Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1QM9
Title	:	NMR, REPRESENTATIVE STRUCTURE
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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:

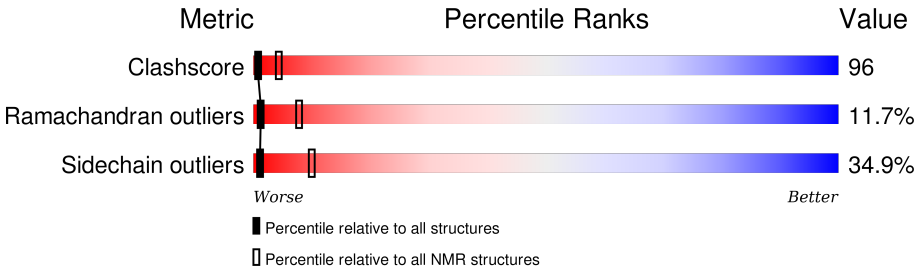
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 >=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	198	21% 48% 26% 5%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3132 atoms, of which 1575 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called POLYPYRIMIDINE TRACT-BINDING PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	198	3132	984	1575	283	285	5	0

There is a discrepancy between the modelled and reference sequences:

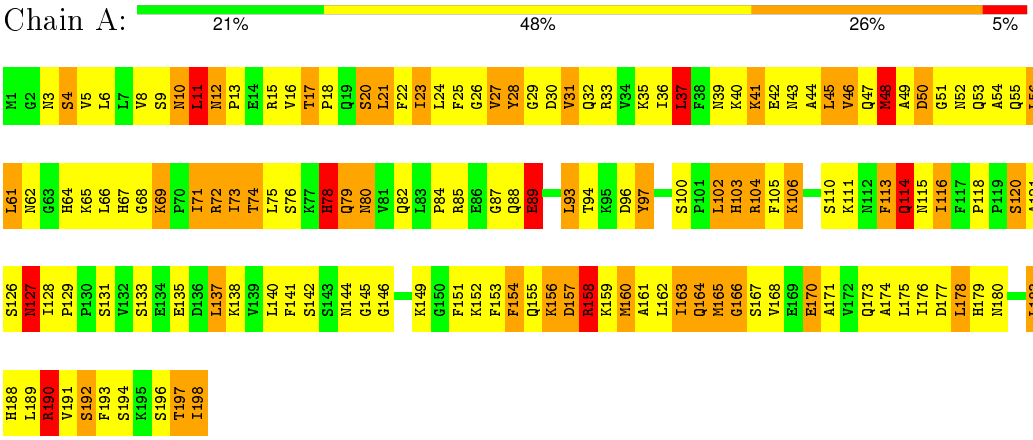
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P26599

4 Residue-property plots (i)

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: POLYPYRIMIDINE TRACT-BINDING PROTEIN

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 100 calculated structures, 1 were deposited, based on the following criterion: *LEAST ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	
AURELIA XPLOR	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 5409
Number of chemical shift lists	1
Total number of shifts	933
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	933
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality

6.1 Standard geometry

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

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	7
All	All	0	7

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	158	ARG	Sidechain
1	A	104	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	190	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	85	ARG	Sidechain
1	A	15	ARG	Sidechain

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	1557	1575	1575	302
All	All	1557	1575	1575	302

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 96.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:5:VAL:HG13	1:A:46:VAL:O	1.10	1.44
1:A:25:PHE:CZ	1:A:61:LEU:HD22	1.04	1.86
1:A:140:LEU:CB	1:A:178:LEU:HD13	1.01	1.86
1:A:5:VAL:HG22	1:A:47:GLN:HA	0.96	1.36
1:A:151:PHE:CB	1:A:163:ILE:HG23	0.94	1.92
1:A:25:PHE:CD1	1:A:61:LEU:HD13	0.93	1.99
1:A:49:ALA:HA	1:A:53:GLN:HB2	0.88	1.46
1:A:102:LEU:O	1:A:102:LEU:HD22	0.88	1.69
1:A:140:LEU:HB2	1:A:178:LEU:HD13	0.85	1.46
1:A:178:LEU:N	1:A:178:LEU:HD23	0.85	1.85
1:A:121:ALA:HB2	1:A:168:VAL:HA	0.83	1.47
1:A:197:THR:O	1:A:198:ILE:HD12	0.83	1.72
1:A:25:PHE:CE1	1:A:61:LEU:HD13	0.82	2.08
1:A:102:LEU:C	1:A:102:LEU:HD22	0.80	1.97
1:A:123:LEU:O	1:A:163:ILE:HD12	0.80	1.76
1:A:140:LEU:HB3	1:A:178:LEU:HD13	0.79	1.54
1:A:36:ILE:C	1:A:37:LEU:HD23	0.77	1.99
1:A:118:PRO:HG2	1:A:198:ILE:HG22	0.77	1.56
1:A:49:ALA:CA	1:A:53:GLN:HB2	0.76	2.10
1:A:4:SER:O	1:A:49:ALA:HB3	0.75	1.81
1:A:49:ALA:O	1:A:51:GLY:N	0.73	2.20
1:A:25:PHE:CE1	1:A:61:LEU:HD22	0.72	2.18
1:A:54:ALA:O	1:A:58:MET:CB	0.72	2.37
1:A:123:LEU:HD11	1:A:191:VAL:CG1	0.71	2.15
1:A:151:PHE:HB2	1:A:163:ILE:HG23	0.71	1.62
1:A:124:HIS:CE1	1:A:161:ALA:N	0.71	2.59
1:A:162:LEU:HD23	1:A:163:ILE:N	0.70	2.01
1:A:175:LEU:HD12	1:A:191:VAL:HB	0.70	1.64
1:A:124:HIS:CE1	1:A:160:MET:HB3	0.69	2.22
1:A:178:LEU:CD2	1:A:178:LEU:N	0.69	2.56
1:A:10:ASN:O	1:A:11:LEU:C	0.68	2.31
1:A:25:PHE:CD1	1:A:61:LEU:CD1	0.67	2.77
1:A:183:LEU:HD23	1:A:183:LEU:N	0.66	2.06
1:A:179:HIS:CE1	1:A:189:LEU:CD1	0.65	2.80
1:A:8:VAL:CG2	1:A:25:PHE:CE2	0.65	2.80
1:A:141:PHE:CD1	1:A:174:ALA:CB	0.65	2.80
1:A:121:ALA:HB3	1:A:165:MET:O	0.64	1.91
1:A:154:PHE:CD1	1:A:154:PHE:N	0.64	2.63
1:A:66:LEU:HD21	1:A:71:ILE:HG12	0.64	1.68
1:A:140:LEU:HB3	1:A:178:LEU:HD22	0.64	1.67
1:A:125:LEU:HG	1:A:137:LEU:HD22	0.63	1.70
1:A:155:GLN:O	1:A:156:LYS:C	0.63	2.36

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:124:HIS:CG	1:A:161:ALA:O	0.63	2.51
1:A:17:THR:HG22	1:A:18:PRO:HD2	0.63	1.69
1:A:54:ALA:HB1	1:A:58:MET:HB2	0.63	1.69
1:A:197:THR:C	1:A:198:ILE:HD12	0.63	2.13
1:A:124:HIS:HA	1:A:161:ALA:O	0.63	1.93
1:A:116:ILE:O	1:A:116:ILE:HG13	0.63	1.93
1:A:140:LEU:CB	1:A:178:LEU:CD1	0.62	2.73
1:A:31:VAL:HA	1:A:47:GLN:O	0.62	1.93
1:A:31:VAL:HG12	1:A:31:VAL:O	0.62	1.94
1:A:12:ASN:CB	1:A:13:PRO:CD	0.62	2.77
1:A:151:PHE:HB3	1:A:163:ILE:HG23	0.62	1.72
1:A:49:ALA:C	1:A:51:GLY:N	0.61	2.49
1:A:141:PHE:CE1	1:A:174:ALA:CB	0.61	2.83
1:A:49:ALA:HB1	1:A:54:ALA:HB2	0.61	1.70
1:A:141:PHE:CE1	1:A:174:ALA:HB1	0.61	2.30
1:A:5:VAL:HG13	1:A:46:VAL:C	0.61	2.15
1:A:154:PHE:CE1	1:A:156:LYS:HB2	0.61	2.31
1:A:141:PHE:CD1	1:A:174:ALA:HB1	0.61	2.31
1:A:25:PHE:O	1:A:28:TYR:CZ	0.61	2.54
1:A:28:TYR:CZ	1:A:48:MET:SD	0.61	2.94
1:A:25:PHE:O	1:A:28:TYR:CE1	0.61	2.54
1:A:189:LEU:O	1:A:189:LEU:HD12	0.60	1.95
1:A:31:VAL:CG1	1:A:31:VAL:O	0.60	2.49
1:A:49:ALA:CB	1:A:54:ALA:HB2	0.60	2.25
1:A:174:ALA:O	1:A:178:LEU:HG	0.60	1.97
1:A:48:MET:HG2	1:A:49:ALA:N	0.60	2.10
1:A:96:ASP:O	1:A:97:TYR:C	0.60	2.40
1:A:49:ALA:HA	1:A:53:GLN:CB	0.60	2.23
1:A:123:LEU:CD1	1:A:191:VAL:HG13	0.59	2.27
1:A:183:LEU:HD21	1:A:187:HIS:NE2	0.59	2.11
1:A:97:TYR:N	1:A:97:TYR:CD1	0.59	2.70
1:A:123:LEU:HD11	1:A:191:VAL:HG13	0.59	1.73
1:A:193:PHE:O	1:A:193:PHE:CG	0.59	2.55
1:A:31:VAL:HA	1:A:48:MET:CB	0.59	2.28
1:A:4:SER:CB	1:A:51:GLY:N	0.59	2.66
1:A:140:LEU:HB3	1:A:178:LEU:CD1	0.58	2.26
1:A:32:GLN:N	1:A:47:GLN:O	0.58	2.36
1:A:114:GLN:O	1:A:114:GLN:CG	0.58	2.52
1:A:123:LEU:HD21	1:A:191:VAL:HG13	0.58	1.75
1:A:10:ASN:O	1:A:12:ASN:N	0.58	2.37
1:A:123:LEU:HD22	1:A:141:PHE:CZ	0.58	2.33
1:A:54:ALA:O	1:A:58:MET:N	0.57	2.36

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:114:GLN:O	1:A:115:ASN:CB	0.57	2.53
1:A:128:ILE:HG23	1:A:129:PRO:HD2	0.57	1.77
1:A:31:VAL:CG2	1:A:46:VAL:HG13	0.57	2.29
1:A:123:LEU:CD2	1:A:191:VAL:HG13	0.57	2.29
1:A:197:THR:O	1:A:198:ILE:CD1	0.57	2.51
1:A:126:SER:O	1:A:127:ASN:C	0.56	2.40
1:A:78:HIS:NE2	1:A:82:GLN:NE2	0.56	2.54
1:A:11:LEU:HD22	1:A:11:LEU:H	0.56	1.60
1:A:140:LEU:O	1:A:145:GLY:N	0.56	2.39
1:A:8:VAL:HG22	1:A:25:PHE:CE2	0.56	2.36
1:A:127:ASN:HB2	1:A:188:HIS:CE1	0.56	2.34
1:A:121:ALA:HB1	1:A:171:ALA:HB2	0.56	1.78
1:A:165:MET:O	1:A:166:GLY:C	0.55	2.44
1:A:102:LEU:HD13	1:A:103:HIS:N	0.55	2.16
1:A:153:PHE:CD1	1:A:161:ALA:HB1	0.55	2.36
1:A:118:PRO:CG	1:A:198:ILE:HG22	0.55	2.28
1:A:37:LEU:CD2	1:A:93:LEU:O	0.55	2.55
1:A:102:LEU:CD1	1:A:102:LEU:N	0.55	2.70
1:A:16:VAL:HG12	1:A:16:VAL:O	0.55	2.01
1:A:176:ILE:O	1:A:180:ASN:CA	0.55	2.54
1:A:188:HIS:ND1	1:A:188:HIS:O	0.54	2.41
1:A:89:GLU:HA	1:A:94:THR:HG21	0.54	1.78
1:A:174:ALA:O	1:A:178:LEU:CG	0.54	2.56
1:A:12:ASN:CB	1:A:13:PRO:HD3	0.54	2.31
1:A:26:GLY:O	1:A:29:GLY:N	0.54	2.39
1:A:49:ALA:O	1:A:50:ASP:C	0.54	2.42
1:A:8:VAL:CG1	1:A:21:LEU:HD11	0.53	2.33
1:A:154:PHE:CE1	1:A:156:LYS:CB	0.53	2.91
1:A:121:ALA:HB1	1:A:171:ALA:CB	0.53	2.33
1:A:154:PHE:CD1	1:A:156:LYS:HB2	0.53	2.39
1:A:125:LEU:HD13	1:A:190:ARG:O	0.53	2.03
1:A:114:GLN:CD	1:A:114:GLN:N	0.53	2.61
1:A:18:PRO:HD3	1:A:36:ILE:HD12	0.53	1.81
1:A:170:GLU:N	1:A:170:GLU:OE1	0.53	2.42
1:A:20:SER:O	1:A:23:ILE:HG22	0.53	2.04
1:A:128:ILE:CG2	1:A:129:PRO:HD2	0.53	2.34
1:A:6:LEU:HD21	1:A:58:MET:HA	0.53	1.80
1:A:48:MET:O	1:A:53:GLN:HG3	0.52	2.04
1:A:4:SER:OG	1:A:51:GLY:N	0.52	2.42
1:A:18:PRO:HD3	1:A:36:ILE:CD1	0.52	2.34
1:A:66:LEU:HD21	1:A:71:ILE:CG1	0.52	2.34
1:A:8:VAL:HG21	1:A:25:PHE:CE2	0.52	2.39

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:66:LEU:HD22	1:A:69:LYS:O	0.52	2.05
1:A:49:ALA:C	1:A:51:GLY:H	0.52	2.08
1:A:88:GLN:O	1:A:89:GLU:CB	0.52	2.58
1:A:153:PHE:HA	1:A:161:ALA:CB	0.51	2.34
1:A:127:ASN:CB	1:A:188:HIS:CE1	0.51	2.93
1:A:162:LEU:HD23	1:A:163:ILE:H	0.51	1.64
1:A:54:ALA:CB	1:A:58:MET:HB2	0.51	2.35
1:A:197:THR:O	1:A:198:ILE:CB	0.51	2.57
1:A:13:PRO:HG2	1:A:16:VAL:CG2	0.51	2.34
1:A:64:HIS:CE1	1:A:66:LEU:HG	0.51	2.39
1:A:155:GLN:O	1:A:156:LYS:O	0.51	2.29
1:A:25:PHE:CZ	1:A:61:LEU:CD2	0.51	2.77
1:A:153:PHE:HA	1:A:161:ALA:HB1	0.51	1.83
1:A:11:LEU:N	1:A:11:LEU:HD22	0.51	2.20
1:A:36:ILE:O	1:A:37:LEU:HD23	0.51	2.05
1:A:48:MET:O	1:A:53:GLN:CG	0.51	2.59
1:A:126:SER:O	1:A:127:ASN:O	0.50	2.29
1:A:140:LEU:HB3	1:A:178:LEU:CD2	0.50	2.36
1:A:154:PHE:O	1:A:160:MET:O	0.50	2.28
1:A:31:VAL:HA	1:A:48:MET:HB2	0.50	1.82
1:A:144:ASN:HB2	1:A:178:LEU:CD2	0.50	2.36
1:A:123:LEU:HD12	1:A:192:SER:C	0.50	2.25
1:A:114:GLN:NE2	1:A:115:ASN:O	0.50	2.45
1:A:186:ASN:C	1:A:187:HIS:CG	0.50	2.82
1:A:102:LEU:C	1:A:102:LEU:CD2	0.50	2.71
1:A:183:LEU:HD23	1:A:183:LEU:H	0.50	1.66
1:A:64:HIS:O	1:A:65:LYS:CB	0.50	2.56
1:A:138:LYS:HE3	1:A:151:PHE:CE1	0.50	2.42
1:A:114:GLN:N	1:A:114:GLN:OE1	0.50	2.44
1:A:102:LEU:CD2	1:A:102:LEU:O	0.50	2.53
1:A:17:THR:CG2	1:A:18:PRO:HD2	0.49	2.37
1:A:56:LEU:O	1:A:60:HIS:CB	0.49	2.60
1:A:175:LEU:HD13	1:A:191:VAL:O	0.49	2.07
1:A:179:HIS:CE1	1:A:189:LEU:HD11	0.49	2.41
1:A:71:ILE:HG13	1:A:71:ILE:O	0.49	2.06
1:A:127:ASN:HB3	1:A:188:HIS:ND1	0.49	2.22
1:A:144:ASN:CB	1:A:178:LEU:CD2	0.49	2.90
1:A:114:GLN:O	1:A:114:GLN:NE2	0.49	2.45
1:A:46:VAL:HG12	1:A:46:VAL:O	0.49	2.07
1:A:123:LEU:CD1	1:A:191:VAL:CG1	0.49	2.89
1:A:189:LEU:O	1:A:189:LEU:CD1	0.49	2.60
1:A:114:GLN:O	1:A:114:GLN:HG2	0.49	2.08

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:4:SER:HB3	1:A:50:ASP:CA	0.49	2.38
1:A:54:ALA:CA	1:A:58:MET:HB2	0.49	2.38
1:A:174:ALA:O	1:A:178:LEU:CB	0.49	2.61
1:A:120:SER:O	1:A:168:VAL:HG22	0.49	2.07
1:A:197:THR:C	1:A:198:ILE:CG1	0.49	2.81
1:A:186:ASN:O	1:A:187:HIS:CB	0.49	2.60
1:A:26:GLY:O	1:A:27:VAL:C	0.49	2.50
1:A:123:LEU:HD11	1:A:191:VAL:HG12	0.49	1.83
1:A:183:LEU:N	1:A:183:LEU:CD2	0.48	2.74
1:A:73:ILE:CG2	1:A:73:ILE:O	0.48	2.60
1:A:124:HIS:CD2	1:A:162:LEU:HB2	0.48	2.43
1:A:26:GLY:O	1:A:28:TYR:N	0.48	2.47
1:A:58:MET:O	1:A:62:ASN:CG	0.48	2.52
1:A:152:LYS:HB3	1:A:154:PHE:CE2	0.48	2.43
1:A:174:ALA:C	1:A:178:LEU:HG	0.48	2.30
1:A:6:LEU:O	1:A:46:VAL:HB	0.47	2.09
1:A:54:ALA:O	1:A:58:MET:HB2	0.47	2.09
1:A:124:HIS:CE1	1:A:161:ALA:C	0.47	2.88
1:A:151:PHE:O	1:A:151:PHE:CG	0.47	2.67
1:A:124:HIS:ND1	1:A:160:MET:HB3	0.47	2.24
1:A:114:GLN:O	1:A:115:ASN:HB2	0.47	2.09
1:A:155:GLN:O	1:A:158:ARG:N	0.47	2.48
1:A:40:LYS:O	1:A:41:LYS:O	0.47	2.33
1:A:11:LEU:CD2	1:A:44:ALA:HB2	0.47	2.39
1:A:54:ALA:O	1:A:58:MET:HB3	0.47	2.06
1:A:23:ILE:CG2	1:A:24:LEU:N	0.47	2.78
1:A:123:LEU:HG	1:A:192:SER:O	0.46	2.09
1:A:69:LYS:CG	1:A:69:LYS:O	0.46	2.63
1:A:66:LEU:CD2	1:A:71:ILE:HG12	0.46	2.39
1:A:18:PRO:O	1:A:22:PHE:CB	0.46	2.63
1:A:48:MET:HG2	1:A:53:GLN:CB	0.46	2.40
1:A:128:ILE:N	1:A:128:ILE:HD12	0.46	2.25
1:A:5:VAL:HG22	1:A:47:GLN:CA	0.46	2.24
1:A:124:HIS:CE1	1:A:161:ALA:CA	0.46	2.98
1:A:197:THR:O	1:A:198:ILE:HB	0.46	2.11
1:A:79:GLN:O	1:A:80:ASN:O	0.46	2.33
1:A:158:ARG:O	1:A:160:MET:SD	0.46	2.73
1:A:189:LEU:O	1:A:189:LEU:CG	0.46	2.63
1:A:124:HIS:CD2	1:A:162:LEU:CB	0.46	2.99
1:A:4:SER:HB3	1:A:51:GLY:N	0.46	2.26
1:A:178:LEU:H	1:A:178:LEU:HD23	0.46	1.65
1:A:197:THR:C	1:A:198:ILE:CD1	0.46	2.83

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:140:LEU:O	1:A:144:ASN:N	0.46	2.49
1:A:102:LEU:CD1	1:A:102:LEU:H	0.45	2.24
1:A:41:LYS:O	1:A:42:GLU:CB	0.45	2.64
1:A:121:ALA:CB	1:A:168:VAL:HA	0.45	2.33
1:A:105:PHE:CG	1:A:106:LYS:N	0.45	2.84
1:A:67:HIS:CD2	1:A:67:HIS:N	0.45	2.84
1:A:30:ASP:HB3	1:A:53:GLN:OE1	0.45	2.11
1:A:31:VAL:HG22	1:A:47:GLN:N	0.45	2.26
1:A:30:ASP:CG	1:A:53:GLN:OE1	0.45	2.55
1:A:123:LEU:CD2	1:A:141:PHE:CZ	0.45	2.99
1:A:193:PHE:O	1:A:193:PHE:CD2	0.45	2.69
1:A:48:MET:C	1:A:53:GLN:HB2	0.45	2.32
1:A:48:MET:CG	1:A:53:GLN:HB3	0.45	2.41
1:A:125:LEU:CG	1:A:137:LEU:HD22	0.45	2.41
1:A:49:ALA:O	1:A:52:ASN:N	0.45	2.50
1:A:12:ASN:HB2	1:A:13:PRO:CD	0.44	2.41
1:A:39:ASN:HB3	1:A:43:ASN:CB	0.44	2.42
1:A:124:HIS:ND1	1:A:161:ALA:O	0.44	2.49
1:A:66:LEU:HD13	1:A:71:ILE:H	0.44	1.72
1:A:185:GLU:O	1:A:186:ASN:CB	0.44	2.64
1:A:36:ILE:C	1:A:37:LEU:CD2	0.44	2.81
1:A:146:GLY:HA3	1:A:170:GLU:CG	0.44	2.43
1:A:25:PHE:CE1	1:A:61:LEU:CD1	0.44	2.92
1:A:137:LEU:HD23	1:A:141:PHE:CE2	0.44	2.48
1:A:157:ASP:HB3	1:A:160:MET:CB	0.44	2.43
1:A:126:SER:HB3	1:A:190:ARG:HB2	0.44	1.90
1:A:153:PHE:CD1	1:A:161:ALA:CB	0.44	3.01
1:A:174:ALA:O	1:A:178:LEU:N	0.44	2.46
1:A:58:MET:O	1:A:62:ASN:HB2	0.43	2.14
1:A:75:LEU:O	1:A:76:SER:C	0.43	2.56
1:A:57:ALA:O	1:A:61:LEU:HB2	0.43	2.14
1:A:121:ALA:CB	1:A:171:ALA:HB2	0.43	2.43
1:A:137:LEU:HA	1:A:140:LEU:HD12	0.43	1.90
1:A:12:ASN:HB2	1:A:13:PRO:HD3	0.43	1.91
1:A:18:PRO:O	1:A:22:PHE:HB2	0.43	2.14
1:A:124:HIS:NE2	1:A:156:LYS:HG2	0.43	2.28
1:A:127:ASN:CB	1:A:188:HIS:ND1	0.43	2.82
1:A:39:ASN:ND2	1:A:39:ASN:N	0.43	2.66
1:A:141:PHE:O	1:A:145:GLY:HA3	0.42	2.13
1:A:174:ALA:CA	1:A:178:LEU:HG	0.42	2.44
1:A:31:VAL:O	1:A:97:TYR:HB3	0.42	2.15
1:A:49:ALA:N	1:A:53:GLN:HB2	0.42	2.28

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:125:LEU:CD2	1:A:191:VAL:HG22	0.42	2.44
1:A:64:HIS:O	1:A:65:LYS:HB3	0.42	2.14
1:A:114:GLN:C	1:A:114:GLN:NE2	0.42	2.73
1:A:154:PHE:CD1	1:A:156:LYS:CB	0.42	3.03
1:A:73:ILE:HG23	1:A:73:ILE:O	0.42	2.15
1:A:125:LEU:HA	1:A:190:ARG:O	0.42	2.15
1:A:140:LEU:O	1:A:144:ASN:HB2	0.42	2.13
1:A:102:LEU:N	1:A:102:LEU:HD13	0.42	2.28
1:A:9:SER:HA	1:A:42:GLU:O	0.42	2.14
1:A:17:THR:CB	1:A:18:PRO:HD2	0.42	2.45
1:A:6:LEU:CD2	1:A:58:MET:HA	0.42	2.45
1:A:5:VAL:HG11	1:A:45:LEU:HD12	0.42	1.91
1:A:54:ALA:O	1:A:55:GLN:C	0.42	2.57
1:A:123:LEU:CG	1:A:192:SER:O	0.42	2.68
1:A:46:VAL:CG1	1:A:48:MET:CE	0.42	2.98
1:A:58:MET:O	1:A:62:ASN:CB	0.41	2.68
1:A:102:LEU:C	1:A:102:LEU:HD13	0.41	2.35
1:A:176:ILE:O	1:A:180:ASN:N	0.41	2.53
1:A:31:VAL:CA	1:A:47:GLN:O	0.41	2.64
1:A:31:VAL:HG23	1:A:46:VAL:HG13	0.41	1.92
1:A:4:SER:OG	1:A:51:GLY:CA	0.41	2.68
1:A:37:LEU:HD22	1:A:93:LEU:H	0.41	1.75
1:A:123:LEU:O	1:A:162:LEU:HA	0.41	2.15
1:A:25:PHE:CE1	1:A:61:LEU:CD2	0.41	2.99
1:A:28:TYR:CD1	1:A:30:ASP:HB2	0.41	2.50
1:A:144:ASN:HB2	1:A:178:LEU:HD22	0.41	1.90
1:A:173:GLN:O	1:A:177:ASP:OD1	0.41	2.39
1:A:31:VAL:CA	1:A:48:MET:HB2	0.41	2.46
1:A:157:ASP:O	1:A:158:ARG:CB	0.41	2.69
1:A:36:ILE:N	1:A:37:LEU:HD23	0.41	2.30
1:A:96:ASP:O	1:A:97:TYR:O	0.41	2.39
1:A:126:SER:CB	1:A:190:ARG:HB2	0.41	2.46
1:A:174:ALA:O	1:A:178:LEU:HB2	0.41	2.15
1:A:9:SER:O	1:A:10:ASN:HB2	0.41	2.15
1:A:22:PHE:O	1:A:26:GLY:N	0.41	2.46
1:A:4:SER:OG	1:A:51:GLY:HA2	0.41	2.15
1:A:28:TYR:OH	1:A:48:MET:SD	0.41	2.78
1:A:49:ALA:HB1	1:A:54:ALA:CB	0.41	2.42
1:A:126:SER:CB	1:A:190:ARG:CB	0.41	2.99
1:A:157:ASP:C	1:A:160:MET:HB2	0.41	2.36
1:A:114:GLN:C	1:A:115:ASN:CG	0.41	2.79
1:A:114:GLN:CD	1:A:114:GLN:C	0.41	2.78

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:25:PHE:HB3	1:A:28:TYR:OH	0.40	2.15
1:A:122:THR:HG22	1:A:162:LEU:CD2	0.40	2.46
1:A:73:ILE:HD13	1:A:74:THR:N	0.40	2.30
1:A:164:GLN:C	1:A:165:MET:HG3	0.40	2.36
1:A:30:ASP:C	1:A:48:MET:HB2	0.40	2.36
1:A:126:SER:OG	1:A:160:MET:CE	0.40	2.69
1:A:49:ALA:HA	1:A:54:ALA:N	0.40	2.32
1:A:167:SER:HB3	1:A:170:GLU:OE2	0.40	2.16

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	196/198 (99%)	145 (74%)	28 (14%)	23 (12%)	1 8
All	All	196/198 (99%)	145 (74%)	28 (14%)	23 (12%)	1 8

All 23 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	89	GLU
1	A	68	GLY
1	A	48	MET
1	A	158	ARG
1	A	41	LYS
1	A	97	TYR
1	A	166	GLY
1	A	106	LYS
1	A	78	HIS
1	A	50	ASP
1	A	127	ASN
1	A	87	GLY
1	A	12	ASN
1	A	84	PRO
1	A	37	LEU

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Mol	Chain	Res	Type
1	A	10	ASN
1	A	80	ASN
1	A	113	PHE
1	A	27	VAL
1	A	114	GLN
1	A	131	SER
1	A	11	LEU
1	A	156	LYS

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	175/175 (100%)	114 (65%)	61 (35%)	1 10
All	All	175/175 (100%)	114 (65%)	61 (35%)	1 10

All 61 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	71	ILE
1	A	17	THR
1	A	89	GLU
1	A	102	LEU
1	A	198	ILE
1	A	4	SER
1	A	48	MET
1	A	178	LEU
1	A	20	SER
1	A	194	SER
1	A	56	LEU
1	A	110	SER
1	A	186	ASN
1	A	103	HIS
1	A	46	VAL
1	A	23	ILE
1	A	93	LEU

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Mol	Chain	Res	Type
1	A	154	PHE
1	A	35	LYS
1	A	142	SER
1	A	123	LEU
1	A	170	GLU
1	A	21	LEU
1	A	133	SER
1	A	159	LYS
1	A	165	MET
1	A	31	VAL
1	A	74	THR
1	A	183	LEU
1	A	125	LEU
1	A	78	HIS
1	A	196	SER
1	A	160	MET
1	A	28	TYR
1	A	197	THR
1	A	127	ASN
1	A	164	GLN
1	A	73	ILE
1	A	122	THR
1	A	190	ARG
1	A	45	LEU
1	A	37	LEU
1	A	61	LEU
1	A	111	LYS
1	A	79	GLN
1	A	120	SER
1	A	104	ARG
1	A	163	ILE
1	A	135	GLU
1	A	157	ASP
1	A	192	SER
1	A	113	PHE
1	A	116	ILE
1	A	100	SER
1	A	72	ARG
1	A	137	LEU
1	A	69	LYS
1	A	114	GLN
1	A	149	LYS

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Mol	Chain	Res	Type
1	A	11	LEU
1	A	3	ASN

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: BMRB entry 5409

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	933
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	933
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 933 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	178	PHE	N	117.42	0.1	1
UNMAPPED	65	THR	H	7.24	0.02	1
UNMAPPED	168	LYS	CA	57.67	0.1	1
UNMAPPED	203	LEU	N	117.98	0.1	1
UNMAPPED	98	LEU	N	124.15	0.1	1
UNMAPPED	42	LEU	C	175.37	0.1	1
UNMAPPED	58	GLN	H	7.38	0.02	1
UNMAPPED	214	THR	H	8.2	0.02	1
UNMAPPED	218	ASP	CA	51.9	0.1	1
UNMAPPED	55	GLY	N	110.28	0.1	1
UNMAPPED	213	CYS	H	8.42	0.02	1
UNMAPPED	27	LYS	CB	28.78	0.1	1
UNMAPPED	203	LEU	CB	42.75	0.1	1
UNMAPPED	201	LEU	CA	57.23	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	17	GLY	H	8.38	0.02	1
UNMAPPED	192	ASP	N	116.72	0.1	1
UNMAPPED	100	THR	N	116.89	0.1	1
UNMAPPED	89	TYR	C	174.14	0.1	1
UNMAPPED	41	GLY	N	103.28	0.1	1
UNMAPPED	230	ASN	H	7.78	0.02	1
UNMAPPED	73	VAL	N	119.65	0.1	1
UNMAPPED	168	LYS	CB	30.94	0.1	1
UNMAPPED	83	LEU	N	125.3	0.1	1
UNMAPPED	197	GLN	H	7.68	0.02	1
UNMAPPED	152	ASN	C	176.05	0.1	1
UNMAPPED	208	ILE	H	8.85	0.02	1
UNMAPPED	232	ASP	CB	39.85	0.1	1
UNMAPPED	202	SER	H	7.58	0.02	1
UNMAPPED	56	LYS	CB	33.15	0.1	1
UNMAPPED	154	PHE	H	7.81	0.02	1
UNMAPPED	142	GLN	C	175.21	0.1	1
UNMAPPED	98	LEU	CB	41.65	0.1	1
UNMAPPED	209	TYR	CA	55.39	0.1	1
UNMAPPED	78	SER	CB	63.57	0.1	1
UNMAPPED	48	THR	N	122.54	0.1	1
UNMAPPED	47	VAL	CB	31.61	0.1	1
UNMAPPED	81	PRO	C	173.6	0.1	1
UNMAPPED	48	THR	CB	67.71	0.1	1
UNMAPPED	223	THR	H	8.32	0.02	1
UNMAPPED	194	VAL	CB	30.28	0.1	1
UNMAPPED	96	LYS	H	8.49	0.02	1
UNMAPPED	232	ASP	N	116.72	0.1	1
UNMAPPED	181	ASN	CA	54.66	0.1	1
UNMAPPED	103	SER	N	120.87	0.1	1
UNMAPPED	101	ASP	CB	40.58	0.1	1
UNMAPPED	34	GLU	CA	60.2	0.1	1
UNMAPPED	215	LEU	CA	55.14	0.1	1
UNMAPPED	231	ASN	C	174.63	0.1	1
UNMAPPED	101	ASP	N	124.08	0.1	1
UNMAPPED	212	CYS	CA	57.42	0.1	1
UNMAPPED	171	THR	H	8.72	0.02	1
UNMAPPED	148	ILE	CA	59.62	0.1	1
UNMAPPED	155	TYR	H	7.2	0.02	1
UNMAPPED	204	ASP	N	120.01	0.1	1
UNMAPPED	28	LEU	CA	52.69	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	74	ASN	N	120.1	0.1	1
UNMAPPED	204	ASP	CB	41.19	0.1	1
UNMAPPED	205	GLY	N	117.79	0.1	1
UNMAPPED	24	HIS	C	173.3	0.1	1
UNMAPPED	209	TYR	C	175.25	0.1	1
UNMAPPED	237	TYR	H	9.01	0.02	1
UNMAPPED	74	ASN	CB	37.52	0.1	1
UNMAPPED	196	ALA	N	121.78	0.1	1
UNMAPPED	43	PRO	C	176.45	0.1	1
UNMAPPED	25	ILE	CA	59.35	0.1	1
UNMAPPED	186	ALA	CA	49.46	0.1	1
UNMAPPED	83	LEU	C	175.65	0.1	1
UNMAPPED	65	THR	C	174.26	0.1	1
UNMAPPED	45	GLY	CA	45.02	0.1	1
UNMAPPED	38	ILE	N	120.04	0.1	1
UNMAPPED	199	ALA	H	8.29	0.02	1
UNMAPPED	153	LEU	H	8.3	0.02	1
UNMAPPED	69	ALA	N	119.91	0.1	1
UNMAPPED	176	ILE	CA	61.0	0.1	1
UNMAPPED	98	LEU	H	8.4	0.02	1
UNMAPPED	143	SER	C	173.83	0.1	1
UNMAPPED	90	ILE	C	173.44	0.1	1
UNMAPPED	69	ALA	CB	18.82	0.1	1
UNMAPPED	156	PRO	CA	62.78	0.1	1
UNMAPPED	28	LEU	N	117.34	0.1	1
UNMAPPED	177	THR	CB	71.41	0.1	1
UNMAPPED	24	HIS	CA	52.53	0.1	1
UNMAPPED	235	ARG	N	121.78	0.1	1
UNMAPPED	220	SER	CA	56.79	0.1	1
UNMAPPED	235	ARG	CB	33.25	0.1	1
UNMAPPED	70	ASN	N	117.79	0.1	1
UNMAPPED	141	GLY	H	8.15	0.02	1
UNMAPPED	163	HIS	H	9.11	0.02	1
UNMAPPED	84	ARG	H	9.45	0.02	1
UNMAPPED	105	ASN	CB	37.9	0.1	1
UNMAPPED	46	LYS	CB	33.53	0.1	1
UNMAPPED	72	MET	C	176.45	0.1	1
UNMAPPED	150	VAL	N	125.56	0.1	1
UNMAPPED	77	THR	C	175.03	0.1	1
UNMAPPED	42	LEU	H	7.16	0.02	1
UNMAPPED	201	LEU	C	180.18	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	90	ILE	CA	59.66	0.1	1
UNMAPPED	186	ALA	H	8.98	0.02	1
UNMAPPED	230	ASN	N	120.89	0.1	1
UNMAPPED	165	ILE	CB	38.29	0.1	1
UNMAPPED	88	ILE	N	118.82	0.1	1
UNMAPPED	245	GLY	CA	44.49	0.1	1
UNMAPPED	229	TYR	CB	42.01	0.1	1
UNMAPPED	177	THR	N	117.42	0.1	1
UNMAPPED	145	VAL	CA	60.34	0.1	1
UNMAPPED	229	TYR	CA	54.57	0.1	1
UNMAPPED	36	GLU	CB	30.31	0.1	1
UNMAPPED	227	VAL	N	125.25	0.1	1
UNMAPPED	195	SER	N	118.62	0.1	1
UNMAPPED	65	THR	CB	72.84	0.1	1
UNMAPPED	36	GLU	N	122.73	0.1	1
UNMAPPED	99	LYS	N	124.15	0.1	1
UNMAPPED	23	ILE	N	131.02	0.1	1
UNMAPPED	239	ARG	CA	52.38	0.1	1
UNMAPPED	65	THR	N	106.16	0.1	1
UNMAPPED	24	HIS	H	9.34	0.02	1
UNMAPPED	21	ARG	N	120.55	0.1	1
UNMAPPED	27	LYS	H	8.55	0.02	1
UNMAPPED	227	VAL	CA	62.05	0.1	1
UNMAPPED	81	PRO	CA	61.81	0.1	1
UNMAPPED	243	PRO	CA	62.36	0.1	1
UNMAPPED	71	THR	N	118.43	0.1	1
UNMAPPED	245	GLY	C	173.21	0.1	1
UNMAPPED	244	SER	CB	64.13	0.1	1
UNMAPPED	219	PHE	CB	39.33	0.1	1
UNMAPPED	218	ASP	CB	44.16	0.1	1
UNMAPPED	229	TYR	N	115.58	0.1	1
UNMAPPED	167	SER	CA	61.73	0.1	1
UNMAPPED	238	THR	N	112.74	0.1	1
UNMAPPED	202	SER	N	113.18	0.1	1
UNMAPPED	41	GLY	H	7.92	0.02	1
UNMAPPED	212	CYS	C	171.7	0.1	1
UNMAPPED	97	GLU	CA	54.99	0.1	1
UNMAPPED	164	GLN	C	178.96	0.1	1
UNMAPPED	208	ILE	CB	38.37	0.1	1
UNMAPPED	227	VAL	CB	33.27	0.1	1
UNMAPPED	68	ALA	C	179.29	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	175	ILE	H	8.75	0.02	1
UNMAPPED	202	SER	CB	64.28	0.1	1
UNMAPPED	56	LYS	H	7.44	0.02	1
UNMAPPED	83	LEU	CA	53.38	0.1	1
UNMAPPED	92	PHE	C	177.1	0.1	1
UNMAPPED	46	LYS	C	174.97	0.1	1
UNMAPPED	93	SER	H	8.79	0.02	1
UNMAPPED	78	SER	H	7.3	0.02	1
UNMAPPED	60	PHE	CA	55.68	0.1	1
UNMAPPED	47	VAL	H	8.03	0.02	1
UNMAPPED	43	PRO	CA	64.03	0.1	1
UNMAPPED	168	LYS	N	120.01	0.1	1
UNMAPPED	48	THR	H	9.17	0.02	1
UNMAPPED	185	GLN	CB	32.35	0.1	1
UNMAPPED	202	SER	C	176.01	0.1	1
UNMAPPED	163	HIS	C	178.65	0.1	1
UNMAPPED	192	ASP	CB	43.86	0.1	1
UNMAPPED	104	PRO	C	176.69	0.1	1
UNMAPPED	147	ARG	N	123.04	0.1	1
UNMAPPED	207	ASN	C	177.47	0.1	1
UNMAPPED	236	ASP	N	126.32	0.1	1
UNMAPPED	176	ILE	C	174.99	0.1	1
UNMAPPED	147	ARG	CB	30.72	0.1	1
UNMAPPED	27	LYS	CA	56.14	0.1	1
UNMAPPED	34	GLU	N	122.86	0.1	1
UNMAPPED	211	ALA	H	8.81	0.02	1
UNMAPPED	30	ILE	CB	37.75	0.1	1
UNMAPPED	205	GLY	H	9.11	0.02	1
UNMAPPED	31	ASP	CA	52.84	0.1	1
UNMAPPED	92	PHE	CA	60.04	0.1	1
UNMAPPED	73	VAL	CA	66.71	0.1	1
UNMAPPED	30	ILE	N	122.67	0.1	1
UNMAPPED	162	LEU	H	7.69	0.02	1
UNMAPPED	234	SER	CA	56.56	0.1	1
UNMAPPED	237	TYR	CB	36.88	0.1	1
UNMAPPED	55	GLY	C	174.37	0.1	1
UNMAPPED	237	TYR	N	125.57	0.1	1
UNMAPPED	71	THR	CA	66.25	0.1	1
UNMAPPED	214	THR	C	174.94	0.1	1
UNMAPPED	75	TYR	N	125.05	0.1	1
UNMAPPED	56	LYS	CA	54.07	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	194	VAL	CA	65.91	0.1	1
UNMAPPED	178	PHE	CB	38.89	0.1	1
UNMAPPED	79	VAL	CB	32.61	0.1	1
UNMAPPED	213	CYS	N	113.69	0.1	1
UNMAPPED	20	SER	H	7.33	0.02	1
UNMAPPED	84	ARG	C	176.68	0.1	1
UNMAPPED	79	VAL	N	124.79	0.1	1
UNMAPPED	39	SER	CA	62.19	0.1	1
UNMAPPED	73	VAL	C	179.0	0.1	1
UNMAPPED	44	PHE	CB	40.04	0.1	1
UNMAPPED	82	VAL	C	175.23	0.1	1
UNMAPPED	234	SER	C	171.46	0.1	1
UNMAPPED	101	ASP	CA	53.61	0.1	1
UNMAPPED	216	ARG	C	176.74	0.1	1
UNMAPPED	215	LEU	C	176.92	0.1	1
UNMAPPED	142	GLN	N	119.94	0.1	1
UNMAPPED	32	VAL	N	119.39	0.1	1
UNMAPPED	47	VAL	C	177.12	0.1	1
UNMAPPED	228	LYS	N	128.47	0.1	1
UNMAPPED	235	ARG	H	8.98	0.02	1
UNMAPPED	210	ASN	H	8.42	0.02	1
UNMAPPED	195	SER	H	7.62	0.02	1
UNMAPPED	56	LYS	C	175.84	0.1	1
UNMAPPED	163	HIS	CB	29.31	0.1	1
UNMAPPED	46	LYS	H	7.51	0.02	1
UNMAPPED	183	GLN	H	7.75	0.02	1
UNMAPPED	186	ALA	N	120.01	0.1	1
UNMAPPED	214	THR	CA	62.46	0.1	1
UNMAPPED	83	LEU	H	8.42	0.02	1
UNMAPPED	69	ALA	C	178.28	0.1	1
UNMAPPED	174	LYS	N	114.45	0.1	1
UNMAPPED	38	ILE	CA	65.18	0.1	1
UNMAPPED	33	THR	H	8.11	0.02	1
UNMAPPED	186	ALA	CB	22.48	0.1	1
UNMAPPED	67	GLU	N	122.35	0.1	1
UNMAPPED	214	THR	CB	70.15	0.1	1
UNMAPPED	39	SER	C	175.3	0.1	1
UNMAPPED	197	GLN	C	178.49	0.1	1
UNMAPPED	82	VAL	CA	59.12	0.1	1
UNMAPPED	89	TYR	CA	56.06	0.1	1
UNMAPPED	149	ILE	CB	40.43	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	86	GLN	N	123.31	0.1	1
UNMAPPED	167	SER	C	174.17	0.1	1
UNMAPPED	76	TYR	CA	58.66	0.1	1
UNMAPPED	141	GLY	C	173.92	0.1	1
UNMAPPED	149	ILE	CA	60.07	0.1	1
UNMAPPED	24	HIS	N	130.25	0.1	1
UNMAPPED	206	GLN	CB	28.49	0.1	1
UNMAPPED	94	ASN	CB	37.97	0.1	1
UNMAPPED	24	HIS	CB	34.53	0.1	1
UNMAPPED	173	LEU	CB	42.67	0.1	1
UNMAPPED	19	PRO	CB	30.77	0.1	1
UNMAPPED	50	LEU	C	173.86	0.1	1
UNMAPPED	70	ASN	CA	56.37	0.1	1
UNMAPPED	94	ASN	N	123.38	0.1	1
UNMAPPED	146	LEU	CA	52.41	0.1	1
UNMAPPED	85	GLY	N	103.99	0.1	1
UNMAPPED	104	PRO	CA	62.73	0.1	1
UNMAPPED	51	LEU	CB	44.72	0.1	1
UNMAPPED	189	GLN	CA	54.0	0.1	1
UNMAPPED	108	ARG	CB	30.39	0.1	1
UNMAPPED	241	ASP	C	176.54	0.1	1
UNMAPPED	244	SER	H	8.56	0.02	1
UNMAPPED	181	ASN	C	174.94	0.1	1
UNMAPPED	49	ASN	H	7.72	0.02	1
UNMAPPED	108	ARG	N	122.41	0.1	1
UNMAPPED	79	VAL	C	174.08	0.1	1
UNMAPPED	224	SER	H	7.28	0.02	1
UNMAPPED	245	GLY	N	111.1	0.1	1
UNMAPPED	31	ASP	C	175.48	0.1	1
UNMAPPED	94	ASN	H	8.75	0.02	1
UNMAPPED	211	ALA	C	176.3	0.1	1
UNMAPPED	58	GLN	CA	52.99	0.1	1
UNMAPPED	153	LEU	N	125.08	0.1	1
UNMAPPED	95	HIS	CA	55.91	0.1	1
UNMAPPED	194	VAL	C	178.72	0.1	1
UNMAPPED	72	MET	CA	58.36	0.1	1
UNMAPPED	63	MET	CB	31.92	0.1	1
UNMAPPED	76	TYR	H	7.79	0.02	1
UNMAPPED	59	ALA	C	174.36	0.1	1
UNMAPPED	96	LYS	CA	56.44	0.1	1
UNMAPPED	65	THR	CA	58.2	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	100	THR	C	174.15	0.1	1
UNMAPPED	61	ILE	CA	58.66	0.1	1
UNMAPPED	168	LYS	H	6.71	0.02	1
UNMAPPED	192	ASP	H	7.72	0.02	1
UNMAPPED	54	LYS	CA	58.82	0.1	1
UNMAPPED	57	ASN	CA	53.76	0.1	1
UNMAPPED	155	TYR	CA	54.79	0.1	1
UNMAPPED	241	ASP	H	8.72	0.02	1
UNMAPPED	170	GLY	C	171.39	0.1	1
UNMAPPED	164	GLN	N	122.6	0.1	1
UNMAPPED	147	ARG	H	8.97	0.02	1
UNMAPPED	91	GLN	CA	53.45	0.1	1
UNMAPPED	30	ILE	H	8.4	0.02	1
UNMAPPED	152	ASN	H	8.98	0.02	1
UNMAPPED	193	PRO	C	178.63	0.1	1
UNMAPPED	232	ASP	C	176.61	0.1	1
UNMAPPED	244	SER	CA	58.91	0.1	1
UNMAPPED	50	LEU	H	8.33	0.02	1
UNMAPPED	97	GLU	N	119.07	0.1	1
UNMAPPED	210	ASN	N	118.74	0.1	1
UNMAPPED	179	THR	C	174.63	0.1	1
UNMAPPED	178	PHE	C	173.26	0.1	1
UNMAPPED	35	GLY	CA	46.48	0.1	1
UNMAPPED	220	SER	C	175.45	0.1	1
UNMAPPED	97	GLU	CB	30.47	0.1	1
UNMAPPED	141	GLY	N	109.96	0.1	1
UNMAPPED	21	ARG	C	174.66	0.1	1
UNMAPPED	223	THR	C	174.3	0.1	1
UNMAPPED	88	ILE	H	7.72	0.02	1
UNMAPPED	228	LYS	C	174.77	0.1	1
UNMAPPED	80	THR	C	172.95	0.1	1
UNMAPPED	151	GLU	CB	31.91	0.1	1
UNMAPPED	178	PHE	H	8.32	0.02	1
UNMAPPED	95	HIS	H	8.28	0.02	1
UNMAPPED	79	VAL	H	7.68	0.02	1
UNMAPPED	16	SER	C	174.71	0.1	1
UNMAPPED	151	GLU	N	127.34	0.1	1
UNMAPPED	20	SER	CB	63.95	0.1	1
UNMAPPED	38	ILE	C	178.97	0.1	1
UNMAPPED	22	VAL	CB	31.54	0.1	1
UNMAPPED	238	THR	C	174.72	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	161	VAL	CA	66.14	0.1	1
UNMAPPED	204	ASP	C	178.29	0.1	1
UNMAPPED	211	ALA	CB	17.88	0.1	1
UNMAPPED	177	THR	H	8.52	0.02	1
UNMAPPED	22	VAL	N	120.94	0.1	1
UNMAPPED	192	ASP	CA	50.51	0.1	1
UNMAPPED	44	PHE	H	7.74	0.02	1
UNMAPPED	26	ARG	CA	53.76	0.1	1
UNMAPPED	57	ASN	H	8.22	0.02	1
UNMAPPED	37	VAL	C	177.77	0.1	1
UNMAPPED	211	ALA	N	124.93	0.1	1
UNMAPPED	233	LYS	CA	56.06	0.1	1
UNMAPPED	102	SER	CA	57.59	0.1	1
UNMAPPED	31	ASP	N	119.39	0.1	1
UNMAPPED	76	TYR	C	175.59	0.1	1
UNMAPPED	210	ASN	CB	37.85	0.1	1
UNMAPPED	30	ILE	CA	62.42	0.1	1
UNMAPPED	242	LEU	CA	54.12	0.1	1
UNMAPPED	195	SER	CB	65.57	0.1	1
UNMAPPED	189	GLN	N	127.9	0.1	1
UNMAPPED	29	PRO	CA	61.65	0.1	1
UNMAPPED	168	LYS	C	177.14	0.1	1
UNMAPPED	70	ASN	C	177.57	0.1	1
UNMAPPED	140	ALA	C	178.45	0.1	1
UNMAPPED	228	LYS	H	8.34	0.02	1
UNMAPPED	83	LEU	CB	46.17	0.1	1
UNMAPPED	169	PHE	CB	39.93	0.1	1
UNMAPPED	146	LEU	C	175.61	0.1	1
UNMAPPED	35	GLY	H	8.67	0.02	1
UNMAPPED	225	LEU	C	175.54	0.1	1
UNMAPPED	33	THR	CB	71.54	0.1	1
UNMAPPED	71	THR	CB	67.71	0.1	1
UNMAPPED	182	ASN	H	8.83	0.02	1
UNMAPPED	33	THR	N	117.34	0.1	1
UNMAPPED	96	LYS	C	176.01	0.1	1
UNMAPPED	78	SER	N	117.66	0.1	1
UNMAPPED	227	VAL	C	175.03	0.1	1
UNMAPPED	79	VAL	CA	60.23	0.1	1
UNMAPPED	47	VAL	N	126.4	0.1	1
UNMAPPED	30	ILE	C	175.48	0.1	1
UNMAPPED	68	ALA	CA	54.76	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	105	ASN	C	175.04	0.1	1
UNMAPPED	206	GLN	H	8.06	0.02	1
UNMAPPED	72	MET	N	124.6	0.1	1
UNMAPPED	39	SER	CB	62.34	0.1	1
UNMAPPED	29	PRO	C	177.55	0.1	1
UNMAPPED	142	GLN	CA	55.26	0.1	1
UNMAPPED	44	PHE	CA	57.29	0.1	1
UNMAPPED	103	SER	CB	62.73	0.1	1
UNMAPPED	173	LEU	H	9.12	0.02	1
UNMAPPED	242	LEU	H	6.9	0.02	1
UNMAPPED	201	LEU	H	7.74	0.02	1
UNMAPPED	140	ALA	CA	52.54	0.1	1
UNMAPPED	216	ARG	CA	53.74	0.1	1
UNMAPPED	225	LEU	CA	52.73	0.1	1
UNMAPPED	174	LYS	C	175.01	0.1	1
UNMAPPED	51	LEU	H	9.1	0.02	1
UNMAPPED	108	ARG	H	8.19	0.02	1
UNMAPPED	85	GLY	H	8.34	0.02	1
UNMAPPED	163	HIS	CA	62.11	0.1	1
UNMAPPED	172	VAL	C	175.3	0.1	1
UNMAPPED	49	ASN	CB	41.73	0.1	1
UNMAPPED	224	SER	N	113.69	0.1	1
UNMAPPED	155	TYR	C	172.44	0.1	1
UNMAPPED	207	ASN	CA	52.16	0.1	1
UNMAPPED	217	ILE	CB	41.34	0.1	1
UNMAPPED	67	GLU	CA	59.73	0.1	1
UNMAPPED	224	SER	CB	64.28	0.1	1
UNMAPPED	196	ALA	CB	17.43	0.1	1
UNMAPPED	62	GLU	CA	53.76	0.1	1
UNMAPPED	175	ILE	CB	42.38	0.1	1
UNMAPPED	38	ILE	CB	37.75	0.1	1
UNMAPPED	34	GLU	C	178.76	0.1	1
UNMAPPED	45	GLY	C	170.12	0.1	1
UNMAPPED	230	ASN	C	174.83	0.1	1
UNMAPPED	245	GLY	H	7.64	0.02	1
UNMAPPED	160	ASP	CB	40.37	0.1	1
UNMAPPED	179	THR	CA	60.94	0.1	1
UNMAPPED	63	MET	H	8.75	0.02	1
UNMAPPED	76	TYR	CB	36.67	0.1	1
UNMAPPED	35	GLY	C	177.01	0.1	1
UNMAPPED	231	ASN	CA	52.57	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	158	THR	H	6.62	0.02	1
UNMAPPED	68	ALA	H	8.38	0.02	1
UNMAPPED	223	THR	CA	61.79	0.1	1
UNMAPPED	99	LYS	C	176.23	0.1	1
UNMAPPED	28	LEU	CB	41.27	0.1	1
UNMAPPED	94	ASN	CA	53.15	0.1	1
UNMAPPED	87	PRO	CA	62.04	0.1	1
UNMAPPED	161	VAL	C	178.4	0.1	1
UNMAPPED	152	ASN	N	120.0	0.1	1
UNMAPPED	16	SER	CA	57.9	0.1	1
UNMAPPED	215	LEU	H	8.86	0.02	1
UNMAPPED	225	LEU	H	8.01	0.02	1
UNMAPPED	152	ASN	CB	35.87	0.1	1
UNMAPPED	162	LEU	C	179.27	0.1	1
UNMAPPED	180	LYS	CA	55.58	0.1	1
UNMAPPED	52	MET	H	9.11	0.02	1
UNMAPPED	236	ASP	H	8.91	0.02	1
UNMAPPED	105	ASN	N	119.65	0.1	1
UNMAPPED	46	LYS	N	120.16	0.1	1
UNMAPPED	50	LEU	CB	44.79	0.1	1
UNMAPPED	207	ASN	H	8.45	0.02	1
UNMAPPED	50	LEU	N	124.08	0.1	1
UNMAPPED	97	GLU	H	7.89	0.02	1
UNMAPPED	174	LYS	H	7.14	0.02	1
UNMAPPED	52	MET	CA	53.76	0.1	1
UNMAPPED	25	ILE	H	9.18	0.02	1
UNMAPPED	86	GLN	CA	51.38	0.1	1
UNMAPPED	165	ILE	N	119.12	0.1	1
UNMAPPED	88	ILE	CB	39.12	0.1	1
UNMAPPED	170	GLY	N	107.5	0.1	1
UNMAPPED	151	GLU	H	9.04	0.02	1
UNMAPPED	77	THR	CA	64.26	0.1	1
UNMAPPED	95	HIS	CB	30.24	0.1	1
UNMAPPED	22	VAL	H	8.56	0.02	1
UNMAPPED	158	THR	CA	59.19	0.1	1
UNMAPPED	218	ASP	C	175.05	0.1	1
UNMAPPED	198	HIS	N	118.74	0.1	1
UNMAPPED	197	GLN	CA	59.13	0.1	1
UNMAPPED	23	ILE	CB	39.66	0.1	1
UNMAPPED	57	ASN	CB	36.29	0.1	1
UNMAPPED	159	LEU	CB	41.34	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	198	HIS	CB	28.94	0.1	1
UNMAPPED	55	GLY	H	8.91	0.02	1
UNMAPPED	159	LEU	N	122.53	0.1	1
UNMAPPED	17	GLY	N	111.63	0.1	1
UNMAPPED	45	GLY	H	7.57	0.02	1
UNMAPPED	160	ASP	CA	57.32	0.1	1
UNMAPPED	200	LYS	CA	60.34	0.1	1
UNMAPPED	229	TYR	H	7.08	0.02	1
UNMAPPED	191	ALA	N	120.45	0.1	1
UNMAPPED	64	ASN	CA	55.91	0.1	1
UNMAPPED	98	LEU	C	176.06	0.1	1
UNMAPPED	216	ARG	CB	29.53	0.1	1
UNMAPPED	36	GLU	H	7.63	0.02	1
UNMAPPED	179	THR	CB	70.07	0.1	1
UNMAPPED	93	SER	CB	63.95	0.1	1
UNMAPPED	42	LEU	CA	57.29	0.1	1
UNMAPPED	71	THR	H	8.6	0.02	1
UNMAPPED	208	ILE	N	123.61	0.1	1
UNMAPPED	90	ILE	H	8.28	0.02	1
UNMAPPED	182	ASN	CB	37.55	0.1	1
UNMAPPED	93	SER	C	174.95	0.1	1
UNMAPPED	194	VAL	H	8.47	0.02	1
UNMAPPED	182	ASN	N	111.6	0.1	1
UNMAPPED	226	ASN	CB	38.89	0.1	1
UNMAPPED	37	VAL	CB	30.54	0.1	1
UNMAPPED	183	GLN	CB	31.31	0.1	1
UNMAPPED	188	LEU	CA	54.15	0.1	1
UNMAPPED	67	GLU	C	178.9	0.1	1
UNMAPPED	97	GLU	C	175.21	0.1	1
UNMAPPED	107	ALA	CB	18.89	0.1	1
UNMAPPED	22	VAL	CA	61.42	0.1	1
UNMAPPED	203	LEU	CA	54.76	0.1	1
UNMAPPED	165	ILE	C	178.32	0.1	1
UNMAPPED	161	VAL	CB	31.31	0.1	1
UNMAPPED	169	PHE	C	175.05	0.1	1
UNMAPPED	39	SER	H	7.86	0.02	1
UNMAPPED	86	GLN	C	172.27	0.1	1
UNMAPPED	236	ASP	C	178.27	0.1	1
UNMAPPED	98	LEU	CA	53.91	0.1	1
UNMAPPED	103	SER	H	8.28	0.02	1
UNMAPPED	239	ARG	H	6.84	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	201	LEU	CB	41.41	0.1	1
UNMAPPED	218	ASP	N	127.08	0.1	1
UNMAPPED	60	PHE	C	175.08	0.1	1
UNMAPPED	216	ARG	H	9.0	0.02	1
UNMAPPED	201	LEU	N	117.1	0.1	1
UNMAPPED	100	THR	CA	60.81	0.1	1
UNMAPPED	145	VAL	CB	31.17	0.1	1
UNMAPPED	29	PRO	CB	31.31	0.1	1
UNMAPPED	187	LEU	H	9.01	0.02	1
UNMAPPED	145	VAL	N	122.41	0.1	1
UNMAPPED	243	PRO	CB	32.06	0.1	1
UNMAPPED	41	GLY	CA	45.41	0.1	1
UNMAPPED	217	ILE	H	8.84	0.02	1
UNMAPPED	167	SER	H	8.38	0.02	1
UNMAPPED	27	LYS	C	175.1	0.1	1
UNMAPPED	196	ALA	H	6.41	0.02	1
UNMAPPED	203	LEU	C	177.38	0.1	1
UNMAPPED	75	TYR	CB	37.97	0.1	1
UNMAPPED	232	ASP	CA	55.77	0.1	1
UNMAPPED	61	ILE	H	9.18	0.02	1
UNMAPPED	209	TYR	N	116.78	0.1	1
UNMAPPED	78	SER	CA	59.12	0.1	1
UNMAPPED	236	ASP	CA	52.13	0.1	1
UNMAPPED	244	SER	C	176.21	0.1	1
UNMAPPED	74	ASN	C	178.25	0.1	1
UNMAPPED	209	TYR	CB	40.16	0.1	1
UNMAPPED	80	THR	CA	60.27	0.1	1
UNMAPPED	149	ILE	N	128.99	0.1	1
UNMAPPED	188	LEU	H	8.48	0.02	1
UNMAPPED	80	THR	CB	69.16	0.1	1
UNMAPPED	68	ALA	CB	19.43	0.1	1
UNMAPPED	229	TYR	C	174.19	0.1	1
UNMAPPED	96	LYS	CB	32.38	0.1	1
UNMAPPED	181	ASN	CB	36.81	0.1	1
UNMAPPED	103	SER	CA	56.14	0.1	1
UNMAPPED	212	CYS	N	114.32	0.1	1
UNMAPPED	148	ILE	CB	40.99	0.1	1
UNMAPPED	96	LYS	N	123.44	0.1	1
UNMAPPED	31	ASP	H	8.3	0.02	1
UNMAPPED	225	LEU	CB	43.05	0.1	1
UNMAPPED	92	PHE	H	8.85	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	191	ALA	CA	54.03	0.1	1
UNMAPPED	148	ILE	N	129.9	0.1	1
UNMAPPED	204	ASP	CA	57.42	0.1	1
UNMAPPED	205	GLY	CA	45.5	0.1	1
UNMAPPED	100	THR	H	8.17	0.02	1
UNMAPPED	207	ASN	N	121.08	0.1	1
UNMAPPED	189	GLN	H	8.84	0.02	1
UNMAPPED	74	ASN	CA	55.98	0.1	1
UNMAPPED	26	ARG	C	174.01	0.1	1
UNMAPPED	148	ILE	H	9.38	0.02	1
UNMAPPED	207	ASN	CB	38.81	0.1	1
UNMAPPED	196	ALA	CA	54.92	0.1	1
UNMAPPED	174	LYS	CB	39.19	0.1	1
UNMAPPED	25	ILE	CB	38.82	0.1	1
UNMAPPED	62	GLU	CB	33.07	0.1	1
UNMAPPED	185	GLN	C	172.81	0.1	1
UNMAPPED	154	PHE	C	174.79	0.1	1
UNMAPPED	179	THR	N	115.65	0.1	1
UNMAPPED	103	SER	C	175.2	0.1	1
UNMAPPED	147	ARG	C	175.03	0.1	1
UNMAPPED	189	GLN	CB	31.02	0.1	1
UNMAPPED	170	GLY	H	7.32	0.02	1
UNMAPPED	71	THR	C	175.78	0.1	1
UNMAPPED	69	ALA	CA	54.99	0.1	1
UNMAPPED	176	ILE	CB	42.15	0.1	1
UNMAPPED	223	THR	N	109.77	0.1	1
UNMAPPED	156	PRO	CB	31.39	0.1	1
UNMAPPED	191	ALA	CB	18.4	0.1	1
UNMAPPED	180	LYS	CB	34.8	0.1	1
UNMAPPED	215	LEU	CB	42.44	0.1	1
UNMAPPED	23	ILE	H	9.44	0.02	1
UNMAPPED	87	PRO	CB	31.54	0.1	1
UNMAPPED	159	LEU	H	8.87	0.02	1
UNMAPPED	198	HIS	H	8.12	0.02	1
UNMAPPED	242	LEU	N	121.71	0.1	1
UNMAPPED	235	ARG	CA	55.11	0.1	1
UNMAPPED	188	LEU	C	173.46	0.1	1
UNMAPPED	160	ASP	N	116.91	0.1	1
UNMAPPED	220	SER	CB	63.91	0.1	1
UNMAPPED	105	ASN	CA	52.84	0.1	1
UNMAPPED	40	LEU	CA	56.06	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	150	VAL	CA	60.65	0.1	1
UNMAPPED	44	PHE	C	175.05	0.1	1
UNMAPPED	50	LEU	CA	53.84	0.1	1
UNMAPPED	64	ASN	H	9.07	0.02	1
UNMAPPED	228	LYS	CB	33.37	0.1	1
UNMAPPED	166	PHE	C	181.09	0.1	1
UNMAPPED	213	CYS	C	173.77	0.1	1
UNMAPPED	165	ILE	CA	64.46	0.1	1
UNMAPPED	228	LYS	CA	56.85	0.1	1
UNMAPPED	90	ILE	CB	40.2	0.1	1
UNMAPPED	144	PRO	CA	62.05	0.1	1
UNMAPPED	240	PRO	CA	63.69	0.1	1
UNMAPPED	89	TYR	H	7.68	0.02	1
UNMAPPED	172	VAL	CA	62.43	0.1	1
UNMAPPED	182	ASN	C	174.12	0.1	1
UNMAPPED	82	VAL	H	7.72	0.02	1
UNMAPPED	37	VAL	H	7.41	0.02	1
UNMAPPED	17	GLY	C	173.33	0.1	1
UNMAPPED	63	MET	N	124.28	0.1	1
UNMAPPED	107	ALA	H	8.24	0.02	1
UNMAPPED	62	GLU	C	174.95	0.1	1
UNMAPPED	161	VAL	H	7.49	0.02	1
UNMAPPED	40	LEU	C	179.58	0.1	1
UNMAPPED	195	SER	C	174.99	0.1	1
UNMAPPED	222	LEU	CA	54.98	0.1	1
UNMAPPED	150	VAL	C	175.5	0.1	1
UNMAPPED	218	ASP	H	8.87	0.02	1
UNMAPPED	230	ASN	CA	50.6	0.1	1
UNMAPPED	23	ILE	CA	58.82	0.1	1
UNMAPPED	53	LEU	CA	52.92	0.1	1
UNMAPPED	239	ARG	CB	30.65	0.1	1
UNMAPPED	146	LEU	H	9.09	0.02	1
UNMAPPED	226	ASN	H	8.68	0.02	1
UNMAPPED	81	PRO	CB	30.01	0.1	1
UNMAPPED	70	ASN	H	8.84	0.02	1
UNMAPPED	36	GLU	C	178.55	0.1	1
UNMAPPED	59	ALA	CA	50.77	0.1	1
UNMAPPED	64	ASN	N	118.17	0.1	1
UNMAPPED	145	VAL	H	8.39	0.02	1
UNMAPPED	94	ASN	C	175.16	0.1	1
UNMAPPED	167	SER	N	121.27	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	211	ALA	CA	52.6	0.1	1
UNMAPPED	227	VAL	H	8.08	0.02	1
UNMAPPED	42	LEU	N	121.64	0.1	1
UNMAPPED	208	ILE	CA	64.17	0.1	1
UNMAPPED	167	SER	CB	60.84	0.1	1
UNMAPPED	91	GLN	C	174.65	0.1	1
UNMAPPED	18	VAL	CA	58.97	0.1	1
UNMAPPED	238	THR	H	9.23	0.02	1
UNMAPPED	52	MET	N	127.55	0.1	1
UNMAPPED	75	TYR	H	8.29	0.02	1
UNMAPPED	222	LEU	C	177.3	0.1	1
UNMAPPED	19	PRO	C	175.3	0.1	1
UNMAPPED	172	VAL	H	9.01	0.02	1
UNMAPPED	53	LEU	C	176.96	0.1	1
UNMAPPED	60	PHE	N	119.14	0.1	1
UNMAPPED	106	GLN	C	175.35	0.1	1
UNMAPPED	157	VAL	N	123.54	0.1	1
UNMAPPED	226	ASN	CA	51.9	0.1	1
UNMAPPED	188	LEU	CB	45.37	0.1	1
UNMAPPED	60	PHE	CB	41.88	0.1	1
UNMAPPED	99	LYS	H	8.07	0.02	1
UNMAPPED	185	GLN	CA	53.2	0.1	1
UNMAPPED	66	GLU	CA	59.12	0.1	1
UNMAPPED	184	PHE	H	8.96	0.02	1
UNMAPPED	172	VAL	N	131.76	0.1	1
UNMAPPED	219	PHE	C	176.76	0.1	1
UNMAPPED	147	ARG	CA	55.01	0.1	1
UNMAPPED	27	LYS	N	115.93	0.1	1
UNMAPPED	206	GLN	N	120.32	0.1	1
UNMAPPED	31	ASP	CB	38.89	0.1	1
UNMAPPED	92	PHE	CB	39.35	0.1	1
UNMAPPED	59	ALA	H	8.86	0.02	1
UNMAPPED	45	GLY	N	107.52	0.1	1
UNMAPPED	157	VAL	C	174.37	0.1	1
UNMAPPED	100	THR	CB	68.93	0.1	1
UNMAPPED	234	SER	CB	66.51	0.1	1
UNMAPPED	92	PHE	N	121.51	0.1	1
UNMAPPED	73	VAL	CB	31.08	0.1	1
UNMAPPED	63	MET	C	177.68	0.1	1
UNMAPPED	234	SER	N	115.39	0.1	1
UNMAPPED	240	PRO	CB	31.17	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	237	TYR	CA	61.57	0.1	1
UNMAPPED	143	SER	H	7.56	0.02	1
UNMAPPED	56	LYS	N	117.85	0.1	1
UNMAPPED	62	GLU	H	8.58	0.02	1
UNMAPPED	160	ASP	C	179.25	0.1	1
UNMAPPED	75	TYR	CA	61.73	0.1	1
UNMAPPED	66	GLU	C	178.64	0.1	1
UNMAPPED	177	THR	CA	59.45	0.1	1
UNMAPPED	64	ASN	C	175.01	0.1	1
UNMAPPED	194	VAL	N	122.28	0.1	1
UNMAPPED	233	LYS	CB	33.32	0.1	1
UNMAPPED	178	PHE	CA	56.56	0.1	1
UNMAPPED	179	THR	H	8.37	0.02	1
UNMAPPED	190	TYR	CA	58.66	0.1	1
UNMAPPED	184	PHE	C	174.72	0.1	1
UNMAPPED	148	ILE	C	174.64	0.1	1
UNMAPPED	233	LYS	N	119.0	0.1	1
UNMAPPED	72	MET	CB	32.0	0.1	1
UNMAPPED	39	SER	N	115.67	0.1	1
UNMAPPED	80	THR	H	8.1	0.02	1
UNMAPPED	32	VAL	CA	61.42	0.1	1
UNMAPPED	102	SER	H	8.18	0.02	1
UNMAPPED	243	PRO	C	176.43	0.1	1
UNMAPPED	34	GLU	H	9.28	0.02	1
UNMAPPED	186	ALA	C	175.99	0.1	1
UNMAPPED	141	GLY	CA	44.96	0.1	1
UNMAPPED	220	SER	H	8.57	0.02	1
UNMAPPED	22	VAL	C	174.36	0.1	1
UNMAPPED	157	VAL	CB	32.65	0.1	1
UNMAPPED	75	TYR	C	177.96	0.1	1
UNMAPPED	169	PHE	CA	57.99	0.1	1
UNMAPPED	88	ILE	C	173.62	0.1	1
UNMAPPED	49	ASN	N	119.46	0.1	1
UNMAPPED	151	GLU	C	177.18	0.1	1
UNMAPPED	217	ILE	N	126.32	0.1	1
UNMAPPED	241	ASP	CA	53.46	0.1	1
UNMAPPED	175	ILE	CA	60.81	0.1	1
UNMAPPED	174	LYS	CA	54.69	0.1	1
UNMAPPED	36	GLU	CA	58.36	0.1	1
UNMAPPED	82	VAL	N	119.46	0.1	1
UNMAPPED	89	TYR	CB	40.5	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	200	LYS	N	118.62	0.1	1
UNMAPPED	82	VAL	CB	35.37	0.1	1
UNMAPPED	89	TYR	N	120.23	0.1	1
UNMAPPED	231	ASN	N	124.43	0.1	1
UNMAPPED	222	LEU	CB	41.34	0.1	1
UNMAPPED	208	ILE	C	175.96	0.1	1
UNMAPPED	200	LYS	CB	31.91	0.1	1
UNMAPPED	190	TYR	H	8.86	0.02	1
UNMAPPED	76	TYR	N	117.34	0.1	1
UNMAPPED	158	THR	CB	71.63	0.1	1
UNMAPPED	241	ASP	CB	39.93	0.1	1
UNMAPPED	19	PRO	CA	62.42	0.1	1
UNMAPPED	206	GLN	CA	54.47	0.1	1
UNMAPPED	99	LYS	CA	55.14	0.1	1
UNMAPPED	191	ALA	H	8.26	0.02	1
UNMAPPED	142	GLN	H	7.62	0.02	1
UNMAPPED	32	VAL	H	6.94	0.02	1
UNMAPPED	146	LEU	CB	44.38	0.1	1
UNMAPPED	173	LEU	CA	56.56	0.1	1
UNMAPPED	226	ASN	C	178.18	0.1	1
UNMAPPED	212	CYS	H	7.84	0.02	1
UNMAPPED	203	LEU	H	8.0	0.02	1
UNMAPPED	70	ASN	CB	38.97	0.1	1
UNMAPPED	40	LEU	N	121.26	0.1	1
UNMAPPED	146	LEU	N	126.32	0.1	1
UNMAPPED	85	GLY	CA	44.87	0.1	1
UNMAPPED	160	ASP	H	8.04	0.02	1
UNMAPPED	21	ARG	CA	56.06	0.1	1
UNMAPPED	51	LEU	CA	53.53	0.1	1
UNMAPPED	40	LEU	CB	42.11	0.1	1
UNMAPPED	108	ARG	CA	55.29	0.1	1
UNMAPPED	150	VAL	CB	31.39	0.1	1
UNMAPPED	230	ASN	CB	38.59	0.1	1
UNMAPPED	185	GLN	H	8.08	0.02	1
UNMAPPED	171	THR	C	174.06	0.1	1
UNMAPPED	233	LYS	C	176.36	0.1	1
UNMAPPED	171	THR	N	117.48	0.1	1
UNMAPPED	197	GLN	CB	27.68	0.1	1
UNMAPPED	48	THR	C	175.07	0.1	1
UNMAPPED	67	GLU	H	8.78	0.02	1
UNMAPPED	28	LEU	H	7.79	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	199	ALA	CA	54.66	0.1	1
UNMAPPED	154	PHE	CB	38.16	0.1	1
UNMAPPED	205	GLY	C	174.41	0.1	1
UNMAPPED	21	ARG	CB	30.85	0.1	1
UNMAPPED	153	LEU	CA	54.76	0.1	1
UNMAPPED	239	ARG	C	173.26	0.1	1
UNMAPPED	206	GLN	C	175.14	0.1	1
UNMAPPED	172	VAL	CB	31.17	0.1	1
UNMAPPED	86	GLN	H	7.96	0.02	1
UNMAPPED	231	ASN	CB	37.03	0.1	1
UNMAPPED	63	MET	CA	51.31	0.1	1
UNMAPPED	95	HIS	N	120.3	0.1	1
UNMAPPED	237	TYR	C	176.94	0.1	1
UNMAPPED	217	ILE	C	173.66	0.1	1
UNMAPPED	60	PHE	H	9.18	0.02	1
UNMAPPED	61	ILE	N	120.55	0.1	1
UNMAPPED	193	PRO	CB	31.76	0.1	1
UNMAPPED	52	MET	C	175.19	0.1	1
UNMAPPED	99	LYS	CB	32.46	0.1	1
UNMAPPED	54	LYS	N	125.44	0.1	1
UNMAPPED	53	LEU	N	128.84	0.1	1
UNMAPPED	231	ASN	H	9.42	0.02	1
UNMAPPED	154	PHE	CA	56.47	0.1	1
UNMAPPED	61	ILE	CB	41.65	0.1	1
UNMAPPED	184	PHE	CB	40.15	0.1	1
UNMAPPED	190	TYR	CB	41.56	0.1	1
UNMAPPED	54	LYS	CB	31.69	0.1	1
UNMAPPED	53	LEU	CB	40.43	0.1	1
UNMAPPED	171	THR	CA	63.06	0.1	1
UNMAPPED	57	ASN	N	117.92	0.1	1
UNMAPPED	155	TYR	CB	40.09	0.1	1
UNMAPPED	91	GLN	N	123.89	0.1	1
UNMAPPED	59	ALA	N	121.32	0.1	1
UNMAPPED	184	PHE	N	128.98	0.1	1
UNMAPPED	190	TYR	C	175.61	0.1	1
UNMAPPED	164	GLN	CA	59.48	0.1	1
UNMAPPED	180	LYS	H	8.34	0.02	1
UNMAPPED	91	GLN	CB	32.76	0.1	1
UNMAPPED	59	ALA	CB	23.95	0.1	1
UNMAPPED	199	ALA	C	178.96	0.1	1
UNMAPPED	244	SER	N	114.76	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	164	GLN	H	8.39	0.02	1
UNMAPPED	153	LEU	C	176.61	0.1	1
UNMAPPED	234	SER	H	7.84	0.02	1
UNMAPPED	219	PHE	H	8.79	0.02	1
UNMAPPED	214	THR	N	121.4	0.1	1
UNMAPPED	73	VAL	H	8.12	0.02	1
UNMAPPED	187	LEU	CA	52.98	0.1	1
UNMAPPED	32	VAL	C	173.53	0.1	1
UNMAPPED	155	TYR	N	119.18	0.1	1
UNMAPPED	216	ARG	N	124.43	0.1	1
UNMAPPED	106	GLN	CB	28.93	0.1	1
UNMAPPED	143	SER	CB	65.54	0.1	1
UNMAPPED	162	LEU	N	118.49	0.1	1
UNMAPPED	35	GLY	N	105.59	0.1	1
UNMAPPED	18	VAL	CB	32.15	0.1	1
UNMAPPED	143	SER	N	117.92	0.1	1
UNMAPPED	162	LEU	CB	40.77	0.1	1
UNMAPPED	77	THR	H	7.59	0.02	1
UNMAPPED	151	GLU	CA	54.69	0.1	1
UNMAPPED	233	LYS	H	8.72	0.02	1
UNMAPPED	37	VAL	N	120.61	0.1	1
UNMAPPED	183	GLN	N	119.31	0.1	1
UNMAPPED	185	GLN	N	127.59	0.1	1
UNMAPPED	66	GLU	N	124.08	0.1	1
UNMAPPED	20	SER	CA	55.91	0.1	1
UNMAPPED	107	ALA	N	126.78	0.1	1
UNMAPPED	33	THR	C	175.59	0.1	1
UNMAPPED	240	PRO	C	177.03	0.1	1
UNMAPPED	26	ARG	CB	33.99	0.1	1
UNMAPPED	66	GLU	CB	28.7	0.1	1
UNMAPPED	72	MET	H	7.78	0.02	1
UNMAPPED	164	GLN	CB	27.47	0.1	1
UNMAPPED	102	SER	CB	63.11	0.1	1
UNMAPPED	26	ARG	N	125.05	0.1	1
UNMAPPED	158	THR	C	175.5	0.1	1
UNMAPPED	34	GLU	CB	28.7	0.1	1
UNMAPPED	25	ILE	C	174.47	0.1	1
UNMAPPED	55	GLY	CA	45.33	0.1	1
UNMAPPED	102	SER	N	117.6	0.1	1
UNMAPPED	84	ARG	N	123.95	0.1	1
UNMAPPED	157	VAL	H	7.92	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	169	PHE	H	7.03	0.02	1
UNMAPPED	195	SER	CA	61.89	0.1	1
UNMAPPED	23	ILE	C	173.73	0.1	1
UNMAPPED	219	PHE	N	120.39	0.1	1
UNMAPPED	64	ASN	CB	37.06	0.1	1
UNMAPPED	210	ASN	CA	55.8	0.1	1
UNMAPPED	33	THR	CA	59.43	0.1	1
UNMAPPED	49	ASN	C	171.92	0.1	1
UNMAPPED	101	ASP	C	175.94	0.1	1
UNMAPPED	200	LYS	C	178.27	0.1	1
UNMAPPED	190	TYR	N	128.47	0.1	1
UNMAPPED	145	VAL	C	175.41	0.1	1
UNMAPPED	41	GLY	C	173.55	0.1	1
UNMAPPED	159	LEU	C	178.77	0.1	1
UNMAPPED	84	ARG	CA	55.98	0.1	1
UNMAPPED	47	VAL	CA	61.27	0.1	1
UNMAPPED	200	LYS	H	7.96	0.02	1
UNMAPPED	187	LEU	CB	44.9	0.1	1
UNMAPPED	48	THR	CA	61.96	0.1	1
UNMAPPED	18	VAL	C	174.5	0.1	1
UNMAPPED	58	GLN	N	114.38	0.1	1
UNMAPPED	238	THR	CB	69.33	0.1	1
UNMAPPED	68	ALA	N	125.88	0.1	1
UNMAPPED	44	PHE	N	113.74	0.1	1
UNMAPPED	219	PHE	CA	58.78	0.1	1
UNMAPPED	78	SER	C	173.49	0.1	1
UNMAPPED	58	GLN	CB	34.91	0.1	1
UNMAPPED	140	ALA	CB	18.4	0.1	1
UNMAPPED	142	GLN	CB	28.86	0.1	1
UNMAPPED	32	VAL	CB	31.31	0.1	1
UNMAPPED	106	GLN	CA	55.37	0.1	1
UNMAPPED	212	CYS	CB	29.53	0.1	1
UNMAPPED	169	PHE	N	113.81	0.1	1
UNMAPPED	225	LEU	N	121.65	0.1	1
UNMAPPED	163	HIS	N	120.07	0.1	1
UNMAPPED	157	VAL	CA	62.27	0.1	1
UNMAPPED	49	ASN	CA	52.69	0.1	1
UNMAPPED	40	LEU	H	7.48	0.02	1
UNMAPPED	150	VAL	H	7.96	0.02	1
UNMAPPED	217	ILE	CA	60.34	0.1	1
UNMAPPED	28	LEU	C	175.01	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	224	SER	CA	57.01	0.1	1
UNMAPPED	175	ILE	N	120.45	0.1	1
UNMAPPED	107	ALA	C	177.32	0.1	1
UNMAPPED	67	GLU	CB	28.55	0.1	1
UNMAPPED	187	LEU	N	122.15	0.1	1
UNMAPPED	232	ASP	H	8.68	0.02	1
UNMAPPED	93	SER	CA	56.6	0.1	1
UNMAPPED	25	ILE	N	129.54	0.1	1
UNMAPPED	62	GLU	N	128.45	0.1	1
UNMAPPED	104	PRO	CB	31.38	0.1	1
UNMAPPED	106	GLN	N	122.16	0.1	1
UNMAPPED	86	GLN	CB	29.93	0.1	1
UNMAPPED	187	LEU	C	175.1	0.1	1
UNMAPPED	202	SER	CA	61.35	0.1	1
UNMAPPED	196	ALA	C	178.8	0.1	1
UNMAPPED	223	THR	CB	69.18	0.1	1
UNMAPPED	20	SER	C	173.08	0.1	1
UNMAPPED	93	SER	N	116.82	0.1	1
UNMAPPED	21	ARG	H	8.51	0.02	1
UNMAPPED	173	LEU	N	127.27	0.1	1
UNMAPPED	101	ASP	H	8.33	0.02	1
UNMAPPED	54	LYS	H	8.39	0.02	1
UNMAPPED	53	LEU	H	8.4	0.02	1
UNMAPPED	80	THR	N	122.99	0.1	1
UNMAPPED	236	ASP	CB	41.26	0.1	1
UNMAPPED	152	ASN	CA	53.74	0.1	1
UNMAPPED	16	SER	CB	63.34	0.1	1
UNMAPPED	51	LEU	N	129.41	0.1	1
UNMAPPED	61	ILE	C	172.6	0.1	1
UNMAPPED	91	GLN	H	8.39	0.02	1
UNMAPPED	162	LEU	CA	57.86	0.1	1
UNMAPPED	220	SER	N	118.49	0.1	1
UNMAPPED	215	LEU	N	128.47	0.1	1
UNMAPPED	46	LYS	CA	54.3	0.1	1
UNMAPPED	18	VAL	N	123.44	0.1	1
UNMAPPED	204	ASP	H	7.45	0.02	1
UNMAPPED	180	LYS	N	127.52	0.1	1
UNMAPPED	58	GLN	C	174.14	0.1	1
UNMAPPED	177	THR	C	173.12	0.1	1
UNMAPPED	74	ASN	H	8.34	0.02	1
UNMAPPED	235	ARG	C	173.9	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	106	GLN	H	8.16	0.02	1
UNMAPPED	38	ILE	H	8.47	0.02	1
UNMAPPED	199	ALA	N	123.92	0.1	1
UNMAPPED	149	ILE	C	175.09	0.1	1
UNMAPPED	18	VAL	H	8.12	0.02	1
UNMAPPED	242	LEU	C	175.48	0.1	1
UNMAPPED	52	MET	CB	32.46	0.1	1
UNMAPPED	199	ALA	CB	18.99	0.1	1
UNMAPPED	90	ILE	N	126.07	0.1	1
UNMAPPED	153	LEU	CB	40.01	0.1	1
UNMAPPED	57	ASN	C	173.91	0.1	1
UNMAPPED	77	THR	CB	68.47	0.1	1
UNMAPPED	88	ILE	CA	58.43	0.1	1
UNMAPPED	87	PRO	C	176.27	0.1	1
UNMAPPED	170	GLY	CA	44.8	0.1	1
UNMAPPED	182	ASN	CA	54.57	0.1	1
UNMAPPED	77	THR	N	114.96	0.1	1
UNMAPPED	158	THR	N	114.64	0.1	1
UNMAPPED	154	PHE	N	127.27	0.1	1
UNMAPPED	69	ALA	H	7.45	0.02	1
UNMAPPED	193	PRO	CA	64.77	0.1	1
UNMAPPED	213	CYS	CA	59.8	0.1	1
UNMAPPED	197	GLN	N	118.49	0.1	1
UNMAPPED	226	ASN	N	122.91	0.1	1
UNMAPPED	26	ARG	H	8.82	0.02	1
UNMAPPED	66	GLU	H	9.3	0.02	1
UNMAPPED	198	HIS	CA	57.42	0.1	1
UNMAPPED	184	PHE	CA	58.62	0.1	1
UNMAPPED	171	THR	CB	69.18	0.1	1
UNMAPPED	239	ARG	N	122.6	0.1	1
UNMAPPED	159	LEU	CA	59.29	0.1	1
UNMAPPED	17	GLY	CA	44.26	0.1	1
UNMAPPED	209	TYR	H	7.1	0.02	1
UNMAPPED	224	SER	C	172.48	0.1	1
UNMAPPED	183	GLN	CA	54.34	0.1	1
UNMAPPED	84	ARG	CB	27.4	0.1	1
UNMAPPED	105	ASN	H	8.36	0.02	1
UNMAPPED	241	ASP	N	117.48	0.1	1
UNMAPPED	183	GLN	C	174.72	0.1	1
UNMAPPED	173	LEU	C	177.3	0.1	1
UNMAPPED	42	LEU	CB	39.51	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	143	SER	CA	54.38	0.1	1
UNMAPPED	161	VAL	N	122.79	0.1	1
UNMAPPED	238	THR	CA	61.79	0.1	1
UNMAPPED	210	ASN	C	175.83	0.1	1
UNMAPPED	85	GLY	C	173.27	0.1	1
UNMAPPED	165	ILE	H	7.97	0.02	1
UNMAPPED	51	LEU	C	174.88	0.1	1
UNMAPPED	198	HIS	C	177.63	0.1	1
UNMAPPED	108	ARG	C	174.82	0.1	1
UNMAPPED	37	VAL	CA	66.1	0.1	1
UNMAPPED	242	LEU	CB	39.33	0.1	1
UNMAPPED	43	PRO	CB	29.93	0.1	1
UNMAPPED	102	SER	C	174.14	0.1	1
UNMAPPED	20	SER	N	116.44	0.1	1
UNMAPPED	107	ALA	CA	51.92	0.1	1
UNMAPPED	149	ILE	H	9.15	0.02	1
UNMAPPED	188	LEU	N	125.19	0.1	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	197	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	185	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	189	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	181	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 2483. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/970 (0%)	0/386 (0%)	0/396 (0%)	0/188 (0%)
Sidechain	0/1328 (0%)	0/783 (0%)	0/480 (0%)	0/65 (0%)
Aromatic	0/185 (0%)	0/103 (0%)	0/72 (0%)	0/10 (0%)
Overall	0/2483 (0%)	0/1272 (0%)	0/948 (0%)	0/263 (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 2483. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/970 (0%)	0/386 (0%)	0/396 (0%)	0/188 (0%)
Sidechain	0/1328 (0%)	0/783 (0%)	0/480 (0%)	0/65 (0%)
Aromatic	0/185 (0%)	0/103 (0%)	0/72 (0%)	0/10 (0%)
Overall	0/2483 (0%)	0/1272 (0%)	0/948 (0%)	0/263 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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.