



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 6, 2016 – 04:22 PM EST

PDB ID : 2N9X  
Title : LC3 FUNDC1 complex structure  
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Deposited on : 2015-12-14

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

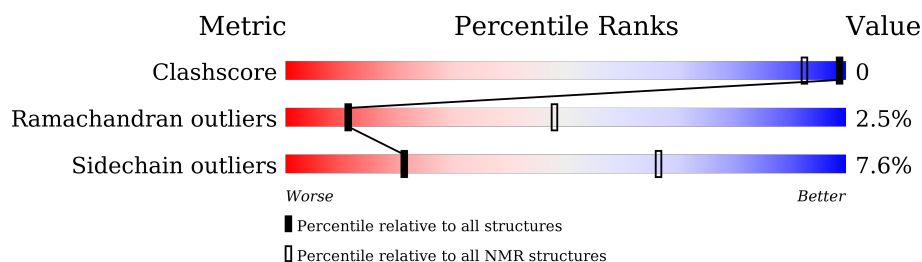
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 3%.

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	120	 90% 7% .
2	B	17	 53% 18% 29%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:117, B:12-B:23 (128)	0.61	11

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 2 single-model clusters were found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 2271 atoms, of which 1130 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Microtubule-associated proteins 1A/1B light chain 3B.

Mol	Chain	Residues	Atoms						Trace
1	A	120	Total	C	H	N	O	S	0
			2010	634	1015	173	184	4	

- Molecule 2 is a protein called FUN14 domain-containing protein 1.

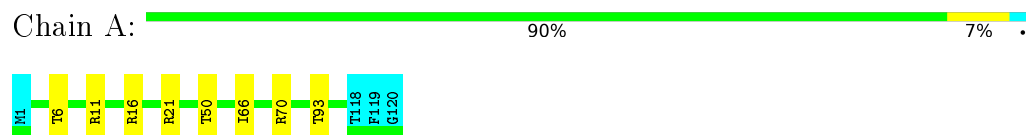
Mol	Chain	Residues	Atoms					Trace
2	B	17	Total	C	H	N	O	0
			261	89	115	17	40	

## 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: Microtubule-associated proteins 1A/1B light chain 3B



- Molecule 2: FUN14 domain-containing protein 1

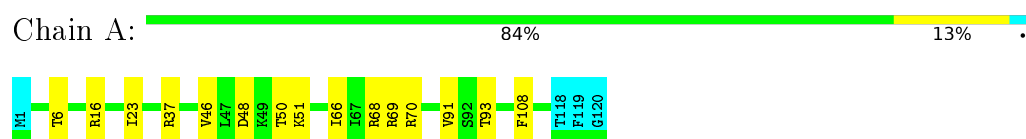


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

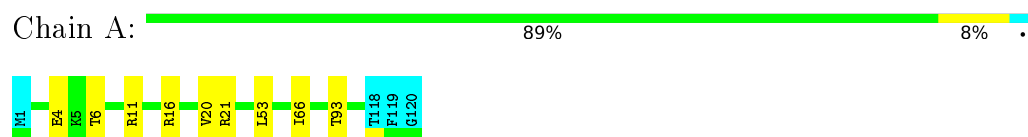


- Molecule 2: FUN14 domain-containing protein 1



### 4.2.2 Score per residue for model 2

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

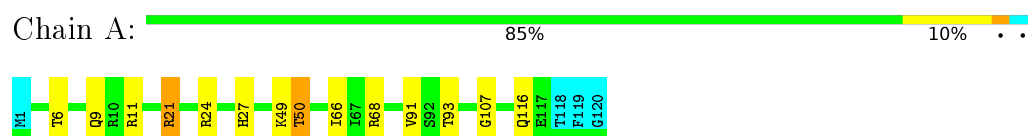


- Molecule 2: FUN14 domain-containing protein 1

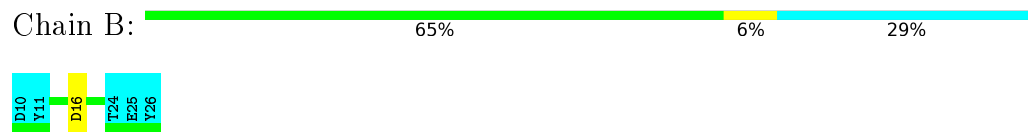


### 4.2.3 Score per residue for model 3

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

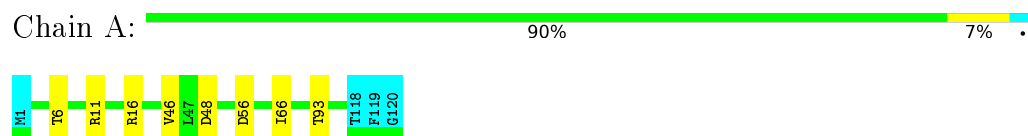


- Molecule 2: FUN14 domain-containing protein 1

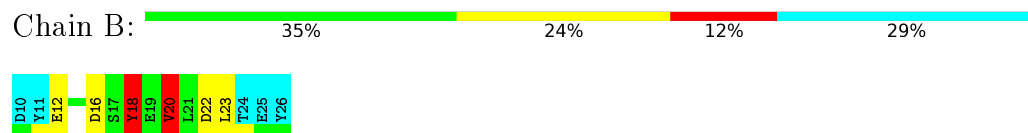


### 4.2.4 Score per residue for model 4

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B



- Molecule 2: FUN14 domain-containing protein 1



### 4.2.5 Score per residue for model 5

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

Chain A:  88% 9%




- Molecule 2: FUN14 domain-containing protein 1

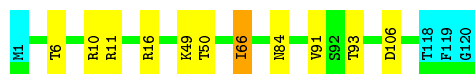
Chain B:  41% 29% 29%



### 4.2.6 Score per residue for model 6

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

Chain A:  88% 8%




- Molecule 2: FUN14 domain-containing protein 1

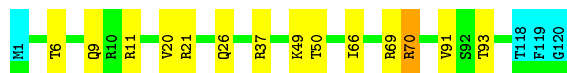
Chain B:  47% 12% 12% 29%



### 4.2.7 Score per residue for model 7

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

Chain A:  85% 11%



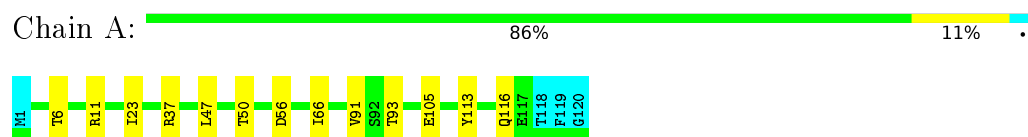
- Molecule 2: FUN14 domain-containing protein 1

Chain B:  41% 29% 29%

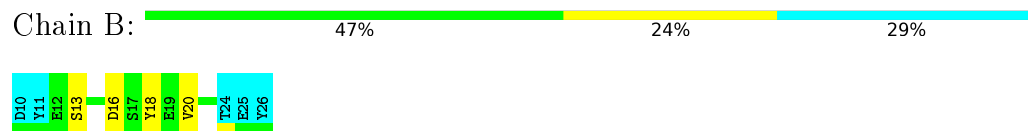


### 4.2.8 Score per residue for model 8

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

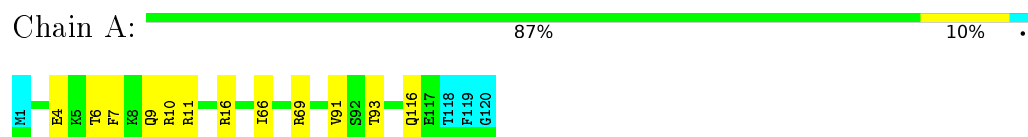


- Molecule 2: FUN14 domain-containing protein 1

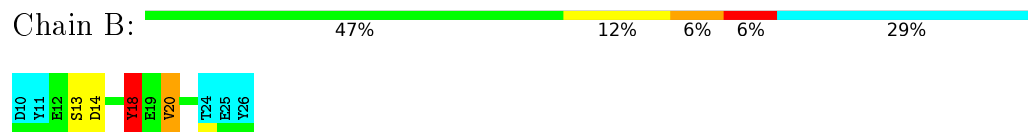


### 4.2.9 Score per residue for model 9

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

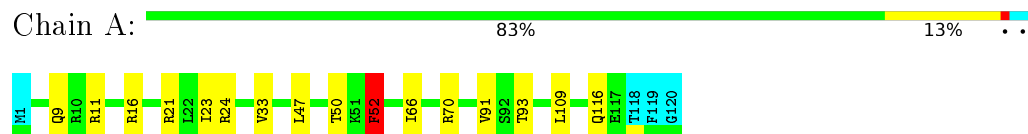


- Molecule 2: FUN14 domain-containing protein 1



### 4.2.10 Score per residue for model 10

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B



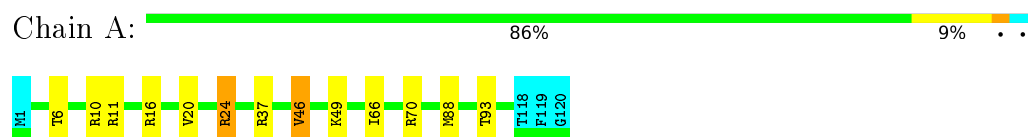
- Molecule 2: FUN14 domain-containing protein 1



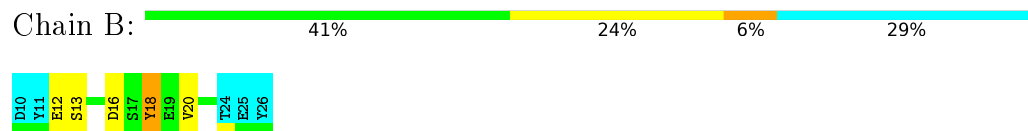


#### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

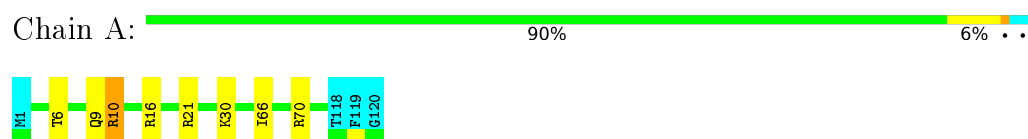


- Molecule 2: FUN14 domain-containing protein 1



#### 4.2.12 Score per residue for model 12

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

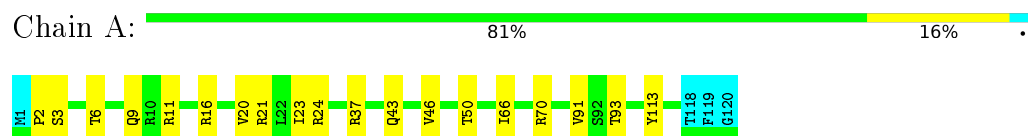


- Molecule 2: FUN14 domain-containing protein 1

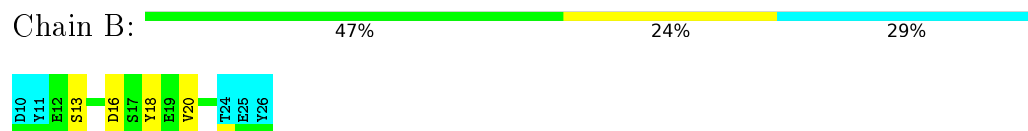


#### 4.2.13 Score per residue for model 13

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

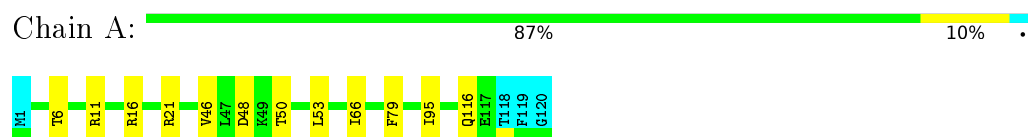


- Molecule 2: FUN14 domain-containing protein 1

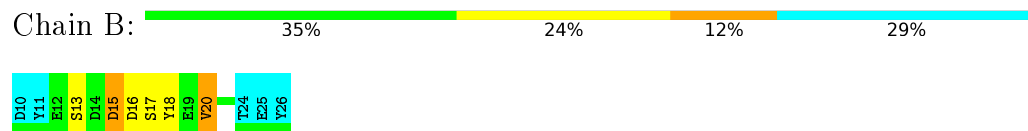


#### 4.2.14 Score per residue for model 14

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

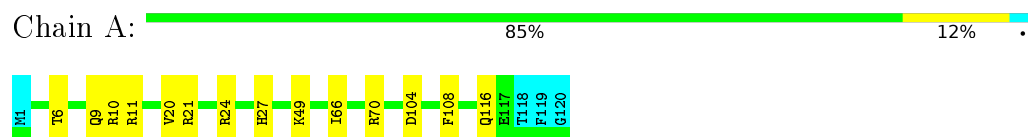


- Molecule 2: FUN14 domain-containing protein 1



#### 4.2.15 Score per residue for model 15

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

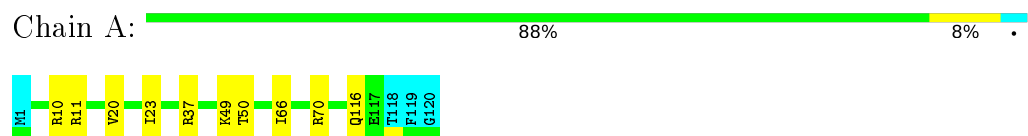


- Molecule 2: FUN14 domain-containing protein 1

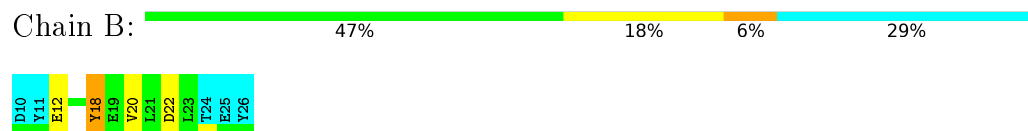


#### 4.2.16 Score per residue for model 16

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

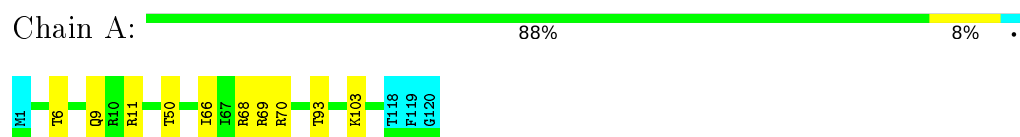


- Molecule 2: FUN14 domain-containing protein 1



#### 4.2.17 Score per residue for model 17

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

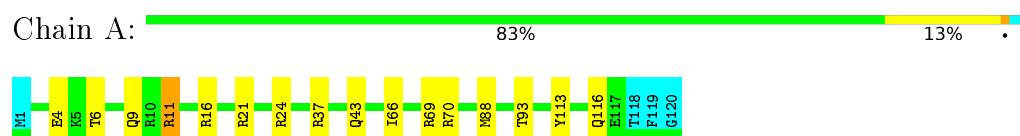


- Molecule 2: FUN14 domain-containing protein 1



#### 4.2.18 Score per residue for model 18

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

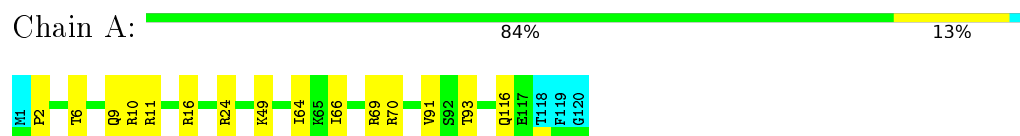


- Molecule 2: FUN14 domain-containing protein 1

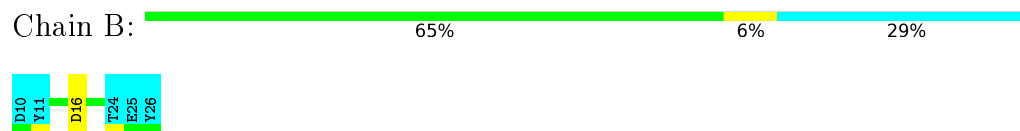


#### 4.2.19 Score per residue for model 19

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B




- Molecule 2: FUN14 domain-containing protein 1



#### 4.2.20 Score per residue for model 20

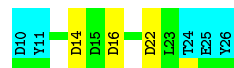
- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

Chain A:  88% 9% .



- Molecule 2: FUN14 domain-containing protein 1

Chain B:  53% 18% 29%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
AMBER	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)	2n9x_cs.cif
Number of chemical shift lists	1
Total number of shifts	1620
Number of shifts mapped to atoms	92
Number of unparsed shifts	1528
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

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	0.76±0.00	0±0/983 (0.0±0.0%)	1.11±0.03	5±2/1324 (0.3±0.2%)
2	B	0.77±0.02	0±0/98 (0.0±0.0%)	1.37±0.15	1±1/134 (0.6±0.8%)
All	All	0.76	0/21620 (0.0%)	1.14	107/29160 (0.4%)

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	0.1±0.3
2	B	0.0±0.0	0.1±0.3
All	All	0	4

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	18	TYR	CB-CG-CD1	-9.42	115.35	121.00	4	7
1	A	70	ARG	NE-CZ-NH1	8.95	124.77	120.30	11	10
1	A	16	ARG	NE-CZ-NH1	8.93	124.76	120.30	6	9
1	A	11	ARG	NE-CZ-NH1	8.22	124.41	120.30	19	6
1	A	11	ARG	NE-CZ-NH2	8.13	124.37	120.30	5	12
1	A	10	ARG	NE-CZ-NH2	7.98	124.29	120.30	6	3
1	A	24	ARG	NE-CZ-NH1	7.79	124.19	120.30	13	4
2	B	18	TYR	CB-CG-CD2	-7.78	116.33	121.00	11	7
1	A	21	ARG	NE-CZ-NH1	6.75	123.68	120.30	3	6
1	A	16	ARG	NE-CZ-NH2	6.71	123.66	120.30	11	5
1	A	21	ARG	NE-CZ-NH2	6.57	123.58	120.30	10	7
1	A	69	ARG	NE-CZ-NH1	6.49	123.55	120.30	17	6
1	A	37	ARG	NE-CZ-NH1	6.47	123.54	120.30	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	ARG	NE-CZ-NH2	6.13	123.36	120.30	5	2
1	A	37	ARG	NE-CZ-NH2	5.68	123.14	120.30	16	1
2	B	15	ASP	CB-CG-OD1	5.63	123.36	118.30	6	1
1	A	10	ARG	NE-CZ-NH1	5.62	123.11	120.30	19	4
2	B	22	ASP	CB-CA-C	5.59	121.58	110.40	4	1
1	A	68	ARG	NE-CZ-NH1	5.59	123.09	120.30	1	3
1	A	52	PHE	CB-CG-CD2	5.41	124.59	120.80	10	1
1	A	70	ARG	NE-CZ-NH2	5.26	122.93	120.30	16	2
1	A	24	ARG	NH1-CZ-NH2	-5.26	113.62	119.40	13	1
1	A	52	PHE	CB-CG-CD1	-5.18	117.17	120.80	10	1
1	A	70	ARG	NH1-CZ-NH2	-5.16	113.72	119.40	13	1
1	A	37	ARG	CD-NE-CZ	5.16	130.83	123.60	13	1
1	A	16	ARG	NH1-CZ-NH2	-5.07	113.82	119.40	6	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)
2	B	18	TYR	Sidechain	2
1	A	68	ARG	Sidechain	1
1	A	24	ARG	Sidechain	1

## 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	964	985	982	0±1
2	B	97	78	78	0±0
All	All	21220	21260	21200	6

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
1:A:53:LEU:H	2:B:20:VAL:HG11	0.59	1.57	2	1
1:A:66:ILE:HD12	2:B:21:LEU:CD2	0.46	2.40	6	1
2:B:18:TYR:CG	2:B:20:VAL:HG22	0.46	2.46	9	2
1:A:33:VAL:HG23	1:A:52:PHE:CD2	0.43	2.49	10	1
1:A:33:VAL:HG23	1:A:52:PHE:CG	0.41	2.50	10	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	116/120 (97%)	109±2 (94±2%)	6±2 (5±2%)	1±1 (1±1%)	24	71
2	B	12/17 (71%)	7±1 (61±9%)	3±1 (22±11%)	2±1 (17±9%)	0	3
All	All	2560/2740 (93%)	2323 (91%)	172 (7%)	65 (3%)	11	48

All 20 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	16	ASP	12
2	B	13	SER	7
2	B	20	VAL	7
2	B	14	ASP	7
1	A	46	VAL	6
1	A	4	GLU	3
2	B	22	ASP	3
1	A	48	ASP	3
2	B	12	GLU	2
1	A	2	PRO	2
2	B	17	SER	2
1	A	47	LEU	2
1	A	108	PHE	2
1	A	3	SER	1
1	A	42	LYS	1
1	A	105	GLU	1
1	A	107	GLY	1

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Mol	Chain	Res	Type	Models (Total)
2	B	15	ASP	1
1	A	49	LYS	1
1	A	50	THR	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	110/113 (97%)	102±2 (93±2%)	8±2 (7±2%)	24 69
2	B	12/17 (71%)	10±1 (86±8%)	2±1 (14±8%)	8 49
All	All	2440/2600 (94%)	2255 (92%)	185 (8%)	21 66

All 47 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	66	ILE	20
1	A	6	THR	17
1	A	93	THR	14
2	B	20	VAL	12
2	B	18	TYR	11
1	A	116	GLN	10
1	A	50	THR	10
1	A	91	VAL	10
1	A	9	GLN	10
1	A	49	LYS	8
1	A	20	VAL	6
1	A	23	ILE	6
2	B	23	LEU	4
1	A	113	TYR	3
1	A	56	ASP	2
1	A	21	ARG	2
1	A	33	VAL	2
1	A	27	HIS	2
1	A	37	ARG	2
1	A	24	ARG	2
1	A	43	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	11	ARG	2
1	A	10	ARG	2
1	A	88	MET	2
1	A	109	LEU	2
1	A	64	ILE	1
1	A	51	LYS	1
2	B	14	ASP	1
1	A	53	LEU	1
1	A	70	ARG	1
1	A	106	ASP	1
2	B	21	LEU	1
1	A	108	PHE	1
1	A	52	PHE	1
2	B	12	GLU	1
1	A	7	PHE	1
1	A	30	LYS	1
2	B	22	ASP	1
1	A	84	ASN	1
1	A	79	PHE	1
1	A	104	ASP	1
2	B	13	SER	1
1	A	26	GLN	1
1	A	46	VAL	1
2	B	15	ASP	1
1	A	103	LYS	1
1	A	95	ILE	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 4% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2n9x\_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	1620
Number of shifts mapped to atoms	92
Number of unparsed shifts	1528
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 1528 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	1	MET	H	8.337	?	1
2	?	1	MET	HA	4.783	?	1
3	?	1	MET	HB2	1.940	?	2
4	?	1	MET	HB3	2.048	?	2
5	?	1	MET	HG2	2.555	?	2
6	?	1	MET	HG3	2.636	?	2
7	?	1	MET	CA	53.141	?	1
8	?	1	MET	CB	32.499	?	1
9	?	1	MET	CG	32.169	?	1
10	?	1	MET	CE	17.188	?	1
11	?	1	MET	N	121.523	?	1
12	?	2	PRO	HA	4.424	?	1
13	?	2	PRO	HB2	1.919	?	2
14	?	2	PRO	HB3	2.299	?	2
15	?	2	PRO	HG2	2.000	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	2	PRO	HG3	2.041	?	2
17	?	2	PRO	HD2	3.689	?	2
18	?	2	PRO	HD3	3.811	?	2
19	?	2	PRO	C	176.917	?	1
20	?	2	PRO	CA	63.418	?	1
21	?	2	PRO	CB	32.160	?	1
22	?	2	PRO	CG	27.458	?	1
23	?	2	PRO	CD	50.650	?	1
24	?	3	SER	H	8.366	?	1
25	?	3	SER	HA	4.389	?	1
26	?	3	SER	HB2	3.828	?	2
27	?	3	SER	HB3	3.888	?	2
28	?	3	SER	C	174.762	?	1
29	?	3	SER	CA	58.472	?	1
30	?	3	SER	CB	63.913	?	1
31	?	3	SER	N	116.273	?	1
32	?	4	GLU	H	8.513	?	1
33	?	4	GLU	HA	4.289	?	1
34	?	4	GLU	HB2	1.936	?	2
35	?	4	GLU	HB3	2.066	?	2
36	?	4	GLU	HG2	2.226	?	2
37	?	4	GLU	HG3	2.272	?	2
38	?	4	GLU	C	176.545	?	1
39	?	4	GLU	CA	56.785	?	1
40	?	4	GLU	CB	30.200	?	1
41	?	4	GLU	CG	36.361	?	1
42	?	4	GLU	N	123.959	?	1
43	?	5	LYS	H	8.198	?	1
44	?	5	LYS	HA	4.508	?	1
45	?	5	LYS	HB2	1.704	?	2
46	?	5	LYS	HB3	1.704	?	2
47	?	5	LYS	HG2	1.317	?	2
48	?	5	LYS	HG3	1.497	?	2
49	?	5	LYS	HD2	1.522	?	2
50	?	5	LYS	HD3	1.555	?	2
51	?	5	LYS	HE2	2.899	?	2
52	?	5	LYS	HE3	2.899	?	2
53	?	5	LYS	C	177.178	?	1
54	?	5	LYS	CA	56.000	?	1
55	?	5	LYS	CB	34.758	?	1
56	?	5	LYS	CG	25.642	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	5	LYS	CD	29.460	?	1
58	?	5	LYS	CE	42.195	?	1
59	?	5	LYS	N	122.165	?	1
60	?	6	THR	H	8.423	?	1
61	?	6	THR	HA	4.426	?	1
62	?	6	THR	HB	5.051	?	1
63	?	6	THR	MG	1.238	?	1
64	?	6	THR	MG	1.238	?	1
65	?	6	THR	MG	1.238	?	1
66	?	6	THR	C	175.570	?	1
67	?	6	THR	CA	61.120	?	1
68	?	6	THR	CB	69.871	?	1
69	?	6	THR	CG2	21.863	?	1
70	?	6	THR	N	115.586	?	1
71	?	7	PHE	H	10.276	?	1
72	?	7	PHE	HA	3.935	?	1
73	?	7	PHE	HB2	2.989	?	2
74	?	7	PHE	HB3	3.073	?	2
75	?	7	PHE	HD1	7.206	?	3
76	?	7	PHE	HD2	7.206	?	3
77	?	7	PHE	HE1	6.863	?	3
78	?	7	PHE	HE2	6.863	?	3
79	?	7	PHE	CA	63.687	?	1
80	?	7	PHE	CB	39.656	?	1
81	?	7	PHE	CD1	131.908	?	3
82	?	7	PHE	CD2	131.908	?	3
83	?	7	PHE	CE1	131.720	?	3
84	?	7	PHE	CE2	131.720	?	3
85	?	7	PHE	N	126.100	?	1
86	?	8	LYS	H	8.707	?	1
87	?	8	LYS	HA	3.800	?	1
88	?	8	LYS	HB2	1.669	?	2
89	?	8	LYS	HB3	1.693	?	2
90	?	8	LYS	HG2	1.304	?	2
91	?	8	LYS	HG3	1.700	?	2
92	?	8	LYS	HD2	1.370	?	2
93	?	8	LYS	HD3	1.470	?	2
94	?	8	LYS	HE2	2.176	?	2
95	?	8	LYS	HE3	2.696	?	2
96	?	8	LYS	CA	59.944	?	1
97	?	8	LYS	CB	33.852	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	8	LYS	CG	26.785	?	1
99	?	8	LYS	CD	30.830	?	1
100	?	8	LYS	CE	41.740	?	1
101	?	8	LYS	N	115.026	?	1
102	?	9	GLN	H	7.343	?	1
103	?	9	GLN	HA	4.178	?	1
104	?	9	GLN	HB2	1.988	?	2
105	?	9	GLN	HB3	2.257	?	2
106	?	9	GLN	HG2	2.331	?	2
107	?	9	GLN	HG3	2.331	?	2
108	?	9	GLN	HE21	7.535	?	2
109	?	9	GLN	HE22	6.907	?	2
110	?	9	GLN	C	173.193	?	1
111	?	9	GLN	CA	56.741	?	1
112	?	9	GLN	CB	30.065	?	1
113	?	9	GLN	CG	34.593	?	1
114	?	9	GLN	CD	180.206	?	1
115	?	9	GLN	N	113.774	?	1
116	?	9	GLN	NE2	112.123	?	1
117	?	10	ARG	H	7.912	?	1
118	?	10	ARG	HA	4.248	?	1
119	?	10	ARG	HB2	1.606	?	2
120	?	10	ARG	HB3	1.844	?	2
121	?	10	ARG	HG2	1.413	?	2
122	?	10	ARG	HG3	1.708	?	2
123	?	10	ARG	HD2	3.139	?	2
124	?	10	ARG	HD3	3.139	?	2
125	?	10	ARG	CA	57.555	?	1
126	?	10	ARG	CB	31.771	?	1
127	?	10	ARG	CG	27.985	?	1
128	?	10	ARG	CD	43.386	?	1
129	?	10	ARG	N	119.156	?	1
130	?	11	ARG	H	7.341	?	1
131	?	11	ARG	HA	4.685	?	1
132	?	11	ARG	HB2	0.910	?	2
133	?	11	ARG	HB3	1.360	?	2
134	?	11	ARG	HG2	1.156	?	2
135	?	11	ARG	HG3	1.264	?	2
136	?	11	ARG	HD2	2.921	?	2
137	?	11	ARG	HD3	2.921	?	2
138	?	11	ARG	HE	7.758	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	11	ARG	CA	53.161	?	1
140	?	11	ARG	CB	32.773	?	1
141	?	11	ARG	CG	26.292	?	1
142	?	11	ARG	CD	43.032	?	1
143	?	11	ARG	N	120.777	?	1
144	?	11	ARG	NE	85.37	?	1
145	?	12	THR	H	8.855	?	1
146	?	12	THR	HA	4.358	?	1
147	?	12	THR	HB	4.776	?	1
148	?	12	THR	MG	1.345	?	1
149	?	12	THR	MG	1.345	?	1
150	?	12	THR	MG	1.345	?	1
151	?	12	THR	C	175.056	?	1
152	?	12	THR	CA	61.795	?	1
153	?	12	THR	CB	71.050	?	1
154	?	12	THR	CG2	22.095	?	1
155	?	12	THR	N	116.696	?	1
156	?	13	PHE	H	9.221	?	1
157	?	13	PHE	HA	4.043	?	1
158	?	13	PHE	HB2	2.998	?	2
159	?	13	PHE	HB3	3.356	?	2
160	?	13	PHE	HD1	7.313	?	3
161	?	13	PHE	HD2	7.313	?	3
162	?	13	PHE	HE1	7.185	?	3
163	?	13	PHE	HE2	7.185	?	3
164	?	13	PHE	C	176.234	?	1
165	?	13	PHE	CA	62.947	?	1
166	?	13	PHE	CB	39.571	?	1
167	?	13	PHE	CD1	132.080	?	3
168	?	13	PHE	CD2	132.080	?	3
169	?	13	PHE	CE1	130.033	?	3
170	?	13	PHE	CE2	130.033	?	3
171	?	13	PHE	N	123.894	?	1
172	?	14	GLU	H	9.002	?	1
173	?	14	GLU	HA	3.812	?	1
174	?	14	GLU	HB2	1.975	?	2
175	?	14	GLU	HB3	2.084	?	2
176	?	14	GLU	HG2	2.406	?	2
177	?	14	GLU	HG3	2.546	?	2
178	?	14	GLU	CA	60.699	?	1
179	?	14	GLU	CB	28.943	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	14	GLU	CG	37.516	?	1
181	?	14	GLU	N	116.516	?	1
182	?	15	GLN	H	7.706	?	1
183	?	15	GLN	HA	4.024	?	1
184	?	15	GLN	HB2	1.861	?	2
185	?	15	GLN	HB3	2.405	?	2
186	?	15	GLN	HG2	2.352	?	2
187	?	15	GLN	HG3	2.501	?	2
188	?	15	GLN	HE21	7.535	?	2
189	?	15	GLN	HE22	6.824	?	2
190	?	15	GLN	C	175.263	?	1
191	?	15	GLN	CA	58.800	?	1
192	?	15	GLN	CB	29.300	?	1
193	?	15	GLN	CG	34.900	?	1
194	?	15	GLN	N	119.291	?	1
195	?	15	GLN	NE2	112.277	?	1
196	?	16	ARG	H	8.567	?	1
197	?	16	ARG	HA	4.235	?	1
198	?	16	ARG	HB2	1.756	?	2
199	?	16	ARG	HB3	2.308	?	2
200	?	16	ARG	HG2	1.644	?	2
201	?	16	ARG	HG3	1.644	?	2
202	?	16	ARG	HD2	3.061	?	2
203	?	16	ARG	HD3	3.295	?	2
204	?	16	ARG	HE	7.285	?	1
205	?	16	ARG	CA	61.660	?	1
206	?	16	ARG	CB	30.877	?	1
207	?	16	ARG	CG	27.271	?	1
208	?	16	ARG	CD	42.454	?	1
209	?	16	ARG	N	122.883	?	1
210	?	16	ARG	NE	84.15	?	1
211	?	17	VAL	H	8.430	?	1
212	?	17	VAL	HA	3.865	?	1
213	?	17	VAL	HB	1.715	?	1
214	?	17	VAL	MG2	0.500	?	2
215	?	17	VAL	MG2	0.500	?	2
216	?	17	VAL	MG2	0.500	?	2
217	?	17	VAL	C	174.213	?	1
218	?	17	VAL	CA	65.550	?	1
219	?	17	VAL	CB	32.171	?	1
220	?	17	VAL	CG1	21.028	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	17	VAL	CG2	23.026	?	2
222	?	17	VAL	N	118.523	?	1
223	?	18	GLU	H	7.423	?	1
224	?	18	GLU	HA	4.212	?	1
225	?	18	GLU	HB2	2.029	?	2
226	?	18	GLU	HB3	2.029	?	2
227	?	18	GLU	HG2	2.342	?	2
228	?	18	GLU	HG3	2.342	?	2
229	?	18	GLU	C	175.758	?	1
230	?	18	GLU	CA	58.488	?	1
231	?	18	GLU	CB	29.360	?	1
232	?	18	GLU	CG	35.316	?	1
233	?	18	GLU	N	120.170	?	1
234	?	19	ASP	H	7.955	?	1
235	?	19	ASP	HA	4.384	?	1
236	?	19	ASP	HB2	3.253	?	2
237	?	19	ASP	HB3	3.253	?	2
238	?	19	ASP	C	177.016	?	1
239	?	19	ASP	CA	56.900	?	1
240	?	19	ASP	CB	41.884	?	1
241	?	19	ASP	N	121.273	?	1
242	?	20	VAL	H	7.818	?	1
243	?	20	VAL	HA	3.232	?	1
244	?	20	VAL	HB	1.781	?	1
245	?	20	VAL	MG2	0.684	?	2
246	?	20	VAL	MG2	0.684	?	2
247	?	20	VAL	MG2	0.684	?	2
248	?	20	VAL	C	173.876	?	1
249	?	20	VAL	CA	66.128	?	1
250	?	20	VAL	CB	31.099	?	1
251	?	20	VAL	CG1	21.705	?	2
252	?	20	VAL	CG2	21.705	?	2
253	?	20	VAL	N	119.523	?	1
254	?	21	ARG	H	8.037	?	1
255	?	21	ARG	HA	3.803	?	1
256	?	21	ARG	HB2	1.862	?	2
257	?	21	ARG	HB3	1.958	?	2
258	?	21	ARG	HG2	1.496	?	2
259	?	21	ARG	HG3	1.689	?	2
260	?	21	ARG	HD2	3.063	?	2
261	?	21	ARG	HD3	3.257	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	21	ARG	HE	7.837	?	1
263	?	21	ARG	CA	59.934	?	1
264	?	21	ARG	CB	30.076	?	1
265	?	21	ARG	CG	27.235	?	1
266	?	21	ARG	CD	43.202	?	1
267	?	21	ARG	N	120.310	?	1
268	?	21	ARG	NE	84.15	?	1
269	?	22	LEU	H	8.050	?	1
270	?	22	LEU	HA	4.094	?	1
271	?	22	LEU	HB2	1.610	?	2
272	?	22	LEU	HB3	1.901	?	2
273	?	22	LEU	HG	1.725	?	1
274	?	22	LEU	MD1	0.953	?	2
275	?	22	LEU	MD1	0.953	?	2
276	?	22	LEU	MD1	0.953	?	2
277	?	22	LEU	MD2	0.890	?	2
278	?	22	LEU	MD2	0.890	?	2
279	?	22	LEU	MD2	0.890	?	2
280	?	22	LEU	C	177.626	?	1
281	?	22	LEU	CA	57.738	?	1
282	?	22	LEU	CB	42.222	?	1
283	?	22	LEU	CG	27.038	?	1
284	?	22	LEU	CD1	25.068	?	2
285	?	22	LEU	CD2	23.729	?	2
286	?	22	LEU	N	118.660	?	1
287	?	23	ILE	H	8.390	?	1
288	?	23	ILE	HA	4.122	?	1
289	?	23	ILE	HB	1.727	?	1
290	?	23	ILE	HG12	0.216	?	2
291	?	23	ILE	HG13	1.094	?	2
292	?	23	ILE	MG	0.897	?	1
293	?	23	ILE	MG	0.897	?	1
294	?	23	ILE	MG	0.897	?	1
295	?	23	ILE	MD	0.734	?	1
296	?	23	ILE	MD	0.734	?	1
297	?	23	ILE	MD	0.734	?	1
298	?	23	ILE	C	176.226	?	1
299	?	23	ILE	CA	61.243	?	1
300	?	23	ILE	CB	38.268	?	1
301	?	23	ILE	CG1	30.232	?	1
302	?	23	ILE	CG2	19.253	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	23	ILE	CD1	14.290	?	1
304	?	23	ILE	N	122.825	?	1
305	?	24	ARG	H	8.540	?	1
306	?	24	ARG	HA	4.017	?	1
307	?	24	ARG	HB2	1.795	?	2
308	?	24	ARG	HB3	1.959	?	2
309	?	24	ARG	HG2	1.647	?	2
310	?	24	ARG	HG3	1.822	?	2
311	?	24	ARG	HD2	3.062	?	2
312	?	24	ARG	HD3	3.293	?	2
313	?	24	ARG	CA	57.684	?	1
314	?	24	ARG	CB	28.817	?	1
315	?	24	ARG	CG	27.228	?	1
316	?	24	ARG	CD	42.556	?	1
317	?	24	ARG	N	122.365	?	1
318	?	25	GLU	H	7.287	?	1
319	?	25	GLU	HA	4.044	?	1
320	?	25	GLU	HB2	2.140	?	2
321	?	25	GLU	HB3	2.140	?	2
322	?	25	GLU	HG2	2.204	?	2
323	?	25	GLU	HG3	2.423	?	2
324	?	25	GLU	CA	58.680	?	1
325	?	25	GLU	CB	29.850	?	1
326	?	25	GLU	CG	36.360	?	1
327	?	25	GLU	N	118.383	?	1
328	?	26	GLN	H	7.423	?	1
329	?	26	GLN	HA	3.948	?	1
330	?	26	GLN	HB2	1.740	?	2
331	?	26	GLN	HB3	1.964	?	2
332	?	26	GLN	HG2	2.134	?	2
333	?	26	GLN	HG3	2.426	?	2
334	?	26	GLN	HE21	7.395	?	2
335	?	26	GLN	HE22	6.785	?	2
336	?	26	GLN	C	176.221	?	1
337	?	26	GLN	CA	57.638	?	1
338	?	26	GLN	CB	30.320	?	1
339	?	26	GLN	CG	33.994	?	1
340	?	26	GLN	N	117.165	?	1
341	?	26	GLN	NE2	111.731	?	1
342	?	27	HIS	H	8.254	?	1
343	?	27	HIS	HA	4.866	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	27	HIS	HB2	2.533	?	2
345	?	27	HIS	HB3	2.910	?	2
346	?	27	HIS	HD2	6.617	?	1
347	?	27	HIS	CA	53.305	?	1
348	?	27	HIS	CB	30.917	?	1
349	?	27	HIS	CD2	119.533	?	1
350	?	27	HIS	N	117.140	?	1
351	?	28	PRO	HA	4.609	?	1
352	?	28	PRO	HB2	2.018	?	2
353	?	28	PRO	HB3	2.447	?	2
354	?	28	PRO	HG2	1.918	?	2
355	?	28	PRO	HG3	1.918	?	2
356	?	28	PRO	HD2	3.252	?	2
357	?	28	PRO	HD3	3.590	?	2
358	?	28	PRO	CA	64.881	?	1
359	?	28	PRO	CB	32.554	?	1
360	?	28	PRO	CG	27.270	?	1
361	?	28	PRO	CD	50.249	?	1
362	?	29	THR	H	7.764	?	1
363	?	29	THR	HA	4.644	?	1
364	?	29	THR	HB	4.726	?	1
365	?	29	THR	MG	1.168	?	1
366	?	29	THR	MG	1.168	?	1
367	?	29	THR	MG	1.168	?	1
368	?	29	THR	C	172.933	?	1
369	?	29	THR	CA	60.600	?	1
370	?	29	THR	CB	68.520	?	1
371	?	29	THR	CG2	21.450	?	1
372	?	29	THR	N	107.339	?	1
373	?	30	LYS	H	7.478	?	1
374	?	30	LYS	HA	4.926	?	1
375	?	30	LYS	HB2	1.210	?	2
376	?	30	LYS	HB3	1.539	?	2
377	?	30	LYS	HG2	1.122	?	2
378	?	30	LYS	HG3	1.462	?	2
379	?	30	LYS	HD2	1.660	?	2
380	?	30	LYS	HD3	1.660	?	2
381	?	30	LYS	HE2	2.901	?	2
382	?	30	LYS	HE3	2.901	?	2
383	?	30	LYS	C	175.010	?	1
384	?	30	LYS	CA	53.740	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	30	LYS	CB	36.445	?	1
386	?	30	LYS	CG	25.560	?	1
387	?	30	LYS	CD	29.536	?	1
388	?	30	LYS	CE	42.021	?	1
389	?	30	LYS	N	118.273	?	1
390	?	31	ILE	H	9.235	?	1
391	?	31	ILE	HA	4.139	?	1
392	?	31	ILE	HB	1.767	?	1
393	?	31	ILE	HG12	0.953	?	2
394	?	31	ILE	HG13	1.318	?	2
395	?	31	ILE	MG	0.404	?	1
396	?	31	ILE	MG	0.404	?	1
397	?	31	ILE	MG	0.404	?	1
398	?	31	ILE	MD	0.326	?	1
399	?	31	ILE	MD	0.326	?	1
400	?	31	ILE	MD	0.326	?	1
401	?	31	ILE	CA	54.669	?	1
402	?	31	ILE	CB	38.427	?	1
403	?	31	ILE	CG1	27.860	?	1
404	?	31	ILE	CG2	16.998	?	1
405	?	31	ILE	CD1	10.032	?	1
406	?	31	ILE	N	123.498	?	1
407	?	32	PRO	HA	5.212	?	1
408	?	32	PRO	HB2	1.761	?	2
409	?	32	PRO	HB3	2.308	?	2
410	?	32	PRO	HG2	1.656	?	2
411	?	32	PRO	HG3	2.600	?	2
412	?	32	PRO	HD2	3.304	?	2
413	?	32	PRO	HD3	3.518	?	2
414	?	32	PRO	C	174.832	?	1
415	?	32	PRO	CA	61.678	?	1
416	?	32	PRO	CB	30.993	?	1
417	?	32	PRO	CG	27.170	?	1
418	?	32	PRO	CD	50.220	?	1
419	?	33	VAL	H	9.289	?	1
420	?	33	VAL	HA	5.234	?	1
421	?	33	VAL	HB	1.886	?	1
422	?	33	VAL	MG2	0.884	?	2
423	?	33	VAL	MG2	0.884	?	2
424	?	33	VAL	MG2	0.884	?	2
425	?	33	VAL	CA	59.611	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	33	VAL	CB	35.711	?	1
427	?	33	VAL	CG1	22.503	?	2
428	?	33	VAL	CG2	22.740	?	2
429	?	33	VAL	N	124.964	?	1
430	?	34	ILE	H	8.594	?	1
431	?	34	ILE	HA	4.742	?	1
432	?	34	ILE	HB	1.407	?	1
433	?	34	ILE	HG12	-0.197	?	2
434	?	34	ILE	HG13	0.311	?	2
435	?	34	ILE	MG	0.503	?	1
436	?	34	ILE	MG	0.503	?	1
437	?	34	ILE	MG	0.503	?	1
438	?	34	ILE	MD	-1.118	?	1
439	?	34	ILE	MD	-1.118	?	1
440	?	34	ILE	MD	-1.118	?	1
441	?	34	ILE	CA	56.330	?	1
442	?	34	ILE	CB	36.629	?	1
443	?	34	ILE	CG1	24.974	?	1
444	?	34	ILE	CG2	16.717	?	1
445	?	34	ILE	CD1	9.011	?	1
446	?	34	ILE	N	127.908	?	1
447	?	35	ILE	H	8.545	?	1
448	?	35	ILE	HA	4.879	?	1
449	?	35	ILE	HB	1.742	?	1
450	?	35	ILE	HG12	0.749	?	2
451	?	35	ILE	HG13	1.588	?	2
452	?	35	ILE	MG	0.774	?	1
453	?	35	ILE	MG	0.774	?	1
454	?	35	ILE	MG	0.774	?	1
455	?	35	ILE	MD	0.133	?	1
456	?	35	ILE	MD	0.133	?	1
457	?	35	ILE	MD	0.133	?	1
458	?	35	ILE	C	176.126	?	1
459	?	35	ILE	CA	60.923	?	1
460	?	35	ILE	CB	38.968	?	1
461	?	35	ILE	CG1	27.809	?	1
462	?	35	ILE	CG2	18.006	?	1
463	?	35	ILE	CD1	12.193	?	1
464	?	35	ILE	N	125.405	?	1
465	?	36	GLU	H	8.363	?	1
466	?	36	GLU	HA	4.789	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	36	GLU	HB2	1.935	?	2
468	?	36	GLU	HB3	2.215	?	2
469	?	36	GLU	HG2	2.302	?	2
470	?	36	GLU	HG3	2.302	?	2
471	?	36	GLU	C	173.645	?	1
472	?	36	GLU	CA	54.282	?	1
473	?	36	GLU	CB	35.401	?	1
474	?	36	GLU	CG	39.320	?	1
475	?	36	GLU	N	124.153	?	1
476	?	37	ARG	H	8.853	?	1
477	?	37	ARG	HA	2.804	?	1
478	?	37	ARG	HB2	1.521	?	2
479	?	37	ARG	HB3	1.816	?	2
480	?	37	ARG	HG2	1.133	?	2
481	?	37	ARG	HG3	1.877	?	2
482	?	37	ARG	HD2	2.840	?	2
483	?	37	ARG	HD3	3.091	?	2
484	?	37	ARG	HE	7.061	?	1
485	?	37	ARG	C	176.456	?	1
486	?	37	ARG	CA	56.120	?	1
487	?	37	ARG	CB	31.500	?	1
488	?	37	ARG	CG	26.483	?	1
489	?	37	ARG	CD	44.211	?	1
490	?	37	ARG	N	123.957	?	1
491	?	37	ARG	NE	84.15	?	1
492	?	38	TYR	H	8.663	?	1
493	?	38	TYR	HA	4.311	?	1
494	?	38	TYR	HB2	2.762	?	2
495	?	38	TYR	HB3	2.980	?	2
496	?	38	TYR	HD1	6.999	?	3
497	?	38	TYR	HD2	6.999	?	3
498	?	38	TYR	HE1	6.628	?	3
499	?	38	TYR	HE2	6.628	?	3
500	?	38	TYR	CA	57.907	?	1
501	?	38	TYR	CB	39.567	?	1
502	?	38	TYR	CD1	133.220	?	3
503	?	38	TYR	CD2	133.220	?	3
504	?	38	TYR	CE1	118.220	?	3
505	?	38	TYR	CE2	118.220	?	3
506	?	38	TYR	N	129.636	?	1
507	?	39	LYS	H	8.389	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	?	39	LYS	HA	3.848	?	1
509	?	39	LYS	HB2	1.524	?	2
510	?	39	LYS	HB3	1.640	?	2
511	?	39	LYS	HG2	1.115	?	2
512	?	39	LYS	HG3	1.170	?	2
513	?	39	LYS	HD2	1.564	?	2
514	?	39	LYS	HD3	1.564	?	2
515	?	39	LYS	HE2	2.900	?	2
516	?	39	LYS	HE3	2.900	?	2
517	?	39	LYS	CA	58.986	?	1
518	?	39	LYS	CB	31.777	?	1
519	?	39	LYS	CG	23.959	?	1
520	?	39	LYS	CD	29.180	?	1
521	?	39	LYS	CE	42.020	?	1
522	?	39	LYS	N	130.772	?	1
523	?	40	GLY	H	5.643	?	1
524	?	40	GLY	HA2	3.350	?	2
525	?	40	GLY	HA3	3.963	?	2
526	?	40	GLY	C	173.407	?	1
527	?	40	GLY	CA	44.796	?	1
528	?	40	GLY	N	106.013	?	1
529	?	41	GLU	H	7.464	?	1
530	?	41	GLU	HA	4.265	?	1
531	?	41	GLU	HB2	2.097	?	2
532	?	41	GLU	HB3	2.471	?	2
533	?	41	GLU	HG2	2.273	?	2
534	?	41	GLU	HG3	2.470	?	2
535	?	41	GLU	C	176.231	?	1
536	?	41	GLU	CA	56.365	?	1
537	?	41	GLU	CB	31.077	?	1
538	?	41	GLU	CG	37.422	?	1
539	?	41	GLU	N	123.519	?	1
540	?	42	LYS	H	8.895	?	1
541	?	42	LYS	HA	4.669	?	1
542	?	42	LYS	HB2	1.712	?	2
543	?	42	LYS	HB3	1.981	?	2
544	?	42	LYS	HG2	1.403	?	2
545	?	42	LYS	HG3	1.510	?	2
546	?	42	LYS	HD2	1.634	?	2
547	?	42	LYS	HD3	1.675	?	2
548	?	42	LYS	HE2	2.974	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	?	42	LYS	HE3	2.974	?	2
550	?	42	LYS	C	177.170	?	1
551	?	42	LYS	CA	55.750	?	1
552	?	42	LYS	CB	34.929	?	1
553	?	42	LYS	CG	24.462	?	1
554	?	42	LYS	CD	28.642	?	1
555	?	42	LYS	CE	42.296	?	1
556	?	42	LYS	N	124.405	?	1
557	?	43	GLN	H	8.459	?	1
558	?	43	GLN	HA	4.541	?	1
559	?	43	GLN	HB2	2.192	?	2
560	?	43	GLN	HB3	2.291	?	2
561	?	43	GLN	HG2	2.393	?	2
562	?	43	GLN	HG3	2.475	?	2
563	?	43	GLN	HE21	7.644	?	2
564	?	43	GLN	HE22	6.855	?	2
565	?	43	GLN	C	177.260	?	1
566	?	43	GLN	CA	57.566	?	1
567	?	43	GLN	CB	30.620	?	1
568	?	43	GLN	CG	34.210	?	1
569	?	43	GLN	CD	180.237	?	1
570	?	43	GLN	N	119.903	?	1
571	?	43	GLN	NE2	112.541	?	1
572	?	44	LEU	H	9.002	?	1
573	?	44	LEU	HA	4.726	?	1
574	?	44	LEU	HB2	1.688	?	2
575	?	44	LEU	HB3	1.796	?	2
576	?	44	LEU	HG	2.038	?	1
577	?	44	LEU	MD1	1.156	?	2
578	?	44	LEU	MD1	1.156	?	2
579	?	44	LEU	MD1	1.156	?	2
580	?	44	LEU	MD2	1.225	?	2
581	?	44	LEU	MD2	1.225	?	2
582	?	44	LEU	MD2	1.225	?	2
583	?	44	LEU	CA	53.165	?	1
584	?	44	LEU	CB	43.444	?	1
585	?	44	LEU	CG	27.500	?	1
586	?	44	LEU	CD1	28.382	?	2
587	?	44	LEU	CD2	24.527	?	2
588	?	44	LEU	N	121.272	?	1
589	?	45	PRO	HA	4.722	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	?	45	PRO	HB2	2.028	?	2
591	?	45	PRO	HB3	2.435	?	2
592	?	45	PRO	HG2	2.066	?	2
593	?	45	PRO	HG3	2.191	?	2
594	?	45	PRO	HD2	3.434	?	2
595	?	45	PRO	HD3	4.016	?	2
596	?	45	PRO	CA	62.169	?	1
597	?	45	PRO	CB	32.722	?	1
598	?	45	PRO	CG	27.197	?	1
599	?	45	PRO	CD	50.436	?	1
600	?	46	VAL	H	8.349	?	1
601	?	46	VAL	HA	4.009	?	1
602	?	46	VAL	HB	2.095	?	1
603	?	46	VAL	MG2	0.977	?	2
604	?	46	VAL	MG2	0.977	?	2
605	?	46	VAL	MG2	0.977	?	2
606	?	46	VAL	C	173.416	?	1
607	?	46	VAL	CA	62.413	?	1
608	?	46	VAL	CB	33.087	?	1
609	?	46	VAL	CG1	20.480	?	2
610	?	46	VAL	CG2	21.274	?	2
611	?	46	VAL	N	118.403	?	1
612	?	47	LEU	H	8.064	?	1
613	?	47	LEU	HA	4.452	?	1
614	?	47	LEU	HB2	1.984	?	2
615	?	47	LEU	HB3	2.057	?	2
616	?	47	LEU	HG	2.043	?	1
617	?	47	LEU	MD1	0.892	?	2
618	?	47	LEU	MD1	0.892	?	2
619	?	47	LEU	MD1	0.892	?	2
620	?	47	LEU	MD2	0.892	?	2
621	?	47	LEU	MD2	0.892	?	2
622	?	47	LEU	MD2	0.892	?	2
623	?	47	LEU	CA	54.758	?	1
624	?	47	LEU	CB	44.076	?	1
625	?	47	LEU	CG	27.063	?	1
626	?	47	LEU	CD1	25.167	?	2
627	?	47	LEU	CD2	25.167	?	2
628	?	47	LEU	N	128.653	?	1
629	?	48	ASP	H	8.649	?	1
630	?	48	ASP	HA	4.347	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	?	48	ASP	HB2	2.737	?	2
632	?	48	ASP	HB3	2.802	?	2
633	?	48	ASP	CA	55.600	?	1
634	?	48	ASP	CB	40.407	?	1
635	?	48	ASP	N	121.042	?	1
636	?	49	LYS	H	7.287	?	1
637	?	49	LYS	HA	4.541	?	1
638	?	49	LYS	HB2	1.349	?	2
639	?	49	LYS	HB3	1.442	?	2
640	?	49	LYS	HG2	1.224	?	2
641	?	49	LYS	HG3	1.224	?	2
642	?	49	LYS	HD2	1.478	?	2
643	?	49	LYS	HD3	1.645	?	2
644	?	49	LYS	HE2	2.831	?	2
645	?	49	LYS	HE3	2.853	?	2
646	?	49	LYS	C	179.744	?	1
647	?	49	LYS	CA	54.099	?	1
648	?	49	LYS	CB	35.378	?	1
649	?	49	LYS	CG	24.456	?	1
650	?	49	LYS	CD	28.177	?	1
651	?	49	LYS	CE	42.277	?	1
652	?	49	LYS	N	118.877	?	1
653	?	50	THR	H	8.064	?	1
654	?	50	THR	HA	4.628	?	1
655	?	50	THR	HB	3.772	?	1
656	?	50	THR	MG	1.140	?	1
657	?	50	THR	MG	1.140	?	1
658	?	50	THR	MG	1.140	?	1
659	?	50	THR	CA	63.920	?	1
660	?	50	THR	CB	71.365	?	1
661	?	50	THR	CG2	22.902	?	1
662	?	50	THR	N	114.691	?	1
663	?	51	LYS	H	7.192	?	1
664	?	51	LYS	HA	4.570	?	1
665	?	51	LYS	HB2	1.029	?	2
666	?	51	LYS	HB3	1.143	?	2
667	?	51	LYS	HG2	0.448	?	2
668	?	51	LYS	HG3	0.927	?	2
669	?	51	LYS	HD2	1.182	?	2
670	?	51	LYS	HD3	1.361	?	2
671	?	51	LYS	HE2	1.886	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	?	51	LYS	HE3	1.970	?	2
673	?	51	LYS	CA	54.997	?	1
674	?	51	LYS	CB	32.700	?	1
675	?	51	LYS	CG	23.780	?	1
676	?	51	LYS	CD	29.601	?	1
677	?	51	LYS	CE	40.951	?	1
678	?	51	LYS	N	120.273	?	1
679	?	52	PHE	H	9.466	?	1
680	?	52	PHE	HA	5.503	?	1
681	?	52	PHE	HB2	2.656	?	2
682	?	52	PHE	HB3	2.749	?	2
683	?	52	PHE	HD1	7.024	?	3
684	?	52	PHE	HD2	7.024	?	3
685	?	52	PHE	HE1	6.918	?	3
686	?	52	PHE	HE2	6.918	?	3
687	?	52	PHE	HZ	7.203	?	1
688	?	52	PHE	CA	56.104	?	1
689	?	52	PHE	CB	43.188	?	1
690	?	52	PHE	CD1	132.470	?	3
691	?	52	PHE	CD2	132.470	?	3
692	?	52	PHE	CE1	132.095	?	3
693	?	52	PHE	CE2	132.095	?	3
694	?	52	PHE	CZ	131.345	?	1
695	?	52	PHE	N	121.816	?	1
696	?	53	LEU	H	8.608	?	1
697	?	53	LEU	HA	5.135	?	1
698	?	53	LEU	HB2	0.868	?	2
699	?	53	LEU	HB3	1.345	?	2
700	?	53	LEU	HG	1.154	?	1
701	?	53	LEU	MD1	-0.123	?	2
702	?	53	LEU	MD1	-0.123	?	2
703	?	53	LEU	MD1	-0.123	?	2
704	?	53	LEU	MD2	0.283	?	2
705	?	53	LEU	MD2	0.283	?	2
706	?	53	LEU	MD2	0.283	?	2
707	?	53	LEU	C	175.042	?	1
708	?	53	LEU	CA	52.916	?	1
709	?	53	LEU	CB	45.242	?	1
710	?	53	LEU	CG	26.278	?	1
711	?	53	LEU	CD1	24.542	?	2
712	?	53	LEU	CD2	22.865	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	?	53	LEU	N	120.846	?	1
714	?	54	VAL	H	8.801	?	1
715	?	54	VAL	HA	4.755	?	1
716	?	54	VAL	HB	1.918	?	1
717	?	54	VAL	MG2	0.845	?	2
718	?	54	VAL	MG2	0.845	?	2
719	?	54	VAL	MG2	0.845	?	2
720	?	54	VAL	CA	58.622	?	1
721	?	54	VAL	CB	35.150	?	1
722	?	54	VAL	CG1	21.430	?	2
723	?	54	VAL	CG2	21.845	?	2
724	?	54	VAL	N	123.773	?	1
725	?	55	PRO	HA	4.435	?	1
726	?	55	PRO	HB2	1.649	?	2
727	?	55	PRO	HB3	2.592	?	2
728	?	55	PRO	HG2	2.125	?	2
729	?	55	PRO	HG3	2.164	?	2
730	?	55	PRO	HD2	3.497	?	2
731	?	55	PRO	HD3	4.070	?	2
732	?	55	PRO	C	176.427	?	1
733	?	55	PRO	CA	64.298	?	1
734	?	55	PRO	CB	32.822	?	1
735	?	55	PRO	CG	28.218	?	1
736	?	55	PRO	CD	51.693	?	1
737	?	56	ASP	H	8.336	?	1
738	?	56	ASP	HA	3.880	?	1
739	?	56	ASP	HB2	2.406	?	2
740	?	56	ASP	HB3	2.747	?	2
741	?	56	ASP	CA	56.742	?	1
742	?	56	ASP	CB	40.481	?	1
743	?	56	ASP	N	121.214	?	1
744	?	57	HIS	H	7.464	?	1
745	?	57	HIS	HA	4.772	?	1
746	?	57	HIS	HB2	3.063	?	2
747	?	57	HIS	HB3	3.390	?	2
748	?	57	HIS	HD2	7.094	?	1
749	?	57	HIS	C	174.806	?	1
750	?	57	HIS	CA	55.688	?	1
751	?	57	HIS	CB	30.450	?	1
752	?	57	HIS	CD2	119.720	?	1
753	?	57	HIS	N	114.277	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	?	58	VAL	H	7.261	?	1
755	?	58	VAL	HA	3.909	?	1
756	?	58	VAL	HB	2.014	?	1
757	?	58	VAL	MG2	0.789	?	2
758	?	58	VAL	MG2	0.789	?	2
759	?	58	VAL	MG2	0.789	?	2
760	?	58	VAL	C	177.148	?	1
761	?	58	VAL	CA	62.900	?	1
762	?	58	VAL	CB	32.320	?	1
763	?	58	VAL	CG1	22.474	?	2
764	?	58	VAL	CG2	21.570	?	2
765	?	58	VAL	N	123.531	?	1
766	?	59	ASN	H	8.819	?	1
767	?	59	ASN	HA	5.174	?	1
768	?	59	ASN	HB2	2.630	?	2
769	?	59	ASN	HB3	2.856	?	2
770	?	59	ASN	HD21	7.470	?	2
771	?	59	ASN	HD22	6.933	?	2
772	?	59	ASN	C	175.176	?	1
773	?	59	ASN	CA	51.374	?	1
774	?	59	ASN	CB	40.038	?	1
775	?	59	ASN	N	124.147	?	1
776	?	59	ASN	ND2	112.449	?	1
777	?	60	MET	H	8.023	?	1
778	?	60	MET	HA	4.425	?	1
779	?	60	MET	HB2	2.054	?	2
780	?	60	MET	HB3	2.273	?	2
781	?	60	MET	HG2	2.775	?	2
782	?	60	MET	HG3	2.797	?	2
783	?	60	MET	CA	57.271	?	1
784	?	60	MET	CB	30.063	?	1
785	?	60	MET	CG	32.309	?	1
786	?	60	MET	CE	16.336	?	1
787	?	60	MET	N	117.583	?	1
788	?	61	SER	H	8.350	?	1
789	?	61	SER	HA	4.138	?	1
790	?	61	SER	HB2	3.894	?	2
791	?	61	SER	HB3	3.894	?	2
792	?	61	SER	C	178.809	?	1
793	?	61	SER	CA	61.553	?	1
794	?	61	SER	CB	62.581	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	?	61	SER	N	115.027	?	1
796	?	62	GLU	H	7.994	?	1
797	?	62	GLU	HA	3.979	?	1
798	?	62	GLU	HB2	1.899	?	2
799	?	62	GLU	HB3	2.350	?	2
800	?	62	GLU	HG2	2.269	?	2
801	?	62	GLU	HG3	2.435	?	2
802	?	62	GLU	C	176.456	?	1
803	?	62	GLU	CA	58.726	?	1
804	?	62	GLU	CB	29.700	?	1
805	?	62	GLU	CG	36.491	?	1
806	?	62	GLU	N	123.657	?	1
807	?	63	LEU	H	8.223	?	1
808	?	63	LEU	HA	3.949	?	1
809	?	63	LEU	HB2	1.242	?	2
810	?	63	LEU	HB3	2.096	?	2
811	?	63	LEU	HG	1.415	?	1
812	?	63	LEU	MD1	0.776	?	2
813	?	63	LEU	MD1	0.776	?	2
814	?	63	LEU	MD1	0.776	?	2
815	?	63	LEU	MD2	0.700	?	2
816	?	63	LEU	MD2	0.700	?	2
817	?	63	LEU	MD2	0.700	?	2
818	?	63	LEU	C	178.113	?	1
819	?	63	LEU	CA	57.860	?	1
820	?	63	LEU	CB	41.526	?	1
821	?	63	LEU	CG	27.066	?	1
822	?	63	LEU	CD1	26.674	?	2
823	?	63	LEU	CD2	23.801	?	2
824	?	63	LEU	N	121.225	?	1
825	?	64	ILE	H	8.301	?	1
826	?	64	ILE	HA	3.375	?	1
827	?	64	ILE	HB	1.956	?	1
828	?	64	ILE	HG12	1.031	?	2
829	?	64	ILE	HG13	1.912	?	2
830	?	64	ILE	MG	0.929	?	1
831	?	64	ILE	MG	0.929	?	1
832	?	64	ILE	MG	0.929	?	1
833	?	64	ILE	MD	0.969	?	1
834	?	64	ILE	MD	0.969	?	1
835	?	64	ILE	MD	0.969	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	?	64	ILE	CA	66.723	?	1
837	?	64	ILE	CB	38.161	?	1
838	?	64	ILE	CG1	31.642	?	1
839	?	64	ILE	CG2	17.340	?	1
840	?	64	ILE	CD1	13.987	?	1
841	?	64	ILE	N	119.273	?	1
842	?	65	LYS	H	7.300	?	1
843	?	65	LYS	HA	3.703	?	1
844	?	65	LYS	HB2	1.894	?	2
845	?	65	LYS	HB3	1.937	?	2
846	?	65	LYS	HG2	1.318	?	2
847	?	65	LYS	HG3	1.608	?	2
848	?	65	LYS	HD2	1.660	?	2
849	?	65	LYS	HD3	1.660	?	2
850	?	65	LYS	HE2	2.898	?	2
851	?	65	LYS	HE3	2.898	?	2
852	?	65	LYS	C	173.869	?	1
853	?	65	LYS	CA	60.451	?	1
854	?	65	LYS	CB	32.300	?	1
855	?	65	LYS	CG	25.511	?	1
856	?	65	LYS	CD	29.615	?	1
857	?	65	LYS	CE	42.000	?	1
858	?	65	LYS	N	119.143	?	1
859	?	66	ILE	H	8.048	?	1
860	?	66	ILE	HA	3.541	?	1
861	?	66	ILE	HB	1.945	?	1
862	?	66	ILE	HG12	0.983	?	2
863	?	66	ILE	HG13	1.787	?	2
864	?	66	ILE	MG	0.805	?	1
865	?	66	ILE	MG	0.805	?	1
866	?	66	ILE	MG	0.805	?	1
867	?	66	ILE	MD	0.681	?	1
868	?	66	ILE	MD	0.681	?	1
869	?	66	ILE	MD	0.681	?	1
870	?	66	ILE	C	176.459	?	1
871	?	66	ILE	CA	65.290	?	1
872	?	66	ILE	CB	38.254	?	1
873	?	66	ILE	CG1	28.908	?	1
874	?	66	ILE	CG2	17.914	?	1
875	?	66	ILE	CD1	13.715	?	1
876	?	66	ILE	N	120.527	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	?	67	ILE	H	8.308	?	1
878	?	67	ILE	HA	3.336	?	1
879	?	67	ILE	HB	1.626	?	1
880	?	67	ILE	HG12	0.994	?	2
881	?	67	ILE	HG13	1.276	?	2
882	?	67	ILE	MG	0.490	?	1
883	?	67	ILE	MG	0.490	?	1
884	?	67	ILE	MG	0.490	?	1
885	?	67	ILE	MD	0.353	?	1
886	?	67	ILE	MD	0.353	?	1
887	?	67	ILE	MD	0.353	?	1
888	?	67	ILE	C	178.102	?	1
889	?	67	ILE	CA	63.952	?	1
890	?	67	ILE	CB	35.891	?	1
891	?	67	ILE	CG1	27.822	?	1
892	?	67	ILE	CG2	18.726	?	1
893	?	67	ILE	CD1	11.388	?	1
894	?	67	ILE	N	121.527	?	1
895	?	68	ARG	H	8.336	?	1
896	?	68	ARG	HA	2.970	?	1
897	?	68	ARG	HB2	1.550	?	2
898	?	68	ARG	HB3	1.550	?	2
899	?	68	ARG	HG2	0.542	?	2
900	?	68	ARG	HG3	1.292	?	2
901	?	68	ARG	HD2	2.765	?	2
902	?	68	ARG	HD3	3.200	?	2
903	?	68	ARG	HE	7.094	?	1
904	?	68	ARG	C	172.723	?	1
905	?	68	ARG	CA	60.704	?	1
906	?	68	ARG	CB	30.320	?	1
907	?	68	ARG	CG	28.906	?	1
908	?	68	ARG	CD	43.382	?	1
909	?	68	ARG	N	119.384	?	1
910	?	68	ARG	NE	82.40	?	1
911	?	69	ARG	H	7.432	?	1
912	?	69	ARG	HA	4.138	?	1
913	?	69	ARG	HB2	1.853	?	2
914	?	69	ARG	HB3	1.931	?	2
915	?	69	ARG	HG2	1.587	?	2
916	?	69	ARG	HG3	1.675	?	2
917	?	69	ARG	HD2	3.137	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	?	69	ARG	HD3	3.137	?	2
919	?	69	ARG	HE	7.245	?	1
920	?	69	ARG	C	172.480	?	1
921	?	69	ARG	CA	58.645	?	1
922	?	69	ARG	CB	29.779	?	1
923	?	69	ARG	CG	27.176	?	1
924	?	69	ARG	CD	43.415	?	1
925	?	69	ARG	N	117.648	?	1
926	?	69	ARG	NE	85.40	?	1
927	?	70	ARG	H	8.212	?	1
928	?	70	ARG	HA	4.074	?	1
929	?	70	ARG	HB2	1.855	?	2
930	?	70	ARG	HB3	1.855	?	2
931	?	70	ARG	HG2	1.586	?	2
932	?	70	ARG	HG3	1.675	?	2
933	?	70	ARG	HD2	3.134	?	2
934	?	70	ARG	HD3	3.188	?	2
935	?	70	ARG	HE	7.245	?	1
936	?	70	ARG	C	178.799	?	1
937	?	70	ARG	CA	58.385	?	1
938	?	70	ARG	CB	30.043	?	1
939	?	70	ARG	CG	27.193	?	1
940	?	70	ARG	CD	43.403	?	1
941	?	70	ARG	N	124.006	?	1
942	?	70	ARG	NE	85.357	?	1
943	?	71	LEU	H	7.750	?	1
944	?	71	LEU	HA	4.085	?	1
945	?	71	LEU	HB2	1.333	?	2
946	?	71	LEU	HB3	1.483	?	2
947	?	71	LEU	HG	1.388	?	1
948	?	71	LEU	MD1	0.270	?	2
949	?	71	LEU	MD1	0.270	?	2
950	?	71	LEU	MD1	0.270	?	2
951	?	71	LEU	MD2	0.641	?	2
952	?	71	LEU	MD2	0.641	?	2
953	?	71	LEU	MD2	0.641	?	2
954	?	71	LEU	CA	55.063	?	1
955	?	71	LEU	CB	43.100	?	1
956	?	71	LEU	CG	26.413	?	1
957	?	71	LEU	CD1	27.358	?	2
958	?	71	LEU	CD2	23.240	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
959	?	71	LEU	N	117.764	?	1
960	?	72	GLN	H	7.751	?	1
961	?	72	GLN	HA	3.839	?	1
962	?	72	GLN	HB2	2.178	?	2
963	?	72	GLN	HB3	2.218	?	2
964	?	72	GLN	HG2	2.233	?	2
965	?	72	GLN	HG3	2.233	?	2
966	?	72	GLN	HE21	7.569	?	2
967	?	72	GLN	HE22	6.812	?	2
968	?	72	GLN	C	175.744	?	1
969	?	72	GLN	CA	56.409	?	1
970	?	72	GLN	CB	25.959	?	1
971	?	72	GLN	CG	34.345	?	1
972	?	72	GLN	CD	181.391	?	1
973	?	72	GLN	N	115.522	?	1
974	?	72	GLN	NE2	113.046	?	1
975	?	73	LEU	H	7.573	?	1
976	?	73	LEU	HA	4.254	?	1
977	?	73	LEU	HB2	1.278	?	2
978	?	73	LEU	HB3	1.328	?	2
979	?	73	LEU	HG	1.595	?	1
980	?	73	LEU	MD1	0.516	?	2
981	?	73	LEU	MD1	0.516	?	2
982	?	73	LEU	MD1	0.516	?	2
983	?	73	LEU	MD2	0.679	?	2
984	?	73	LEU	MD2	0.679	?	2
985	?	73	LEU	MD2	0.679	?	2
986	?	73	LEU	C	178.568	?	1
987	?	73	LEU	CA	54.468	?	1
988	?	73	LEU	CB	42.050	?	1
989	?	73	LEU	CG	26.014	?	1
990	?	73	LEU	CD1	26.342	?	2
991	?	73	LEU	CD2	22.684	?	2
992	?	73	LEU	N	115.900	?	1
993	?	74	ASN	H	8.949	?	1
994	?	74	ASN	HA	4.684	?	1
995	?	74	ASN	HB2	2.812	?	2
996	?	74	ASN	HB3	2.912	?	2
997	?	74	ASN	HD21	7.712	?	2
998	?	74	ASN	HD22	7.037	?	2
999	?	74	ASN	C	174.122	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1000	?	74	ASN	CA	52.724	?	1
1001	?	74	ASN	CB	39.579	?	1
1002	?	74	ASN	CG	176.501	?	1
1003	?	74	ASN	N	122.154	?	1
1004	?	74	ASN	ND2	114.905	?	1
1005	?	75	ALA	H	8.690	?	1
1006	?	75	ALA	HA	3.972	?	1
1007	?	75	ALA	C	178.113	?	1
1008	?	75	ALA	CA	54.900	?	1
1009	?	75	ALA	CB	18.708	?	1
1010	?	75	ALA	N	124.274	?	1
1011	?	76	ASN	H	8.340	?	1
1012	?	76	ASN	HA	4.589	?	1
1013	?	76	ASN	HB2	2.833	?	2
1014	?	76	ASN	HB3	2.833	?	2
1015	?	76	ASN	HD21	7.558	?	2
1016	?	76	ASN	HD22	6.876	?	2
1017	?	76	ASN	C	175.515	?	1
1018	?	76	ASN	CA	53.276	?	1
1019	?	76	ASN	CB	38.343	?	1
1020	?	76	ASN	CG	177.365	?	1
1021	?	76	ASN	N	112.911	?	1
1022	?	76	ASN	ND2	113.151	?	1
1023	?	77	GLN	H	7.546	?	1
1024	?	77	GLN	HA	4.287	?	1
1025	?	77	GLN	HB2	2.001	?	2
1026	?	77	GLN	HB3	2.161	?	2
1027	?	77	GLN	HG2	2.324	?	2
1028	?	77	GLN	HG3	2.397	?	2
1029	?	77	GLN	HE21	8.224	?	2
1030	?	77	GLN	HE22	7.315	?	2
1031	?	77	GLN	C	175.053	?	1
1032	?	77	GLN	CA	55.856	?	1
1033	?	77	GLN	CB	30.320	?	1
1034	?	77	GLN	CG	35.101	?	1
1035	?	77	GLN	CD	180.151	?	1
1036	?	77	GLN	N	121.144	?	1
1037	?	77	GLN	NE2	115.368	?	1
1038	?	78	ALA	H	8.730	?	1
1039	?	78	ALA	HA	4.179	?	1
1040	?	78	ALA	C	176.453	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1041	?	78	ALA	CA	52.852	?	1
1042	?	78	ALA	CB	20.074	?	1
1043	?	78	ALA	N	131.146	?	1
1044	?	79	PHE	H	7.601	?	1
1045	?	79	PHE	HA	4.453	?	1
1046	?	79	PHE	HB2	2.570	?	2
1047	?	79	PHE	HB3	2.753	?	2
1048	?	79	PHE	HD1	6.905	?	3
1049	?	79	PHE	HD2	6.905	?	3
1050	?	79	PHE	HE1	6.763	?	3
1051	?	79	PHE	HE2	6.763	?	3
1052	?	79	PHE	HZ	6.577	?	1
1053	?	79	PHE	C	171.834	?	1
1054	?	79	PHE	CA	59.115	?	1
1055	?	79	PHE	CB	42.246	?	1
1056	?	79	PHE	CD1	131.533	?	3
1057	?	79	PHE	CD2	131.533	?	3
1058	?	79	PHE	CE1	129.845	?	3
1059	?	79	PHE	CE2	129.845	?	3
1060	?	79	PHE	CZ	128.908	?	1
1061	?	79	PHE	N	119.860	?	1
1062	?	80	PHE	H	8.504	?	1
1063	?	80	PHE	HA	4.396	?	1
1064	?	80	PHE	HB2	2.409	?	2
1065	?	80	PHE	HB3	2.777	?	2
1066	?	80	PHE	HD1	6.920	?	3
1067	?	80	PHE	HD2	6.920	?	3
1068	?	80	PHE	HE1	7.203	?	3
1069	?	80	PHE	HE2	7.203	?	3
1070	?	80	PHE	HZ	7.272	?	1
1071	?	80	PHE	C	173.169	?	1
1072	?	80	PHE	CA	56.859	?	1
1073	?	80	PHE	CB	41.946	?	1
1074	?	80	PHE	CD1	132.100	?	3
1075	?	80	PHE	CD2	132.100	?	3
1076	?	80	PHE	CE1	131.345	?	3
1077	?	80	PHE	CE2	131.345	?	3
1078	?	80	PHE	CZ	130.220	?	1
1079	?	80	PHE	N	126.800	?	1
1080	?	81	LEU	H	8.159	?	1
1081	?	81	LEU	HA	4.902	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1082	?	81	LEU	HB2	1.235	?	2
1083	?	81	LEU	HB3	1.682	?	2
1084	?	81	LEU	HG	1.461	?	1
1085	?	81	LEU	MD1	0.846	?	2
1086	?	81	LEU	MD1	0.846	?	2
1087	?	81	LEU	MD1	0.846	?	2
1088	?	81	LEU	MD2	0.891	?	2
1089	?	81	LEU	MD2	0.891	?	2
1090	?	81	LEU	MD2	0.891	?	2
1091	?	81	LEU	CA	53.108	?	1
1092	?	81	LEU	CB	45.781	?	1
1093	?	81	LEU	CG	27.020	?	1
1094	?	81	LEU	CD1	26.021	?	2
1095	?	81	LEU	CD2	24.840	?	2
1096	?	81	LEU	N	122.590	?	1
1097	?	82	LEU	H	9.347	?	1
1098	?	82	LEU	HA	4.807	?	1
1099	?	82	LEU	HB2	0.992	?	2
1100	?	82	LEU	HB3	1.507	?	2
1101	?	82	LEU	HG	1.220	?	1
1102	?	82	LEU	MD1	0.501	?	2
1103	?	82	LEU	MD1	0.501	?	2
1104	?	82	LEU	MD1	0.501	?	2
1105	?	82	LEU	MD2	0.489	?	2
1106	?	82	LEU	MD2	0.489	?	2
1107	?	82	LEU	MD2	0.489	?	2
1108	?	82	LEU	C	174.204	?	1
1109	?	82	LEU	CA	54.200	?	1
1110	?	82	LEU	CB	43.650	?	1
1111	?	82	LEU	CG	27.678	?	1
1112	?	82	LEU	CD1	24.763	?	2
1113	?	82	LEU	CD2	24.455	?	2
1114	?	82	LEU	N	126.414	?	1
1115	?	83	VAL	H	8.676	?	1
1116	?	83	VAL	HA	4.466	?	1
1117	?	83	VAL	HB	2.005	?	1
1118	?	83	VAL	MG2	0.972	?	2
1119	?	83	VAL	MG2	0.972	?	2
1120	?	83	VAL	MG2	0.972	?	2
1121	?	83	VAL	C	175.891	?	1
1122	?	83	VAL	CA	61.339	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1123	?	83	VAL	CB	34.013	?	1
1124	?	83	VAL	CG1	21.791	?	2
1125	?	83	VAL	CG2	21.791	?	2
1126	?	83	VAL	N	123.910	?	1
1127	?	84	ASN	H	9.630	?	1
1128	?	84	ASN	HA	4.384	?	1
1129	?	84	ASN	HB2	2.905	?	2
1130	?	84	ASN	HB3	3.264	?	2
1131	?	84	ASN	HD21	8.541	?	2
1132	?	84	ASN	HD22	7.131	?	2
1133	?	84	ASN	CA	54.494	?	1
1134	?	84	ASN	CB	37.933	?	1
1135	?	84	ASN	N	127.149	?	1
1136	?	84	ASN	ND2	116.358	?	1
1137	?	85	GLY	H	8.670	?	1
1138	?	85	GLY	HA2	3.383	?	2
1139	?	85	GLY	HA3	4.027	?	2
1140	?	85	GLY	C	175.112	?	1
1141	?	85	GLY	CA	45.624	?	1
1142	?	85	GLY	N	101.905	?	1
1143	?	86	HIS	H	7.927	?	1
1144	?	86	HIS	HA	5.039	?	1
1145	?	86	HIS	HB2	3.224	?	2
1146	?	86	HIS	HB3	3.320	?	2
1147	?	86	HIS	HD2	7.245	?	1
1148	?	86	HIS	CA	53.890	?	1
1149	?	86	HIS	CB	30.888	?	1
1150	?	86	HIS	CD2	121.408	?	1
1151	?	86	HIS	N	117.905	?	1
1152	?	87	SER	H	8.927	?	1
1153	?	87	SER	HA	4.397	?	1
1154	?	87	SER	HB2	3.894	?	2
1155	?	87	SER	HB3	3.894	?	2
1156	?	87	SER	C	175.275	?	1
1157	?	87	SER	CA	58.414	?	1
1158	?	87	SER	CB	63.772	?	1
1159	?	87	SER	N	118.646	?	1
1160	?	88	MET	H	9.088	?	1
1161	?	88	MET	HA	4.851	?	1
1162	?	88	MET	HB2	2.011	?	2
1163	?	88	MET	HB3	2.158	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1164	?	88	MET	HG2	2.628	?	2
1165	?	88	MET	HG3	2.628	?	2
1166	?	88	MET	C	178.796	?	1
1167	?	88	MET	CA	54.727	?	1
1168	?	88	MET	CB	33.309	?	1
1169	?	88	MET	CG	32.674	?	1
1170	?	88	MET	CE	18.593	?	1
1171	?	88	MET	N	126.013	?	1
1172	?	89	VAL	H	8.144	?	1
1173	?	89	VAL	HA	4.057	?	1
1174	?	89	VAL	HB	2.192	?	1
1175	?	89	VAL	MG2	1.047	?	2
1176	?	89	VAL	MG2	1.047	?	2
1177	?	89	VAL	MG2	1.047	?	2
1178	?	89	VAL	C	176.695	?	1
1179	?	89	VAL	CA	63.592	?	1
1180	?	89	VAL	CB	32.422	?	1
1181	?	89	VAL	CG1	21.099	?	2
1182	?	89	VAL	CG2	21.099	?	2
1183	?	89	VAL	N	121.153	?	1
1184	?	90	SER	H	8.322	?	1
1185	?	90	SER	HA	4.561	?	1
1186	?	90	SER	HB2	3.934	?	2
1187	?	90	SER	HB3	4.043	?	2
1188	?	90	SER	C	173.898	?	1
1189	?	90	SER	CA	57.895	?	1
1190	?	90	SER	CB	63.133	?	1
1191	?	90	SER	N	116.778	?	1
1192	?	91	VAL	H	8.036	?	1
1193	?	91	VAL	HA	4.286	?	1
1194	?	91	VAL	HB	2.275	?	1
1195	?	91	VAL	MG2	1.041	?	2
1196	?	91	VAL	MG2	1.041	?	2
1197	?	91	VAL	MG2	1.041	?	2
1198	?	91	VAL	CA	62.846	?	1
1199	?	91	VAL	CB	32.069	?	1
1200	?	91	VAL	CG1	19.561	?	2
1201	?	91	VAL	CG2	21.577	?	2
1202	?	91	VAL	N	120.735	?	1
1203	?	92	SER	H	8.470	?	1
1204	?	92	SER	HA	4.549	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1205	?	92	SER	HB2	3.896	?	2
1206	?	92	SER	HB3	4.016	?	2
1207	?	92	SER	CA	57.813	?	1
1208	?	92	SER	CB	63.488	?	1
1209	?	92	SER	N	118.146	?	1
1210	?	93	THR	H	7.382	?	1
1211	?	93	THR	HA	4.467	?	1
1212	?	93	THR	HB	3.812	?	1
1213	?	93	THR	MG	1.414	?	1
1214	?	93	THR	MG	1.414	?	1
1215	?	93	THR	MG	1.414	?	1
1216	?	93	THR	CA	61.005	?	1
1217	?	93	THR	CB	70.592	?	1
1218	?	93	THR	CG2	22.133	?	1
1219	?	93	THR	N	119.747	?	1
1220	?	94	PRO	HA	4.424	?	1
1221	?	94	PRO	HB2	2.108	?	2
1222	?	94	PRO	HB3	2.468	?	2
1223	?	94	PRO	HG2	2.118	?	2
1224	?	94	PRO	HG3	2.159	?	2
1225	?	94	PRO	HD2	3.812	?	2
1226	?	94	PRO	HD3	4.074	?	2
1227	?	94	PRO	CA	63.060	?	1
1228	?	94	PRO	CB	32.798	?	1
1229	?	94	PRO	CG	28.178	?	1
1230	?	94	PRO	CD	51.727	?	1
1231	?	95	ILE	H	9.358	?	1
1232	?	95	ILE	HA	3.984	?	1
1233	?	95	ILE	HB	1.756	?	1
1234	?	95	ILE	HG12	1.198	?	2
1235	?	95	ILE	HG13	1.375	?	2
1236	?	95	ILE	MG	0.911	?	1
1237	?	95	ILE	MG	0.911	?	1
1238	?	95	ILE	MG	0.911	?	1
1239	?	95	ILE	MD	0.693	?	1
1240	?	95	ILE	MD	0.693	?	1
1241	?	95	ILE	MD	0.693	?	1
1242	?	95	ILE	CA	63.963	?	1
1243	?	95	ILE	CB	38.200	?	1
1244	?	95	ILE	CG1	29.374	?	1
1245	?	95	ILE	CG2	18.034	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1246	?	95	ILE	CD1	14.619	?	1
1247	?	95	ILE	N	124.894	?	1
1248	?	96	SER	H	8.202	?	1
1249	?	96	SER	HA	4.004	?	1
1250	?	96	SER	HB2	4.016	?	2
1251	?	96	SER	HB3	4.016	?	2
1252	?	96	SER	CA	61.700	?	1
1253	?	96	SER	CB	61.400	?	1
1254	?	96	SER	N	117.523	?	1
1255	?	97	GLU	H	7.301	?	1
1256	?	97	GLU	HA	4.282	?	1
1257	?	97	GLU	HB2	2.107	?	2
1258	?	97	GLU	HB3	2.151	?	2
1259	?	97	GLU	HG2	2.267	?	2
1260	?	97	GLU	HG3	2.367	?	2
1261	?	97	GLU	CA	58.700	?	1
1262	?	97	GLU	CB	29.800	?	1
1263	?	97	GLU	CG	36.510	?	1
1264	?	97	GLU	N	123.657	?	1
1265	?	98	VAL	H	7.410	?	1
1266	?	98	VAL	HA	3.797	?	1
1267	?	98	VAL	HB	2.165	?	1
1268	?	98	VAL	MG2	1.068	?	2
1269	?	98	VAL	MG2	1.068	?	2
1270	?	98	VAL	MG2	1.068	?	2
1271	?	98	VAL	CA	65.949	?	1
1272	?	98	VAL	CB	32.186	?	1
1273	?	98	VAL	CG1	21.800	?	2
1274	?	98	VAL	CG2	22.126	?	2
1275	?	98	VAL	N	121.907	?	1
1276	?	99	TYR	H	9.071	?	1
1277	?	99	TYR	HA	4.016	?	1
1278	?	99	TYR	HB2	3.037	?	2
1279	?	99	TYR	HB3	3.158	?	2
1280	?	99	TYR	HD1	7.108	?	3
1281	?	99	TYR	HD2	7.108	?	3
1282	?	99	TYR	HE1	6.905	?	3
1283	?	99	TYR	HE2	6.905	?	3
1284	?	99	TYR	C	175.741	?	1
1285	?	99	TYR	CA	62.229	?	1
1286	?	99	TYR	CB	38.967	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1287	?	99	TYR	CD1	133.783	?	3
1288	?	99	TYR	CD2	133.783	?	3
1289	?	99	TYR	CE1	118.033	?	3
1290	?	99	TYR	CE2	118.033	?	3
1291	?	99	TYR	N	119.526	?	1
1292	?	100	GLU	H	7.342	?	1
1293	?	100	GLU	HA	3.850	?	1
1294	?	100	GLU	HB2	2.136	?	2
1295	?	100	GLU	HB3	2.136	?	2
1296	?	100	GLU	HG2	2.494	?	2
1297	?	100	GLU	HG3	2.494	?	2
1298	?	100	GLU	C	178.094	?	1
1299	?	100	GLU	CA	58.920	?	1
1300	?	100	GLU	CB	29.481	?	1
1301	?	100	GLU	CG	35.630	?	1
1302	?	100	GLU	N	114.405	?	1
1303	?	101	SER	H	7.410	?	1
1304	?	101	SER	HA	4.529	?	1
1305	?	101	SER	HB2	3.989	?	2
1306	?	101	SER	HB3	3.989	?	2
1307	?	101	SER	C	176.681	?	1
1308	?	101	SER	CA	60.313	?	1
1309	?	101	SER	CB	64.703	?	1
1310	?	101	SER	N	109.656	?	1
1311	?	102	GLU	H	8.500	?	1
1312	?	102	GLU	HA	4.721	?	1
1313	?	102	GLU	HB2	1.658	?	2
1314	?	102	GLU	HB3	2.272	?	2
1315	?	102	GLU	HG2	2.246	?	2
1316	?	102	GLU	HG3	2.398	?	2
1317	?	102	GLU	CA	55.592	?	1
1318	?	102	GLU	CB	30.564	?	1
1319	?	102	GLU	CG	35.035	?	1
1320	?	102	GLU	N	117.283	?	1
1321	?	103	LYS	H	7.777	?	1
1322	?	103	LYS	HA	4.179	?	1
1323	?	103	LYS	HB2	1.291	?	2
1324	?	103	LYS	HB3	1.445	?	2
1325	?	103	LYS	HG2	1.038	?	2
1326	?	103	LYS	HG3	1.038	?	2
1327	?	103	LYS	HD2	0.570	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1328	?	103	LYS	HD3	1.114	?	2
1329	?	103	LYS	HE2	2.708	?	2
1330	?	103	LYS	HE3	2.761	?	2
1331	?	103	LYS	C	175.032	?	1
1332	?	103	LYS	CA	57.154	?	1
1333	?	103	LYS	CB	32.238	?	1
1334	?	103	LYS	CG	22.612	?	1
1335	?	103	LYS	CD	29.129	?	1
1336	?	103	LYS	CE	42.335	?	1
1337	?	103	LYS	N	118.772	?	1
1338	?	104	ASP	H	9.030	?	1
1339	?	104	ASP	HA	5.032	?	1
1340	?	104	ASP	HB2	3.213	?	2
1341	?	104	ASP	HB3	3.900	?	2
1342	?	104	ASP	C	177.548	?	1
1343	?	104	ASP	CA	53.882	?	1
1344	?	104	ASP	CB	43.420	?	1
1345	?	104	ASP	N	124.024	?	1
1346	?	105	GLU	H	8.894	?	1
1347	?	105	GLU	HA	4.179	?	1
1348	?	105	GLU	HB2	2.208	?	2
1349	?	105	GLU	HB3	2.208	?	2
1350	?	105	GLU	HG2	2.506	?	2
1351	?	105	GLU	HG3	2.506	?	2
1352	?	105	GLU	CA	59.526	?	1
1353	?	105	GLU	CB	30.036	?	1
1354	?	105	GLU	CG	36.569	?	1
1355	?	105	GLU	N	125.669	?	1
1356	?	106	ASP	H	9.838	?	1
1357	?	106	ASP	HA	4.180	?	1
1358	?	106	ASP	HB2	2.653	?	2
1359	?	106	ASP	HB3	2.840	?	2
1360	?	106	ASP	C	176.018	?	1
1361	?	106	ASP	CA	54.750	?	1
1362	?	106	ASP	CB	40.250	?	1
1363	?	106	ASP	N	119.257	?	1
1364	?	107	GLY	H	7.945	?	1
1365	?	107	GLY	HA2	3.388	?	2
1366	?	107	GLY	HA3	4.453	?	2
1367	?	107	GLY	CA	45.125	?	1
1368	?	107	GLY	N	106.307	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1369	?	108	PHE	H	9.739	?	1
1370	?	108	PHE	HA	4.670	?	1
1371	?	108	PHE	HB2	2.082	?	2
1372	?	108	PHE	HB3	3.531	?	2
1373	?	108	PHE	HD1	7.103	?	3
1374	?	108	PHE	HD2	7.103	?	3
1375	?	108	PHE	HE1	7.276	?	3
1376	?	108	PHE	HE2	7.276	?	3
1377	?	108	PHE	C	179.501	?	1
1378	?	108	PHE	CA	60.288	?	1
1379	?	108	PHE	CB	40.506	?	1
1380	?	108	PHE	CD1	131.908	?	3
1381	?	108	PHE	CD2	131.908	?	3
1382	?	108	PHE	CE1	130.408	?	3
1383	?	108	PHE	CE2	130.408	?	3
1384	?	108	PHE	N	124.389	?	1
1385	?	109	LEU	H	7.968	?	1
1386	?	109	LEU	HA	5.038	?	1
1387	?	109	LEU	HB2	1.491	?	2
1388	?	109	LEU	HB3	2.280	?	2
1389	?	109	LEU	HG	1.500	?	1
1390	?	109	LEU	MD1	0.843	?	2
1391	?	109	LEU	MD1	0.843	?	2
1392	?	109	LEU	MD1	0.843	?	2
1393	?	109	LEU	MD2	0.953	?	2
1394	?	109	LEU	MD2	0.953	?	2
1395	?	109	LEU	MD2	0.953	?	2
1396	?	109	LEU	CA	53.479	?	1
1397	?	109	LEU	CB	45.197	?	1
1398	?	109	LEU	CG	27.232	?	1
1399	?	109	LEU	CD1	26.700	?	2
1400	?	109	LEU	CD2	24.690	?	2
1401	?	109	LEU	N	120.814	?	1
1402	?	110	TYR	H	9.349	?	1
1403	?	110	TYR	HA	4.907	?	1
1404	?	110	TYR	HB2	2.947	?	2
1405	?	110	TYR	HB3	3.058	?	2
1406	?	110	TYR	HD1	7.345	?	3
1407	?	110	TYR	HD2	7.345	?	3
1408	?	110	TYR	HE1	7.257	?	3
1409	?	110	TYR	HE2	7.257	?	3

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1410	?	110	TYR	CA	59.259	?	1
1411	?	110	TYR	CB	39.469	?	1
1412	?	110	TYR	CD1	132.845	?	3
1413	?	110	TYR	CD2	132.845	?	3
1414	?	110	TYR	CE1	119.345	?	3
1415	?	110	TYR	CE2	119.345	?	3
1416	?	110	TYR	N	127.403	?	1
1417	?	111	MET	H	9.575	?	1
1418	?	111	MET	HA	5.543	?	1
1419	?	111	MET	HB2	1.958	?	2
1420	?	111	MET	HB3	1.958	?	2
1421	?	111	MET	HG2	2.452	?	2
1422	?	111	MET	HG3	2.452	?	2
1423	?	111	MET	CA	54.341	?	1
1424	?	111	MET	CB	36.894	?	1
1425	?	111	MET	CG	33.578	?	1
1426	?	111	MET	CE	19.131	?	1
1427	?	111	MET	N	120.344	?	1
1428	?	112	VAL	H	8.730	?	1
1429	?	112	VAL	HA	5.938	?	1
1430	?	112	VAL	HB	1.926	?	1
1431	?	112	VAL	MG2	1.033	?	2
1432	?	112	VAL	MG2	1.033	?	2
1433	?	112	VAL	MG2	1.033	?	2
1434	?	112	VAL	C	176.696	?	1
1435	?	112	VAL	CA	59.068	?	1
1436	?	112	VAL	CB	36.180	?	1
1437	?	112	VAL	CG1	21.350	?	2
1438	?	112	VAL	CG2	21.780	?	2
1439	?	112	VAL	N	121.026	?	1
1440	?	113	TYR	H	8.172	?	1
1441	?	113	TYR	HA	6.143	?	1
1442	?	113	TYR	HB2	2.443	?	2
1443	?	113	TYR	HB3	2.737	?	2
1444	?	113	TYR	HD1	6.834	?	3
1445	?	113	TYR	HD2	6.834	?	3
1446	?	113	TYR	HE1	6.687	?	3
1447	?	113	TYR	HE2	6.687	?	3
1448	?	113	TYR	C	173.533	?	1
1449	?	113	TYR	CA	54.165	?	1
1450	?	113	TYR	CB	43.667	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1451	?	113	TYR	CD1	133.783	?	3
1452	?	113	TYR	CD2	133.783	?	3
1453	?	113	TYR	CE1	117.095	?	3
1454	?	113	TYR	CE2	117.095	?	3
1455	?	113	TYR	N	119.995	?	1
1456	?	114	ALA	H	8.499	?	1
1457	?	114	ALA	HA	4.750	?	1
1458	?	114	ALA	C	176.007	?	1
1459	?	114	ALA	CA	51.356	?	1
1460	?	114	ALA	CB	24.623	?	1
1461	?	114	ALA	N	120.454	?	1
1462	?	115	SER	H	9.823	?	1
1463	?	115	SER	HA	4.505	?	1
1464	?	115	SER	HB2	3.893	?	2
1465	?	115	SER	HB3	4.316	?	2
1466	?	115	SER	C	172.860	?	1
1467	?	115	SER	CA	58.837	?	1
1468	?	115	SER	CB	63.798	?	1
1469	?	115	SER	N	115.279	?	1
1470	?	116	GLN	H	7.165	?	1
1471	?	116	GLN	HA	4.453	?	1
1472	?	116	GLN	HB2	1.754	?	2
1473	?	116	GLN	HB3	1.969	?	2
1474	?	116	GLN	HG2	2.015	?	2
1475	?	116	GLN	HG3	2.082	?	2
1476	?	116	GLN	HE21	7.510	?	2
1477	?	116	GLN	HE22	6.854	?	2
1478	?	116	GLN	C	173.181	?	1
1479	?	116	GLN	CA	54.024	?	1
1480	?	116	GLN	CB	32.179	?	1
1481	?	116	GLN	CG	33.347	?	1
1482	?	116	GLN	CD	180.452	?	1
1483	?	116	GLN	N	117.398	?	1
1484	?	116	GLN	NE2	113.241	?	1
1485	?	117	GLU	H	7.873	?	1
1486	?	117	GLU	HA	3.224	?	1
1487	?	117	GLU	HB2	1.120	?	2
1488	?	117	GLU	HB3	1.255	?	2
1489	?	117	GLU	HG2	1.510	?	2
1490	?	117	GLU	HG3	1.660	?	2
1491	?	117	GLU	C	175.451	?	1

*Continued on next page...*



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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1492	?	117	GLU	CA	56.917	?	1
1493	?	117	GLU	CB	30.206	?	1
1494	?	117	GLU	CG	36.398	?	1
1495	?	117	GLU	N	118.885	?	1
1496	?	118	THR	H	6.988	?	1
1497	?	118	THR	HA	4.074	?	1
1498	?	118	THR	HB	3.921	?	1
1499	?	118	THR	MG	0.911	?	1
1500	?	118	THR	MG	0.911	?	1
1501	?	118	THR	MG	0.911	?	1
1502	?	118	THR	C	173.234	?	1
1503	?	118	THR	CA	60.300	?	1
1504	?	118	THR	CB	70.118	?	1
1505	?	118	THR	CG2	21.250	?	1
1506	?	118	THR	N	110.883	?	1
1507	?	119	PHE	H	8.122	?	1
1508	?	119	PHE	HA	4.397	?	1
1509	?	119	PHE	HB2	2.638	?	2
1510	?	119	PHE	HB3	2.984	?	2
1511	?	119	PHE	HD1	6.754	?	3
1512	?	119	PHE	HD2	6.754	?	3
1513	?	119	PHE	HE1	6.758	?	3
1514	?	119	PHE	HE2	6.758	?	3
1515	?	119	PHE	HZ	6.768	?	1
1516	?	119	PHE	C	175.045	?	1
1517	?	119	PHE	CA	56.810	?	1
1518	?	119	PHE	CB	39.349	?	1
1519	?	119	PHE	CD1	131.533	?	3
1520	?	119	PHE	CD2	131.533	?	3
1521	?	119	PHE	CE1	130.780	?	3
1522	?	119	PHE	CE2	130.780	?	3
1523	?	119	PHE	CZ	129.283	?	1
1524	?	119	PHE	N	122.773	?	1
1525	?	120	GLY	H	7.845	?	1
1526	?	120	GLY	HA3	3.758	?	2
1527	?	120	GLY	CA	46.177	?	1
1528	?	120	GLY	N	116.195	?	1

### 7.1.2 Chemical shift referencing ⓘ

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

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 54 atoms were assigned a chemical shift out of a possible 1685. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	19/628 (3%)	19/250 (8%)	0/256 (0%)	0/122 (0%)
Sidechain	31/939 (3%)	31/551 (6%)	0/341 (0%)	0/47 (0%)
Aromatic	4/118 (3%)	4/62 (6%)	0/50 (0%)	0/6 (0%)
Overall	54/1685 (3%)	54/863 (6%)	0/647 (0%)	0/175 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 77 atoms were assigned a chemical shift out of a possible 1791. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	27/673 (4%)	27/268 (10%)	0/274 (0%)	0/131 (0%)
Sidechain	38/975 (4%)	38/572 (7%)	0/356 (0%)	0/47 (0%)
Aromatic	12/143 (8%)	12/75 (16%)	0/62 (0%)	0/6 (0%)
Overall	77/1791 (4%)	77/915 (8%)	0/692 (0%)	0/184 (0%)

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

There are no statistically unusual chemical shifts.

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

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 B:

