135	GLN	NE2	112.038	0.400	1
1260	?	135	GLN	HE21	7.285	0.020	2
1261	?	135	GLN	HE22	6.765	0.020	2
1262	?	135	GLN	C	178.594	0.400	1
1263	?	136	GLN	N	118.513	0.400	1
1264	?	136	GLN	H	7.900	0.020	1
1265	?	136	GLN	CA	58.210	0.400	1
1266	?	136	GLN	HA	4.048	0.020	1
1267	?	136	GLN	CB	28.396	0.400	1
1268	?	136	GLN	HB2	2.142	0.020	2
1269	?	136	GLN	HB3	2.142	0.020	2
1270	?	136	GLN	CG	34.152	0.400	1
1271	?	136	GLN	HG2	2.512	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1272	?	136	GLN	HG3	2.512	0.020	2
1273	?	136	GLN	C	178.597	0.400	1
1274	?	137	GLN	N	117.373	0.400	1
1275	?	137	GLN	H	7.935	0.020	1
1276	?	137	GLN	CA	57.369	0.400	1
1277	?	137	GLN	HA	3.869	0.020	1
1278	?	137	GLN	CB	28.361	0.400	1
1279	?	137	GLN	HB2	2.002	0.020	2
1280	?	137	GLN	HB3	2.002	0.020	2
1281	?	137	GLN	CG	33.617	0.400	1
1282	?	137	GLN	HG2	2.000	0.020	2
1283	?	137	GLN	HG3	2.000	0.020	2
1284	?	137	GLN	C	178.363	0.400	1
1285	?	138	GLN	N	118.243	0.400	1
1286	?	138	GLN	H	7.709	0.020	1
1287	?	138	GLN	CA	57.852	0.400	1
1288	?	138	GLN	HA	4.142	0.020	1
1289	?	138	GLN	CB	28.516	0.400	1
1290	?	138	GLN	HB2	2.161	0.020	2
1291	?	138	GLN	HB3	2.161	0.020	2
1292	?	138	GLN	CG	34.000	0.400	1
1293	?	138	GLN	HG2	2.478	0.020	2
1294	?	138	GLN	HG3	2.478	0.020	2
1295	?	138	GLN	C	177.503	0.400	1
1296	?	139	LEU	N	118.586	0.400	1
1297	?	139	LEU	H	7.484	0.020	1
1298	?	139	LEU	CA	56.031	0.400	1
1299	?	139	LEU	HA	4.268	0.020	1
1300	?	139	LEU	CB	42.078	0.400	1
1301	?	139	LEU	HB2	1.780	0.020	2
1302	?	139	LEU	HB3	1.647	0.020	2
1303	?	139	LEU	CG	26.962	0.400	1
1304	?	139	LEU	HG	1.750	0.020	1
1305	?	139	LEU	HD1	0.924	0.020	2
1306	?	139	LEU	HD1	0.924	0.020	2
1307	?	139	LEU	HD1	0.924	0.020	2
1308	?	139	LEU	HD2	0.924	0.020	2
1309	?	139	LEU	HD2	0.924	0.020	2
1310	?	139	LEU	HD2	0.924	0.020	2
1311	?	139	LEU	CD1	25.189	0.400	1
1312	?	139	LEU	CD2	23.004	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1313	?	139	LEU	C	177.835	0.400	1
1314	?	140	LEU	N	118.753	0.400	1
1315	?	140	LEU	H	7.532	0.020	1
1316	?	140	LEU	CA	55.149	0.400	1
1317	?	140	LEU	HA	4.341	0.020	1
1318	?	140	LEU	CB	42.380	0.400	1
1319	?	140	LEU	HB2	1.755	0.020	2
1320	?	140	LEU	HB3	1.599	0.020	2
1321	?	140	LEU	CG	26.624	0.400	1
1322	?	140	LEU	HG	1.731	0.020	1
1323	?	140	LEU	HD1	0.840	0.020	2
1324	?	140	LEU	HD1	0.840	0.020	2
1325	?	140	LEU	HD1	0.840	0.020	2
1326	?	140	LEU	HD2	0.840	0.020	2
1327	?	140	LEU	HD2	0.840	0.020	2
1328	?	140	LEU	HD2	0.840	0.020	2
1329	?	140	LEU	CD1	25.299	0.400	1
1330	?	140	LEU	CD2	22.837	0.400	1
1331	?	140	LEU	C	177.207	0.400	1
1332	?	141	GLN	N	119.878	0.400	1
1333	?	141	GLN	H	7.675	0.020	1
1334	?	141	GLN	CA	56.161	0.400	1
1335	?	141	GLN	HA	4.359	0.020	1
1336	?	141	GLN	CB	29.534	0.400	1
1337	?	141	GLN	HB2	2.213	0.020	2
1338	?	141	GLN	HB3	2.051	0.020	2
1339	?	141	GLN	CG	34.003	0.400	1
1340	?	141	GLN	HG2	2.457	0.020	2
1341	?	141	GLN	HG3	2.457	0.020	2
1342	?	141	GLN	C	174.910	0.400	1
1343	?	142	ARG	N	127.959	0.400	1
1344	?	142	ARG	H	7.955	0.020	1
1345	?	142	ARG	CA	57.568	0.400	1
1346	?	142	ARG	HA	4.140	0.020	1
1347	?	142	ARG	CB	31.701	0.400	1
1348	?	142	ARG	HB2	1.590	0.020	2
1349	?	142	ARG	HB3	1.756	0.020	2
1350	?	142	ARG	CD	43.483	0.400	1
1351	?	142	ARG	HD2	2.888	0.020	2
1352	?	142	ARG	HD3	2.861	0.020	2
1353	?	142	ARG	C	180.825	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1354	?	1001	SER	CA	59.385	0.400	1
1355	?	1001	SER	HA	4.455	0.020	1
1356	?	1001	SER	CB	63.702	0.400	1
1357	?	1001	SER	HB2	3.908	0.020	2
1358	?	1001	SER	HB3	3.908	0.020	2
1359	?	1001	SER	C	174.696	0.400	1
1360	?	1002	ASP	N	121.276	0.400	1
1361	?	1002	ASP	H	8.555	0.020	1
1362	?	1002	ASP	CA	54.685	0.400	1
1363	?	1002	ASP	HA	4.683	0.020	1
1364	?	1002	ASP	CB	40.974	0.400	1
1365	?	1002	ASP	HB2	2.759	0.020	2
1366	?	1002	ASP	HB3	2.644	0.020	2
1367	?	1002	ASP	C	175.828	0.400	1
1368	?	1003	ASP	N	119.296	0.400	1
1369	?	1003	ASP	H	8.004	0.020	1
1370	?	1003	ASP	CA	54.119	0.400	1
1371	?	1003	ASP	HA	4.580	0.020	1
1372	?	1003	ASP	CB	41.305	0.400	1
1373	?	1003	ASP	HB2	2.630	0.020	2
1374	?	1003	ASP	HB3	2.630	0.020	2
1375	?	1003	ASP	C	175.884	0.400	1
1376	?	1004	GLU	N	120.922	0.400	1
1377	?	1004	GLU	H	7.945	0.020	1
1378	?	1004	GLU	CA	56.871	0.400	1
1379	?	1004	GLU	HA	4.135	0.020	1
1380	?	1004	GLU	CB	30.780	0.400	1
1381	?	1004	GLU	HB2	1.959	0.020	2
1382	?	1004	GLU	HB3	1.959	0.020	2
1383	?	1004	GLU	CG	36.283	0.400	1
1384	?	1004	GLU	HG2	2.181	0.020	2
1385	?	1004	GLU	HG3	2.261	0.020	2
1386	?	1004	GLU	C	174.979	0.400	1
1387	?	1005	LEU	N	124.551	0.400	1
1388	?	1005	LEU	H	8.042	0.020	1
1389	?	1005	LEU	CA	54.871	0.400	1
1390	?	1005	LEU	HA	4.539	0.020	1
1391	?	1005	LEU	CB	42.841	0.400	1
1392	?	1005	LEU	HB2	1.487	0.020	2
1393	?	1005	LEU	HB3	1.351	0.020	2
1394	?	1005	LEU	CG	27.198	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1395	?	1005	LEU	HG	1.290	0.020	1
1396	?	1005	LEU	CD1	25.427	0.400	1
1397	?	1005	LEU	HD11	0.788	0.020	2
1398	?	1005	LEU	HD12	0.788	0.020	2
1399	?	1005	LEU	HD13	0.788	0.020	2
1400	?	1005	LEU	CD2	24.146	0.400	1
1401	?	1005	LEU	HD21	0.689	0.020	2
1402	?	1005	LEU	HD22	0.689	0.020	2
1403	?	1005	LEU	HD23	0.689	0.020	2
1404	?	1005	LEU	C	175.305	0.400	1
1405	?	1006	LEU	N	127.945	0.400	1
1406	?	1006	LEU	H	8.799	0.020	1
1407	?	1006	LEU	CA	53.517	0.400	1
1408	?	1006	LEU	HA	4.512	0.020	1
1409	?	1006	LEU	CB	45.589	0.400	1
1410	?	1006	LEU	HB2	0.968	0.020	2
1411	?	1006	LEU	HB3	1.274	0.020	2
1412	?	1006	LEU	CG	26.950	0.400	1
1413	?	1006	LEU	CD1	24.896	0.400	1
1414	?	1006	LEU	HD11	0.330	0.020	2
1415	?	1006	LEU	HD12	0.330	0.020	2
1416	?	1006	LEU	HD13	0.330	0.020	2
1417	?	1006	LEU	CD2	23.410	0.400	1
1418	?	1006	LEU	HD21	0.514	0.020	2
1419	?	1006	LEU	HD22	0.514	0.020	2
1420	?	1006	LEU	HD23	0.514	0.020	2
1421	?	1006	LEU	C	174.919	0.400	1
1422	?	1007	TYR	N	117.176	0.400	1
1423	?	1007	TYR	H	8.583	0.020	1
1424	?	1007	TYR	CA	57.432	0.400	1
1425	?	1007	TYR	HA	5.157	0.020	1
1426	?	1007	TYR	CB	40.944	0.400	1
1427	?	1007	TYR	HB2	2.840	0.020	2
1428	?	1007	TYR	HB3	2.617	0.020	2
1429	?	1007	TYR	CD1	132.591	0.400	1
1430	?	1007	TYR	HD1	6.845	0.020	1
1431	?	1007	TYR	CE1	118.012	0.400	1
1432	?	1007	TYR	HE1	6.743	0.020	1
1433	?	1007	TYR	HE2	6.743	0.020	1
1434	?	1007	TYR	HD2	6.845	0.020	1
1435	?	1007	TYR	C	175.335	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1436	?	1008	LEU	N	128.094	0.400	1
1437	?	1008	LEU	H	9.308	0.020	1
1438	?	1008	LEU	CA	51.618	0.400	1
1439	?	1008	LEU	HA	5.152	0.020	1
1440	?	1008	LEU	CB	45.412	0.400	1
1441	?	1008	LEU	HB2	2.014	0.020	2
1442	?	1008	LEU	HB3	1.395	0.020	2
1443	?	1008	LEU	CD1	27.204	0.400	1
1444	?	1008	LEU	HD11	0.589	0.020	2
1445	?	1008	LEU	HD12	0.589	0.020	2
1446	?	1008	LEU	HD13	0.589	0.020	2
1447	?	1008	LEU	CD2	25.251	0.400	1
1448	?	1008	LEU	HD21	0.662	0.020	2
1449	?	1008	LEU	HD22	0.662	0.020	2
1450	?	1008	LEU	HD23	0.662	0.020	2
1451	?	1008	LEU	C	173.946	0.400	1
1452	?	1009	PRO	CD	51.406	0.400	1
1453	?	1009	PRO	CA	62.090	0.400	1
1454	?	1009	PRO	HA	4.527	0.020	1
1455	?	1009	PRO	CB	31.873	0.400	1
1456	?	1009	PRO	HB2	1.757	0.020	2
1457	?	1009	PRO	HB3	1.919	0.020	2
1458	?	1009	PRO	CG	27.887	0.400	1
1459	?	1009	PRO	HG2	2.163	0.020	2
1460	?	1009	PRO	HG3	2.158	0.020	2
1461	?	1009	PRO	HD2	3.864	0.020	2
1462	?	1009	PRO	HD3	4.392	0.020	2
1463	?	1009	PRO	C	176.758	0.400	1
1464	?	1010	VAL	N	124.047	0.400	1
1465	?	1010	VAL	H	9.193	0.020	1
1466	?	1010	VAL	CA	61.618	0.400	1
1467	?	1010	VAL	HA	4.209	0.020	1
1468	?	1010	VAL	CB	35.669	0.400	1
1469	?	1010	VAL	HB	1.959	0.020	1
1470	?	1010	VAL	HG1	0.914	0.020	2
1471	?	1010	VAL	HG1	0.914	0.020	2
1472	?	1010	VAL	HG1	0.914	0.020	2
1473	?	1010	VAL	HG2	0.914	0.020	2
1474	?	1010	VAL	HG2	0.914	0.020	2
1475	?	1010	VAL	HG2	0.914	0.020	2
1476	?	1010	VAL	CG1	22.539	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1477	?	1010	VAL	C	173.446	0.400	1
1478	?	1011	ARG	N	127.433	0.400	1
1479	?	1011	ARG	H	9.053	0.020	1
1480	?	1011	ARG	CA	55.367	0.400	1
1481	?	1011	ARG	HA	4.699	0.020	1
1482	?	1011	ARG	CB	30.605	0.400	1
1483	?	1011	ARG	HB2	1.813	0.020	2
1484	?	1011	ARG	HB3	1.632	0.020	2
1485	?	1011	ARG	CG	27.566	0.400	1
1486	?	1011	ARG	HG2	1.523	0.020	2
1487	?	1011	ARG	HG3	1.523	0.020	2
1488	?	1011	ARG	CD	43.376	0.400	1
1489	?	1011	ARG	HD2	3.164	0.020	2
1490	?	1011	ARG	HD3	3.164	0.020	2
1491	?	1011	ARG	NE	134.864	0.400	1
1492	?	1011	ARG	HE	7.298	0.020	1
1493	?	1011	ARG	C	176.092	0.400	1
1494	?	1012	GLY	N	115.279	0.400	1
1495	?	1012	GLY	H	8.614	0.020	1
1496	?	1012	GLY	CA	44.951	0.400	1
1497	?	1012	GLY	HA2	4.507	0.020	2
1498	?	1012	GLY	HA3	3.770	0.020	2
1499	?	1012	GLY	C	173.823	0.400	1
1500	?	1013	ARG	N	125.500	0.400	1
1501	?	1013	ARG	H	8.774	0.020	1
1502	?	1013	ARG	CA	59.204	0.400	1
1503	?	1013	ARG	HA	3.852	0.020	1
1504	?	1013	ARG	CB	29.767	0.400	1
1505	?	1013	ARG	HB2	1.895	0.020	2
1506	?	1013	ARG	HB3	1.895	0.020	2
1507	?	1013	ARG	CG	27.031	0.400	1
1508	?	1013	ARG	HG2	1.690	0.020	2
1509	?	1013	ARG	HG3	1.690	0.020	2
1510	?	1013	ARG	CD	42.716	0.400	1
1511	?	1013	ARG	HD2	3.196	0.020	2
1512	?	1013	ARG	HD3	3.196	0.020	2
1513	?	1013	ARG	NE	134.051	0.400	1
1514	?	1013	ARG	HE	7.620	0.020	1
1515	?	1013	ARG	C	177.793	0.400	1
1516	?	1014	GLU	N	119.254	0.400	1
1517	?	1014	GLU	H	8.888	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1518	?	1014	GLU	CA	60.362	0.400	1
1519	?	1014	GLU	HA	4.082	0.020	1
1520	?	1014	GLU	CB	28.959	0.400	1
1521	?	1014	GLU	HB2	2.037	0.020	2
1522	?	1014	GLU	HB3	2.037	0.020	2
1523	?	1014	GLU	CG	36.906	0.400	1
1524	?	1014	GLU	HG2	2.306	0.020	2
1525	?	1014	GLU	HG3	2.306	0.020	2
1526	?	1014	GLU	C	179.794	0.400	1
1527	?	1015	THR	N	117.699	0.400	1
1528	?	1015	THR	H	7.958	0.020	1
1529	?	1015	THR	CA	66.498	0.400	1
1530	?	1015	THR	HA	3.784	0.020	1
1531	?	1015	THR	CB	67.813	0.400	1
1532	?	1015	THR	HB	4.058	0.020	1
1533	?	1015	THR	CG2	23.072	0.400	1
1534	?	1015	THR	HG21	1.188	0.020	1
1535	?	1015	THR	HG22	1.188	0.020	1
1536	?	1015	THR	HG23	1.188	0.020	1
1537	?	1015	THR	C	175.457	0.400	1
1538	?	1016	TYR	N	122.365	0.400	1
1539	?	1016	TYR	H	8.042	0.020	1
1540	?	1016	TYR	CA	63.096	0.400	1
1541	?	1016	TYR	HA	3.742	0.020	1
1542	?	1016	TYR	CB	39.224	0.400	1
1543	?	1016	TYR	HB2	3.237	0.020	2
1544	?	1016	TYR	HB3	2.820	0.020	2
1545	?	1016	TYR	CD1	133.116	0.400	1
1546	?	1016	TYR	HD1	6.777	0.020	1
1547	?	1016	TYR	CE1	118.368	0.400	1
1548	?	1016	TYR	HE1	6.677	0.020	1
1549	?	1016	TYR	HE2	6.677	0.020	1
1550	?	1016	TYR	HD2	6.777	0.020	1
1551	?	1016	TYR	C	175.895	0.400	1
1552	?	1017	GLU	N	116.940	0.400	1
1553	?	1017	GLU	H	8.713	0.020	1
1554	?	1017	GLU	CA	59.879	0.400	1
1555	?	1017	GLU	HA	3.827	0.020	1
1556	?	1017	GLU	CB	29.245	0.400	1
1557	?	1017	GLU	HB2	2.124	0.020	2
1558	?	1017	GLU	HB3	2.124	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1559	?	1017	GLU	CG	37.199	0.400	1
1560	?	1017	GLU	HG2	2.684	0.020	2
1561	?	1017	GLU	HG3	2.426	0.020	2
1562	?	1017	GLU	C	179.448	0.400	1
1563	?	1018	MET	N	118.965	0.400	1
1564	?	1018	MET	H	7.505	0.020	1
1565	?	1018	MET	CA	58.815	0.400	1
1566	?	1018	MET	HA	4.291	0.020	1
1567	?	1018	MET	CB	32.736	0.400	1
1568	?	1018	MET	HB2	2.575	0.020	2
1569	?	1018	MET	HB3	2.421	0.020	2
1570	?	1018	MET	HG2	2.219	0.020	2
1571	?	1018	MET	HG3	2.219	0.020	2
1572	?	1018	MET	CE	18.011	0.400	1
1573	?	1018	MET	HE1	2.013	0.020	1
1574	?	1018	MET	HE2	2.013	0.020	1
1575	?	1018	MET	HE3	2.013	0.020	1
1576	?	1018	MET	C	178.050	0.400	1
1577	?	1019	LEU	N	117.499	0.400	1
1578	?	1019	LEU	H	8.151	0.020	1
1579	?	1019	LEU	CA	57.561	0.400	1
1580	?	1019	LEU	HA	3.823	0.020	1
1581	?	1019	LEU	CB	41.755	0.400	1
1582	?	1019	LEU	HB2	1.066	0.020	2
1583	?	1019	LEU	HB3	1.787	0.020	2
1584	?	1019	LEU	CG	27.231	0.400	1
1585	?	1019	LEU	HG	1.442	0.020	1
1586	?	1019	LEU	HD1	0.670	0.020	2
1587	?	1019	LEU	HD1	0.670	0.020	2
1588	?	1019	LEU	HD1	0.670	0.020	2
1589	?	1019	LEU	HD2	0.670	0.020	2
1590	?	1019	LEU	HD2	0.670	0.020	2
1591	?	1019	LEU	HD2	0.670	0.020	2
1592	?	1019	LEU	CD1	22.993	0.400	1
1593	?	1019	LEU	C	178.443	0.400	1
1594	?	1020	LEU	N	120.873	0.400	1
1595	?	1020	LEU	H	8.649	0.020	1
1596	?	1020	LEU	CA	58.702	0.400	1
1597	?	1020	LEU	HA	3.764	0.020	1
1598	?	1020	LEU	CB	41.865	0.400	1
1599	?	1020	LEU	HB2	1.247	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1600	?	1020	LEU	HB3	1.247	0.020	2
1601	?	1020	LEU	CG	26.812	0.400	1
1602	?	1020	LEU	HG	1.430	0.020	1
1603	?	1020	LEU	HD1	0.846	0.020	2
1604	?	1020	LEU	HD1	0.846	0.020	2
1605	?	1020	LEU	HD1	0.846	0.020	2
1606	?	1020	LEU	HD2	0.846	0.020	2
1607	?	1020	LEU	HD2	0.846	0.020	2
1608	?	1020	LEU	HD2	0.846	0.020	2
1609	?	1020	LEU	CD1	24.962	0.400	1
1610	?	1020	LEU	C	178.475	0.400	1
1611	?	1021	GLU	N	118.433	0.400	1
1612	?	1021	GLU	H	7.379	0.020	1
1613	?	1021	GLU	CA	59.700	0.400	1
1614	?	1021	GLU	HA	4.061	0.020	1
1615	?	1021	GLU	CB	29.294	0.400	1
1616	?	1021	GLU	HB2	2.069	0.020	2
1617	?	1021	GLU	HB3	2.179	0.020	2
1618	?	1021	GLU	CG	35.703	0.400	1
1619	?	1021	GLU	HG2	2.208	0.020	2
1620	?	1021	GLU	HG3	2.436	0.020	2
1621	?	1021	GLU	C	179.572	0.400	1
1622	?	1022	ILE	N	116.978	0.400	1
1623	?	1022	ILE	H	7.649	0.020	1
1624	?	1022	ILE	CA	64.520	0.400	1
1625	?	1022	ILE	HA	3.715	0.020	1
1626	?	1022	ILE	CB	37.912	0.400	1
1627	?	1022	ILE	HB	1.807	0.020	1
1628	?	1022	ILE	CG2	18.339	0.400	1
1629	?	1022	ILE	HG21	0.784	0.020	1
1630	?	1022	ILE	HG22	0.784	0.020	1
1631	?	1022	ILE	HG23	0.784	0.020	1
1632	?	1022	ILE	CG1	28.189	0.400	1
1633	?	1022	ILE	HG12	1.728	0.020	2
1634	?	1022	ILE	HG13	1.136	0.020	2
1635	?	1022	ILE	CD1	13.936	0.400	1
1636	?	1022	ILE	HD11	0.746	0.020	1
1637	?	1022	ILE	HD12	0.746	0.020	1
1638	?	1022	ILE	HD13	0.746	0.020	1
1639	?	1022	ILE	C	177.909	0.400	1
1640	?	1023	LYS	N	122.631	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1641	?	1023	LYS	H	9.094	0.020	1
1642	?	1023	LYS	CA	60.543	0.400	1
1643	?	1023	LYS	HA	3.708	0.020	1
1644	?	1023	LYS	CB	32.495	0.400	1
1645	?	1023	LYS	HB2	2.042	0.020	2
1646	?	1023	LYS	HB3	2.042	0.020	2
1647	?	1023	LYS	CG	25.116	0.400	1
1648	?	1023	LYS	HG2	1.468	0.020	2
1649	?	1023	LYS	HG3	1.468	0.020	2
1650	?	1023	LYS	CD	29.918	0.400	1
1651	?	1023	LYS	HD2	1.866	0.020	2
1652	?	1023	LYS	HD3	1.477	0.020	2
1653	?	1023	LYS	CE	42.419	0.400	1
1654	?	1023	LYS	HE2	2.979	0.020	2
1655	?	1023	LYS	HE3	2.979	0.020	2
1656	?	1023	LYS	C	177.322	0.400	1
1657	?	1024	GLU	N	117.756	0.400	1
1658	?	1024	GLU	H	8.320	0.020	1
1659	?	1024	GLU	CA	59.767	0.400	1
1660	?	1024	GLU	HA	4.241	0.020	1
1661	?	1024	GLU	CB	29.767	0.400	1
1662	?	1024	GLU	HB2	2.261	0.020	2
1663	?	1024	GLU	HB3	2.261	0.020	2
1664	?	1024	GLU	CG	37.220	0.400	1
1665	?	1024	GLU	HG2	2.252	0.020	2
1666	?	1024	GLU	HG3	2.562	0.020	2
1667	?	1024	GLU	C	177.755	0.400	1
1668	?	1025	SER	N	114.010	0.400	1
1669	?	1025	SER	H	7.425	0.020	1
1670	?	1025	SER	CA	62.272	0.400	1
1671	?	1025	SER	HA	4.174	0.020	1
1672	?	1025	SER	CB	63.277	0.400	1
1673	?	1025	SER	HB2	3.973	0.020	2
1674	?	1025	SER	HB3	3.767	0.020	2
1675	?	1025	SER	C	175.840	0.400	1
1676	?	1026	LEU	N	122.202	0.400	1
1677	?	1026	LEU	H	7.625	0.020	1
1678	?	1026	LEU	CA	57.999	0.400	1
1679	?	1026	LEU	HA	4.045	0.020	1
1680	?	1026	LEU	CB	42.710	0.400	1
1681	?	1026	LEU	HB2	1.481	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1682	?	1026	LEU	HB3	1.481	0.020	2
1683	?	1026	LEU	CG	26.763	0.400	1
1684	?	1026	LEU	HG	1.821	0.020	1
1685	?	1026	LEU	CD1	22.608	0.400	1
1686	?	1026	LEU	HD11	0.855	0.020	2
1687	?	1026	LEU	HD12	0.855	0.020	2
1688	?	1026	LEU	HD13	0.855	0.020	2
1689	?	1026	LEU	C	180.418	0.400	1
1690	?	1027	GLU	N	118.591	0.400	1
1691	?	1027	GLU	H	8.593	0.020	1
1692	?	1027	GLU	CA	59.636	0.400	1
1693	?	1027	GLU	HA	4.079	0.020	1
1694	?	1027	GLU	CB	29.557	0.400	1
1695	?	1027	GLU	CG	38.354	0.400	1
1696	?	1027	GLU	HG2	2.789	0.020	2
1697	?	1027	GLU	HG3	2.346	0.020	2
1698	?	1027	GLU	C	180.128	0.400	1
1699	?	1028	LEU	N	119.793	0.400	1
1700	?	1028	LEU	H	8.468	0.020	1
1701	?	1028	LEU	CA	57.289	0.400	1
1702	?	1028	LEU	HA	3.967	0.020	1
1703	?	1028	LEU	CB	41.847	0.400	1
1704	?	1028	LEU	HB2	1.817	0.020	2
1705	?	1028	LEU	HB3	1.227	0.020	2
1706	?	1028	LEU	CD1	26.940	0.400	1
1707	?	1028	LEU	HD11	0.657	0.020	2
1708	?	1028	LEU	HD12	0.657	0.020	2
1709	?	1028	LEU	HD13	0.657	0.020	2
1710	?	1028	LEU	CD2	23.989	0.400	1
1711	?	1028	LEU	HD21	0.469	0.020	2
1712	?	1028	LEU	HD22	0.469	0.020	2
1713	?	1028	LEU	HD23	0.469	0.020	2
1714	?	1028	LEU	C	178.567	0.400	1
1715	?	1029	MET	N	115.804	0.400	1
1716	?	1029	MET	H	7.279	0.020	1
1717	?	1029	MET	CA	58.463	0.400	1
1718	?	1029	MET	HA	3.928	0.020	1
1719	?	1029	MET	CB	33.047	0.400	1
1720	?	1029	MET	HB2	2.098	0.020	2
1721	?	1029	MET	HB3	2.012	0.020	2
1722	?	1029	MET	CG	31.955	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1723	?	1029	MET	HG2	2.587	0.020	2
1724	?	1029	MET	HG3	2.688	0.020	2
1725	?	1029	MET	CE	17.262	0.400	1
1726	?	1029	MET	HE1	1.943	0.020	1
1727	?	1029	MET	HE2	1.943	0.020	1
1728	?	1029	MET	HE3	1.943	0.020	1
1729	?	1029	MET	C	177.907	0.400	1
1730	?	1030	GLN	N	114.048	0.400	1
1731	?	1030	GLN	H	7.138	0.020	1
1732	?	1030	GLN	CA	56.935	0.400	1
1733	?	1030	GLN	HA	4.120	0.020	1
1734	?	1030	GLN	CB	28.342	0.400	1
1735	?	1030	GLN	HB2	1.969	0.020	2
1736	?	1030	GLN	HB3	1.881	0.020	2
1737	?	1030	GLN	CG	33.415	0.400	1
1738	?	1030	GLN	HG2	2.253	0.020	2
1739	?	1030	GLN	HG3	2.253	0.020	2
1740	?	1030	GLN	C	176.520	0.400	1
1741	?	1031	TYR	N	117.000	0.400	1
1742	?	1031	TYR	H	7.764	0.020	1
1743	?	1031	TYR	CA	58.425	0.400	1
1744	?	1031	TYR	HA	4.483	0.020	1
1745	?	1031	TYR	CB	38.492	0.400	1
1746	?	1031	TYR	HB2	3.313	0.020	2
1747	?	1031	TYR	HB3	2.928	0.020	2
1748	?	1031	TYR	CD1	133.087	0.400	1
1749	?	1031	TYR	HD1	7.258	0.020	1
1750	?	1031	TYR	HE1	6.796	0.020	1
1751	?	1031	TYR	HE2	6.796	0.020	1
1752	?	1031	TYR	HD2	7.258	0.020	1
1753	?	1031	TYR	C	176.095	0.400	1
1754	?	1032	LEU	N	120.517	0.400	1
1755	?	1032	LEU	H	7.368	0.020	1
1756	?	1032	LEU	CA	52.337	0.400	1
1757	?	1032	LEU	HA	2.906	0.020	1
1758	?	1032	LEU	CB	42.269	0.400	1
1759	?	1032	LEU	HB2	1.920	0.020	2
1760	?	1032	LEU	HB3	1.920	0.020	2
1761	?	1032	LEU	CG	27.404	0.400	1
1762	?	1032	LEU	HG	0.871	0.020	1
1763	?	1032	LEU	C	174.141	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1764	?	1033	PRO	CD	50.551	0.400	1
1765	?	1033	PRO	HD2	3.520	0.020	2
1766	?	1033	PRO	HD3	4.007	0.020	2
1767	?	1034	GLN	HA	4.547	0.020	1
1768	?	1034	GLN	CB	32.286	0.400	1
1769	?	1034	GLN	HB2	2.429	0.020	2
1770	?	1034	GLN	HB3	1.806	0.020	2
1771	?	1035	HIS	N	124.090	0.400	1
1772	?	1035	HIS	H	8.869	0.020	1
1773	?	1035	HIS	CA	59.366	0.400	1
1774	?	1035	HIS	HA	4.472	0.020	1
1775	?	1035	HIS	CB	29.512	0.400	1
1776	?	1035	HIS	HB2	3.298	0.020	2
1777	?	1035	HIS	HB3	3.115	0.020	2
1778	?	1035	HIS	CD2	120.025	0.400	1
1779	?	1035	HIS	CE1	138.550	0.400	1
1780	?	1035	HIS	HD2	7.146	0.020	1
1781	?	1035	HIS	HE1	7.927	0.020	1
1782	?	1035	HIS	C	177.836	0.400	1
1783	?	1036	THR	N	119.182	0.400	1
1784	?	1036	THR	H	7.138	0.020	1
1785	?	1036	THR	CA	66.606	0.400	1
1786	?	1036	THR	HA	3.946	0.020	1
1787	?	1036	THR	CB	68.598	0.400	1
1788	?	1036	THR	HB	4.157	0.020	1
1789	?	1036	THR	CG2	22.866	0.400	1
1790	?	1036	THR	HG21	1.251	0.020	1
1791	?	1036	THR	HG22	1.251	0.020	1
1792	?	1036	THR	HG23	1.251	0.020	1
1793	?	1036	THR	C	176.029	0.400	1
1794	?	1037	ILE	N	122.903	0.400	1
1795	?	1037	ILE	H	7.193	0.020	1
1796	?	1037	ILE	CA	65.667	0.400	1
1797	?	1037	ILE	HA	3.562	0.020	1
1798	?	1037	ILE	CB	38.204	0.400	1
1799	?	1037	ILE	HB	1.917	0.020	1
1800	?	1037	ILE	CG2	16.687	0.400	1
1801	?	1037	ILE	HG21	0.812	0.020	1
1802	?	1037	ILE	HG22	0.812	0.020	1
1803	?	1037	ILE	HG23	0.812	0.020	1
1804	?	1037	ILE	CG1	29.223	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1805	?	1037	ILE	HG12	0.897	0.020	2
1806	?	1037	ILE	HG13	1.513	0.020	2
1807	?	1037	ILE	CD1	13.468	0.400	1
1808	?	1037	ILE	HD11	0.823	0.020	1
1809	?	1037	ILE	HD12	0.823	0.020	1
1810	?	1037	ILE	HD13	0.823	0.020	1
1811	?	1037	ILE	C	177.685	0.400	1
1812	?	1038	GLU	N	118.719	0.400	1
1813	?	1038	GLU	H	8.578	0.020	1
1814	?	1038	GLU	CA	59.745	0.400	1
1815	?	1038	GLU	HA	4.049	0.020	1
1816	?	1038	GLU	CB	29.441	0.400	1
1817	?	1038	GLU	HB2	2.098	0.020	2
1818	?	1038	GLU	HB3	2.098	0.020	2
1819	?	1038	GLU	CG	36.448	0.400	1
1820	?	1038	GLU	HG2	2.410	0.020	2
1821	?	1038	GLU	HG3	2.341	0.020	2
1822	?	1038	GLU	C	179.575	0.400	1
1823	?	1039	THR	N	116.297	0.400	1
1824	?	1039	THR	H	8.124	0.020	1
1825	?	1039	THR	CA	66.989	0.400	1
1826	?	1039	THR	HA	3.936	0.020	1
1827	?	1039	THR	CB	68.845	0.400	1
1828	?	1039	THR	HB	4.264	0.020	1
1829	?	1039	THR	CG2	21.508	0.400	1
1830	?	1039	THR	HG21	1.245	0.020	1
1831	?	1039	THR	HG22	1.245	0.020	1
1832	?	1039	THR	HG23	1.245	0.020	1
1833	?	1039	THR	C	176.203	0.400	1
1834	?	1040	TYR	N	123.453	0.400	1
1835	?	1040	TYR	H	7.730	0.020	1
1836	?	1040	TYR	CA	61.902	0.400	1
1837	?	1040	TYR	HA	4.223	0.020	1
1838	?	1040	TYR	CB	38.583	0.400	1
1839	?	1040	TYR	HB2	3.329	0.020	2
1840	?	1040	TYR	HB3	3.094	0.020	2
1841	?	1040	TYR	CD1	133.346	0.400	1
1842	?	1040	TYR	HD1	7.059	0.020	1
1843	?	1040	TYR	CE1	118.182	0.400	1
1844	?	1040	TYR	HE1	6.793	0.020	1
1845	?	1040	TYR	HE2	6.793	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1846	?	1040	TYR	HD2	7.059	0.020	1
1847	?	1040	TYR	C	178.058	0.400	1
1848	?	1041	ARG	N	119.944	0.400	1
1849	?	1041	ARG	H	8.635	0.020	1
1850	?	1041	ARG	CA	60.487	0.400	1
1851	?	1041	ARG	HA	3.802	0.020	1
1852	?	1041	ARG	CB	30.078	0.400	1
1853	?	1041	ARG	HB2	1.950	0.020	2
1854	?	1041	ARG	HB3	1.950	0.020	2
1855	?	1041	ARG	CG	29.165	0.400	1
1856	?	1041	ARG	HG2	1.782	0.020	2
1857	?	1041	ARG	HG3	1.782	0.020	2
1858	?	1041	ARG	CD	43.879	0.400	1
1859	?	1041	ARG	HD2	3.051	0.020	2
1860	?	1041	ARG	HD3	3.051	0.020	2
1861	?	1041	ARG	NE	136.898	0.400	1
1862	?	1041	ARG	HE	8.491	0.020	1
1863	?	1041	ARG	C	179.552	0.400	1
1864	?	1042	GLN	N	119.455	0.400	1
1865	?	1042	GLN	H	8.225	0.020	1
1866	?	1042	GLN	CA	58.828	0.400	1
1867	?	1042	GLN	HA	4.083	0.020	1
1868	?	1042	GLN	CB	28.352	0.400	1
1869	?	1042	GLN	CG	33.973	0.400	1
1870	?	1042	GLN	HG2	2.568	0.020	2
1871	?	1042	GLN	HG3	2.365	0.020	2
1872	?	1042	GLN	C	178.700	0.400	1
1873	?	1043	GLN	N	118.905	0.400	1
1874	?	1043	GLN	H	7.894	0.020	1
1875	?	1043	GLN	CA	58.347	0.400	1
1876	?	1043	GLN	HA	4.088	0.020	1
1877	?	1043	GLN	CB	28.179	0.400	1
1878	?	1043	GLN	CG	34.038	0.400	1
1879	?	1043	GLN	HG2	2.565	0.020	2
1880	?	1043	GLN	HG3	2.370	0.020	2
1881	?	1043	GLN	C	178.664	0.400	1
1882	?	1044	GLN	N	117.762	0.400	1
1883	?	1044	GLN	H	8.034	0.020	1
1884	?	1044	GLN	CA	57.285	0.400	1
1885	?	1044	GLN	HA	3.947	0.020	1
1886	?	1044	GLN	CB	28.161	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1887	?	1044	GLN	CG	33.561	0.400	1
1888	?	1044	GLN	HG2	2.027	0.020	2
1889	?	1044	GLN	HG3	2.027	0.020	2
1890	?	1044	GLN	C	178.320	0.400	1
1891	?	1045	GLN	N	119.382	0.400	1
1892	?	1045	GLN	H	7.997	0.020	1
1893	?	1045	GLN	CA	58.171	0.400	1
1894	?	1045	GLN	HA	4.191	0.020	1
1895	?	1045	GLN	CB	28.493	0.400	1
1896	?	1045	GLN	HB2	2.196	0.020	2
1897	?	1045	GLN	HB3	2.196	0.020	2
1898	?	1045	GLN	CG	33.959	0.400	1
1899	?	1045	GLN	HG2	2.475	0.020	2
1900	?	1045	GLN	HG3	2.475	0.020	2
1901	?	1045	GLN	C	177.742	0.400	1
1902	?	1046	GLN	N	118.664	0.400	1
1903	?	1046	GLN	H	7.870	0.020	1
1904	?	1046	GLN	CA	57.685	0.400	1
1905	?	1046	GLN	HA	4.196	0.020	1
1906	?	1046	GLN	CB	28.743	0.400	1
1907	?	1046	GLN	HB2	2.143	0.020	2
1908	?	1046	GLN	HB3	2.143	0.020	2
1909	?	1046	GLN	CG	34.010	0.400	1
1910	?	1046	GLN	HG2	2.452	0.020	2
1911	?	1046	GLN	HG3	2.452	0.020	2
1912	?	1046	GLN	C	177.540	0.400	1
1913	?	1047	GLN	N	118.622	0.400	1
1914	?	1047	GLN	H	8.043	0.020	1
1915	?	1047	GLN	CA	57.328	0.400	1
1916	?	1047	GLN	CB	28.925	0.400	1
1917	?	1047	GLN	C	177.073	0.400	1
1918	?	1048	HIS	CA	57.913	0.400	1
1919	?	1048	HIS	HA	4.573	0.020	1
1920	?	1048	HIS	CB	30.219	0.400	1
1921	?	1048	HIS	HB2	3.184	0.020	2
1922	?	1048	HIS	HB3	3.300	0.020	2
1923	?	1048	HIS	CD2	121.459	0.400	1
1924	?	1048	HIS	HD2	7.207	0.020	1
1925	?	1048	HIS	C	176.277	0.400	1
1926	?	1049	GLN	N	119.554	0.400	1
1927	?	1049	GLN	H	8.117	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1928	?	1049	GLN	CA	57.545	0.400	1
1929	?	1049	GLN	HA	4.215	0.020	1
1930	?	1049	GLN	CB	28.874	0.400	1
1931	?	1049	GLN	HB2	2.093	0.020	2
1932	?	1049	GLN	HB3	2.093	0.020	2
1933	?	1049	GLN	CG	33.945	0.400	1
1934	?	1049	GLN	HG2	2.385	0.020	2
1935	?	1049	GLN	HG3	2.385	0.020	2
1936	?	1049	GLN	C	176.896	0.400	1
1937	?	1050	HIS	N	118.665	0.400	1
1938	?	1050	HIS	H	8.138	0.020	1
1939	?	1050	HIS	CA	57.300	0.400	1
1940	?	1050	HIS	HA	4.548	0.020	1
1941	?	1050	HIS	CB	30.189	0.400	1
1942	?	1050	HIS	HB2	3.148	0.020	2
1943	?	1050	HIS	HB3	3.148	0.020	2
1944	?	1050	HIS	CD2	120.038	0.400	1
1945	?	1050	HIS	HD2	7.035	0.020	1
1946	?	1050	HIS	C	176.265	0.400	1
1947	?	1051	LEU	N	121.208	0.400	1
1948	?	1051	LEU	H	7.809	0.020	1
1949	?	1051	LEU	CA	56.203	0.400	1
1950	?	1051	LEU	HA	4.170	0.020	1
1951	?	1051	LEU	CB	42.144	0.400	1
1952	?	1051	LEU	HB2	1.629	0.020	2
1953	?	1051	LEU	HB3	1.629	0.020	2
1954	?	1051	LEU	CG	26.996	0.400	1
1955	?	1051	LEU	HG	1.458	0.020	1
1956	?	1051	LEU	HD1	0.822	0.020	2
1957	?	1051	LEU	HD1	0.822	0.020	2
1958	?	1051	LEU	HD1	0.822	0.020	2
1959	?	1051	LEU	HD2	0.822	0.020	2
1960	?	1051	LEU	HD2	0.822	0.020	2
1961	?	1051	LEU	HD2	0.822	0.020	2
1962	?	1051	LEU	CD1	25.037	0.400	1
1963	?	1051	LEU	CD2	23.883	0.400	1
1964	?	1051	LEU	C	177.627	0.400	1
1965	?	1052	LEU	N	120.700	0.400	1
1966	?	1052	LEU	H	7.924	0.020	1
1967	?	1052	LEU	CA	55.993	0.400	1
1968	?	1052	LEU	HA	4.178	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1969	?	1052	LEU	CB	42.118	0.400	1
1970	?	1052	LEU	HB2	1.564	0.020	2
1971	?	1052	LEU	HB3	1.564	0.020	2
1972	?	1052	LEU	CG	26.999	0.400	1
1973	?	1052	LEU	HG	1.562	0.020	1
1974	?	1052	LEU	HD1	0.830	0.020	2
1975	?	1052	LEU	HD1	0.830	0.020	2
1976	?	1052	LEU	HD1	0.830	0.020	2
1977	?	1052	LEU	HD2	0.830	0.020	2
1978	?	1052	LEU	HD2	0.830	0.020	2
1979	?	1052	LEU	HD2	0.830	0.020	2
1980	?	1052	LEU	CD1	25.008	0.400	1
1981	?	1052	LEU	CD2	23.567	0.400	1
1982	?	1052	LEU	C	177.799	0.400	1
1983	?	1053	GLN	N	119.631	0.400	1
1984	?	1053	GLN	H	7.986	0.020	1
1985	?	1053	GLN	CA	56.492	0.400	1
1986	?	1053	GLN	HA	4.215	0.020	1
1987	?	1053	GLN	CB	29.202	0.400	1
1988	?	1053	GLN	HB2	2.086	0.020	2
1989	?	1053	GLN	HB3	2.013	0.020	2
1990	?	1053	GLN	CG	33.904	0.400	1
1991	?	1053	GLN	HG2	2.352	0.020	2
1992	?	1053	GLN	HG3	2.352	0.020	2
1993	?	1053	GLN	C	176.327	0.400	1
1994	?	1054	LYS	N	121.278	0.400	1
1995	?	1054	LYS	H	8.053	0.020	1
1996	?	1054	LYS	CA	56.680	0.400	1
1997	?	1054	LYS	HA	4.227	0.020	1
1998	?	1054	LYS	CB	32.898	0.400	1
1999	?	1054	LYS	HB2	1.795	0.020	2
2000	?	1054	LYS	HB3	1.735	0.020	2
2001	?	1054	LYS	CG	24.731	0.400	1
2002	?	1054	LYS	HG2	1.404	0.020	2
2003	?	1054	LYS	HG3	1.358	0.020	2
2004	?	1054	LYS	CD	29.071	0.400	1
2005	?	1054	LYS	HD2	1.622	0.020	2
2006	?	1054	LYS	HD3	1.622	0.020	2
2007	?	1054	LYS	CE	42.176	0.400	1
2008	?	1054	LYS	HE2	2.931	0.020	2
2009	?	1054	LYS	HE3	2.931	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2010	?	1054	LYS	C	176.812	0.400	1
2011	?	1055	GLN	N	120.539	0.400	1
2012	?	1055	GLN	H	8.249	0.020	1
2013	?	1055	GLN	CA	56.199	0.400	1
2014	?	1055	GLN	HA	4.322	0.020	1
2015	?	1055	GLN	CB	29.392	0.400	1
2016	?	1055	GLN	HB2	2.081	0.020	2
2017	?	1055	GLN	HB3	1.959	0.020	2
2018	?	1055	GLN	CG	33.814	0.400	1
2019	?	1055	GLN	HG2	2.296	0.020	2
2020	?	1055	GLN	HG3	2.296	0.020	2
2021	?	1055	GLN	C	176.291	0.400	1
2022	?	1056	THR	N	114.334	0.400	1
2023	?	1056	THR	H	8.063	0.020	1
2024	?	1056	THR	CA	62.075	0.400	1
2025	?	1056	THR	HA	4.347	0.020	1
2026	?	1056	THR	CB	69.852	0.400	1
2027	?	1056	THR	HB	4.233	0.020	1
2028	?	1056	THR	CG2	21.600	0.400	1
2029	?	1056	THR	HG21	1.196	0.020	1
2030	?	1056	THR	HG22	1.196	0.020	1
2031	?	1056	THR	HG23	1.196	0.020	1
2032	?	1056	THR	C	174.526	0.400	1
2033	?	1057	SER	N	117.856	0.400	1
2034	?	1057	SER	H	8.163	0.020	1
2035	?	1057	SER	CA	58.405	0.400	1
2036	?	1057	SER	HA	4.502	0.020	1
2037	?	1057	SER	CB	63.949	0.400	1
2038	?	1057	SER	HB2	3.868	0.020	2
2039	?	1057	SER	HB3	3.868	0.020	2
2040	?	1057	SER	C	174.275	0.400	1
2041	?	1058	ILE	N	122.144	0.400	1
2042	?	1058	ILE	H	8.049	0.020	1
2043	?	1058	ILE	CA	61.275	0.400	1
2044	?	1058	ILE	HA	4.194	0.020	1
2045	?	1058	ILE	CB	38.820	0.400	1
2046	?	1058	ILE	HB	1.856	0.020	1
2047	?	1058	ILE	CG2	17.571	0.400	1
2048	?	1058	ILE	HG21	0.881	0.020	1
2049	?	1058	ILE	HG22	0.881	0.020	1
2050	?	1058	ILE	HG23	0.881	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2051	?	1058	ILE	CG1	27.288	0.400	1
2052	?	1058	ILE	HG12	1.445	0.020	2
2053	?	1058	ILE	HG13	1.162	0.020	2
2054	?	1058	ILE	CD1	13.017	0.400	1
2055	?	1058	ILE	HD11	0.827	0.020	1
2056	?	1058	ILE	HD12	0.827	0.020	1
2057	?	1058	ILE	HD13	0.827	0.020	1
2058	?	1058	ILE	C	176.006	0.400	1
2059	?	1059	GLN	N	124.842	0.400	1
2060	?	1059	GLN	H	8.327	0.020	1
2061	?	1059	GLN	CA	55.845	0.400	1
2062	?	1059	GLN	HA	4.416	0.020	1
2063	?	1059	GLN	CB	29.748	0.400	1
2064	?	1059	GLN	HB2	2.143	0.020	2
2065	?	1059	GLN	HB3	1.985	0.020	2
2066	?	1059	GLN	CG	33.916	0.400	1
2067	?	1059	GLN	HG2	2.367	0.020	2
2068	?	1059	GLN	HG3	2.367	0.020	2
2069	?	1059	GLN	C	174.974	0.400	1
2070	?	1060	SER	N	123.632	0.400	1
2071	?	1060	SER	H	7.961	0.020	1
2072	?	1060	SER	CA	60.023	0.400	1
2073	?	1060	SER	HA	4.267	0.020	1
2074	?	1060	SER	CB	64.970	0.400	1
2075	?	1060	SER	HB2	3.837	0.020	2
2076	?	1060	SER	HB3	3.837	0.020	2
2077	?	1094	SER	CA	58.711	0.400	1
2078	?	1094	SER	CB	63.860	0.400	1
2079	?	1094	SER	HB2	3.928	0.020	2
2080	?	1094	SER	HB3	3.890	0.020	2
2081	?	1095	ASP	N	122.025	0.400	1
2082	?	1095	ASP	H	8.562	0.020	1
2083	?	1095	ASP	CA	54.810	0.400	1
2084	?	1095	ASP	HA	4.639	0.020	1
2085	?	1095	ASP	CB	41.016	0.400	1
2086	?	1095	ASP	HB2	2.764	0.020	2
2087	?	1095	ASP	HB3	2.665	0.020	2
2088	?	1095	ASP	C	176.278	0.400	1
2089	?	1096	GLU	N	120.066	0.400	1
2090	?	1096	GLU	H	8.250	0.020	1
2091	?	1096	GLU	CA	56.585	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2092	?	1096	GLU	HA	4.298	0.020	1
2093	?	1096	GLU	CB	30.397	0.400	1
2094	?	1096	GLU	HB2	2.122	0.020	2
2095	?	1096	GLU	HB3	1.905	0.020	2
2096	?	1096	GLU	CG	36.418	0.400	1
2097	?	1096	GLU	HG2	2.250	0.020	2
2098	?	1096	GLU	HG3	2.250	0.020	2
2099	?	1096	GLU	C	176.192	0.400	1
2100	?	1097	ASP	N	121.351	0.400	1
2101	?	1097	ASP	H	8.201	0.020	1
2102	?	1097	ASP	CA	54.406	0.400	1
2103	?	1097	ASP	HA	4.573	0.020	1
2104	?	1097	ASP	CB	41.369	0.400	1
2105	?	1097	ASP	HB2	2.601	0.020	2
2106	?	1097	ASP	HB3	2.601	0.020	2
2107	?	1097	ASP	C	174.498	0.400	1
2108	?	1098	THR	N	114.380	0.400	1
2109	?	1098	THR	H	7.557	0.020	1
2110	?	1098	THR	CA	62.159	0.400	1
2111	?	1098	THR	HA	4.655	0.020	1
2112	?	1098	THR	CB	70.272	0.400	1
2113	?	1098	THR	HB	3.722	0.020	1
2114	?	1098	THR	CG2	21.804	0.400	1
2115	?	1098	THR	HG21	0.862	0.020	1
2116	?	1098	THR	HG22	0.862	0.020	1
2117	?	1098	THR	HG23	0.862	0.020	1
2118	?	1098	THR	C	172.624	0.400	1
2119	?	1099	TYR	N	124.760	0.400	1
2120	?	1099	TYR	H	8.926	0.020	1
2121	?	1099	TYR	CA	56.835	0.400	1
2122	?	1099	TYR	HA	4.350	0.020	1
2123	?	1099	TYR	CB	42.581	0.400	1
2124	?	1099	TYR	HB2	2.104	0.020	2
2125	?	1099	TYR	HB3	2.104	0.020	2
2126	?	1099	TYR	CD1	133.400	0.400	1
2127	?	1099	TYR	HD1	6.485	0.020	1
2128	?	1099	TYR	CE1	117.091	0.400	1
2129	?	1099	TYR	HE1	6.445	0.020	1
2130	?	1099	TYR	HE2	6.445	0.020	1
2131	?	1099	TYR	HD2	6.485	0.020	1
2132	?	1099	TYR	C	174.022	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2133	?	1100	TYR	N	118.700	0.400	1
2134	?	1100	TYR	H	8.401	0.020	1
2135	?	1100	TYR	CA	57.289	0.400	1
2136	?	1100	TYR	HA	5.441	0.020	1
2137	?	1100	TYR	CB	41.584	0.400	1
2138	?	1100	TYR	HB2	2.920	0.020	2
2139	?	1100	TYR	HB3	2.821	0.020	2
2140	?	1100	TYR	CD1	133.033	0.400	1
2141	?	1100	TYR	HD1	6.984	0.020	1
2142	?	1100	TYR	CE1	118.034	0.400	1
2143	?	1100	TYR	HE1	6.663	0.020	1
2144	?	1100	TYR	HE2	6.663	0.020	1
2145	?	1100	TYR	HD2	6.984	0.020	1
2146	?	1100	TYR	C	174.891	0.400	1
2147	?	1101	LEU	N	121.632	0.400	1
2148	?	1101	LEU	H	9.204	0.020	1
2149	?	1101	LEU	CA	54.498	0.400	1
2150	?	1101	LEU	HA	4.992	0.020	1
2151	?	1101	LEU	CB	46.266	0.400	1
2152	?	1101	LEU	HB2	1.854	0.020	2
2153	?	1101	LEU	HB3	1.620	0.020	2
2154	?	1101	LEU	CG	26.939	0.400	1
2155	?	1101	LEU	HG	1.775	0.020	1
2156	?	1101	LEU	CD1	26.375	0.400	1
2157	?	1101	LEU	HD11	0.819	0.020	2
2158	?	1101	LEU	HD12	0.819	0.020	2
2159	?	1101	LEU	HD13	0.819	0.020	2
2160	?	1101	LEU	CD2	27.073	0.400	1
2161	?	1101	LEU	HD21	0.776	0.020	2
2162	?	1101	LEU	HD22	0.776	0.020	2
2163	?	1101	LEU	HD23	0.776	0.020	2
2164	?	1101	LEU	C	174.466	0.400	1
2165	?	1102	GLN	N	123.532	0.400	1
2166	?	1102	GLN	H	9.013	0.020	1
2167	?	1102	GLN	CA	54.374	0.400	1
2168	?	1102	GLN	HA	5.080	0.020	1
2169	?	1102	GLN	CB	31.382	0.400	1
2170	?	1102	GLN	HB2	1.817	0.020	2
2171	?	1102	GLN	HB3	1.936	0.020	2
2172	?	1102	GLN	CG	34.225	0.400	1
2173	?	1102	GLN	HG2	1.993	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2174	?	1102	GLN	HG3	1.993	0.020	2
2175	?	1102	GLN	NE2	111.543	0.400	1
2176	?	1102	GLN	HE21	6.763	0.020	2
2177	?	1102	GLN	HE22	7.171	0.020	2
2178	?	1102	GLN	C	174.509	0.400	1
2179	?	1103	VAL	N	124.091	0.400	1
2180	?	1103	VAL	H	9.159	0.020	1
2181	?	1103	VAL	CA	60.198	0.400	1
2182	?	1103	VAL	HA	4.599	0.020	1
2183	?	1103	VAL	CB	35.603	0.400	1
2184	?	1103	VAL	HB	1.858	0.020	1
2185	?	1103	VAL	CG1	22.465	0.400	1
2186	?	1103	VAL	HG11	0.974	0.020	2
2187	?	1103	VAL	HG12	0.974	0.020	2
2188	?	1103	VAL	HG13	0.974	0.020	2
2189	?	1103	VAL	CG2	20.695	0.400	1
2190	?	1103	VAL	HG21	0.942	0.020	2
2191	?	1103	VAL	HG22	0.942	0.020	2
2192	?	1103	VAL	HG23	0.942	0.020	2
2193	?	1103	VAL	C	172.608	0.400	1
2194	?	1104	ARG	N	129.114	0.400	1
2195	?	1104	ARG	H	9.324	0.020	1
2196	?	1104	ARG	CA	55.820	0.400	1
2197	?	1104	ARG	HA	4.890	0.020	1
2198	?	1104	ARG	CB	31.257	0.400	1
2199	?	1104	ARG	HB2	1.824	0.020	2
2200	?	1104	ARG	HB3	1.699	0.020	2
2201	?	1104	ARG	CG	27.514	0.400	1
2202	?	1104	ARG	HG2	1.595	0.020	2
2203	?	1104	ARG	HG3	1.595	0.020	2
2204	?	1104	ARG	CD	43.493	0.400	1
2205	?	1104	ARG	HD2	3.221	0.020	2
2206	?	1104	ARG	HD3	3.221	0.020	2
2207	?	1104	ARG	NE	136.282	0.400	1
2208	?	1104	ARG	HE	8.184	0.020	1
2209	?	1104	ARG	C	176.488	0.400	1
2210	?	1105	GLY	N	114.585	0.400	1
2211	?	1105	GLY	H	8.813	0.020	1
2212	?	1105	GLY	CA	44.970	0.400	1
2213	?	1105	GLY	HA2	4.696	0.020	2
2214	?	1105	GLY	HA3	3.911	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2215	?	1105	GLY	C	176.498	0.400	1
2216	?	1106	ARG	N	127.937	0.400	1
2217	?	1106	ARG	H	8.866	0.020	1
2218	?	1106	ARG	CA	59.637	0.400	1
2219	?	1106	ARG	HA	3.525	0.020	1
2220	?	1106	ARG	CB	29.841	0.400	1
2221	?	1106	ARG	HB2	2.044	0.020	2
2222	?	1106	ARG	HB3	1.862	0.020	2
2223	?	1106	ARG	CG	26.877	0.400	1
2224	?	1106	ARG	HG2	1.693	0.020	2
2225	?	1106	ARG	HG3	1.693	0.020	2
2226	?	1106	ARG	CD	42.924	0.400	1
2227	?	1106	ARG	HD2	3.112	0.020	2
2228	?	1106	ARG	HD3	3.112	0.020	2
2229	?	1106	ARG	C	177.603	0.400	1
2230	?	1107	LYS	N	119.095	0.400	1
2231	?	1107	LYS	H	8.556	0.020	1
2232	?	1107	LYS	CA	59.527	0.400	1
2233	?	1107	LYS	HA	4.024	0.020	1
2234	?	1107	LYS	CB	31.368	0.400	1
2235	?	1107	LYS	HB2	1.864	0.020	2
2236	?	1107	LYS	HB3	1.765	0.020	2
2237	?	1107	LYS	CG	24.515	0.400	1
2238	?	1107	LYS	HG2	1.478	0.020	2
2239	?	1107	LYS	HG3	1.355	0.020	2
2240	?	1107	LYS	CD	29.078	0.400	1
2241	?	1107	LYS	HD2	1.688	0.020	2
2242	?	1107	LYS	HD3	1.688	0.020	2
2243	?	1107	LYS	CE	42.151	0.400	1
2244	?	1107	LYS	HE2	2.947	0.020	2
2245	?	1107	LYS	HE3	2.947	0.020	2
2246	?	1107	LYS	C	178.726	0.400	1
2247	?	1108	ASN	N	116.769	0.400	1
2248	?	1108	ASN	H	7.617	0.020	1
2249	?	1108	ASN	CA	55.393	0.400	1
2250	?	1108	ASN	HA	4.402	0.020	1
2251	?	1108	ASN	CB	37.528	0.400	1
2252	?	1108	ASN	HB2	2.957	0.020	2
2253	?	1108	ASN	HB3	2.268	0.020	2
2254	?	1108	ASN	ND2	114.634	0.400	1
2255	?	1108	ASN	HD21	6.624	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2256	?	1108	ASN	C	176.932	0.400	1
2257	?	1109	PHE	N	120.646	0.400	1
2258	?	1109	PHE	H	8.051	0.020	1
2259	?	1109	PHE	CA	61.430	0.400	1
2260	?	1109	PHE	HA	3.901	0.020	1
2261	?	1109	PHE	CB	39.099	0.400	1
2262	?	1109	PHE	HB2	2.594	0.020	2
2263	?	1109	PHE	HB3	2.724	0.020	2
2264	?	1109	PHE	CD1	131.521	0.400	1
2265	?	1109	PHE	HD1	6.635	0.020	1
2266	?	1109	PHE	CE1	131.117	0.400	1
2267	?	1109	PHE	HE1	7.213	0.020	1
2268	?	1109	PHE	HE2	7.213	0.020	1
2269	?	1109	PHE	HD2	6.635	0.020	1
2270	?	1109	PHE	C	175.757	0.400	1
2271	?	1110	GLU	N	117.509	0.400	1
2272	?	1110	GLU	H	8.364	0.020	1
2273	?	1110	GLU	CA	59.873	0.400	1
2274	?	1110	GLU	HA	3.505	0.020	1
2275	?	1110	GLU	CB	29.177	0.400	1
2276	?	1110	GLU	HB2	2.096	0.020	2
2277	?	1110	GLU	HB3	1.930	0.020	2
2278	?	1110	GLU	CG	37.152	0.400	1
2279	?	1110	GLU	HG2	2.176	0.020	2
2280	?	1110	GLU	HG3	2.534	0.020	2
2281	?	1110	GLU	C	180.017	0.400	1
2282	?	1111	ILE	N	119.260	0.400	1
2283	?	1111	ILE	H	7.670	0.020	1
2284	?	1111	ILE	CA	65.580	0.400	1
2285	?	1111	ILE	HA	3.644	0.020	1
2286	?	1111	ILE	CB	38.429	0.400	1
2287	?	1111	ILE	HB	1.833	0.020	1
2288	?	1111	ILE	CG2	17.073	0.400	1
2289	?	1111	ILE	HG21	0.806	0.020	1
2290	?	1111	ILE	HG22	0.806	0.020	1
2291	?	1111	ILE	HG23	0.806	0.020	1
2292	?	1111	ILE	CG1	29.459	0.400	1
2293	?	1111	ILE	HG12	1.833	0.020	2
2294	?	1111	ILE	HG13	0.984	0.020	2
2295	?	1111	ILE	CD1	13.733	0.400	1
2296	?	1111	ILE	HD11	0.840	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2297	?	1111	ILE	HD12	0.840	0.020	1
2298	?	1111	ILE	HD13	0.840	0.020	1
2299	?	1111	ILE	C	177.344	0.400	1
2300	?	1112	LEU	N	117.913	0.400	1
2301	?	1112	LEU	H	7.937	0.020	1
2302	?	1112	LEU	CA	58.221	0.400	1
2303	?	1112	LEU	HA	3.804	0.020	1
2304	?	1112	LEU	CB	41.337	0.400	1
2305	?	1112	LEU	HB2	1.150	0.020	2
2306	?	1112	LEU	HB3	1.150	0.020	2
2307	?	1112	LEU	CG	26.751	0.400	1
2308	?	1112	LEU	HG	1.828	0.020	1
2309	?	1112	LEU	CD1	23.470	0.400	1
2310	?	1112	LEU	HD11	0.731	0.020	2
2311	?	1112	LEU	HD12	0.731	0.020	2
2312	?	1112	LEU	HD13	0.731	0.020	2
2313	?	1112	LEU	C	178.883	0.400	1
2314	?	1113	MET	N	118.279	0.400	1
2315	?	1113	MET	H	8.659	0.020	1
2316	?	1113	MET	CA	57.871	0.400	1
2317	?	1113	MET	HA	4.032	0.020	1
2318	?	1113	MET	CB	31.907	0.400	1
2319	?	1113	MET	HB2	1.904	0.020	2
2320	?	1113	MET	HB3	1.843	0.020	2
2321	?	1113	MET	CG	31.572	0.400	1
2322	?	1113	MET	HG2	1.821	0.020	2
2323	?	1113	MET	HG3	1.716	0.020	2
2324	?	1113	MET	CE	16.833	0.400	1
2325	?	1113	MET	HE1	1.883	0.020	1
2326	?	1113	MET	HE2	1.883	0.020	1
2327	?	1113	MET	HE3	1.883	0.020	1
2328	?	1113	MET	C	178.742	0.400	1
2329	?	1114	LYS	N	120.560	0.400	1
2330	?	1114	LYS	H	7.381	0.020	1
2331	?	1114	LYS	CA	59.346	0.400	1
2332	?	1114	LYS	HA	4.023	0.020	1
2333	?	1114	LYS	CB	32.224	0.400	1
2334	?	1114	LYS	HB2	1.911	0.020	2
2335	?	1114	LYS	HB3	1.817	0.020	2
2336	?	1114	LYS	CG	25.296	0.400	1
2337	?	1114	LYS	HG2	1.377	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2338	?	1114	LYS	HG3	1.547	0.020	2
2339	?	1114	LYS	CD	29.305	0.400	1
2340	?	1114	LYS	HD2	1.633	0.020	2
2341	?	1114	LYS	HD3	1.633	0.020	2
2342	?	1114	LYS	CE	42.200	0.400	1
2343	?	1114	LYS	HE2	2.890	0.020	2
2344	?	1114	LYS	HE3	2.890	0.020	2
2345	?	1114	LYS	C	179.072	0.400	1
2346	?	1115	LEU	N	118.891	0.400	1
2347	?	1115	LEU	H	7.688	0.020	1
2348	?	1115	LEU	CA	56.462	0.400	1
2349	?	1115	LEU	HA	4.345	0.020	1
2350	?	1115	LEU	CB	41.718	0.400	1
2351	?	1115	LEU	HB2	1.644	0.020	2
2352	?	1115	LEU	HB3	1.234	0.020	2
2353	?	1115	LEU	CG	26.351	0.400	1
2354	?	1115	LEU	HG	0.721	0.020	1
2355	?	1115	LEU	CD1	24.109	0.400	1
2356	?	1115	LEU	HD11	0.695	0.020	2
2357	?	1115	LEU	HD12	0.695	0.020	2
2358	?	1115	LEU	HD13	0.695	0.020	2
2359	?	1115	LEU	C	177.923	0.400	1
2360	?	1116	LYS	N	121.250	0.400	1
2361	?	1116	LYS	H	8.884	0.020	1
2362	?	1116	LYS	CA	60.465	0.400	1
2363	?	1116	LYS	HA	3.730	0.020	1
2364	?	1116	LYS	CB	33.137	0.400	1
2365	?	1116	LYS	HB2	2.102	0.020	2
2366	?	1116	LYS	HB3	1.897	0.020	2
2367	?	1116	LYS	CG	24.741	0.400	1
2368	?	1116	LYS	HG2	1.413	0.020	2
2369	?	1116	LYS	HG3	1.581	0.020	2
2370	?	1116	LYS	CD	30.050	0.400	1
2371	?	1116	LYS	HD2	1.682	0.020	2
2372	?	1116	LYS	HD3	1.925	0.020	2
2373	?	1116	LYS	CE	43.381	0.400	1
2374	?	1116	LYS	C	177.059	0.400	1
2375	?	1117	GLU	N	116.755	0.400	1
2376	?	1117	GLU	H	7.660	0.020	1
2377	?	1117	GLU	CA	58.898	0.400	1
2378	?	1117	GLU	HA	4.276	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2379	?	1117	GLU	CB	30.277	0.400	1
2380	?	1117	GLU	HB2	2.250	0.020	2
2381	?	1117	GLU	HB3	2.250	0.020	2
2382	?	1117	GLU	CG	37.309	0.400	1
2383	?	1117	GLU	HG2	2.037	0.020	2
2384	?	1117	GLU	HG3	2.353	0.020	2
2385	?	1117	GLU	C	177.169	0.400	1
2386	?	1118	SER	N	114.369	0.400	1
2387	?	1118	SER	H	7.659	0.020	1
2388	?	1118	SER	CA	62.553	0.400	1
2389	?	1118	SER	HA	4.169	0.020	1
2390	?	1118	SER	CB	62.632	0.400	1
2391	?	1118	SER	HB2	3.738	0.020	2
2392	?	1118	SER	HB3	3.818	0.020	2
2393	?	1118	SER	C	177.177	0.400	1
2394	?	1119	LEU	N	123.247	0.400	1
2395	?	1119	LEU	H	8.486	0.020	1
2396	?	1119	LEU	CA	58.379	0.400	1
2397	?	1119	LEU	HA	4.039	0.020	1
2398	?	1119	LEU	CB	40.787	0.400	1
2399	?	1119	LEU	HB2	1.787	0.020	2
2400	?	1119	LEU	HB3	1.417	0.020	2
2401	?	1119	LEU	CG	25.848	0.400	1
2402	?	1119	LEU	HG	0.689	0.020	1
2403	?	1119	LEU	CD1	21.773	0.400	1
2404	?	1119	LEU	HD11	0.852	0.020	2
2405	?	1119	LEU	HD12	0.852	0.020	2
2406	?	1119	LEU	HD13	0.852	0.020	2
2407	?	1119	LEU	C	180.394	0.400	1
2408	?	1120	GLU	N	117.672	0.400	1
2409	?	1120	GLU	H	8.410	0.020	1
2410	?	1120	GLU	CA	59.795	0.400	1
2411	?	1120	GLU	HA	4.069	0.020	1
2412	?	1120	GLU	CB	29.567	0.400	1
2413	?	1120	GLU	HB2	2.296	0.020	2
2414	?	1120	GLU	HB3	2.026	0.020	2
2415	?	1120	GLU	CG	38.477	0.400	1
2416	?	1120	GLU	HG2	2.886	0.020	2
2417	?	1120	GLU	HG3	2.341	0.020	2
2418	?	1120	GLU	C	180.268	0.400	1
2419	?	1121	LEU	N	119.445	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2420	?	1121	LEU	H	8.323	0.020	1
2421	?	1121	LEU	CA	57.093	0.400	1
2422	?	1121	LEU	HA	3.865	0.020	1
2423	?	1121	LEU	CB	41.526	0.400	1
2424	?	1121	LEU	HB2	1.085	0.020	2
2425	?	1121	LEU	HB3	1.741	0.020	2
2426	?	1121	LEU	CG	27.031	0.400	1
2427	?	1121	LEU	HG	1.749	0.020	1
2428	?	1121	LEU	CD1	23.424	0.400	1
2429	?	1121	LEU	HD11	0.447	0.020	2
2430	?	1121	LEU	HD12	0.447	0.020	2
2431	?	1121	LEU	HD13	0.447	0.020	2
2432	?	1121	LEU	CD2	27.068	0.400	1
2433	?	1121	LEU	HD21	0.496	0.020	2
2434	?	1121	LEU	HD22	0.496	0.020	2
2435	?	1121	LEU	HD23	0.496	0.020	2
2436	?	1121	LEU	C	179.058	0.400	1
2437	?	1122	MET	N	118.025	0.400	1
2438	?	1122	MET	H	7.662	0.020	1
2439	?	1122	MET	CA	58.894	0.400	1
2440	?	1122	MET	HA	4.002	0.020	1
2441	?	1122	MET	CB	31.981	0.400	1
2442	?	1122	MET	HB2	2.705	0.020	2
2443	?	1122	MET	HB3	2.515	0.020	2
2444	?	1122	MET	CG	32.264	0.400	1
2445	?	1122	MET	HG2	2.194	0.020	2
2446	?	1122	MET	HG3	2.114	0.020	2
2447	?	1122	MET	CE	17.346	0.400	1
2448	?	1122	MET	HE1	2.024	0.020	1
2449	?	1122	MET	HE2	2.024	0.020	1
2450	?	1122	MET	HE3	2.024	0.020	1
2451	?	1122	MET	C	178.224	0.400	1
2452	?	1123	GLU	N	115.784	0.400	1
2453	?	1123	GLU	H	7.235	0.020	1
2454	?	1123	GLU	CA	57.957	0.400	1
2455	?	1123	GLU	HA	4.157	0.020	1
2456	?	1123	GLU	CB	29.809	0.400	1
2457	?	1123	GLU	HB2	2.130	0.020	2
2458	?	1123	GLU	HB3	2.130	0.020	2
2459	?	1123	GLU	CG	36.187	0.400	1
2460	?	1123	GLU	HG2	2.390	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2461	?	1123	GLU	HG3	2.390	0.020	2
2462	?	1123	GLU	C	176.954	0.400	1
2463	?	1124	LEU	N	117.445	0.400	1
2464	?	1124	LEU	H	7.964	0.020	1
2465	?	1124	LEU	CA	54.748	0.400	1
2466	?	1124	LEU	HA	4.308	0.020	1
2467	?	1124	LEU	CB	42.099	0.400	1
2468	?	1124	LEU	HB2	1.905	0.020	2
2469	?	1124	LEU	HB3	1.905	0.020	2
2470	?	1124	LEU	CG	27.458	0.400	1
2471	?	1124	LEU	HG	1.667	0.020	1
2472	?	1124	LEU	HD1	0.895	0.020	2
2473	?	1124	LEU	HD1	0.895	0.020	2
2474	?	1124	LEU	HD1	0.895	0.020	2
2475	?	1124	LEU	HD2	0.895	0.020	2
2476	?	1124	LEU	HD2	0.895	0.020	2
2477	?	1124	LEU	HD2	0.895	0.020	2
2478	?	1124	LEU	CD1	25.800	0.400	1
2479	?	1124	LEU	CD2	22.551	0.400	1
2480	?	1124	LEU	C	177.537	0.400	1
2481	?	1125	VAL	N	122.935	0.400	1
2482	?	1125	VAL	H	7.375	0.020	1
2483	?	1125	VAL	CA	61.225	0.400	1
2484	?	1125	VAL	HA	3.932	0.020	1
2485	?	1125	VAL	CB	32.131	0.400	1
2486	?	1125	VAL	HB	2.038	0.020	1
2487	?	1125	VAL	HG1	0.958	0.020	2
2488	?	1125	VAL	HG1	0.958	0.020	2
2489	?	1125	VAL	HG1	0.958	0.020	2
2490	?	1125	VAL	HG2	0.958	0.020	2
2491	?	1125	VAL	HG2	0.958	0.020	2
2492	?	1125	VAL	HG2	0.958	0.020	2
2493	?	1125	VAL	C	174.154	0.400	1
2494	?	1126	PRO	CD	51.276	0.400	1
2495	?	1126	PRO	CA	63.358	0.400	1
2496	?	1126	PRO	HA	4.393	0.020	1
2497	?	1126	PRO	CB	33.330	0.400	1
2498	?	1126	PRO	HB2	1.917	0.020	2
2499	?	1126	PRO	HB3	2.490	0.020	2
2500	?	1126	PRO	CG	27.975	0.400	1
2501	?	1126	PRO	HG2	2.195	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2502	?	1126	PRO	HG3	2.105	0.020	2
2503	?	1126	PRO	HD2	4.219	0.020	2
2504	?	1126	PRO	HD3	3.564	0.020	2
2505	?	1126	PRO	C	177.633	0.400	1
2506	?	1127	GLN	N	125.241	0.400	1
2507	?	1127	GLN	H	8.993	0.020	1
2508	?	1127	GLN	CA	60.076	0.400	1
2509	?	1127	GLN	HA	3.959	0.020	1
2510	?	1127	GLN	CB	26.139	0.400	1
2511	?	1127	GLN	HB2	2.279	0.020	2
2512	?	1127	GLN	HB3	2.141	0.020	2
2513	?	1127	GLN	C	174.012	0.400	1
2514	?	1128	PRO	CD	50.402	0.400	1
2515	?	1128	PRO	CA	66.248	0.400	1
2516	?	1128	PRO	HA	4.427	0.020	1
2517	?	1128	PRO	CB	31.154	0.400	1
2518	?	1128	PRO	HB2	2.415	0.020	2
2519	?	1128	PRO	HB3	1.764	0.020	2
2520	?	1128	PRO	CG	28.668	0.400	1
2521	?	1128	PRO	HG2	2.016	0.020	2
2522	?	1128	PRO	HG3	2.016	0.020	2
2523	?	1128	PRO	HD2	3.821	0.020	2
2524	?	1128	PRO	HD3	3.515	0.020	2
2525	?	1128	PRO	C	179.719	0.400	1
2526	?	1129	LEU	N	116.655	0.400	1
2527	?	1129	LEU	H	7.220	0.020	1
2528	?	1129	LEU	CA	57.174	0.400	1
2529	?	1129	LEU	HA	4.162	0.020	1
2530	?	1129	LEU	CB	41.264	0.400	1
2531	?	1129	LEU	HB2	1.204	0.020	2
2532	?	1129	LEU	HB3	1.732	0.020	2
2533	?	1129	LEU	CG	27.511	0.400	1
2534	?	1129	LEU	HG	1.571	0.020	1
2535	?	1129	LEU	CD1	24.993	0.400	1
2536	?	1129	LEU	HD11	0.871	0.020	2
2537	?	1129	LEU	HD12	0.871	0.020	2
2538	?	1129	LEU	HD13	0.871	0.020	2
2539	?	1129	LEU	CD2	23.290	0.400	1
2540	?	1129	LEU	HD21	0.761	0.020	2
2541	?	1129	LEU	HD22	0.761	0.020	2
2542	?	1129	LEU	HD23	0.761	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2543	?	1129	LEU	C	178.871	0.400	1
2544	?	1130	VAL	N	121.976	0.400	1
2545	?	1130	VAL	H	7.465	0.020	1
2546	?	1130	VAL	CA	67.124	0.400	1
2547	?	1130	VAL	HA	3.471	0.020	1
2548	?	1130	VAL	CB	31.438	0.400	1
2549	?	1130	VAL	HB	2.220	0.020	1
2550	?	1130	VAL	HG1	0.936	0.020	2
2551	?	1130	VAL	HG1	0.936	0.020	2
2552	?	1130	VAL	HG1	0.936	0.020	2
2553	?	1130	VAL	HG2	0.936	0.020	2
2554	?	1130	VAL	HG2	0.936	0.020	2
2555	?	1130	VAL	HG2	0.936	0.020	2
2556	?	1130	VAL	CG1	22.511	0.400	1
2557	?	1130	VAL	CG2	21.028	0.400	1
2558	?	1130	VAL	C	178.353	0.400	1
2559	?	1131	ASP	N	118.845	0.400	1
2560	?	1131	ASP	H	8.605	0.020	1
2561	?	1131	ASP	CA	57.796	0.400	1
2562	?	1131	ASP	HA	4.365	0.020	1
2563	?	1131	ASP	CB	40.198	0.400	1
2564	?	1131	ASP	HB2	2.672	0.020	2
2565	?	1131	ASP	HB3	2.672	0.020	2
2566	?	1131	ASP	C	179.398	0.400	1
2567	?	1132	SER	N	115.275	0.400	1
2568	?	1132	SER	H	7.817	0.020	1
2569	?	1132	SER	CA	61.726	0.400	1
2570	?	1132	SER	HA	4.239	0.020	1
2571	?	1132	SER	CB	62.897	0.400	1
2572	?	1132	SER	HB2	3.980	0.020	2
2573	?	1132	SER	HB3	4.028	0.020	2
2574	?	1132	SER	C	179.406	0.400	1
2575	?	1133	TYR	N	124.425	0.400	1
2576	?	1133	TYR	H	8.247	0.020	1
2577	?	1133	TYR	CA	61.719	0.400	1
2578	?	1133	TYR	HA	4.175	0.020	1
2579	?	1133	TYR	CB	38.434	0.400	1
2580	?	1133	TYR	HB2	3.291	0.020	2
2581	?	1133	TYR	HB3	3.059	0.020	2
2582	?	1133	TYR	CD1	133.170	0.400	1
2583	?	1133	TYR	HD1	7.085	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2584	?	1133	TYR	CE1	117.977	0.400	1
2585	?	1133	TYR	HE1	6.801	0.020	1
2586	?	1133	TYR	HE2	6.801	0.020	1
2587	?	1133	TYR	HD2	7.085	0.020	1
2588	?	1133	TYR	C	178.220	0.400	1
2589	?	1134	ARG	N	119.750	0.400	1
2590	?	1134	ARG	H	8.731	0.020	1
2591	?	1134	ARG	CA	60.458	0.400	1
2592	?	1134	ARG	HA	3.734	0.020	1
2593	?	1134	ARG	CB	29.662	0.400	1
2594	?	1134	ARG	HB2	1.791	0.020	2
2595	?	1134	ARG	HB3	2.157	0.020	2
2596	?	1134	ARG	CD	43.719	0.400	1
2597	?	1134	ARG	HD2	3.185	0.020	2
2598	?	1134	ARG	HD3	3.185	0.020	2
2599	?	1134	ARG	NE	135.124	0.400	1
2600	?	1134	ARG	HE	7.364	0.020	1
2601	?	1134	ARG	C	179.611	0.400	1
2602	?	1135	GLN	N	119.346	0.400	1
2603	?	1135	GLN	H	8.063	0.020	1
2604	?	1135	GLN	CA	58.813	0.400	1
2605	?	1135	GLN	HA	4.078	0.020	1
2606	?	1135	GLN	CB	28.394	0.400	1
2607	?	1135	GLN	HB2	2.085	0.020	2
2608	?	1135	GLN	HB3	1.918	0.020	2
2609	?	1135	GLN	CG	34.014	0.400	1
2610	?	1135	GLN	HG2	2.531	0.020	2
2611	?	1135	GLN	HG3	2.410	0.020	2
2612	?	1135	GLN	NE2	112.038	0.400	1
2613	?	1135	GLN	HE21	7.285	0.020	2
2614	?	1135	GLN	HE22	6.765	0.020	2
2615	?	1135	GLN	C	178.594	0.400	1
2616	?	1136	GLN	N	118.513	0.400	1
2617	?	1136	GLN	H	7.900	0.020	1
2618	?	1136	GLN	CA	58.210	0.400	1
2619	?	1136	GLN	HA	4.048	0.020	1
2620	?	1136	GLN	CB	28.396	0.400	1
2621	?	1136	GLN	HB2	2.142	0.020	2
2622	?	1136	GLN	HB3	2.142	0.020	2
2623	?	1136	GLN	CG	34.152	0.400	1
2624	?	1136	GLN	HG2	2.512	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2625	?	1136	GLN	HG3	2.512	0.020	2
2626	?	1136	GLN	C	178.597	0.400	1
2627	?	1137	GLN	N	117.373	0.400	1
2628	?	1137	GLN	H	7.935	0.020	1
2629	?	1137	GLN	CA	57.369	0.400	1
2630	?	1137	GLN	HA	3.869	0.020	1
2631	?	1137	GLN	CB	28.361	0.400	1
2632	?	1137	GLN	HB2	2.002	0.020	2
2633	?	1137	GLN	HB3	2.002	0.020	2
2634	?	1137	GLN	CG	33.617	0.400	1
2635	?	1137	GLN	HG2	2.000	0.020	2
2636	?	1137	GLN	HG3	2.000	0.020	2
2637	?	1137	GLN	C	178.363	0.400	1
2638	?	1138	GLN	N	118.243	0.400	1
2639	?	1138	GLN	H	7.709	0.020	1
2640	?	1138	GLN	CA	57.852	0.400	1
2641	?	1138	GLN	HA	4.142	0.020	1
2642	?	1138	GLN	CB	28.516	0.400	1
2643	?	1138	GLN	HB2	2.161	0.020	2
2644	?	1138	GLN	HB3	2.161	0.020	2
2645	?	1138	GLN	CG	34.000	0.400	1
2646	?	1138	GLN	HG2	2.478	0.020	2
2647	?	1138	GLN	HG3	2.478	0.020	2
2648	?	1138	GLN	C	177.503	0.400	1
2649	?	1139	LEU	N	118.586	0.400	1
2650	?	1139	LEU	H	7.484	0.020	1
2651	?	1139	LEU	CA	56.031	0.400	1
2652	?	1139	LEU	HA	4.268	0.020	1
2653	?	1139	LEU	CB	42.078	0.400	1
2654	?	1139	LEU	HB2	1.780	0.020	2
2655	?	1139	LEU	HB3	1.647	0.020	2
2656	?	1139	LEU	CG	26.962	0.400	1
2657	?	1139	LEU	HG	1.750	0.020	1
2658	?	1139	LEU	HD1	0.924	0.020	2
2659	?	1139	LEU	HD1	0.924	0.020	2
2660	?	1139	LEU	HD1	0.924	0.020	2
2661	?	1139	LEU	HD2	0.924	0.020	2
2662	?	1139	LEU	HD2	0.924	0.020	2
2663	?	1139	LEU	HD2	0.924	0.020	2
2664	?	1139	LEU	CD1	25.189	0.400	1
2665	?	1139	LEU	CD2	23.004	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2666	?	1139	LEU	C	177.835	0.400	1
2667	?	1140	LEU	N	118.753	0.400	1
2668	?	1140	LEU	H	7.532	0.020	1
2669	?	1140	LEU	CA	55.149	0.400	1
2670	?	1140	LEU	HA	4.341	0.020	1
2671	?	1140	LEU	CB	42.380	0.400	1
2672	?	1140	LEU	HB2	1.755	0.020	2
2673	?	1140	LEU	HB3	1.599	0.020	2
2674	?	1140	LEU	CG	26.624	0.400	1
2675	?	1140	LEU	HG	1.731	0.020	1
2676	?	1140	LEU	HD1	0.840	0.020	2
2677	?	1140	LEU	HD1	0.840	0.020	2
2678	?	1140	LEU	HD1	0.840	0.020	2
2679	?	1140	LEU	HD2	0.840	0.020	2
2680	?	1140	LEU	HD2	0.840	0.020	2
2681	?	1140	LEU	HD2	0.840	0.020	2
2682	?	1140	LEU	CD1	25.299	0.400	1
2683	?	1140	LEU	CD2	22.837	0.400	1
2684	?	1140	LEU	C	177.207	0.400	1
2685	?	1141	GLN	N	119.878	0.400	1
2686	?	1141	GLN	H	7.675	0.020	1
2687	?	1141	GLN	CA	56.161	0.400	1
2688	?	1141	GLN	HA	4.359	0.020	1
2689	?	1141	GLN	CB	29.534	0.400	1
2690	?	1141	GLN	HB2	2.213	0.020	2
2691	?	1141	GLN	HB3	2.051	0.020	2
2692	?	1141	GLN	CG	34.003	0.400	1
2693	?	1141	GLN	HG2	2.457	0.020	2
2694	?	1141	GLN	HG3	2.457	0.020	2
2695	?	1141	GLN	C	174.910	0.400	1
2696	?	1142	ARG	N	127.959	0.400	1
2697	?	1142	ARG	H	7.955	0.020	1
2698	?	1142	ARG	CA	57.568	0.400	1
2699	?	1142	ARG	HA	4.140	0.020	1
2700	?	1142	ARG	CB	31.701	0.400	1
2701	?	1142	ARG	HB2	1.590	0.020	2
2702	?	1142	ARG	HB3	1.756	0.020	2
2703	?	1142	ARG	CD	43.483	0.400	1
2704	?	1142	ARG	HD2	2.888	0.020	2
2705	?	1142	ARG	HD3	2.861	0.020	2
2706	?	1142	ARG	C	180.825	0.400	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	58	-0.56 ± 0.13	Should be applied
$^{13}\text{C}_\beta$	58	0.03 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	57	-0.15 ± 0.11	None needed (< 0.5 ppm)
^{15}N	55	-0.80 ± 0.35	Should be applied

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 20%, i.e. 475 atoms were assigned a chemical shift out of a possible 2338. 4 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	203/828 (25%)	81/330 (25%)	82/336 (24%)	40/162 (25%)
Sidechain	245/1366 (18%)	151/804 (19%)	91/492 (18%)	3/70 (4%)
Aromatic	27/144 (19%)	18/74 (24%)	9/68 (13%)	0/2 (0%)
Overall	475/2338 (20%)	250/1208 (21%)	182/896 (20%)	43/234 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 22%, i.e. 652 atoms were assigned a chemical shift out of a possible 2986. 6 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	283/1084 (26%)	113/432 (26%)	115/440 (26%)	55/212 (26%)
Sidechain	338/1730 (20%)	209/1020 (20%)	126/618 (20%)	3/92 (3%)
Aromatic	31/172 (18%)	20/90 (22%)	11/76 (14%)	0/6 (0%)
Overall	652/2986 (22%)	342/1542 (22%)	252/1134 (22%)	58/310 (19%)

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 containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	41	ARG	NE	136.90	92.63 – 76.73	32.8
1	A	11	ARG	NE	134.86	92.63 – 76.73	31.6
1	A	13	ARG	NE	134.05	92.63 – 76.73	31.1

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

