



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:36 AM BST

PDB ID : 2O10  
Title : Solution structure of the N-terminal LIM domain of MLP/CRP3  
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Deposited on : 2006-11-28

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

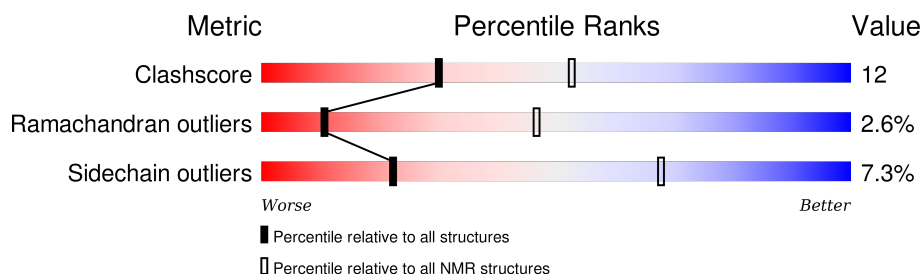
# 1 Overall quality at a glance

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	60	 68% 28% . .

## 2 Ensemble composition and analysis

This entry contains 19 models. Model 13 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:8-A:66 (59)	0.38	13

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 4 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 911 atoms, of which 442 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Muscle LIM protein.

Mol	Chain	Residues	Atoms						Trace
1	A	60	Total	C	H	N	O	S	0
			909	286	442	87	85	9	

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

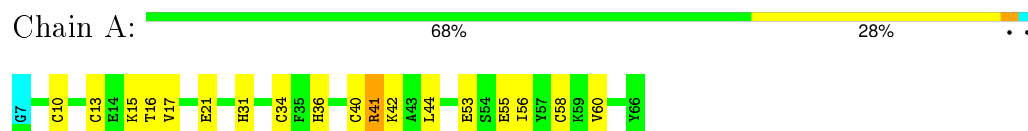
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

## 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: Muscle LIM protein

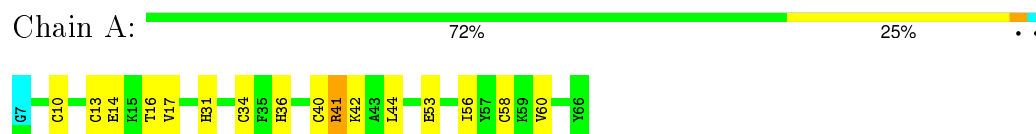


### 4.2 Scores per residue for each member of the ensemble

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

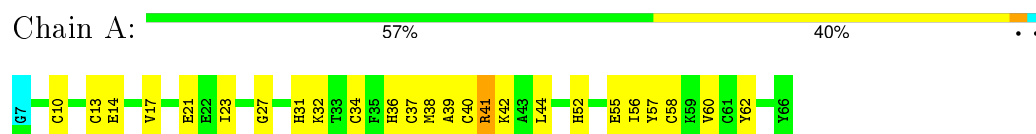
#### 4.2.1 Score per residue for model 1

- Molecule 1: Muscle LIM protein



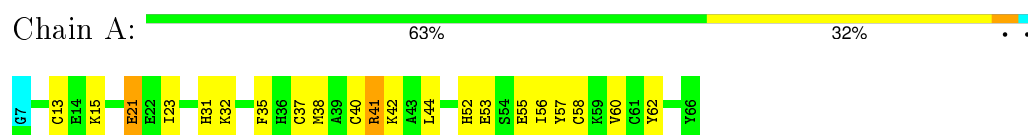
#### 4.2.2 Score per residue for model 2

- Molecule 1: Muscle LIM protein



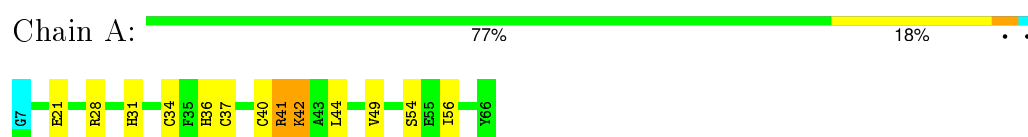
### 4.2.3 Score per residue for model 3

- Molecule 1: Muscle LIM protein



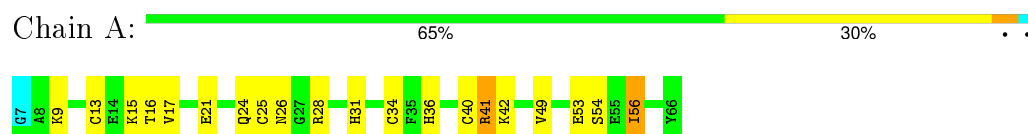
### 4.2.4 Score per residue for model 4

- Molecule 1: Muscle LIM protein



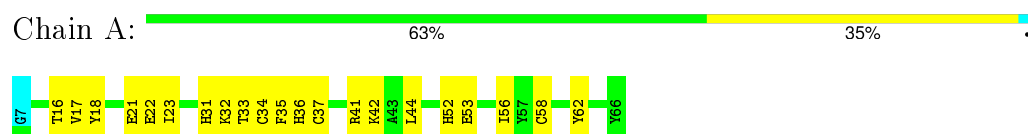
### 4.2.5 Score per residue for model 5

- Molecule 1: Muscle LIM protein



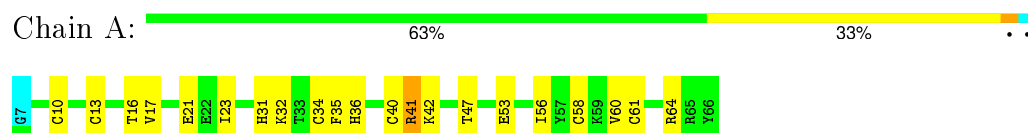
### 4.2.6 Score per residue for model 6

- Molecule 1: Muscle LIM protein



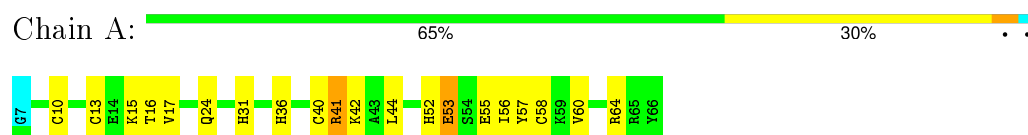
### 4.2.7 Score per residue for model 7

- Molecule 1: Muscle LIM protein



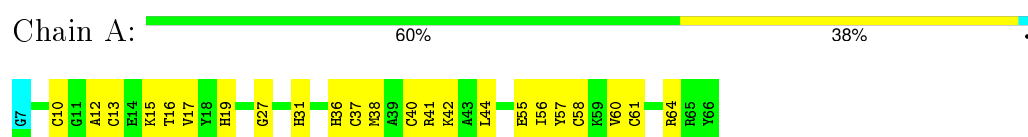
### 4.2.8 Score per residue for model 8

- Molecule 1: Muscle LIM protein



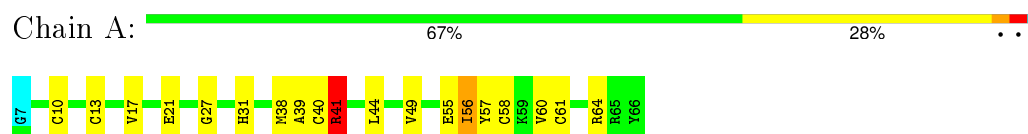
### 4.2.9 Score per residue for model 9

- Molecule 1: Muscle LIM protein



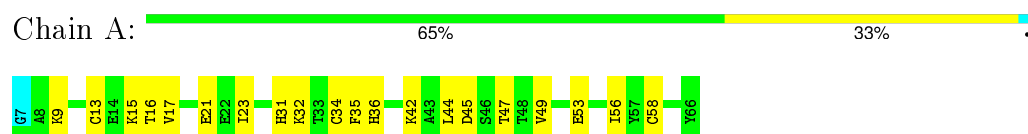
### 4.2.10 Score per residue for model 10

- Molecule 1: Muscle LIM protein



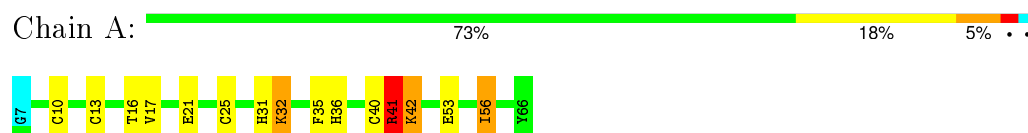
### 4.2.11 Score per residue for model 11

- Molecule 1: Muscle LIM protein



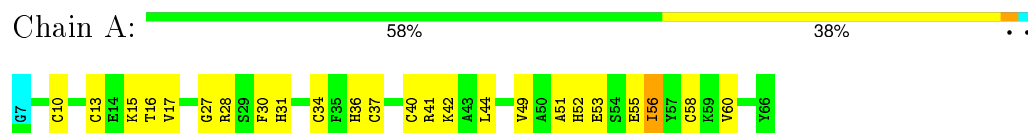
### 4.2.12 Score per residue for model 12

- Molecule 1: Muscle LIM protein



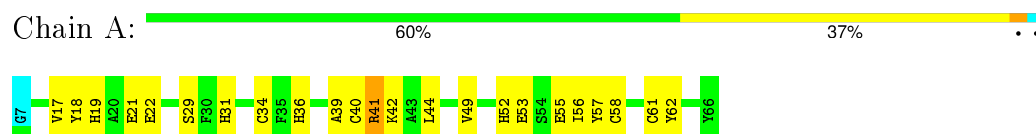
#### 4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Muscle LIM protein



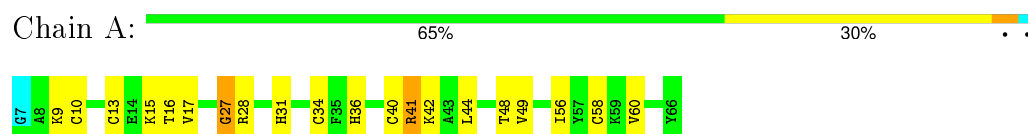
#### 4.2.14 Score per residue for model 14

- Molecule 1: Muscle LIM protein



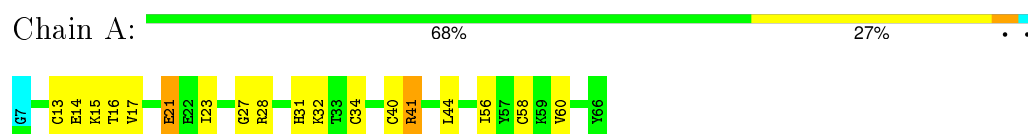
#### 4.2.15 Score per residue for model 15

- Molecule 1: Muscle LIM protein



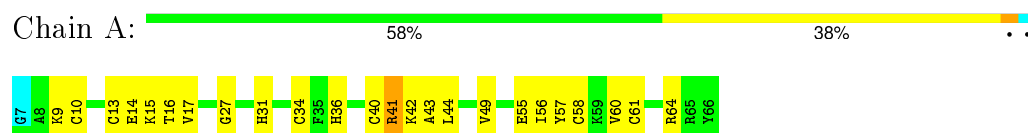
#### 4.2.16 Score per residue for model 16

- Molecule 1: Muscle LIM protein



#### 4.2.17 Score per residue for model 17

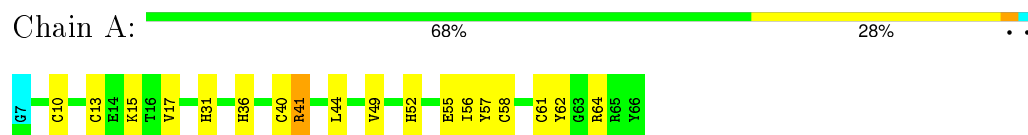
- Molecule 1: Muscle LIM protein





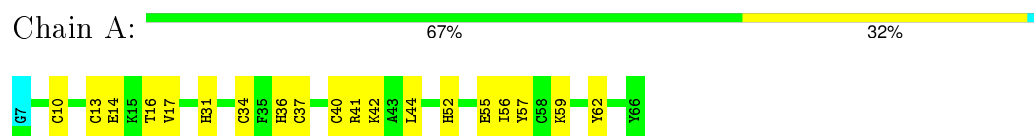
#### 4.2.18 Score per residue for model 18

- Molecule 1: Muscle LIM protein



#### 4.2.19 Score per residue for model 19

- Molecule 1: Muscle LIM protein



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 19 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
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)	BMRB entry 15059
Number of chemical shift lists	1
Total number of shifts	1500
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1500
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 ⓘ

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

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	463	439	436	11±2
All	All	8835	8341	8284	203

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:HIS:HB2	1:A:62:TYR:HE1	0.75	1.41	19	4
1:A:31:HIS:HB2	1:A:34:CYS:SG	0.69	2.28	4	13
1:A:17:VAL:HG22	1:A:31:HIS:CD2	0.66	2.24	9	17
1:A:58:CYS:SG	1:A:60:VAL:HG22	0.66	2.30	15	1
1:A:52:HIS:HB2	1:A:62:TYR:HE2	0.65	1.52	3	2
1:A:44:LEU:HD11	1:A:58:CYS:HA	0.63	1.70	6	12
1:A:55:GLU:HB3	1:A:57:TYR:CE1	0.62	2.30	18	2
1:A:58:CYS:SG	1:A:60:VAL:HB	0.62	2.34	2	9
1:A:55:GLU:HB3	1:A:57:TYR:CE2	0.61	2.30	8	7
1:A:55:GLU:HB3	1:A:57:TYR:HE1	0.61	1.56	18	1
1:A:10:CYS:HB3	1:A:13:CYS:HB2	0.60	1.73	15	10
1:A:40:CYS:SG	1:A:42:LYS:HB2	0.60	2.36	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:CYS:HA	1:A:64:ARG:HG2	0.57	1.75	17	2
1:A:23:ILE:HG21	1:A:35:PHE:CD1	0.57	2.34	11	4
1:A:61:CYS:HA	1:A:64:ARG:HB3	0.57	1.75	7	2
1:A:52:HIS:CD2	1:A:53:GLU:HG2	0.57	2.34	13	2
1:A:36:HIS:HB2	1:A:42:LYS:O	0.56	2.00	9	15
1:A:13:CYS:HB3	1:A:15:LYS:HG2	0.56	1.76	5	2
1:A:40:CYS:O	1:A:41:ARG:HB2	0.55	2.01	8	9
1:A:52:HIS:HB2	1:A:62:TYR:CE1	0.55	2.32	19	1
1:A:37:CYS:O	1:A:41:ARG:HD3	0.55	2.01	6	2
1:A:19:HIS:HA	1:A:22:GLU:HB2	0.54	1.77	14	1
1:A:13:CYS:HB3	1:A:15:LYS:HG3	0.53	1.80	3	5
1:A:21:GLU:O	1:A:31:HIS:HA	0.53	2.04	11	4
1:A:15:LYS:HB2	1:A:31:HIS:HE1	0.52	1.63	18	1
1:A:23:ILE:HD12	1:A:32:LYS:HA	0.52	1.81	3	5
1:A:40:CYS:SG	1:A:41:ARG:N	0.51	2.81	18	13
1:A:10:CYS:HB3	1:A:13:CYS:O	0.51	2.06	10	2
1:A:21:GLU:HB2	1:A:32:LYS:HB3	0.50	1.82	12	1
1:A:38:MET:HB3	1:A:56:ILE:O	0.50	2.06	10	1
1:A:39:ALA:HB2	1:A:57:TYR:CD1	0.49	2.43	10	2
1:A:42:LYS:HD3	1:A:58:CYS:HB2	0.49	1.84	15	1
1:A:28:ARG:HD2	1:A:54:SER:OG	0.48	2.08	4	1
1:A:38:MET:HA	1:A:41:ARG:NH1	0.48	2.24	3	1
1:A:23:ILE:CD1	1:A:32:LYS:HA	0.47	2.39	16	1
1:A:18:TYR:O	1:A:22:GLU:HB2	0.47	2.10	14	2
1:A:61:CYS:HA	1:A:64:ARG:CG	0.47	2.39	17	1
1:A:13:CYS:HB3	1:A:15:LYS:H	0.47	1.70	9	2
1:A:25:CYS:HG	1:A:35:PHE:HE1	0.47	1.53	12	1
1:A:61:CYS:HA	1:A:64:ARG:CD	0.46	2.39	17	1
1:A:12:ALA:HB2	1:A:38:MET:SD	0.46	2.50	9	1
1:A:61:CYS:HA	1:A:64:ARG:HE	0.46	1.71	9	1
1:A:37:CYS:O	1:A:41:ARG:HA	0.46	2.11	6	4
1:A:55:GLU:HB3	1:A:57:TYR:HE2	0.45	1.68	2	2
1:A:37:CYS:N	1:A:44:LEU:HD23	0.45	2.27	9	6
1:A:21:GLU:HG3	1:A:31:HIS:CD2	0.44	2.47	3	1
1:A:51:ALA:HA	1:A:55:GLU:O	0.44	2.13	13	1
1:A:49:VAL:HG23	1:A:56:ILE:HG13	0.44	1.90	5	2
1:A:45:ASP:O	1:A:49:VAL:HG12	0.44	2.13	11	1
1:A:39:ALA:HB3	1:A:61:CYS:SG	0.43	2.52	14	1
1:A:35:PHE:O	1:A:56:ILE:HD11	0.43	2.13	12	1
1:A:19:HIS:HA	1:A:22:GLU:CB	0.43	2.43	14	1
1:A:61:CYS:SG	1:A:64:ARG:NH1	0.43	2.91	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:NZ	1:A:59:LYS:HB2	0.42	2.29	19	1
1:A:60:VAL:O	1:A:64:ARG:HG3	0.42	2.14	8	1
1:A:10:CYS:CB	1:A:13:CYS:HB2	0.42	2.45	1	1
1:A:26:ASN:ND2	1:A:54:SER:HA	0.42	2.29	5	1
1:A:28:ARG:HA	1:A:28:ARG:HE	0.42	1.74	16	1
1:A:24:GLN:HA	1:A:28:ARG:O	0.41	2.15	5	1
1:A:25:CYS:SG	1:A:35:PHE:HE1	0.41	2.39	12	1
1:A:36:HIS:CB	1:A:43:ALA:HA	0.41	2.45	17	1
1:A:44:LEU:HD12	1:A:49:VAL:HA	0.41	1.93	10	2
1:A:27:GLY:C	1:A:28:ARG:HD2	0.41	2.36	15	1
1:A:42:LYS:HB2	1:A:42:LYS:NZ	0.41	2.31	4	1
1:A:28:ARG:HB2	1:A:30:PHE:CE2	0.40	2.52	13	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	58/60 (97%)	52±1 (89±3%)	5±1 (9±2%)	2±1 (3±1%)	11	47
All	All	1102/1140 (97%)	979 (89%)	94 (9%)	29 (3%)	11	47

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	41	ARG	13
1	A	53	GLU	9
1	A	27	GLY	7

### 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	49/49 (100%)	45±1 (93±2%)	4±1 (7±2%)	22	68
All	All	931/931 (100%)	863 (93%)	68 (7%)	22	68

All 18 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	56	ILE	19
1	A	16	THR	13
1	A	21	GLU	7
1	A	14	GLU	5
1	A	9	LYS	4
1	A	49	VAL	4
1	A	41	ARG	3
1	A	42	LYS	2
1	A	47	THR	2
1	A	24	GLN	1
1	A	25	CYS	1
1	A	33	THR	1
1	A	19	HIS	1
1	A	38	MET	1
1	A	29	SER	1
1	A	32	LYS	1
1	A	48	THR	1
1	A	36	HIS	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

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

### 7.1 Chemical shift list 1

File name: BMRB entry 15059

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	1500
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1500
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 1500 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	164	GLY	N	105.728	-1.0	1
UNMAPPED	182	GLY	H	8.411	-1.0	1
UNMAPPED	133	VAL	HG23	0.33	-1.0	2
UNMAPPED	56	ILE	CG2	19.19	-1.0	1
UNMAPPED	79	CYS	H	8.079	-1.0	1
UNMAPPED	4	TRP	HE1	10.113	-1.0	1
UNMAPPED	131	GLU	HB2	2.479	-1.0	2
UNMAPPED	74	GLY	CA	45.323	-1.0	1
UNMAPPED	29	SER	HB2	3.34	-1.0	2
UNMAPPED	127	VAL	HG13	0.396	-1.0	2
UNMAPPED	43	ALA	CB	18.564	-1.0	1
UNMAPPED	75	GLN	HB3	1.915	-1.0	2
UNMAPPED	158	ASN	HD22	6.87	-1.0	2
UNMAPPED	52	HIS	H	8.565	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	134	MET	HB2	1.867	-1.0	2
UNMAPPED	192	LYS	HA	4.31	-1.0	1
UNMAPPED	149	ILE	CA	62.704	-1.0	1
UNMAPPED	64	ARG	CA	58.239	-1.0	1
UNMAPPED	179	THR	HG23	1.119	-1.0	1
UNMAPPED	149	ILE	HD11	0.828	-1.0	1
UNMAPPED	123	CYS	CA	57.392	-1.0	1
UNMAPPED	20	ALA	HB3	1.348	-1.0	1
UNMAPPED	17	VAL	N	127.587	-1.0	1
UNMAPPED	48	THR	HA	4.431	-1.0	1
UNMAPPED	61	CYS	HB2	3.145	-1.0	2
UNMAPPED	26	ASN	HD22	6.9	-1.0	2
UNMAPPED	154	LEU	CD2	22.45	-1.0	2
UNMAPPED	41	ARG	CG	26.619	-1.0	1
UNMAPPED	35	PHE	HB3	2.602	-1.0	2
UNMAPPED	126	SER	H	8.65	-1.0	1
UNMAPPED	125	LYS	HB2	2.01	-1.0	2
UNMAPPED	22	GLU	CG	36.53	-1.0	1
UNMAPPED	15	LYS	HG3	1.481	-1.0	2
UNMAPPED	163	ASP	HB3	2.619	-1.0	2
UNMAPPED	29	SER	N	116.988	-1.0	1
UNMAPPED	154	LEU	HB3	0.538	-1.0	2
UNMAPPED	77	ALA	H	8.194	-1.0	1
UNMAPPED	41	ARG	HB2	2.095	-1.0	2
UNMAPPED	62	TYR	CB	39.278	-1.0	1
UNMAPPED	140	TRP	HB2	3.233	-1.0	2
UNMAPPED	62	TYR	HB2	2.976	-1.0	2
UNMAPPED	69	LYS	CG	24.734	-1.0	1
UNMAPPED	159	VAL	HG22	0.837	-1.0	2
UNMAPPED	25	CYS	HB2	2.776	-1.0	2
UNMAPPED	49	VAL	HB	1.809	-1.0	1
UNMAPPED	66	TYR	H	8.01	-1.0	1
UNMAPPED	79	CYS	CB	28.08	-1.0	1
UNMAPPED	19	HIS	HB2	3.06	-1.0	2
UNMAPPED	23	ILE	HD11	0.487	-1.0	1
UNMAPPED	166	LEU	N	121.023	-1.0	1
UNMAPPED	60	VAL	N	121.083	-1.0	1
UNMAPPED	56	ILE	HG13	0.592	-1.0	9
UNMAPPED	166	LEU	HD11	1.03	-1.0	2
UNMAPPED	39	ALA	CA	53.981	-1.0	1
UNMAPPED	62	TYR	HE1	6.636	-1.0	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	52	HIS	CB	32.391	-1.0	1
UNMAPPED	68	PRO	HG2	1.963	-1.0	2
UNMAPPED	48	THR	H	7.707	-1.0	1
UNMAPPED	189	GLN	NE2	112.6	-1.0	1
UNMAPPED	50	ALA	HB1	0.678	-1.0	1
UNMAPPED	161	ASP	CA	52.735	-1.0	1
UNMAPPED	188	GLN	N	122.469	-1.0	1
UNMAPPED	158	ASN	HB2	2.896	-1.0	2
UNMAPPED	172	TYR	CD1	133.369	-1.0	3
UNMAPPED	193	LYS	H	8.005	-1.0	1
UNMAPPED	70	GLY	CA	45.24	-1.0	1
UNMAPPED	16	THR	CB	69.088	-1.0	1
UNMAPPED	42	LYS	CA	57.606	-1.0	1
UNMAPPED	116	GLU	CA	56.454	-1.0	1
UNMAPPED	64	ARG	N	119.156	-1.0	1
UNMAPPED	166	LEU	HD21	0.159	-1.0	2
UNMAPPED	119	LYS	HE2	2.841	-1.0	2
UNMAPPED	56	ILE	HG22	0.252	-1.0	2
UNMAPPED	123	CYS	N	113.797	-1.0	1
UNMAPPED	132	LYS	CG	24.428	-1.0	1
UNMAPPED	3	ASN	CA	52.921	-1.0	1
UNMAPPED	178	PRO	HB2	2.23	-1.0	2
UNMAPPED	17	VAL	CA	59.44	-1.0	1
UNMAPPED	170	VAL	HG21	0.93	-1.0	2
UNMAPPED	167	TYR	HE1	6.767	-1.0	3
UNMAPPED	146	ARG	CG	27.379	-1.0	1
UNMAPPED	7	GLY	CA	44.786	-1.0	1
UNMAPPED	67	GLY	CA	44.776	-1.0	1
UNMAPPED	32	LYS	CD	29.755	-1.0	1
UNMAPPED	187	THR	HB	4.137	-1.0	1
UNMAPPED	61	CYS	CA	64.549	-1.0	1
UNMAPPED	77	ALA	HB2	1.316	-1.0	1
UNMAPPED	1	MET	CA	55.004	-1.0	1
UNMAPPED	57	TYR	N	118.674	-1.0	1
UNMAPPED	170	VAL	HG12	1.073	-1.0	2
UNMAPPED	62	TYR	H	8.784	-1.0	1
UNMAPPED	48	THR	CB	70.389	-1.0	1
UNMAPPED	176	PHE	HD1	6.544	-1.0	3
UNMAPPED	134	MET	CG	31.476	-1.0	1
UNMAPPED	159	VAL	HG13	0.673	-1.0	2
UNMAPPED	47	THR	HG21	1.177	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	82	THR	CG2	21.437	-1.0	1
UNMAPPED	66	TYR	CB	38.836	-1.0	1
UNMAPPED	49	VAL	HG12	1.007	-1.0	2
UNMAPPED	66	TYR	HB3	1.457	-1.0	2
UNMAPPED	146	ARG	H	7.499	-1.0	1
UNMAPPED	34	CYS	CA	60.334	-1.0	1
UNMAPPED	157	THR	HB	4.317	-1.0	1
UNMAPPED	189	GLN	CA	55.734	-1.0	1
UNMAPPED	122	ARG	HA	4.418	-1.0	1
UNMAPPED	175	ASN	HB2	1.652	-1.0	2
UNMAPPED	29	SER	CA	58.382	-1.0	1
UNMAPPED	33	THR	HG21	1.292	-1.0	1
UNMAPPED	29	SER	HA	4.777	-1.0	1
UNMAPPED	58	CYS	HB3	2.73	-1.0	2
UNMAPPED	47	THR	CB	69.379	-1.0	1
UNMAPPED	158	ASN	N	119.939	-1.0	1
UNMAPPED	52	HIS	HA	4.515	-1.0	1
UNMAPPED	162	LYS	HB2	1.615	-1.0	2
UNMAPPED	171	CYS	HB3	2.874	-1.0	2
UNMAPPED	15	LYS	CG	25.31	-1.0	1
UNMAPPED	60	VAL	HA	3.696	-1.0	1
UNMAPPED	38	MET	HE2	2.33	-1.0	1
UNMAPPED	12	ALA	CA	53.264	-1.0	1
UNMAPPED	19	HIS	HA	4.16	-1.0	1
UNMAPPED	28	ARG	CD	43.394	-1.0	1
UNMAPPED	35	PHE	CD1	132.759	-1.0	3
UNMAPPED	129	ALA	CA	56.01	-1.0	1
UNMAPPED	82	THR	HG22	1.123	-1.0	1
UNMAPPED	152	LYS	HA	4.188	-1.0	1
UNMAPPED	162	LYS	CB	34.91	-1.0	1
UNMAPPED	185	GLY	HA2	3.867	-1.0	2
UNMAPPED	36	HIS	HB2	2.465	-1.0	2
UNMAPPED	16	THR	H	8.422	-1.0	1
UNMAPPED	16	THR	HG23	0.58	-1.0	1
UNMAPPED	153	SER	CB	63.266	-1.0	1
UNMAPPED	145	PHE	CA	57.27	-1.0	1
UNMAPPED	141	HIS	H	7.768	-1.0	1
UNMAPPED	71	ILE	CA	61.21	-1.0	1
UNMAPPED	134	MET	HA	5.34	-1.0	1
UNMAPPED	114	PHE	CB	39.58	-1.0	1
UNMAPPED	159	VAL	CB	33.142	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	142	LYS	HG2	1.407	-1.0	2
UNMAPPED	188	GLN	HA	4.294	-1.0	1
UNMAPPED	142	LYS	HA	3.966	-1.0	1
UNMAPPED	160	THR	HG22	0.451	-1.0	1
UNMAPPED	71	ILE	HG21	0.805	-1.0	2
UNMAPPED	43	ALA	N	127.466	-1.0	1
UNMAPPED	33	THR	CB	68.133	-1.0	1
UNMAPPED	42	LYS	N	124.455	-1.0	1
UNMAPPED	56	ILE	H	7.559	-1.0	1
UNMAPPED	31	HIS	CA	59.506	-1.0	1
UNMAPPED	132	LYS	HA	4.321	-1.0	1
UNMAPPED	71	ILE	HG12	1.339	-1.0	9
UNMAPPED	130	ALA	HB3	1.419	-1.0	1
UNMAPPED	137	GLY	HA3	3.57	-1.0	2
UNMAPPED	145	PHE	HB2	3.234	-1.0	2
UNMAPPED	61	CYS	N	125.66	-1.0	1
UNMAPPED	130	ALA	HB1	1.419	-1.0	1
UNMAPPED	133	VAL	H	8.995	-1.0	1
UNMAPPED	185	GLY	CA	45.246	-1.0	1
UNMAPPED	1	MET	N	119.758	-1.0	1
UNMAPPED	59	LYS	CG	26.289	-1.0	1
UNMAPPED	141	HIS	CD2	118.12	-1.0	1
UNMAPPED	163	ASP	CB	40.035	-1.0	1
UNMAPPED	133	VAL	HG12	0.511	-1.0	2
UNMAPPED	174	LYS	CA	58.356	-1.0	1
UNMAPPED	154	LEU	HG	1.142	-1.0	1
UNMAPPED	5	GLY	CA	45.358	-1.0	1
UNMAPPED	186	LEU	CB	42.445	-1.0	1
UNMAPPED	14	GLU	N	115.904	-1.0	1
UNMAPPED	81	SER	CA	57.897	-1.0	1
UNMAPPED	122	ARG	HG2	1.983	-1.0	2
UNMAPPED	113	LYS	CA	56.098	-1.0	1
UNMAPPED	35	PHE	H	7.486	-1.0	1
UNMAPPED	24	GLN	N	125.057	-1.0	1
UNMAPPED	4	TRP	HA	4.599	-1.0	1
UNMAPPED	157	THR	CA	54.479	-1.0	1
UNMAPPED	130	ALA	N	117.049	-1.0	1
UNMAPPED	119	LYS	HB3	1.137	-1.0	2
UNMAPPED	122	ARG	CB	30.324	-1.0	1
UNMAPPED	134	MET	HE3	1.687	-1.0	1
UNMAPPED	153	SER	H	8.655	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	164	GLY	H	9.017	-1.0	1
UNMAPPED	37	CYS	N	121.083	-1.0	1
UNMAPPED	56	ILE	CA	59.862	-1.0	1
UNMAPPED	169	LYS	CB	32.771	-1.0	1
UNMAPPED	159	VAL	H	7.606	-1.0	1
UNMAPPED	41	ARG	HD2	3.014	-1.0	2
UNMAPPED	152	LYS	N	123.552	-1.0	1
UNMAPPED	139	PRO	HG3	1.788	-1.0	2
UNMAPPED	36	HIS	N	120.36	-1.0	1
UNMAPPED	181	ILE	H	7.934	-1.0	1
UNMAPPED	77	ALA	HA	4.244	-1.0	1
UNMAPPED	1	MET	HB2	1.914	-1.0	2
UNMAPPED	162	LYS	HA	4.389	-1.0	1
UNMAPPED	23	ILE	CD1	13.146	-1.0	1
UNMAPPED	119	LYS	H	8.07	-1.0	1
UNMAPPED	131	GLU	HB3	2.235	-1.0	2
UNMAPPED	56	ILE	CG1	24.111	-1.0	1
UNMAPPED	190	VAL	HG13	0.861	-1.0	2
UNMAPPED	172	TYR	HE1	6.42	-1.0	3
UNMAPPED	42	LYS	HB2	2.007	-1.0	2
UNMAPPED	175	ASN	HA	4.217	-1.0	1
UNMAPPED	173	ALA	HB3	1.499	-1.0	1
UNMAPPED	188	GLN	CG	33.812	-1.0	1
UNMAPPED	31	HIS	N	119.638	-1.0	1
UNMAPPED	131	GLU	CG	36.754	-1.0	1
UNMAPPED	16	THR	N	118.072	-1.0	1
UNMAPPED	57	TYR	HD1	7.242	-1.0	3
UNMAPPED	154	LEU	HD21	0.468	-1.0	2
UNMAPPED	192	LYS	HG2	1.365	-1.0	2
UNMAPPED	178	PRO	HD2	3.598	-1.0	2
UNMAPPED	169	LYS	HG2	1.42	-1.0	2
UNMAPPED	26	ASN	HD21	7.798	-1.0	2
UNMAPPED	73	TYR	HA	4.441	-1.0	1
UNMAPPED	127	VAL	HB	1.289	-1.0	1
UNMAPPED	41	ARG	CB	26.984	-1.0	1
UNMAPPED	71	ILE	CD1	13.149	-1.0	1
UNMAPPED	35	PHE	CB	37.17	-1.0	1
UNMAPPED	131	GLU	H	7.709	-1.0	1
UNMAPPED	179	THR	N	111.99	-1.0	1
UNMAPPED	10	CYS	HB3	2.271	-1.0	2
UNMAPPED	189	GLN	CB	29.553	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	57	TYR	CB	44.903	-1.0	1
UNMAPPED	153	SER	HB2	3.867	-1.0	2
UNMAPPED	44	LEU	CA	52.975	-1.0	1
UNMAPPED	115	GLY	CA	45.182	-1.0	1
UNMAPPED	118	GLU	CG	36.723	-1.0	1
UNMAPPED	42	LYS	HB3	1.601	-1.0	2
UNMAPPED	181	ILE	HD13	0.787	-1.0	1
UNMAPPED	14	GLU	CA	58.311	-1.0	1
UNMAPPED	160	THR	CG2	21.785	-1.0	1
UNMAPPED	169	LYS	H	8.242	-1.0	1
UNMAPPED	62	TYR	CE1	118.471	-1.0	3
UNMAPPED	174	LYS	HE2	2.837	-1.0	2
UNMAPPED	113	LYS	N	120.542	-1.0	1
UNMAPPED	172	TYR	CB	38.681	-1.0	1
UNMAPPED	61	CYS	H	8.914	-1.0	1
UNMAPPED	21	GLU	HB2	2.493	-1.0	2
UNMAPPED	158	ASN	CB	39.358	-1.0	1
UNMAPPED	1	MET	H	8.372	-1.0	1
UNMAPPED	157	THR	N	108.739	-1.0	1
UNMAPPED	143	THR	HA	4.107	-1.0	1
UNMAPPED	82	THR	H	8.13	-1.0	1
UNMAPPED	36	HIS	HA	4.786	-1.0	1
UNMAPPED	79	CYS	CA	58.404	-1.0	1
UNMAPPED	120	CYS	HA	4.704	-1.0	1
UNMAPPED	181	ILE	HG13	1.078	-1.0	9
UNMAPPED	126	SER	HB2	3.55	-1.0	2
UNMAPPED	39	ALA	CB	20.762	-1.0	1
UNMAPPED	72	GLY	CA	45.084	-1.0	1
UNMAPPED	148	ALA	HB1	1.229	-1.0	1
UNMAPPED	23	ILE	HA	4.104	-1.0	1
UNMAPPED	124	GLY	HA2	4.019	-1.0	2
UNMAPPED	49	VAL	HG22	0.7	-1.0	2
UNMAPPED	43	ALA	HB2	1.311	-1.0	1
UNMAPPED	153	SER	N	118.374	-1.0	1
UNMAPPED	37	CYS	H	8.765	-1.0	1
UNMAPPED	14	GLU	HA	4.0	-1.0	1
UNMAPPED	38	MET	HA	4.027	-1.0	1
UNMAPPED	26	ASN	ND2	112.422	-1.0	1
UNMAPPED	179	THR	CG2	21.637	-1.0	1
UNMAPPED	114	PHE	N	121.385	-1.0	1
UNMAPPED	188	GLN	HE21	7.5	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	27	GLY	H	8.793	-1.0	1
UNMAPPED	41	ARG	H	7.814	-1.0	1
UNMAPPED	146	ARG	HB3	1.154	-1.0	2
UNMAPPED	65	ARG	H	7.165	-1.0	1
UNMAPPED	16	THR	CA	64.459	-1.0	1
UNMAPPED	53	GLU	HA	3.52	-1.0	1
UNMAPPED	155	GLU	CA	55.326	-1.0	1
UNMAPPED	71	ILE	HD11	0.781	-1.0	1
UNMAPPED	56	ILE	HG21	0.252	-1.0	2
UNMAPPED	140	TRP	CE3	119.79	-1.0	1
UNMAPPED	142	LYS	CB	32.204	-1.0	1
UNMAPPED	190	VAL	HB	1.995	-1.0	1
UNMAPPED	146	ARG	CD	43.594	-1.0	1
UNMAPPED	17	VAL	HA	3.997	-1.0	1
UNMAPPED	61	CYS	CB	30.023	-1.0	1
UNMAPPED	168	CYS	CA	57.418	-1.0	1
UNMAPPED	68	PRO	HA	4.301	-1.0	1
UNMAPPED	60	VAL	HG13	1.015	-1.0	2
UNMAPPED	158	ASN	H	7.942	-1.0	1
UNMAPPED	1	MET	CB	32.536	-1.0	1
UNMAPPED	190	VAL	CG1	20.942	-1.0	1
UNMAPPED	65	ARG	HB2	0.805	-1.0	2
UNMAPPED	125	LYS	HE2	2.942	-1.0	2
UNMAPPED	16	THR	HB	3.668	-1.0	1
UNMAPPED	13	CYS	HA	4.932	-1.0	1
UNMAPPED	170	VAL	HG11	1.073	-1.0	2
UNMAPPED	115	GLY	N	111.027	-1.0	1
UNMAPPED	170	VAL	HA	3.749	-1.0	1
UNMAPPED	133	VAL	CG2	20.503	-1.0	1
UNMAPPED	49	VAL	HG11	1.007	-1.0	2
UNMAPPED	190	VAL	H	8.196	-1.0	1
UNMAPPED	176	PHE	HA	4.612	-1.0	1
UNMAPPED	34	CYS	HB3	3.137	-1.0	2
UNMAPPED	56	ILE	HD11	-0.103	-1.0	1
UNMAPPED	75	GLN	CA	55.776	-1.0	1
UNMAPPED	189	GLN	HB2	2.03	-1.0	2
UNMAPPED	15	LYS	CD	28.736	-1.0	1
UNMAPPED	75	GLN	HA	4.282	-1.0	1
UNMAPPED	124	GLY	N	113.436	-1.0	1
UNMAPPED	130	ALA	CB	18.875	-1.0	1
UNMAPPED	119	LYS	CE	42.264	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	171	CYS	CB	30.051	-1.0	1
UNMAPPED	37	CYS	CB	30.935	-1.0	1
UNMAPPED	78	GLY	CA	45.253	-1.0	1
UNMAPPED	184	GLY	HA2	3.833	-1.0	2
UNMAPPED	151	GLY	HA2	4.111	-1.0	2
UNMAPPED	169	LYS	N	119.458	-1.0	1
UNMAPPED	152	LYS	CB	33.893	-1.0	1
UNMAPPED	57	TYR	HA	5.871	-1.0	1
UNMAPPED	10	CYS	H	8.19	-1.0	1
UNMAPPED	188	GLN	NE2	112.6	-1.0	1
UNMAPPED	30	PHE	CE1	132.449	-1.0	3
UNMAPPED	145	PHE	CB	36.954	-1.0	1
UNMAPPED	142	LYS	H	9.276	-1.0	1
UNMAPPED	71	ILE	CB	38.529	-1.0	1
UNMAPPED	159	VAL	CA	58.483	-1.0	1
UNMAPPED	167	TYR	H	8.146	-1.0	1
UNMAPPED	64	ARG	HA	3.928	-1.0	1
UNMAPPED	56	ILE	HA	4.372	-1.0	1
UNMAPPED	149	ILE	HG13	1.339	-1.0	9
UNMAPPED	117	SER	CB	64.151	-1.0	1
UNMAPPED	66	TYR	HD1	6.288	-1.0	3
UNMAPPED	7	GLY	HA2	3.727	-1.0	2
UNMAPPED	138	LYS	CA	52.733	-1.0	1
UNMAPPED	147	CYS	HB2	3.236	-1.0	2
UNMAPPED	147	CYS	CA	59.547	-1.0	1
UNMAPPED	31	HIS	CB	30.663	-1.0	1
UNMAPPED	155	GLU	N	118.253	-1.0	1
UNMAPPED	176	PHE	H	8.045	-1.0	1
UNMAPPED	127	VAL	CA	60.977	-1.0	1
UNMAPPED	48	THR	CA	61.077	-1.0	1
UNMAPPED	51	ALA	HB3	1.262	-1.0	1
UNMAPPED	51	ALA	CB	21.719	-1.0	1
UNMAPPED	60	VAL	CG2	22.304	-1.0	2
UNMAPPED	71	ILE	HA	4.073	-1.0	1
UNMAPPED	129	ALA	HB2	1.396	-1.0	1
UNMAPPED	141	HIS	HA	4.661	-1.0	1
UNMAPPED	145	PHE	HE1	6.36	-1.0	3
UNMAPPED	157	THR	HG21	1.159	-1.0	1
UNMAPPED	59	LYS	CD	29.23	-1.0	1
UNMAPPED	69	LYS	HA	4.252	-1.0	1
UNMAPPED	31	HIS	HA	4.63	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	54	SER	N	117.831	-1.0	1
UNMAPPED	176	PHE	HB2	2.795	-1.0	2
UNMAPPED	37	CYS	HA	3.785	-1.0	1
UNMAPPED	19	HIS	CA	59.528	-1.0	1
UNMAPPED	143	THR	CA	63.746	-1.0	1
UNMAPPED	4	TRP	N	121.685	-1.0	1
UNMAPPED	154	LEU	HD13	-0.16	-1.0	2
UNMAPPED	113	LYS	CB	33.823	-1.0	1
UNMAPPED	174	LYS	HD2	1.64	-1.0	2
UNMAPPED	75	GLN	HE22	6.813	-1.0	2
UNMAPPED	53	GLU	H	8.905	-1.0	1
UNMAPPED	115	GLY	H	8.426	-1.0	1
UNMAPPED	69	LYS	N	120.481	-1.0	1
UNMAPPED	145	PHE	H	7.381	-1.0	1
UNMAPPED	169	LYS	CA	60.135	-1.0	1
UNMAPPED	26	ASN	CB	38.031	-1.0	1
UNMAPPED	4	TRP	CD1	127.168	-1.0	1
UNMAPPED	128	TYR	CE1	118.089	-1.0	3
UNMAPPED	80	LEU	CG	26.892	-1.0	1
UNMAPPED	139	PRO	CA	62.121	-1.0	1
UNMAPPED	59	LYS	HB2	1.854	-1.0	2
UNMAPPED	176	PHE	CB	39.211	-1.0	1
UNMAPPED	149	ILE	H	8.957	-1.0	1
UNMAPPED	9	LYS	CB	33.256	-1.0	1
UNMAPPED	51	ALA	H	8.26	-1.0	1
UNMAPPED	42	LYS	HG2	1.446	-1.0	2
UNMAPPED	3	ASN	ND2	112.648	-1.0	1
UNMAPPED	42	LYS	HA	4.168	-1.0	1
UNMAPPED	120	CYS	H	7.864	-1.0	1
UNMAPPED	36	HIS	CD2	124.062	-1.0	1
UNMAPPED	21	GLU	CG	36.512	-1.0	1
UNMAPPED	131	GLU	HA	4.51	-1.0	1
UNMAPPED	125	LYS	HD2	1.599	-1.0	2
UNMAPPED	50	ALA	HB3	0.678	-1.0	1
UNMAPPED	181	ILE	CG2	17.533	-1.0	1
UNMAPPED	147	CYS	N	122.95	-1.0	1
UNMAPPED	174	LYS	HG2	1.41	-1.0	2
UNMAPPED	9	LYS	HB2	1.432	-1.0	2
UNMAPPED	2	ALA	N	125.419	-1.0	1
UNMAPPED	140	TRP	HE1	9.91	-1.0	1
UNMAPPED	154	LEU	HD22	0.468	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	127	VAL	N	124.757	-1.0	1
UNMAPPED	48	THR	N	111.448	-1.0	1
UNMAPPED	20	ALA	HA	4.023	-1.0	1
UNMAPPED	4	TRP	CH2	124.683	-1.0	1
UNMAPPED	132	LYS	N	120.542	-1.0	1
UNMAPPED	36	HIS	HD2	6.529	-1.0	1
UNMAPPED	82	THR	HB	4.247	-1.0	1
UNMAPPED	192	LYS	CD	29.118	-1.0	1
UNMAPPED	120	CYS	HB3	2.285	-1.0	2
UNMAPPED	77	ALA	CA	52.586	-1.0	1
UNMAPPED	80	LEU	HD23	0.805	-1.0	2
UNMAPPED	133	VAL	HB	1.561	-1.0	1
UNMAPPED	122	ARG	HD2	3.468	-1.0	2
UNMAPPED	118	GLU	CB	30.645	-1.0	1
UNMAPPED	19	HIS	N	120.842	-1.0	1
UNMAPPED	9	LYS	HE2	2.831	-1.0	2
UNMAPPED	134	MET	N	122.348	-1.0	1
UNMAPPED	127	VAL	HG22	0.082	-1.0	2
UNMAPPED	26	ASN	H	9.587	-1.0	1
UNMAPPED	140	TRP	HA	5.063	-1.0	1
UNMAPPED	125	LYS	CG	25.427	-1.0	1
UNMAPPED	21	GLU	CB	30.741	-1.0	1
UNMAPPED	191	GLU	CA	56.356	-1.0	1
UNMAPPED	80	LEU	CD1	24.867	-1.0	2
UNMAPPED	27	GLY	HA3	3.547	-1.0	2
UNMAPPED	131	GLU	HG2	2.36	-1.0	2
UNMAPPED	80	LEU	HD11	0.854	-1.0	2
UNMAPPED	143	THR	HB	4.347	-1.0	1
UNMAPPED	66	TYR	HA	4.412	-1.0	1
UNMAPPED	44	LEU	HD12	0.432	-1.0	2
UNMAPPED	15	LYS	HB2	2.031	-1.0	2
UNMAPPED	162	LYS	H	8.924	-1.0	1
UNMAPPED	12	ALA	HB2	1.752	-1.0	1
UNMAPPED	4	TRP	HZ3	7.066	-1.0	1
UNMAPPED	4	TRP	CZ2	114.743	-1.0	1
UNMAPPED	23	ILE	N	125.66	-1.0	1
UNMAPPED	120	CYS	CB	31.804	-1.0	1
UNMAPPED	119	LYS	HG2	1.1	-1.0	2
UNMAPPED	132	LYS	HE2	2.717	-1.0	2
UNMAPPED	165	GLU	N	121.264	-1.0	1
UNMAPPED	60	VAL	CB	32.305	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	27	GLY	N	104.342	-1.0	1
UNMAPPED	23	ILE	HB	1.191	-1.0	1
UNMAPPED	186	LEU	HD21	0.83	-1.0	2
UNMAPPED	52	HIS	HD2	6.735	-1.0	1
UNMAPPED	65	ARG	CD	42.751	-1.0	1
UNMAPPED	65	ARG	HD2	2.445	-1.0	2
UNMAPPED	11	GLY	HA2	3.792	-1.0	2
UNMAPPED	68	PRO	CG	27.23	-1.0	1
UNMAPPED	140	TRP	CA	54.689	-1.0	1
UNMAPPED	172	TYR	HA	3.74	-1.0	1
UNMAPPED	192	LYS	HD2	1.614	-1.0	2
UNMAPPED	127	VAL	HG12	0.396	-1.0	2
UNMAPPED	117	SER	N	116.447	-1.0	1
UNMAPPED	75	GLN	HB2	2.107	-1.0	2
UNMAPPED	19	HIS	CD2	120.645	-1.0	1
UNMAPPED	8	ALA	N	124.214	-1.0	1
UNMAPPED	23	ILE	CG1	28.076	-1.0	1
UNMAPPED	155	GLU	CB	32.002	-1.0	1
UNMAPPED	71	ILE	HD12	0.781	-1.0	1
UNMAPPED	118	GLU	H	8.358	-1.0	1
UNMAPPED	64	ARG	CB	30.745	-1.0	1
UNMAPPED	190	VAL	HA	4.047	-1.0	1
UNMAPPED	123	CYS	CB	32.103	-1.0	1
UNMAPPED	169	LYS	HB2	1.851	-1.0	2
UNMAPPED	146	ARG	CA	53.189	-1.0	1
UNMAPPED	17	VAL	HB	0.959	-1.0	1
UNMAPPED	61	CYS	HB3	2.794	-1.0	2
UNMAPPED	39	ALA	HB1	1.775	-1.0	1
UNMAPPED	66	TYR	CD1	133.07	-1.0	3
UNMAPPED	174	LYS	N	115.483	-1.0	1
UNMAPPED	1	MET	CG	31.771	-1.0	1
UNMAPPED	69	LYS	HB3	1.685	-1.0	2
UNMAPPED	35	PHE	HB2	3.314	-1.0	2
UNMAPPED	44	LEU	CD2	25.842	-1.0	1
UNMAPPED	127	VAL	H	8.464	-1.0	1
UNMAPPED	139	PRO	HB3	1.355	-1.0	2
UNMAPPED	54	SER	CB	63.773	-1.0	1
UNMAPPED	178	PRO	CG	27.37	-1.0	1
UNMAPPED	64	ARG	HB2	1.71	-1.0	2
UNMAPPED	79	CYS	HA	4.427	-1.0	1
UNMAPPED	66	TYR	N	115.543	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	4	TRP	CB	29.378	-1.0	1
UNMAPPED	15	LYS	HG2	1.581	-1.0	2
UNMAPPED	191	GLU	N	125.118	-1.0	1
UNMAPPED	163	ASP	HB2	2.947	-1.0	2
UNMAPPED	154	LEU	HB2	0.81	-1.0	2
UNMAPPED	121	PRO	HG2	0.673	-1.0	2
UNMAPPED	3	ASN	HD22	6.813	-1.0	2
UNMAPPED	171	CYS	CA	65.022	-1.0	1
UNMAPPED	62	TYR	CA	61.686	-1.0	1
UNMAPPED	140	TRP	HB3	2.682	-1.0	2
UNMAPPED	80	LEU	HG	1.593	-1.0	1
UNMAPPED	25	CYS	HB3	2.546	-1.0	2
UNMAPPED	49	VAL	HA	4.24	-1.0	1
UNMAPPED	58	CYS	CA	57.56	-1.0	1
UNMAPPED	49	VAL	CA	61.2	-1.0	1
UNMAPPED	26	ASN	N	129.393	-1.0	1
UNMAPPED	152	LYS	CE	41.957	-1.0	1
UNMAPPED	27	GLY	CA	45.439	-1.0	1
UNMAPPED	166	LEU	HD12	1.03	-1.0	2
UNMAPPED	46	SER	CB	62.81	-1.0	1
UNMAPPED	114	PHE	H	8.27	-1.0	1
UNMAPPED	121	PRO	CA	63.903	-1.0	1
UNMAPPED	50	ALA	HA	4.233	-1.0	1
UNMAPPED	52	HIS	CA	56.31	-1.0	1
UNMAPPED	189	GLN	H	8.442	-1.0	1
UNMAPPED	34	CYS	H	7.574	-1.0	1
UNMAPPED	140	TRP	HD1	7.615	-1.0	1
UNMAPPED	9	LYS	N	119.638	-1.0	1
UNMAPPED	3	ASN	HA	4.546	-1.0	1
UNMAPPED	38	MET	HG2	2.84	-1.0	2
UNMAPPED	135	GLY	H	9.068	-1.0	1
UNMAPPED	56	ILE	HB	0.937	-1.0	1
UNMAPPED	72	GLY	H	8.43	-1.0	1
UNMAPPED	55	GLU	CA	54.988	-1.0	1
UNMAPPED	68	PRO	CB	32.003	-1.0	1
UNMAPPED	187	THR	CB	69.74	-1.0	1
UNMAPPED	1	MET	HA	4.318	-1.0	1
UNMAPPED	147	CYS	CB	31.232	-1.0	1
UNMAPPED	149	ILE	HA	4.219	-1.0	1
UNMAPPED	33	THR	N	106.51	-1.0	1
UNMAPPED	2	ALA	CB	18.985	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	42	LYS	CB	33.553	-1.0	1
UNMAPPED	127	VAL	CB	32.92	-1.0	1
UNMAPPED	17	VAL	HG11	0.387	-1.0	2
UNMAPPED	3	ASN	CB	38.577	-1.0	1
UNMAPPED	170	VAL	HG22	0.93	-1.0	2
UNMAPPED	50	ALA	N	131.441	-1.0	1
UNMAPPED	188	GLN	HG2	2.27	-1.0	2
UNMAPPED	164	GLY	HA3	3.732	-1.0	2
UNMAPPED	32	LYS	CG	25.997	-1.0	1
UNMAPPED	32	LYS	HB3	1.89	-1.0	2
UNMAPPED	77	ALA	HB3	1.316	-1.0	1
UNMAPPED	157	THR	HG22	1.159	-1.0	1
UNMAPPED	23	ILE	HG23	-0.086	-1.0	2
UNMAPPED	116	GLU	HA	4.269	-1.0	1
UNMAPPED	166	LEU	CD2	21.523	-1.0	2
UNMAPPED	28	ARG	H	7.857	-1.0	1
UNMAPPED	66	TYR	CA	57.52	-1.0	1
UNMAPPED	76	GLY	H	8.436	-1.0	1
UNMAPPED	66	TYR	HB2	2.797	-1.0	2
UNMAPPED	34	CYS	CB	31.352	-1.0	1
UNMAPPED	113	LYS	CG	24.745	-1.0	1
UNMAPPED	172	TYR	HB2	3.014	-1.0	2
UNMAPPED	35	PHE	CE1	130.274	-1.0	3
UNMAPPED	71	ILE	CG1	27.05	-1.0	1
UNMAPPED	175	ASN	HB3	1.22	-1.0	2
UNMAPPED	33	THR	HG22	1.292	-1.0	1
UNMAPPED	168	CYS	H	9.653	-1.0	1
UNMAPPED	80	LEU	HD22	0.805	-1.0	2
UNMAPPED	47	THR	CA	62.897	-1.0	1
UNMAPPED	174	LYS	H	7.639	-1.0	1
UNMAPPED	128	TYR	N	128.731	-1.0	1
UNMAPPED	165	GLU	HB2	1.886	-1.0	2
UNMAPPED	171	CYS	HB2	3.11	-1.0	2
UNMAPPED	24	GLN	CB	30.104	-1.0	1
UNMAPPED	60	VAL	HB	2.236	-1.0	1
UNMAPPED	38	MET	HE3	2.33	-1.0	1
UNMAPPED	122	ARG	N	118.012	-1.0	1
UNMAPPED	119	LYS	CA	54.235	-1.0	1
UNMAPPED	20	ALA	H	8.141	-1.0	1
UNMAPPED	23	ILE	CB	40.444	-1.0	1
UNMAPPED	49	VAL	N	120.24	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	132	LYS	HB3	1.497	-1.0	2
UNMAPPED	73	TYR	HE1	6.757	-1.0	3
UNMAPPED	154	LEU	CG	26.6	-1.0	1
UNMAPPED	26	ASN	HA	4.45	-1.0	1
UNMAPPED	177	GLY	HA2	4.09	-1.0	2
UNMAPPED	82	THR	HG23	1.123	-1.0	1
UNMAPPED	17	VAL	HG23	0.11	-1.0	2
UNMAPPED	165	GLU	CB	32.696	-1.0	1
UNMAPPED	48	THR	HG21	1.192	-1.0	1
UNMAPPED	179	THR	CB	69.719	-1.0	1
UNMAPPED	187	THR	H	8.134	-1.0	1
UNMAPPED	36	HIS	CB	32.968	-1.0	1
UNMAPPED	147	CYS	H	8.458	-1.0	1
UNMAPPED	28	ARG	HB2	1.866	-1.0	2
UNMAPPED	57	TYR	HB3	2.839	-1.0	2
UNMAPPED	42	LYS	H	8.478	-1.0	1
UNMAPPED	117	SER	HB2	3.713	-1.0	2
UNMAPPED	73	TYR	CB	38.674	-1.0	1
UNMAPPED	16	THR	HG22	0.58	-1.0	1
UNMAPPED	140	TRP	CH2	124.29	-1.0	1
UNMAPPED	173	ALA	CA	54.669	-1.0	1
UNMAPPED	140	TRP	CZ3	122.39	-1.0	1
UNMAPPED	167	TYR	HD1	7.04	-1.0	3
UNMAPPED	168	CYS	HB3	2.728	-1.0	2
UNMAPPED	133	VAL	N	124.757	-1.0	1
UNMAPPED	53	GLU	HB2	2.18	-1.0	2
UNMAPPED	160	THR	HG23	0.451	-1.0	1
UNMAPPED	71	ILE	HG22	0.805	-1.0	2
UNMAPPED	181	ILE	CG1	27.161	-1.0	1
UNMAPPED	143	THR	HG23	1.265	-1.0	1
UNMAPPED	131	GLU	CA	55.6	-1.0	1
UNMAPPED	6	GLY	H	7.673	-1.0	1
UNMAPPED	9	LYS	HG3	1.071	-1.0	2
UNMAPPED	57	TYR	CD1	133.07	-1.0	3
UNMAPPED	25	CYS	H	9.031	-1.0	1
UNMAPPED	49	VAL	CG1	19.188	-1.0	2
UNMAPPED	28	ARG	HD2	3.093	-1.0	2
UNMAPPED	14	GLU	H	7.927	-1.0	1
UNMAPPED	168	CYS	HA	5.022	-1.0	1
UNMAPPED	170	VAL	CG1	22.729	-1.0	2
UNMAPPED	50	ALA	CA	51.309	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	172	TYR	CE1	118.389	-1.0	3
UNMAPPED	161	ASP	H	8.247	-1.0	1
UNMAPPED	192	LYS	CG	24.678	-1.0	1
UNMAPPED	137	GLY	HA2	4.117	-1.0	2
UNMAPPED	145	PHE	HB3	2.557	-1.0	2
UNMAPPED	75	GLN	NE2	112.648	-1.0	1
UNMAPPED	41	ARG	N	116.386	-1.0	1
UNMAPPED	174	LYS	CB	33.012	-1.0	1
UNMAPPED	35	PHE	N	125.539	-1.0	1
UNMAPPED	70	GLY	H	8.179	-1.0	1
UNMAPPED	163	ASP	CA	55.641	-1.0	1
UNMAPPED	133	VAL	HG13	0.511	-1.0	2
UNMAPPED	55	GLU	HA	4.416	-1.0	1
UNMAPPED	23	ILE	H	8.939	-1.0	1
UNMAPPED	125	LYS	CB	34.467	-1.0	1
UNMAPPED	112	ALA	HB3	1.268	-1.0	1
UNMAPPED	37	CYS	HB3	2.767	-1.0	2
UNMAPPED	78	GLY	HA2	3.873	-1.0	2
UNMAPPED	144	CYS	HA	4.352	-1.0	1
UNMAPPED	171	CYS	HA	3.847	-1.0	1
UNMAPPED	191	GLU	CB	30.53	-1.0	1
UNMAPPED	36	HIS	H	7.293	-1.0	1
UNMAPPED	135	GLY	HA3	3.318	-1.0	2
UNMAPPED	157	THR	CB	69.499	-1.0	1
UNMAPPED	73	TYR	HD1	7.025	-1.0	3
UNMAPPED	73	TYR	H	7.997	-1.0	1
UNMAPPED	119	LYS	N	120.421	-1.0	1
UNMAPPED	40	CYS	HB2	3.249	-1.0	2
UNMAPPED	30	PHE	HB3	2.467	-1.0	2
UNMAPPED	45	ASP	CB	43.05	-1.0	1
UNMAPPED	169	LYS	CE	42.18	-1.0	1
UNMAPPED	166	LEU	HG	-0.515	-1.0	1
UNMAPPED	166	LEU	CG	25.765	-1.0	1
UNMAPPED	41	ARG	HG2	1.396	-1.0	2
UNMAPPED	130	ALA	HA	4.166	-1.0	1
UNMAPPED	39	ALA	N	123.973	-1.0	1
UNMAPPED	141	HIS	HD2	7.372	-1.0	1
UNMAPPED	165	GLU	HG2	2.153	-1.0	2
UNMAPPED	142	LYS	HE2	2.9	-1.0	2
UNMAPPED	1	MET	HE3	1.98	-1.0	1
UNMAPPED	173	ALA	N	120.542	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	125	LYS	HG2	1.402	-1.0	2
UNMAPPED	55	GLU	HG2	2.405	-1.0	2
UNMAPPED	49	VAL	H	7.367	-1.0	1
UNMAPPED	134	MET	HG2	2.605	-1.0	2
UNMAPPED	129	ALA	H	8.555	-1.0	1
UNMAPPED	166	LEU	H	8.467	-1.0	1
UNMAPPED	64	ARG	HD2	3.026	-1.0	2
UNMAPPED	127	VAL	HG11	0.396	-1.0	2
UNMAPPED	53	GLU	HG3	1.673	-1.0	2
UNMAPPED	179	THR	H	8.178	-1.0	1
UNMAPPED	64	ARG	CG	27.719	-1.0	1
UNMAPPED	176	PHE	HZ	6.943	-1.0	1
UNMAPPED	149	ILE	HD13	0.828	-1.0	1
UNMAPPED	190	VAL	CA	62.231	-1.0	1
UNMAPPED	3	ASN	N	117.59	-1.0	1
UNMAPPED	25	CYS	HA	4.409	-1.0	1
UNMAPPED	68	PRO	HB3	1.818	-1.0	2
UNMAPPED	127	VAL	HA	3.928	-1.0	1
UNMAPPED	7	GLY	N	108.557	-1.0	1
UNMAPPED	59	LYS	HD2	1.613	-1.0	2
UNMAPPED	60	VAL	HG12	1.015	-1.0	2
UNMAPPED	35	PHE	CA	57.679	-1.0	1
UNMAPPED	12	ALA	HB1	1.752	-1.0	1
UNMAPPED	75	GLN	H	8.178	-1.0	1
UNMAPPED	157	THR	H	7.449	-1.0	1
UNMAPPED	73	TYR	HB2	2.923	-1.0	2
UNMAPPED	57	TYR	CA	56.382	-1.0	1
UNMAPPED	44	LEU	CB	44.891	-1.0	1
UNMAPPED	140	TRP	HZ2	7.28	-1.0	1
UNMAPPED	8	ALA	HB1	1.123	-1.0	1
UNMAPPED	181	ILE	HD12	0.787	-1.0	1
UNMAPPED	45	ASP	H	7.717	-1.0	1
UNMAPPED	34	CYS	N	118.072	-1.0	1
UNMAPPED	189	GLN	N	122.228	-1.0	1
UNMAPPED	75	GLN	CG	33.71	-1.0	1
UNMAPPED	48	THR	CG2	22.558	-1.0	1
UNMAPPED	158	ASN	CA	52.62	-1.0	1
UNMAPPED	125	LYS	HA	4.679	-1.0	1
UNMAPPED	158	ASN	HA	4.853	-1.0	1
UNMAPPED	3	ASN	HD21	7.493	-1.0	2
UNMAPPED	73	TYR	CD1	133.07	-1.0	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	59	LYS	H	8.675	-1.0	1
UNMAPPED	69	LYS	CE	42.061	-1.0	1
UNMAPPED	175	ASN	HD22	7.016	-1.0	2
UNMAPPED	160	THR	H	8.465	-1.0	1
UNMAPPED	58	CYS	CB	31.243	-1.0	1
UNMAPPED	49	VAL	CB	32.319	-1.0	1
UNMAPPED	23	ILE	HD13	0.487	-1.0	1
UNMAPPED	81	SER	H	8.332	-1.0	1
UNMAPPED	126	SER	HB3	3.46	-1.0	2
UNMAPPED	41	ARG	HA	4.085	-1.0	1
UNMAPPED	148	ALA	HB2	1.229	-1.0	1
UNMAPPED	146	ARG	HD2	3.072	-1.0	2
UNMAPPED	32	LYS	HG2	1.39	-1.0	2
UNMAPPED	152	LYS	CG	24.827	-1.0	1
UNMAPPED	193	LYS	CA	57.902	-1.0	1
UNMAPPED	40	CYS	CB	32.635	-1.0	1
UNMAPPED	49	VAL	HG23	0.7	-1.0	2
UNMAPPED	152	LYS	HG2	1.421	-1.0	2
UNMAPPED	43	ALA	HB1	1.311	-1.0	1
UNMAPPED	73	TYR	N	120.24	-1.0	1
UNMAPPED	62	TYR	CD1	133.381	-1.0	3
UNMAPPED	133	VAL	HG22	0.33	-1.0	2
UNMAPPED	47	THR	HA	4.514	-1.0	1
UNMAPPED	145	PHE	N	123.914	-1.0	1
UNMAPPED	154	LEU	H	7.731	-1.0	1
UNMAPPED	71	ILE	N	119.397	-1.0	1
UNMAPPED	116	GLU	HG2	2.176	-1.0	2
UNMAPPED	55	GLU	CB	32.299	-1.0	1
UNMAPPED	68	PRO	CA	63.353	-1.0	1
UNMAPPED	4	TRP	NE1	129.518	-1.0	1
UNMAPPED	60	VAL	CA	66.396	-1.0	1
UNMAPPED	42	LYS	CG	24.497	-1.0	1
UNMAPPED	116	GLU	CG	36.292	-1.0	1
UNMAPPED	81	SER	HB2	3.814	-1.0	2
UNMAPPED	170	VAL	CB	32.341	-1.0	1
UNMAPPED	186	LEU	HD11	0.88	-1.0	2
UNMAPPED	44	LEU	H	7.615	-1.0	1
UNMAPPED	172	TYR	HD1	6.742	-1.0	3
UNMAPPED	141	HIS	N	116.808	-1.0	1
UNMAPPED	132	LYS	CE	41.815	-1.0	1
UNMAPPED	45	ASP	HB3	2.708	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	152	LYS	HE2	3.028	-1.0	2
UNMAPPED	43	ALA	H	8.687	-1.0	1
UNMAPPED	167	TYR	CD1	133.369	-1.0	3
UNMAPPED	121	PRO	CG	27.576	-1.0	1
UNMAPPED	35	PHE	CZ	129.032	-1.0	1
UNMAPPED	53	GLU	CA	58.513	-1.0	1
UNMAPPED	27	GLY	HA2	4.067	-1.0	2
UNMAPPED	15	LYS	H	8.193	-1.0	1
UNMAPPED	144	CYS	HB2	3.342	-1.0	2
UNMAPPED	165	GLU	HA	4.803	-1.0	1
UNMAPPED	134	MET	CE	14.776	-1.0	1
UNMAPPED	151	GLY	CA	46.257	-1.0	1
UNMAPPED	58	CYS	HA	5.174	-1.0	1
UNMAPPED	112	ALA	CB	19.33	-1.0	1
UNMAPPED	133	VAL	CG1	20.503	-1.0	1
UNMAPPED	132	LYS	HD2	1.546	-1.0	2
UNMAPPED	50	ALA	CB	20.367	-1.0	1
UNMAPPED	5	GLY	N	110.966	-1.0	1
UNMAPPED	125	LYS	N	120.06	-1.0	1
UNMAPPED	177	GLY	H	7.479	-1.0	1
UNMAPPED	63	GLY	H	7.92	-1.0	1
UNMAPPED	189	GLN	HA	4.292	-1.0	1
UNMAPPED	73	TYR	CE1	118.471	-1.0	3
UNMAPPED	175	ASN	ND2	113.889	-1.0	1
UNMAPPED	24	GLN	CA	54.308	-1.0	1
UNMAPPED	15	LYS	CE	42.246	-1.0	1
UNMAPPED	130	ALA	CA	54.075	-1.0	1
UNMAPPED	180	GLY	H	8.189	-1.0	1
UNMAPPED	69	LYS	CB	32.713	-1.0	1
UNMAPPED	37	CYS	CA	59.905	-1.0	1
UNMAPPED	154	LEU	CB	42.405	-1.0	1
UNMAPPED	127	VAL	CG1	20.802	-1.0	2
UNMAPPED	152	LYS	CA	57.298	-1.0	1
UNMAPPED	35	PHE	HE1	6.392	-1.0	3
UNMAPPED	48	THR	HG22	1.192	-1.0	1
UNMAPPED	80	LEU	CA	55.146	-1.0	1
UNMAPPED	36	HIS	CA	52.991	-1.0	1
UNMAPPED	4	TRP	HB2	3.19	-1.0	2
UNMAPPED	193	LYS	N	127.404	-1.0	1
UNMAPPED	15	LYS	HA	4.706	-1.0	1
UNMAPPED	73	TYR	CA	58.509	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	82	THR	CA	61.364	-1.0	1
UNMAPPED	52	HIS	CE1	138.661	-1.0	1
UNMAPPED	34	CYS	HA	4.437	-1.0	1
UNMAPPED	122	ARG	HB2	2.29	-1.0	2
UNMAPPED	143	THR	CG2	22.425	-1.0	1
UNMAPPED	186	LEU	HA	4.362	-1.0	1
UNMAPPED	2	ALA	HB3	1.189	-1.0	1
UNMAPPED	147	CYS	HB3	2.671	-1.0	2
UNMAPPED	44	LEU	CD1	21.781	-1.0	2
UNMAPPED	176	PHE	CD1	132.24	-1.0	3
UNMAPPED	60	VAL	CG1	21.033	-1.0	2
UNMAPPED	159	VAL	HA	4.282	-1.0	1
UNMAPPED	129	ALA	HB1	1.396	-1.0	1
UNMAPPED	132	LYS	CB	34.543	-1.0	1
UNMAPPED	55	GLU	HB2	2.018	-1.0	2
UNMAPPED	192	LYS	CB	33.113	-1.0	1
UNMAPPED	149	ILE	HB	2.47	-1.0	1
UNMAPPED	145	PHE	HZ	6.751	-1.0	1
UNMAPPED	167	TYR	HB2	3.261	-1.0	2
UNMAPPED	6	GLY	HA2	3.775	-1.0	2
UNMAPPED	174	LYS	CE	42.017	-1.0	1
UNMAPPED	53	GLU	N	124.214	-1.0	1
UNMAPPED	140	TRP	CD1	128.85	-1.0	1
UNMAPPED	59	LYS	CE	42.188	-1.0	1
UNMAPPED	159	VAL	CG2	20.16	-1.0	2
UNMAPPED	128	TYR	CD1	133.089	-1.0	3
UNMAPPED	151	GLY	N	111.509	-1.0	1
UNMAPPED	150	CYS	CA	59.275	-1.0	1
UNMAPPED	176	PHE	HB3	1.613	-1.0	2
UNMAPPED	44	LEU	N	121.324	-1.0	1
UNMAPPED	118	GLU	N	122.469	-1.0	1
UNMAPPED	19	HIS	CB	29.643	-1.0	1
UNMAPPED	154	LEU	HA	4.379	-1.0	1
UNMAPPED	125	LYS	CA	54.985	-1.0	1
UNMAPPED	134	MET	CB	30.667	-1.0	1
UNMAPPED	154	LEU	HD12	-0.16	-1.0	2
UNMAPPED	191	GLU	CG	36.254	-1.0	1
UNMAPPED	30	PHE	HA	5.686	-1.0	1
UNMAPPED	24	GLN	HB2	1.799	-1.0	2
UNMAPPED	30	PHE	CA	55.858	-1.0	1
UNMAPPED	75	GLN	HE21	7.493	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	134	MET	HE1	1.687	-1.0	1
UNMAPPED	161	ASP	HB2	2.355	-1.0	2
UNMAPPED	114	PHE	HB2	3.09	-1.0	2
UNMAPPED	179	THR	HB	4.222	-1.0	1
UNMAPPED	28	ARG	CA	54.536	-1.0	1
UNMAPPED	120	CYS	N	127.045	-1.0	1
UNMAPPED	169	LYS	HD2	1.64	-1.0	2
UNMAPPED	47	THR	H	8.949	-1.0	1
UNMAPPED	6	GLY	CA	45.108	-1.0	1
UNMAPPED	43	ALA	HA	3.632	-1.0	1
UNMAPPED	68	PRO	CD	49.63	-1.0	1
UNMAPPED	188	GLN	HB3	1.903	-1.0	2
UNMAPPED	20	ALA	CA	54.128	-1.0	1
UNMAPPED	8	ALA	HA	4.261	-1.0	1
UNMAPPED	81	SER	HA	4.443	-1.0	1
UNMAPPED	54	SER	HA	4.574	-1.0	1
UNMAPPED	170	VAL	H	7.774	-1.0	1
UNMAPPED	180	GLY	HA2	3.879	-1.0	2
UNMAPPED	33	THR	HB	4.476	-1.0	1
UNMAPPED	18	TYR	HE1	6.73	-1.0	3
UNMAPPED	50	ALA	HB2	0.678	-1.0	1
UNMAPPED	188	GLN	HB2	2.022	-1.0	2
UNMAPPED	9	LYS	HB3	1.251	-1.0	2
UNMAPPED	154	LEU	HD23	0.468	-1.0	2
UNMAPPED	64	ARG	CD	43.265	-1.0	1
UNMAPPED	60	VAL	HG22	0.856	-1.0	2
UNMAPPED	19	HIS	H	8.557	-1.0	1
UNMAPPED	141	HIS	CB	30.841	-1.0	1
UNMAPPED	23	ILE	CG2	15.81	-1.0	1
UNMAPPED	31	HIS	HE1	7.15	-1.0	1
UNMAPPED	28	ARG	HG2	1.613	-1.0	2
UNMAPPED	140	TRP	H	8.744	-1.0	1
UNMAPPED	166	LEU	HB2	1.14	-1.0	2
UNMAPPED	59	LYS	HG3	1.312	-1.0	2
UNMAPPED	120	CYS	HB2	3.324	-1.0	2
UNMAPPED	116	GLU	CB	30.506	-1.0	1
UNMAPPED	32	LYS	N	126.744	-1.0	1
UNMAPPED	77	ALA	CB	19.191	-1.0	1
UNMAPPED	33	THR	H	8.162	-1.0	1
UNMAPPED	44	LEU	HD23	1.276	-1.0	2
UNMAPPED	52	HIS	HB3	2.583	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	146	ARG	HG2	1.23	-1.0	2
UNMAPPED	188	GLN	H	8.33	-1.0	1
UNMAPPED	56	ILE	CB	41.184	-1.0	1
UNMAPPED	150	CYS	N	118.735	-1.0	1
UNMAPPED	140	TRP	NE1	130.159	-1.0	1
UNMAPPED	118	GLU	CA	56.209	-1.0	1
UNMAPPED	60	VAL	HG23	0.856	-1.0	2
UNMAPPED	127	VAL	HG23	0.082	-1.0	2
UNMAPPED	14	GLU	HB2	2.264	-1.0	2
UNMAPPED	24	GLN	HA	5.158	-1.0	1
UNMAPPED	65	ARG	HA	3.733	-1.0	1
UNMAPPED	80	LEU	HD12	0.854	-1.0	2
UNMAPPED	148	ALA	HA	3.908	-1.0	1
UNMAPPED	44	LEU	HD13	0.432	-1.0	2
UNMAPPED	175	ASN	HD21	7.115	-1.0	2
UNMAPPED	80	LEU	HA	4.353	-1.0	1
UNMAPPED	122	ARG	CG	26.392	-1.0	1
UNMAPPED	4	TRP	HZ2	7.4	-1.0	1
UNMAPPED	28	ARG	N	120.962	-1.0	1
UNMAPPED	4	TRP	CZ3	122.198	-1.0	1
UNMAPPED	38	MET	H	9.015	-1.0	1
UNMAPPED	120	CYS	CA	55.874	-1.0	1
UNMAPPED	135	GLY	CA	45.903	-1.0	1
UNMAPPED	76	GLY	N	110.123	-1.0	1
UNMAPPED	65	ARG	HG2	0.866	-1.0	2
UNMAPPED	12	ALA	HA	4.822	-1.0	1
UNMAPPED	149	ILE	HG23	0.896	-1.0	2
UNMAPPED	24	GLN	HG2	2.132	-1.0	2
UNMAPPED	65	ARG	CG	26.869	-1.0	1
UNMAPPED	128	TYR	H	9.0	-1.0	1
UNMAPPED	46	SER	CA	62.81	-1.0	1
UNMAPPED	150	CYS	HB2	3.202	-1.0	2
UNMAPPED	20	ALA	N	118.915	-1.0	1
UNMAPPED	47	THR	HB	4.315	-1.0	1
UNMAPPED	178	PRO	HA	4.367	-1.0	1
UNMAPPED	140	TRP	CB	31.908	-1.0	1
UNMAPPED	4	TRP	HE3	7.52	-1.0	1
UNMAPPED	113	LYS	H	8.163	-1.0	1
UNMAPPED	80	LEU	CD2	23.208	-1.0	2
UNMAPPED	175	ASN	CA	54.788	-1.0	1
UNMAPPED	186	LEU	HG	1.62	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	121	PRO	HD2	3.78	-1.0	2
UNMAPPED	42	LYS	CD	29.539	-1.0	1
UNMAPPED	187	THR	N	114.881	-1.0	1
UNMAPPED	176	PHE	HE1	6.42	-1.0	3
UNMAPPED	188	GLN	CB	29.629	-1.0	1
UNMAPPED	186	LEU	HD12	0.88	-1.0	2
UNMAPPED	71	ILE	HD13	0.781	-1.0	1
UNMAPPED	69	LYS	HE2	2.869	-1.0	2
UNMAPPED	18	TYR	CA	57.685	-1.0	1
UNMAPPED	123	CYS	HB2	3.17	-1.0	2
UNMAPPED	179	THR	HG21	1.119	-1.0	1
UNMAPPED	41	ARG	CA	57.915	-1.0	1
UNMAPPED	146	ARG	CB	34.971	-1.0	1
UNMAPPED	63	GLY	N	105.787	-1.0	1
UNMAPPED	20	ALA	HB1	1.348	-1.0	1
UNMAPPED	39	ALA	HA	4.797	-1.0	1
UNMAPPED	4	TRP	CE3	121.266	-1.0	1
UNMAPPED	69	LYS	HB2	1.782	-1.0	2
UNMAPPED	139	PRO	HB2	1.753	-1.0	2
UNMAPPED	54	SER	CA	58.432	-1.0	1
UNMAPPED	186	LEU	N	121.505	-1.0	1
UNMAPPED	30	PHE	HB2	3.0	-1.0	2
UNMAPPED	38	MET	CB	31.698	-1.0	1
UNMAPPED	78	GLY	H	8.424	-1.0	1
UNMAPPED	178	PRO	CD	49.797	-1.0	1
UNMAPPED	40	CYS	HA	4.89	-1.0	1
UNMAPPED	121	PRO	HB2	1.989	-1.0	2
UNMAPPED	22	GLU	CA	56.801	-1.0	1
UNMAPPED	4	TRP	CA	57.367	-1.0	1
UNMAPPED	161	ASP	HA	5.526	-1.0	1
UNMAPPED	181	ILE	HA	4.1	-1.0	1
UNMAPPED	10	CYS	HA	4.028	-1.0	1
UNMAPPED	21	GLU	HG2	2.385	-1.0	2
UNMAPPED	56	ILE	HD13	-0.103	-1.0	1
UNMAPPED	10	CYS	CA	57.951	-1.0	1
UNMAPPED	118	GLU	HG2	2.115	-1.0	2
UNMAPPED	128	TYR	CB	38.568	-1.0	1
UNMAPPED	150	CYS	H	8.347	-1.0	1
UNMAPPED	69	LYS	CA	55.9	-1.0	1
UNMAPPED	76	GLY	CA	45.185	-1.0	1
UNMAPPED	167	TYR	CA	55.914	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	179	THR	CA	61.628	-1.0	1
UNMAPPED	166	LEU	HD13	1.03	-1.0	2
UNMAPPED	30	PHE	H	8.813	-1.0	1
UNMAPPED	121	PRO	CB	32.667	-1.0	1
UNMAPPED	46	SER	HA	4.222	-1.0	1
UNMAPPED	82	THR	CB	69.37	-1.0	1
UNMAPPED	26	ASN	HB2	3.199	-1.0	2
UNMAPPED	152	LYS	HD2	1.656	-1.0	2
UNMAPPED	32	LYS	HE2	2.872	-1.0	2
UNMAPPED	141	HIS	CE1	139.02	-1.0	1
UNMAPPED	192	LYS	HB2	1.767	-1.0	2
UNMAPPED	5	GLY	HA2	3.804	-1.0	2
UNMAPPED	38	MET	HG3	2.517	-1.0	2
UNMAPPED	133	VAL	CB	34.526	-1.0	1
UNMAPPED	3	ASN	HB2	2.613	-1.0	2
UNMAPPED	187	THR	CA	61.958	-1.0	1
UNMAPPED	15	LYS	HE2	2.979	-1.0	2
UNMAPPED	2	ALA	CA	52.431	-1.0	1
UNMAPPED	38	MET	HB3	1.519	-1.0	2
UNMAPPED	140	TRP	HH2	7.24	-1.0	1
UNMAPPED	116	GLU	HB2	1.938	-1.0	2
UNMAPPED	8	ALA	CB	20.532	-1.0	1
UNMAPPED	149	ILE	N	118.735	-1.0	1
UNMAPPED	166	LEU	HD23	0.159	-1.0	2
UNMAPPED	151	GLY	H	7.595	-1.0	1
UNMAPPED	17	VAL	HG12	0.387	-1.0	2
UNMAPPED	160	THR	HB	3.436	-1.0	1
UNMAPPED	132	LYS	CA	57.162	-1.0	1
UNMAPPED	63	GLY	CA	46.732	-1.0	1
UNMAPPED	123	CYS	H	7.513	-1.0	1
UNMAPPED	170	VAL	HG23	0.93	-1.0	2
UNMAPPED	46	SER	N	114.097	-1.0	1
UNMAPPED	152	LYS	HB2	1.973	-1.0	2
UNMAPPED	164	GLY	HA2	4.22	-1.0	2
UNMAPPED	32	LYS	HB2	1.999	-1.0	2
UNMAPPED	157	THR	HG23	1.159	-1.0	1
UNMAPPED	77	ALA	N	123.853	-1.0	1
UNMAPPED	23	ILE	HG22	-0.086	-1.0	2
UNMAPPED	122	ARG	H	8.059	-1.0	1
UNMAPPED	150	CYS	CB	32.294	-1.0	1
UNMAPPED	149	ILE	CD1	12.121	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	134	MET	CA	52.848	-1.0	1
UNMAPPED	22	GLU	N	120.722	-1.0	1
UNMAPPED	159	VAL	HG11	0.673	-1.0	2
UNMAPPED	47	THR	HG23	1.177	-1.0	1
UNMAPPED	187	THR	CG2	21.785	-1.0	1
UNMAPPED	23	ILE	HG12	1.161	-1.0	9
UNMAPPED	113	LYS	CD	29.139	-1.0	1
UNMAPPED	148	ALA	CA	54.79	-1.0	1
UNMAPPED	189	GLN	CG	33.807	-1.0	1
UNMAPPED	71	ILE	CG2	17.366	-1.0	1
UNMAPPED	145	PHE	CE1	130.83	-1.0	3
UNMAPPED	13	CYS	HB3	2.936	-1.0	2
UNMAPPED	33	THR	HG23	1.292	-1.0	1
UNMAPPED	10	CYS	N	126.141	-1.0	1
UNMAPPED	30	PHE	CB	43.367	-1.0	1
UNMAPPED	11	GLY	CA	46.785	-1.0	1
UNMAPPED	39	ALA	HB2	1.775	-1.0	1
UNMAPPED	134	MET	HE2	1.687	-1.0	1
UNMAPPED	15	LYS	CA	54.945	-1.0	1
UNMAPPED	181	ILE	CB	38.692	-1.0	1
UNMAPPED	119	LYS	CB	33.795	-1.0	1
UNMAPPED	189	GLN	HB3	1.909	-1.0	2
UNMAPPED	23	ILE	CA	59.951	-1.0	1
UNMAPPED	129	ALA	HA	3.79	-1.0	1
UNMAPPED	76	GLY	HA2	3.883	-1.0	2
UNMAPPED	132	LYS	HB2	1.699	-1.0	2
UNMAPPED	166	LEU	HA	4.547	-1.0	1
UNMAPPED	166	LEU	CA	53.582	-1.0	1
UNMAPPED	45	ASP	N	116.988	-1.0	1
UNMAPPED	17	VAL	HG22	0.11	-1.0	2
UNMAPPED	165	GLU	CA	53.924	-1.0	1
UNMAPPED	144	CYS	H	7.506	-1.0	1
UNMAPPED	173	ALA	HA	4.01	-1.0	1
UNMAPPED	69	LYS	HD2	1.553	-1.0	2
UNMAPPED	28	ARG	HB3	1.58	-1.0	2
UNMAPPED	57	TYR	HB2	3.712	-1.0	2
UNMAPPED	8	ALA	H	8.073	-1.0	1
UNMAPPED	128	TYR	HB2	3.24	-1.0	2
UNMAPPED	130	ALA	H	8.335	-1.0	1
UNMAPPED	16	THR	HG21	0.58	-1.0	1
UNMAPPED	128	TYR	HD1	7.2	-1.0	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	171	CYS	H	8.998	-1.0	1
UNMAPPED	145	PHE	CD1	132.52	-1.0	3
UNMAPPED	173	ALA	CB	18.174	-1.0	1
UNMAPPED	168	CYS	HB2	3.469	-1.0	2
UNMAPPED	161	ASP	N	122.589	-1.0	1
UNMAPPED	140	TRP	N	117.049	-1.0	1
UNMAPPED	174	LYS	HB2	1.733	-1.0	2
UNMAPPED	64	ARG	HG3	1.481	-1.0	2
UNMAPPED	47	THR	CG2	21.833	-1.0	1
UNMAPPED	152	LYS	H	8.49	-1.0	1
UNMAPPED	18	TYR	HB2	3.174	-1.0	2
UNMAPPED	21	GLU	CA	54.993	-1.0	1
UNMAPPED	53	GLU	HB3	1.951	-1.0	2
UNMAPPED	71	ILE	HG23	0.805	-1.0	2
UNMAPPED	44	LEU	HG	-0.234	-1.0	1
UNMAPPED	143	THR	HG22	1.265	-1.0	1
UNMAPPED	131	GLU	CB	31.194	-1.0	1
UNMAPPED	70	GLY	N	109.4	-1.0	1
UNMAPPED	9	LYS	HG2	1.167	-1.0	2
UNMAPPED	140	TRP	HE3	7.389	-1.0	1
UNMAPPED	116	GLU	N	120.301	-1.0	1
UNMAPPED	155	GLU	HB2	2.213	-1.0	2
UNMAPPED	49	VAL	CG2	22.794	-1.0	2
UNMAPPED	57	TYR	H	7.938	-1.0	1
UNMAPPED	170	VAL	CG2	21.566	-1.0	2
UNMAPPED	146	ARG	N	121.866	-1.0	1
UNMAPPED	172	TYR	H	8.982	-1.0	1
UNMAPPED	67	GLY	N	108.918	-1.0	1
UNMAPPED	117	SER	H	8.307	-1.0	1
UNMAPPED	166	LEU	CD1	25.838	-1.0	2
UNMAPPED	80	LEU	HD21	0.805	-1.0	2
UNMAPPED	54	SER	H	8.4	-1.0	1
UNMAPPED	59	LYS	CA	60.366	-1.0	1
UNMAPPED	38	MET	HE1	2.33	-1.0	1
UNMAPPED	52	HIS	HE1	7.715	-1.0	1
UNMAPPED	22	GLU	HB2	1.939	-1.0	2
UNMAPPED	38	MET	N	130.116	-1.0	1
UNMAPPED	31	HIS	CD2	119.403	-1.0	1
UNMAPPED	142	LYS	HB2	1.857	-1.0	2
UNMAPPED	125	LYS	CE	42.351	-1.0	1
UNMAPPED	148	ALA	N	133.308	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	112	ALA	HB2	1.268	-1.0	1
UNMAPPED	37	CYS	HB2	3.328	-1.0	2
UNMAPPED	33	THR	CG2	22.158	-1.0	1
UNMAPPED	39	ALA	H	9.276	-1.0	1
UNMAPPED	144	CYS	CB	31.953	-1.0	1
UNMAPPED	191	GLU	HA	4.212	-1.0	1
UNMAPPED	135	GLY	HA2	4.296	-1.0	2
UNMAPPED	15	LYS	N	119.638	-1.0	1
UNMAPPED	126	SER	CA	59.779	-1.0	1
UNMAPPED	14	GLU	HG2	2.084	-1.0	2
UNMAPPED	12	ALA	N	123.733	-1.0	1
UNMAPPED	79	CYS	HB2	2.838	-1.0	2
UNMAPPED	173	ALA	H	7.771	-1.0	1
UNMAPPED	129	ALA	N	123.793	-1.0	1
UNMAPPED	45	ASP	CA	52.674	-1.0	1
UNMAPPED	58	CYS	N	116.386	-1.0	1
UNMAPPED	169	LYS	CD	29.467	-1.0	1
UNMAPPED	186	LEU	HD23	0.83	-1.0	2
UNMAPPED	167	TYR	HA	5.608	-1.0	1
UNMAPPED	65	ARG	CB	31.435	-1.0	1
UNMAPPED	139	PRO	CD	49.584	-1.0	1
UNMAPPED	1	MET	HE2	1.98	-1.0	1
UNMAPPED	36	HIS	HE1	7.776	-1.0	1
UNMAPPED	152	LYS	CD	29.586	-1.0	1
UNMAPPED	9	LYS	CG	24.428	-1.0	1
UNMAPPED	190	VAL	HG11	0.861	-1.0	2
UNMAPPED	123	CYS	HA	4.934	-1.0	1
UNMAPPED	134	MET	HG3	2.303	-1.0	2
UNMAPPED	40	CYS	H	8.795	-1.0	1
UNMAPPED	29	SER	HB3	3.109	-1.0	2
UNMAPPED	57	TYR	CE1	118.781	-1.0	3
UNMAPPED	55	GLU	N	120.842	-1.0	1
UNMAPPED	67	GLY	HA2	4.089	-1.0	2
UNMAPPED	173	ALA	HB1	1.499	-1.0	1
UNMAPPED	53	GLU	HG2	1.842	-1.0	2
UNMAPPED	149	ILE	CB	37.946	-1.0	1
UNMAPPED	32	LYS	HA	3.957	-1.0	1
UNMAPPED	179	THR	HG22	1.119	-1.0	1
UNMAPPED	149	ILE	HD12	0.828	-1.0	1
UNMAPPED	190	VAL	CB	32.905	-1.0	1
UNMAPPED	162	LYS	CA	56.553	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	20	ALA	HB2	1.348	-1.0	1
UNMAPPED	68	PRO	HB2	2.204	-1.0	2
UNMAPPED	154	LEU	CD1	26.6	-1.0	1
UNMAPPED	51	ALA	HA	5.056	-1.0	1
UNMAPPED	185	GLY	N	108.257	-1.0	1
UNMAPPED	169	LYS	HA	3.911	-1.0	1
UNMAPPED	59	LYS	N	119.276	-1.0	1
UNMAPPED	66	TYR	HE1	6.22	-1.0	3
UNMAPPED	62	TYR	HD1	6.835	-1.0	3
UNMAPPED	180	GLY	CA	45.436	-1.0	1
UNMAPPED	38	MET	CA	59.124	-1.0	1
UNMAPPED	140	TRP	HZ3	7.07	-1.0	1
UNMAPPED	178	PRO	CA	63.374	-1.0	1
UNMAPPED	181	ILE	HD11	0.787	-1.0	1
UNMAPPED	14	GLU	CG	36.688	-1.0	1
UNMAPPED	81	SER	N	116.988	-1.0	1
UNMAPPED	192	LYS	HE2	2.928	-1.0	2
UNMAPPED	50	ALA	H	9.039	-1.0	1
UNMAPPED	181	ILE	HB	1.8	-1.0	1
UNMAPPED	18	TYR	HD1	7.157	-1.0	3
UNMAPPED	186	LEU	HB2	1.6	-1.0	2
UNMAPPED	10	CYS	CB	31.107	-1.0	1
UNMAPPED	126	SER	N	116.928	-1.0	1
UNMAPPED	128	TYR	CA	57.41	-1.0	1
UNMAPPED	42	LYS	HE2	3.022	-1.0	2
UNMAPPED	41	ARG	HB3	1.939	-1.0	2
UNMAPPED	62	TYR	HB3	2.88	-1.0	2
UNMAPPED	69	LYS	CD	28.854	-1.0	1
UNMAPPED	159	VAL	HG23	0.837	-1.0	2
UNMAPPED	119	LYS	HD2	1.38	-1.0	2
UNMAPPED	71	ILE	H	7.944	-1.0	1
UNMAPPED	167	TYR	CB	43.776	-1.0	1
UNMAPPED	154	LEU	N	125.479	-1.0	1
UNMAPPED	23	ILE	HD12	0.487	-1.0	1
UNMAPPED	56	ILE	HG12	1.349	-1.0	9
UNMAPPED	148	ALA	HB3	1.229	-1.0	1
UNMAPPED	181	ILE	CD1	13.221	-1.0	1
UNMAPPED	31	HIS	H	8.518	-1.0	1
UNMAPPED	54	SER	HB2	4.012	-1.0	2
UNMAPPED	133	VAL	HG21	0.33	-1.0	2
UNMAPPED	137	GLY	CA	44.946	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	186	LEU	CD1	25.018	-1.0	2
UNMAPPED	4	TRP	HH2	7.149	-1.0	1
UNMAPPED	9	LYS	CE	41.845	-1.0	1
UNMAPPED	133	VAL	CA	60.481	-1.0	1
UNMAPPED	163	ASP	HA	4.336	-1.0	1
UNMAPPED	158	ASN	HB3	2.756	-1.0	2
UNMAPPED	22	GLU	HG3	1.726	-1.0	2
UNMAPPED	69	LYS	H	8.386	-1.0	1
UNMAPPED	131	GLU	N	114.76	-1.0	1
UNMAPPED	8	ALA	CA	50.993	-1.0	1
UNMAPPED	56	ILE	HG23	0.252	-1.0	2
UNMAPPED	132	LYS	CD	29.887	-1.0	1
UNMAPPED	5	GLY	H	8.295	-1.0	1
UNMAPPED	17	VAL	CB	33.133	-1.0	1
UNMAPPED	45	ASP	HB2	3.16	-1.0	2
UNMAPPED	11	GLY	H	8.497	-1.0	1
UNMAPPED	192	LYS	N	124.034	-1.0	1
UNMAPPED	17	VAL	H	8.741	-1.0	1
UNMAPPED	32	LYS	CE	42.055	-1.0	1
UNMAPPED	23	ILE	HG21	-0.086	-1.0	2
UNMAPPED	186	LEU	CD2	23.436	-1.0	2
UNMAPPED	181	ILE	HG22	0.827	-1.0	2
UNMAPPED	132	LYS	HG2	1.088	-1.0	2
UNMAPPED	53	GLU	CB	26.714	-1.0	1
UNMAPPED	180	GLY	N	110.786	-1.0	1
UNMAPPED	170	VAL	HG13	1.073	-1.0	2
UNMAPPED	159	VAL	HG12	0.673	-1.0	2
UNMAPPED	112	ALA	CA	52.576	-1.0	1
UNMAPPED	49	VAL	HG13	1.007	-1.0	2
UNMAPPED	187	THR	HG22	1.124	-1.0	1
UNMAPPED	114	PHE	HA	4.542	-1.0	1
UNMAPPED	148	ALA	CB	18.926	-1.0	1
UNMAPPED	24	GLN	HE22	6.557	-1.0	2
UNMAPPED	29	SER	CB	64.98	-1.0	1
UNMAPPED	40	CYS	HB3	2.625	-1.0	2
UNMAPPED	58	CYS	HB2	3.457	-1.0	2
UNMAPPED	144	CYS	N	119.458	-1.0	1
UNMAPPED	35	PHE	HD1	6.538	-1.0	3
UNMAPPED	12	ALA	CB	20.885	-1.0	1
UNMAPPED	119	LYS	CG	24.665	-1.0	1
UNMAPPED	9	LYS	H	8.218	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	43	ALA	CA	53.347	-1.0	1
UNMAPPED	21	GLU	N	114.459	-1.0	1
UNMAPPED	79	CYS	N	118.794	-1.0	1
UNMAPPED	154	LEU	CA	54.0	-1.0	1
UNMAPPED	127	VAL	CG2	20.7	-1.0	2
UNMAPPED	82	THR	HG21	1.123	-1.0	1
UNMAPPED	115	GLY	HA2	3.811	-1.0	2
UNMAPPED	17	VAL	HG21	0.11	-1.0	2
UNMAPPED	72	GLY	N	112.311	-1.0	1
UNMAPPED	48	THR	HG23	1.192	-1.0	1
UNMAPPED	80	LEU	CB	42.295	-1.0	1
UNMAPPED	18	TYR	CD1	133.07	-1.0	3
UNMAPPED	65	ARG	N	117.349	-1.0	1
UNMAPPED	25	CYS	CA	58.889	-1.0	1
UNMAPPED	153	SER	CA	59.81	-1.0	1
UNMAPPED	160	THR	CA	61.821	-1.0	1
UNMAPPED	112	ALA	HA	3.818	-1.0	1
UNMAPPED	114	PHE	CA	58.097	-1.0	1
UNMAPPED	66	TYR	CE1	118.781	-1.0	3
UNMAPPED	191	GLU	HB2	1.895	-1.0	2
UNMAPPED	117	SER	HA	4.362	-1.0	1
UNMAPPED	167	TYR	CE1	118.089	-1.0	3
UNMAPPED	160	THR	HG21	0.451	-1.0	1
UNMAPPED	30	PHE	HD1	7.102	-1.0	3
UNMAPPED	143	THR	HG21	1.265	-1.0	1
UNMAPPED	2	ALA	HB2	1.189	-1.0	1
UNMAPPED	145	PHE	HA	4.102	-1.0	1
UNMAPPED	57	TYR	HE1	6.828	-1.0	3
UNMAPPED	56	ILE	CD1	14.367	-1.0	1
UNMAPPED	51	ALA	HB1	1.262	-1.0	1
UNMAPPED	71	ILE	HG13	1.068	-1.0	9
UNMAPPED	159	VAL	HB	1.9	-1.0	1
UNMAPPED	1	MET	HG2	2.446	-1.0	2
UNMAPPED	148	ALA	H	9.05	-1.0	1
UNMAPPED	178	PRO	HB3	1.9	-1.0	2
UNMAPPED	13	CYS	H	8.019	-1.0	1
UNMAPPED	29	SER	H	8.476	-1.0	1
UNMAPPED	167	TYR	HB3	2.742	-1.0	2
UNMAPPED	168	CYS	N	121.144	-1.0	1
UNMAPPED	36	HIS	CE1	137.729	-1.0	1
UNMAPPED	174	LYS	CD	29.507	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	32	LYS	CB	32.115	-1.0	1
UNMAPPED	2	ALA	H	8.244	-1.0	1
UNMAPPED	191	GLU	HG2	2.171	-1.0	2
UNMAPPED	56	ILE	N	115.302	-1.0	1
UNMAPPED	159	VAL	CG1	23.444	-1.0	2
UNMAPPED	3	ASN	H	8.239	-1.0	1
UNMAPPED	82	THR	HA	4.315	-1.0	1
UNMAPPED	112	ALA	HB1	1.268	-1.0	1
UNMAPPED	128	TYR	HA	4.628	-1.0	1
UNMAPPED	122	ARG	HG3	1.744	-1.0	2
UNMAPPED	154	LEU	HD11	-0.16	-1.0	2
UNMAPPED	7	GLY	H	8.008	-1.0	1
UNMAPPED	144	CYS	CA	60.906	-1.0	1
UNMAPPED	60	VAL	H	7.814	-1.0	1
UNMAPPED	80	LEU	H	8.373	-1.0	1
UNMAPPED	75	GLN	N	119.638	-1.0	1
UNMAPPED	149	ILE	CG2	17.732	-1.0	1
UNMAPPED	44	LEU	HB2	0.685	-1.0	2
UNMAPPED	190	VAL	N	121.987	-1.0	1
UNMAPPED	118	GLU	HB2	1.787	-1.0	2
UNMAPPED	124	GLY	CA	46.5	-1.0	1
UNMAPPED	119	LYS	HB2	1.43	-1.0	2
UNMAPPED	114	PHE	HB3	2.97	-1.0	2
UNMAPPED	16	THR	CG2	21.866	-1.0	1
UNMAPPED	28	ARG	CB	32.934	-1.0	1
UNMAPPED	32	LYS	HD2	1.698	-1.0	2
UNMAPPED	177	GLY	CA	44.803	-1.0	1
UNMAPPED	31	HIS	HD2	7.44	-1.0	1
UNMAPPED	62	TYR	HA	3.372	-1.0	1
UNMAPPED	139	PRO	HG2	1.959	-1.0	2
UNMAPPED	17	VAL	CG2	20.6	-1.0	2
UNMAPPED	65	ARG	CA	57.626	-1.0	1
UNMAPPED	80	LEU	HB2	1.585	-1.0	2
UNMAPPED	25	CYS	N	123.01	-1.0	1
UNMAPPED	24	GLN	H	8.42	-1.0	1
UNMAPPED	139	PRO	CG	26.654	-1.0	1
UNMAPPED	1	MET	HE1	1.98	-1.0	1
UNMAPPED	160	THR	N	122.348	-1.0	1
UNMAPPED	64	ARG	H	7.359	-1.0	1
UNMAPPED	114	PHE	HD1	7.184	-1.0	3
UNMAPPED	9	LYS	CD	28.768	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	20	ALA	CB	18.531	-1.0	1
UNMAPPED	192	LYS	CA	56.066	-1.0	1
UNMAPPED	159	VAL	N	118.976	-1.0	1
UNMAPPED	2	ALA	HA	4.119	-1.0	1
UNMAPPED	13	CYS	CB	31.69	-1.0	1
UNMAPPED	165	GLU	H	7.828	-1.0	1
UNMAPPED	157	THR	CG2	21.736	-1.0	1
UNMAPPED	138	LYS	N	120.542	-1.0	1
UNMAPPED	33	THR	HA	4.316	-1.0	1
UNMAPPED	173	ALA	HB2	1.499	-1.0	1
UNMAPPED	32	LYS	H	9.26	-1.0	1
UNMAPPED	46	SER	HB2	3.971	-1.0	2
UNMAPPED	83	ASP	HA	4.642	-1.0	1
UNMAPPED	60	VAL	HG21	0.856	-1.0	2
UNMAPPED	141	HIS	CA	59.255	-1.0	1
UNMAPPED	4	TRP	H	8.056	-1.0	1
UNMAPPED	21	GLU	H	7.68	-1.0	1
UNMAPPED	166	LEU	HB3	0.479	-1.0	2
UNMAPPED	70	GLY	HA2	3.851	-1.0	2
UNMAPPED	59	LYS	HG2	1.493	-1.0	2
UNMAPPED	74	GLY	H	8.372	-1.0	1
UNMAPPED	24	GLN	NE2	111.253	-1.0	1
UNMAPPED	44	LEU	HD22	1.276	-1.0	2
UNMAPPED	52	HIS	HB2	3.051	-1.0	2
UNMAPPED	83	ASP	CB	41.093	-1.0	1
UNMAPPED	10	CYS	HB2	3.343	-1.0	2
UNMAPPED	186	LEU	CG	27.061	-1.0	1
UNMAPPED	140	TRP	CZ2	114.45	-1.0	1
UNMAPPED	18	TYR	H	8.983	-1.0	1
UNMAPPED	8	ALA	HB3	1.123	-1.0	1
UNMAPPED	14	GLU	CB	27.361	-1.0	1
UNMAPPED	46	SER	H	8.883	-1.0	1
UNMAPPED	172	TYR	CA	62.217	-1.0	1
UNMAPPED	9	LYS	HA	3.976	-1.0	1
UNMAPPED	21	GLU	HB3	2.276	-1.0	2
UNMAPPED	181	ILE	HG23	0.827	-1.0	2
UNMAPPED	156	SER	CB	62.962	-1.0	1
UNMAPPED	124	GLY	H	8.238	-1.0	1
UNMAPPED	80	LEU	HD13	0.854	-1.0	2
UNMAPPED	122	ARG	CD	41.831	-1.0	1
UNMAPPED	186	LEU	CA	55.351	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	40	CYS	CA	59.558	-1.0	1
UNMAPPED	125	LYS	H	8.297	-1.0	1
UNMAPPED	177	GLY	N	108.618	-1.0	1
UNMAPPED	22	GLU	H	7.115	-1.0	1
UNMAPPED	181	ILE	HG12	1.341	-1.0	9
UNMAPPED	65	ARG	HG3	0.588	-1.0	2
UNMAPPED	121	PRO	CD	51.483	-1.0	1
UNMAPPED	149	ILE	HG22	0.896	-1.0	2
UNMAPPED	139	PRO	HD2	3.498	-1.0	2
UNMAPPED	80	LEU	N	124.576	-1.0	1
UNMAPPED	24	GLN	HG3	2.035	-1.0	2
UNMAPPED	124	GLY	HA3	3.75	-1.0	2
UNMAPPED	35	PHE	HA	4.123	-1.0	1
UNMAPPED	30	PHE	HE1	7.216	-1.0	3
UNMAPPED	49	VAL	HG21	0.7	-1.0	2
UNMAPPED	145	PHE	CZ	128.85	-1.0	1
UNMAPPED	12	ALA	H	9.165	-1.0	1
UNMAPPED	43	ALA	HB3	1.311	-1.0	1
UNMAPPED	18	TYR	HA	4.581	-1.0	1
UNMAPPED	82	THR	N	115.061	-1.0	1
UNMAPPED	150	CYS	HB3	2.638	-1.0	2
UNMAPPED	188	GLN	HE22	6.8	-1.0	2
UNMAPPED	150	CYS	HA	4.775	-1.0	1
UNMAPPED	175	ASN	CB	40.051	-1.0	1
UNMAPPED	8	ALA	HB2	1.123	-1.0	1
UNMAPPED	146	ARG	HB2	1.29	-1.0	2
UNMAPPED	121	PRO	HD3	2.133	-1.0	2
UNMAPPED	158	ASN	HD21	7.533	-1.0	2
UNMAPPED	42	LYS	CE	41.788	-1.0	1
UNMAPPED	188	GLN	CA	55.752	-1.0	1
UNMAPPED	186	LEU	HD13	0.88	-1.0	2
UNMAPPED	142	LYS	CA	60.818	-1.0	1
UNMAPPED	30	PHE	CD1	132.449	-1.0	3
UNMAPPED	18	TYR	CB	38.542	-1.0	1
UNMAPPED	123	CYS	HB3	2.824	-1.0	2
UNMAPPED	38	MET	CG	34.259	-1.0	1
UNMAPPED	19	HIS	HD2	6.943	-1.0	1
UNMAPPED	187	THR	HG23	1.124	-1.0	1
UNMAPPED	48	THR	HB	4.415	-1.0	1
UNMAPPED	141	HIS	HE1	7.285	-1.0	1
UNMAPPED	168	CYS	CB	31.026	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	41	ARG	CD	42.342	-1.0	1
UNMAPPED	1	MET	CE	16.657	-1.0	1
UNMAPPED	181	ILE	HG21	0.827	-1.0	2
UNMAPPED	65	ARG	HB3	0.556	-1.0	2
UNMAPPED	53	GLU	CG	35.457	-1.0	1
UNMAPPED	16	THR	HA	4.014	-1.0	1
UNMAPPED	155	GLU	HA	4.57	-1.0	1
UNMAPPED	21	GLU	HA	4.497	-1.0	1
UNMAPPED	170	VAL	HB	2.277	-1.0	1
UNMAPPED	189	GLN	HG2	2.28	-1.0	2
UNMAPPED	44	LEU	CG	25.711	-1.0	1
UNMAPPED	38	MET	CE	17.588	-1.0	1
UNMAPPED	187	THR	HG21	1.124	-1.0	1
UNMAPPED	52	HIS	CD2	120.645	-1.0	1
UNMAPPED	121	PRO	HB3	1.149	-1.0	2
UNMAPPED	172	TYR	N	120.542	-1.0	1
UNMAPPED	22	GLU	CB	32.305	-1.0	1
UNMAPPED	24	GLN	HE21	7.282	-1.0	2
UNMAPPED	34	CYS	HB2	3.427	-1.0	2
UNMAPPED	67	GLY	H	7.471	-1.0	1
UNMAPPED	21	GLU	HG3	2.288	-1.0	2
UNMAPPED	56	ILE	HD12	-0.103	-1.0	1
UNMAPPED	75	GLN	CB	29.343	-1.0	1
UNMAPPED	121	PRO	HA	3.976	-1.0	1
UNMAPPED	24	GLN	CG	33.749	-1.0	1
UNMAPPED	30	PHE	N	117.951	-1.0	1
UNMAPPED	169	LYS	HE2	2.884	-1.0	2
UNMAPPED	119	LYS	CD	28.613	-1.0	1
UNMAPPED	181	ILE	N	119.337	-1.0	1
UNMAPPED	182	GLY	CA	45.037	-1.0	1
UNMAPPED	151	GLY	HA3	3.774	-1.0	2
UNMAPPED	165	GLU	CG	36.446	-1.0	1
UNMAPPED	145	PHE	HD1	6.398	-1.0	3
UNMAPPED	175	ASN	H	7.405	-1.0	1
UNMAPPED	61	CYS	HA	3.697	-1.0	1
UNMAPPED	176	PHE	CZ	129.416	-1.0	1
UNMAPPED	128	TYR	HB3	2.849	-1.0	2
UNMAPPED	25	CYS	CB	28.88	-1.0	1
UNMAPPED	189	GLN	HE21	7.5	-1.0	2
UNMAPPED	26	ASN	HB3	2.523	-1.0	2
UNMAPPED	160	THR	CB	70.832	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	22	GLU	HG2	1.951	-1.0	2
UNMAPPED	58	CYS	H	9.429	-1.0	1
UNMAPPED	186	LEU	H	8.125	-1.0	1
UNMAPPED	178	PRO	HG2	1.98	-1.0	2
UNMAPPED	161	ASP	CB	43.838	-1.0	1
UNMAPPED	149	ILE	HG12	1.644	-1.0	9
UNMAPPED	13	CYS	N	116.024	-1.0	1
UNMAPPED	117	SER	CA	58.159	-1.0	1
UNMAPPED	44	LEU	HA	4.385	-1.0	1
UNMAPPED	55	GLU	CG	35.94	-1.0	1
UNMAPPED	118	GLU	HA	4.179	-1.0	1
UNMAPPED	178	PRO	CB	32.251	-1.0	1
UNMAPPED	2	ALA	HB1	1.189	-1.0	1
UNMAPPED	138	LYS	CB	34.327	-1.0	1
UNMAPPED	38	MET	HB2	2.118	-1.0	2
UNMAPPED	142	LYS	N	126.443	-1.0	1
UNMAPPED	158	ASN	ND2	110.106	-1.0	1
UNMAPPED	153	SER	HA	4.187	-1.0	1
UNMAPPED	166	LEU	HD22	0.159	-1.0	2
UNMAPPED	17	VAL	HG13	0.387	-1.0	2
UNMAPPED	83	ASP	H	8.299	-1.0	1
UNMAPPED	51	ALA	HB2	1.262	-1.0	1
UNMAPPED	160	THR	HA	4.348	-1.0	1
UNMAPPED	51	ALA	CA	50.749	-1.0	1
UNMAPPED	141	HIS	HB2	3.613	-1.0	2
UNMAPPED	71	ILE	HB	1.775	-1.0	1
UNMAPPED	129	ALA	HB3	1.396	-1.0	1
UNMAPPED	176	PHE	CE1	130.446	-1.0	3
UNMAPPED	31	HIS	HB2	3.552	-1.0	2
UNMAPPED	191	GLU	H	8.466	-1.0	1
UNMAPPED	174	LYS	CG	25.077	-1.0	1
UNMAPPED	32	LYS	CA	61.131	-1.0	1
UNMAPPED	187	THR	HA	4.33	-1.0	1
UNMAPPED	77	ALA	HB1	1.316	-1.0	1
UNMAPPED	147	CYS	HA	3.7	-1.0	1
UNMAPPED	138	LYS	HA	4.26	-1.0	1
UNMAPPED	83	ASP	N	122.889	-1.0	1
UNMAPPED	119	LYS	HA	4.097	-1.0	1
UNMAPPED	143	THR	CB	68.803	-1.0	1
UNMAPPED	47	THR	HG22	1.177	-1.0	1
UNMAPPED	128	TYR	HE1	6.789	-1.0	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	23	ILE	HG13	0.701	-1.0	9
UNMAPPED	78	GLY	N	108.316	-1.0	1
UNMAPPED	113	LYS	CE	42.122	-1.0	1
UNMAPPED	13	CYS	HB2	3.288	-1.0	2
UNMAPPED	159	VAL	HG21	0.837	-1.0	2
UNMAPPED	4	TRP	HD1	7.17	-1.0	1
UNMAPPED	149	ILE	CG1	28.112	-1.0	1
UNMAPPED	185	GLY	H	7.896	-1.0	1
UNMAPPED	190	VAL	HG12	0.861	-1.0	2
UNMAPPED	22	GLU	HA	4.282	-1.0	1
UNMAPPED	171	CYS	N	124.757	-1.0	1
UNMAPPED	15	LYS	CB	33.658	-1.0	1
UNMAPPED	62	TYR	N	119.999	-1.0	1
UNMAPPED	181	ILE	CA	61.411	-1.0	1
UNMAPPED	60	VAL	HG11	1.015	-1.0	2
UNMAPPED	182	GLY	N	112.231	-1.0	1
UNMAPPED	40	CYS	N	119.156	-1.0	1
UNMAPPED	28	ARG	CG	28.109	-1.0	1
UNMAPPED	35	PHE	HZ	6.836	-1.0	1
UNMAPPED	28	ARG	HA	4.479	-1.0	1
UNMAPPED	26	ASN	CA	53.86	-1.0	1
UNMAPPED	129	ALA	CB	18.688	-1.0	1
UNMAPPED	166	LEU	CB	43.731	-1.0	1
UNMAPPED	135	GLY	N	108.979	-1.0	1
UNMAPPED	17	VAL	CG1	20.485	-1.0	2
UNMAPPED	170	VAL	CA	66.083	-1.0	1
UNMAPPED	138	LYS	H	7.758	-1.0	1
UNMAPPED	52	HIS	N	120.842	-1.0	1
UNMAPPED	68	PRO	HD2	3.576	-1.0	2
UNMAPPED	139	PRO	CB	32.536	-1.0	1
UNMAPPED	63	GLY	HA2	3.761	-1.0	2
UNMAPPED	126	SER	HA	4.267	-1.0	1
UNMAPPED	176	PHE	CA	56.975	-1.0	1
UNMAPPED	116	GLU	H	8.144	-1.0	1
UNMAPPED	83	ASP	HB2	2.633	-1.0	2
UNMAPPED	9	LYS	CA	55.0	-1.0	1
UNMAPPED	164	GLY	CA	45.574	-1.0	1
UNMAPPED	64	ARG	HG2	1.685	-1.0	2
UNMAPPED	13	CYS	CA	58.996	-1.0	1
UNMAPPED	18	TYR	HB3	2.754	-1.0	2
UNMAPPED	31	HIS	CE1	138.351	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	175	ASN	N	114.279	-1.0	1
UNMAPPED	15	LYS	HD2	1.662	-1.0	2
UNMAPPED	74	GLY	HA2	3.818	-1.0	2
UNMAPPED	74	GLY	N	110.966	-1.0	1
UNMAPPED	162	LYS	N	121.866	-1.0	1
UNMAPPED	33	THR	CA	63.217	-1.0	1
UNMAPPED	174	LYS	HA	3.93	-1.0	1
UNMAPPED	59	LYS	HA	3.775	-1.0	1
UNMAPPED	155	GLU	HB3	1.89	-1.0	2
UNMAPPED	39	ALA	HB3	1.775	-1.0	1
UNMAPPED	51	ALA	N	124.696	-1.0	1
UNMAPPED	18	TYR	N	129.273	-1.0	1
UNMAPPED	192	LYS	CE	42.174	-1.0	1
UNMAPPED	18	TYR	CE1	118.16	-1.0	3
UNMAPPED	6	GLY	N	107.955	-1.0	1
UNMAPPED	130	ALA	HB2	1.419	-1.0	1
UNMAPPED	44	LEU	HD21	1.276	-1.0	2
UNMAPPED	83	ASP	CA	54.436	-1.0	1
UNMAPPED	59	LYS	CB	32.345	-1.0	1
UNMAPPED	133	VAL	HA	4.156	-1.0	1
UNMAPPED	184	GLY	CA	45.497	-1.0	1
UNMAPPED	75	GLN	HG2	2.269	-1.0	2
UNMAPPED	133	VAL	HG11	0.511	-1.0	2
UNMAPPED	72	GLY	HA2	3.792	-1.0	2
UNMAPPED	127	VAL	HG21	0.082	-1.0	2
UNMAPPED	146	ARG	HA	4.8	-1.0	1
UNMAPPED	132	LYS	H	7.102	-1.0	1
UNMAPPED	125	LYS	CD	28.921	-1.0	1
UNMAPPED	192	LYS	H	8.399	-1.0	1
UNMAPPED	81	SER	CB	63.752	-1.0	1
UNMAPPED	47	THR	N	113.254	-1.0	1
UNMAPPED	156	SER	CA	61.627	-1.0	1
UNMAPPED	59	LYS	HE2	2.821	-1.0	2
UNMAPPED	139	PRO	HA	4.981	-1.0	1
UNMAPPED	44	LEU	HD11	0.432	-1.0	2
UNMAPPED	126	SER	CB	63.987	-1.0	1
UNMAPPED	122	ARG	CA	57.117	-1.0	1
UNMAPPED	12	ALA	HB3	1.752	-1.0	1
UNMAPPED	11	GLY	N	115.302	-1.0	1
UNMAPPED	155	GLU	H	8.367	-1.0	1
UNMAPPED	134	MET	H	8.177	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	169	LYS	CG	25.709	-1.0	1
UNMAPPED	167	TYR	N	116.206	-1.0	1
UNMAPPED	170	VAL	N	121.144	-1.0	1
UNMAPPED	55	GLU	H	8.664	-1.0	1
UNMAPPED	149	ILE	HG21	0.896	-1.0	2
UNMAPPED	186	LEU	HD22	0.83	-1.0	2
UNMAPPED	69	LYS	HG2	1.36	-1.0	2
UNMAPPED	176	PHE	N	116.326	-1.0	1
UNMAPPED	65	ARG	HD3	2.337	-1.0	2
UNMAPPED	11	GLY	HA3	3.045	-1.0	2

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	163	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	139	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	153	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)

### 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 715. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/295 (0%)	0/118 (0%)	0/118 (0%)	0/59 (0%)
Sidechain	0/339 (0%)	0/202 (0%)	0/118 (0%)	0/19 (0%)
Aromatic	0/81 (0%)	0/42 (0%)	0/32 (0%)	0/7 (0%)
Overall	0/715 (0%)	0/362 (0%)	0/268 (0%)	0/85 (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 720. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/300 (0%)	0/120 (0%)	0/120 (0%)	0/60 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Sidechain	0/339 (0%)	0/202 (0%)	0/118 (0%)	0/19 (0%)
Aromatic	0/81 (0%)	0/42 (0%)	0/32 (0%)	0/7 (0%)
Overall	0/720 (0%)	0/364 (0%)	0/270 (0%)	0/86 (0%)

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

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
???	UNMAPPED	166	LEU	HG	-0.52	3.16 – -0.14	-6.1
???	UNMAPPED	44	LEU	HG	-0.23	3.16 – -0.14	-5.3

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

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