Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:36 PM BST

PDB ID	:	1KOS
Title	:	SOLUTION NMR STRUCTURE OF AN ANALOG OF THE YEAST TRNA PHE T STEM LOOP CONTAINING RIBOTHYMIDINE AT ITS NATURALLY OCCURRING POSITION
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Deposited on	:	1999-05-03

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

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

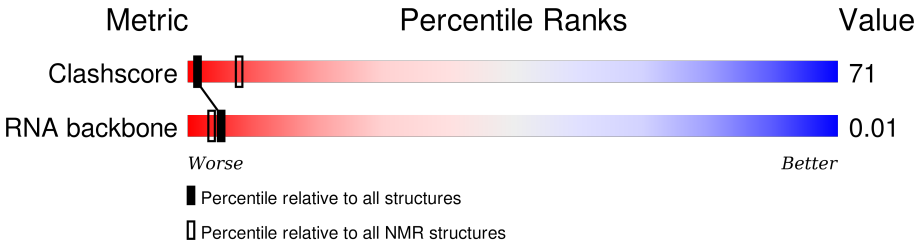
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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
RNA backbone	3027	600

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

Mol	Chain	Length	Quality of chain
1	A	17	6% 18% 76%

2 Ensemble composition and analysis (i)

This entry contains 8 models. This entry does not contain protein, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 543 atoms, of which 187 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	17	543	161	187	60	119	16	0

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: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 

4.2.2 Score per residue for model 2

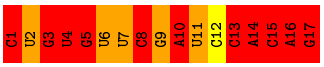
• Molecule 1: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 

4.2.3 Score per residue for model 3

• Molecule 1: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 



4.2.4 Score per residue for model 4

• Molecule 1: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 

4.2.5 Score per residue for model 5

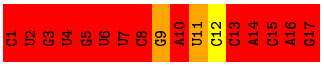
• Molecule 1: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 

4.2.6 Score per residue for model 6

• Molecule 1: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 



4.2.7 Score per residue for model 7

• Molecule 1: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 

4.2.8 Score per residue for model 8

• Molecule 1: 5'-R(*CP*UP*GP*UP*GP*(5MU)P*UP*CP*GP*AP*UP*(CH)P*CP*AP*CP*AP*G)- 3'

Chain A: 

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY AND SIMULATED ANNEALING*.

Of the 50 calculated structures, 8 were deposited, based on the following criterion: *LOWEST ENERGY STRUCTURES*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
X-PLOR	structure solution	

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 4984
Number of chemical shift lists	1
Total number of shifts	1712
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1712
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: 5MU, CH

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	1.91±0.03	9±1/350 (2.5±0.3%)	3.34±0.07	61±4/541 (11.2±0.8%)
All	All	1.91	71/2800 (2.5%)	3.34	486/4328 (11.2%)

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	0.1±0.3	0.0±0.0
All	All	1	0

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	5	G	N9-C8	-11.48	1.29	1.37	2	8
1	A	3	G	N9-C8	-8.69	1.31	1.37	6	8
1	A	17	G	N9-C8	-8.28	1.32	1.37	4	8
1	A	17	G	N9-C4	-7.09	1.32	1.38	2	6
1	A	15	C	N1-C6	-6.91	1.33	1.37	2	8
1	A	13	C	N1-C6	-6.79	1.33	1.37	7	3
1	A	1	C	C2'-C1'	-6.50	1.46	1.53	7	7
1	A	5	G	C2'-C1'	-6.31	1.46	1.53	2	6
1	A	8	C	C3'-C2'	-6.18	1.46	1.52	7	7
1	A	3	G	C2'-C1'	-6.10	1.46	1.53	5	2
1	A	16	A	N9-C8	-6.00	1.32	1.37	7	4
1	A	1	C	C4-C5	-5.59	1.38	1.43	4	4

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	16	A	O4'-C1'-N9	19.91	124.13	108.20	2	8
1	A	1	C	O4'-C1'-N1	19.41	123.73	108.20	8	8
1	A	17	G	N9-C1'-C2'	-17.47	91.28	114.00	6	8
1	A	4	U	O4'-C1'-N1	13.79	119.23	108.20	5	8
1	A	11	U	O4'-C1'-N1	13.69	119.15	108.20	2	8
1	A	3	G	O4'-C1'-N9	13.10	118.68	108.20	6	7
1	A	13	C	O4'-C1'-C2'	-12.49	93.31	105.80	5	2
1	A	13	C	C5'-C4'-O4'	12.41	123.99	109.10	4	8
1	A	16	A	N9-C1'-C2'	-12.03	98.37	114.00	4	8
1	A	7	U	C5'-C4'-O4'	11.98	123.47	109.10	1	8
1	A	3	G	N9-C1'-C2'	-11.71	98.77	114.00	7	8
1	A	5	G	N7-C8-N9	11.55	118.88	113.10	4	8
1	A	3	G	C3'-C2'-C1'	11.25	110.50	101.50	3	8
1	A	15	C	C3'-C2'-C1'	11.12	110.40	101.50	8	8
1	A	3	G	N7-C8-N9	11.10	118.65	113.10	2	8
1	A	1	C	C3'-C2'-C1'	10.47	109.88	101.50	6	7
1	A	8	C	C3'-C2'-C1'	10.29	109.74	101.50	3	7
1	A	16	A	C3'-C2'-C1'	10.22	109.68	101.50	4	8
1	A	1	C	N1-C1'-C2'	-10.17	100.78	114.00	8	7
1	A	17	G	C1'-O4'-C4'	-10.00	101.90	109.90	4	7
1	A	1	C	C1'-O4'-C4'	-9.41	102.37	109.90	1	8
1	A	1	C	O4'-C1'-C2'	-9.28	96.52	105.80	2	8
1	A	3	G	C1'-O4'-C4'	-9.24	102.51	109.90	6	5
1	A	4	U	P-O3'-C3'	9.18	130.72	119.70	3	8
1	A	5	G	N9-C1'-C2'	-9.12	101.97	112.00	8	6
1	A	14	A	N7-C8-N9	8.84	118.22	113.80	8	7
1	A	17	G	C5-N7-C8	-8.84	99.88	104.30	2	8
1	A	5	G	C5-N7-C8	-8.81	99.90	104.30	7	8
1	A	17	G	O4'-C1'-N9	8.75	115.20	108.20	6	1
1	A	14	A	C5'-C4'-O4'	8.65	119.48	109.10	7	7
1	A	1	C	P-O3'-C3'	8.62	130.05	119.70	8	7
1	A	10	A	O4'-C1'-N9	8.40	114.92	108.20	3	8
1	A	7	U	C4'-C3'-C2'	-8.40	94.20	102.60	7	8
1	A	7	U	N1-C1'-C2'	-8.33	102.84	112.00	3	2
1	A	3	G	C5-N7-C8	-8.32	100.14	104.30	4	8
1	A	14	A	C2'-C3'-O3'	8.31	127.79	109.50	7	6
1	A	15	C	O4'-C1'-N1	8.27	114.81	108.20	8	6
1	A	15	C	N1-C1'-C2'	-8.16	103.02	112.00	3	8
1	A	17	G	N7-C8-N9	8.14	117.17	113.10	4	8
1	A	13	C	P-O3'-C3'	8.04	129.35	119.70	7	2
1	A	13	C	C2'-C3'-O3'	8.01	127.12	109.50	4	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	11	U	C1'-O4'-C4'	-7.95	103.54	109.90	8	1
1	A	15	C	P-O3'-C3'	7.84	129.11	119.70	1	6
1	A	8	C	O4'-C1'-N1	7.69	114.35	108.20	8	6
1	A	15	C	N3-C4-N4	7.67	123.37	118.00	7	7
1	A	5	G	C3'-C2'-C1'	7.63	107.60	101.50	1	3
1	A	14	A	C3'-C2'-C1'	7.62	107.60	101.50	6	6
1	A	2	U	P-O3'-C3'	7.53	128.74	119.70	5	2
1	A	5	G	C2'-C3'-O3'	7.52	126.05	109.50	7	2
1	A	14	A	N9-C1'-C2'	-7.45	103.81	112.00	8	2
1	A	9	G	N7-C8-N9	7.32	116.76	113.10	5	8
1	A	16	A	O4'-C1'-C2'	-7.22	98.58	105.80	6	4
1	A	2	U	O4'-C1'-N1	7.20	113.96	108.20	7	4
1	A	10	A	P-O3'-C3'	7.20	128.34	119.70	4	1
1	A	2	U	P-O5'-C5'	7.07	132.21	120.90	2	1
1	A	9	G	P-O3'-C3'	7.05	128.16	119.70	3	6
1	A	5	G	C5'-C4'-O4'	7.04	117.55	109.10	1	1
1	A	15	C	C5-C4-N4	-6.99	115.31	120.20	1	7
1	A	2	U	O4'-C1'-C2'	-6.93	98.87	105.80	7	4
1	A	1	C	N3-C4-N4	6.92	122.85	118.00	4	8
1	A	1	C	C5-C4-N4	-6.88	115.39	120.20	4	8
1	A	14	A	N1-C6-N6	6.81	122.69	118.60	8	2
1	A	3	G	P-O3'-C3'	6.71	127.76	119.70	8	7
1	A	14	A	C5-N7-C8	-6.68	100.56	103.90	8	2
1	A	13	C	N1-C1'-C2'	-6.65	104.68	112.00	4	5
1	A	8	C	P-O3'-C3'	6.58	127.59	119.70	2	4
1	A	1	C	C4'-C3'-C2'	-6.48	96.12	102.60	2	1
1	A	5	G	C4-N9-C1'	6.37	134.78	126.50	5	4
1	A	2	U	C1'-O4'-C4'	-6.36	104.81	109.90	6	2
1	A	17	G	P-O5'-C5'	6.36	131.07	120.90	2	1
1	A	1	C	C2'-C3'-O3'	6.35	123.87	113.70	2	1
1	A	4	U	O4'-C1'-C2'	-6.30	99.50	105.80	5	4
1	A	6	5MU	P-O3'-C3'	6.30	127.27	119.70	7	4
1	A	3	G	N3-C2-N2	6.29	124.31	119.90	5	5
1	A	5	G	C4'-C3'-C2'	6.24	108.84	102.60	7	3
1	A	13	C	C4'-C3'-C2'	-6.24	96.36	102.60	4	1
1	A	13	C	P-O5'-C5'	6.20	130.81	120.90	5	1
1	A	3	G	C5'-C4'-O4'	6.18	116.52	109.10	6	2
1	A	4	U	C3'-C2'-C1'	6.09	106.37	101.50	7	4
1	A	2	U	C5'-C4'-O4'	6.03	116.33	109.10	7	3
1	A	10	A	N7-C8-N9	5.98	116.79	113.80	2	8
1	A	13	C	C1'-O4'-C4'	-5.97	105.13	109.90	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	14	A	C5-C6-N6	-5.93	118.96	123.70	8	1
1	A	16	A	C1'-O4'-C4'	-5.91	105.17	109.90	8	4
1	A	7	U	P-O3'-C3'	5.91	126.79	119.70	1	1
1	A	9	G	O4'-C1'-N9	-5.88	103.50	108.20	5	7
1	A	16	A	P-O3'-C3'	5.84	126.70	119.70	2	1
1	A	5	G	O4'-C1'-N9	-5.80	103.56	108.20	3	1
1	A	17	G	C3'-C2'-O2'	5.78	130.05	113.30	2	7
1	A	15	C	N1-C2-O2	5.75	122.35	118.90	5	2
1	A	5	G	C8-N9-C1'	-5.73	119.55	127.00	5	1
1	A	14	A	P-O5'-C5'	5.73	130.07	120.90	7	1
1	A	16	A	P-O5'-C5'	5.60	129.86	120.90	8	1
1	A	5	G	C4'-C3'-O3'	5.56	124.12	113.00	8	1
1	A	5	G	C1'-C2'-O2'	-5.50	94.09	110.60	8	3
1	A	9	G	P-O5'-C5'	5.49	129.68	120.90	4	1
1	A	7	U	C6-N1-C1'	-5.40	113.64	121.20	1	2
1	A	14	A	P-O3'-C3'	5.38	126.16	119.70	1	1
1	A	14	A	O4'-C1'-C2'	-5.38	100.42	105.80	2	2
1	A	9	G	C5-N7-C8	-5.29	101.65	104.30	5	5
1	A	15	C	C4'-C3'-C2'	-5.25	97.34	102.60	4	1
1	A	13	C	C6-N1-C2	5.18	122.37	120.30	7	2
1	A	13	C	C3'-C2'-C1'	5.09	105.57	101.50	5	1
1	A	1	C	C1'-C2'-O2'	-5.08	95.35	110.60	1	1
1	A	1	C	C5'-C4'-O4'	5.08	115.19	109.10	2	1
1	A	7	U	C2-N1-C1'	5.03	123.74	117.70	4	1
1	A	17	G	N3-C4-C5	5.03	131.12	128.60	2	1
1	A	16	A	N7-C8-N9	5.01	116.31	113.80	8	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	8	C	C2'	1

There are no planarity outliers.

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	356	187	186	38±3
All	All	2848	1496	1494	308

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 71.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:G:O2'	1:A:6:5MU:H2'	0.97	1.59	5	4
1:A:6:5MU:O2'	1:A:7:U:H5"	0.92	1.63	4	1
1:A:14:A:HO2'	1:A:15:C:H6	0.92	1.06	5	6
1:A:6:5MU:O2'	1:A:7:U:H5'	0.84	1.73	3	1
1:A:5:G:HO2'	1:A:6:5MU:H2'	0.77	1.33	2	2
1:A:1:C:O2'	1:A:2:U:C6	0.76	2.39	8	7
1:A:13:C:O2'	1:A:14:A:H5'	0.69	1.88	4	3
1:A:5:G:N3	1:A:14:A:C2	0.66	2.64	6	8
1:A:5:G:H4'	1:A:6:5MU:H71	0.65	1.67	8	4
1:A:5:G:C3'	1:A:6:5MU:H71	0.65	2.22	6	3
1:A:14:A:C5	1:A:15:C:C4	0.63	2.86	4	7
1:A:5:G:O2'	1:A:6:5MU:C6	0.63	2.51	5	7
1:A:13:C:H2'	1:A:14:A:C8	0.63	2.29	7	1
1:A:14:A:O2'	1:A:15:C:C6	0.62	2.52	2	8
1:A:12:CH:OP2	1:A:12:CH:H6	0.62	1.93	5	1
1:A:5:G:C4	1:A:6:5MU:H72	0.62	2.30	3	1
1:A:11:U:H5'	1:A:12:CH:O5'	0.61	1.95	2	2
1:A:14:A:O2'	1:A:15:C:H6	0.61	1.77	7	6
1:A:3:G:O2'	1:A:4:U:C6	0.61	2.54	3	8
1:A:11:U:H4'	1:A:12:CH:OP2	0.60	1.96	4	2
1:A:5:G:C5	1:A:6:5MU:H72	0.60	2.31	3	1
1:A:5:G:O3'	1:A:6:5MU:H3'	0.59	1.97	7	3
1:A:6:5MU:O2'	1:A:7:U:C6	0.59	2.56	1	4
1:A:5:G:C2	1:A:6:5MU:C4	0.59	2.91	4	1
1:A:5:G:C4'	1:A:6:5MU:H71	0.59	2.28	8	5
1:A:4:U:H1'	1:A:5:G:O4'	0.59	1.98	3	3
1:A:13:C:H2'	1:A:13:C:OP2	0.58	1.99	5	1
1:A:15:C:C5	1:A:16:A:N7	0.57	2.72	7	8
1:A:5:G:O2'	1:A:6:5MU:C2'	0.57	2.53	8	1
1:A:1:C:O2'	1:A:2:U:C5	0.57	2.57	2	1
1:A:12:CH:O4'	1:A:13:C:H5	0.57	1.83	7	5
1:A:1:C:O2'	1:A:2:U:H5	0.57	1.83	2	1
1:A:4:U:C2	1:A:5:G:C8	0.56	2.93	8	3
1:A:16:A:O2'	1:A:17:G:C8	0.56	2.57	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:C:C2'	1:A:2:U:C6	0.56	2.89	6	6
1:A:5:G:HO2'	1:A:6:5MU:C2'	0.55	2.14	8	2
1:A:7:U:H3'	1:A:7:U:OP2	0.55	2.02	6	1
1:A:12:CH:OP1	1:A:13:C:C5	0.54	2.60	4	1
1:A:5:G:N3	1:A:14:A:N1	0.54	2.56	3	5
1:A:10:A:O3'	1:A:12:CH:H5'	0.54	2.02	8	3
1:A:3:G:H2'	1:A:4:U:C6	0.54	2.38	6	8
1:A:15:C:N4	1:A:16:A:N6	0.53	2.57	1	7
1:A:3:G:C5	1:A:4:U:C4	0.53	2.97	8	8
1:A:13:C:O2'	1:A:14:A:H8	0.53	1.87	8	3
1:A:5:G:N2	1:A:14:A:C5	0.52	2.78	1	3
1:A:12:CH:O4'	1:A:13:C:C5	0.52	2.63	2	6
1:A:2:U:C2	1:A:3:G:N7	0.52	2.78	8	8
1:A:6:5MU:H73	1:A:8:C:OP2	0.51	2.04	3	1
1:A:6:5MU:O4'	1:A:7:U:H5	0.51	1.87	8	1
1:A:13:C:HO2'	1:A:14:A:H8	0.51	1.44	8	2
1:A:6:5MU:C5	1:A:7:U:O2'	0.51	2.64	3	1
1:A:5:G:O2'	1:A:6:5MU:H6	0.51	1.87	5	4
1:A:5:G:O3'	1:A:6:5MU:H71	0.51	2.06	2	2
1:A:5:G:N2	1:A:14:A:C4	0.50	2.79	4	3
1:A:5:G:C2	1:A:14:A:C6	0.50	2.99	4	5
1:A:15:C:C4	1:A:16:A:N7	0.50	2.80	7	5
1:A:2:U:C2	1:A:3:G:C5	0.50	2.99	6	3
1:A:3:G:C2'	1:A:4:U:C6	0.50	2.94	8	8
1:A:2:U:OP2	1:A:2:U:H3'	0.49	2.07	5	2
1:A:16:A:N6	1:A:17:G:C6	0.49	2.80	7	2
1:A:10:A:OP2	1:A:10:A:H3'	0.49	2.06	6	1
1:A:4:U:H4'	1:A:5:G:OP1	0.49	2.07	5	2
1:A:13:C:C2'	1:A:14:A:C8	0.49	2.95	7	1
1:A:5:G:C2	1:A:7:U:O2'	0.49	2.66	7	1
1:A:1:C:H4'	1:A:2:U:OP1	0.48	2.08	3	4
1:A:14:A:O2'	1:A:15:C:H5"	0.48	2.08	1	3
1:A:3:G:N2	1:A:15:C:N3	0.48	2.59	4	6
1:A:5:G:N2	1:A:14:A:C6	0.47	2.82	1	1
1:A:5:G:C2'	1:A:6:5MU:H2'	0.47	2.39	7	2
1:A:5:G:H4'	1:A:6:5MU:OP1	0.47	2.09	4	1
1:A:6:5MU:O2'	1:A:7:U:C5	0.47	2.68	1	1
1:A:12:CH:OP1	1:A:13:C:H5	0.47	1.90	4	2
1:A:11:U:O2'	1:A:12:CH:H5	0.47	2.10	8	1
1:A:16:A:O2'	1:A:17:G:O4'	0.47	2.33	8	7
1:A:15:C:C4	1:A:16:A:C5	0.47	3.03	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:U:H2'	1:A:12:CH:C6	0.46	2.40	5	1
1:A:15:C:O2'	1:A:16:A:O4'	0.46	2.32	8	3
1:A:7:U:P	1:A:7:U:H2'	0.46	2.51	2	1
1:A:5:G:H4'	1:A:6:5MU:C5M	0.46	2.40	6	1
1:A:7:U:OP2	1:A:7:U:H2'	0.45	2.11	8	2
1:A:13:C:O2'	1:A:14:A:C8	0.45	2.68	8	2
1:A:2:U:HO2'	1:A:3:G:H8	0.44	1.53	8	2
1:A:5:G:C2	1:A:14:A:N1	0.44	2.86	7	2
1:A:2:U:H3'	1:A:2:U:OP2	0.44	2.13	6	2
1:A:14:A:C8	1:A:15:C:C5	0.43	3.07	5	1
1:A:3:G:O2'	1:A:4:U:O4'	0.43	2.36	7	3
1:A:5:G:H5"	1:A:6:5MU:OP2	0.43	2.13	3	1
1:A:5:G:C2	1:A:6:5MU:O4	0.43	2.72	3	1
1:A:6:5MU:O2'	1:A:7:U:H6	0.43	1.93	4	1
1:A:2:U:OP2	1:A:2:U:H2'	0.43	2.14	2	1
1:A:3:G:H4'	1:A:4:U:OP1	0.43	2.13	7	1
1:A:6:5MU:H4'	1:A:7:U:OP1	0.42	2.13	5	1
1:A:14:A:C2	1:A:15:C:C2	0.42	3.06	7	3
1:A:5:G:H2'	1:A:6:5MU:C6	0.42	2.48	3	1
1:A:7:U:H1'	1:A:8:C:OP1	0.42	2.14	6	1
1:A:2:U:H1'	1:A:3:G:C8	0.42	2.49	6	1
1:A:12:CH:H2'	1:A:12:CH:OP2	0.42	2.15	5	1
1:A:14:A:C6	1:A:15:C:C4	0.42	3.08	7	1
1:A:2:U:C2	1:A:3:G:C8	0.42	3.08	3	3
1:A:5:G:C2'	1:A:6:5MU:C6	0.42	3.03	3	2
1:A:1:C:C6	1:A:1:C:O2'	0.42	2.72	2	1
1:A:7:U:H6	1:A:7:U:O5'	0.41	1.97	2	1
1:A:14:A:C4	1:A:15:C:C4	0.41	3.09	4	1
1:A:6:5MU:H4'	1:A:7:U:O5'	0.41	2.16	8	1
1:A:5:G:O2'	1:A:6:5MU:O4'	0.40	2.39	4	1
1:A:1:C:HO2'	1:A:2:U:H5	0.40	1.52	2	1
1:A:11:U:H5'	1:A:12:CH:C5'	0.40	2.46	1	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

There are no protein molecules in this entry.

6.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	16/17 (94%)	14±1 (90±4%)	9±1 (59±6%)	0.01±0.01
All	All	128/136 (94%)	115 (90%)	75 (59%)	0.01

The overall RNA backbone suiteness is 0.01.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	9	G	8
1	A	15	C	8
1	A	16	A	8
1	A	11	U	8
1	A	10	A	8
1	A	6	5MU	8
1	A	5	G	8
1	A	14	A	8
1	A	13	C	8
1	A	4	U	8
1	A	8	C	8
1	A	3	G	8
1	A	2	U	8
1	A	7	U	6
1	A	17	G	5

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	14	A	8
1	A	13	C	8
1	A	4	U	8
1	A	1	C	8
1	A	3	G	8
1	A	2	U	8
1	A	15	C	6
1	A	6	5MU	6
1	A	7	U	4
1	A	8	C	4

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Mol	Chain	Res	Type	Models (Total)
1	A	16	A	3
1	A	10	A	2
1	A	9	G	2

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	CH	A	12	1	13,21,22	1.11±0.07	0±0 (0±0%)
1	5MU	A	6	1	12,22,23	1.75±0.13	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	CH	A	12	1	16,30,33	1.23±0.29	0±0 (0±2%)
1	5MU	A	6	1	15,32,35	2.87±0.75	2±1 (11±7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CH	A	12	1	-	0±0,3,25,26	0±0,2,2,2
1	5MU	A	6	1	-	0±0,3,25,26	0±0,2,2,2

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	6	5MU	O4'-C1'-N1	10.40	127.86	108.10	1	5
1	A	6	5MU	C4'-O4'-C1'	6.42	102.84	109.64	1	3
1	A	6	5MU	C5M-C5-C4	6.41	127.65	120.79	3	2
1	A	6	5MU	O2'-C2'-C3'	5.44	129.45	111.86	8	4
1	A	12	CH	O4'-C1'-N1	5.20	117.99	108.10	5	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4984

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	1712
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1712
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- Chain not found in structure. All 1712 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	40	THR	HG23	1.268	-1.0	1
UNMAPPED	101	VAL	HG12	0.899	-1.0	1
UNMAPPED	37	SER	CB	64.267	-1.0	1
UNMAPPED	39	ILE	HG13	0.91	-1.0	2
UNMAPPED	130	GLY	N	108.216	-1.0	1
UNMAPPED	69	LEU	HB2	1.7	-1.0	2
UNMAPPED	32	MET	HG2	2.269	-1.0	2
UNMAPPED	54	ASN	HB2	2.81	-1.0	2
UNMAPPED	25	PHE	CB	45.19	-1.0	1
UNMAPPED	72	SER	HB2	3.968	-1.0	2
UNMAPPED	117	LYS	CE	42.25	-1.0	1
UNMAPPED	67	LYS	CB	33.668	-1.0	1
UNMAPPED	21	GLN	C	179.0	-1.0	1
UNMAPPED	133	ILE	HA	4.07	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	98	VAL	CA	63.249	-1.0	1
UNMAPPED	78	MET	H	7.22	-1.0	1
UNMAPPED	94	LEU	HD13	0.912	-1.0	1
UNMAPPED	111	LEU	CA	55.156	-1.0	1
UNMAPPED	10	GLU	HG3	2.228	-1.0	2
UNMAPPED	104	ILE	CG2	18.708	-1.0	1
UNMAPPED	41	PRO	HD2	4.05	-1.0	2
UNMAPPED	26	ASP	HB2	2.84	-1.0	2
UNMAPPED	14	LEU	CA	54.396	-1.0	1
UNMAPPED	12	GLU	H	8.71	-1.0	1
UNMAPPED	18	ILE	HG22	1.138	-1.0	1
UNMAPPED	37	SER	C	179.3	-1.0	1
UNMAPPED	8	LEU	CB	43.031	-1.0	1
UNMAPPED	133	ILE	N	127.314	-1.0	1
UNMAPPED	23	LEU	HD12	0.59	-1.0	1
UNMAPPED	31	GLU	HG3	2.12	-1.0	2
UNMAPPED	82	ILE	N	128.01	-1.0	1
UNMAPPED	54	ASN	CA	52.028	-1.0	1
UNMAPPED	93	PHE	CD1	133.204	-1.0	3
UNMAPPED	130	GLY	C	178.9	-1.0	1
UNMAPPED	30	ILE	HG13	1.435	-1.0	2
UNMAPPED	72	SER	H	8.18	-1.0	1
UNMAPPED	144	GLU	HB2	2.17	-1.0	2
UNMAPPED	138	ILE	CG2	16.65	-1.0	1
UNMAPPED	20	GLU	HB2	2.215	-1.0	2
UNMAPPED	21	GLN	H	8.24	-1.0	1
UNMAPPED	64	ASN	H	9.19	-1.0	1
UNMAPPED	38	ASP	H	8.3	-1.0	1
UNMAPPED	68	ILE	CG1	28.517	-1.0	1
UNMAPPED	34	ILE	HD12	0.76	-1.0	1
UNMAPPED	100	GLY	H	7.28	-1.0	1
UNMAPPED	121	LYS	CG	26.235	-1.0	1
UNMAPPED	79	LYS	H	7.85	-1.0	1
UNMAPPED	138	ILE	HA	3.79	-1.0	1
UNMAPPED	133	ILE	CG1	27.3	-1.0	1
UNMAPPED	76	GLN	CG	34.676	-1.0	1
UNMAPPED	49	VAL	HB	2.14	-1.0	1
UNMAPPED	135	TYR	CB	37.995	-1.0	1
UNMAPPED	40	THR	CA	61.0	-1.0	1
UNMAPPED	6	ASP	N	120.946	-1.0	1
UNMAPPED	148	LYS	HD2	1.85	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	142	ILE	HG13	1.19	-1.0	2
UNMAPPED	11	PHE	HA	4.975	-1.0	1
UNMAPPED	126	VAL	HB	1.85	-1.0	1
UNMAPPED	19	ASP	CB	39.659	-1.0	1
UNMAPPED	114	VAL	C	176.4	-1.0	1
UNMAPPED	2	LYS	CE	42.478	-1.0	1
UNMAPPED	8	LEU	HD21	0.909	-1.0	1
UNMAPPED	140	LYS	HB2	1.74	-1.0	2
UNMAPPED	132	LEU	CA	54.475	-1.0	1
UNMAPPED	105	THR	C	175.9	-1.0	1
UNMAPPED	111	LEU	HD12	0.95	-1.0	1
UNMAPPED	63	VAL	HG13	0.91	-1.0	1
UNMAPPED	69	LEU	HA	4.148	-1.0	1
UNMAPPED	116	ASP	CB	40.9	-1.0	1
UNMAPPED	23	LEU	CD2	22.8	-1.0	1
UNMAPPED	104	ILE	CG1	26.174	-1.0	1
UNMAPPED	133	ILE	HG21	0.315	-1.0	1
UNMAPPED	82	ILE	CG2	18.473	-1.0	1
UNMAPPED	130	GLY	CA	45.979	-1.0	1
UNMAPPED	84	ALA	HB3	1.202	-1.0	1
UNMAPPED	12	GLU	CB	32.501	-1.0	1
UNMAPPED	34	ILE	HG22	0.83	-1.0	1
UNMAPPED	56	ARG	CA	57.106	-1.0	1
UNMAPPED	106	GLU	HG2	2.498	-1.0	2
UNMAPPED	84	ALA	HA	5.398	-1.0	1
UNMAPPED	70	GLY	CA	46.774	-1.0	1
UNMAPPED	111	LEU	N	128.382	-1.0	1
UNMAPPED	86	THR	HB	4.33	-1.0	1
UNMAPPED	7	ALA	HB2	1.419	-1.0	1
UNMAPPED	7	ALA	CA	52.912	-1.0	1
UNMAPPED	133	ILE	C	177.6	-1.0	1
UNMAPPED	142	ILE	H	8.39	-1.0	1
UNMAPPED	47	HIS	H	7.79	-1.0	1
UNMAPPED	94	LEU	N	128.194	-1.0	1
UNMAPPED	114	VAL	HG11	0.91	-1.0	2
UNMAPPED	101	VAL	N	125.2	-1.0	1
UNMAPPED	14	LEU	HG	1.425	-1.0	1
UNMAPPED	105	THR	HB	4.48	-1.0	1
UNMAPPED	134	ILE	C	179.2	-1.0	1
UNMAPPED	108	GLN	CB	30.438	-1.0	1
UNMAPPED	93	PHE	HB2	2.813	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	38	ASP	CB	41.432	-1.0	1
UNMAPPED	146	THR	C	177.6	-1.0	1
UNMAPPED	52	VAL	CA	59.106	-1.0	1
UNMAPPED	48	PHE	CD1	131.8	-1.0	3
UNMAPPED	142	ILE	N	121.06	-1.0	1
UNMAPPED	92	GLY	H	8.95	-1.0	1
UNMAPPED	75	GLU	CA	60.252	-1.0	1
UNMAPPED	20	GLU	CB	28.5	-1.0	1
UNMAPPED	79	LYS	CB	35.415	-1.0	1
UNMAPPED	45	SER	HA	3.81	-1.0	1
UNMAPPED	141	ILE	HB	2.01	-1.0	1
UNMAPPED	135	TYR	H	8.57	-1.0	1
UNMAPPED	40	THR	HB	4.06	-1.0	1
UNMAPPED	132	LEU	C	176.8	-1.0	1
UNMAPPED	91	VAL	CA	60.496	-1.0	1
UNMAPPED	19	ASP	H	10.6	-1.0	1
UNMAPPED	128	THR	CA	60.314	-1.0	1
UNMAPPED	142	ILE	HD12	0.75	-1.0	1
UNMAPPED	120	LYS	C	176.3	-1.0	1
UNMAPPED	62	VAL	CA	61.04	-1.0	1
UNMAPPED	114	VAL	CG1	22.03	-1.0	1
UNMAPPED	62	VAL	HA	4.667	-1.0	1
UNMAPPED	5	ALA	C	175.0	-1.0	1
UNMAPPED	73	PHE	HA	4.898	-1.0	1
UNMAPPED	17	GLU	HB2	1.84	-1.0	2
UNMAPPED	48	PHE	HB2	3.4	-1.0	2
UNMAPPED	78	MET	HB3	2.62	-1.0	2
UNMAPPED	93	PHE	CA	56.635	-1.0	1
UNMAPPED	40	THR	N	127.925	-1.0	1
UNMAPPED	110	ASP	CA	53.354	-1.0	1
UNMAPPED	148	LYS	CE	42.6	-1.0	1
UNMAPPED	85	ARG	HG2	1.46	-1.0	2
UNMAPPED	103	ARG	HB3	1.51	-1.0	2
UNMAPPED	62	VAL	HG12	0.816	-1.0	1
UNMAPPED	90	GLU	HG3	1.78	-1.0	2
UNMAPPED	16	PHE	C	173.3	-1.0	1
UNMAPPED	50	GLU	HB3	2.168	-1.0	2
UNMAPPED	81	ILE	HG22	0.542	-1.0	1
UNMAPPED	95	VAL	HG21	0.466	-1.0	1
UNMAPPED	55	LEU	CB	44.042	-1.0	1
UNMAPPED	64	ASN	HB2	3.06	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	112	THR	H	8.45	-1.0	1
UNMAPPED	115	SER	HB2	3.85	-1.0	1
UNMAPPED	44	LYS	CD	29.474	-1.0	1
UNMAPPED	71	ILE	CA	59.809	-1.0	1
UNMAPPED	98	VAL	HB	2.18	-1.0	1
UNMAPPED	75	GLU	C	174.7	-1.0	1
UNMAPPED	69	LEU	HD11	0.585	-1.0	1
UNMAPPED	16	PHE	HB3	3.12	-1.0	2
UNMAPPED	30	ILE	CA	60.048	-1.0	1
UNMAPPED	100	GLY	HA2	4.6	-1.0	2
UNMAPPED	71	ILE	HG21	0.988	-1.0	1
UNMAPPED	134	ILE	CA	61.795	-1.0	1
UNMAPPED	25	PHE	N	117.948	-1.0	1
UNMAPPED	151	VAL	N	124.267	-1.0	1
UNMAPPED	7	ALA	N	125.613	-1.0	1
UNMAPPED	116	ASP	HB2	2.69	-1.0	2
UNMAPPED	99	LEU	HD21	1.04	-1.0	1
UNMAPPED	8	LEU	HA	4.404	-1.0	1
UNMAPPED	36	LYS	CG	25.163	-1.0	1
UNMAPPED	109	LEU	HA	4.72	-1.0	1
UNMAPPED	95	VAL	CG1	22.962	-1.0	1
UNMAPPED	104	ILE	HG21	0.632	-1.0	1
UNMAPPED	102	LEU	C	178.1	-1.0	1
UNMAPPED	94	LEU	CA	55.722	-1.0	1
UNMAPPED	55	LEU	HD12	0.87	-1.0	1
UNMAPPED	71	ILE	HG12	1.701	-1.0	2
UNMAPPED	148	LYS	HG3	1.26	-1.0	2
UNMAPPED	135	TYR	HB3	2.52	-1.0	2
UNMAPPED	39	ILE	HD12	0.72	-1.0	1
UNMAPPED	23	LEU	HA	5.01	-1.0	1
UNMAPPED	25	PHE	CD1	131.355	-1.0	3
UNMAPPED	61	PRO	HA	4.872	-1.0	1
UNMAPPED	105	THR	HG23	1.226	-1.0	1
UNMAPPED	52	VAL	N	115.094	-1.0	1
UNMAPPED	90	GLU	HA	5.264	-1.0	1
UNMAPPED	120	LYS	CB	31.79	-1.0	1
UNMAPPED	58	ARG	HB2	1.616	-1.0	2
UNMAPPED	150	GLY	N	112.007	-1.0	1
UNMAPPED	81	ILE	HD11	0.758	-1.0	1
UNMAPPED	103	ARG	CG	28.238	-1.0	1
UNMAPPED	147	VAL	H	7.87	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	103	ARG	N	125.444	-1.0	1
UNMAPPED	38	ASP	CA	55.1	-1.0	1
UNMAPPED	3	THR	CA	61.906	-1.0	1
UNMAPPED	95	VAL	C	179.0	-1.0	1
UNMAPPED	82	ILE	HD12	0.083	-1.0	1
UNMAPPED	117	LYS	HD2	1.49	-1.0	2
UNMAPPED	118	PHE	HB3	2.89	-1.0	1
UNMAPPED	22	ALA	H	8.71	-1.0	1
UNMAPPED	23	LEU	HD22	0.27	-1.0	1
UNMAPPED	83	VAL	H	9.21	-1.0	1
UNMAPPED	18	ILE	HG12	0.7	-1.0	2
UNMAPPED	17	GLU	CA	54.8	-1.0	1
UNMAPPED	85	ARG	CD	44.018	-1.0	1
UNMAPPED	144	GLU	HG3	2.26	-1.0	2
UNMAPPED	6	ASP	CB	41.481	-1.0	1
UNMAPPED	121	LYS	HA	4.09	-1.0	1
UNMAPPED	36	LYS	H	8.05	-1.0	1
UNMAPPED	16	PHE	HE1	6.557	-1.0	3
UNMAPPED	34	ILE	H	9.14	-1.0	1
UNMAPPED	11	PHE	CE1	130.754	-1.0	3
UNMAPPED	75	GLU	CB	29.838	-1.0	1
UNMAPPED	146	THR	HA	4.31	-1.0	1
UNMAPPED	118	PHE	HD1	7.189	-1.0	1
UNMAPPED	13	VAL	C	179.4	-1.0	1
UNMAPPED	118	PHE	H	7.92	-1.0	1
UNMAPPED	101	VAL	HG11	0.899	-1.0	1
UNMAPPED	9	LYS	CE	42.621	-1.0	1
UNMAPPED	121	LYS	H	7.82	-1.0	1
UNMAPPED	91	VAL	HB	1.625	-1.0	1
UNMAPPED	136	LEU	CG	27.635	-1.0	1
UNMAPPED	142	ILE	CG1	30.767	-1.0	1
UNMAPPED	138	ILE	C	177.4	-1.0	1
UNMAPPED	97	ARG	CA	54.92	-1.0	1
UNMAPPED	133	ILE	CD1	14.476	-1.0	1
UNMAPPED	63	VAL	HB	2.008	-1.0	1
UNMAPPED	86	THR	CA	60.043	-1.0	1
UNMAPPED	81	ILE	HG12	1.594	-1.0	2
UNMAPPED	53	ILE	HG22	0.944	-1.0	1
UNMAPPED	63	VAL	CG2	21.5	-1.0	1
UNMAPPED	113	ASN	HA	4.72	-1.0	1
UNMAPPED	60	ILE	HG12	1.391	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	59	ILE	HD11	0.722	-1.0	1
UNMAPPED	111	LEU	CB	42.039	-1.0	1
UNMAPPED	78	MET	HE1	1.993	-1.0	1
UNMAPPED	128	THR	CG2	20.771	-1.0	1
UNMAPPED	40	THR	HA	4.719	-1.0	1
UNMAPPED	131	ARG	HB2	1.7	-1.0	2
UNMAPPED	104	ILE	CD1	13.851	-1.0	1
UNMAPPED	5	ALA	H	8.205	-1.0	1
UNMAPPED	27	VAL	HB	2.14	-1.0	1
UNMAPPED	65	LEU	HD23	0.685	-1.0	1
UNMAPPED	21	GLN	HA	4.463	-1.0	1
UNMAPPED	146	THR	N	115.184	-1.0	1
UNMAPPED	70	GLY	HA3	3.99	-1.0	2
UNMAPPED	126	VAL	HG23	0.63	-1.0	1
UNMAPPED	146	THR	H	7.79	-1.0	1
UNMAPPED	60	ILE	HD13	0.625	-1.0	1
UNMAPPED	71	ILE	CD1	13.925	-1.0	1
UNMAPPED	23	LEU	HD11	0.59	-1.0	1
UNMAPPED	113	ASN	CB	39.6	-1.0	1
UNMAPPED	29	ASN	HA	4.95	-1.0	1
UNMAPPED	89	VAL	N	122.068	-1.0	1
UNMAPPED	96	ASP	N	121.59	-1.0	1
UNMAPPED	32	MET	HB3	1.955	-1.0	2
UNMAPPED	148	LYS	HA	4.04	-1.0	1
UNMAPPED	13	VAL	HG23	0.49	-1.0	1
UNMAPPED	150	GLY	CA	45.792	-1.0	1
UNMAPPED	132	LEU	CD1	25.02	-1.0	2
UNMAPPED	4	LEU	HG	0.745	-1.0	1
UNMAPPED	138	ILE	CG1	29.769	-1.0	1
UNMAPPED	66	ALA	HB2	1.509	-1.0	1
UNMAPPED	6	ASP	H	8.091	-1.0	1
UNMAPPED	125	LEU	CB	45.653	-1.0	1
UNMAPPED	83	VAL	HG13	0.74	-1.0	2
UNMAPPED	141	ILE	HD13	0.924	-1.0	1
UNMAPPED	50	GLU	CB	31.036	-1.0	1
UNMAPPED	131	ARG	H	7.89	-1.0	1
UNMAPPED	149	GLU	CG	36.27	-1.0	1
UNMAPPED	68	ILE	CG2	17.162	-1.0	1
UNMAPPED	86	THR	HG23	1.117	-1.0	1
UNMAPPED	28	ASP	CA	57.354	-1.0	1
UNMAPPED	5	ALA	HB1	1.398	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	74	ASP	HB2	2.556	-1.0	2
UNMAPPED	50	GLU	HA	4.435	-1.0	1
UNMAPPED	12	GLU	HB2	1.92	-1.0	2
UNMAPPED	17	GLU	N	119.656	-1.0	1
UNMAPPED	118	PHE	CB	39.556	-1.0	1
UNMAPPED	133	ILE	CG2	17.774	-1.0	1
UNMAPPED	58	ARG	HG2	1.91	-1.0	2
UNMAPPED	125	LEU	HD11	0.758	-1.0	1
UNMAPPED	119	GLY	HA2	3.98	-1.0	1
UNMAPPED	94	LEU	HD21	0.78	-1.0	1
UNMAPPED	124	GLY	HA2	4.49	-1.0	2
UNMAPPED	101	VAL	HB	1.96	-1.0	1
UNMAPPED	8	LEU	HD22	0.909	-1.0	1
UNMAPPED	60	ILE	HB	1.73	-1.0	1
UNMAPPED	39	ILE	CG2	17.833	-1.0	1
UNMAPPED	111	LEU	H	8.88	-1.0	1
UNMAPPED	91	VAL	HG11	0.38	-1.0	1
UNMAPPED	83	VAL	N	131.726	-1.0	1
UNMAPPED	123	LYS	N	125.149	-1.0	1
UNMAPPED	141	ILE	HG23	0.875	-1.0	1
UNMAPPED	133	ILE	HG22	0.315	-1.0	1
UNMAPPED	97	ARG	N	113.276	-1.0	1
UNMAPPED	108	GLN	H	7.95	-1.0	1
UNMAPPED	65	LEU	HA	4.03	-1.0	1
UNMAPPED	86	THR	N	120.01	-1.0	1
UNMAPPED	46	ARG	N	123.799	-1.0	1
UNMAPPED	34	ILE	HG21	0.83	-1.0	1
UNMAPPED	132	LEU	HG	1.52	-1.0	1
UNMAPPED	56	ARG	CD	43.998	-1.0	1
UNMAPPED	109	LEU	CD1	25.292	-1.0	1
UNMAPPED	87	LYS	C	176.7	-1.0	1
UNMAPPED	56	ARG	HA	3.881	-1.0	1
UNMAPPED	25	PHE	CE1	131.093	-1.0	3
UNMAPPED	122	SER	H	7.69	-1.0	1
UNMAPPED	89	VAL	HB	2.084	-1.0	1
UNMAPPED	7	ALA	CB	19.635	-1.0	1
UNMAPPED	23	LEU	CB	46.7	-1.0	1
UNMAPPED	3	THR	CG2	22.002	-1.0	1
UNMAPPED	61	PRO	CB	33.03	-1.0	1
UNMAPPED	71	ILE	HD11	0.889	-1.0	1
UNMAPPED	142	ILE	HG21	0.84	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	28	ASP	HA	4.431	-1.0	1
UNMAPPED	69	LEU	CA	55.52	-1.0	1
UNMAPPED	90	GLU	C	178.0	-1.0	1
UNMAPPED	4	LEU	HB2	1.668	-1.0	2
UNMAPPED	145	ILE	CG2	17.924	-1.0	1
UNMAPPED	87	LYS	CG	25.077	-1.0	1
UNMAPPED	124	GLY	N	106.656	-1.0	1
UNMAPPED	18	ILE	CG2	18.319	-1.0	1
UNMAPPED	125	LEU	C	176.9	-1.0	1
UNMAPPED	52	VAL	CB	36.197	-1.0	1
UNMAPPED	61	PRO	HD3	3.906	-1.0	2
UNMAPPED	79	LYS	CG	25.8	-1.0	1
UNMAPPED	145	ILE	CD1	15.759	-1.0	1
UNMAPPED	68	ILE	HG13	0.29	-1.0	2
UNMAPPED	33	VAL	HA	4.819	-1.0	1
UNMAPPED	120	LYS	N	124.931	-1.0	1
UNMAPPED	49	VAL	HG11	0.96	-1.0	1
UNMAPPED	14	LEU	H	9.39	-1.0	1
UNMAPPED	33	VAL	CG1	21.5	-1.0	2
UNMAPPED	105	THR	H	8.12	-1.0	1
UNMAPPED	63	VAL	HG23	0.76	-1.0	1
UNMAPPED	128	THR	CB	70.137	-1.0	1
UNMAPPED	86	THR	CG2	21.721	-1.0	1
UNMAPPED	12	GLU	C	176.3	-1.0	1
UNMAPPED	123	LYS	CD	29.671	-1.0	1
UNMAPPED	128	THR	HB	4.04	-1.0	1
UNMAPPED	114	VAL	CG2	21.521	-1.0	1
UNMAPPED	58	ARG	HD2	3.26	-1.0	2
UNMAPPED	60	ILE	H	8.94	-1.0	1
UNMAPPED	62	VAL	HB	1.65	-1.0	1
UNMAPPED	103	ARG	HG3	1.39	-1.0	2
UNMAPPED	102	LEU	HD21	0.72	-1.0	1
UNMAPPED	13	VAL	HG11	0.521	-1.0	1
UNMAPPED	126	VAL	C	178.3	-1.0	1
UNMAPPED	109	LEU	HD21	0.78	-1.0	1
UNMAPPED	16	PHE	CD1	132.85	-1.0	3
UNMAPPED	99	LEU	N	129.985	-1.0	1
UNMAPPED	55	LEU	HD23	0.812	-1.0	1
UNMAPPED	115	SER	CB	63.907	-1.0	1
UNMAPPED	44	LYS	HD3	1.64	-1.0	2
UNMAPPED	126	VAL	CG2	21.555	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	22	ALA	HB1	1.291	-1.0	1
UNMAPPED	144	GLU	CB	29.82	-1.0	1
UNMAPPED	127	LYS	CD	27.778	-1.0	1
UNMAPPED	126	VAL	HG12	0.686	-1.0	1
UNMAPPED	141	ILE	CA	65.769	-1.0	1
UNMAPPED	107	ASN	N	116.698	-1.0	1
UNMAPPED	122	SER	CB	65.913	-1.0	1
UNMAPPED	81	ILE	HG21	0.542	-1.0	1
UNMAPPED	2	LYS	CA	56.789	-1.0	1
UNMAPPED	7	ALA	H	8.02	-1.0	1
UNMAPPED	44	LYS	CA	56.849	-1.0	1
UNMAPPED	71	ILE	CB	40.278	-1.0	1
UNMAPPED	47	HIS	HB2	3.12	-1.0	2
UNMAPPED	98	VAL	HA	4.271	-1.0	1
UNMAPPED	68	ILE	HD11	0.56	-1.0	1
UNMAPPED	4	LEU	HD13	0.951	-1.0	1
UNMAPPED	111	LEU	HA	4.65	-1.0	1
UNMAPPED	2	LYS	HD2	1.717	-1.0	2
UNMAPPED	10	GLU	HB2	1.857	-1.0	2
UNMAPPED	138	ILE	HD11	0.07	-1.0	1
UNMAPPED	130	GLY	HA3	3.76	-1.0	2
UNMAPPED	132	LEU	H	8.35	-1.0	1
UNMAPPED	36	LYS	CB	32.779	-1.0	1
UNMAPPED	14	LEU	HB2	2.03	-1.0	2
UNMAPPED	44	LYS	HG2	1.43	-1.0	2
UNMAPPED	142	ILE	CD1	13.03	-1.0	1
UNMAPPED	94	LEU	HA	4.42	-1.0	1
UNMAPPED	71	ILE	HA	4.845	-1.0	1
UNMAPPED	59	ILE	HG12	1.459	-1.0	2
UNMAPPED	125	LEU	CD1	25.268	-1.0	1
UNMAPPED	105	THR	CB	72.034	-1.0	1
UNMAPPED	80	SER	CB	66.477	-1.0	1
UNMAPPED	10	GLU	CA	54.96	-1.0	1
UNMAPPED	145	ILE	HD12	0.873	-1.0	1
UNMAPPED	8	LEU	HB3	1.474	-1.0	2
UNMAPPED	88	ASP	HB3	2.632	-1.0	2
UNMAPPED	128	THR	H	8.04	-1.0	1
UNMAPPED	141	ILE	C	175.7	-1.0	1
UNMAPPED	78	MET	N	121.789	-1.0	1
UNMAPPED	96	ASP	CB	40.521	-1.0	1
UNMAPPED	62	VAL	HG22	0.969	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	59	ILE	CG1	22.048	-1.0	1
UNMAPPED	109	LEU	H	7.32	-1.0	1
UNMAPPED	103	ARG	HB2	1.66	-1.0	2
UNMAPPED	50	GLU	CG	35.754	-1.0	1
UNMAPPED	98	VAL	CG1	22.492	-1.0	1
UNMAPPED	8	LEU	CD2	24.98	-1.0	1
UNMAPPED	32	MET	N	114.613	-1.0	1
UNMAPPED	131	ARG	CD	43.7	-1.0	1
UNMAPPED	134	ILE	HG22	0.545	-1.0	1
UNMAPPED	80	SER	C	178.2	-1.0	1
UNMAPPED	39	ILE	CG1	27.798	-1.0	1
UNMAPPED	121	LYS	N	117.053	-1.0	1
UNMAPPED	89	VAL	HG23	0.888	-1.0	1
UNMAPPED	52	VAL	HG22	0.67	-1.0	1
UNMAPPED	18	ILE	HD13	1.029	-1.0	1
UNMAPPED	85	ARG	CG	26.96	-1.0	1
UNMAPPED	110	ASP	HB3	2.55	-1.0	2
UNMAPPED	95	VAL	HB	2.23	-1.0	1
UNMAPPED	95	VAL	CB	36.6	-1.0	1
UNMAPPED	17	GLU	HG3	1.754	-1.0	2
UNMAPPED	148	LYS	CA	57.025	-1.0	1
UNMAPPED	77	LYS	CB	34.335	-1.0	1
UNMAPPED	98	VAL	HG21	0.95	-1.0	1
UNMAPPED	107	ASN	CA	55.135	-1.0	1
UNMAPPED	149	GLU	HA	4.38	-1.0	1
UNMAPPED	107	ASN	HB2	2.87	-1.0	2
UNMAPPED	28	ASP	HB2	2.631	-1.0	2
UNMAPPED	9	LYS	CB	33.494	-1.0	1
UNMAPPED	117	LYS	CG	24.755	-1.0	1
UNMAPPED	136	LEU	CB	44.31	-1.0	1
UNMAPPED	125	LEU	HD22	0.88	-1.0	1
UNMAPPED	52	VAL	CG2	18.471	-1.0	1
UNMAPPED	97	ARG	CB	32.919	-1.0	1
UNMAPPED	13	VAL	CG2	18.754	-1.0	1
UNMAPPED	76	GLN	H	8.52	-1.0	1
UNMAPPED	20	GLU	HG2	2.1	-1.0	2
UNMAPPED	17	GLU	H	8.88	-1.0	1
UNMAPPED	80	SER	H	8.35	-1.0	1
UNMAPPED	104	ILE	HB	1.46	-1.0	1
UNMAPPED	133	ILE	HD12	0.524	-1.0	1
UNMAPPED	117	LYS	N	121.976	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	9	LYS	CG	25.3	-1.0	1
UNMAPPED	9	LYS	HB2	1.776	-1.0	2
UNMAPPED	111	LEU	CG	27.635	-1.0	1
UNMAPPED	116	ASP	N	125.865	-1.0	1
UNMAPPED	78	MET	HE2	1.993	-1.0	1
UNMAPPED	23	LEU	N	127.524	-1.0	1
UNMAPPED	40	THR	CG2	21.262	-1.0	1
UNMAPPED	29	ASN	HB2	3.216	-1.0	2
UNMAPPED	151	VAL	HG13	0.883	-1.0	2
UNMAPPED	13	VAL	CG1	21.888	-1.0	1
UNMAPPED	85	ARG	HD2	3.207	-1.0	2
UNMAPPED	136	LEU	HA	4.71	-1.0	1
UNMAPPED	26	ASP	H	9.43	-1.0	1
UNMAPPED	97	ARG	HA	4.7	-1.0	1
UNMAPPED	9	LYS	C	177.3	-1.0	1
UNMAPPED	21	GLN	CA	54.777	-1.0	1
UNMAPPED	98	VAL	C	177.5	-1.0	1
UNMAPPED	14	LEU	HD11	0.986	-1.0	2
UNMAPPED	111	LEU	C	174.9	-1.0	1
UNMAPPED	59	ILE	C	176.2	-1.0	1
UNMAPPED	101	VAL	HG23	0.974	-1.0	1
UNMAPPED	33	VAL	HG11	0.91	-1.0	1
UNMAPPED	36	LYS	HG2	1.36	-1.0	2
UNMAPPED	100	GLY	CA	44.6	-1.0	1
UNMAPPED	27	VAL	HG22	1.075	-1.0	1
UNMAPPED	106	GLU	C	175.4	-1.0	1
UNMAPPED	82	ILE	CB	40.497	-1.0	1
UNMAPPED	107	ASN	C	176.7	-1.0	1
UNMAPPED	64	ASN	HA	4.636	-1.0	1
UNMAPPED	9	LYS	HE2	3.02	-1.0	2
UNMAPPED	129	ASP	C	176.8	-1.0	1
UNMAPPED	30	ILE	HG23	0.785	-1.0	1
UNMAPPED	99	LEU	HB2	1.85	-1.0	2
UNMAPPED	149	GLU	CB	30.59	-1.0	1
UNMAPPED	104	ILE	HD13	0.324	-1.0	1
UNMAPPED	30	ILE	N	121.536	-1.0	1
UNMAPPED	5	ALA	HB2	1.398	-1.0	1
UNMAPPED	134	ILE	HG23	0.545	-1.0	1
UNMAPPED	119	GLY	CA	47.279	-1.0	1
UNMAPPED	76	GLN	CA	57.906	-1.0	1
UNMAPPED	11	PHE	H	8.94	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	132	LEU	HD12	0.92	-1.0	1
UNMAPPED	146	THR	HG22	1.21	-1.0	1
UNMAPPED	136	LEU	H	9.0	-1.0	1
UNMAPPED	122	SER	HB3	3.56	-1.0	2
UNMAPPED	143	GLU	CA	59.865	-1.0	1
UNMAPPED	135	TYR	N	133.62	-1.0	1
UNMAPPED	80	SER	HB2	3.553	-1.0	2
UNMAPPED	148	LYS	N	125.324	-1.0	1
UNMAPPED	132	LEU	HB2	1.71	-1.0	2
UNMAPPED	90	GLU	CA	55.033	-1.0	1
UNMAPPED	94	LEU	HD22	0.78	-1.0	1
UNMAPPED	133	ILE	H	9.04	-1.0	1
UNMAPPED	60	ILE	HA	4.75	-1.0	1
UNMAPPED	132	LEU	CG	27.49	-1.0	1
UNMAPPED	73	PHE	HB2	3.141	-1.0	2
UNMAPPED	91	VAL	HG12	0.38	-1.0	1
UNMAPPED	69	LEU	HG	0.92	-1.0	1
UNMAPPED	67	LYS	HE2	3.029	-1.0	2
UNMAPPED	43	PRO	CG	27.8	-1.0	1
UNMAPPED	106	GLU	CA	59.843	-1.0	1
UNMAPPED	40	THR	H	8.91	-1.0	1
UNMAPPED	39	ILE	HG12	1.44	-1.0	2
UNMAPPED	147	VAL	CB	32.764	-1.0	1
UNMAPPED	74	ASP	H	9.23	-1.0	1
UNMAPPED	56	ARG	CG	28.032	-1.0	1
UNMAPPED	116	ASP	C	175.6	-1.0	1
UNMAPPED	139	ASP	HB2	2.77	-1.0	2
UNMAPPED	109	LEU	CD2	27.471	-1.0	1
UNMAPPED	140	LYS	HA	4.11	-1.0	1
UNMAPPED	61	PRO	C	177.7	-1.0	1
UNMAPPED	143	GLU	CG	36.455	-1.0	1
UNMAPPED	27	VAL	C	174.2	-1.0	1
UNMAPPED	67	LYS	CA	59.289	-1.0	1
UNMAPPED	149	GLU	HG3	2.01	-1.0	2
UNMAPPED	147	VAL	N	123.635	-1.0	1
UNMAPPED	98	VAL	CB	32.8	-1.0	1
UNMAPPED	23	LEU	CA	53.857	-1.0	1
UNMAPPED	61	PRO	CG	27.494	-1.0	1
UNMAPPED	135	TYR	C	178.0	-1.0	1
UNMAPPED	94	LEU	HD12	0.912	-1.0	1
UNMAPPED	71	ILE	HD12	0.889	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	54	ASN	HA	5.185	-1.0	1
UNMAPPED	82	ILE	H	8.94	-1.0	1
UNMAPPED	36	LYS	N	123.713	-1.0	1
UNMAPPED	142	ILE	HG22	0.84	-1.0	1
UNMAPPED	59	ILE	HB	1.85	-1.0	1
UNMAPPED	56	ARG	C	176.8	-1.0	1
UNMAPPED	41	PRO	HD3	3.8	-1.0	2
UNMAPPED	21	GLN	N	123.645	-1.0	1
UNMAPPED	64	ASN	HB3	2.74	-1.0	2
UNMAPPED	109	LEU	CG	21.556	-1.0	1
UNMAPPED	31	GLU	CG	35.166	-1.0	1
UNMAPPED	105	THR	HA	5.135	-1.0	1
UNMAPPED	105	THR	N	113.904	-1.0	1
UNMAPPED	80	SER	N	118.733	-1.0	1
UNMAPPED	18	ILE	HG21	1.138	-1.0	1
UNMAPPED	141	ILE	CD1	13.347	-1.0	1
UNMAPPED	98	VAL	HG13	1.1	-1.0	1
UNMAPPED	8	LEU	CA	55.084	-1.0	1
UNMAPPED	19	ASP	HA	4.221	-1.0	1
UNMAPPED	149	GLU	H	8.33	-1.0	1
UNMAPPED	100	GLY	N	106.581	-1.0	1
UNMAPPED	31	GLU	HG2	2.3	-1.0	2
UNMAPPED	38	ASP	N	123.755	-1.0	1
UNMAPPED	95	VAL	HG11	0.582	-1.0	1
UNMAPPED	39	ILE	CA	61.023	-1.0	1
UNMAPPED	48	PHE	HA	4.539	-1.0	1
UNMAPPED	55	LEU	H	8.95	-1.0	1
UNMAPPED	136	LEU	HD13	0.53	-1.0	2
UNMAPPED	16	PHE	HD1	6.775	-1.0	3
UNMAPPED	15	SER	C	178.2	-1.0	1
UNMAPPED	73	PHE	HD1	7.241	-1.0	3
UNMAPPED	123	LYS	CG	25.751	-1.0	1
UNMAPPED	82	ILE	HG23	0.82	-1.0	1
UNMAPPED	67	LYS	HD2	1.74	-1.0	2
UNMAPPED	137	ASP	CA	52.506	-1.0	1
UNMAPPED	9	LYS	HD2	1.48	-1.0	2
UNMAPPED	79	LYS	HD2	2.24	-1.0	2
UNMAPPED	48	PHE	CE1	133.636	-1.0	3
UNMAPPED	121	LYS	HB2	1.95	-1.0	2
UNMAPPED	13	VAL	HA	5.211	-1.0	1
UNMAPPED	150	GLY	H	8.28	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	60	ILE	HG21	0.721	-1.0	1
UNMAPPED	49	VAL	HA	4.17	-1.0	1
UNMAPPED	135	TYR	CA	54.08	-1.0	1
UNMAPPED	49	VAL	CA	63.791	-1.0	1
UNMAPPED	40	THR	CB	70.4	-1.0	1
UNMAPPED	148	LYS	HD3	1.69	-1.0	2
UNMAPPED	126	VAL	CG1	21.874	-1.0	1
UNMAPPED	95	VAL	N	117.317	-1.0	1
UNMAPPED	74	ASP	CB	43.24	-1.0	1
UNMAPPED	127	LYS	CG	29.772	-1.0	1
UNMAPPED	46	ARG	H	8.29	-1.0	1
UNMAPPED	112	THR	HG23	1.238	-1.0	1
UNMAPPED	2	LYS	CD	29.481	-1.0	1
UNMAPPED	56	ARG	HG2	1.62	-1.0	2
UNMAPPED	14	LEU	CB	44.542	-1.0	1
UNMAPPED	6	ASP	HB2	2.707	-1.0	2
UNMAPPED	27	VAL	HG13	1.014	-1.0	1
UNMAPPED	44	LYS	CB	32.046	-1.0	1
UNMAPPED	111	LEU	HD13	0.95	-1.0	1
UNMAPPED	9	LYS	N	124.633	-1.0	1
UNMAPPED	63	VAL	HG12	0.91	-1.0	1
UNMAPPED	94	LEU	H	8.28	-1.0	1
UNMAPPED	36	LYS	HE2	2.73	-1.0	2
UNMAPPED	106	GLU	N	122.363	-1.0	1
UNMAPPED	4	LEU	HD21	0.903	-1.0	1
UNMAPPED	55	LEU	CA	53.772	-1.0	1
UNMAPPED	151	VAL	CA	64.0	-1.0	1
UNMAPPED	142	ILE	HB	2.06	-1.0	1
UNMAPPED	97	ARG	HG3	1.55	-1.0	2
UNMAPPED	16	PHE	CA	56.544	-1.0	1
UNMAPPED	44	LYS	HB2	1.84	-1.0	2
UNMAPPED	135	TYR	HE1	6.53	-1.0	3
UNMAPPED	8	LEU	HG	0.762	-1.0	1
UNMAPPED	36	LYS	CA	57.511	-1.0	1
UNMAPPED	86	THR	HA	4.56	-1.0	1
UNMAPPED	91	VAL	CG2	21.699	-1.0	1
UNMAPPED	7	ALA	HB3	1.419	-1.0	1
UNMAPPED	30	ILE	C	177.2	-1.0	1
UNMAPPED	114	VAL	CA	63.128	-1.0	1
UNMAPPED	66	ALA	CA	55.663	-1.0	1
UNMAPPED	60	ILE	HD11	0.625	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	73	PHE	CE1	130.69	-1.0	3
UNMAPPED	143	GLU	H	8.05	-1.0	1
UNMAPPED	11	PHE	HB3	2.915	-1.0	2
UNMAPPED	105	THR	CA	60.277	-1.0	1
UNMAPPED	129	ASP	HA	4.38	-1.0	1
UNMAPPED	77	LYS	HG2	1.49	-1.0	2
UNMAPPED	42	VAL	H	8.186	-1.0	1
UNMAPPED	84	ALA	CA	50.112	-1.0	1
UNMAPPED	108	GLN	CA	56.626	-1.0	1
UNMAPPED	94	LEU	C	177.1	-1.0	1
UNMAPPED	65	LEU	HD11	0.785	-1.0	1
UNMAPPED	25	PHE	HA	5.602	-1.0	1
UNMAPPED	39	ILE	N	123.439	-1.0	1
UNMAPPED	128	THR	HG21	0.952	-1.0	1
UNMAPPED	69	LEU	H	7.64	-1.0	1
UNMAPPED	62	VAL	HG21	0.969	-1.0	1
UNMAPPED	5	ALA	HA	4.271	-1.0	1
UNMAPPED	59	ILE	CG2	17.976	-1.0	1
UNMAPPED	34	ILE	C	177.6	-1.0	1
UNMAPPED	60	ILE	CB	41.1	-1.0	1
UNMAPPED	53	ILE	HB	1.88	-1.0	1
UNMAPPED	99	LEU	HD11	0.733	-1.0	1
UNMAPPED	71	ILE	CG1	25.781	-1.0	1
UNMAPPED	98	VAL	CG2	22.579	-1.0	1
UNMAPPED	118	PHE	HA	4.77	-1.0	1
UNMAPPED	103	ARG	CB	31.349	-1.0	1
UNMAPPED	68	ILE	HG21	0.709	-1.0	1
UNMAPPED	149	GLU	N	122.731	-1.0	1
UNMAPPED	142	ILE	HD13	0.75	-1.0	1
UNMAPPED	89	VAL	H	7.96	-1.0	1
UNMAPPED	74	ASP	C	175.1	-1.0	1
UNMAPPED	2	LYS	HA	4.51	-1.0	1
UNMAPPED	125	LEU	HA	5.2	-1.0	2
UNMAPPED	78	MET	HB2	2.921	-1.0	2
UNMAPPED	44	LYS	H	8.21	-1.0	1
UNMAPPED	37	SER	H	8.14	-1.0	1
UNMAPPED	85	ARG	CB	34.067	-1.0	1
UNMAPPED	24	ALA	HB1	0.89	-1.0	1
UNMAPPED	49	VAL	N	124.047	-1.0	1
UNMAPPED	95	VAL	CA	59.329	-1.0	1
UNMAPPED	58	ARG	CD	43.7	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	148	LYS	CB	33.283	-1.0	1
UNMAPPED	127	LYS	HA	4.98	-1.0	1
UNMAPPED	64	ASN	CA	52.739	-1.0	1
UNMAPPED	98	VAL	HG22	0.95	-1.0	1
UNMAPPED	65	LEU	HD12	0.785	-1.0	1
UNMAPPED	56	ARG	HD2	3.2	-1.0	2
UNMAPPED	62	VAL	HG13	0.816	-1.0	1
UNMAPPED	131	ARG	N	122.463	-1.0	1
UNMAPPED	145	ILE	HD11	0.873	-1.0	1
UNMAPPED	50	GLU	HB2	2.28	-1.0	2
UNMAPPED	20	GLU	H	8.54	-1.0	1
UNMAPPED	109	LEU	HB2	1.67	-1.0	2
UNMAPPED	108	GLN	C	178.1	-1.0	1
UNMAPPED	97	ARG	CG	26.303	-1.0	1
UNMAPPED	30	ILE	HD13	0.698	-1.0	1
UNMAPPED	5	ALA	CA	53.265	-1.0	1
UNMAPPED	33	VAL	HG23	0.84	-1.0	1
UNMAPPED	123	LYS	HA	4.38	-1.0	1
UNMAPPED	145	ILE	HG23	0.888	-1.0	1
UNMAPPED	83	VAL	C	178.9	-1.0	1
UNMAPPED	149	GLU	C	176.1	-1.0	1
UNMAPPED	141	ILE	H	7.82	-1.0	1
UNMAPPED	34	ILE	CG2	27.226	-1.0	1
UNMAPPED	43	PRO	HD2	4.7	-1.0	2
UNMAPPED	134	ILE	HD13	0.655	-1.0	1
UNMAPPED	16	PHE	N	123.872	-1.0	1
UNMAPPED	38	ASP	HB3	2.6	-1.0	2
UNMAPPED	71	ILE	HG22	0.988	-1.0	1
UNMAPPED	91	VAL	HG23	0.519	-1.0	1
UNMAPPED	138	ILE	HG12	0.88	-1.0	2
UNMAPPED	2	LYS	H	8.719	-1.0	1
UNMAPPED	98	VAL	N	125.56	-1.0	1
UNMAPPED	39	ILE	HG21	0.682	-1.0	1
UNMAPPED	66	ALA	N	123.306	-1.0	1
UNMAPPED	108	GLN	HG2	2.44	-1.0	2
UNMAPPED	151	VAL	HB	2.08	-1.0	1
UNMAPPED	104	ILE	HG22	0.632	-1.0	1
UNMAPPED	55	LEU	HD13	0.87	-1.0	1
UNMAPPED	148	LYS	HG2	1.47	-1.0	2
UNMAPPED	135	TYR	HB2	3.17	-1.0	2
UNMAPPED	39	ILE	HD13	0.72	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	87	LYS	N	124.404	-1.0	1
UNMAPPED	49	VAL	HG12	0.96	-1.0	1
UNMAPPED	50	GLU	H	9.05	-1.0	1
UNMAPPED	67	LYS	C	173.2	-1.0	1
UNMAPPED	71	ILE	C	177.6	-1.0	1
UNMAPPED	105	THR	HG22	1.226	-1.0	1
UNMAPPED	147	VAL	HG13	0.98	-1.0	2
UNMAPPED	108	GLN	HB2	2.32	-1.0	2
UNMAPPED	84	ALA	N	134.925	-1.0	1
UNMAPPED	33	VAL	HG12	0.91	-1.0	1
UNMAPPED	118	PHE	CD1	131.449	-1.0	1
UNMAPPED	70	GLY	H	7.98	-1.0	1
UNMAPPED	43	PRO	HB2	2.36	-1.0	2
UNMAPPED	21	GLN	HG2	2.244	-1.0	2
UNMAPPED	16	PHE	CE1	131.09	-1.0	3
UNMAPPED	47	HIS	HD1	8.538	-1.0	3
UNMAPPED	137	ASP	HA	4.58	-1.0	1
UNMAPPED	138	ILE	HG23	0.89	-1.0	1
UNMAPPED	102	LEU	CA	53.988	-1.0	1
UNMAPPED	12	GLU	HG3	2.037	-1.0	2
UNMAPPED	125	LEU	N	122.689	-1.0	1
UNMAPPED	149	GLU	CA	56.897	-1.0	1
UNMAPPED	3	THR	CB	70.536	-1.0	1
UNMAPPED	28	ASP	CB	40.754	-1.0	1
UNMAPPED	3	THR	HB	4.429	-1.0	1
UNMAPPED	151	VAL	H	7.54	-1.0	1
UNMAPPED	82	ILE	HD13	0.083	-1.0	1
UNMAPPED	23	LEU	HD23	0.27	-1.0	1
UNMAPPED	94	LEU	CD1	25.494	-1.0	2
UNMAPPED	144	GLU	HA	4.21	-1.0	1
UNMAPPED	17	GLU	CB	35.5	-1.0	1
UNMAPPED	124	GLY	C	173.7	-1.0	1
UNMAPPED	144	GLU	HG2	2.41	-1.0	2
UNMAPPED	115	SER	CA	58.949	-1.0	1
UNMAPPED	6	ASP	CA	55.009	-1.0	1
UNMAPPED	34	ILE	N	126.659	-1.0	1
UNMAPPED	6	ASP	HA	4.58	-1.0	1
UNMAPPED	68	ILE	H	7.08	-1.0	1
UNMAPPED	104	ILE	HG12	0.76	-1.0	2
UNMAPPED	115	SER	N	120.383	-1.0	1
UNMAPPED	113	ASN	HB2	2.8	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	85	ARG	HB2	1.723	-1.0	2
UNMAPPED	53	ILE	CA	59.538	-1.0	1
UNMAPPED	76	GLN	HG3	2.43	-1.0	1
UNMAPPED	43	PRO	CD	51.2	-1.0	1
UNMAPPED	5	ALA	N	126.186	-1.0	1
UNMAPPED	125	LEU	HD21	0.88	-1.0	1
UNMAPPED	53	ILE	HD11	0.643	-1.0	1
UNMAPPED	99	LEU	H	8.97	-1.0	1
UNMAPPED	42	VAL	N	119.582	-1.0	1
UNMAPPED	106	GLU	CB	30.169	-1.0	1
UNMAPPED	106	GLU	HB2	2.3	-1.0	2
UNMAPPED	123	LYS	CA	56.642	-1.0	1
UNMAPPED	147	VAL	HB	2.16	-1.0	1
UNMAPPED	63	VAL	HA	5.056	-1.0	1
UNMAPPED	127	LYS	H	8.7	-1.0	1
UNMAPPED	53	ILE	HG23	0.944	-1.0	1
UNMAPPED	138	ILE	CB	38.119	-1.0	1
UNMAPPED	140	LYS	CA	57.862	-1.0	1
UNMAPPED	8	LEU	HD12	0.973	-1.0	1
UNMAPPED	59	ILE	HD12	0.722	-1.0	1
UNMAPPED	104	ILE	H	8.78	-1.0	1
UNMAPPED	110	ASP	C	176.1	-1.0	1
UNMAPPED	55	LEU	HG	1.4	-1.0	1
UNMAPPED	59	ILE	HA	4.717	-1.0	1
UNMAPPED	10	GLU	HA	4.957	-1.0	1
UNMAPPED	29	ASN	C	179.0	-1.0	1
UNMAPPED	27	VAL	HA	4.047	-1.0	1
UNMAPPED	87	LYS	CA	59.055	-1.0	1
UNMAPPED	144	GLU	CG	36.458	-1.0	1
UNMAPPED	28	ASP	H	8.81	-1.0	1
UNMAPPED	126	VAL	HG22	0.63	-1.0	1
UNMAPPED	134	ILE	CG2	17.613	-1.0	1
UNMAPPED	97	ARG	C	178.6	-1.0	1
UNMAPPED	102	LEU	HD11	0.658	-1.0	1
UNMAPPED	3	THR	H	8.349	-1.0	1
UNMAPPED	78	MET	CE	18.607	-1.0	1
UNMAPPED	81	ILE	CD1	15.302	-1.0	1
UNMAPPED	122	SER	C	197.1	-1.0	1
UNMAPPED	111	LEU	CD2	23.816	-1.0	1
UNMAPPED	76	GLN	HA	4.17	-1.0	1
UNMAPPED	32	MET	HB2	2.28	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	75	GLU	N	128.728	-1.0	1
UNMAPPED	39	ILE	CB	39.982	-1.0	1
UNMAPPED	66	ALA	HB3	1.509	-1.0	1
UNMAPPED	35	GLU	HA	4.51	-1.0	1
UNMAPPED	35	GLU	HG3	1.983	-1.0	2
UNMAPPED	83	VAL	HG12	0.74	-1.0	2
UNMAPPED	141	ILE	HD12	0.924	-1.0	1
UNMAPPED	73	PHE	CB	41.268	-1.0	1
UNMAPPED	132	LEU	HD11	0.92	-1.0	1
UNMAPPED	143	GLU	HA	4.0	-1.0	1
UNMAPPED	32	MET	CE	17.621	-1.0	1
UNMAPPED	84	ALA	H	9.4	-1.0	1
UNMAPPED	128	THR	N	120.082	-1.0	1
UNMAPPED	48	PHE	C	177.6	-1.0	1
UNMAPPED	13	VAL	HB	1.934	-1.0	1
UNMAPPED	60	ILE	HG22	0.721	-1.0	1
UNMAPPED	26	ASP	HA	5.011	-1.0	1
UNMAPPED	49	VAL	CB	32.295	-1.0	1
UNMAPPED	26	ASP	CA	57.6	-1.0	1
UNMAPPED	130	GLY	H	8.44	-1.0	1
UNMAPPED	127	LYS	CB	33.039	-1.0	1
UNMAPPED	79	LYS	HA	4.67	-1.0	1
UNMAPPED	101	VAL	CG1	21.659	-1.0	1
UNMAPPED	14	LEU	CD1	24.261	-1.0	2
UNMAPPED	18	ILE	CB	41.9	-1.0	1
UNMAPPED	2	LYS	CG	25.077	-1.0	1
UNMAPPED	101	VAL	HA	4.91	-1.0	1
UNMAPPED	8	LEU	HD23	0.909	-1.0	1
UNMAPPED	49	VAL	HG23	0.888	-1.0	1
UNMAPPED	63	VAL	HG11	0.91	-1.0	1
UNMAPPED	48	PHE	CB	38.433	-1.0	1
UNMAPPED	141	ILE	HG22	0.875	-1.0	1
UNMAPPED	32	MET	H	7.72	-1.0	1
UNMAPPED	4	LEU	HD22	0.903	-1.0	1
UNMAPPED	111	LEU	HG	1.85	-1.0	1
UNMAPPED	48	PHE	HD1	7.097	-1.0	3
UNMAPPED	84	ALA	HB1	1.202	-1.0	1
UNMAPPED	35	GLU	CA	57.1	-1.0	1
UNMAPPED	64	ASN	N	125.117	-1.0	1
UNMAPPED	112	THR	HA	4.24	-1.0	1
UNMAPPED	142	ILE	HA	3.72	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	16	PHE	CB	41.072	-1.0	1
UNMAPPED	59	ILE	HG21	0.77	-1.0	1
UNMAPPED	140	LYS	N	121.574	-1.0	1
UNMAPPED	45	SER	N	117.95	-1.0	1
UNMAPPED	55	LEU	CD2	25.591	-1.0	1
UNMAPPED	133	ILE	CA	60.242	-1.0	1
UNMAPPED	44	LYS	C	176.8	-1.0	1
UNMAPPED	117	LYS	HB2	1.41	-1.0	2
UNMAPPED	89	VAL	HA	4.355	-1.0	1
UNMAPPED	52	VAL	HB	1.98	-1.0	1
UNMAPPED	66	ALA	CB	19.402	-1.0	1
UNMAPPED	39	ILE	H	8.24	-1.0	1
UNMAPPED	82	ILE	HG21	0.82	-1.0	1
UNMAPPED	110	ASP	HA	4.94	-1.0	1
UNMAPPED	114	VAL	HG13	0.91	-1.0	2
UNMAPPED	109	LEU	HD13	0.92	-1.0	1
UNMAPPED	14	LEU	HA	4.776	-1.0	1
UNMAPPED	10	GLU	CG	36.438	-1.0	1
UNMAPPED	53	ILE	HG13	1.981	-1.0	2
UNMAPPED	73	PHE	H	7.51	-1.0	1
UNMAPPED	61	PRO	HG3	1.798	-1.0	2
UNMAPPED	25	PHE	H	8.23	-1.0	1
UNMAPPED	60	ILE	N	131.371	-1.0	1
UNMAPPED	91	VAL	H	8.72	-1.0	1
UNMAPPED	84	ALA	CB	23.912	-1.0	1
UNMAPPED	24	ALA	CA	51.533	-1.0	1
UNMAPPED	133	ILE	HG12	1.34	-1.0	2
UNMAPPED	78	MET	CB	32.682	-1.0	1
UNMAPPED	69	LEU	CD2	18.69	-1.0	1
UNMAPPED	79	LYS	CD	29.159	-1.0	1
UNMAPPED	68	ILE	HG12	1.28	-1.0	2
UNMAPPED	33	VAL	HB	1.63	-1.0	1
UNMAPPED	136	LEU	HB2	2.05	-1.0	2
UNMAPPED	143	GLU	N	123.236	-1.0	1
UNMAPPED	41	PRO	CD	50.3	-1.0	1
UNMAPPED	99	LEU	HD12	0.733	-1.0	1
UNMAPPED	13	VAL	HG22	0.49	-1.0	1
UNMAPPED	56	ARG	HB3	1.86	-1.0	2
UNMAPPED	103	ARG	CA	55.659	-1.0	1
UNMAPPED	85	ARG	C	177.1	-1.0	1
UNMAPPED	45	SER	HB2	3.93	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	122	SER	CA	56.396	-1.0	1
UNMAPPED	3	THR	N	118.988	-1.0	1
UNMAPPED	128	THR	HA	4.64	-1.0	1
UNMAPPED	90	GLU	HB2	1.98	-1.0	2
UNMAPPED	127	LYS	C	176.9	-1.0	1
UNMAPPED	29	ASN	H	7.92	-1.0	1
UNMAPPED	13	VAL	HG12	0.521	-1.0	1
UNMAPPED	69	LEU	HD21	1.51	-1.0	1
UNMAPPED	27	VAL	CG1	22.261	-1.0	1
UNMAPPED	121	LYS	CB	32.063	-1.0	1
UNMAPPED	24	ALA	HB2	0.89	-1.0	1
UNMAPPED	147	VAL	CG1	21.5	-1.0	2
UNMAPPED	26	ASP	N	123.758	-1.0	1
UNMAPPED	47	HIS	HA	4.34	-1.0	1
UNMAPPED	109	LEU	HD22	0.78	-1.0	1
UNMAPPED	55	LEU	HD22	0.812	-1.0	1
UNMAPPED	83	VAL	CB	31.782	-1.0	1
UNMAPPED	148	LYS	CG	25.298	-1.0	1
UNMAPPED	102	LEU	H	9.12	-1.0	1
UNMAPPED	87	LYS	HB3	1.852	-1.0	2
UNMAPPED	22	ALA	HB2	1.291	-1.0	1
UNMAPPED	89	VAL	HG13	0.806	-1.0	1
UNMAPPED	96	ASP	C	175.7	-1.0	1
UNMAPPED	126	VAL	HG13	0.686	-1.0	1
UNMAPPED	93	PHE	HD1	7.059	-1.0	3
UNMAPPED	95	VAL	HG23	0.466	-1.0	1
UNMAPPED	102	LEU	HG	1.393	-1.0	1
UNMAPPED	66	ALA	H	8.32	-1.0	1
UNMAPPED	114	VAL	HB	2.028	-1.0	1
UNMAPPED	81	ILE	H	9.05	-1.0	1
UNMAPPED	88	ASP	C	177.3	-1.0	1
UNMAPPED	35	GLU	N	126.267	-1.0	1
UNMAPPED	136	LEU	N	131.942	-1.0	1
UNMAPPED	68	ILE	HD12	0.56	-1.0	1
UNMAPPED	69	LEU	HD13	0.585	-1.0	1
UNMAPPED	4	LEU	HD12	0.951	-1.0	1
UNMAPPED	141	ILE	HG21	0.875	-1.0	1
UNMAPPED	4	LEU	CG	27.279	-1.0	1
UNMAPPED	39	ILE	CD1	14.265	-1.0	1
UNMAPPED	142	ILE	CG2	18.02	-1.0	1
UNMAPPED	123	LYS	C	177.5	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	99	LEU	HD23	1.04	-1.0	1
UNMAPPED	4	LEU	C	175.5	-1.0	1
UNMAPPED	53	ILE	H	8.58	-1.0	1
UNMAPPED	109	LEU	HG	1.71	-1.0	1
UNMAPPED	141	ILE	CG2	18.298	-1.0	1
UNMAPPED	89	VAL	C	179.4	-1.0	1
UNMAPPED	49	VAL	H	7.74	-1.0	1
UNMAPPED	75	GLU	HB2	2.246	-1.0	2
UNMAPPED	109	LEU	N	122.028	-1.0	1
UNMAPPED	125	LEU	CD2	25.616	-1.0	1
UNMAPPED	77	LYS	HA	4.327	-1.0	1
UNMAPPED	44	LYS	HB3	2.024	-1.0	2
UNMAPPED	8	LEU	HB2	1.676	-1.0	2
UNMAPPED	92	GLY	HA2	5.183	-1.0	2
UNMAPPED	57	GLY	H	8.2	-1.0	1
UNMAPPED	140	LYS	H	7.58	-1.0	1
UNMAPPED	43	PRO	C	175.9	-1.0	1
UNMAPPED	86	THR	CB	70.497	-1.0	1
UNMAPPED	81	ILE	C	177.4	-1.0	1
UNMAPPED	96	ASP	CA	57.974	-1.0	1
UNMAPPED	68	ILE	HB	1.824	-1.0	1
UNMAPPED	47	HIS	CB	31.6	-1.0	1
UNMAPPED	81	ILE	HD13	0.758	-1.0	1
UNMAPPED	102	LEU	CB	45.281	-1.0	1
UNMAPPED	13	VAL	CB	35.078	-1.0	1
UNMAPPED	34	ILE	HA	4.692	-1.0	1
UNMAPPED	65	LEU	CD1	23.141	-1.0	1
UNMAPPED	3	THR	HA	4.267	-1.0	1
UNMAPPED	17	GLU	C	176.6	-1.0	1
UNMAPPED	2	LYS	HG2	1.474	-1.0	2
UNMAPPED	22	ALA	CA	51.574	-1.0	1
UNMAPPED	88	ASP	CA	54.994	-1.0	1
UNMAPPED	17	GLU	CG	36.4	-1.0	1
UNMAPPED	81	ILE	CB	41.256	-1.0	1
UNMAPPED	52	VAL	HG23	0.67	-1.0	1
UNMAPPED	18	ILE	HD12	1.029	-1.0	1
UNMAPPED	143	GLU	CB	29.97	-1.0	1
UNMAPPED	110	ASP	HB2	2.95	-1.0	2
UNMAPPED	18	ILE	CA	62.765	-1.0	1
UNMAPPED	18	ILE	HA	4.092	-1.0	1
UNMAPPED	73	PHE	CD1	133.31	-1.0	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	17	GLU	HG2	2.036	-1.0	2
UNMAPPED	134	ILE	CD1	12.974	-1.0	1
UNMAPPED	90	GLU	CG	36.349	-1.0	1
UNMAPPED	119	GLY	C	177.2	-1.0	1
UNMAPPED	52	VAL	HG13	0.707	-1.0	1
UNMAPPED	30	ILE	CD1	11.0	-1.0	1
UNMAPPED	121	LYS	C	177.4	-1.0	1
UNMAPPED	53	ILE	CB	42.268	-1.0	1
UNMAPPED	116	ASP	HA	4.46	-1.0	1
UNMAPPED	43	PRO	CA	64.035	-1.0	1
UNMAPPED	86	THR	C	179.0	-1.0	1
UNMAPPED	93	PHE	CE1	130.936	-1.0	3
UNMAPPED	53	ILE	HD12	0.643	-1.0	1
UNMAPPED	117	LYS	CD	29.1	-1.0	1
UNMAPPED	136	LEU	CA	54.869	-1.0	1
UNMAPPED	106	GLU	CG	35.56	-1.0	1
UNMAPPED	2	LYS	HE2	3.03	-1.0	2
UNMAPPED	147	VAL	HA	4.09	-1.0	1
UNMAPPED	147	VAL	CA	63.535	-1.0	1
UNMAPPED	113	ASN	C	177.7	-1.0	1
UNMAPPED	104	ILE	HA	4.72	-1.0	1
UNMAPPED	36	LYS	HA	4.0	-1.0	1
UNMAPPED	43	PRO	HG2	2.06	-1.0	2
UNMAPPED	66	ALA	HA	3.871	-1.0	1
UNMAPPED	8	LEU	H	8.01	-1.0	1
UNMAPPED	133	ILE	HD13	0.524	-1.0	1
UNMAPPED	140	LYS	CB	32.534	-1.0	1
UNMAPPED	67	LYS	N	118.306	-1.0	1
UNMAPPED	29	ASN	CB	39.269	-1.0	1
UNMAPPED	19	ASP	HB2	3.261	-1.0	2
UNMAPPED	148	LYS	C	175.7	-1.0	1
UNMAPPED	78	MET	HE3	1.993	-1.0	1
UNMAPPED	130	GLY	HA2	4.04	-1.0	2
UNMAPPED	112	THR	CB	70.0	-1.0	1
UNMAPPED	16	PHE	HA	5.132	-1.0	1
UNMAPPED	72	SER	CB	64.191	-1.0	1
UNMAPPED	122	SER	HA	4.91	-1.0	1
UNMAPPED	79	LYS	HB2	1.98	-1.0	2
UNMAPPED	31	GLU	CA	57.65	-1.0	1
UNMAPPED	139	ASP	CA	58.361	-1.0	1
UNMAPPED	27	VAL	CA	65.757	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	8	LEU	CG	27.27	-1.0	1
UNMAPPED	21	GLN	CB	30.367	-1.0	1
UNMAPPED	132	LEU	HD21	1.52	-1.0	1
UNMAPPED	126	VAL	HG21	0.63	-1.0	1
UNMAPPED	13	VAL	H	8.91	-1.0	1
UNMAPPED	94	LEU	HD11	0.912	-1.0	1
UNMAPPED	102	LEU	HD12	0.658	-1.0	1
UNMAPPED	99	LEU	CD2	25.067	-1.0	1
UNMAPPED	131	ARG	HA	4.58	-1.0	1
UNMAPPED	15	SER	HB2	3.726	-1.0	2
UNMAPPED	111	LEU	CD1	25.565	-1.0	1
UNMAPPED	151	VAL	HA	4.08	-1.0	1
UNMAPPED	27	VAL	HG23	1.075	-1.0	1
UNMAPPED	32	MET	HE3	1.994	-1.0	1
UNMAPPED	11	PHE	N	123.118	-1.0	1
UNMAPPED	81	ILE	HA	4.86	-1.0	1
UNMAPPED	69	LEU	CG	26.997	-1.0	1
UNMAPPED	3	THR	HG21	1.234	-1.0	1
UNMAPPED	65	LEU	H	7.63	-1.0	1
UNMAPPED	120	LYS	CG	25.218	-1.0	1
UNMAPPED	8	LEU	C	175.8	-1.0	1
UNMAPPED	99	LEU	HG	1.41	-1.0	1
UNMAPPED	115	SER	H	8.38	-1.0	1
UNMAPPED	63	VAL	CA	59.521	-1.0	1
UNMAPPED	145	ILE	HG12	1.28	-1.0	2
UNMAPPED	73	PHE	CA	56.588	-1.0	1
UNMAPPED	2	LYS	HB2	1.838	-1.0	2
UNMAPPED	30	ILE	HG22	0.785	-1.0	1
UNMAPPED	117	LYS	HA	4.06	-1.0	1
UNMAPPED	38	ASP	C	177.3	-1.0	1
UNMAPPED	86	THR	HG21	1.117	-1.0	1
UNMAPPED	11	PHE	CD1	132.539	-1.0	3
UNMAPPED	22	ALA	N	131.377	-1.0	1
UNMAPPED	5	ALA	HB3	1.398	-1.0	1
UNMAPPED	39	ILE	C	176.9	-1.0	1
UNMAPPED	88	ASP	N	118.285	-1.0	1
UNMAPPED	76	GLN	CB	29.024	-1.0	1
UNMAPPED	71	ILE	HB	2.331	-1.0	1
UNMAPPED	146	THR	HG23	1.21	-1.0	1
UNMAPPED	125	LEU	HD13	0.758	-1.0	1
UNMAPPED	26	ASP	CB	41.9	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	75	GLU	HA	4.165	-1.0	1
UNMAPPED	80	SER	HB3	3.338	-1.0	2
UNMAPPED	150	GLY	HA3	4.08	-1.0	2
UNMAPPED	137	ASP	C	177.1	-1.0	1
UNMAPPED	112	THR	C	177.8	-1.0	1
UNMAPPED	74	ASP	N	123.141	-1.0	1
UNMAPPED	94	LEU	HD23	0.78	-1.0	1
UNMAPPED	47	HIS	CD2	136.675	-1.0	3
UNMAPPED	139	ASP	C	173.8	-1.0	1
UNMAPPED	114	VAL	H	7.91	-1.0	1
UNMAPPED	131	ARG	CG	26.789	-1.0	1
UNMAPPED	91	VAL	HG13	0.38	-1.0	1
UNMAPPED	59	ILE	CB	37.255	-1.0	1
UNMAPPED	145	ILE	H	7.71	-1.0	1
UNMAPPED	109	LEU	C	177.0	-1.0	1
UNMAPPED	40	THR	HG21	1.268	-1.0	1
UNMAPPED	44	LYS	N	120.579	-1.0	1
UNMAPPED	14	LEU	CG	27.027	-1.0	1
UNMAPPED	51	GLY	CA	45.509	-1.0	1
UNMAPPED	12	GLU	CG	36.74	-1.0	1
UNMAPPED	123	LYS	H	8.85	-1.0	1
UNMAPPED	59	ILE	HG22	0.77	-1.0	1
UNMAPPED	68	ILE	CA	64.293	-1.0	1
UNMAPPED	139	ASP	HB3	2.64	-1.0	2
UNMAPPED	33	VAL	N	123.927	-1.0	1
UNMAPPED	55	LEU	CD1	24.907	-1.0	1
UNMAPPED	63	VAL	C	178.1	-1.0	1
UNMAPPED	151	VAL	CB	33.3	-1.0	1
UNMAPPED	77	LYS	HB2	2.007	-1.0	2
UNMAPPED	51	GLY	HA3	3.908	-1.0	2
UNMAPPED	71	ILE	HD13	0.889	-1.0	1
UNMAPPED	142	ILE	HG23	0.84	-1.0	1
UNMAPPED	82	ILE	HG22	0.82	-1.0	1
UNMAPPED	65	LEU	CB	42.7	-1.0	1
UNMAPPED	129	ASP	HB3	2.57	-1.0	2
UNMAPPED	139	ASP	N	124.208	-1.0	1
UNMAPPED	87	LYS	CE	42.33	-1.0	1
UNMAPPED	75	GLU	HG2	2.485	-1.0	2
UNMAPPED	55	LEU	N	129.918	-1.0	1
UNMAPPED	98	VAL	HG12	1.1	-1.0	1
UNMAPPED	108	GLN	CG	35.8	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	126	VAL	CB	34.123	-1.0	1
UNMAPPED	78	MET	CA	56.794	-1.0	1
UNMAPPED	58	ARG	C	178.0	-1.0	1
UNMAPPED	60	ILE	CA	57.6	-1.0	1
UNMAPPED	47	HIS	N	124.479	-1.0	1
UNMAPPED	13	VAL	HG21	0.49	-1.0	1
UNMAPPED	63	VAL	HG21	0.76	-1.0	1
UNMAPPED	50	GLU	N	128.836	-1.0	1
UNMAPPED	74	ASP	HA	4.718	-1.0	1
UNMAPPED	112	THR	CG2	22.107	-1.0	1
UNMAPPED	37	SER	HA	4.49	-1.0	1
UNMAPPED	25	PHE	HB2	3.641	-1.0	2
UNMAPPED	113	ASN	H	8.37	-1.0	1
UNMAPPED	137	ASP	CB	41.544	-1.0	1
UNMAPPED	102	LEU	HD23	0.72	-1.0	1
UNMAPPED	69	LEU	HD22	1.51	-1.0	1
UNMAPPED	121	LYS	CA	58.27	-1.0	1
UNMAPPED	59	ILE	H	8.32	-1.0	1
UNMAPPED	145	ILE	CB	38.787	-1.0	1
UNMAPPED	77	LYS	HE2	3.04	-1.0	2
UNMAPPED	85	ARG	N	120.279	-1.0	1
UNMAPPED	125	LEU	H	8.45	-1.0	1
UNMAPPED	137	ASP	HB2	3.05	-1.0	2
UNMAPPED	74	ASP	CA	52.771	-1.0	1
UNMAPPED	105	THR	CG2	22.508	-1.0	1
UNMAPPED	95	VAL	HG12	0.582	-1.0	1
UNMAPPED	78	MET	HA	4.69	-1.0	1
UNMAPPED	57	GLY	HA3	3.624	-1.0	2
UNMAPPED	112	THR	HG22	1.238	-1.0	1
UNMAPPED	15	SER	CA	56.502	-1.0	1
UNMAPPED	56	ARG	HG3	1.4	-1.0	2
UNMAPPED	88	ASP	H	8.25	-1.0	1
UNMAPPED	114	VAL	HA	4.08	-1.0	1
UNMAPPED	27	VAL	HG12	1.014	-1.0	1
UNMAPPED	121	LYS	HG2	1.25	-1.0	2
UNMAPPED	79	LYS	CA	56.388	-1.0	1
UNMAPPED	68	ILE	N	120.869	-1.0	1
UNMAPPED	65	LEU	C	178.2	-1.0	1
UNMAPPED	97	ARG	HG2	1.83	-1.0	2
UNMAPPED	82	ILE	HB	1.747	-1.0	1
UNMAPPED	31	GLU	HB2	1.96	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	126	VAL	H	9.3	-1.0	1
UNMAPPED	138	ILE	HD13	0.07	-1.0	1
UNMAPPED	81	ILE	CG2	18.315	-1.0	1
UNMAPPED	38	ASP	HA	4.65	-1.0	1
UNMAPPED	91	VAL	CG1	21.11	-1.0	1
UNMAPPED	32	MET	HE2	1.994	-1.0	1
UNMAPPED	112	THR	N	116.646	-1.0	1
UNMAPPED	120	LYS	H	8.76	-1.0	1
UNMAPPED	110	ASP	N	126.445	-1.0	1
UNMAPPED	11	PHE	HB2	3.178	-1.0	2
UNMAPPED	7	ALA	C	175.4	-1.0	1
UNMAPPED	4	LEU	HA	4.354	-1.0	1
UNMAPPED	18	ILE	H	8.21	-1.0	1
UNMAPPED	54	ASN	N	123.3	-1.0	1
UNMAPPED	137	ASP	H	8.4	-1.0	1
UNMAPPED	23	LEU	H	8.79	-1.0	1
UNMAPPED	68	ILE	HA	3.596	-1.0	1
UNMAPPED	87	LYS	HG2	1.47	-1.0	2
UNMAPPED	97	ARG	HB2	2.13	-1.0	2
UNMAPPED	47	HIS	CA	57.6	-1.0	1
UNMAPPED	32	MET	HE1	1.994	-1.0	1
UNMAPPED	139	ASP	H	7.77	-1.0	1
UNMAPPED	27	VAL	H	8.02	-1.0	1
UNMAPPED	12	GLU	HG2	2.253	-1.0	2
UNMAPPED	53	ILE	HA	4.71	-1.0	1
UNMAPPED	125	LEU	HB3	1.52	-1.0	1
UNMAPPED	71	ILE	CG2	17.909	-1.0	1
UNMAPPED	34	ILE	HB	1.962	-1.0	1
UNMAPPED	96	ASP	HB3	2.76	-1.0	2
UNMAPPED	103	ARG	CD	43.568	-1.0	1
UNMAPPED	34	ILE	CB	41.694	-1.0	1
UNMAPPED	103	ARG	HD2	3.16	-1.0	2
UNMAPPED	22	ALA	CB	20.089	-1.0	1
UNMAPPED	13	VAL	N	117.231	-1.0	1
UNMAPPED	119	GLY	N	112.11	-1.0	1
UNMAPPED	88	ASP	CB	42.374	-1.0	1
UNMAPPED	101	VAL	C	176.9	-1.0	1
UNMAPPED	89	VAL	HG21	0.888	-1.0	1
UNMAPPED	120	LYS	HA	4.38	-1.0	1
UNMAPPED	128	THR	C	179.3	-1.0	1
UNMAPPED	18	ILE	HD11	1.029	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	62	VAL	C	177.7	-1.0	1
UNMAPPED	76	GLN	N	117.87	-1.0	1
UNMAPPED	85	ARG	CA	54.748	-1.0	1
UNMAPPED	85	ARG	HA	5.418	-1.0	1
UNMAPPED	63	VAL	H	9.08	-1.0	1
UNMAPPED	32	MET	CA	55.701	-1.0	1
UNMAPPED	58	ARG	CG	27.11	-1.0	1
UNMAPPED	4	LEU	H	8.359	-1.0	1
UNMAPPED	61	PRO	HB2	2.247	-1.0	2
UNMAPPED	98	VAL	HG23	0.95	-1.0	1
UNMAPPED	102	LEU	CD2	24.068	-1.0	1
UNMAPPED	15	SER	N	123.634	-1.0	1
UNMAPPED	132	LEU	N	126.311	-1.0	1
UNMAPPED	77	LYS	HD2	2.3	-1.0	2
UNMAPPED	59	ILE	N	125.711	-1.0	1
UNMAPPED	117	LYS	CA	58.032	-1.0	1
UNMAPPED	89	VAL	CG1	21.719	-1.0	1
UNMAPPED	97	ARG	CD	43.776	-1.0	1
UNMAPPED	30	ILE	HD12	0.698	-1.0	1
UNMAPPED	5	ALA	CB	19.553	-1.0	1
UNMAPPED	33	VAL	HG22	0.84	-1.0	1
UNMAPPED	145	ILE	HG22	0.888	-1.0	1
UNMAPPED	134	ILE	HD12	0.655	-1.0	1
UNMAPPED	56	ARG	N	124.918	-1.0	1
UNMAPPED	144	GLU	H	7.54	-1.0	1
UNMAPPED	140	LYS	CG	25.04	-1.0	1
UNMAPPED	38	ASP	HB2	2.72	-1.0	2
UNMAPPED	102	LEU	HB2	1.391	-1.0	2
UNMAPPED	71	ILE	HG23	0.988	-1.0	1
UNMAPPED	138	ILE	N	127.094	-1.0	1
UNMAPPED	117	LYS	HG3	0.95	-1.0	2
UNMAPPED	37	SER	HB2	3.86	-1.0	2
UNMAPPED	70	GLY	N	110.113	-1.0	1
UNMAPPED	9	LYS	HG2	1.394	-1.0	2
UNMAPPED	91	VAL	HG22	0.519	-1.0	1
UNMAPPED	64	ASN	C	178.2	-1.0	1
UNMAPPED	112	THR	CA	63.8	-1.0	1
UNMAPPED	39	ILE	HG22	0.682	-1.0	1
UNMAPPED	92	GLY	N	113.372	-1.0	1
UNMAPPED	43	PRO	HA	4.385	-1.0	1
UNMAPPED	104	ILE	HG23	0.632	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	82	ILE	CD1	14.89	-1.0	1
UNMAPPED	25	PHE	HE1	6.564	-1.0	3
UNMAPPED	51	GLY	H	7.67	-1.0	1
UNMAPPED	139	ASP	CB	40.72	-1.0	1
UNMAPPED	101	VAL	CA	62.56	-1.0	1
UNMAPPED	27	VAL	CB	32.742	-1.0	1
UNMAPPED	21	GLN	CG	34.589	-1.0	1
UNMAPPED	132	LEU	HD22	1.52	-1.0	1
UNMAPPED	14	LEU	HD13	0.986	-1.0	2
UNMAPPED	99	LEU	CD1	28.242	-1.0	1
UNMAPPED	105	THR	HG21	1.226	-1.0	1
UNMAPPED	147	VAL	HG12	0.98	-1.0	2
UNMAPPED	136	LEU	CD1	23.206	-1.0	2
UNMAPPED	101	VAL	HG21	0.974	-1.0	1
UNMAPPED	45	SER	H	8.06	-1.0	1
UNMAPPED	59	ILE	CD1	11.721	-1.0	1
UNMAPPED	33	VAL	HG13	0.91	-1.0	1
UNMAPPED	142	ILE	CA	65.26	-1.0	1
UNMAPPED	94	LEU	HB3	1.435	-1.0	2
UNMAPPED	146	THR	CG2	23.0	-1.0	1
UNMAPPED	81	ILE	HB	1.72	-1.0	1
UNMAPPED	43	PRO	HB3	1.88	-1.0	2
UNMAPPED	3	THR	HG22	1.234	-1.0	1
UNMAPPED	125	LEU	HG	1.63	-1.0	1
UNMAPPED	17	GLU	HA	5.558	-1.0	1
UNMAPPED	87	LYS	HD2	1.71	-1.0	2
UNMAPPED	32	MET	C	180.4	-1.0	1
UNMAPPED	63	VAL	CB	35.24	-1.0	1
UNMAPPED	138	ILE	HG22	0.89	-1.0	1
UNMAPPED	93	PHE	CB	41.515	-1.0	1
UNMAPPED	143	GLU	HG2	2.44	-1.0	2
UNMAPPED	91	VAL	N	123.068	-1.0	1
UNMAPPED	30	ILE	HG21	0.785	-1.0	1
UNMAPPED	57	GLY	CA	45.755	-1.0	1
UNMAPPED	36	LYS	HB2	1.77	-1.0	2
UNMAPPED	62	VAL	N	122.908	-1.0	1
UNMAPPED	134	ILE	HG21	0.545	-1.0	1
UNMAPPED	54	ASN	H	8.37	-1.0	1
UNMAPPED	137	ASP	N	121.871	-1.0	1
UNMAPPED	3	THR	C	178.2	-1.0	1
UNMAPPED	93	PHE	N	124.155	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	141	ILE	HG12	1.92	-1.0	2
UNMAPPED	12	GLU	CA	55.358	-1.0	1
UNMAPPED	106	GLU	H	8.81	-1.0	1
UNMAPPED	21	GLN	HB2	2.152	-1.0	2
UNMAPPED	4	LEU	CD1	25.232	-1.0	1
UNMAPPED	118	PHE	CE1	131.601	-1.0	1
UNMAPPED	127	LYS	N	130.232	-1.0	1
UNMAPPED	23	LEU	HB3	0.186	-1.0	1
UNMAPPED	77	LYS	CG	25.894	-1.0	1
UNMAPPED	81	ILE	HG13	1.409	-1.0	2
UNMAPPED	113	ASN	HB3	2.71	-1.0	2
UNMAPPED	80	SER	HA	5.165	-1.0	1
UNMAPPED	76	GLN	HG2	2.476	-1.0	2
UNMAPPED	40	THR	HG22	1.268	-1.0	1
UNMAPPED	101	VAL	HG13	0.899	-1.0	1
UNMAPPED	37	SER	CA	57.996	-1.0	1
UNMAPPED	72	SER	HA	4.299	-1.0	1
UNMAPPED	147	VAL	C	176.4	-1.0	1
UNMAPPED	106	GLU	HB3	2.26	-1.0	2
UNMAPPED	150	GLY	HA2	5.38	-1.0	2
UNMAPPED	95	VAL	H	8.86	-1.0	1
UNMAPPED	54	ASN	HB3	2.41	-1.0	2
UNMAPPED	23	LEU	C	178.4	-1.0	1
UNMAPPED	134	ILE	N	129.383	-1.0	1
UNMAPPED	138	ILE	CA	64.332	-1.0	1
UNMAPPED	25	PHE	CA	53.993	-1.0	1
UNMAPPED	72	SER	HB3	3.908	-1.0	2
UNMAPPED	45	SER	CB	64.5	-1.0	1
UNMAPPED	8	LEU	HD11	0.973	-1.0	1
UNMAPPED	15	SER	H	8.92	-1.0	1
UNMAPPED	106	GLU	HG3	2.533	-1.0	2
UNMAPPED	27	VAL	CG2	21.7	-1.0	1
UNMAPPED	59	ILE	HD13	0.722	-1.0	1
UNMAPPED	92	GLY	CA	43.855	-1.0	1
UNMAPPED	10	GLU	HG2	2.187	-1.0	2
UNMAPPED	20	GLU	CA	58.1	-1.0	1
UNMAPPED	114	VAL	N	121.586	-1.0	1
UNMAPPED	34	ILE	CD1	14.136	-1.0	1
UNMAPPED	77	LYS	CA	56.603	-1.0	1
UNMAPPED	19	ASP	C	178.0	-1.0	1
UNMAPPED	86	THR	H	8.6	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	79	LYS	HG2	1.48	-1.0	2
UNMAPPED	144	GLU	N	119.136	-1.0	1
UNMAPPED	65	LEU	HD21	0.685	-1.0	1
UNMAPPED	35	GLU	H	8.64	-1.0	1
UNMAPPED	18	ILE	C	177.3	-1.0	1
UNMAPPED	83	VAL	HB	2.059	-1.0	1
UNMAPPED	23	LEU	HD13	0.59	-1.0	1
UNMAPPED	69	LEU	CD1	22.021	-1.0	1
UNMAPPED	54	ASN	CB	39.791	-1.0	1
UNMAPPED	30	ILE	HA	4.222	-1.0	1
UNMAPPED	30	ILE	HG12	1.799	-1.0	2
UNMAPPED	95	VAL	HG13	0.582	-1.0	1
UNMAPPED	121	LYS	HE2	3.04	-1.0	2
UNMAPPED	134	ILE	HA	4.09	-1.0	1
UNMAPPED	83	VAL	CG1	21.752	-1.0	2
UNMAPPED	131	ARG	HD2	3.05	-1.0	2
UNMAPPED	12	GLU	HA	5.388	-1.0	1
UNMAPPED	76	GLN	HB2	2.164	-1.0	2
UNMAPPED	35	GLU	HG2	2.344	-1.0	2
UNMAPPED	83	VAL	HG11	0.74	-1.0	2
UNMAPPED	57	GLY	N	107.685	-1.0	1
UNMAPPED	141	ILE	HD11	0.924	-1.0	1
UNMAPPED	49	VAL	CG1	22.042	-1.0	2
UNMAPPED	30	ILE	CG2	17.584	-1.0	1
UNMAPPED	145	ILE	HD13	0.873	-1.0	1
UNMAPPED	34	ILE	HD13	0.76	-1.0	1
UNMAPPED	50	GLU	HG2	1.49	-1.0	2
UNMAPPED	25	PHE	C	176.9	-1.0	1
UNMAPPED	49	VAL	C	176.8	-1.0	1
UNMAPPED	122	SER	N	113.291	-1.0	1
UNMAPPED	71	ILE	H	7.83	-1.0	1
UNMAPPED	60	ILE	HG23	0.721	-1.0	1
UNMAPPED	92	GLY	C	172.9	-1.0	1
UNMAPPED	95	VAL	HG22	0.466	-1.0	1
UNMAPPED	87	LYS	HE2	3.02	-1.0	2
UNMAPPED	70	GLY	C	177.5	-1.0	1
UNMAPPED	127	LYS	CA	55.503	-1.0	1
UNMAPPED	104	ILE	C	178.3	-1.0	1
UNMAPPED	101	VAL	CG2	22.576	-1.0	1
UNMAPPED	135	TYR	HD1	6.738	-1.0	3
UNMAPPED	19	ASP	CA	55.75	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	15	SER	CB	67.13	-1.0	1
UNMAPPED	59	ILE	CA	60.037	-1.0	1
UNMAPPED	132	LEU	CB	43.275	-1.0	1
UNMAPPED	27	VAL	HG11	1.014	-1.0	1
UNMAPPED	143	GLU	HB2	2.17	-1.0	2
UNMAPPED	37	SER	N	121.903	-1.0	1
UNMAPPED	93	PHE	H	9.46	-1.0	1
UNMAPPED	48	PHE	CA	58.305	-1.0	1
UNMAPPED	4	LEU	HD23	0.903	-1.0	1
UNMAPPED	65	LEU	HG	1.514	-1.0	1
UNMAPPED	84	ALA	HB2	1.202	-1.0	1
UNMAPPED	35	GLU	CB	30.68	-1.0	1
UNMAPPED	25	PHE	HD1	7.208	-1.0	3
UNMAPPED	58	ARG	H	7.82	-1.0	1
UNMAPPED	112	THR	HB	4.72	-1.0	1
UNMAPPED	34	ILE	HG23	0.83	-1.0	1
UNMAPPED	82	ILE	HA	4.324	-1.0	1
UNMAPPED	56	ARG	CB	30.492	-1.0	1
UNMAPPED	147	VAL	HG11	0.98	-1.0	2
UNMAPPED	67	LYS	HA	4.248	-1.0	1
UNMAPPED	14	LEU	C	177.5	-1.0	1
UNMAPPED	81	ILE	CG1	28.511	-1.0	1
UNMAPPED	133	ILE	CB	40.763	-1.0	1
UNMAPPED	117	LYS	HB3	1.22	-1.0	2
UNMAPPED	133	ILE	HG23	0.315	-1.0	1
UNMAPPED	7	ALA	HB1	1.419	-1.0	1
UNMAPPED	52	VAL	HA	5.424	-1.0	1
UNMAPPED	96	ASP	H	7.97	-1.0	1
UNMAPPED	20	GLU	N	114.058	-1.0	1
UNMAPPED	93	PHE	HE1	7.387	-1.0	3
UNMAPPED	54	ASN	C	177.9	-1.0	1
UNMAPPED	143	GLU	C	174.7	-1.0	1
UNMAPPED	114	VAL	HG12	0.91	-1.0	2
UNMAPPED	109	LEU	HD12	0.92	-1.0	1
UNMAPPED	71	ILE	N	115.981	-1.0	1
UNMAPPED	146	THR	CA	63.285	-1.0	1
UNMAPPED	84	ALA	C	178.2	-1.0	1
UNMAPPED	53	ILE	HG12	0.82	-1.0	2
UNMAPPED	109	LEU	CB	43.984	-1.0	1
UNMAPPED	12	GLU	N	121.261	-1.0	1
UNMAPPED	61	PRO	HG2	2.11	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	68	ILE	HD13	0.56	-1.0	1
UNMAPPED	24	ALA	CB	22.476	-1.0	1
UNMAPPED	89	VAL	CA	62.273	-1.0	1
UNMAPPED	7	ALA	HA	4.323	-1.0	1
UNMAPPED	104	ILE	CA	58.949	-1.0	1
UNMAPPED	65	LEU	HD13	0.785	-1.0	1
UNMAPPED	16	PHE	HB2	3.25	-1.0	2
UNMAPPED	79	LYS	CE	42.4	-1.0	1
UNMAPPED	49	VAL	HG13	0.96	-1.0	1
UNMAPPED	87	LYS	H	8.8	-1.0	1
UNMAPPED	99	LEU	HD13	0.733	-1.0	1
UNMAPPED	56	ARG	HB2	2.01	-1.0	2
UNMAPPED	102	LEU	N	129.766	-1.0	1
UNMAPPED	135	TYR	CD1	130.652	-1.0	3
UNMAPPED	77	LYS	H	7.65	-1.0	1
UNMAPPED	68	ILE	HG23	0.709	-1.0	1
UNMAPPED	67	LYS	HG2	1.54	-1.0	2
UNMAPPED	142	ILE	HD11	0.75	-1.0	1
UNMAPPED	138	ILE	HB	1.62	-1.0	1
UNMAPPED	15	SER	HA	5.599	-1.0	1
UNMAPPED	62	VAL	CB	44.0	-1.0	1
UNMAPPED	132	LEU	HA	4.92	-1.0	1
UNMAPPED	48	PHE	HB3	3.03	-1.0	2
UNMAPPED	13	VAL	HG13	0.521	-1.0	1
UNMAPPED	4	LEU	CB	42.594	-1.0	1
UNMAPPED	9	LYS	H	8.42	-1.0	1
UNMAPPED	24	ALA	C	176.9	-1.0	1
UNMAPPED	90	GLU	H	7.68	-1.0	1
UNMAPPED	24	ALA	HB3	0.89	-1.0	1
UNMAPPED	81	ILE	N	123.571	-1.0	1
UNMAPPED	97	ARG	H	7.27	-1.0	1
UNMAPPED	109	LEU	HD23	0.78	-1.0	1
UNMAPPED	55	LEU	HD21	0.812	-1.0	1
UNMAPPED	149	GLU	HB2	2.11	-1.0	2
UNMAPPED	58	ARG	CB	31.861	-1.0	1
UNMAPPED	148	LYS	CD	29.47	-1.0	1
UNMAPPED	87	LYS	HB2	1.955	-1.0	2
UNMAPPED	22	ALA	HB3	1.291	-1.0	1
UNMAPPED	19	ASP	N	134.895	-1.0	1
UNMAPPED	56	ARG	H	9.08	-1.0	1
UNMAPPED	102	LEU	CD1	25.844	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	89	VAL	HG12	0.806	-1.0	1
UNMAPPED	68	ILE	CD1	14.271	-1.0	1
UNMAPPED	62	VAL	HG11	0.816	-1.0	1
UNMAPPED	90	GLU	HG2	2.17	-1.0	2
UNMAPPED	108	GLN	HA	4.41	-1.0	1
UNMAPPED	103	ARG	C	177.1	-1.0	1
UNMAPPED	81	ILE	HG23	0.542	-1.0	1
UNMAPPED	83	VAL	CA	63.044	-1.0	1
UNMAPPED	8	LEU	HD13	0.973	-1.0	1
UNMAPPED	22	ALA	HA	5.032	-1.0	1
UNMAPPED	117	LYS	CB	33.016	-1.0	1
UNMAPPED	53	ILE	N	117.0	-1.0	1
UNMAPPED	97	ARG	HD2	3.16	-1.0	2
UNMAPPED	44	LYS	CG	25.314	-1.0	1
UNMAPPED	145	ILE	HG21	0.888	-1.0	1
UNMAPPED	116	ASP	CA	55.9	-1.0	1
UNMAPPED	46	ARG	CA	56.1	-1.0	1
UNMAPPED	73	PHE	HE1	6.98	-1.0	3
UNMAPPED	69	LEU	HD12	0.585	-1.0	1
UNMAPPED	4	LEU	HD11	0.951	-1.0	1
UNMAPPED	30	ILE	CB	36.265	-1.0	1
UNMAPPED	100	GLY	HA3	3.9	-1.0	2
UNMAPPED	134	ILE	CB	37.742	-1.0	1
UNMAPPED	24	ALA	H	7.8	-1.0	1
UNMAPPED	99	LEU	HD22	1.04	-1.0	1
UNMAPPED	29	ASN	N	115.678	-1.0	1
UNMAPPED	48	PHE	HE1	7.31	-1.0	3
UNMAPPED	95	VAL	CG2	18.474	-1.0	1
UNMAPPED	53	ILE	CD1	14.55	-1.0	1
UNMAPPED	69	LEU	N	118.138	-1.0	1
UNMAPPED	94	LEU	CB	44.733	-1.0	1
UNMAPPED	71	ILE	HG13	1.15	-1.0	2
UNMAPPED	101	VAL	CB	33.018	-1.0	1
UNMAPPED	52	VAL	C	177.7	-1.0	1
UNMAPPED	72	SER	N	119.171	-1.0	1
UNMAPPED	92	GLY	HA3	2.815	-1.0	2
UNMAPPED	141	ILE	CG1	21.2	-1.0	1
UNMAPPED	31	GLU	C	176.6	-1.0	1
UNMAPPED	33	VAL	H	8.46	-1.0	1
UNMAPPED	62	VAL	H	8.81	-1.0	1
UNMAPPED	136	LEU	HD11	0.53	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	107	ASN	HA	4.7	-1.0	1
UNMAPPED	135	TYR	HA	4.771	-1.0	1
UNMAPPED	120	LYS	CA	57.26	-1.0	1
UNMAPPED	11	PHE	CB	40.847	-1.0	1
UNMAPPED	111	LEU	HB2	1.73	-1.0	2
UNMAPPED	133	ILE	HD11	0.524	-1.0	1
UNMAPPED	81	ILE	HD12	0.758	-1.0	1
UNMAPPED	114	VAL	CB	33.072	-1.0	1
UNMAPPED	31	GLU	H	9.44	-1.0	1
UNMAPPED	138	ILE	HG21	0.89	-1.0	1
UNMAPPED	131	ARG	C	178.5	-1.0	1
UNMAPPED	93	PHE	C	177.9	-1.0	1
UNMAPPED	13	VAL	CA	58.694	-1.0	1
UNMAPPED	65	LEU	CD2	26.626	-1.0	1
UNMAPPED	82	ILE	HD11	0.083	-1.0	1
UNMAPPED	118	PHE	HB2	3.14	-1.0	1
UNMAPPED	23	LEU	HD21	0.27	-1.0	1
UNMAPPED	124	GLY	CA	45.5	-1.0	1
UNMAPPED	75	GLU	H	9.43	-1.0	1
UNMAPPED	117	LYS	H	7.85	-1.0	1
UNMAPPED	81	ILE	CA	60.156	-1.0	1
UNMAPPED	138	ILE	CD1	13.9	-1.0	1
UNMAPPED	99	LEU	CA	56.033	-1.0	1
UNMAPPED	135	TYR	CE1	118.25	-1.0	3
UNMAPPED	18	ILE	HB	1.675	-1.0	1
UNMAPPED	30	ILE	H	7.83	-1.0	1
UNMAPPED	134	ILE	H	8.08	-1.0	1
UNMAPPED	77	LYS	CD	29.804	-1.0	1
UNMAPPED	53	ILE	C	179.3	-1.0	1
UNMAPPED	52	VAL	HG12	0.707	-1.0	1
UNMAPPED	11	PHE	HE1	6.796	-1.0	3
UNMAPPED	146	THR	HB	3.63	-1.0	1
UNMAPPED	145	ILE	CG1	27.728	-1.0	1
UNMAPPED	2	LYS	N	126.969	-1.0	1
UNMAPPED	98	VAL	H	9.02	-1.0	1
UNMAPPED	43	PRO	CB	32.432	-1.0	1
UNMAPPED	125	LEU	HD23	0.88	-1.0	1
UNMAPPED	9	LYS	CD	29.496	-1.0	1
UNMAPPED	87	LYS	CB	31.018	-1.0	1
UNMAPPED	53	ILE	HD13	0.643	-1.0	1
UNMAPPED	67	LYS	HB2	1.956	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	91	VAL	HA	4.402	-1.0	1
UNMAPPED	101	VAL	H	8.62	-1.0	1
UNMAPPED	22	ALA	C	175.9	-1.0	1
UNMAPPED	139	ASP	HA	4.34	-1.0	1
UNMAPPED	140	LYS	C	173.3	-1.0	1
UNMAPPED	20	GLU	C	177.4	-1.0	1
UNMAPPED	53	ILE	HG21	0.944	-1.0	1
UNMAPPED	63	VAL	CG1	21.582	-1.0	1
UNMAPPED	45	SER	CA	58.7	-1.0	1
UNMAPPED	33	VAL	CB	34.1	-1.0	1
UNMAPPED	18	ILE	CD1	15.11	-1.0	1
UNMAPPED	29	ASN	CA	54.261	-1.0	1
UNMAPPED	19	ASP	HB3	2.644	-1.0	2
UNMAPPED	55	LEU	HA	4.666	-1.0	1
UNMAPPED	136	LEU	HD12	0.53	-1.0	2
UNMAPPED	62	VAL	CG1	22.685	-1.0	2
UNMAPPED	151	VAL	HG11	0.883	-1.0	2
UNMAPPED	68	ILE	C	175.6	-1.0	1
UNMAPPED	129	ASP	CB	40.371	-1.0	1
UNMAPPED	72	SER	CA	59.749	-1.0	1
UNMAPPED	65	LEU	N	129.615	-1.0	1
UNMAPPED	136	LEU	HG	1.25	-1.0	1
UNMAPPED	65	LEU	HD22	0.685	-1.0	1
UNMAPPED	31	GLU	CB	31.556	-1.0	1
UNMAPPED	10	GLU	N	123.489	-1.0	1
UNMAPPED	83	VAL	HA	4.542	-1.0	1
UNMAPPED	70	GLY	HA2	4.122	-1.0	2
UNMAPPED	136	LEU	C	178.1	-1.0	1
UNMAPPED	23	LEU	HG	0.75	-1.0	1
UNMAPPED	60	ILE	HD12	0.625	-1.0	1
UNMAPPED	99	LEU	C	175.6	-1.0	1
UNMAPPED	102	LEU	HD13	0.658	-1.0	1
UNMAPPED	113	ASN	CA	54.3	-1.0	1
UNMAPPED	24	ALA	N	119.222	-1.0	1
UNMAPPED	126	VAL	N	125.178	-1.0	1
UNMAPPED	30	ILE	HB	2.321	-1.0	1
UNMAPPED	67	LYS	H	7.15	-1.0	1
UNMAPPED	134	ILE	HB	1.78	-1.0	1
UNMAPPED	106	GLU	HA	4.13	-1.0	1
UNMAPPED	66	ALA	HB1	1.509	-1.0	1
UNMAPPED	110	ASP	H	9.14	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	32	MET	HA	4.7	-1.0	1
UNMAPPED	9	LYS	HA	4.271	-1.0	1
UNMAPPED	32	MET	CG	31.024	-1.0	1
UNMAPPED	104	ILE	HD11	0.324	-1.0	1
UNMAPPED	86	THR	HG22	1.117	-1.0	1
UNMAPPED	74	ASP	HB3	2.804	-1.0	2
UNMAPPED	134	ILE	CG1	27.268	-1.0	1
UNMAPPED	35	GLU	HB2	2.1	-1.0	2
UNMAPPED	26	ASP	C	175.4	-1.0	1
UNMAPPED	118	PHE	CA	57.377	-1.0	1
UNMAPPED	45	SER	C	177.9	-1.0	1
UNMAPPED	39	ILE	HB	1.679	-1.0	1
UNMAPPED	145	ILE	N	116.52	-1.0	1
UNMAPPED	125	LEU	HD12	0.758	-1.0	1
UNMAPPED	119	GLY	HA3	3.91	-1.0	1
UNMAPPED	58	ARG	N	123.415	-1.0	1
UNMAPPED	88	ASP	HA	4.685	-1.0	1
UNMAPPED	82	ILE	HG12	1.466	-1.0	2
UNMAPPED	72	SER	C	180.3	-1.0	1
UNMAPPED	104	ILE	N	124.0	-1.0	1
UNMAPPED	124	GLY	HA3	3.91	-1.0	2
UNMAPPED	44	LYS	HE2	3.23	-1.0	2
UNMAPPED	73	PHE	C	179.7	-1.0	1
UNMAPPED	69	LEU	C	176.4	-1.0	1
UNMAPPED	49	VAL	HG21	0.888	-1.0	1
UNMAPPED	47	HIS	HE1	7.11	-1.0	3
UNMAPPED	129	ASP	H	8.79	-1.0	1
UNMAPPED	75	GLU	CG	36.044	-1.0	1
UNMAPPED	59	ILE	HG23	0.77	-1.0	1
UNMAPPED	68	ILE	CB	37.987	-1.0	1
UNMAPPED	128	THR	HG22	0.952	-1.0	1
UNMAPPED	96	ASP	HA	5.3	-1.0	1
UNMAPPED	4	LEU	N	127.087	-1.0	1
UNMAPPED	118	PHE	HE1	7.253	-1.0	1
UNMAPPED	67	LYS	CG	26.867	-1.0	1
UNMAPPED	133	ILE	HB	1.59	-1.0	1
UNMAPPED	61	PRO	CA	62.664	-1.0	1
UNMAPPED	51	GLY	HA2	4.198	-1.0	2
UNMAPPED	68	ILE	HG22	0.709	-1.0	1
UNMAPPED	125	LEU	CA	53.7	-1.0	1
UNMAPPED	69	LEU	CB	43.256	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	65	LEU	CA	57.3	-1.0	1
UNMAPPED	65	LEU	HB2	1.929	-1.0	2
UNMAPPED	129	ASP	HB2	2.87	-1.0	2
UNMAPPED	109	LEU	HD11	0.92	-1.0	1
UNMAPPED	87	LYS	HA	3.911	-1.0	1
UNMAPPED	146	THR	CB	70.015	-1.0	1
UNMAPPED	110	ASP	CB	42.531	-1.0	1
UNMAPPED	118	PHE	C	175.8	-1.0	1
UNMAPPED	148	LYS	HB2	2.13	-1.0	2
UNMAPPED	87	LYS	CD	29.58	-1.0	1
UNMAPPED	109	LEU	CA	54.722	-1.0	1
UNMAPPED	150	GLY	C	179.6	-1.0	1
UNMAPPED	98	VAL	HG11	1.1	-1.0	1
UNMAPPED	138	ILE	H	8.34	-1.0	1
UNMAPPED	103	ARG	H	8.34	-1.0	1
UNMAPPED	113	ASN	N	123.318	-1.0	1
UNMAPPED	126	VAL	CA	61.02	-1.0	1
UNMAPPED	89	VAL	CB	35.0	-1.0	1
UNMAPPED	104	ILE	CB	41.184	-1.0	1
UNMAPPED	61	PRO	HD2	4.77	-1.0	2
UNMAPPED	85	ARG	H	8.79	-1.0	1
UNMAPPED	145	ILE	C	176.2	-1.0	1
UNMAPPED	10	GLU	H	8.01	-1.0	1
UNMAPPED	148	LYS	H	8.2	-1.0	1
UNMAPPED	63	VAL	HG22	0.76	-1.0	1
UNMAPPED	148	LYS	HE2	3.0	-1.0	2
UNMAPPED	25	PHE	HB3	2.84	-1.0	2
UNMAPPED	50	GLU	CA	56.546	-1.0	1
UNMAPPED	103	ARG	HG2	1.43	-1.0	2
UNMAPPED	118	PHE	N	117.322	-1.0	1
UNMAPPED	143	GLU	HG3	2.24	-1.0	2
UNMAPPED	102	LEU	HD22	0.72	-1.0	1
UNMAPPED	69	LEU	HD23	1.51	-1.0	1
UNMAPPED	145	ILE	CA	63.401	-1.0	1
UNMAPPED	78	MET	C	177.1	-1.0	1
UNMAPPED	141	ILE	CB	38.029	-1.0	1
UNMAPPED	58	ARG	CA	55.11	-1.0	1
UNMAPPED	44	LYS	HD2	1.7	-1.0	2
UNMAPPED	90	GLU	N	126.755	-1.0	1
UNMAPPED	144	GLU	CA	59.015	-1.0	1
UNMAPPED	89	VAL	HG11	0.806	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	127	LYS	CE	25.241	-1.0	1
UNMAPPED	126	VAL	HG11	0.686	-1.0	1
UNMAPPED	24	ALA	HA	5.323	-1.0	1
UNMAPPED	126	VAL	HA	4.55	-1.0	1
UNMAPPED	31	GLU	HA	4.395	-1.0	1
UNMAPPED	57	GLY	HA2	4.271	-1.0	2
UNMAPPED	112	THR	HG21	1.238	-1.0	1
UNMAPPED	28	ASP	C	175.9	-1.0	1
UNMAPPED	2	LYS	CB	33.532	-1.0	1
UNMAPPED	102	LEU	HA	4.75	-1.0	1
UNMAPPED	55	LEU	C	177.5	-1.0	1
UNMAPPED	10	GLU	HB3	2.067	-1.0	2
UNMAPPED	111	LEU	HD11	0.95	-1.0	1
UNMAPPED	10	GLU	C	177.6	-1.0	1
UNMAPPED	23	LEU	CD1	27.12	-1.0	1
UNMAPPED	82	ILE	CG1	27.042	-1.0	1
UNMAPPED	20	GLU	HA	3.936	-1.0	1
UNMAPPED	4	LEU	CA	55.829	-1.0	1
UNMAPPED	107	ASN	H	8.14	-1.0	1
UNMAPPED	31	GLU	HB3	1.836	-1.0	2
UNMAPPED	138	ILE	HD12	0.07	-1.0	1
UNMAPPED	52	VAL	H	8.88	-1.0	1
UNMAPPED	34	ILE	HD11	0.76	-1.0	1
UNMAPPED	73	PHE	N	116.821	-1.0	1
UNMAPPED	44	LYS	HA	4.121	-1.0	1
UNMAPPED	129	ASP	N	126.767	-1.0	1
UNMAPPED	77	LYS	C	176.1	-1.0	1
UNMAPPED	59	ILE	HG13	0.732	-1.0	2
UNMAPPED	31	GLU	N	129.991	-1.0	1
UNMAPPED	80	SER	CA	58.426	-1.0	1
UNMAPPED	91	VAL	C	180.8	-1.0	1
UNMAPPED	66	ALA	C	176.2	-1.0	1
UNMAPPED	27	VAL	N	121.388	-1.0	1
UNMAPPED	10	GLU	CB	32.75	-1.0	1
UNMAPPED	16	PHE	H	9.05	-1.0	1
UNMAPPED	8	LEU	N	121.896	-1.0	1
UNMAPPED	88	ASP	HB2	2.77	-1.0	2
UNMAPPED	119	GLY	H	8.18	-1.0	1
UNMAPPED	144	GLU	C	174.7	-1.0	1
UNMAPPED	11	PHE	CA	56.257	-1.0	1
UNMAPPED	87	LYS	HG3	1.44	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	128	THR	HG23	0.952	-1.0	1
UNMAPPED	62	VAL	HG23	0.969	-1.0	1
UNMAPPED	141	ILE	HA	3.57	-1.0	1
UNMAPPED	60	ILE	CD1	14.645	-1.0	1
UNMAPPED	63	VAL	N	125.075	-1.0	1
UNMAPPED	39	ILE	HA	4.352	-1.0	1
UNMAPPED	125	LEU	HB2	1.68	-1.0	2
UNMAPPED	8	LEU	CD1	25.604	-1.0	1
UNMAPPED	96	ASP	HB2	2.9	-1.0	2
UNMAPPED	91	VAL	CB	36.064	-1.0	1
UNMAPPED	34	ILE	CA	59.65	-1.0	1
UNMAPPED	11	PHE	HD1	7.059	-1.0	3
UNMAPPED	89	VAL	HG22	0.888	-1.0	1
UNMAPPED	52	VAL	HG21	0.67	-1.0	1
UNMAPPED	99	LEU	CB	42.015	-1.0	1
UNMAPPED	2	LYS	C	176.7	-1.0	1
UNMAPPED	57	GLY	C	178.8	-1.0	1
UNMAPPED	95	VAL	HA	4.72	-1.0	1
UNMAPPED	141	ILE	N	121.995	-1.0	1
UNMAPPED	61	PRO	HB3	1.81	-1.0	2
UNMAPPED	145	ILE	HB	2.13	-1.0	1
UNMAPPED	82	ILE	C	177.5	-1.0	1
UNMAPPED	52	VAL	HG11	0.707	-1.0	1
UNMAPPED	107	ASN	CB	38.015	-1.0	1
UNMAPPED	79	LYS	HE2	3.1	-1.0	2
UNMAPPED	151	VAL	CG1	20.637	-1.0	2
UNMAPPED	50	GLU	C	176.1	-1.0	1
UNMAPPED	18	ILE	N	123.423	-1.0	1
UNMAPPED	115	SER	HA	4.01	-1.0	1
UNMAPPED	9	LYS	CA	57.032	-1.0	1
UNMAPPED	89	VAL	CG2	21.42	-1.0	1
UNMAPPED	55	LEU	HB2	1.697	-1.0	2
UNMAPPED	52	VAL	CG1	21.638	-1.0	1
UNMAPPED	30	ILE	HD11	0.698	-1.0	1
UNMAPPED	33	VAL	HG21	0.84	-1.0	1
UNMAPPED	131	ARG	CB	33.376	-1.0	1
UNMAPPED	123	LYS	CB	33.953	-1.0	1
UNMAPPED	51	GLY	N	108.488	-1.0	1
UNMAPPED	11	PHE	C	179.3	-1.0	1
UNMAPPED	76	GLN	C	175.4	-1.0	1
UNMAPPED	79	LYS	C	175.9	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	134	ILE	HD11	0.655	-1.0	1
UNMAPPED	100	GLY	C	179.7	-1.0	1
UNMAPPED	18	ILE	HG23	1.138	-1.0	1
UNMAPPED	64	ASN	CB	37.737	-1.0	1
UNMAPPED	142	ILE	HG12	1.76	-1.0	2
UNMAPPED	33	VAL	CA	62.032	-1.0	1
UNMAPPED	117	LYS	HG2	1.002	-1.0	2
UNMAPPED	37	SER	HB3	3.73	-1.0	2
UNMAPPED	91	VAL	HG21	0.519	-1.0	1
UNMAPPED	20	GLU	CG	36.7	-1.0	1
UNMAPPED	39	ILE	HG23	0.682	-1.0	1
UNMAPPED	29	ASN	HB3	2.384	-1.0	2
UNMAPPED	151	VAL	HG12	0.883	-1.0	2
UNMAPPED	129	ASP	CA	55.786	-1.0	1
UNMAPPED	55	LEU	HD11	0.87	-1.0	1
UNMAPPED	39	ILE	HD11	0.72	-1.0	1
UNMAPPED	117	LYS	C	175.4	-1.0	1
UNMAPPED	132	LEU	HD23	1.52	-1.0	1
UNMAPPED	14	LEU	N	125.643	-1.0	1
UNMAPPED	14	LEU	HD12	0.986	-1.0	2
UNMAPPED	77	LYS	N	118.908	-1.0	1
UNMAPPED	145	ILE	HA	4.2	-1.0	1
UNMAPPED	131	ARG	HG2	1.53	-1.0	2
UNMAPPED	108	GLN	N	119.998	-1.0	1
UNMAPPED	101	VAL	HG22	0.974	-1.0	1
UNMAPPED	116	ASP	H	8.49	-1.0	1
UNMAPPED	124	GLY	H	7.85	-1.0	1
UNMAPPED	149	GLU	HG2	2.31	-1.0	2
UNMAPPED	47	HIS	CE1	119.615	-1.0	3
UNMAPPED	142	ILE	CB	36.74	-1.0	1
UNMAPPED	27	VAL	HG21	1.075	-1.0	1
UNMAPPED	94	LEU	HB2	1.696	-1.0	2
UNMAPPED	82	ILE	CA	61.064	-1.0	1
UNMAPPED	79	LYS	N	124.661	-1.0	1
UNMAPPED	3	THR	HG23	1.234	-1.0	1
UNMAPPED	117	LYS	HE2	2.87	-1.0	2
UNMAPPED	99	LEU	HA	4.48	-1.0	1
UNMAPPED	102	LEU	CG	27.149	-1.0	1
UNMAPPED	28	ASP	N	121.676	-1.0	1
UNMAPPED	32	MET	CB	35.751	-1.0	1
UNMAPPED	104	ILE	HD12	0.324	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	49	VAL	HG22	0.888	-1.0	1
UNMAPPED	58	ARG	HA	4.537	-1.0	1
UNMAPPED	103	ARG	HA	4.957	-1.0	1
UNMAPPED	33	VAL	C	177.5	-1.0	1
UNMAPPED	132	LEU	HD13	0.92	-1.0	1
UNMAPPED	146	THR	HG21	1.21	-1.0	1
UNMAPPED	122	SER	HB2	3.69	-1.0	2
UNMAPPED	4	LEU	CD2	23.98	-1.0	1
UNMAPPED	90	GLU	CB	33.513	-1.0	1
UNMAPPED	23	LEU	HB2	1.384	-1.0	1
UNMAPPED	115	SER	C	177.1	-1.0	1
UNMAPPED	93	PHE	HA	5.237	-1.0	1
UNMAPPED	6	ASP	C	176.7	-1.0	1
UNMAPPED	131	ARG	CA	55.223	-1.0	1
UNMAPPED	73	PHE	HB3	2.996	-1.0	2
UNMAPPED	51	GLY	C	174.0	-1.0	1
UNMAPPED	60	ILE	CG2	16.846	-1.0	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	148	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	138	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	140	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	146	0.00 ± 0.00	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 281. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/281 (0%)	0/161 (0%)	0/101 (0%)	0/19 (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 281. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/281 (0%)	0/161 (0%)	0/101 (0%)	0/19 (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, *ppm*	Expected range, *ppm*	Z-score
???	UNMAPPED	127	LYS	CE	25.24	46.00 – 37.80	-20.3
???	UNMAPPED	122	SER	C	197.10	183.48 – 165.88	12.7
???	UNMAPPED	47	HIS	CE1	119.61	149.70 – 125.30	-7.3
???	UNMAPPED	34	ILE	CG2	27.23	24.63 – 10.43	6.8
???	UNMAPPED	62	VAL	CB	44.00	41.76 – 23.66	6.2

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.