



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 01:03 AM BST

PDB ID : 2LDU  
Title : Solution NMR Structure of Heat shock factor protein 1 DNA binding domain from homo sapiens, Northeast Structural Genomics Consortium Target HR3023C  
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Deposited on : 2011-06-01

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

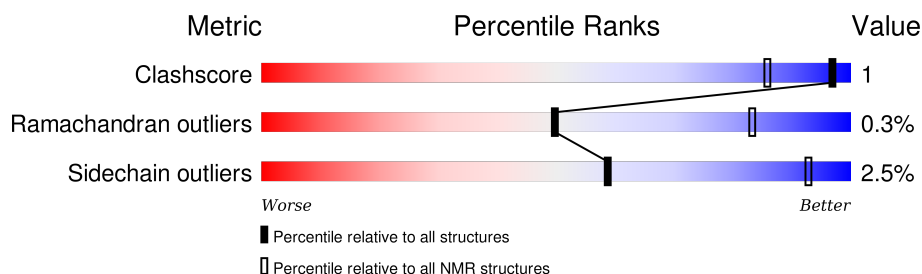
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	125	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:17-A:85, A:96-A:119 (93)	0.36	1

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 5 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2002 atoms, of which 987 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock factor protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	125	Total	C	H	N	O	S	0
			2002	645	987	185	179	6	

There are 11 discrepancies between the modelled and reference sequences:

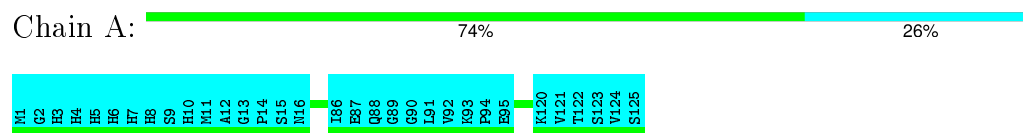
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q00613
A	2	GLY	-	EXPRESSION TAG	UNP Q00613
A	3	HIS	-	EXPRESSION TAG	UNP Q00613
A	4	HIS	-	EXPRESSION TAG	UNP Q00613
A	5	HIS	-	EXPRESSION TAG	UNP Q00613
A	6	HIS	-	EXPRESSION TAG	UNP Q00613
A	7	HIS	-	EXPRESSION TAG	UNP Q00613
A	8	HIS	-	EXPRESSION TAG	UNP Q00613
A	9	SER	-	EXPRESSION TAG	UNP Q00613
A	10	HIS	-	EXPRESSION TAG	UNP Q00613
A	11	MET	-	EXPRESSION TAG	UNP Q00613

## 4 Residue-property plots

### 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: Heat shock factor protein 1

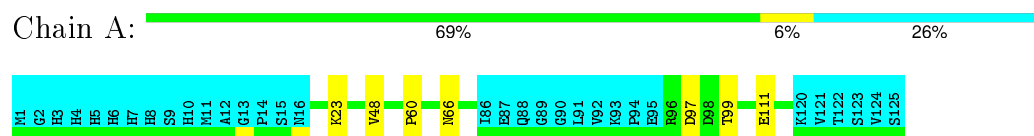


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

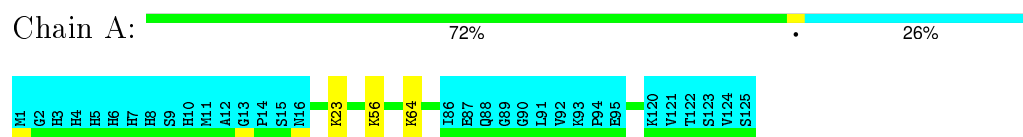
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Heat shock factor protein 1



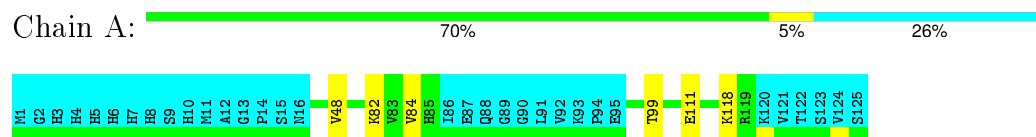
#### 4.2.2 Score per residue for model 2

- Molecule 1: Heat shock factor protein 1



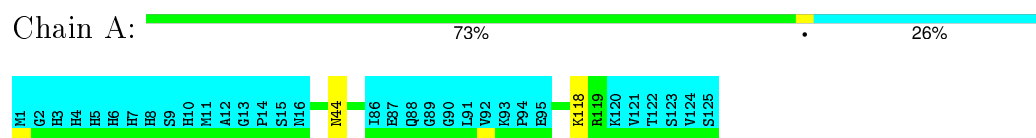
### 4.2.3 Score per residue for model 3

- Molecule 1: Heat shock factor protein 1



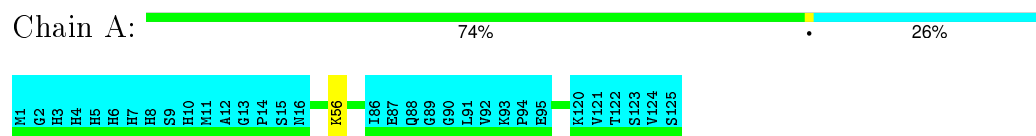
### 4.2.4 Score per residue for model 4

- Molecule 1: Heat shock factor protein 1



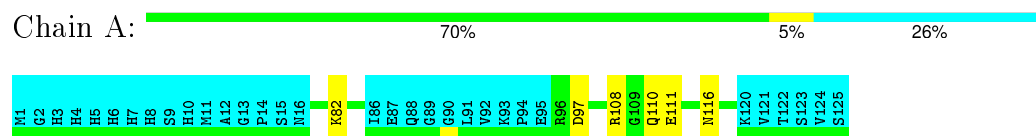
### 4.2.5 Score per residue for model 5

- Molecule 1: Heat shock factor protein 1



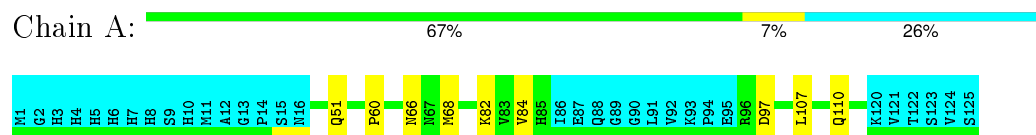
### 4.2.6 Score per residue for model 6

- Molecule 1: Heat shock factor protein 1



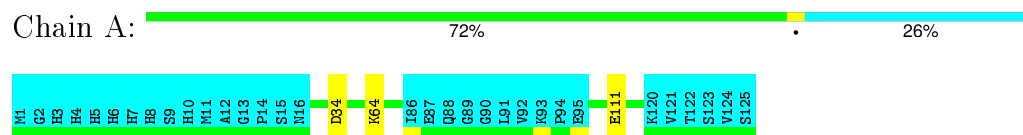
### 4.2.7 Score per residue for model 7

- Molecule 1: Heat shock factor protein 1



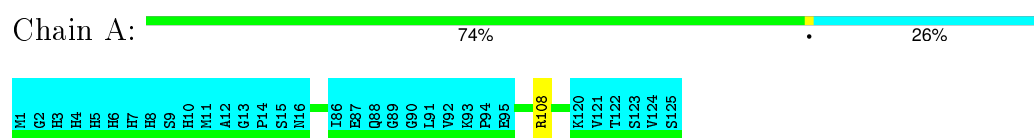
### 4.2.8 Score per residue for model 8

- Molecule 1: Heat shock factor protein 1



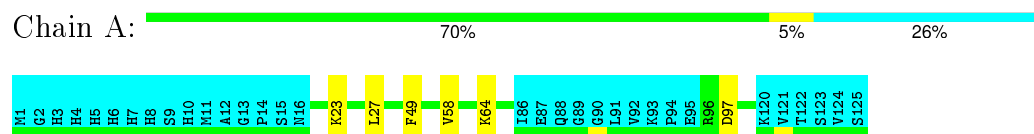
### 4.2.9 Score per residue for model 9

- Molecule 1: Heat shock factor protein 1



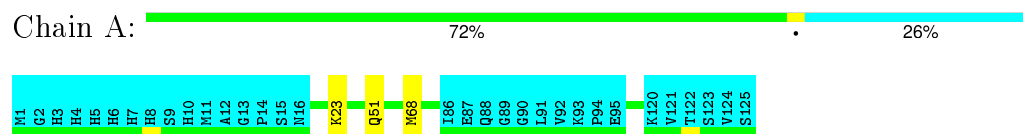
### 4.2.10 Score per residue for model 10

- Molecule 1: Heat shock factor protein 1



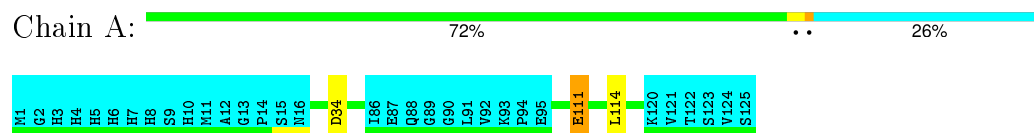
### 4.2.11 Score per residue for model 11

- Molecule 1: Heat shock factor protein 1



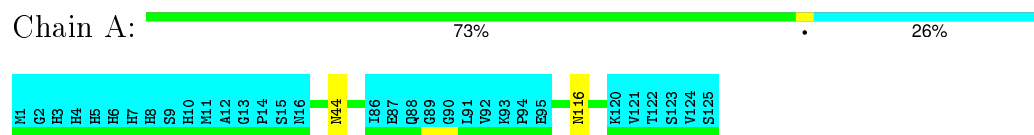
### 4.2.12 Score per residue for model 12

- Molecule 1: Heat shock factor protein 1



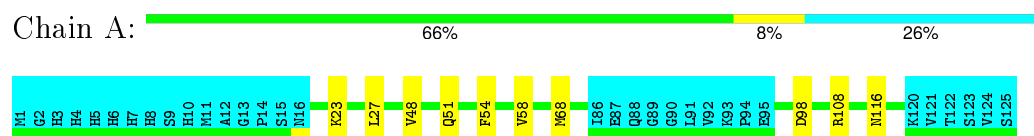
### 4.2.13 Score per residue for model 13

- Molecule 1: Heat shock factor protein 1



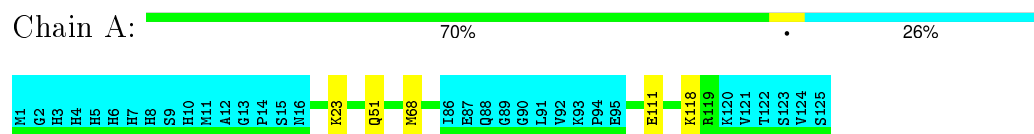
### 4.2.14 Score per residue for model 14

- Molecule 1: Heat shock factor protein 1



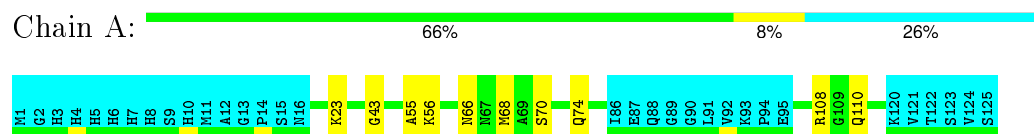
### 4.2.15 Score per residue for model 15

- Molecule 1: Heat shock factor protein 1



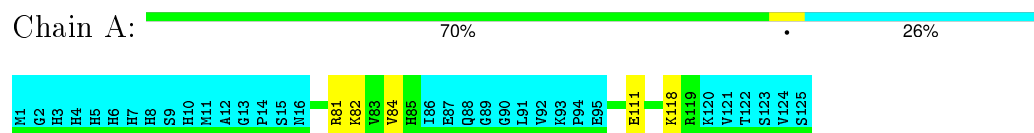
### 4.2.16 Score per residue for model 16

- Molecule 1: Heat shock factor protein 1



### 4.2.17 Score per residue for model 17

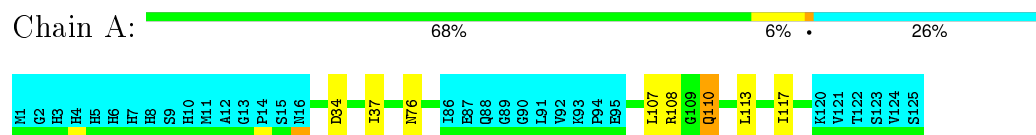
- Molecule 1: Heat shock factor protein 1





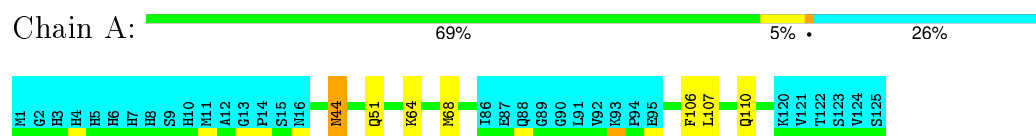
#### 4.2.18 Score per residue for model 18

- Molecule 1: Heat shock factor protein 1



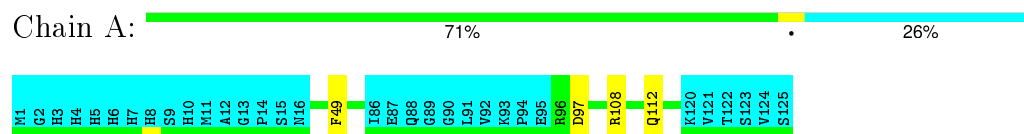
#### 4.2.19 Score per residue for model 19

- Molecule 1: Heat shock factor protein 1



#### 4.2.20 Score per residue for model 20

- Molecule 1: Heat shock factor protein 1



## 5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
TALOS+	geometry optimization	
CYANA	refinement	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2ldu_cs.str
Number of chemical shift lists	1
Total number of shifts	1478
Number of shifts mapped to atoms	0
Number of unparsed shifts	1478
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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	772	752	748	1±1
All	All	15440	15040	14960	29

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:GLN:HB3	1:A:68:MET:SD	0.60	2.35	19	5
1:A:82:LYS:HE2	1:A:84:VAL:HB	0.47	1.85	3	2
1:A:107:LEU:HB2	1:A:110:GLN:HB3	0.46	1.86	19	2
1:A:44:ASN:HA	1:A:106:PHE:O	0.45	2.11	19	1
1:A:49:PHE:HA	1:A:97:ASP:O	0.44	2.13	20	2
1:A:27:LEU:HD11	1:A:58:VAL:CG1	0.44	2.43	10	1
1:A:27:LEU:HD11	1:A:58:VAL:HG13	0.43	1.89	14	1
1:A:111:GLU:HA	1:A:114:LEU:HG	0.43	1.90	12	1
1:A:54:PHE:O	1:A:58:VAL:HB	0.43	2.14	14	1
1:A:60:PRO:HG3	1:A:66:ASN:ND2	0.42	2.29	7	2
1:A:48:VAL:O	1:A:98:ASP:HA	0.42	2.15	14	1
1:A:82:LYS:HE3	1:A:84:VAL:HG22	0.41	1.92	7	1
1:A:43:GLY:HA3	1:A:108:ARG:HD2	0.41	1.91	16	1
1:A:55:ALA:HB1	1:A:66:ASN:O	0.41	2.15	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:VAL:HB	1:A:99:THR:HB	0.41	1.91	3	2
1:A:70:SER:O	1:A:74:GLN:HG2	0.41	2.16	16	1
1:A:113:LEU:O	1:A:117:ILE:HG13	0.41	2.16	18	1
1:A:107:LEU:HB2	1:A:110:GLN:HB2	0.40	1.94	18	1
1:A:55:ALA:HB2	1:A:68:MET:HB2	0.40	1.93	16	1
1:A:34:ASP:HA	1:A:37:ILE:O	0.40	2.17	18	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	93/125 (74%)	88±2 (95±2%)	5±1 (5±2%)	0±1 (0±1%)	50	83
All	All	1860/2500 (74%)	1764 (95%)	90 (5%)	6 (0%)	50	83

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

Mol	Chain	Res	Type	Models (Total)
1	A	108	ARG	3
1	A	97	ASP	2
1	A	44	ASN	1

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/112 (76%)	83±1 (98±1%)	2±1 (2±1%)	59	93
All	All	1700/2240 (76%)	1658 (98%)	42 (2%)	59	93

All 15 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	111	GLU	7
1	A	23	LYS	7
1	A	118	LYS	4
1	A	64	LYS	4
1	A	56	LYS	3
1	A	110	GLN	3
1	A	116	ASN	3
1	A	44	ASN	2
1	A	34	ASP	2
1	A	108	ARG	2
1	A	97	ASP	1
1	A	112	GLN	1
1	A	76	ASN	1
1	A	82	LYS	1
1	A	81	ARG	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

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

### 7.1 Chemical shift list 1

File name: 2ldu\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1478
Number of shifts mapped to atoms	0
Number of unparsed shifts	1478
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Entity instance (chain) must be specified. All 1478 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	.	10	HIS	HA	4.651	0.020	1
2	.	10	HIS	HB2	3.178	0.020	2
3	.	10	HIS	HB3	3.125	0.020	2
4	.	10	HIS	HD2	7.074	0.020	1
5	.	10	HIS	C	174.834	0.400	1
6	.	10	HIS	CA	56.324	0.400	1
7	.	10	HIS	CB	29.942	0.400	1
8	.	11	MET	H	8.251	0.020	1
9	.	11	MET	HA	4.420	0.020	1
10	.	11	MET	HB2	1.898	0.020	2
11	.	11	MET	HB3	2.053	0.020	2
12	.	11	MET	HG2	2.422	0.020	2
13	.	11	MET	HG3	2.465	0.020	2
14	.	11	MET	HE1	2.040	0.020	1
15	.	11	MET	HE2	2.040	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	.	11	MET	HE3	2.040	0.020	1
17	.	11	MET	C	175.345	0.400	1
18	.	11	MET	CA	55.337	0.400	1
19	.	11	MET	CB	32.700	0.400	1
20	.	11	MET	CG	32.070	0.400	1
21	.	11	MET	CE	16.722	0.400	1
22	.	11	MET	N	121.689	0.400	1
23	.	12	ALA	H	8.333	0.020	1
24	.	12	ALA	HA	4.346	0.020	1
25	.	12	ALA	HB1	1.388	0.020	1
26	.	12	ALA	HB2	1.388	0.020	1
27	.	12	ALA	HB3	1.388	0.020	1
28	.	12	ALA	C	177.388	0.400	1
29	.	12	ALA	CA	52.148	0.400	1
30	.	12	ALA	CB	19.248	0.400	1
31	.	12	ALA	N	125.404	0.400	1
32	.	13	GLY	H	8.194	0.020	1
33	.	13	GLY	HA2	4.019	0.020	2
34	.	13	GLY	HA3	4.127	0.020	2
35	.	13	GLY	CA	44.168	0.400	1
36	.	13	GLY	N	108.257	0.400	1
37	.	14	PRO	HA	4.451	0.020	1
38	.	14	PRO	HB2	2.272	0.020	2
39	.	14	PRO	HB3	1.933	0.020	2
40	.	14	PRO	HG2	1.986	0.020	1
41	.	14	PRO	HG3	1.986	0.020	1
42	.	14	PRO	HD2	3.581	0.020	1
43	.	14	PRO	HD3	3.580	0.020	1
44	.	14	PRO	C	177.058	0.400	1
45	.	14	PRO	CA	62.750	0.400	1
46	.	14	PRO	CB	32.000	0.400	1
47	.	14	PRO	CG	26.753	0.400	1
48	.	14	PRO	CD	49.414	0.400	1
49	.	15	SER	H	8.514	0.020	1
50	.	15	SER	HA	4.443	0.020	1
51	.	15	SER	HB2	3.892	0.020	2
52	.	15	SER	HB3	3.802	0.020	2
53	.	15	SER	HG	4.838	0.020	1
54	.	15	SER	C	174.263	0.400	1
55	.	15	SER	CA	58.017	0.400	1
56	.	15	SER	CB	63.851	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	.	15	SER	N	115.934	0.400	1
58	.	16	ASN	H	8.699	0.020	1
59	.	16	ASN	HA	4.754	0.020	1
60	.	16	ASN	HB2	2.880	0.020	2
61	.	16	ASN	HB3	2.752	0.020	2
62	.	16	ASN	HD21	7.653	0.020	2
63	.	16	ASN	HD22	6.920	0.020	2
64	.	16	ASN	C	174.443	0.400	1
65	.	16	ASN	CA	53.177	0.400	1
66	.	16	ASN	CB	38.667	0.400	1
67	.	16	ASN	N	121.161	0.400	1
68	.	16	ASN	ND2	112.830	0.400	1
69	.	17	VAL	H	8.041	0.020	1
70	.	17	VAL	HA	4.320	0.020	1
71	.	17	VAL	HB	1.823	0.020	1
72	.	17	VAL	HG11	0.958	0.020	2
73	.	17	VAL	HG12	0.958	0.020	2
74	.	17	VAL	HG13	0.958	0.020	2
75	.	17	VAL	HG21	0.848	0.020	2
76	.	17	VAL	HG22	0.848	0.020	2
77	.	17	VAL	HG23	0.848	0.020	2
78	.	17	VAL	CA	60.194	0.400	1
79	.	17	VAL	CB	33.284	0.400	1
80	.	17	VAL	CG1	21.578	0.400	1
81	.	17	VAL	CG2	21.865	0.400	1
82	.	17	VAL	N	123.030	0.400	1
83	.	18	PRO	HA	4.445	0.020	1
84	.	18	PRO	HB2	1.874	0.020	2
85	.	18	PRO	HB3	2.654	0.020	2
86	.	18	PRO	HG2	2.283	0.020	2
87	.	18	PRO	HG3	2.207	0.020	2
88	.	18	PRO	HD2	3.859	0.020	2
89	.	18	PRO	HD3	4.110	0.020	2
90	.	18	PRO	C	177.028	0.400	1
91	.	18	PRO	CA	63.697	0.400	1
92	.	18	PRO	CB	32.536	0.400	1
93	.	18	PRO	CG	27.757	0.400	1
94	.	18	PRO	CD	51.611	0.400	1
95	.	19	ALA	H	8.788	0.020	1
96	.	19	ALA	HA	4.229	0.020	1
97	.	19	ALA	HB1	1.560	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	.	19	ALA	HB2	1.560	0.020	1
99	.	19	ALA	HB3	1.560	0.020	1
100	.	19	ALA	C	178.711	0.400	1
101	.	19	ALA	CA	54.970	0.400	1
102	.	19	ALA	CB	18.202	0.400	1
103	.	19	ALA	N	128.241	0.400	1
104	.	20	PHE	H	8.923	0.020	1
105	.	20	PHE	HA	4.278	0.020	1
106	.	20	PHE	HB2	3.608	0.020	2
107	.	20	PHE	HB3	2.514	0.020	2
108	.	20	PHE	HD1	6.983	0.020	1
109	.	20	PHE	HD2	6.983	0.020	1
110	.	20	PHE	HE1	6.553	0.020	1
111	.	20	PHE	HE2	6.553	0.020	1
112	.	20	PHE	HZ	6.282	0.020	1
113	.	20	PHE	C	176.126	0.400	1
114	.	20	PHE	CA	62.138	0.400	1
115	.	20	PHE	CB	40.680	0.400	1
116	.	20	PHE	CD1	132.362	0.400	1
117	.	20	PHE	CD2	132.453	0.400	1
118	.	20	PHE	CE1	130.180	0.400	1
119	.	20	PHE	CE2	129.965	0.400	1
120	.	20	PHE	CZ	128.875	0.400	1
121	.	20	PHE	N	115.643	0.400	1
122	.	21	LEU	H	7.066	0.020	1
123	.	21	LEU	HA	3.853	0.020	1
124	.	21	LEU	HB2	1.336	0.020	2
125	.	21	LEU	HB3	1.958	0.020	2
126	.	21	LEU	HG	1.253	0.020	1
127	.	21	LEU	HD11	0.755	0.020	2
128	.	21	LEU	HD12	0.755	0.020	2
129	.	21	LEU	HD13	0.755	0.020	2
130	.	21	LEU	HD21	0.644	0.020	2
131	.	21	LEU	HD22	0.644	0.020	2
132	.	21	LEU	HD23	0.644	0.020	2
133	.	21	LEU	C	178.531	0.400	1
134	.	21	LEU	CA	56.716	0.400	1
135	.	21	LEU	CB	42.416	0.400	1
136	.	21	LEU	CG	26.928	0.400	1
137	.	21	LEU	CD1	26.062	0.400	1
138	.	21	LEU	CD2	21.915	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	.	21	LEU	N	113.210	0.400	1
140	.	22	THR	H	7.516	0.020	1
141	.	22	THR	HA	3.888	0.020	1
142	.	22	THR	HB	4.124	0.020	1
143	.	22	THR	HG21	1.207	0.020	1
144	.	22	THR	HG22	1.207	0.020	1
145	.	22	THR	HG23	1.207	0.020	1
146	.	22	THR	C	177.719	0.400	1
147	.	22	THR	CA	66.257	0.400	1
148	.	22	THR	CB	68.035	0.400	1
149	.	22	THR	CG2	22.151	0.400	1
150	.	22	THR	N	115.147	0.400	1
151	.	23	LYS	H	8.733	0.020	1
152	.	23	LYS	HA	4.021	0.020	1
153	.	23	LYS	HB2	1.918	0.020	2
154	.	23	LYS	HB3	1.446	0.020	2
155	.	23	LYS	HG2	1.583	0.020	2
156	.	23	LYS	HG3	1.348	0.020	2
157	.	23	LYS	HD2	1.583	0.020	1
158	.	23	LYS	HD3	1.583	0.020	1
159	.	23	LYS	HE2	2.934	0.020	2
160	.	23	LYS	HE3	2.883	0.020	2
161	.	23	LYS	C	178.380	0.400	1
162	.	23	LYS	CA	59.496	0.400	1
163	.	23	LYS	CB	32.700	0.400	1
164	.	23	LYS	CG	25.367	0.400	1
165	.	23	LYS	CD	28.780	0.400	1
166	.	23	LYS	CE	41.946	0.400	1
167	.	23	LYS	N	123.281	0.400	1
168	.	24	LEU	H	8.318	0.020	1
169	.	24	LEU	HA	3.857	0.020	1
170	.	24	LEU	HB2	1.750	0.020	2
171	.	24	LEU	HB3	0.932	0.020	2
172	.	24	LEU	HG	1.056	0.020	1
173	.	24	LEU	HD11	0.478	0.020	2
174	.	24	LEU	HD12	0.478	0.020	2
175	.	24	LEU	HD13	0.478	0.020	2
176	.	24	LEU	HD21	-0.151	0.020	2
177	.	24	LEU	HD22	-0.151	0.020	2
178	.	24	LEU	HD23	-0.151	0.020	2
179	.	24	LEU	C	176.970	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	.	24	LEU	CA	58.054	0.400	1
181	.	24	LEU	CB	41.420	0.400	1
182	.	24	LEU	CG	26.062	0.400	1
183	.	24	LEU	CD1	22.280	0.400	1
184	.	24	LEU	CD2	26.410	0.400	1
185	.	24	LEU	N	119.466	0.400	1
186	.	25	TRP	H	8.832	0.020	1
187	.	25	TRP	HA	3.806	0.020	1
188	.	25	TRP	HB2	3.378	0.020	2
189	.	25	TRP	HB3	3.488	0.020	2
190	.	25	TRP	HD1	7.939	0.020	1
191	.	25	TRP	HE3	7.316	0.020	1
192	.	25	TRP	HZ2	7.262	0.020	1
193	.	25	TRP	HZ3	7.073	0.020	1
194	.	25	TRP	HH2	7.235	0.020	1
195	.	25	TRP	C	176.100	0.400	1
196	.	25	TRP	CA	63.250	0.400	1
197	.	25	TRP	CB	29.890	0.400	1
198	.	25	TRP	CD1	126.600	0.400	1
199	.	25	TRP	CE3	120.164	0.400	1
200	.	25	TRP	CZ2	113.743	0.400	1
201	.	25	TRP	CZ3	122.462	0.400	1
202	.	25	TRP	CH2	124.772	0.400	1
203	.	25	TRP	N	119.688	0.400	1
204	.	26	THR	H	8.465	0.020	1
205	.	26	THR	HA	3.802	0.020	1
206	.	26	THR	HB	4.396	0.020	1
207	.	26	THR	HG21	1.423	0.020	1
208	.	26	THR	HG22	1.423	0.020	1
209	.	26	THR	HG23	1.423	0.020	1
210	.	26	THR	C	175.375	0.400	1
211	.	26	THR	CA	66.923	0.400	1
212	.	26	THR	CB	68.666	0.400	1
213	.	26	THR	CG2	21.440	0.400	1
214	.	26	THR	N	117.620	0.400	1
215	.	27	LEU	H	8.265	0.020	1
216	.	27	LEU	HA	3.858	0.020	1
217	.	27	LEU	HB2	1.652	0.020	2
218	.	27	LEU	HB3	1.103	0.020	2
219	.	27	LEU	HG	1.274	0.020	1
220	.	27	LEU	HD11	0.206	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	.	27	LEU	HD12	0.206	0.020	2
222	.	27	LEU	HD13	0.206	0.020	2
223	.	27	LEU	HD21	0.493	0.020	2
224	.	27	LEU	HD22	0.493	0.020	2
225	.	27	LEU	HD23	0.493	0.020	2
226	.	27	LEU	C	178.921	0.400	1
227	.	27	LEU	CA	57.839	0.400	1
228	.	27	LEU	CB	41.284	0.400	1
229	.	27	LEU	CG	26.199	0.400	1
230	.	27	LEU	CD1	23.282	0.400	1
231	.	27	LEU	CD2	25.717	0.400	1
232	.	27	LEU	N	123.846	0.400	1
233	.	28	VAL	H	8.441	0.020	1
234	.	28	VAL	HA	2.762	0.020	1
235	.	28	VAL	HB	0.922	0.020	1
236	.	28	VAL	HG11	-1.060	0.020	2
237	.	28	VAL	HG12	-1.060	0.020	2
238	.	28	VAL	HG13	-1.060	0.020	2
239	.	28	VAL	HG21	-0.065	0.020	2
240	.	28	VAL	HG22	-0.065	0.020	2
241	.	28	VAL	HG23	-0.065	0.020	2
242	.	28	VAL	C	179.252	0.400	1
243	.	28	VAL	CA	66.611	0.400	1
244	.	28	VAL	CB	31.114	0.400	1
245	.	28	VAL	CG1	20.092	0.400	1
246	.	28	VAL	CG2	21.889	0.400	1
247	.	28	VAL	N	119.567	0.400	1
248	.	29	SER	H	7.297	0.020	1
249	.	29	SER	HA	4.059	0.020	1
250	.	29	SER	HB2	3.655	0.020	2
251	.	29	SER	HB3	3.711	0.020	2
252	.	29	SER	C	172.429	0.400	1
253	.	29	SER	CA	60.865	0.400	1
254	.	29	SER	CB	63.451	0.400	1
255	.	29	SER	N	112.180	0.400	1
256	.	30	ASP	H	7.422	0.020	1
257	.	30	ASP	HA	4.576	0.020	1
258	.	30	ASP	HB2	2.799	0.020	2
259	.	30	ASP	HB3	3.054	0.020	2
260	.	30	ASP	CA	52.025	0.400	1
261	.	30	ASP	CB	41.052	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	.	30	ASP	N	123.540	0.400	1
263	.	31	PRO	HA	4.645	0.020	1
264	.	31	PRO	HB2	2.411	0.020	2
265	.	31	PRO	HB3	2.044	0.020	2
266	.	31	PRO	HG2	2.074	0.020	2
267	.	31	PRO	HG3	2.119	0.020	2
268	.	31	PRO	HD2	4.089	0.020	1
269	.	31	PRO	HD3	4.090	0.020	1
270	.	31	PRO	C	179.643	0.400	1
271	.	31	PRO	CA	63.621	0.400	1
272	.	31	PRO	CB	31.572	0.400	1
273	.	31	PRO	CG	27.140	0.400	1
274	.	31	PRO	CD	50.808	0.400	1
275	.	32	ASP	H	8.744	0.020	1
276	.	32	ASP	HA	4.555	0.020	1
277	.	32	ASP	HB2	2.837	0.020	2
278	.	32	ASP	HB3	2.721	0.020	2
279	.	32	ASP	C	178.290	0.400	1
280	.	32	ASP	CA	56.033	0.400	1
281	.	32	ASP	CB	40.166	0.400	1
282	.	32	ASP	N	117.536	0.400	1
283	.	33	THR	H	7.611	0.020	1
284	.	33	THR	HA	4.696	0.020	1
285	.	33	THR	HB	4.682	0.020	1
286	.	33	THR	HG21	1.166	0.020	1
287	.	33	THR	HG22	1.166	0.020	1
288	.	33	THR	HG23	1.166	0.020	1
289	.	33	THR	C	175.735	0.400	1
290	.	33	THR	CA	60.423	0.400	1
291	.	33	THR	CB	70.089	0.400	1
292	.	33	THR	CG2	21.440	0.400	1
293	.	33	THR	N	106.489	0.400	1
294	.	34	ASP	H	7.388	0.020	1
295	.	34	ASP	HA	4.750	0.020	1
296	.	34	ASP	HB2	2.886	0.020	2
297	.	34	ASP	HB3	2.737	0.020	2
298	.	34	ASP	C	175.705	0.400	1
299	.	34	ASP	CA	57.087	0.400	1
300	.	34	ASP	CB	40.366	0.400	1
301	.	34	ASP	N	122.431	0.400	1
302	.	35	ALA	H	8.486	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	.	35	ALA	HA	4.129	0.020	1
304	.	35	ALA	HB1	1.378	0.020	1
305	.	35	ALA	HB2	1.378	0.020	1
306	.	35	ALA	HB3	1.378	0.020	1
307	.	35	ALA	C	177.599	0.400	1
308	.	35	ALA	CA	54.189	0.400	1
309	.	35	ALA	CB	18.079	0.400	1
310	.	35	ALA	N	120.157	0.400	1
311	.	36	LEU	H	8.204	0.020	1
312	.	36	LEU	HA	5.065	0.020	1
313	.	36	LEU	HB2	1.921	0.020	2
314	.	36	LEU	HB3	1.828	0.020	2
315	.	36	LEU	HG	1.677	0.020	1
316	.	36	LEU	HD11	1.115	0.020	2
317	.	36	LEU	HD12	1.115	0.020	2
318	.	36	LEU	HD13	1.115	0.020	2
319	.	36	LEU	HD21	0.970	0.020	2
320	.	36	LEU	HD22	0.970	0.020	2
321	.	36	LEU	HD23	0.970	0.020	2
322	.	36	LEU	C	175.104	0.400	1
323	.	36	LEU	CA	55.632	0.400	1
324	.	36	LEU	CB	46.180	0.400	1
325	.	36	LEU	CG	27.110	0.400	1
326	.	36	LEU	CD1	24.100	0.400	1
327	.	36	LEU	CD2	26.244	0.400	1
328	.	36	LEU	N	115.101	0.400	1
329	.	37	ILE	H	8.753	0.020	1
330	.	37	ILE	HA	5.700	0.020	1
331	.	37	ILE	HB	1.936	0.020	1
332	.	37	ILE	HG12	0.579	0.020	2
333	.	37	ILE	HG13	1.818	0.020	2
334	.	37	ILE	HG21	0.984	0.020	1
335	.	37	ILE	HG22	0.984	0.020	1
336	.	37	ILE	HG23	0.984	0.020	1
337	.	37	ILE	HD11	0.602	0.020	1
338	.	37	ILE	HD12	0.602	0.020	1
339	.	37	ILE	HD13	0.602	0.020	1
340	.	37	ILE	C	173.361	0.400	1
341	.	37	ILE	CA	59.125	0.400	1
342	.	37	ILE	CB	38.008	0.400	1
343	.	37	ILE	CG1	28.225	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	.	37	ILE	CG2	14.135	0.400	1
345	.	37	ILE	CD1	13.894	0.400	1
346	.	37	ILE	N	116.260	0.400	1
347	.	38	CYS	H	8.474	0.020	1
348	.	38	CYS	HA	5.168	0.020	1
349	.	38	CYS	HB2	3.089	0.020	2
350	.	38	CYS	HB3	3.243	0.020	2
351	.	38	CYS	C	173.421	0.400	1
352	.	38	CYS	CA	54.740	0.400	1
353	.	38	CYS	CB	33.069	0.400	1
354	.	38	CYS	N	122.579	0.400	1
355	.	39	TRP	H	8.885	0.020	1
356	.	39	TRP	HA	5.049	0.020	1
357	.	39	TRP	HB2	3.222	0.020	2
358	.	39	TRP	HB3	3.618	0.020	2
359	.	39	TRP	HD1	7.375	0.020	1
360	.	39	TRP	HE1	9.105	0.020	1
361	.	39	TRP	HE3	7.938	0.020	1
362	.	39	TRP	HZ2	5.618	0.020	1
363	.	39	TRP	HZ3	7.186	0.020	1
364	.	39	TRP	HH2	5.950	0.020	1
365	.	39	TRP	C	178.591	0.400	1
366	.	39	TRP	CA	57.584	0.400	1
367	.	39	TRP	CB	31.321	0.400	1
368	.	39	TRP	CD1	126.248	0.400	1
369	.	39	TRP	CE3	120.637	0.400	1
370	.	39	TRP	CZ2	111.793	0.400	1
371	.	39	TRP	CZ3	121.967	0.400	1
372	.	39	TRP	CH2	127.182	0.400	1
373	.	39	TRP	N	122.577	0.400	1
374	.	39	TRP	NE1	127.438	0.400	1
375	.	40	SER	H	9.322	0.020	1
376	.	40	SER	HA	4.832	0.020	1
377	.	40	SER	HB2	4.163	0.020	2
378	.	40	SER	HB3	4.427	0.020	2
379	.	40	SER	CA	57.574	0.400	1
380	.	40	SER	CB	62.096	0.400	1
381	.	40	SER	N	118.682	0.400	1
382	.	41	PRO	HA	4.426	0.020	1
383	.	41	PRO	HB2	2.470	0.020	2
384	.	41	PRO	HB3	2.019	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	.	41	PRO	HG2	2.131	0.020	2
386	.	41	PRO	HG3	2.247	0.020	2
387	.	41	PRO	HD2	4.049	0.020	2
388	.	41	PRO	HD3	4.013	0.020	2
389	.	41	PRO	C	178.951	0.400	1
390	.	41	PRO	CA	66.217	0.400	1
391	.	41	PRO	CB	31.448	0.400	1
392	.	41	PRO	CG	27.838	0.400	1
393	.	41	PRO	CD	50.280	0.400	1
394	.	42	SER	H	8.351	0.020	1
395	.	42	SER	HA	4.391	0.020	1
396	.	42	SER	HB2	3.997	0.020	2
397	.	42	SER	HB3	4.000	0.020	2
398	.	42	SER	C	175.766	0.400	1
399	.	42	SER	CA	59.213	0.400	1
400	.	42	SER	CB	63.510	0.400	1
401	.	42	SER	N	110.051	0.400	1
402	.	43	GLY	H	8.472	0.020	1
403	.	43	GLY	HA2	3.467	0.020	2
404	.	43	GLY	HA3	3.900	0.020	2
405	.	43	GLY	C	172.129	0.400	1
406	.	43	GLY	CA	45.827	0.400	1
407	.	43	GLY	N	110.191	0.400	1
408	.	44	ASN	H	7.849	0.020	1
409	.	44	ASN	HA	5.295	0.020	1
410	.	44	ASN	HB2	3.058	0.020	2
411	.	44	ASN	HB3	2.825	0.020	2
412	.	44	ASN	HD21	7.542	0.020	2
413	.	44	ASN	HD22	6.912	0.020	2
414	.	44	ASN	C	175.405	0.400	1
415	.	44	ASN	CA	52.332	0.400	1
416	.	44	ASN	CB	38.597	0.400	1
417	.	44	ASN	N	113.354	0.400	1
418	.	44	ASN	ND2	111.488	0.400	1
419	.	45	SER	H	8.595	0.020	1
420	.	45	SER	HA	5.637	0.020	1
421	.	45	SER	HB2	4.163	0.020	2
422	.	45	SER	HB3	4.075	0.020	2
423	.	45	SER	C	171.949	0.400	1
424	.	45	SER	CA	57.060	0.400	1
425	.	45	SER	CB	64.228	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	.	45	SER	N	114.334	0.400	1
427	.	46	PHE	H	9.267	0.020	1
428	.	46	PHE	HA	5.854	0.020	1
429	.	46	PHE	HB2	2.497	0.020	2
430	.	46	PHE	HB3	2.862	0.020	2
431	.	46	PHE	HD1	6.958	0.020	1
432	.	46	PHE	HD2	6.958	0.020	1
433	.	46	PHE	HE1	6.646	0.020	1
434	.	46	PHE	HE2	6.646	0.020	1
435	.	46	PHE	HZ	6.480	0.020	1
436	.	46	PHE	C	171.558	0.400	1
437	.	46	PHE	CA	55.656	0.400	1
438	.	46	PHE	CB	43.457	0.400	1
439	.	46	PHE	CD1	132.307	0.400	1
440	.	46	PHE	CD2	132.507	0.400	1
441	.	46	PHE	CE1	130.378	0.400	1
442	.	46	PHE	CE2	130.600	0.400	1
443	.	46	PHE	CZ	127.971	0.400	1
444	.	46	PHE	N	115.412	0.400	1
445	.	47	HIS	H	9.287	0.020	1
446	.	47	HIS	HA	5.050	0.020	1
447	.	47	HIS	HB2	1.924	0.020	2
448	.	47	HIS	HB3	2.489	0.020	2
449	.	47	HIS	HD2	6.658	0.020	1
450	.	47	HIS	HE1	8.040	0.020	1
451	.	47	HIS	C	173.511	0.400	1
452	.	47	HIS	CA	54.118	0.400	1
453	.	47	HIS	CB	32.516	0.400	1
454	.	47	HIS	CD2	119.840	0.400	1
455	.	47	HIS	CE1	136.445	0.400	1
456	.	47	HIS	N	118.235	0.400	1
457	.	48	VAL	H	8.744	0.020	1
458	.	48	VAL	HA	4.563	0.020	1
459	.	48	VAL	HB	1.619	0.020	1
460	.	48	VAL	HG11	0.153	0.020	2
461	.	48	VAL	HG12	0.153	0.020	2
462	.	48	VAL	HG13	0.153	0.020	2
463	.	48	VAL	HG21	0.587	0.020	2
464	.	48	VAL	HG22	0.587	0.020	2
465	.	48	VAL	HG23	0.587	0.020	2
466	.	48	VAL	C	175.555	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	.	48	VAL	CA	60.926	0.400	1
468	.	48	VAL	CB	33.518	0.400	1
469	.	48	VAL	CG1	20.134	0.400	1
470	.	48	VAL	CG2	20.867	0.400	1
471	.	48	VAL	N	119.188	0.400	1
472	.	49	PHE	H	9.128	0.020	1
473	.	49	PHE	HA	5.414	0.020	1
474	.	49	PHE	HB2	3.161	0.020	2
475	.	49	PHE	HB3	3.027	0.020	2
476	.	49	PHE	HD1	7.105	0.020	1
477	.	49	PHE	HD2	7.105	0.020	1
478	.	49	PHE	HE1	7.135	0.020	1
479	.	49	PHE	HE2	7.135	0.020	1
480	.	49	PHE	HZ	6.714	0.020	1
481	.	49	PHE	C	174.203	0.400	1
482	.	49	PHE	CA	55.908	0.400	1
483	.	49	PHE	CB	41.065	0.400	1
484	.	49	PHE	CD1	131.283	0.400	1
485	.	49	PHE	CD2	131.496	0.400	1
486	.	49	PHE	CE1	131.029	0.400	1
487	.	49	PHE	CE2	131.074	0.400	1
488	.	49	PHE	CZ	128.328	0.400	1
489	.	49	PHE	N	129.318	0.400	1
490	.	50	ASP	H	7.884	0.020	1
491	.	50	ASP	HA	4.522	0.020	1
492	.	50	ASP	HB2	2.507	0.020	2
493	.	50	ASP	HB3	3.385	0.020	2
494	.	50	ASP	C	176.246	0.400	1
495	.	50	ASP	CA	53.832	0.400	1
496	.	50	ASP	CB	40.199	0.400	1
497	.	50	ASP	N	114.807	0.400	1
498	.	51	GLN	H	9.425	0.020	1
499	.	51	GLN	HA	3.997	0.020	1
500	.	51	GLN	HB2	2.280	0.020	1
501	.	51	GLN	HB3	2.280	0.020	1
502	.	51	GLN	HG2	2.465	0.020	2
503	.	51	GLN	HG3	2.553	0.020	2
504	.	51	GLN	HE21	7.575	0.020	2
505	.	51	GLN	HE22	6.773	0.020	2
506	.	51	GLN	C	177.929	0.400	1
507	.	51	GLN	CA	59.924	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	.	51	GLN	CB	28.666	0.400	1
509	.	51	GLN	CG	34.141	0.400	1
510	.	51	GLN	N	121.212	0.400	1
511	.	51	GLN	NE2	110.752	0.400	1
512	.	52	GLY	H	9.188	0.020	1
513	.	52	GLY	HA2	3.962	0.020	2
514	.	52	GLY	HA3	4.018	0.020	2
515	.	52	GLY	C	176.307	0.400	1
516	.	52	GLY	CA	46.879	0.400	1
517	.	52	GLY	N	108.889	0.400	1
518	.	53	GLN	H	7.959	0.020	1
519	.	53	GLN	HA	4.238	0.020	1
520	.	53	GLN	HB2	2.168	0.020	1
521	.	53	GLN	HB3	2.168	0.020	1
522	.	53	GLN	HG2	2.492	0.020	2
523	.	53	GLN	HG3	2.446	0.020	2
524	.	53	GLN	HE21	7.928	0.020	2
525	.	53	GLN	HE22	6.862	0.020	2
526	.	53	GLN	C	178.320	0.400	1
527	.	53	GLN	CA	58.013	0.400	1
528	.	53	GLN	CB	28.361	0.400	1
529	.	53	GLN	CG	33.515	0.400	1
530	.	53	GLN	N	123.993	0.400	1
531	.	53	GLN	NE2	111.869	0.400	1
532	.	54	PHE	H	9.209	0.020	1
533	.	54	PHE	HA	4.072	0.020	1
534	.	54	PHE	HB2	3.336	0.020	2
535	.	54	PHE	HB3	3.204	0.020	2
536	.	54	PHE	HD1	7.071	0.020	1
537	.	54	PHE	HD2	7.071	0.020	1
538	.	54	PHE	HE1	6.663	0.020	1
539	.	54	PHE	HE2	6.663	0.020	1
540	.	54	PHE	HZ	6.255	0.020	1
541	.	54	PHE	C	177.599	0.400	1
542	.	54	PHE	CA	61.965	0.400	1
543	.	54	PHE	CB	39.524	0.400	1
544	.	54	PHE	CD1	131.366	0.400	1
545	.	54	PHE	CD2	131.584	0.400	1
546	.	54	PHE	CE1	130.518	0.400	1
547	.	54	PHE	CE2	130.600	0.400	1
548	.	54	PHE	CZ	128.600	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	.	54	PHE	N	121.568	0.400	1
550	.	55	ALA	H	8.849	0.020	1
551	.	55	ALA	HA	3.756	0.020	1
552	.	55	ALA	HB1	1.572	0.020	1
553	.	55	ALA	HB2	1.572	0.020	1
554	.	55	ALA	HB3	1.572	0.020	1
555	.	55	ALA	C	176.216	0.400	1
556	.	55	ALA	CA	54.398	0.400	1
557	.	55	ALA	CB	18.489	0.400	1
558	.	55	ALA	N	121.199	0.400	1
559	.	56	LYS	H	7.161	0.020	1
560	.	56	LYS	HA	4.217	0.020	1
561	.	56	LYS	HB2	1.964	0.020	2
562	.	56	LYS	HB3	1.876	0.020	2
563	.	56	LYS	HG2	1.587	0.020	2
564	.	56	LYS	HG3	1.474	0.020	2
565	.	56	LYS	HD2	1.719	0.020	1
566	.	56	LYS	HD3	1.719	0.020	1
567	.	56	LYS	HE2	3.009	0.020	1
568	.	56	LYS	HE3	3.009	0.020	1
569	.	56	LYS	C	177.809	0.400	1
570	.	56	LYS	CA	57.898	0.400	1
571	.	56	LYS	CB	34.056	0.400	1
572	.	56	LYS	CG	24.910	0.400	1
573	.	56	LYS	CD	29.095	0.400	1
574	.	56	LYS	CE	41.780	0.400	1
575	.	56	LYS	N	112.691	0.400	1
576	.	57	GLU	H	8.362	0.020	1
577	.	57	GLU	HA	4.455	0.020	1
578	.	57	GLU	HB2	1.935	0.020	2
579	.	57	GLU	HB3	2.060	0.020	2
580	.	57	GLU	HG2	2.333	0.020	2
581	.	57	GLU	HG3	2.171	0.020	2
582	.	57	GLU	C	177.208	0.400	1
583	.	57	GLU	CA	57.268	0.400	1
584	.	57	GLU	CB	32.008	0.400	1
585	.	57	GLU	CG	35.753	0.400	1
586	.	57	GLU	N	113.775	0.400	1
587	.	58	VAL	H	7.846	0.020	1
588	.	58	VAL	HA	4.037	0.020	1
589	.	58	VAL	HB	1.598	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	.	58	VAL	HG11	0.688	0.020	2
591	.	58	VAL	HG12	0.688	0.020	2
592	.	58	VAL	HG13	0.688	0.020	2
593	.	58	VAL	HG21	1.001	0.020	2
594	.	58	VAL	HG22	1.001	0.020	2
595	.	58	VAL	HG23	1.001	0.020	2
596	.	58	VAL	C	176.667	0.400	1
597	.	58	VAL	CA	64.712	0.400	1
598	.	58	VAL	CB	31.597	0.400	1
599	.	58	VAL	CG1	23.496	0.400	1
600	.	58	VAL	CG2	22.955	0.400	1
601	.	58	VAL	N	119.325	0.400	1
602	.	59	LEU	H	7.112	0.020	1
603	.	59	LEU	HA	3.895	0.020	1
604	.	59	LEU	HB2	1.845	0.020	2
605	.	59	LEU	HB3	1.222	0.020	2
606	.	59	LEU	HG	0.829	0.020	1
607	.	59	LEU	HD11	0.615	0.020	2
608	.	59	LEU	HD12	0.615	0.020	2
609	.	59	LEU	HD13	0.615	0.020	2
610	.	59	LEU	HD21	0.179	0.020	2
611	.	59	LEU	HD22	0.179	0.020	2
612	.	59	LEU	HD23	0.179	0.020	2
613	.	59	LEU	CA	60.000	0.400	1
614	.	59	LEU	CB	38.352	0.400	1
615	.	59	LEU	CG	25.587	0.400	1
616	.	59	LEU	CD1	24.730	0.400	1
617	.	59	LEU	CD2	24.100	0.400	1
618	.	59	LEU	N	117.593	0.400	1
619	.	60	PRO	HA	4.093	0.020	1
620	.	60	PRO	HB2	2.107	0.020	2
621	.	60	PRO	HB3	1.623	0.020	2
622	.	60	PRO	HG2	1.908	0.020	2
623	.	60	PRO	HG3	1.741	0.020	2
624	.	60	PRO	HD2	3.822	0.020	2
625	.	60	PRO	HD3	2.865	0.020	2
626	.	60	PRO	C	178.771	0.400	1
627	.	60	PRO	CA	65.984	0.400	1
628	.	60	PRO	CB	30.984	0.400	1
629	.	60	PRO	CG	28.276	0.400	1
630	.	60	PRO	CD	50.593	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	.	61	LYS	H	6.726	0.020	1
632	.	61	LYS	HA	3.862	0.020	1
633	.	61	LYS	HB2	1.756	0.020	2
634	.	61	LYS	HB3	1.572	0.020	2
635	.	61	LYS	HG2	1.193	0.020	2
636	.	61	LYS	HG3	0.705	0.020	2
637	.	61	LYS	HD2	1.572	0.020	2
638	.	61	LYS	HD3	1.518	0.020	2
639	.	61	LYS	HE2	2.824	0.020	1
640	.	61	LYS	HE3	2.824	0.020	1
641	.	61	LYS	C	177.058	0.400	1
642	.	61	LYS	CA	58.328	0.400	1
643	.	61	LYS	CB	32.625	0.400	1
644	.	61	LYS	CG	24.910	0.400	1
645	.	61	LYS	CD	29.103	0.400	1
646	.	61	LYS	CE	41.780	0.400	1
647	.	61	LYS	N	115.571	0.400	1
648	.	62	TYR	H	7.452	0.020	1
649	.	62	TYR	HA	4.082	0.020	1
650	.	62	TYR	HB2	1.811	0.020	2
651	.	62	TYR	HB3	2.052	0.020	2
652	.	62	TYR	HD1	7.031	0.020	1
653	.	62	TYR	HD2	7.031	0.020	1
654	.	62	TYR	HE1	6.685	0.020	1
655	.	62	TYR	HE2	6.685	0.020	1
656	.	62	TYR	C	175.390	0.400	1
657	.	62	TYR	CA	59.968	0.400	1
658	.	62	TYR	CB	40.388	0.400	1
659	.	62	TYR	CD1	133.230	0.400	1
660	.	62	TYR	CD2	133.253	0.400	1
661	.	62	TYR	CE1	118.051	0.400	1
662	.	62	TYR	CE2	117.910	0.400	1
663	.	62	TYR	N	113.391	0.400	1
664	.	63	PHE	H	8.421	0.020	1
665	.	63	PHE	HA	4.947	0.020	1
666	.	63	PHE	HB2	3.572	0.020	2
667	.	63	PHE	HB3	2.478	0.020	2
668	.	63	PHE	HD1	7.394	0.020	1
669	.	63	PHE	HD2	7.394	0.020	1
670	.	63	PHE	HE1	7.047	0.020	1
671	.	63	PHE	HE2	7.047	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	.	63	PHE	HZ	6.653	0.020	1
673	.	63	PHE	C	174.443	0.400	1
674	.	63	PHE	CA	55.140	0.400	1
675	.	63	PHE	CB	40.930	0.400	1
676	.	63	PHE	CD1	132.181	0.400	1
677	.	63	PHE	CD2	132.291	0.400	1
678	.	63	PHE	CE1	131.070	0.400	1
679	.	63	PHE	CE2	131.220	0.400	1
680	.	63	PHE	CZ	128.194	0.400	1
681	.	63	PHE	N	115.028	0.400	1
682	.	64	LYS	H	7.769	0.020	1
683	.	64	LYS	HA	4.175	0.020	1
684	.	64	LYS	HB2	2.010	0.020	1
685	.	64	LYS	HB3	2.010	0.020	1
686	.	64	LYS	HG2	1.257	0.020	2
687	.	64	LYS	HG3	1.333	0.020	2
688	.	64	LYS	HD2	1.642	0.020	2
689	.	64	LYS	HD3	1.639	0.020	2
690	.	64	LYS	HE2	2.938	0.020	1
691	.	64	LYS	HE3	2.938	0.020	1
692	.	64	LYS	C	174.864	0.400	1
693	.	64	LYS	CA	57.244	0.400	1
694	.	64	LYS	CB	29.070	0.400	1
695	.	64	LYS	CG	24.910	0.400	1
696	.	64	LYS	CD	28.780	0.400	1
697	.	64	LYS	CE	41.941	0.400	1
698	.	64	LYS	N	115.083	0.400	1
699	.	65	HIS	H	7.406	0.020	1
700	.	65	HIS	HA	4.702	0.020	1
701	.	65	HIS	HB2	3.220	0.020	2
702	.	65	HIS	HB3	3.157	0.020	2
703	.	65	HIS	HD2	6.978	0.020	1
704	.	65	HIS	HE1	7.732	0.020	1
705	.	65	HIS	C	172.309	0.400	1
706	.	65	HIS	CA	55.620	0.400	1
707	.	65	HIS	CB	32.550	0.400	1
708	.	65	HIS	CD2	118.439	0.400	1
709	.	65	HIS	CE1	138.301	0.400	1
710	.	65	HIS	N	114.996	0.400	1
711	.	66	ASN	H	8.077	0.020	1
712	.	66	ASN	HA	5.007	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	.	66	ASN	HB2	2.620	0.020	2
714	.	66	ASN	HB3	3.141	0.020	2
715	.	66	ASN	HD21	7.453	0.020	2
716	.	66	ASN	HD22	6.857	0.020	2
717	.	66	ASN	CA	51.765	0.400	1
718	.	66	ASN	CB	39.532	0.400	1
719	.	66	ASN	N	115.813	0.400	1
720	.	66	ASN	ND2	110.696	0.400	1
721	.	67	ASN	H	8.078	0.020	1
722	.	67	ASN	HA	4.879	0.020	1
723	.	67	ASN	HB2	2.817	0.020	2
724	.	67	ASN	HB3	3.142	0.020	2
725	.	67	ASN	HD21	7.640	0.020	2
726	.	67	ASN	HD22	6.944	0.020	2
727	.	67	ASN	C	174.563	0.400	1
728	.	67	ASN	CA	52.736	0.400	1
729	.	67	ASN	CB	40.106	0.400	1
730	.	67	ASN	ND2	112.430	0.400	1
731	.	68	MET	H	9.152	0.020	1
732	.	68	MET	HA	4.387	0.020	1
733	.	68	MET	HB2	2.012	0.020	2
734	.	68	MET	HB3	2.359	0.020	2
735	.	68	MET	HG2	3.011	0.020	2
736	.	68	MET	HG3	2.807	0.020	2
737	.	68	MET	HE1	2.098	0.020	1
738	.	68	MET	HE2	2.098	0.020	1
739	.	68	MET	HE3	2.098	0.020	1
740	.	68	MET	C	177.208	0.400	1
741	.	68	MET	CA	57.479	0.400	1
742	.	68	MET	CB	32.003	0.400	1
743	.	68	MET	CG	32.070	0.400	1
744	.	68	MET	CE	16.765	0.400	1
745	.	68	MET	N	125.636	0.400	1
746	.	69	ALA	H	8.451	0.020	1
747	.	69	ALA	HA	4.161	0.020	1
748	.	69	ALA	HB1	1.476	0.020	1
749	.	69	ALA	HB2	1.476	0.020	1
750	.	69	ALA	HB3	1.476	0.020	1
751	.	69	ALA	C	181.025	0.400	1
752	.	69	ALA	CA	55.202	0.400	1
753	.	69	ALA	CB	17.281	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	.	69	ALA	N	120.436	0.400	1
755	.	70	SER	H	8.080	0.020	1
756	.	70	SER	HA	4.096	0.020	1
757	.	70	SER	HB2	3.792	0.020	2
758	.	70	SER	HB3	3.709	0.020	2
759	.	70	SER	C	176.096	0.400	1
760	.	70	SER	CA	60.871	0.400	1
761	.	70	SER	CB	62.384	0.400	1
762	.	70	SER	N	114.621	0.400	1
763	.	71	PHE	H	7.663	0.020	1
764	.	71	PHE	HA	4.253	0.020	1
765	.	71	PHE	HB2	3.081	0.020	2
766	.	71	PHE	HB3	3.638	0.020	2
767	.	71	PHE	HD1	7.076	0.020	1
768	.	71	PHE	HD2	7.076	0.020	1
769	.	71	PHE	HE1	6.649	0.020	1
770	.	71	PHE	HE2	6.649	0.020	1
771	.	71	PHE	HZ	6.256	0.020	1
772	.	71	PHE	C	175.916	0.400	1
773	.	71	PHE	CA	60.688	0.400	1
774	.	71	PHE	CB	39.795	0.400	1
775	.	71	PHE	CD1	132.050	0.400	1
776	.	71	PHE	CD2	131.987	0.400	1
777	.	71	PHE	CE1	130.429	0.400	1
778	.	71	PHE	CE2	130.600	0.400	1
779	.	71	PHE	CZ	128.594	0.400	1
780	.	71	PHE	N	124.107	0.400	1
781	.	72	VAL	H	8.712	0.020	1
782	.	72	VAL	HA	3.114	0.020	1
783	.	72	VAL	HB	2.134	0.020	1
784	.	72	VAL	HG11	1.009	0.020	2
785	.	72	VAL	HG12	1.009	0.020	2
786	.	72	VAL	HG13	1.009	0.020	2
787	.	72	VAL	HG21	1.243	0.020	2
788	.	72	VAL	HG22	1.243	0.020	2
789	.	72	VAL	HG23	1.243	0.020	2
790	.	72	VAL	C	177.629	0.400	1
791	.	72	VAL	CA	66.527	0.400	1
792	.	72	VAL	CB	31.434	0.400	1
793	.	72	VAL	CG1	21.329	0.400	1
794	.	72	VAL	CG2	23.452	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	.	72	VAL	N	118.726	0.400	1
796	.	73	ARG	H	8.044	0.020	1
797	.	73	ARG	HA	4.006	0.020	1
798	.	73	ARG	HB2	1.919	0.020	2
799	.	73	ARG	HB3	1.846	0.020	2
800	.	73	ARG	HG2	1.508	0.020	2
801	.	73	ARG	HG3	1.747	0.020	2
802	.	73	ARG	HD2	3.169	0.020	1
803	.	73	ARG	HD3	3.169	0.020	1
804	.	73	ARG	C	178.981	0.400	1
805	.	73	ARG	CA	59.712	0.400	1
806	.	73	ARG	CB	29.567	0.400	1
807	.	73	ARG	CG	27.605	0.400	1
808	.	73	ARG	CD	43.213	0.400	1
809	.	73	ARG	N	120.255	0.400	1
810	.	74	GLN	H	7.421	0.020	1
811	.	74	GLN	HA	3.725	0.020	1
812	.	74	GLN	HB2	1.003	0.020	2
813	.	74	GLN	HB3	1.616	0.020	2
814	.	74	GLN	HG2	1.846	0.020	2
815	.	74	GLN	HG3	1.649	0.020	2
816	.	74	GLN	HE21	6.723	0.020	2
817	.	74	GLN	HE22	6.645	0.020	2
818	.	74	GLN	C	177.599	0.400	1
819	.	74	GLN	CA	58.855	0.400	1
820	.	74	GLN	CB	27.766	0.400	1
821	.	74	GLN	CG	33.720	0.400	1
822	.	74	GLN	N	119.507	0.400	1
823	.	74	GLN	NE2	111.277	0.400	1
824	.	75	LEU	H	7.439	0.020	1
825	.	75	LEU	HA	3.672	0.020	1
826	.	75	LEU	HB2	1.571	0.020	2
827	.	75	LEU	HB3	0.582	0.020	2
828	.	75	LEU	HG	0.659	0.020	1
829	.	75	LEU	HD11	-0.761	0.020	2
830	.	75	LEU	HD12	-0.761	0.020	2
831	.	75	LEU	HD13	-0.761	0.020	2
832	.	75	LEU	HD21	-0.522	0.020	2
833	.	75	LEU	HD22	-0.522	0.020	2
834	.	75	LEU	HD23	-0.522	0.020	2
835	.	75	LEU	C	180.123	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	.	75	LEU	CA	57.877	0.400	1
837	.	75	LEU	CB	39.877	0.400	1
838	.	75	LEU	CG	24.832	0.400	1
839	.	75	LEU	CD1	24.730	0.400	1
840	.	75	LEU	CD2	21.859	0.400	1
841	.	75	LEU	N	117.285	0.400	1
842	.	76	ASN	H	8.536	0.020	1
843	.	76	ASN	HA	4.553	0.020	1
844	.	76	ASN	HB2	2.869	0.020	2
845	.	76	ASN	HB3	2.916	0.020	2
846	.	76	ASN	HD21	7.520	0.020	2
847	.	76	ASN	HD22	6.919	0.020	2
848	.	76	ASN	C	179.282	0.400	1
849	.	76	ASN	CA	56.481	0.400	1
850	.	76	ASN	CB	38.536	0.400	1
851	.	76	ASN	N	118.452	0.400	1
852	.	76	ASN	ND2	110.650	0.400	1
853	.	77	MET	H	8.185	0.020	1
854	.	77	MET	HA	4.133	0.020	1
855	.	77	MET	HB2	2.056	0.020	2
856	.	77	MET	HB3	1.896	0.020	2
857	.	77	MET	HG2	2.419	0.020	2
858	.	77	MET	HG3	2.298	0.020	2
859	.	77	MET	HE1	1.823	0.020	1
860	.	77	MET	HE2	1.823	0.020	1
861	.	77	MET	HE3	1.823	0.020	1
862	.	77	MET	C	176.637	0.400	1
863	.	77	MET	CA	58.104	0.400	1
864	.	77	MET	CB	31.974	0.400	1
865	.	77	MET	CG	31.605	0.400	1
866	.	77	MET	CE	16.765	0.400	1
867	.	77	MET	N	121.614	0.400	1
868	.	78	TYR	H	7.505	0.020	1
869	.	78	TYR	HA	4.765	0.020	1
870	.	78	TYR	HB2	2.819	0.020	2
871	.	78	TYR	HB3	3.685	0.020	2
872	.	78	TYR	HD1	7.099	0.020	1
873	.	78	TYR	HD2	7.099	0.020	1
874	.	78	TYR	HE1	6.669	0.020	1
875	.	78	TYR	HE2	6.669	0.020	1
876	.	78	TYR	C	174.413	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	.	78	TYR	CA	59.191	0.400	1
878	.	78	TYR	CB	38.851	0.400	1
879	.	78	TYR	CD1	133.230	0.400	1
880	.	78	TYR	CD2	133.253	0.400	1
881	.	78	TYR	CE1	117.541	0.400	1
882	.	78	TYR	CE2	117.788	0.400	1
883	.	78	TYR	N	115.682	0.400	1
884	.	79	GLY	H	7.954	0.020	1
885	.	79	GLY	HA2	3.909	0.020	2
886	.	79	GLY	HA3	4.296	0.020	2
887	.	79	GLY	C	176.066	0.400	1
888	.	79	GLY	CA	46.149	0.400	1
889	.	79	GLY	N	103.999	0.400	1
890	.	80	PHE	H	8.316	0.020	1
891	.	80	PHE	HA	4.620	0.020	1
892	.	80	PHE	HB2	2.999	0.020	2
893	.	80	PHE	HB3	2.605	0.020	2
894	.	80	PHE	HD1	7.333	0.020	1
895	.	80	PHE	HD2	7.333	0.020	1
896	.	80	PHE	HE1	6.709	0.020	1
897	.	80	PHE	HE2	6.709	0.020	1
898	.	80	PHE	HZ	6.249	0.020	1
899	.	80	PHE	C	175.856	0.400	1
900	.	80	PHE	CA	58.796	0.400	1
901	.	80	PHE	CB	39.896	0.400	1
902	.	80	PHE	CD1	131.969	0.400	1
903	.	80	PHE	CD2	132.159	0.400	1
904	.	80	PHE	CE1	130.716	0.400	1
905	.	80	PHE	CE2	130.600	0.400	1
906	.	80	PHE	CZ	129.140	0.400	1
907	.	80	PHE	N	118.914	0.400	1
908	.	81	ARG	H	9.166	0.020	1
909	.	81	ARG	HA	4.790	0.020	1
910	.	81	ARG	HB2	1.868	0.020	2
911	.	81	ARG	HB3	1.784	0.020	2
912	.	81	ARG	HG2	1.642	0.020	1
913	.	81	ARG	HG3	1.642	0.020	1
914	.	81	ARG	HD2	3.195	0.020	2
915	.	81	ARG	HD3	3.197	0.020	2
916	.	81	ARG	C	174.984	0.400	1
917	.	81	ARG	CA	54.212	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	.	81	ARG	CB	33.145	0.400	1
919	.	81	ARG	CG	27.310	0.400	1
920	.	81	ARG	CD	43.100	0.400	1
921	.	81	ARG	N	121.147	0.400	1
922	.	82	LYS	H	8.627	0.020	1
923	.	82	LYS	HA	4.534	0.020	1
924	.	82	LYS	HB2	1.483	0.020	2
925	.	82	LYS	HB3	1.559	0.020	2
926	.	82	LYS	HG2	0.790	0.020	2
927	.	82	LYS	HG3	0.953	0.020	2
928	.	82	LYS	HD2	1.520	0.020	2
929	.	82	LYS	HD3	1.484	0.020	2
930	.	82	LYS	HE2	2.822	0.020	1
931	.	82	LYS	HE3	2.822	0.020	1
932	.	82	LYS	C	176.096	0.400	1
933	.	82	LYS	CA	55.127	0.400	1
934	.	82	LYS	CB	33.460	0.400	1
935	.	82	LYS	CG	24.645	0.400	1
936	.	82	LYS	CD	29.200	0.400	1
937	.	82	LYS	CE	41.544	0.400	1
938	.	82	LYS	N	124.110	0.400	1
939	.	83	VAL	H	8.521	0.020	1
940	.	83	VAL	HA	3.799	0.020	1
941	.	83	VAL	HB	1.461	0.020	1
942	.	83	VAL	HG11	0.543	0.020	2
943	.	83	VAL	HG12	0.543	0.020	2
944	.	83	VAL	HG13	0.543	0.020	2
945	.	83	VAL	HG21	0.629	0.020	2
946	.	83	VAL	HG22	0.629	0.020	2
947	.	83	VAL	HG23	0.629	0.020	2
948	.	83	VAL	C	174.714	0.400	1
949	.	83	VAL	CA	61.983	0.400	1
950	.	83	VAL	CB	32.778	0.400	1
951	.	83	VAL	CG1	20.385	0.400	1
952	.	83	VAL	CG2	20.817	0.400	1
953	.	83	VAL	N	128.638	0.400	1
954	.	84	VAL	H	8.309	0.020	1
955	.	84	VAL	HA	3.957	0.020	1
956	.	84	VAL	HB	1.918	0.020	1
957	.	84	VAL	HG11	0.841	0.020	2
958	.	84	VAL	HG12	0.841	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
959	.	84	VAL	HG13	0.841	0.020	2
960	.	84	VAL	HG21	0.869	0.020	2
961	.	84	VAL	HG22	0.869	0.020	2
962	.	84	VAL	HG23	0.869	0.020	2
963	.	84	VAL	C	175.495	0.400	1
964	.	84	VAL	CA	61.897	0.400	1
965	.	84	VAL	CB	32.476	0.400	1
966	.	84	VAL	CG1	20.767	0.400	1
967	.	84	VAL	CG2	20.718	0.400	1
968	.	84	VAL	N	127.052	0.400	1
969	.	85	HIS	H	8.675	0.020	1
970	.	85	HIS	HA	4.800	0.020	1
971	.	85	HIS	HB2	3.206	0.020	2
972	.	85	HIS	HB3	3.115	0.020	2
973	.	85	HIS	HD2	7.078	0.020	1
974	.	85	HIS	HE1	8.281	0.020	1
975	.	85	HIS	C	174.473	0.400	1
976	.	85	HIS	CA	55.079	0.400	1
977	.	85	HIS	CB	29.967	0.400	1
978	.	85	HIS	CD2	119.727	0.400	1
979	.	85	HIS	CE1	136.914	0.400	1
980	.	85	HIS	N	125.850	0.400	1
981	.	86	ILE	H	8.418	0.020	1
982	.	86	ILE	HA	4.227	0.020	1
983	.	86	ILE	HB	1.856	0.020	1
984	.	86	ILE	HG12	1.471	0.020	2
985	.	86	ILE	HG13	1.190	0.020	2
986	.	86	ILE	HG21	0.888	0.020	1
987	.	86	ILE	HG22	0.888	0.020	1
988	.	86	ILE	HG23	0.888	0.020	1
989	.	86	ILE	HD11	0.860	0.020	1
990	.	86	ILE	HD12	0.860	0.020	1
991	.	86	ILE	HD13	0.860	0.020	1
992	.	86	ILE	C	175.820	0.400	1
993	.	86	ILE	CA	60.976	0.400	1
994	.	86	ILE	CB	39.047	0.400	1
995	.	86	ILE	CG1	26.982	0.400	1
996	.	86	ILE	CG2	17.360	0.400	1
997	.	86	ILE	CD1	12.478	0.400	1
998	.	86	ILE	N	123.030	0.400	1
999	.	87	GLU	H	8.778	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1000	.	87	GLU	HA	4.353	0.020	1
1001	.	87	GLU	HB2	2.072	0.020	2
1002	.	87	GLU	HB3	1.951	0.020	2
1003	.	87	GLU	HG2	2.292	0.020	2
1004	.	87	GLU	HG3	2.290	0.020	2
1005	.	87	GLU	C	176.186	0.400	1
1006	.	87	GLU	CA	55.984	0.400	1
1007	.	87	GLU	CB	30.029	0.400	1
1008	.	87	GLU	CG	36.010	0.400	1
1009	.	87	GLU	N	126.020	0.400	1
1010	.	88	GLN	H	8.644	0.020	1
1011	.	88	GLN	HA	4.331	0.020	1
1012	.	88	GLN	HB2	2.153	0.020	2
1013	.	88	GLN	HB3	2.004	0.020	2
1014	.	88	GLN	HG2	2.388	0.020	2
1015	.	88	GLN	HG3	2.392	0.020	2
1016	.	88	GLN	HE21	7.593	0.020	2
1017	.	88	GLN	HE22	6.882	0.020	2
1018	.	88	GLN	C	176.390	0.400	1
1019	.	88	GLN	CA	56.184	0.400	1
1020	.	88	GLN	CB	29.228	0.400	1
1021	.	88	GLN	CG	33.720	0.400	1
1022	.	88	GLN	N	122.181	0.400	1
1023	.	88	GLN	NE2	112.211	0.400	1
1024	.	89	GLY	H	8.625	0.020	1
1025	.	89	GLY	HA2	3.956	0.020	2
1026	.	89	GLY	HA3	4.002	0.020	2
1027	.	89	GLY	C	174.593	0.400	1
1028	.	89	GLY	CA	45.239	0.400	1
1029	.	89	GLY	N	110.175	0.400	1
1030	.	90	GLY	H	8.337	0.020	1
1031	.	90	GLY	HA2	3.958	0.020	2
1032	.	90	GLY	HA3	3.974	0.020	2
1033	.	90	GLY	C	173.842	0.400	1
1034	.	90	GLY	CA	45.109	0.400	1
1035	.	90	GLY	N	108.580	0.400	1
1036	.	91	LEU	H	8.099	0.020	1
1037	.	91	LEU	HA	4.361	0.020	1
1038	.	91	LEU	HB2	1.650	0.020	2
1039	.	91	LEU	HB3	1.593	0.020	2
1040	.	91	LEU	HG	1.606	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1041	.	91	LEU	HD11	0.928	0.020	2
1042	.	91	LEU	HD12	0.928	0.020	2
1043	.	91	LEU	HD13	0.928	0.020	2
1044	.	91	LEU	HD21	0.866	0.020	2
1045	.	91	LEU	HD22	0.866	0.020	2
1046	.	91	LEU	HD23	0.866	0.020	2
1047	.	91	LEU	C	177.148	0.400	1
1048	.	91	LEU	CA	55.204	0.400	1
1049	.	91	LEU	CB	42.440	0.400	1
1050	.	91	LEU	CG	26.770	0.400	1
1051	.	91	LEU	CD1	24.730	0.400	1
1052	.	91	LEU	CD2	23.170	0.400	1
1053	.	91	LEU	N	121.292	0.400	1
1054	.	92	VAL	H	8.079	0.020	1
1055	.	92	VAL	HA	4.074	0.020	1
1056	.	92	VAL	HB	2.027	0.020	1
1057	.	92	VAL	HG11	0.922	0.020	1
1058	.	92	VAL	HG12	0.922	0.020	1
1059	.	92	VAL	HG13	0.922	0.020	1
1060	.	92	VAL	HG21	0.923	0.020	1
1061	.	92	VAL	HG22	0.923	0.020	1
1062	.	92	VAL	HG23	0.923	0.020	1
1063	.	92	VAL	C	175.690	0.400	1
1064	.	92	VAL	CA	62.179	0.400	1
1065	.	92	VAL	CB	32.842	0.400	1
1066	.	92	VAL	CG1	20.767	0.400	1
1067	.	92	VAL	CG2	20.718	0.400	1
1068	.	92	VAL	N	120.593	0.400	1
1069	.	93	LYS	H	8.390	0.020	1
1070	.	93	LYS	HA	4.625	0.020	1
1071	.	93	LYS	HB2	1.733	0.020	2
1072	.	93	LYS	HB3	1.851	0.020	2
1073	.	93	LYS	HG2	1.435	0.020	2
1074	.	93	LYS	HG3	1.476	0.020	2
1075	.	93	LYS	HD2	1.703	0.020	1
1076	.	93	LYS	HD3	1.703	0.020	1
1077	.	93	LYS	HE2	3.013	0.020	2
1078	.	93	LYS	HE3	3.018	0.020	2
1079	.	93	LYS	CA	53.879	0.400	1
1080	.	93	LYS	CB	32.463	0.400	1
1081	.	93	LYS	CG	24.181	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1082	.	93	LYS	CD	28.780	0.400	1
1083	.	93	LYS	CE	41.780	0.400	1
1084	.	93	LYS	N	126.113	0.400	1
1085	.	94	PRO	HA	4.449	0.020	1
1086	.	94	PRO	HB2	1.979	0.020	2
1087	.	94	PRO	HB3	2.344	0.020	2
1088	.	94	PRO	HG2	2.036	0.020	2
1089	.	94	PRO	HG3	2.076	0.020	2
1090	.	94	PRO	HD2	3.701	0.020	2
1091	.	94	PRO	HD3	3.826	0.020	2
1092	.	94	PRO	C	176.998	0.400	1
1093	.	94	PRO	CA	62.894	0.400	1
1094	.	94	PRO	CB	32.003	0.400	1
1095	.	94	PRO	CG	27.140	0.400	1
1096	.	94	PRO	CD	50.547	0.400	1
1097	.	95	GLU	H	8.659	0.020	1
1098	.	95	GLU	HA	4.253	0.020	1
1099	.	95	GLU	HB2	2.074	0.020	2
1100	.	95	GLU	HB3	1.967	0.020	2
1101	.	95	GLU	HG2	2.283	0.020	2
1102	.	95	GLU	HG3	2.337	0.020	2
1103	.	95	GLU	C	176.337	0.400	1
1104	.	95	GLU	CA	57.205	0.400	1
1105	.	95	GLU	CB	30.017	0.400	1
1106	.	95	GLU	CG	36.010	0.400	1
1107	.	95	GLU	N	121.342	0.400	1
1108	.	96	ARG	H	8.136	0.020	1
1109	.	96	ARG	HA	4.476	0.020	1
1110	.	96	ARG	HB2	1.838	0.020	2
1111	.	96	ARG	HB3	1.925	0.020	2
1112	.	96	ARG	HG2	1.693	0.020	1
1113	.	96	ARG	HG3	1.692	0.020	1
1114	.	96	ARG	HD2	3.171	0.020	1
1115	.	96	ARG	HD3	3.172	0.020	1
1116	.	96	ARG	HE	7.328	0.020	1
1117	.	96	ARG	C	175.134	0.400	1
1118	.	96	ARG	CA	55.352	0.400	1
1119	.	96	ARG	CB	31.111	0.400	1
1120	.	96	ARG	CG	26.601	0.400	1
1121	.	96	ARG	CD	43.364	0.400	1
1122	.	96	ARG	N	119.745	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1123	.	96	ARG	NE	84.336	0.400	1
1124	.	97	ASP	H	8.445	0.020	1
1125	.	97	ASP	HA	4.602	0.020	1
1126	.	97	ASP	HB2	2.850	0.020	2
1127	.	97	ASP	HB3	2.767	0.020	2
1128	.	97	ASP	C	174.383	0.400	1
1129	.	97	ASP	CA	54.295	0.400	1
1130	.	97	ASP	CB	41.420	0.400	1
1131	.	97	ASP	N	121.784	0.400	1
1132	.	98	ASP	H	7.992	0.020	1
1133	.	98	ASP	HA	5.093	0.020	1
1134	.	98	ASP	HB2	2.779	0.020	2
1135	.	98	ASP	HB3	2.777	0.020	2
1136	.	98	ASP	C	175.525	0.400	1
1137	.	98	ASP	CA	53.590	0.400	1
1138	.	98	ASP	CB	42.852	0.400	1
1139	.	98	ASP	N	120.991	0.400	1
1140	.	99	THR	H	8.581	0.020	1
1141	.	99	THR	HA	4.241	0.020	1
1142	.	99	THR	HB	3.621	0.020	1
1143	.	99	THR	HG21	0.580	0.020	1
1144	.	99	THR	HG22	0.580	0.020	1
1145	.	99	THR	HG23	0.580	0.020	1
1146	.	99	THR	C	170.326	0.400	1
1147	.	99	THR	CA	61.723	0.400	1
1148	.	99	THR	CB	69.838	0.400	1
1149	.	99	THR	CG2	22.159	0.400	1
1150	.	99	THR	N	123.427	0.400	1
1151	.	100	GLU	H	8.604	0.020	1
1152	.	100	GLU	HA	4.783	0.020	1
1153	.	100	GLU	HB2	1.051	0.020	2
1154	.	100	GLU	HB3	1.753	0.020	2
1155	.	100	GLU	HG2	1.265	0.020	2
1156	.	100	GLU	HG3	1.582	0.020	2
1157	.	100	GLU	C	173.301	0.400	1
1158	.	100	GLU	CA	52.795	0.400	1
1159	.	100	GLU	CB	32.974	0.400	1
1160	.	100	GLU	CG	34.829	0.400	1
1161	.	100	GLU	N	129.229	0.400	1
1162	.	101	PHE	H	8.363	0.020	1
1163	.	101	PHE	HA	5.393	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1164	.	101	PHE	HB2	2.382	0.020	2
1165	.	101	PHE	HB3	1.286	0.020	2
1166	.	101	PHE	HD1	6.455	0.020	1
1167	.	101	PHE	HD2	6.455	0.020	1
1168	.	101	PHE	HE1	6.885	0.020	1
1169	.	101	PHE	HE2	6.885	0.020	1
1170	.	101	PHE	HZ	6.954	0.020	1
1171	.	101	PHE	C	174.804	0.400	1
1172	.	101	PHE	CA	55.882	0.400	1
1173	.	101	PHE	CB	44.143	0.400	1
1174	.	101	PHE	CD1	131.737	0.400	1
1175	.	101	PHE	CD2	131.832	0.400	1
1176	.	101	PHE	CE1	130.308	0.400	1
1177	.	101	PHE	CE2	130.084	0.400	1
1178	.	101	PHE	CZ	129.294	0.400	1
1179	.	101	PHE	N	122.583	0.400	1
1180	.	102	GLN	H	8.945	0.020	1
1181	.	102	GLN	HA	5.440	0.020	1
1182	.	102	GLN	HB2	1.943	0.020	2
1183	.	102	GLN	HB3	1.992	0.020	2
1184	.	102	GLN	HG2	2.486	0.020	2
1185	.	102	GLN	HG3	2.280	0.020	2
1186	.	102	GLN	HE21	7.223	0.020	2
1187	.	102	GLN	HE22	6.672	0.020	2
1188	.	102	GLN	C	174.052	0.400	1
1189	.	102	GLN	CA	54.603	0.400	1
1190	.	102	GLN	CB	32.742	0.400	1
1191	.	102	GLN	CG	32.820	0.400	1
1192	.	102	GLN	N	116.182	0.400	1
1193	.	102	GLN	NE2	108.779	0.400	1
1194	.	103	HIS	H	10.118	0.020	1
1195	.	103	HIS	HA	4.595	0.020	1
1196	.	103	HIS	HB2	2.385	0.020	2
1197	.	103	HIS	HB3	1.517	0.020	2
1198	.	103	HIS	HD2	6.402	0.020	1
1199	.	103	HIS	HE1	7.685	0.020	1
1200	.	103	HIS	CA	55.382	0.400	1
1201	.	103	HIS	CB	34.518	0.400	1
1202	.	103	HIS	CD2	118.369	0.400	1
1203	.	103	HIS	CE1	137.382	0.400	1
1204	.	103	HIS	N	127.562	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1205	.	104	PRO	HA	4.458	0.020	1
1206	.	104	PRO	HB2	2.066	0.020	2
1207	.	104	PRO	HB3	2.398	0.020	2
1208	.	104	PRO	HG2	1.854	0.020	2
1209	.	104	PRO	HG3	1.908	0.020	2
1210	.	104	PRO	HD2	3.419	0.020	2
1211	.	104	PRO	HD3	2.451	0.020	2
1212	.	104	PRO	C	177.509	0.400	1
1213	.	104	PRO	CA	64.890	0.400	1
1214	.	104	PRO	CB	32.625	0.400	1
1215	.	104	PRO	CG	27.140	0.400	1
1216	.	104	PRO	CD	50.913	0.400	1
1217	.	105	CYS	H	11.462	0.020	1
1218	.	105	CYS	HA	4.656	0.020	1
1219	.	105	CYS	HB2	2.533	0.020	2
1220	.	105	CYS	HB3	3.604	0.020	2
1221	.	105	CYS	C	171.919	0.400	1
1222	.	105	CYS	CA	58.328	0.400	1
1223	.	105	CYS	CB	28.250	0.400	1
1224	.	105	CYS	N	117.508	0.400	1
1225	.	106	PHE	H	8.281	0.020	1
1226	.	106	PHE	HA	4.943	0.020	1
1227	.	106	PHE	HB2	2.433	0.020	2
1228	.	106	PHE	HB3	3.853	0.020	2
1229	.	106	PHE	HD1	7.545	0.020	1
1230	.	106	PHE	HD2	7.545	0.020	1
1231	.	106	PHE	C	171.648	0.400	1
1232	.	106	PHE	CA	56.687	0.400	1
1233	.	106	PHE	CB	42.468	0.400	1
1234	.	106	PHE	CD1	132.785	0.400	1
1235	.	106	PHE	CD2	132.796	0.400	1
1236	.	106	PHE	N	126.227	0.400	1
1237	.	107	LEU	H	9.542	0.020	1
1238	.	107	LEU	HA	4.992	0.020	1
1239	.	107	LEU	HB2	1.373	0.020	2
1240	.	107	LEU	HB3	1.404	0.020	2
1241	.	107	LEU	HG	1.455	0.020	1
1242	.	107	LEU	HD11	0.868	0.020	2
1243	.	107	LEU	HD12	0.868	0.020	2
1244	.	107	LEU	HD13	0.868	0.020	2
1245	.	107	LEU	HD21	1.093	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1246	.	107	LEU	HD22	1.093	0.020	2
1247	.	107	LEU	HD23	1.093	0.020	2
1248	.	107	LEU	C	176.970	0.400	1
1249	.	107	LEU	CA	53.406	0.400	1
1250	.	107	LEU	CB	47.013	0.400	1
1251	.	107	LEU	CG	26.770	0.400	1
1252	.	107	LEU	CD1	25.622	0.400	1
1253	.	107	LEU	CD2	24.100	0.400	1
1254	.	107	LEU	N	123.183	0.400	1
1255	.	108	ARG	H	7.220	0.020	1
1256	.	108	ARG	HA	2.642	0.020	1
1257	.	108	ARG	HB2	-0.409	0.020	2
1258	.	108	ARG	HB3	1.131	0.020	2
1259	.	108	ARG	CA	57.415	0.400	1
1260	.	108	ARG	CB	29.890	0.400	1
1261	.	108	ARG	CG	26.089	0.400	1
1262	.	108	ARG	CD	43.664	0.400	1
1263	.	108	ARG	N	125.016	0.400	1
1264	.	110	GLN	HA	5.083	0.020	1
1265	.	110	GLN	HB2	2.184	0.020	2
1266	.	110	GLN	HB3	1.745	0.020	2
1267	.	110	GLN	HG2	2.160	0.020	2
1268	.	110	GLN	HG3	2.203	0.020	2
1269	.	110	GLN	HE21	7.418	0.020	2
1270	.	110	GLN	HE22	6.732	0.020	2
1271	.	110	GLN	C	176.757	0.400	1
1272	.	110	GLN	CA	53.021	0.400	1
1273	.	110	GLN	CB	28.461	0.400	1
1274	.	110	GLN	CG	32.553	0.400	1
1275	.	110	GLN	NE2	112.072	0.400	1
1276	.	111	GLU	H	8.879	0.020	1
1277	.	111	GLU	HA	2.492	0.020	1
1278	.	111	GLU	HG2	1.686	0.020	2
1279	.	111	GLU	HG3	1.085	0.020	2
1280	.	111	GLU	C	177.839	0.400	1
1281	.	111	GLU	CA	58.922	0.400	1
1282	.	111	GLU	CB	28.348	0.400	1
1283	.	111	GLU	CG	35.169	0.400	1
1284	.	111	GLU	N	126.825	0.400	1
1285	.	112	GLN	H	8.920	0.020	1
1286	.	112	GLN	HA	3.956	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1287	.	112	GLN	HB2	2.003	0.020	1
1288	.	112	GLN	HB3	2.004	0.020	1
1289	.	112	GLN	HG2	2.238	0.020	2
1290	.	112	GLN	HG3	2.469	0.020	2
1291	.	112	GLN	HE21	7.576	0.020	2
1292	.	112	GLN	HE22	7.027	0.020	2
1293	.	112	GLN	C	177.449	0.400	1
1294	.	112	GLN	CA	57.918	0.400	1
1295	.	112	GLN	CB	26.466	0.400	1
1296	.	112	GLN	CG	33.041	0.400	1
1297	.	112	GLN	N	118.103	0.400	1
1298	.	112	GLN	NE2	111.575	0.400	1
1299	.	113	LEU	H	7.311	0.020	1
1300	.	113	LEU	HA	4.159	0.020	1
1301	.	113	LEU	HB2	1.809	0.020	2
1302	.	113	LEU	HB3	1.735	0.020	2
1303	.	113	LEU	HG	1.725	0.020	1
1304	.	113	LEU	HD11	0.989	0.020	2
1305	.	113	LEU	HD12	0.989	0.020	2
1306	.	113	LEU	HD13	0.989	0.020	2
1307	.	113	LEU	HD21	0.907	0.020	2
1308	.	113	LEU	HD22	0.907	0.020	2
1309	.	113	LEU	HD23	0.907	0.020	2
1310	.	113	LEU	C	178.110	0.400	1
1311	.	113	LEU	CA	55.809	0.400	1
1312	.	113	LEU	CB	42.088	0.400	1
1313	.	113	LEU	CG	26.882	0.400	1
1314	.	113	LEU	CD1	26.110	0.400	1
1315	.	113	LEU	CD2	22.448	0.400	1
1316	.	113	LEU	N	117.706	0.400	1
1317	.	114	LEU	H	7.565	0.020	1
1318	.	114	LEU	HA	3.962	0.020	1
1319	.	114	LEU	HB2	1.315	0.020	2
1320	.	114	LEU	HB3	1.848	0.020	2
1321	.	114	LEU	HG	1.835	0.020	1
1322	.	114	LEU	HD11	0.596	0.020	2
1323	.	114	LEU	HD12	0.596	0.020	2
1324	.	114	LEU	HD13	0.596	0.020	2
1325	.	114	LEU	HD21	1.078	0.020	2
1326	.	114	LEU	HD22	1.078	0.020	2
1327	.	114	LEU	HD23	1.078	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1328	.	114	LEU	C	179.011	0.400	1
1329	.	114	LEU	CA	57.286	0.400	1
1330	.	114	LEU	CB	42.321	0.400	1
1331	.	114	LEU	CG	26.359	0.400	1
1332	.	114	LEU	CD1	25.277	0.400	1
1333	.	114	LEU	CD2	24.588	0.400	1
1334	.	114	LEU	N	117.066	0.400	1
1335	.	115	GLU	H	7.434	0.020	1
1336	.	115	GLU	HA	4.002	0.020	1
1337	.	115	GLU	HB2	2.022	0.020	1
1338	.	115	GLU	HB3	2.022	0.020	1
1339	.	115	GLU	HG2	2.234	0.020	2
1340	.	115	GLU	HG3	2.321	0.020	2
1341	.	115	GLU	C	175.705	0.400	1
1342	.	115	GLU	CA	57.884	0.400	1
1343	.	115	GLU	CB	29.296	0.400	1
1344	.	115	GLU	CG	35.347	0.400	1
1345	.	115	GLU	N	114.502	0.400	1
1346	.	116	ASN	H	7.891	0.020	1
1347	.	116	ASN	HA	4.739	0.020	1
1348	.	116	ASN	HB2	3.040	0.020	2
1349	.	116	ASN	HB3	3.169	0.020	2
1350	.	116	ASN	HD21	7.317	0.020	2
1351	.	116	ASN	HD22	7.032	0.020	2
1352	.	116	ASN	C	175.160	0.400	1
1353	.	116	ASN	CA	53.271	0.400	1
1354	.	116	ASN	CB	39.858	0.400	1
1355	.	116	ASN	N	115.327	0.400	1
1356	.	116	ASN	ND2	112.167	0.400	1
1357	.	117	ILE	H	7.453	0.020	1
1358	.	117	ILE	HA	3.857	0.020	1
1359	.	117	ILE	HB	1.922	0.020	1
1360	.	117	ILE	HG12	1.588	0.020	2
1361	.	117	ILE	HG13	0.097	0.020	2
1362	.	117	ILE	HG21	0.830	0.020	1
1363	.	117	ILE	HG22	0.830	0.020	1
1364	.	117	ILE	HG23	0.830	0.020	1
1365	.	117	ILE	HD11	0.608	0.020	1
1366	.	117	ILE	HD12	0.608	0.020	1
1367	.	117	ILE	HD13	0.608	0.020	1
1368	.	117	ILE	C	174.323	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1369	.	117	ILE	CA	63.608	0.400	1
1370	.	117	ILE	CB	36.179	0.400	1
1371	.	117	ILE	CG1	28.333	0.400	1
1372	.	117	ILE	CG2	17.871	0.400	1
1373	.	117	ILE	CD1	13.995	0.400	1
1374	.	117	ILE	N	121.603	0.400	1
1375	.	118	LYS	H	8.434	0.020	1
1376	.	118	LYS	HA	4.776	0.020	1
1377	.	118	LYS	HB2	1.778	0.020	2
1378	.	118	LYS	HB3	1.935	0.020	2
1379	.	118	LYS	HG2	1.513	0.020	2
1380	.	118	LYS	HG3	1.457	0.020	2
1381	.	118	LYS	HD2	1.709	0.020	1
1382	.	118	LYS	HD3	1.709	0.020	1
1383	.	118	LYS	HE2	3.051	0.020	2
1384	.	118	LYS	HE3	3.053	0.020	2
1385	.	118	LYS	C	175.826	0.400	1
1386	.	118	LYS	CA	53.896	0.400	1
1387	.	118	LYS	CB	34.480	0.400	1
1388	.	118	LYS	CG	24.231	0.400	1
1389	.	118	LYS	CD	28.416	0.400	1
1390	.	118	LYS	CE	42.254	0.400	1
1391	.	118	LYS	N	126.655	0.400	1
1392	.	119	ARG	H	8.576	0.020	1
1393	.	119	ARG	HA	4.208	0.020	1
1394	.	119	ARG	HB2	1.673	0.020	2
1395	.	119	ARG	HB3	1.620	0.020	2
1396	.	119	ARG	HG2	1.401	0.020	2
1397	.	119	ARG	HG3	1.314	0.020	2
1398	.	119	ARG	HD2	3.051	0.020	1
1399	.	119	ARG	HD3	3.051	0.020	1
1400	.	119	ARG	C	176.276	0.400	1
1401	.	119	ARG	CA	56.036	0.400	1
1402	.	119	ARG	CB	30.797	0.400	1
1403	.	119	ARG	CG	27.310	0.400	1
1404	.	119	ARG	CD	43.259	0.400	1
1405	.	119	ARG	N	121.431	0.400	1
1406	.	120	LYS	H	8.526	0.020	1
1407	.	120	LYS	HA	4.334	0.020	1
1408	.	120	LYS	HB2	1.811	0.020	2
1409	.	120	LYS	HB3	1.759	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1410	.	120	LYS	HG2	1.490	0.020	2
1411	.	120	LYS	HG3	1.412	0.020	2
1412	.	120	LYS	HD2	1.709	0.020	1
1413	.	120	LYS	HD3	1.709	0.020	1
1414	.	120	LYS	HE2	3.008	0.020	2
1415	.	120	LYS	HE3	3.013	0.020	2
1416	.	120	LYS	C	176.006	0.400	1
1417	.	120	LYS	CA	56.384	0.400	1
1418	.	120	LYS	CB	33.044	0.400	1
1419	.	120	LYS	CG	24.588	0.400	1
1420	.	120	LYS	CD	28.780	0.400	1
1421	.	120	LYS	CE	41.898	0.400	1
1422	.	120	LYS	N	125.409	0.400	1
1423	.	121	VAL	H	8.281	0.020	1
1424	.	121	VAL	HA	4.180	0.020	1
1425	.	121	VAL	HB	2.085	0.020	1
1426	.	121	VAL	HG11	0.941	0.020	1
1427	.	121	VAL	HG12	0.941	0.020	1
1428	.	121	VAL	HG13	0.941	0.020	1
1429	.	121	VAL	HG21	0.941	0.020	1
1430	.	121	VAL	HG22	0.941	0.020	1
1431	.	121	VAL	HG23	0.941	0.020	1
1432	.	121	VAL	C	176.096	0.400	1
1433	.	121	VAL	CA	62.114	0.400	1
1434	.	121	VAL	CB	32.717	0.400	1
1435	.	121	VAL	CG1	20.367	0.400	1
1436	.	121	VAL	CG2	20.427	0.400	1
1437	.	121	VAL	N	122.068	0.400	1
1438	.	122	THR	H	8.228	0.020	1
1439	.	122	THR	HA	4.403	0.020	1
1440	.	122	THR	HB	4.224	0.020	1
1441	.	122	THR	HG21	1.185	0.020	1
1442	.	122	THR	HG22	1.185	0.020	1
1443	.	122	THR	HG23	1.185	0.020	1
1444	.	122	THR	C	174.052	0.400	1
1445	.	122	THR	CA	61.625	0.400	1
1446	.	122	THR	CB	69.922	0.400	1
1447	.	122	THR	CG2	21.440	0.400	1
1448	.	122	THR	N	117.824	0.400	1
1449	.	123	SER	H	8.310	0.020	1
1450	.	123	SER	HA	4.510	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1451	.	123	SER	HB2	3.875	0.020	1
1452	.	123	SER	HB3	3.875	0.020	1
1453	.	123	SER	C	174.052	0.400	1
1454	.	123	SER	CA	57.981	0.400	1
1455	.	123	SER	CB	63.841	0.400	1
1456	.	123	SER	N	118.198	0.400	1
1457	.	124	VAL	H	8.206	0.020	1
1458	.	124	VAL	HA	4.225	0.020	1
1459	.	124	VAL	HB	2.131	0.020	1
1460	.	124	VAL	HG11	0.930	0.020	1
1461	.	124	VAL	HG12	0.930	0.020	1
1462	.	124	VAL	HG13	0.930	0.020	1
1463	.	124	VAL	HG21	0.930	0.020	1
1464	.	124	VAL	HG22	0.930	0.020	1
1465	.	124	VAL	HG23	0.930	0.020	1
1466	.	124	VAL	C	175.134	0.400	1
1467	.	124	VAL	CA	62.240	0.400	1
1468	.	124	VAL	CB	32.672	0.400	1
1469	.	124	VAL	CG1	21.380	0.400	1
1470	.	124	VAL	CG2	21.310	0.400	1
1471	.	124	VAL	N	121.388	0.400	1
1472	.	125	SER	H	7.957	0.020	1
1473	.	125	SER	HA	4.260	0.020	1
1474	.	125	SER	HB2	3.816	0.020	2
1475	.	125	SER	HB3	3.819	0.020	2
1476	.	125	SER	CA	59.978	0.400	1
1477	.	125	SER	CB	64.882	0.400	1
1478	.	125	SER	N	124.616	0.400	1

### 7.1.2 Chemical shift referencing ⓘ

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

### 7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1221. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/455 (0%)	0/181 (0%)	0/186 (0%)	0/88 (0%)
Sidechain	0/613 (0%)	0/363 (0%)	0/218 (0%)	0/32 (0%)
Aromatic	0/153 (0%)	0/81 (0%)	0/62 (0%)	0/10 (0%)
Overall	0/1221 (0%)	0/625 (0%)	0/466 (0%)	0/130 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1599. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/611 (0%)	0/243 (0%)	0/250 (0%)	0/118 (0%)
Sidechain	0/779 (0%)	0/463 (0%)	0/280 (0%)	0/36 (0%)
Aromatic	0/209 (0%)	0/109 (0%)	0/76 (0%)	0/24 (0%)
Overall	0/1599 (0%)	0/815 (0%)	0/606 (0%)	0/178 (0%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_1). RCI is only applicable to proteins.