



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:42 PM BST

PDB ID : 2K7D
Title : NMR Structure of Ca²⁺-bound CaBP1 C-domain
Authors : Ames, J.
Deposited on : 2008-08-08

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

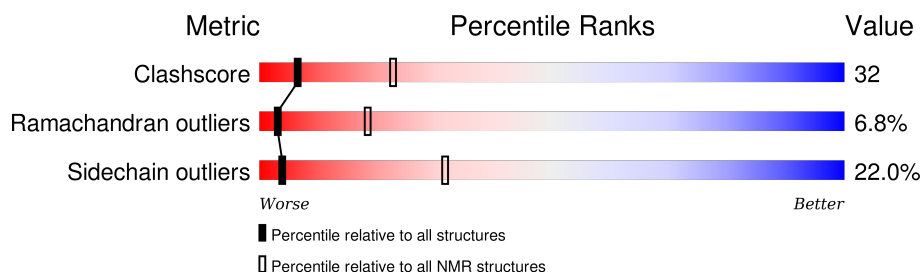
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	72	

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:101-A:167 (67)	0.72	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1143 atoms, of which 559 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	72	Total	C	H	N	O	S	0
			1141	353	559	108	117	4	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

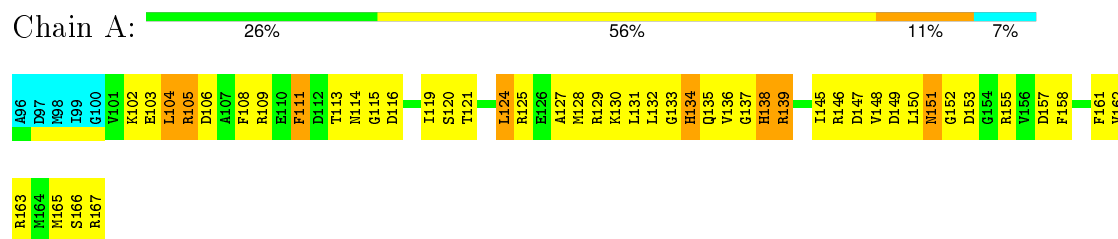
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Calcium-binding protein 1

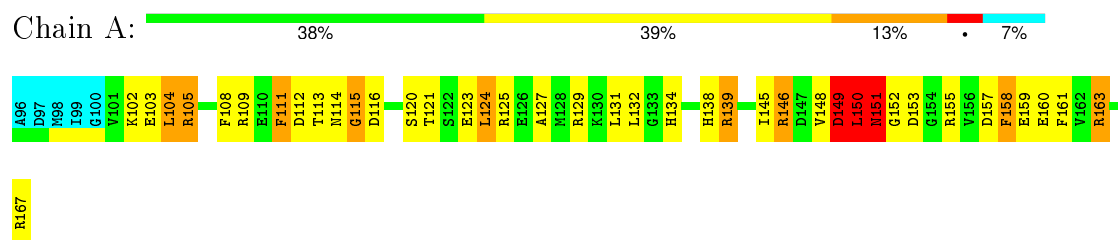


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

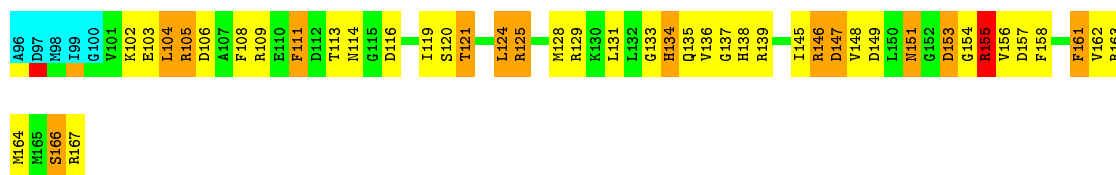
- Molecule 1: Calcium-binding protein 1



4.2.2 Score per residue for model 2

- Molecule 1: Calcium-binding protein 1





4.2.3 Score per residue for model 3

- Molecule 1: Calcium-binding protein 1

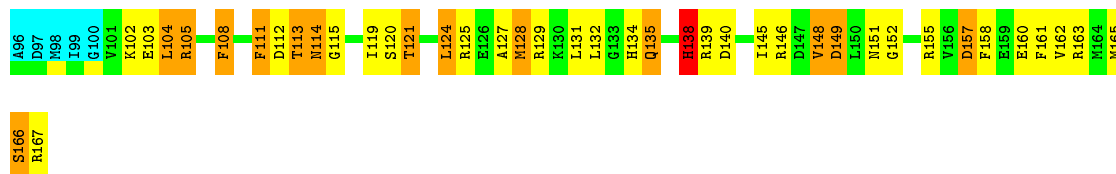
Chain A: 44% 35% 13% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Calcium-binding protein 1

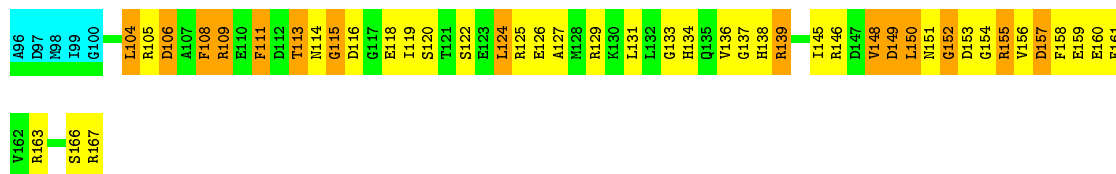
Chain A: 36% 36% 19% 7%



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Calcium-binding protein 1

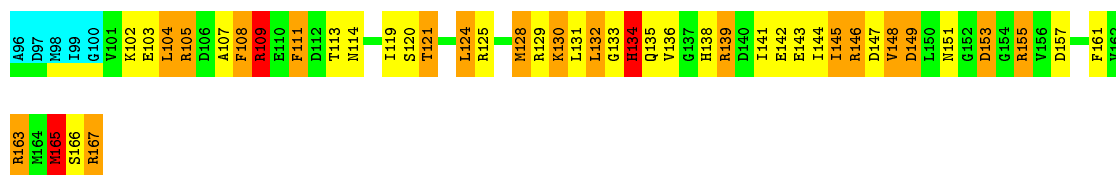
Chain A: 31% 42% 21% 7%



4.2.6 Score per residue for model 6

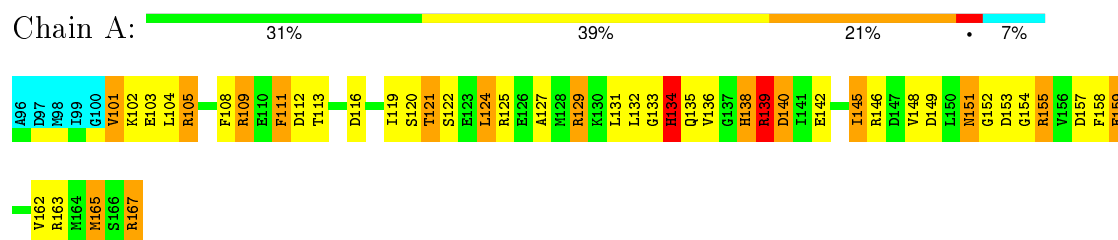
- Molecule 1: Calcium-binding protein 1

Chain A: 32% 32% 25% 7%



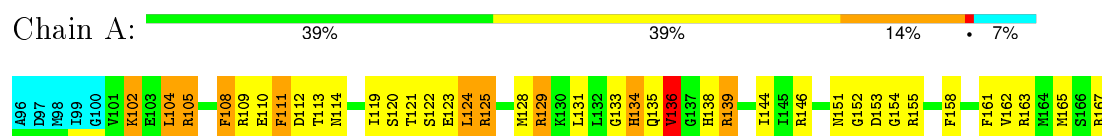
4.2.7 Score per residue for model 7

- Molecule 1: Calcium-binding protein 1



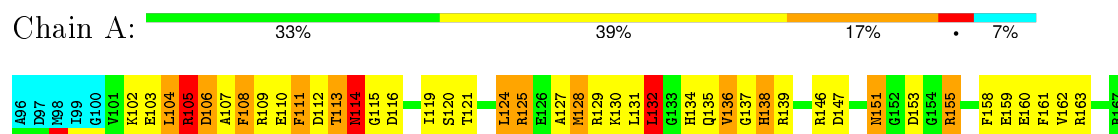
4.2.8 Score per residue for model 8

- Molecule 1: Calcium-binding protein 1



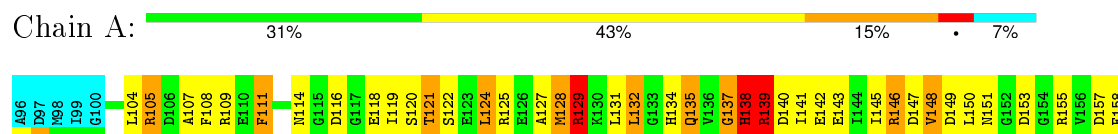
4.2.9 Score per residue for model 9

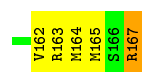
- Molecule 1: Calcium-binding protein 1



4.2.10 Score per residue for model 10

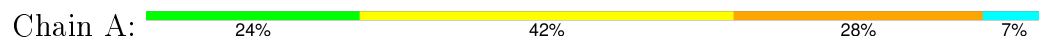
- Molecule 1: Calcium-binding protein 1





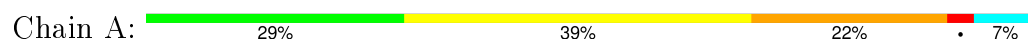
4.2.11 Score per residue for model 11

- Molecule 1: Calcium-binding protein 1



4.2.12 Score per residue for model 12

- Molecule 1: Calcium-binding protein 1



4.2.13 Score per residue for model 13

- Molecule 1: Calcium-binding protein 1



4.2.14 Score per residue for model 14

- Molecule 1: Calcium-binding protein 1





4.2.15 Score per residue for model 15

- Molecule 1: Calcium-binding protein 1



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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 15623
Number of chemical shift lists	1
Total number of shifts	1585
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1585
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:
CA

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	1.14±0.01	2±0/554 (0.4±0.0%)	1.25±0.00	0±0/736 (0.0±0.0%)
All	All	1.14	30/8310 (0.4%)	1.25	0/11040 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	8.7±0.5
All	All	0	130

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	134	HIS	CG-ND1	-6.21	1.25	1.38	5	15
1	A	138	HIS	CG-ND1	-6.17	1.25	1.38	7	15

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	105	ARG	Sidechain	15
1	A	139	ARG	Sidechain	15
1	A	129	ARG	Sidechain	15
1	A	146	ARG	Sidechain	15

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	163	ARG	Sidechain	15
1	A	109	ARG	Sidechain	14
1	A	125	ARG	Sidechain	14
1	A	155	ARG	Sidechain	14
1	A	167	ARG	Sidechain	13

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	549	527	527	35±7
2	A	2	0	0	0±0
All	All	8265	7905	7905	524

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:VAL:HG13	1:A:149:ASP:N	0.89	1.83	4	7
1:A:148:VAL:HG13	1:A:149:ASP:H	0.82	1.35	12	5
1:A:114:ASN:HD22	1:A:114:ASN:H	0.82	1.16	9	1
1:A:114:ASN:ND2	1:A:116:ASP:N	0.76	2.31	14	1
1:A:104:LEU:CD1	1:A:161:PHE:CE2	0.76	2.69	12	10
1:A:132:LEU:HD12	1:A:133:GLY:N	0.75	1.96	14	1
1:A:114:ASN:H	1:A:114:ASN:ND2	0.75	1.78	13	1
1:A:114:ASN:ND2	1:A:115:GLY:N	0.74	2.35	14	1
1:A:130:LYS:C	1:A:131:LEU:HD12	0.74	2.02	6	3
1:A:111:PHE:CD1	1:A:119:ILE:HD13	0.74	2.18	6	10
1:A:124:LEU:HD21	1:A:128:MET:SD	0.74	2.22	13	1
1:A:128:MET:SD	1:A:132:LEU:HD11	0.73	2.23	11	1
1:A:124:LEU:HD11	1:A:128:MET:SD	0.71	2.25	3	3
1:A:112:ASP:OD1	2:A:501:CA:CA	0.71	1.67	1	1
1:A:114:ASN:ND2	1:A:114:ASN:H	0.69	1.83	9	1
1:A:104:LEU:HD12	1:A:161:PHE:CE2	0.69	2.22	2	10
1:A:114:ASN:HD22	1:A:115:GLY:N	0.68	1.86	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:LEU:O	1:A:124:LEU:HD23	0.68	1.88	13	1
1:A:114:ASN:ND2	1:A:114:ASN:N	0.68	2.42	13	2
1:A:114:ASN:N	1:A:114:ASN:ND2	0.68	2.42	9	1
1:A:104:LEU:HD12	1:A:162:VAL:HG22	0.67	1.66	10	4
1:A:148:VAL:CG1	1:A:149:ASP:N	0.67	2.55	4	6
1:A:104:LEU:CD1	1:A:161:PHE:CZ	0.67	2.78	2	2
1:A:118:GLU:CD	1:A:118:GLU:N	0.66	2.49	3	1
1:A:148:VAL:CG1	1:A:149:ASP:H	0.66	2.03	4	2
1:A:105:ARG:NH1	1:A:158:PHE:CG	0.66	2.64	8	1
1:A:131:LEU:CD1	1:A:131:LEU:N	0.65	2.59	4	6
1:A:108:PHE:CZ	1:A:158:PHE:N	0.65	2.65	1	8
1:A:111:PHE:CE1	1:A:119:ILE:HD13	0.65	2.27	7	8
1:A:114:ASN:ND2	1:A:116:ASP:H	0.64	1.90	14	1
1:A:114:ASN:HD22	1:A:114:ASN:N	0.64	1.89	13	1
1:A:132:LEU:CD1	1:A:133:GLY:N	0.64	2.61	14	1
1:A:103:GLU:CG	1:A:104:LEU:N	0.64	2.60	3	2
1:A:151:ASN:HD22	1:A:152:GLY:H	0.63	1.35	11	1
1:A:114:ASN:ND2	1:A:116:ASP:CG	0.62	2.53	14	1
1:A:112:ASP:OD2	1:A:115:GLY:N	0.62	2.33	1	1
1:A:101:VAL:CG1	1:A:102:LYS:N	0.62	2.62	11	1
1:A:116:ASP:OD1	1:A:117:GLY:N	0.62	2.33	12	2
1:A:149:ASP:OD2	1:A:154:GLY:N	0.61	2.33	2	1
1:A:106:ASP:OD1	1:A:106:ASP:N	0.61	2.31	5	2
1:A:151:ASN:ND2	1:A:151:ASN:H	0.61	1.92	11	1
1:A:151:ASN:HD22	1:A:152:GLY:N	0.61	1.93	11	1
1:A:166:SER:OG	1:A:167:ARG:N	0.60	2.34	2	3
1:A:153:ASP:OD2	1:A:155:ARG:N	0.60	2.33	12	2
1:A:135:GLN:CD	1:A:135:GLN:H	0.60	1.99	7	2
1:A:151:ASN:ND2	1:A:152:GLY:H	0.60	1.95	11	1
1:A:124:LEU:HD23	1:A:145:ILE:CD1	0.60	2.27	2	1
1:A:116:ASP:CG	1:A:117:GLY:N	0.60	2.54	11	1
1:A:138:HIS:CD2	1:A:138:HIS:H	0.60	2.10	4	2
1:A:132:LEU:N	1:A:132:LEU:HD12	0.60	2.11	1	1
1:A:111:PHE:CD1	1:A:119:ILE:CD1	0.60	2.85	6	8
1:A:128:MET:SD	1:A:132:LEU:CD1	0.60	2.90	11	1
1:A:151:ASN:CG	1:A:152:GLY:N	0.59	2.55	7	3
1:A:148:VAL:HG22	1:A:149:ASP:N	0.59	2.11	12	3
1:A:147:ASP:OD1	1:A:148:VAL:N	0.59	2.36	13	1
1:A:138:HIS:N	1:A:138:HIS:ND1	0.59	2.51	3	2
1:A:153:ASP:CG	1:A:154:GLY:N	0.59	2.55	8	3
1:A:110:GLU:OE2	1:A:130:LYS:NZ	0.59	2.34	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ASN:ND2	1:A:160:GLU:OE2	0.59	2.34	4	1
1:A:136:VAL:HG23	1:A:136:VAL:O	0.59	1.98	7	1
1:A:131:LEU:N	1:A:131:LEU:CD1	0.59	2.66	10	7
1:A:114:ASN:C	1:A:114:ASN:HD22	0.59	2.01	14	1
1:A:150:LEU:HD23	1:A:150:LEU:N	0.59	2.13	1	1
1:A:158:PHE:O	1:A:162:VAL:HG23	0.58	1.97	14	5
1:A:122:SER:OG	1:A:123:GLU:N	0.58	2.36	8	3
1:A:111:PHE:CE1	1:A:127:ALA:CB	0.58	2.87	10	3
1:A:114:ASN:H	1:A:114:ASN:HD22	0.58	1.36	13	1
1:A:131:LEU:HD12	1:A:131:LEU:N	0.57	2.14	4	8
1:A:149:ASP:OD1	1:A:150:LEU:N	0.57	2.38	1	2
1:A:116:ASP:CG	1:A:117:GLY:H	0.56	2.04	11	1
1:A:138:HIS:CG	1:A:139:ARG:N	0.56	2.72	7	1
1:A:151:ASN:ND2	1:A:153:ASP:OD2	0.56	2.38	5	1
1:A:138:HIS:CD2	1:A:138:HIS:N	0.56	2.73	4	2
1:A:146:ARG:O	1:A:150:LEU:HD21	0.56	2.00	1	1
1:A:114:ASN:HD21	1:A:116:ASP:H	0.56	1.42	14	1
1:A:148:VAL:HG22	1:A:149:ASP:H	0.56	1.60	6	3
1:A:148:VAL:HG11	1:A:156:VAL:CG2	0.56	2.30	13	1
1:A:101:VAL:HG13	1:A:102:LYS:N	0.56	2.15	11	1
1:A:157:ASP:OD1	1:A:158:PHE:N	0.55	2.40	10	2
1:A:148:VAL:HG11	1:A:156:VAL:HG22	0.55	1.79	5	5
1:A:112:ASP:OD1	1:A:114:ASN:ND2	0.55	2.39	9	1
1:A:153:ASP:OD1	1:A:154:GLY:N	0.55	2.40	14	2
1:A:165:MET:O	1:A:167:ARG:N	0.55	2.40	11	2
1:A:132:LEU:HD12	1:A:132:LEU:N	0.55	2.16	12	1
1:A:142:GLU:O	1:A:146:ARG:N	0.55	2.40	10	2
1:A:109:ARG:C	1:A:111:PHE:N	0.55	2.60	12	4
1:A:147:ASP:C	1:A:149:ASP:H	0.55	2.06	10	1
1:A:149:ASP:OD1	1:A:151:ASN:ND2	0.55	2.39	11	1
1:A:104:LEU:HG	1:A:162:VAL:HG22	0.54	1.79	12	3
1:A:124:LEU:HB2	1:A:145:ILE:HD11	0.54	1.78	11	1
1:A:128:MET:O	1:A:132:LEU:N	0.54	2.37	9	3
1:A:149:ASP:OD1	1:A:160:GLU:CG	0.54	2.55	1	1
1:A:108:PHE:CD1	1:A:161:PHE:CD2	0.54	2.96	11	9
1:A:150:LEU:O	1:A:152:GLY:N	0.54	2.41	1	1
1:A:147:ASP:OD1	1:A:147:ASP:C	0.54	2.46	13	1
1:A:125:ARG:O	1:A:129:ARG:N	0.54	2.41	14	3
1:A:112:ASP:C	1:A:114:ASN:H	0.54	2.05	15	1
1:A:157:ASP:O	1:A:159:GLU:N	0.54	2.40	1	2
1:A:149:ASP:H	1:A:150:LEU:HD23	0.54	1.61	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ASP:CG	1:A:107:ALA:N	0.54	2.60	15	1
1:A:153:ASP:OD1	1:A:153:ASP:N	0.54	2.41	13	1
1:A:120:SER:O	1:A:124:LEU:N	0.54	2.41	14	8
1:A:131:LEU:N	1:A:131:LEU:HD12	0.53	2.16	6	3
1:A:146:ARG:O	1:A:148:VAL:N	0.53	2.42	2	1
1:A:102:LYS:O	1:A:105:ARG:N	0.53	2.41	9	11
1:A:151:ASN:OD1	1:A:151:ASN:N	0.53	2.41	15	2
1:A:149:ASP:CG	1:A:150:LEU:H	0.53	2.05	12	2
1:A:151:ASN:OD1	1:A:153:ASP:N	0.53	2.41	7	1
1:A:157:ASP:O	1:A:161:PHE:N	0.53	2.41	12	4
1:A:132:LEU:CD1	1:A:132:LEU:N	0.53	2.72	12	2
1:A:134:HIS:CD2	1:A:134:HIS:N	0.53	2.76	8	1
1:A:124:LEU:C	1:A:124:LEU:HD23	0.52	2.24	13	1
1:A:121:THR:OG1	1:A:122:SER:N	0.52	2.40	13	1
1:A:161:PHE:CD1	1:A:161:PHE:C	0.52	2.82	11	2
1:A:124:LEU:C	1:A:124:LEU:CD1	0.52	2.77	9	4
1:A:150:LEU:C	1:A:152:GLY:N	0.52	2.62	1	1
1:A:106:ASP:OD1	1:A:107:ALA:N	0.52	2.43	15	1
1:A:136:VAL:HG12	1:A:137:GLY:N	0.52	2.19	5	1
1:A:114:ASN:C	1:A:114:ASN:ND2	0.52	2.60	14	1
1:A:138:HIS:O	1:A:140:ASP:N	0.52	2.42	7	1
1:A:124:LEU:O	1:A:127:ALA:N	0.52	2.43	13	10
1:A:129:ARG:O	1:A:131:LEU:N	0.52	2.43	11	1
1:A:147:ASP:O	1:A:149:ASP:N	0.51	2.43	10	1
1:A:133:GLY:O	1:A:135:GLN:N	0.51	2.43	11	2
1:A:114:ASN:HD22	1:A:116:ASP:N	0.51	2.02	14	1
1:A:149:ASP:CG	1:A:150:LEU:N	0.51	2.64	5	3
1:A:151:ASN:N	1:A:151:ASN:ND2	0.51	2.56	11	2
1:A:164:MET:O	1:A:164:MET:SD	0.51	2.69	2	1
1:A:150:LEU:C	1:A:152:GLY:H	0.51	2.07	1	1
1:A:117:GLY:C	1:A:118:GLU:CD	0.51	2.70	11	1
1:A:130:LYS:O	1:A:131:LEU:HD12	0.51	2.04	11	1
1:A:116:ASP:OD1	1:A:116:ASP:N	0.51	2.41	12	2
1:A:124:LEU:CD1	1:A:124:LEU:C	0.51	2.79	1	5
1:A:135:GLN:N	1:A:135:GLN:CD	0.51	2.64	4	1
1:A:106:ASP:C	1:A:106:ASP:OD1	0.51	2.49	15	1
1:A:151:ASN:CG	1:A:152:GLY:H	0.51	2.09	5	1
1:A:104:LEU:HD13	1:A:161:PHE:CE2	0.50	2.41	1	1
1:A:159:GLU:CG	1:A:160:GLU:N	0.50	2.74	9	1
1:A:109:ARG:C	1:A:111:PHE:H	0.50	2.09	12	1
1:A:153:ASP:OD1	1:A:155:ARG:N	0.50	2.37	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:VAL:CG1	1:A:137:GLY:N	0.50	2.75	5	1
1:A:157:ASP:OD1	1:A:157:ASP:N	0.50	2.44	5	1
1:A:112:ASP:O	1:A:114:ASN:N	0.50	2.44	4	2
1:A:165:MET:SD	1:A:165:MET:N	0.50	2.85	7	1
1:A:112:ASP:OD1	1:A:114:ASN:CG	0.50	2.50	9	1
1:A:147:ASP:C	1:A:149:ASP:N	0.50	2.63	10	1
1:A:134:HIS:O	1:A:136:VAL:N	0.50	2.45	2	1
1:A:149:ASP:OD2	1:A:153:ASP:N	0.50	2.44	7	1
1:A:101:VAL:O	1:A:104:LEU:N	0.50	2.45	7	1
1:A:132:LEU:HD12	1:A:132:LEU:C	0.49	2.26	14	1
1:A:163:ARG:CG	1:A:163:ARG:HH11	0.49	2.20	13	1
1:A:109:ARG:O	1:A:111:PHE:N	0.49	2.45	12	1
1:A:134:HIS:CD2	1:A:134:HIS:H	0.49	2.26	12	1
1:A:124:LEU:CB	1:A:145:ILE:HD11	0.49	2.37	11	2
1:A:142:GLU:O	1:A:145:ILE:N	0.49	2.46	12	3
1:A:134:HIS:O	1:A:135:GLN:CB	0.49	2.61	6	1
1:A:112:ASP:C	1:A:114:ASN:N	0.49	2.66	4	2
1:A:153:ASP:CG	1:A:154:GLY:H	0.49	2.10	8	1
1:A:135:GLN:C	1:A:136:VAL:HG23	0.49	2.28	8	1
1:A:153:ASP:CG	1:A:155:ARG:H	0.49	2.08	12	1
1:A:120:SER:CB	1:A:155:ARG:NE	0.48	2.76	5	1
1:A:131:LEU:O	1:A:132:LEU:C	0.48	2.51	9	1
1:A:129:ARG:C	1:A:131:LEU:N	0.48	2.66	11	1
1:A:116:ASP:N	1:A:116:ASP:OD1	0.48	2.33	7	2
1:A:157:ASP:CG	1:A:160:GLU:OE1	0.48	2.52	1	1
1:A:102:LYS:O	1:A:105:ARG:CB	0.48	2.62	15	6
1:A:140:ASP:O	1:A:143:GLU:N	0.48	2.47	10	1
1:A:124:LEU:HD23	1:A:145:ILE:HD11	0.48	1.85	2	2
1:A:112:ASP:OD1	1:A:116:ASP:CG	0.48	2.51	1	1
1:A:149:ASP:C	1:A:149:ASP:OD1	0.48	2.52	1	1
1:A:133:GLY:O	1:A:134:HIS:CG	0.48	2.67	15	2
1:A:138:HIS:C	1:A:140:ASP:N	0.47	2.68	7	2
1:A:111:PHE:CD2	1:A:119:ILE:CD1	0.47	2.97	2	1
1:A:149:ASP:O	1:A:150:LEU:C	0.47	2.52	1	1
1:A:103:GLU:HG3	1:A:104:LEU:N	0.47	2.24	3	2
1:A:140:ASP:C	1:A:142:GLU:N	0.47	2.66	7	1
1:A:130:LYS:HZ2	1:A:130:LYS:CB	0.47	2.23	12	1
1:A:161:PHE:CD1	1:A:161:PHE:O	0.47	2.67	11	1
1:A:138:HIS:ND1	1:A:139:ARG:N	0.47	2.63	10	1
1:A:103:GLU:O	1:A:106:ASP:N	0.47	2.48	12	3
1:A:145:ILE:O	1:A:145:ILE:HG22	0.47	2.09	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:158:PHE:CE1	1:A:162:VAL:CG2	0.47	2.98	9	1
1:A:149:ASP:OD1	1:A:153:ASP:OD2	0.47	2.32	6	1
1:A:129:ARG:NE	1:A:135:GLN:OE1	0.47	2.46	10	1
1:A:111:PHE:CD2	1:A:119:ILE:HD11	0.46	2.45	2	1
1:A:136:VAL:CG2	1:A:137:GLY:N	0.46	2.78	9	1
1:A:136:VAL:HG12	1:A:136:VAL:O	0.46	2.10	6	1
1:A:159:GLU:C	1:A:159:GLU:OE1	0.46	2.53	5	1
1:A:157:ASP:C	1:A:159:GLU:N	0.46	2.67	1	2
1:A:151:ASN:HD21	1:A:153:ASP:CG	0.46	2.13	5	1
1:A:145:ILE:HG22	1:A:145:ILE:O	0.46	2.11	4	1
1:A:157:ASP:OD2	1:A:160:GLU:OE1	0.46	2.34	1	1
1:A:105:ARG:NH1	1:A:158:PHE:CD2	0.46	2.84	8	1
1:A:146:ARG:C	1:A:148:VAL:N	0.46	2.68	2	1
1:A:104:LEU:CD1	1:A:162:VAL:HG22	0.46	2.41	7	2
1:A:135:GLN:CG	1:A:136:VAL:N	0.45	2.79	14	1
1:A:121:THR:O	1:A:124:LEU:N	0.45	2.47	12	1
1:A:140:ASP:O	1:A:142:GLU:N	0.45	2.48	7	1
1:A:149:ASP:OD1	1:A:160:GLU:OE2	0.45	2.34	1	1
1:A:103:GLU:OE1	1:A:103:GLU:C	0.45	2.55	1	1
1:A:135:GLN:CG	1:A:136:VAL:H	0.45	2.24	14	1
1:A:112:ASP:C	1:A:112:ASP:OD1	0.45	2.54	9	1
1:A:148:VAL:HG21	1:A:164:MET:SD	0.45	2.51	10	1
1:A:111:PHE:CE1	1:A:124:LEU:HD13	0.45	2.46	3	1
1:A:159:GLU:HG3	1:A:160:GLU:N	0.45	2.26	9	1
1:A:104:LEU:HD22	1:A:165:MET:SD	0.45	2.51	11	1
1:A:165:MET:C	1:A:167:ARG:N	0.45	2.70	6	1
1:A:144:ILE:HD12	1:A:144:ILE:N	0.45	2.27	6	1
1:A:118:GLU:OE1	1:A:157:ASP:OD2	0.45	2.35	10	1
1:A:157:ASP:O	1:A:158:PHE:C	0.44	2.55	14	8
1:A:114:ASN:OD1	1:A:114:ASN:N	0.44	2.49	5	1
1:A:114:ASN:CG	1:A:116:ASP:OD2	0.44	2.56	14	1
1:A:120:SER:O	1:A:123:GLU:N	0.44	2.50	1	1
1:A:129:ARG:C	1:A:131:LEU:H	0.44	2.16	11	1
1:A:116:ASP:C	1:A:116:ASP:OD1	0.44	2.54	10	1
1:A:144:ILE:CD1	1:A:144:ILE:N	0.44	2.80	6	1
1:A:161:PHE:O	1:A:161:PHE:CD1	0.44	2.71	2	1
1:A:120:SER:O	1:A:121:THR:C	0.44	2.56	11	11
1:A:156:VAL:C	1:A:157:ASP:OD1	0.44	2.55	5	1
1:A:104:LEU:HD12	1:A:161:PHE:CD2	0.44	2.47	1	2
1:A:104:LEU:O	1:A:107:ALA:N	0.44	2.51	10	1
1:A:137:GLY:O	1:A:139:ARG:N	0.44	2.51	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:ASP:OD2	1:A:115:GLY:CA	0.44	2.65	1	1
1:A:112:ASP:OD1	1:A:116:ASP:OD1	0.44	2.36	1	1
1:A:126:GLU:OE1	1:A:126:GLU:N	0.43	2.51	11	1
1:A:143:GLU:CD	1:A:147:ASP:OD2	0.43	2.57	6	1
1:A:149:ASP:OD1	1:A:160:GLU:CD	0.43	2.56	1	1
1:A:124:LEU:O	1:A:125:ARG:C	0.43	2.56	13	5
1:A:165:MET:O	1:A:166:SER:C	0.43	2.57	4	1
1:A:130:LYS:NZ	1:A:130:LYS:CB	0.43	2.79	12	1
1:A:150:LEU:CD1	1:A:151:ASN:ND2	0.43	2.82	3	1
1:A:125:ARG:O	1:A:129:ARG:CB	0.43	2.67	14	1
1:A:112:ASP:OD1	1:A:123:GLU:OE1	0.43	2.37	8	1
1:A:128:MET:HG3	1:A:141:ILE:HG22	0.43	1.91	12	1
1:A:142:GLU:OE1	1:A:142:GLU:N	0.43	2.51	14	1
1:A:138:HIS:O	1:A:139:ARG:C	0.43	2.57	11	1
1:A:148:VAL:CG2	1:A:149:ASP:H	0.43	2.26	12	1
1:A:114:ASN:HD21	1:A:116:ASP:N	0.42	2.03	14	1
1:A:114:ASN:HD21	1:A:123:GLU:CD	0.42	2.16	8	1
1:A:114:ASN:ND2	1:A:115:GLY:H	0.42	2.12	5	1
1:A:145:ILE:CG2	1:A:145:ILE:O	0.42	2.66	4	1
1:A:102:LYS:O	1:A:103:GLU:C	0.42	2.57	13	7
1:A:140:ASP:OD1	1:A:140:ASP:N	0.42	2.53	7	1
1:A:107:ALA:O	1:A:108:PHE:C	0.42	2.58	6	2
1:A:136:VAL:HG23	1:A:137:GLY:N	0.42	2.29	11	1
1:A:114:ASN:ND2	1:A:123:GLU:OE2	0.42	2.42	8	1
1:A:141:ILE:CG1	1:A:142:GLU:N	0.42	2.82	6	2
1:A:152:GLY:O	1:A:153:ASP:C	0.42	2.57	8	1
1:A:149:ASP:OD1	1:A:155:ARG:N	0.42	2.53	6	1
1:A:118:GLU:OE2	1:A:157:ASP:OD2	0.42	2.37	5	1
1:A:151:ASN:ND2	1:A:151:ASN:N	0.42	2.68	2	1
1:A:141:ILE:HG13	1:A:142:GLU:N	0.42	2.30	10	3
1:A:111:PHE:CG	1:A:119:ILE:CD1	0.41	3.02	2	3
1:A:135:GLN:C	1:A:136:VAL:HG12	0.41	2.34	9	1
1:A:104:LEU:O	1:A:105:ARG:C	0.41	2.58	10	1
1:A:153:ASP:C	1:A:153:ASP:OD1	0.41	2.59	7	1
1:A:150:LEU:N	1:A:150:LEU:CD2	0.41	2.82	1	1
1:A:114:ASN:CG	1:A:115:GLY:H	0.41	2.17	5	1
1:A:145:ILE:O	1:A:145:ILE:CG2	0.41	2.68	1	1
1:A:159:GLU:OE1	1:A:160:GLU:N	0.41	2.53	5	1
1:A:128:MET:SD	1:A:132:LEU:HB2	0.41	2.56	6	1
1:A:101:VAL:O	1:A:102:LYS:C	0.41	2.58	14	2
1:A:124:LEU:CD1	1:A:128:MET:SD	0.41	3.09	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:THR:HG22	1:A:138:HIS:NE2	0.41	2.30	15	1
1:A:138:HIS:O	1:A:141:ILE:N	0.41	2.54	11	1
1:A:151:ASN:N	1:A:151:ASN:OD1	0.41	2.50	5	1
1:A:149:ASP:C	1:A:151:ASN:H	0.41	2.19	13	1
1:A:136:VAL:CG2	1:A:136:VAL:O	0.41	2.67	7	1
1:A:147:ASP:O	1:A:148:VAL:C	0.41	2.60	3	1
1:A:113:THR:HG21	1:A:126:GLU:OE2	0.41	2.16	5	1
1:A:143:GLU:OE2	1:A:147:ASP:OD1	0.41	2.38	11	1
1:A:146:ARG:C	1:A:148:VAL:H	0.40	2.19	2	1
1:A:148:VAL:CG2	1:A:149:ASP:N	0.40	2.76	12	1
1:A:145:ILE:CG2	1:A:154:GLY:O	0.40	2.69	5	1
1:A:113:THR:O	1:A:114:ASN:C	0.40	2.59	9	1
1:A:157:ASP:CG	1:A:158:PHE:N	0.40	2.74	12	1
1:A:137:GLY:C	1:A:139:ARG:N	0.40	2.75	15	1
1:A:136:VAL:CG1	1:A:136:VAL:O	0.40	2.70	6	1
1:A:143:GLU:OE1	1:A:147:ASP:OD2	0.40	2.39	6	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	66/72 (92%)	48±3 (73±4%)	13±3 (20±4%)	4±1 (7±2%)	3	18
All	All	990/1080 (92%)	725 (73%)	198 (20%)	67 (7%)	3	18

All 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	152	GLY	6
1	A	115	GLY	6
1	A	135	GLN	5
1	A	134	HIS	5
1	A	149	ASP	5
1	A	137	GLY	4

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Mol	Chain	Res	Type	Models (Total)
1	A	148	VAL	4
1	A	133	GLY	4
1	A	166	SER	4
1	A	136	VAL	3
1	A	150	LEU	3
1	A	153	ASP	2
1	A	101	VAL	2
1	A	151	ASN	2
1	A	113	THR	2
1	A	132	LEU	2
1	A	138	HIS	1
1	A	139	ARG	1
1	A	147	ASP	1
1	A	117	GLY	1
1	A	158	PHE	1
1	A	165	MET	1
1	A	114	ASN	1
1	A	130	LYS	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/62 (95%)	46±2 (78±4%)	13±2 (22±4%)	4	32
All	All	885/930 (95%)	690 (78%)	195 (22%)	4	32

All 46 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	111	PHE	15
1	A	113	THR	13
1	A	124	LEU	13
1	A	151	ASN	12
1	A	104	LEU	11
1	A	114	ASN	10
1	A	128	MET	9

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Mol	Chain	Res	Type	Models (Total)
1	A	108	PHE	9
1	A	153	ASP	8
1	A	121	THR	8
1	A	139	ARG	6
1	A	157	ASP	5
1	A	132	LEU	5
1	A	163	ARG	4
1	A	138	HIS	4
1	A	122	SER	4
1	A	165	MET	4
1	A	136	VAL	3
1	A	167	ARG	3
1	A	106	ASP	3
1	A	148	VAL	3
1	A	109	ARG	3
1	A	130	LYS	3
1	A	110	GLU	3
1	A	102	LYS	3
1	A	105	ARG	2
1	A	147	ASP	2
1	A	149	ASP	2
1	A	145	ILE	2
1	A	150	LEU	2
1	A	140	ASP	2
1	A	129	ARG	2
1	A	161	PHE	2
1	A	116	ASP	2
1	A	155	ARG	2
1	A	112	ASP	1
1	A	159	GLU	1
1	A	118	GLU	1
1	A	126	GLU	1
1	A	146	ARG	1
1	A	164	MET	1
1	A	134	HIS	1
1	A	144	ILE	1
1	A	101	VAL	1
1	A	166	SER	1
1	A	142	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

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

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: BMRB entry 15623

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	1585
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1585
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 1585 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	105	ARG	C	178.91	0.2	1
UNMAPPED	113	THR	C	176.41	0.2	1
UNMAPPED	48	GLY	N	106.09	0.2	1
UNMAPPED	101	VAL	HG12	1.07	0.04	2
UNMAPPED	89	PRO	C	178.73	0.2	1
UNMAPPED	144	ILE	HG23	0.85	0.04	1
UNMAPPED	116	ASP	CB	40.25	0.2	1
UNMAPPED	131	LEU	HB3	1.58	0.04	2
UNMAPPED	92	LEU	CA	55.82	0.2	1
UNMAPPED	119	ILE	CG2	18.37	0.2	1
UNMAPPED	130	LYS	HB2	1.94	0.04	2
UNMAPPED	69	GLN	C	178.76	0.2	1
UNMAPPED	91	LEU	HD11	0.8	0.04	2
UNMAPPED	72	MET	HB3	2.64	0.04	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	111	PHE	H	7.62	0.04	1
UNMAPPED	60	GLU	HA	4.0	0.04	1
UNMAPPED	105	ARG	CB	29.0	0.2	1
UNMAPPED	102	LYS	HG2	1.44	0.04	2
UNMAPPED	82	ASP	N	121.67	0.2	1
UNMAPPED	86	LEU	HD11	0.82	0.04	2
UNMAPPED	45	ARG	HB2	1.9	0.04	2
UNMAPPED	37	ASP	CB	38.76	0.2	1
UNMAPPED	162	VAL	HA	3.01	0.04	1
UNMAPPED	157	ASP	H	8.68	0.04	1
UNMAPPED	59	THR	HG23	1.38	0.04	1
UNMAPPED	51	MET	N	117.96	0.2	1
UNMAPPED	130	LYS	H	7.49	0.04	1
UNMAPPED	151	ASN	C	176.64	0.2	1
UNMAPPED	22	GLU	CG	36.3	0.2	1
UNMAPPED	74	LEU	HD22	0.97	0.04	2
UNMAPPED	92	LEU	HD21	0.75	0.04	2
UNMAPPED	156	VAL	CG2	21.84	0.2	1
UNMAPPED	120	SER	H	9.24	0.04	1
UNMAPPED	72	MET	C	177.71	0.2	1
UNMAPPED	79	ASP	HA	5.51	0.04	1
UNMAPPED	61	MET	CA	58.4	0.2	1
UNMAPPED	61	MET	HA	4.27	0.04	1
UNMAPPED	65	GLU	HB2	2.12	0.04	2
UNMAPPED	150	LEU	CA	56.96	0.2	1
UNMAPPED	163	ARG	CB	29.01	0.2	1
UNMAPPED	71	ASN	CA	56.32	0.2	1
UNMAPPED	106	ASP	HB3	2.68	0.04	2
UNMAPPED	161	PHE	HA	3.97	0.04	1
UNMAPPED	143	GLU	HA	3.97	0.04	1
UNMAPPED	37	ASP	C	175.57	0.2	1
UNMAPPED	94	GLU	HB2	2.37	0.04	2
UNMAPPED	24	ILE	HG23	1.09	0.04	1
UNMAPPED	27	LEU	H	8.12	0.04	1
UNMAPPED	156	VAL	N	126.27	0.2	1
UNMAPPED	91	LEU	HD23	0.78	0.04	2
UNMAPPED	31	PHE	HB3	2.91	0.04	2
UNMAPPED	54	MET	HB3	2.25	0.04	2
UNMAPPED	151	ASN	HB3	2.85	0.04	2
UNMAPPED	83	PHE	HB3	3.36	0.04	2
UNMAPPED	93	ALA	HA	4.26	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	62	GLU	HA	4.07	0.04	1
UNMAPPED	13	SER	N	115.72	0.2	1
UNMAPPED	45	ARG	N	120.97	0.2	1
UNMAPPED	34	PHE	C	176.27	0.2	1
UNMAPPED	70	ILE	CB	38.04	0.2	1
UNMAPPED	121	THR	HA	3.81	0.04	1
UNMAPPED	164	MET	CG	31.67	0.2	1
UNMAPPED	125	ARG	CA	60.22	0.2	1
UNMAPPED	132	LEU	CA	54.99	0.2	1
UNMAPPED	27	LEU	CG	27.4	0.2	1
UNMAPPED	42	ILE	CA	59.88	0.2	1
UNMAPPED	129	ARG	HB2	1.88	0.04	2
UNMAPPED	35	ASP	CB	38.62	0.2	1
UNMAPPED	63	LEU	C	180.07	0.2	1
UNMAPPED	85	GLU	CG	36.14	0.2	1
UNMAPPED	131	LEU	HD11	0.86	0.04	2
UNMAPPED	130	LYS	HA	4.06	0.04	1
UNMAPPED	42	ILE	HG23	0.29	0.04	1
UNMAPPED	124	LEU	CA	57.41	0.2	1
UNMAPPED	30	ALA	HA	4.33	0.04	1
UNMAPPED	131	LEU	CG	26.7	0.2	1
UNMAPPED	78	VAL	CG1	20.99	0.2	1
UNMAPPED	167	ARG	N	127.07	0.2	1
UNMAPPED	120	SER	HA	4.81	0.04	1
UNMAPPED	147	ASP	N	116.82	0.2	1
UNMAPPED	101	VAL	N	119.57	0.2	1
UNMAPPED	91	LEU	HA	4.14	0.04	1
UNMAPPED	45	ARG	HA	4.12	0.04	1
UNMAPPED	83	PHE	HD1	7.104	0.04	3
UNMAPPED	113	THR	HG23	1.28	0.04	1
UNMAPPED	105	ARG	HA	3.99	0.04	1
UNMAPPED	78	VAL	CG2	22.7	0.2	1
UNMAPPED	132	LEU	HB2	1.66	0.04	2
UNMAPPED	38	LYS	HA	3.87	0.04	1
UNMAPPED	148	VAL	HG11	0.97	0.04	2
UNMAPPED	54	MET	N	118.14	0.2	1
UNMAPPED	24	ILE	HG12	1.62	0.04	1
UNMAPPED	141	ILE	HB	1.99	0.04	1
UNMAPPED	26	GLU	C	180.28	0.2	1
UNMAPPED	132	LEU	C	178.47	0.2	1
UNMAPPED	111	PHE	N	116.75	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	146	ARG	H	7.47	0.04	1
UNMAPPED	14	ARG	CB	32.65	0.2	1
UNMAPPED	60	GLU	C	179.48	0.2	1
UNMAPPED	148	VAL	HG21	0.96	0.04	2
UNMAPPED	52	ARG	HD2	3.22	0.04	2
UNMAPPED	63	LEU	CA	57.96	0.2	1
UNMAPPED	27	LEU	CD1	24.15	0.2	1
UNMAPPED	15	LYS	CG	24.81	0.2	1
UNMAPPED	98	MET	CB	33.36	0.2	1
UNMAPPED	117	GLY	H	10.43	0.04	1
UNMAPPED	77	HIS	C	172.27	0.2	1
UNMAPPED	28	ARG	CD	42.74	0.2	1
UNMAPPED	93	ALA	N	121.93	0.2	1
UNMAPPED	14	ARG	HB2	2.02	0.04	2
UNMAPPED	123	GLU	H	7.72	0.04	1
UNMAPPED	70	ILE	C	179.28	0.2	1
UNMAPPED	13	SER	C	174.73	0.2	1
UNMAPPED	57	MET	HB2	1.91	0.04	2
UNMAPPED	90	LYS	HB2	1.63	0.04	2
UNMAPPED	56	TYR	H	7.9	0.04	1
UNMAPPED	145	ILE	HD12	0.72	0.04	1
UNMAPPED	127	ALA	CB	17.43	0.2	1
UNMAPPED	75	GLY	HA2	3.87	0.04	2
UNMAPPED	78	VAL	HG23	1.13	0.04	2
UNMAPPED	41	TYR	CE1	117.91	0.2	3
UNMAPPED	34	PHE	HB2	2.61	0.04	2
UNMAPPED	100	GLY	HA2	4.16	0.04	2
UNMAPPED	59	THR	H	8.66	0.04	1
UNMAPPED	124	LEU	N	122.54	0.2	1
UNMAPPED	45	ARG	HG2	1.63	0.04	2
UNMAPPED	24	ILE	C	178.37	0.2	1
UNMAPPED	117	GLY	HA2	4.29	0.04	2
UNMAPPED	47	LEU	HD11	0.92	0.04	2
UNMAPPED	70	ILE	HG21	0.9	0.04	1
UNMAPPED	104	LEU	HD21	0.87	0.04	2
UNMAPPED	91	LEU	HB2	1.64	0.04	2
UNMAPPED	147	ASP	CA	55.57	0.2	1
UNMAPPED	164	MET	HA	3.93	0.04	1
UNMAPPED	24	ILE	HB	2.17	0.04	1
UNMAPPED	44	CYS	C	176.43	0.2	1
UNMAPPED	80	PHE	CA	61.54	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	149	ASP	C	176.86	0.2	1
UNMAPPED	41	TYR	HE1	6.8	0.04	3
UNMAPPED	72	MET	HA	4.4	0.04	1
UNMAPPED	70	ILE	HG12	1.75	0.04	1
UNMAPPED	37	ASP	N	114.44	0.2	1
UNMAPPED	144	ILE	HB	1.92	0.04	1
UNMAPPED	148	VAL	HA	4.05	0.04	1
UNMAPPED	24	ILE	CG1	28.97	0.2	1
UNMAPPED	97	ASP	HB2	2.6	0.04	2
UNMAPPED	41	TYR	HB2	2.65	0.04	2
UNMAPPED	64	ILE	HA	3.75	0.04	1
UNMAPPED	155	ARG	CB	32.79	0.2	1
UNMAPPED	167	ARG	H	7.28	0.04	1
UNMAPPED	70	ILE	CG1	29.23	0.2	1
UNMAPPED	114	ASN	HB2	3.29	0.04	2
UNMAPPED	111	PHE	CA	57.57	0.2	1
UNMAPPED	47	LEU	CD2	24.81	0.2	1
UNMAPPED	25	GLU	HB2	2.4	0.04	2
UNMAPPED	119	ILE	HD12	0.24	0.04	1
UNMAPPED	51	MET	HB3	2.56	0.04	2
UNMAPPED	57	MET	CA	51.77	0.2	1
UNMAPPED	66	LEU	HA	4.13	0.04	1
UNMAPPED	148	VAL	CG2	21.74	0.2	1
UNMAPPED	17	ARG	CG	26.65	0.2	1
UNMAPPED	66	LEU	CA	58.24	0.2	1
UNMAPPED	65	GLU	N	121.06	0.2	1
UNMAPPED	126	GLU	CA	58.33	0.2	1
UNMAPPED	80	PHE	HD1	6.714	0.04	3
UNMAPPED	87	MET	CA	56.9	0.2	1
UNMAPPED	68	GLN	HG3	2.44	0.04	2
UNMAPPED	78	VAL	HG12	0.99	0.04	2
UNMAPPED	63	LEU	HB2	1.61	0.04	2
UNMAPPED	78	VAL	CA	60.5	0.2	1
UNMAPPED	155	ARG	C	174.41	0.2	1
UNMAPPED	162	VAL	HG13	0.36	0.04	2
UNMAPPED	19	LEU	HA	4.33	0.04	1
UNMAPPED	26	GLU	N	120.33	0.2	1
UNMAPPED	166	SER	HB2	3.87	0.04	2
UNMAPPED	22	GLU	C	179.56	0.2	1
UNMAPPED	148	VAL	HG12	0.97	0.04	2
UNMAPPED	45	ARG	CB	30.0	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	155	ARG	N	118.11	0.2	1
UNMAPPED	74	LEU	HA	4.81	0.04	1
UNMAPPED	101	VAL	HG11	1.07	0.04	2
UNMAPPED	105	ARG	HB2	1.87	0.04	2
UNMAPPED	137	GLY	N	111.89	0.2	1
UNMAPPED	143	GLU	C	178.41	0.2	1
UNMAPPED	104	LEU	H	8.37	0.04	1
UNMAPPED	32	ARG	C	178.9	0.2	1
UNMAPPED	110	GLU	N	117.53	0.2	1
UNMAPPED	19	LEU	HD21	0.74	0.04	2
UNMAPPED	19	LEU	CA	55.2	0.2	1
UNMAPPED	38	LYS	HD2	1.77	0.04	2
UNMAPPED	162	VAL	CG1	23.36	0.2	1
UNMAPPED	99	ILE	CA	61.02	0.2	1
UNMAPPED	16	ASP	N	120.42	0.2	1
UNMAPPED	87	MET	HA	4.34	0.04	1
UNMAPPED	38	LYS	CA	57.36	0.2	1
UNMAPPED	118	GLU	N	116.91	0.2	1
UNMAPPED	12	LEU	HD21	0.89	0.04	2
UNMAPPED	49	ASN	HB2	2.74	0.04	2
UNMAPPED	128	MET	HB3	1.86	0.04	2
UNMAPPED	91	LEU	HD12	0.8	0.04	2
UNMAPPED	50	CYS	HB3	2.21	0.04	2
UNMAPPED	155	ARG	H	8.0	0.04	1
UNMAPPED	167	ARG	CB	31.05	0.2	1
UNMAPPED	70	ILE	CD1	14.58	0.2	1
UNMAPPED	111	PHE	HD1	7.19	0.04	3
UNMAPPED	84	VAL	HG23	0.64	0.04	2
UNMAPPED	109	ARG	HA	3.95	0.04	1
UNMAPPED	86	LEU	HD12	0.82	0.04	2
UNMAPPED	119	ILE	H	9.32	0.04	1
UNMAPPED	124	LEU	H	8.82	0.04	1
UNMAPPED	74	LEU	CD1	22.98	0.2	1
UNMAPPED	78	VAL	C	175.44	0.2	1
UNMAPPED	86	LEU	HD22	0.8	0.04	2
UNMAPPED	86	LEU	CA	56.88	0.2	1
UNMAPPED	93	ALA	HB1	1.49	0.04	1
UNMAPPED	32	ARG	HB2	1.92	0.04	2
UNMAPPED	162	VAL	HB	1.81	0.04	1
UNMAPPED	81	ASP	HA	4.04	0.04	1
UNMAPPED	40	GLY	H	10.38	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	66	LEU	HB3	1.84	0.04	2
UNMAPPED	115	GLY	CA	47.21	0.2	1
UNMAPPED	118	GLU	CG	35.41	0.2	1
UNMAPPED	123	GLU	CG	36.18	0.2	1
UNMAPPED	132	LEU	CD1	22.48	0.2	1
UNMAPPED	29	GLU	HB2	2.16	0.04	2
UNMAPPED	38	LYS	HE2	2.99	0.04	2
UNMAPPED	160	GLU	HG2	2.97	0.04	2
UNMAPPED	109	ARG	H	7.7	0.04	1
UNMAPPED	34	PHE	HD1	7.55	0.04	3
UNMAPPED	52	ARG	CD	43.47	0.2	1
UNMAPPED	14	ARG	N	122.75	0.2	1
UNMAPPED	141	ILE	HD13	0.77	0.04	1
UNMAPPED	124	LEU	HD21	0.95	0.04	2
UNMAPPED	42	ILE	HB	1.94	0.04	1
UNMAPPED	57	MET	N	122.69	0.2	1
UNMAPPED	12	LEU	HD12	0.84	0.04	2
UNMAPPED	66	LEU	N	120.42	0.2	1
UNMAPPED	142	GLU	CA	59.03	0.2	1
UNMAPPED	154	GLY	C	173.36	0.2	1
UNMAPPED	161	PHE	CA	61.21	0.2	1
UNMAPPED	65	GLU	CA	59.85	0.2	1
UNMAPPED	90	LYS	N	114.73	0.2	1
UNMAPPED	126	GLU	N	116.81	0.2	1
UNMAPPED	160	GLU	CA	58.54	0.2	1
UNMAPPED	45	ARG	H	8.35	0.04	1
UNMAPPED	26	GLU	HG2	2.56	0.04	2
UNMAPPED	136	VAL	HG11	0.9	0.04	2
UNMAPPED	99	ILE	HG23	0.95	0.04	1
UNMAPPED	129	ARG	CB	29.59	0.2	1
UNMAPPED	96	ALA	CA	53.07	0.2	1
UNMAPPED	58	PRO	CB	31.9	0.2	1
UNMAPPED	37	ASP	HA	4.46	0.04	1
UNMAPPED	29	GLU	H	8.15	0.04	1
UNMAPPED	101	VAL	HB	2.15	0.04	1
UNMAPPED	32	ARG	N	116.11	0.2	1
UNMAPPED	27	LEU	HD22	0.77	0.04	2
UNMAPPED	83	PHE	C	176.68	0.2	1
UNMAPPED	86	LEU	C	178.5	0.2	1
UNMAPPED	141	ILE	HG23	0.93	0.04	1
UNMAPPED	110	GLU	CA	58.12	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	85	GLU	CB	29.39	0.2	1
UNMAPPED	148	VAL	CB	32.52	0.2	1
UNMAPPED	157	ASP	HB3	2.69	0.04	2
UNMAPPED	124	LEU	HG	1.61	0.04	1
UNMAPPED	121	THR	N	114.3	0.2	1
UNMAPPED	161	PHE	HB2	3.37	0.04	2
UNMAPPED	156	VAL	HA	5.09	0.04	1
UNMAPPED	124	LEU	CB	41.28	0.2	1
UNMAPPED	84	VAL	HG11	0.29	0.04	2
UNMAPPED	69	GLN	CG	33.46	0.2	1
UNMAPPED	44	CYS	HB2	2.98	0.04	2
UNMAPPED	122	SER	H	8.19	0.04	1
UNMAPPED	153	ASP	HA	4.51	0.04	1
UNMAPPED	142	GLU	C	179.28	0.2	1
UNMAPPED	42	ILE	HG13	0.96	0.04	1
UNMAPPED	100	GLY	H	8.48	0.04	1
UNMAPPED	145	ILE	CG2	17.38	0.2	1
UNMAPPED	165	MET	HB2	1.67	0.04	2
UNMAPPED	119	ILE	CD1	14.22	0.2	1
UNMAPPED	32	ARG	HA	3.97	0.04	1
UNMAPPED	96	ALA	C	177.46	0.2	1
UNMAPPED	40	GLY	HA2	4.11	0.04	2
UNMAPPED	86	LEU	N	117.47	0.2	1
UNMAPPED	166	SER	HA	4.52	0.04	1
UNMAPPED	158	PHE	HD1	6.6	0.04	3
UNMAPPED	157	ASP	CA	52.09	0.2	1
UNMAPPED	36	LYS	H	7.91	0.04	1
UNMAPPED	115	GLY	N	108.93	0.2	1
UNMAPPED	145	ILE	CD1	13.17	0.2	1
UNMAPPED	150	LEU	HD21	0.86	0.04	2
UNMAPPED	86	LEU	CD1	24.3	0.2	1
UNMAPPED	110	GLU	HG3	2.04	0.04	2
UNMAPPED	44	CYS	H	8.56	0.04	1
UNMAPPED	126	GLU	HA	4.12	0.04	1
UNMAPPED	43	ASN	CB	39.68	0.2	1
UNMAPPED	14	ARG	CA	56.42	0.2	1
UNMAPPED	127	ALA	HA	3.75	0.04	1
UNMAPPED	24	ILE	CD1	12.05	0.2	1
UNMAPPED	142	GLU	N	119.22	0.2	1
UNMAPPED	27	LEU	CD2	27.07	0.2	1
UNMAPPED	160	GLU	N	121.01	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	52	ARG	HA	4.4	0.04	1
UNMAPPED	15	LYS	CD	29.02	0.2	1
UNMAPPED	53	THR	HG23	1.55	0.04	1
UNMAPPED	112	ASP	HB2	2.6	0.04	2
UNMAPPED	88	GLY	H	8.31	0.04	1
UNMAPPED	159	GLU	HB3	2.14	0.04	2
UNMAPPED	51	MET	CG	33.46	0.2	1
UNMAPPED	141	ILE	CA	62.82	0.2	1
UNMAPPED	85	GLU	H	7.6	0.04	1
UNMAPPED	148	VAL	H	7.72	0.04	1
UNMAPPED	12	LEU	CD1	23.44	0.2	1
UNMAPPED	83	PHE	CB	39.72	0.2	1
UNMAPPED	136	VAL	CA	61.84	0.2	1
UNMAPPED	155	ARG	HD2	2.97	0.04	2
UNMAPPED	76	GLY	C	172.96	0.2	1
UNMAPPED	166	SER	CA	58.27	0.2	1
UNMAPPED	23	GLU	C	178.76	0.2	1
UNMAPPED	122	SER	CB	61.73	0.2	1
UNMAPPED	22	GLU	H	10.03	0.04	1
UNMAPPED	162	VAL	HG23	0.67	0.04	2
UNMAPPED	92	LEU	HB2	1.63	0.04	2
UNMAPPED	59	THR	HA	4.47	0.04	1
UNMAPPED	69	GLN	HG2	2.47	0.04	2
UNMAPPED	78	VAL	H	8.98	0.04	1
UNMAPPED	103	GLU	HB3	2.06	0.04	2
UNMAPPED	135	GLN	N	119.25	0.2	1
UNMAPPED	64	ILE	HD12	0.87	0.04	1
UNMAPPED	33	GLU	HB2	2.05	0.04	2
UNMAPPED	16	ASP	CB	41.25	0.2	1
UNMAPPED	158	PHE	HB3	2.43	0.04	2
UNMAPPED	142	GLU	HG3	2.05	0.04	2
UNMAPPED	88	GLY	HA2	4.17	0.04	2
UNMAPPED	119	ILE	HG21	0.89	0.04	1
UNMAPPED	49	ASN	C	177.49	0.2	1
UNMAPPED	124	LEU	HD13	0.9	0.04	2
UNMAPPED	132	LEU	H	8.22	0.04	1
UNMAPPED	36	LYS	CB	32.26	0.2	1
UNMAPPED	99	ILE	HG12	1.52	0.04	2
UNMAPPED	47	LEU	HG	1.7	0.04	1
UNMAPPED	99	ILE	HB	1.83	0.04	1
UNMAPPED	126	GLU	C	178.7	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	133	GLY	CA	45.89	0.2	1
UNMAPPED	24	ILE	HA	3.78	0.04	1
UNMAPPED	123	GLU	HG2	2.43	0.04	2
UNMAPPED	104	LEU	HB3	1.59	0.04	2
UNMAPPED	99	ILE	HD11	0.84	0.04	1
UNMAPPED	56	TYR	HE1	6.75	0.04	3
UNMAPPED	82	ASP	HB3	3.15	0.04	2
UNMAPPED	80	PHE	HA	3.29	0.04	1
UNMAPPED	159	GLU	HG2	2.31	0.04	2
UNMAPPED	141	ILE	C	176.78	0.2	1
UNMAPPED	97	ASP	C	176.06	0.2	1
UNMAPPED	47	LEU	C	178.57	0.2	1
UNMAPPED	153	ASP	HB3	2.41	0.04	2
UNMAPPED	58	PRO	HG2	0.97	0.04	2
UNMAPPED	148	VAL	HB	2.12	0.04	1
UNMAPPED	136	VAL	C	176.05	0.2	1
UNMAPPED	24	ILE	CG2	17.5	0.2	1
UNMAPPED	166	SER	C	173.13	0.2	1
UNMAPPED	133	GLY	H	7.72	0.04	1
UNMAPPED	26	GLU	CG	36.5	0.2	1
UNMAPPED	107	ALA	HB1	1.66	0.04	1
UNMAPPED	53	THR	CA	66.36	0.2	1
UNMAPPED	155	ARG	CG	25.94	0.2	1
UNMAPPED	149	ASP	HB2	2.93	0.04	2
UNMAPPED	65	GLU	HA	4.07	0.04	1
UNMAPPED	129	ARG	HG2	1.62	0.04	2
UNMAPPED	55	GLY	HA2	4.24	0.04	2
UNMAPPED	71	ASN	HB2	2.74	0.04	2
UNMAPPED	74	LEU	CB	42.9	0.2	1
UNMAPPED	82	ASP	H	8.68	0.04	1
UNMAPPED	91	LEU	C	179.03	0.2	1
UNMAPPED	13	SER	HA	4.43	0.04	1
UNMAPPED	18	SER	C	174.67	0.2	1
UNMAPPED	64	ILE	HG23	0.91	0.04	1
UNMAPPED	117	GLY	HA3	3.6	0.04	2
UNMAPPED	99	ILE	C	175.49	0.2	1
UNMAPPED	133	GLY	HA2	4.08	0.04	2
UNMAPPED	64	ILE	CD1	13.08	0.2	1
UNMAPPED	106	ASP	CB	39.74	0.2	1
UNMAPPED	66	LEU	HD11	0.86	0.04	2
UNMAPPED	115	GLY	H	7.62	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	103	GLU	CA	59.29	0.2	1
UNMAPPED	37	ASP	HB2	3.06	0.04	2
UNMAPPED	86	LEU	CD2	25.71	0.2	1
UNMAPPED	159	GLU	CB	28.67	0.2	1
UNMAPPED	78	VAL	HG11	0.99	0.04	2
UNMAPPED	141	ILE	HG13	1.3	0.04	2
UNMAPPED	15	LYS	C	176.15	0.2	1
UNMAPPED	78	VAL	CB	34.75	0.2	1
UNMAPPED	163	ARG	HA	3.88	0.04	1
UNMAPPED	136	VAL	N	119.69	0.2	1
UNMAPPED	127	ALA	C	179.96	0.2	1
UNMAPPED	18	SER	CB	64.5	0.2	1
UNMAPPED	89	PRO	HB2	1.69	0.04	2
UNMAPPED	86	LEU	HG	1.79	0.04	1
UNMAPPED	89	PRO	CA	65.16	0.2	1
UNMAPPED	25	GLU	CA	59.1	0.2	1
UNMAPPED	95	THR	N	113.59	0.2	1
UNMAPPED	97	ASP	CA	54.86	0.2	1
UNMAPPED	47	LEU	N	121.26	0.2	1
UNMAPPED	27	LEU	N	120.41	0.2	1
UNMAPPED	47	LEU	CA	58.77	0.2	1
UNMAPPED	55	GLY	N	105.41	0.2	1
UNMAPPED	110	GLU	HB3	1.93	0.04	2
UNMAPPED	116	ASP	C	177.57	0.2	1
UNMAPPED	19	LEU	CB	42.38	0.2	1
UNMAPPED	53	THR	C	175.58	0.2	1
UNMAPPED	95	THR	HG23	1.24	0.04	1
UNMAPPED	121	THR	CB	67.86	0.2	1
UNMAPPED	161	PHE	N	123.54	0.2	1
UNMAPPED	116	ASP	N	118.91	0.2	1
UNMAPPED	91	LEU	CA	57.22	0.2	1
UNMAPPED	128	MET	CA	57.1	0.2	1
UNMAPPED	18	SER	CA	57.75	0.2	1
UNMAPPED	135	GLN	HG2	2.22	0.04	2
UNMAPPED	28	ARG	HG3	1.13	0.04	2
UNMAPPED	150	LEU	HD11	0.96	0.04	2
UNMAPPED	31	PHE	HA	3.59	0.04	1
UNMAPPED	79	ASP	H	9.32	0.04	1
UNMAPPED	105	ARG	N	120.49	0.2	1
UNMAPPED	74	LEU	CD2	25.7	0.2	1
UNMAPPED	82	ASP	CB	41.39	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	61	MET	H	8.43	0.04	1
UNMAPPED	86	LEU	CB	43.02	0.2	1
UNMAPPED	101	VAL	HG23	1.02	0.04	2
UNMAPPED	30	ALA	H	7.8	0.04	1
UNMAPPED	16	ASP	HB2	2.65	0.04	2
UNMAPPED	55	GLY	CA	45.29	0.2	1
UNMAPPED	87	MET	C	178.62	0.2	1
UNMAPPED	100	GLY	CA	44.89	0.2	1
UNMAPPED	64	ILE	CG1	29.32	0.2	1
UNMAPPED	53	THR	N	116.94	0.2	1
UNMAPPED	21	PRO	HB3	2.45	0.04	2
UNMAPPED	118	GLU	CB	33.55	0.2	1
UNMAPPED	150	LEU	HB2	1.83	0.04	2
UNMAPPED	78	VAL	HA	5.01	0.04	1
UNMAPPED	103	GLU	HG2	2.5	0.04	2
UNMAPPED	13	SER	HB2	3.87	0.04	2
UNMAPPED	94	GLU	HA	4.4	0.04	1
UNMAPPED	42	ILE	HA	4.99	0.04	1
UNMAPPED	12	LEU	HD11	0.84	0.04	2
UNMAPPED	44	CYS	HA	3.93	0.04	1
UNMAPPED	142	GLU	CB	28.6	0.2	1
UNMAPPED	160	GLU	CB	29.41	0.2	1
UNMAPPED	160	GLU	HB2	2.57	0.04	2
UNMAPPED	15	LYS	HB2	1.76	0.04	2
UNMAPPED	112	ASP	N	118.84	0.2	1
UNMAPPED	163	ARG	N	119.54	0.2	1
UNMAPPED	129	ARG	CA	58.96	0.2	1
UNMAPPED	132	LEU	HD12	0.8	0.04	2
UNMAPPED	128	MET	C	178.18	0.2	1
UNMAPPED	104	LEU	HD12	0.82	0.04	2
UNMAPPED	24	ILE	HD11	0.82	0.04	1
UNMAPPED	83	PHE	N	122.09	0.2	1
UNMAPPED	121	THR	H	8.81	0.04	1
UNMAPPED	12	LEU	HB2	1.63	0.04	2
UNMAPPED	119	ILE	HG12	0.89	0.04	2
UNMAPPED	132	LEU	CG	26.78	0.2	1
UNMAPPED	122	SER	N	115.88	0.2	1
UNMAPPED	87	MET	HG2	1.83	0.04	2
UNMAPPED	167	ARG	HA	4.07	0.04	1
UNMAPPED	42	ILE	HD11	0.33	0.04	1
UNMAPPED	85	GLU	CA	59.16	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	94	GLU	CG	36.45	0.2	1
UNMAPPED	30	ALA	N	122.65	0.2	1
UNMAPPED	46	ASP	H	7.65	0.04	1
UNMAPPED	150	LEU	N	126.57	0.2	1
UNMAPPED	27	LEU	C	178.73	0.2	1
UNMAPPED	31	PHE	C	177.51	0.2	1
UNMAPPED	143	GLU	CG	36.16	0.2	1
UNMAPPED	156	VAL	CA	61.19	0.2	1
UNMAPPED	116	ASP	CA	53.07	0.2	1
UNMAPPED	131	LEU	CA	56.83	0.2	1
UNMAPPED	30	ALA	CB	18.41	0.2	1
UNMAPPED	51	MET	H	8.48	0.04	1
UNMAPPED	26	GLU	H	7.62	0.04	1
UNMAPPED	36	LYS	N	123.54	0.2	1
UNMAPPED	66	LEU	CD1	24.66	0.2	1
UNMAPPED	63	LEU	HD21	0.86	0.04	2
UNMAPPED	19	LEU	HB2	1.64	0.04	2
UNMAPPED	72	MET	HB2	2.14	0.04	2
UNMAPPED	67	SER	CB	62.36	0.2	1
UNMAPPED	146	ARG	CA	58.71	0.2	1
UNMAPPED	145	ILE	CG1	28.69	0.2	1
UNMAPPED	154	GLY	H	10.36	0.04	1
UNMAPPED	23	GLU	H	7.41	0.04	1
UNMAPPED	50	CYS	HA	3.45	0.04	1
UNMAPPED	113	THR	CA	64.89	0.2	1
UNMAPPED	141	ILE	CD1	12.62	0.2	1
UNMAPPED	144	ILE	CD1	13.65	0.2	1
UNMAPPED	151	ASN	HA	4.78	0.04	1
UNMAPPED	77	HIS	H	7.51	0.04	1
UNMAPPED	18	SER	N	115.44	0.2	1
UNMAPPED	160	GLU	H	8.64	0.04	1
UNMAPPED	100	GLY	N	112.75	0.2	1
UNMAPPED	164	MET	HB2	2.2	0.04	2
UNMAPPED	71	ASN	HA	4.33	0.04	1
UNMAPPED	150	LEU	HD22	0.86	0.04	2
UNMAPPED	144	ILE	CG1	28.81	0.2	1
UNMAPPED	126	GLU	HG2	2.37	0.04	2
UNMAPPED	33	GLU	CA	58.69	0.2	1
UNMAPPED	34	PHE	N	114.03	0.2	1
UNMAPPED	74	LEU	HD23	0.97	0.04	2
UNMAPPED	12	LEU	CG	26.72	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	87	MET	HB2	1.41	0.04	2
UNMAPPED	23	GLU	HB2	2.63	0.04	2
UNMAPPED	15	LYS	HG2	1.42	0.04	2
UNMAPPED	119	ILE	CA	59.42	0.2	1
UNMAPPED	17	ARG	HB2	1.88	0.04	2
UNMAPPED	108	PHE	N	118.83	0.2	1
UNMAPPED	163	ARG	CA	59.05	0.2	1
UNMAPPED	121	THR	CG2	22.66	0.2	1
UNMAPPED	106	ASP	N	120.04	0.2	1
UNMAPPED	98	MET	N	119.8	0.2	1
UNMAPPED	89	PRO	HA	4.18	0.04	1
UNMAPPED	122	SER	HA	4.19	0.04	1
UNMAPPED	12	LEU	CD2	25.31	0.2	1
UNMAPPED	91	LEU	HD22	0.78	0.04	2
UNMAPPED	41	TYR	HD1	6.66	0.04	3
UNMAPPED	41	TYR	CA	56.68	0.2	1
UNMAPPED	151	ASN	CA	51.39	0.2	1
UNMAPPED	68	GLN	CG	33.78	0.2	1
UNMAPPED	70	ILE	CA	64.64	0.2	1
UNMAPPED	112	ASP	H	7.52	0.04	1
UNMAPPED	127	ALA	N	121.67	0.2	1
UNMAPPED	42	ILE	CB	40.99	0.2	1
UNMAPPED	30	ALA	C	178.77	0.2	1
UNMAPPED	51	MET	HE3	1.72	0.04	1
UNMAPPED	80	PHE	H	8.47	0.04	1
UNMAPPED	146	ARG	CG	26.72	0.2	1
UNMAPPED	34	PHE	HZ	7.256	0.04	1
UNMAPPED	131	LEU	HD12	0.86	0.04	2
UNMAPPED	70	ILE	HD13	0.74	0.04	1
UNMAPPED	119	ILE	HG22	0.89	0.04	1
UNMAPPED	114	ASN	N	115.79	0.2	1
UNMAPPED	36	LYS	CA	59.27	0.2	1
UNMAPPED	36	LYS	HB2	1.83	0.04	2
UNMAPPED	80	PHE	HZ	7.217	0.04	1
UNMAPPED	92	LEU	HD13	0.73	0.04	2
UNMAPPED	99	ILE	HA	4.2	0.04	1
UNMAPPED	27	LEU	HG	1.99	0.04	1
UNMAPPED	54	MET	H	7.64	0.04	1
UNMAPPED	72	MET	N	117.1	0.2	1
UNMAPPED	34	PHE	CA	60.31	0.2	1
UNMAPPED	110	GLU	H	7.5	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	113	THR	N	118.41	0.2	1
UNMAPPED	144	ILE	H	7.56	0.04	1
UNMAPPED	49	ASN	CB	37.81	0.2	1
UNMAPPED	62	GLU	CG	36.73	0.2	1
UNMAPPED	80	PHE	HB3	2.44	0.04	2
UNMAPPED	155	ARG	CD	43.34	0.2	1
UNMAPPED	123	GLU	N	123.34	0.2	1
UNMAPPED	48	GLY	HA3	3.9	0.04	2
UNMAPPED	37	ASP	CA	52.86	0.2	1
UNMAPPED	28	ARG	H	8.97	0.04	1
UNMAPPED	76	GLY	H	8.17	0.04	1
UNMAPPED	17	ARG	HA	4.41	0.04	1
UNMAPPED	74	LEU	CA	54.65	0.2	1
UNMAPPED	47	LEU	HD21	1.04	0.04	2
UNMAPPED	54	MET	C	175.65	0.2	1
UNMAPPED	98	MET	CA	55.87	0.2	1
UNMAPPED	112	ASP	CB	38.64	0.2	1
UNMAPPED	45	ARG	HD2	3.2	0.04	2
UNMAPPED	87	MET	CG	32.0	0.2	1
UNMAPPED	125	ARG	HG2	1.49	0.04	2
UNMAPPED	71	ASN	C	176.91	0.2	1
UNMAPPED	104	LEU	HA	4.32	0.04	1
UNMAPPED	36	LYS	C	177.25	0.2	1
UNMAPPED	104	LEU	CA	58.04	0.2	1
UNMAPPED	55	GLY	H	7.76	0.04	1
UNMAPPED	41	TYR	N	116.11	0.2	1
UNMAPPED	63	LEU	HD13	0.83	0.04	2
UNMAPPED	38	LYS	H	7.76	0.04	1
UNMAPPED	56	TYR	HD1	6.98	0.04	3
UNMAPPED	89	PRO	CB	32.32	0.2	1
UNMAPPED	19	LEU	CD2	26.46	0.2	1
UNMAPPED	57	MET	HA	4.82	0.04	1
UNMAPPED	28	ARG	HB2	1.8	0.04	2
UNMAPPED	66	LEU	H	8.44	0.04	1
UNMAPPED	98	MET	HG2	2.61	0.04	2
UNMAPPED	60	GLU	CA	60.39	0.2	1
UNMAPPED	145	ILE	HD11	0.72	0.04	1
UNMAPPED	90	LYS	HA	4.0	0.04	1
UNMAPPED	127	ALA	CA	54.57	0.2	1
UNMAPPED	97	ASP	CB	41.13	0.2	1
UNMAPPED	108	PHE	HD1	6.57	0.04	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	119	ILE	HB	1.99	0.04	1
UNMAPPED	145	ILE	HG23	0.87	0.04	1
UNMAPPED	141	ILE	H	8.09	0.04	1
UNMAPPED	164	MET	C	177.5	0.2	1
UNMAPPED	34	PHE	HB3	2.94	0.04	2
UNMAPPED	38	LYS	CG	25.09	0.2	1
UNMAPPED	150	LEU	CB	42.27	0.2	1
UNMAPPED	145	ILE	C	177.15	0.2	1
UNMAPPED	162	VAL	CG2	21.13	0.2	1
UNMAPPED	38	LYS	HG2	1.38	0.04	2
UNMAPPED	40	GLY	CA	45.0	0.2	1
UNMAPPED	91	LEU	CB	41.98	0.2	1
UNMAPPED	128	MET	CB	31.44	0.2	1
UNMAPPED	19	LEU	C	177.54	0.2	1
UNMAPPED	97	ASP	HA	4.61	0.04	1
UNMAPPED	28	ARG	HD2	2.87	0.04	2
UNMAPPED	98	MET	C	176.22	0.2	1
UNMAPPED	94	GLU	H	8.12	0.02	1
UNMAPPED	67	SER	N	114.23	0.2	1
UNMAPPED	27	LEU	HB2	2.54	0.04	2
UNMAPPED	109	ARG	CB	29.85	0.2	1
UNMAPPED	137	GLY	HA2	3.96	0.04	2
UNMAPPED	108	PHE	C	176.82	0.2	1
UNMAPPED	86	LEU	CG	27.2	0.2	1
UNMAPPED	70	ILE	HG13	1.0	0.04	1
UNMAPPED	64	ILE	CG2	16.81	0.2	1
UNMAPPED	144	ILE	HA	3.75	0.04	1
UNMAPPED	153	ASP	CB	40.25	0.2	1
UNMAPPED	97	ASP	HB3	2.75	0.04	2
UNMAPPED	41	TYR	HB3	2.83	0.04	2
UNMAPPED	52	ARG	CB	30.32	0.2	1
UNMAPPED	119	ILE	HD13	0.24	0.04	1
UNMAPPED	156	VAL	HG21	0.81	0.04	2
UNMAPPED	142	GLU	CG	36.08	0.2	1
UNMAPPED	96	ALA	HB3	1.42	0.04	1
UNMAPPED	84	VAL	H	8.3	0.04	1
UNMAPPED	57	MET	CB	31.64	0.2	1
UNMAPPED	17	ARG	CD	43.58	0.2	1
UNMAPPED	25	GLU	HA	4.17	0.04	1
UNMAPPED	66	LEU	CB	42.52	0.2	1
UNMAPPED	12	LEU	HA	4.36	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	162	VAL	N	119.7	0.2	1
UNMAPPED	67	SER	C	176.24	0.2	1
UNMAPPED	90	LYS	CB	31.71	0.2	1
UNMAPPED	126	GLU	CB	29.25	0.2	1
UNMAPPED	103	GLU	HA	4.18	0.04	1
UNMAPPED	129	ARG	CD	43.27	0.2	1
UNMAPPED	104	LEU	N	121.93	0.2	1
UNMAPPED	40	GLY	C	173.3	0.2	1
UNMAPPED	150	LEU	CD2	25.04	0.2	1
UNMAPPED	160	GLU	C	179.58	0.2	1
UNMAPPED	144	ILE	HD11	0.78	0.04	1
UNMAPPED	148	VAL	CG1	23.61	0.2	1
UNMAPPED	136	VAL	HG21	0.92	0.04	2
UNMAPPED	45	ARG	CA	58.84	0.2	1
UNMAPPED	49	ASN	HA	4.49	0.04	1
UNMAPPED	160	GLU	CG	36.81	0.2	1
UNMAPPED	32	ARG	CB	30.44	0.2	1
UNMAPPED	42	ILE	N	119.02	0.2	1
UNMAPPED	94	GLU	CB	30.45	0.2	1
UNMAPPED	84	VAL	C	178.87	0.2	1
UNMAPPED	51	MET	HA	3.94	0.04	1
UNMAPPED	151	ASN	H	7.99	0.04	1
UNMAPPED	148	VAL	N	114.33	0.2	1
UNMAPPED	99	ILE	CB	38.85	0.2	1
UNMAPPED	143	GLU	CB	29.3	0.2	1
UNMAPPED	156	VAL	CB	32.59	0.2	1
UNMAPPED	69	GLN	CA	58.87	0.2	1
UNMAPPED	92	LEU	CG	27.0	0.2	1
UNMAPPED	109	ARG	C	178.3	0.2	1
UNMAPPED	56	TYR	CA	57.17	0.2	1
UNMAPPED	156	VAL	HG13	1.14	0.04	2
UNMAPPED	114	ASN	CB	37.01	0.2	1
UNMAPPED	42	ILE	CD1	13.74	0.2	1
UNMAPPED	112	ASP	HB3	1.73	0.04	2
UNMAPPED	91	LEU	HD13	0.8	0.04	2
UNMAPPED	167	ARG	CA	57.49	0.2	1
UNMAPPED	72	MET	CB	32.99	0.2	1
UNMAPPED	67	SER	CA	61.71	0.2	1
UNMAPPED	84	VAL	HG22	0.64	0.04	2
UNMAPPED	52	ARG	H	7.92	0.04	1
UNMAPPED	31	PHE	N	118.77	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	59	THR	CA	60.67	0.2	1
UNMAPPED	71	ASN	H	8.63	0.04	1
UNMAPPED	86	LEU	HD13	0.82	0.04	2
UNMAPPED	120	SER	CA	56.42	0.2	1
UNMAPPED	98	MET	HB2	2.07	0.04	2
UNMAPPED	84	VAL	CB	31.42	0.2	1
UNMAPPED	97	ASP	H	8.29	0.04	1
UNMAPPED	35	ASP	HB2	2.58	0.04	2
UNMAPPED	86	LEU	HD21	0.8	0.04	2
UNMAPPED	104	LEU	CD2	26.36	0.2	1
UNMAPPED	93	ALA	HB2	1.49	0.04	1
UNMAPPED	126	GLU	H	7.57	0.04	1
UNMAPPED	59	THR	HG21	1.38	0.04	1
UNMAPPED	127	ALA	HB3	0.73	0.04	1
UNMAPPED	34	PHE	H	7.34	0.04	1
UNMAPPED	132	LEU	CD2	25.7	0.2	1
UNMAPPED	74	LEU	HB2	2.36	0.04	2
UNMAPPED	157	ASP	N	127.84	0.2	1
UNMAPPED	147	ASP	H	7.63	0.04	1
UNMAPPED	74	LEU	HD13	0.96	0.04	2
UNMAPPED	161	PHE	HZ	7.02	0.04	1
UNMAPPED	93	ALA	C	177.96	0.2	1
UNMAPPED	102	LYS	H	8.41	0.04	1
UNMAPPED	106	ASP	HA	4.42	0.04	1
UNMAPPED	43	ASN	N	120.24	0.2	1
UNMAPPED	141	ILE	HD12	0.77	0.04	1
UNMAPPED	98	MET	HA	4.49	0.04	1
UNMAPPED	51	MET	HG2	2.95	0.04	2
UNMAPPED	108	PHE	HB3	3.12	0.04	2
UNMAPPED	131	LEU	HD23	0.96	0.04	2
UNMAPPED	158	PHE	H	8.8	0.04	1
UNMAPPED	164	MET	H	7.72	0.04	1
UNMAPPED	32	ARG	H	8.48	0.04	1
UNMAPPED	77	HIS	HB2	2.86	0.04	2
UNMAPPED	144	ILE	C	178.14	0.2	1
UNMAPPED	60	GLU	HB2	2.09	0.04	2
UNMAPPED	147	ASP	HB2	2.72	0.04	2
UNMAPPED	157	ASP	C	176.1	0.2	1
UNMAPPED	41	TYR	CB	42.83	0.2	1
UNMAPPED	151	ASN	CB	36.97	0.2	1
UNMAPPED	101	VAL	CG1	21.68	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	125	ARG	C	178.44	0.2	1
UNMAPPED	17	ARG	H	8.01	0.04	1
UNMAPPED	101	VAL	HA	3.92	0.04	1
UNMAPPED	114	ASN	H	8.05	0.04	1
UNMAPPED	26	GLU	HB2	2.31	0.04	2
UNMAPPED	120	SER	C	175.51	0.2	1
UNMAPPED	58	PRO	C	177.71	0.2	1
UNMAPPED	21	PRO	CG	27.23	0.2	1
UNMAPPED	27	LEU	HD23	0.77	0.04	2
UNMAPPED	141	ILE	HG22	0.93	0.04	1
UNMAPPED	72	MET	H	8.23	0.04	1
UNMAPPED	124	LEU	C	177.77	0.2	1
UNMAPPED	148	VAL	CA	52.65	0.2	1
UNMAPPED	79	ASP	HB2	2.51	0.04	2
UNMAPPED	133	GLY	N	107.32	0.2	1
UNMAPPED	161	PHE	HB3	3.11	0.04	2
UNMAPPED	136	VAL	H	7.92	0.04	1
UNMAPPED	84	VAL	HG12	0.29	0.04	2
UNMAPPED	61	MET	HB2	2.06	0.04	2
UNMAPPED	92	LEU	HA	4.17	0.04	1
UNMAPPED	60	GLU	H	8.87	0.04	1
UNMAPPED	149	ASP	N	119.31	0.2	1
UNMAPPED	130	LYS	N	118.31	0.2	1
UNMAPPED	150	LEU	HA	4.08	0.04	1
UNMAPPED	34	PHE	CB	39.97	0.2	1
UNMAPPED	42	ILE	HG12	1.25	0.04	1
UNMAPPED	59	THR	N	113.11	0.2	1
UNMAPPED	49	ASN	CA	55.86	0.2	1
UNMAPPED	105	ARG	HD2	2.74	0.04	2
UNMAPPED	123	GLU	C	180.41	0.2	1
UNMAPPED	161	PHE	H	8.86	0.04	1
UNMAPPED	26	GLU	CA	60.13	0.2	1
UNMAPPED	33	GLU	H	7.62	0.04	1
UNMAPPED	68	GLN	HB3	2.53	0.04	2
UNMAPPED	56	TYR	CD1	132.82	0.2	3
UNMAPPED	52	ARG	HB2	1.97	0.04	2
UNMAPPED	43	ASN	CA	51.59	0.2	1
UNMAPPED	105	ARG	H	8.7	0.04	1
UNMAPPED	47	LEU	HD22	1.04	0.04	2
UNMAPPED	31	PHE	H	8.64	0.04	1
UNMAPPED	20	ARG	H	9.67	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	77	HIS	CA	53.56	0.2	1
UNMAPPED	50	CYS	C	176.85	0.2	1
UNMAPPED	15	LYS	CE	42.25	0.2	1
UNMAPPED	150	LEU	C	178.44	0.2	1
UNMAPPED	103	GLU	CG	37.21	0.2	1
UNMAPPED	70	ILE	HA	3.73	0.04	1
UNMAPPED	162	VAL	C	179.12	0.2	1
UNMAPPED	125	ARG	HD2	3.18	0.04	2
UNMAPPED	159	GLU	N	117.94	0.2	1
UNMAPPED	60	GLU	HG2	2.38	0.04	2
UNMAPPED	31	PHE	HE1	6.925	0.04	3
UNMAPPED	134	HIS	C	175.08	0.2	1
UNMAPPED	89	PRO	CG	27.62	0.2	1
UNMAPPED	25	GLU	CG	35.68	0.2	1
UNMAPPED	136	VAL	CB	32.65	0.2	1
UNMAPPED	19	LEU	CD1	23.55	0.2	1
UNMAPPED	166	SER	CB	63.61	0.2	1
UNMAPPED	62	GLU	HG2	2.22	0.04	2
UNMAPPED	60	GLU	CB	29.45	0.2	1
UNMAPPED	15	LYS	HA	4.29	0.04	1
UNMAPPED	163	ARG	H	7.47	0.04	1
UNMAPPED	30	ALA	HB1	1.75	0.04	1
UNMAPPED	47	LEU	CG	29.1	0.2	1
UNMAPPED	125	ARG	CD	42.83	0.2	1
UNMAPPED	162	VAL	HG22	0.67	0.04	2
UNMAPPED	30	ALA	HB3	1.75	0.04	1
UNMAPPED	119	ILE	HA	4.95	0.04	1
UNMAPPED	78	VAL	HG21	1.13	0.04	2
UNMAPPED	27	LEU	CB	41.51	0.2	1
UNMAPPED	19	LEU	HD11	0.76	0.04	2
UNMAPPED	24	ILE	CA	64.59	0.2	1
UNMAPPED	43	ASN	HA	5.06	0.04	1
UNMAPPED	114	ASN	HA	4.81	0.04	1
UNMAPPED	64	ILE	HD13	0.87	0.04	1
UNMAPPED	162	VAL	CB	31.14	0.2	1
UNMAPPED	19	LEU	N	123.51	0.2	1
UNMAPPED	16	ASP	CA	54.38	0.2	1
UNMAPPED	165	MET	CG	31.56	0.2	1
UNMAPPED	142	GLU	HG2	2.27	0.04	2
UNMAPPED	147	ASP	C	177.26	0.2	1
UNMAPPED	70	ILE	H	8.63	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	47	LEU	HD13	0.92	0.04	2
UNMAPPED	128	MET	CG	32.9	0.2	1
UNMAPPED	50	CYS	CA	62.85	0.2	1
UNMAPPED	33	GLU	CB	28.96	0.2	1
UNMAPPED	141	ILE	CG2	18.17	0.2	1
UNMAPPED	95	THR	HB	4.33	0.04	1
UNMAPPED	135	GLN	CA	56.03	0.2	1
UNMAPPED	123	GLU	HG3	2.58	0.04	2
UNMAPPED	31	PHE	HB2	3.19	0.04	2
UNMAPPED	89	PRO	HD2	3.42	0.04	2
UNMAPPED	99	ILE	HD12	0.84	0.04	1
UNMAPPED	31	PHE	CB	40.28	0.2	1
UNMAPPED	64	ILE	C	178.86	0.2	1
UNMAPPED	102	LYS	HA	4.01	0.04	1
UNMAPPED	150	LEU	HB3	1.58	0.04	2
UNMAPPED	53	THR	CB	69.37	0.2	1
UNMAPPED	91	LEU	CD2	25.64	0.2	1
UNMAPPED	85	GLU	N	120.25	0.2	1
UNMAPPED	12	LEU	N	122.76	0.2	1
UNMAPPED	158	PHE	HA	3.73	0.04	1
UNMAPPED	71	ASN	HB3	2.91	0.04	2
UNMAPPED	77	HIS	N	116.69	0.2	1
UNMAPPED	66	LEU	HG	1.63	0.04	1
UNMAPPED	66	LEU	CG	27.17	0.2	1
UNMAPPED	118	GLU	HB3	1.84	0.04	2
UNMAPPED	90	LYS	CA	57.61	0.2	1
UNMAPPED	126	GLU	CG	35.51	0.2	1
UNMAPPED	66	LEU	HD12	0.86	0.04	2
UNMAPPED	54	MET	HA	4.58	0.04	1
UNMAPPED	144	ILE	CA	64.57	0.2	1
UNMAPPED	111	PHE	HA	4.43	0.04	1
UNMAPPED	28	ARG	CA	60.22	0.2	1
UNMAPPED	46	ASP	CA	56.41	0.2	1
UNMAPPED	39	ASP	HB2	1.73	0.04	2
UNMAPPED	68	GLN	N	120.68	0.2	1
UNMAPPED	39	ASP	CA	53.08	0.2	1
UNMAPPED	144	ILE	HD12	0.78	0.04	1
UNMAPPED	89	PRO	HB3	2.36	0.04	2
UNMAPPED	136	VAL	HG22	0.92	0.04	2
UNMAPPED	45	ARG	CD	43.71	0.2	1
UNMAPPED	98	MET	H	8.11	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	32	ARG	CA	59.27	0.2	1
UNMAPPED	74	LEU	HG	1.6	0.04	1
UNMAPPED	116	ASP	HA	4.53	0.04	1
UNMAPPED	121	THR	HG23	1.23	0.04	1
UNMAPPED	131	LEU	CD2	25.16	0.2	1
UNMAPPED	73	ASN	H	8.24	0.04	1
UNMAPPED	116	ASP	HB3	2.42	0.04	2
UNMAPPED	64	ILE	CA	65.62	0.2	1
UNMAPPED	24	ILE	N	119.96	0.2	1
UNMAPPED	12	LEU	HD22	0.89	0.04	2
UNMAPPED	110	GLU	HB2	2.03	0.04	2
UNMAPPED	83	PHE	HE1	7.494	0.04	3
UNMAPPED	19	LEU	HD23	0.74	0.04	2
UNMAPPED	131	LEU	CB	42.88	0.2	1
UNMAPPED	36	LYS	HA	3.94	0.04	1
UNMAPPED	121	THR	CA	67.04	0.2	1
UNMAPPED	37	ASP	H	7.94	0.04	1
UNMAPPED	56	TYR	CB	39.58	0.2	1
UNMAPPED	85	GLU	HG2	2.21	0.04	2
UNMAPPED	149	ASP	CB	38.91	0.2	1
UNMAPPED	127	ALA	H	7.86	0.04	1
UNMAPPED	130	LYS	CB	32.53	0.2	1
UNMAPPED	147	ASP	HA	4.47	0.04	1
UNMAPPED	64	ILE	HG13	1.15	0.04	1
UNMAPPED	135	GLN	HA	4.26	0.04	1
UNMAPPED	84	VAL	HG21	0.64	0.04	2
UNMAPPED	28	ARG	HG2	0.99	0.04	2
UNMAPPED	59	THR	CB	71.1	0.2	1
UNMAPPED	132	LEU	HD21	0.8	0.04	2
UNMAPPED	120	SER	CB	65.42	0.2	1
UNMAPPED	17	ARG	C	174.89	0.2	1
UNMAPPED	92	LEU	HD11	0.73	0.04	2
UNMAPPED	135	GLN	HB3	1.94	0.04	2
UNMAPPED	89	PRO	HG3	1.87	0.04	2
UNMAPPED	115	GLY	C	174.79	0.2	1
UNMAPPED	131	LEU	H	8.06	0.04	1
UNMAPPED	113	THR	HA	3.93	0.04	1
UNMAPPED	56	TYR	HA	4.56	0.04	1
UNMAPPED	47	LEU	HB3	1.58	0.04	2
UNMAPPED	144	ILE	HG13	1.04	0.04	1
UNMAPPED	20	ARG	HA	4.58	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	118	GLU	CA	53.64	0.2	1
UNMAPPED	108	PHE	HZ	7.29	0.04	1
UNMAPPED	145	ILE	HG12	1.55	0.04	1
UNMAPPED	103	GLU	HG3	2.32	0.04	2
UNMAPPED	124	LEU	HD23	0.95	0.04	2
UNMAPPED	113	THR	H	7.89	0.04	1
UNMAPPED	161	PHE	HE1	7.13	0.04	3
UNMAPPED	29	GLU	HA	4.06	0.04	1
UNMAPPED	29	GLU	CG	36.2	0.2	1
UNMAPPED	160	GLU	HB3	2.17	0.04	2
UNMAPPED	99	ILE	CG1	27.28	0.2	1
UNMAPPED	136	VAL	HG13	0.9	0.04	2
UNMAPPED	28	ARG	N	122.09	0.2	1
UNMAPPED	132	LEU	HD11	0.8	0.04	2
UNMAPPED	136	VAL	HB	2.06	0.04	1
UNMAPPED	35	ASP	H	7.86	0.04	1
UNMAPPED	76	GLY	N	104.55	0.2	1
UNMAPPED	39	ASP	N	117.4	0.2	1
UNMAPPED	104	LEU	HD13	0.82	0.04	2
UNMAPPED	24	ILE	HD12	0.82	0.04	1
UNMAPPED	153	ASP	HB2	3.08	0.04	2
UNMAPPED	166	SER	N	114.73	0.2	1
UNMAPPED	165	MET	HG2	1.87	0.04	2
UNMAPPED	149	ASP	H	7.97	0.04	1
UNMAPPED	110	GLU	C	178.25	0.2	1
UNMAPPED	27	LEU	HB3	1.7	0.04	2
UNMAPPED	145	ILE	H	8.04	0.04	1
UNMAPPED	144	ILE	HG21	0.85	0.04	1
UNMAPPED	141	ILE	HG21	0.93	0.04	1
UNMAPPED	123	GLU	HB3	2.32	0.04	2
UNMAPPED	159	GLU	CA	59.91	0.2	1
UNMAPPED	42	ILE	HD12	0.33	0.04	1
UNMAPPED	155	ARG	HA	4.83	0.04	1
UNMAPPED	84	VAL	HA	2.99	0.04	1
UNMAPPED	142	GLU	HB2	2.03	0.04	2
UNMAPPED	105	ARG	CD	42.63	0.2	1
UNMAPPED	152	GLY	HA2	3.8	0.04	2
UNMAPPED	30	ALA	CA	55.34	0.2	1
UNMAPPED	63	LEU	HD22	0.86	0.04	2
UNMAPPED	49	ASN	N	119.38	0.2	1
UNMAPPED	19	LEU	HB3	1.4	0.04	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	146	ARG	CB	29.91	0.2	1
UNMAPPED	102	LYS	HB2	1.79	0.04	2
UNMAPPED	14	ARG	H	8.23	0.04	1
UNMAPPED	81	ASP	H	7.6	0.04	1
UNMAPPED	113	THR	CB	68.62	0.2	1
UNMAPPED	33	GLU	HA	3.86	0.04	1
UNMAPPED	158	PHE	C	176.49	0.2	1
UNMAPPED	56	TYR	HB2	2.59	0.04	2
UNMAPPED	86	LEU	HB2	1.33	0.04	2
UNMAPPED	62	GLU	CA	58.97	0.2	1
UNMAPPED	164	MET	HB3	2.03	0.04	2
UNMAPPED	162	VAL	HG11	0.36	0.04	2
UNMAPPED	150	LEU	HD23	0.86	0.04	2
UNMAPPED	125	ARG	HB3	1.91	0.04	2
UNMAPPED	123	GLU	CB	29.27	0.2	1
UNMAPPED	144	ILE	CG2	17.3	0.2	1
UNMAPPED	154	GLY	HA2	4.12	0.04	2
UNMAPPED	22	GLU	CA	59.95	0.2	1
UNMAPPED	92	LEU	HD23	0.75	0.04	2
UNMAPPED	130	LYS	HG2	1.43	0.04	2
UNMAPPED	122	SER	C	177.72	0.2	1
UNMAPPED	43	ASN	HB3	2.9	0.04	2
UNMAPPED	79	ASP	CA	51.56	0.2	1
UNMAPPED	119	ILE	CB	37.71	0.2	1
UNMAPPED	81	ASP	HB3	2.74	0.04	2
UNMAPPED	118	GLU	HG2	2.06	0.04	2
UNMAPPED	17	ARG	HB3	1.76	0.04	2
UNMAPPED	70	ILE	HB	1.86	0.04	1
UNMAPPED	39	ASP	HA	4.7	0.04	1
UNMAPPED	54	MET	HG2	2.8	0.04	2
UNMAPPED	61	MET	C	178.52	0.2	1
UNMAPPED	145	ILE	CB	37.35	0.2	1
UNMAPPED	74	LEU	HB3	1.98	0.04	2
UNMAPPED	23	GLU	HG2	2.32	0.04	2
UNMAPPED	62	GLU	HB2	2.27	0.04	2
UNMAPPED	81	ASP	C	179.67	0.2	1
UNMAPPED	24	ILE	HG21	1.09	0.04	1
UNMAPPED	124	LEU	CD2	23.3	0.2	1
UNMAPPED	38	LYS	C	175.63	0.2	1
UNMAPPED	76	GLY	CA	45.75	0.2	1
UNMAPPED	132	LEU	HB3	1.35	0.04	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	102	LYS	CA	59.12	0.2	1
UNMAPPED	91	LEU	HD21	0.78	0.04	2
UNMAPPED	85	GLU	C	178.47	0.2	1
UNMAPPED	53	THR	HB	4.54	0.04	1
UNMAPPED	51	MET	C	178.08	0.2	1
UNMAPPED	150	LEU	CD1	21.64	0.2	1
UNMAPPED	58	PRO	CG	27.15	0.2	1
UNMAPPED	158	PHE	CA	62.22	0.2	1
UNMAPPED	162	VAL	HG21	0.67	0.04	2
UNMAPPED	48	GLY	CA	47.45	0.2	1
UNMAPPED	97	ASP	N	118.64	0.2	1
UNMAPPED	27	LEU	CA	58.48	0.2	1
UNMAPPED	19	LEU	HD12	0.76	0.04	2
UNMAPPED	51	MET	HE2	1.72	0.04	1
UNMAPPED	54	MET	CA	55.92	0.2	1
UNMAPPED	149	ASP	HA	4.69	0.04	1
UNMAPPED	81	ASP	CB	40.14	0.2	1
UNMAPPED	56	TYR	CE1	117.92	0.2	3
UNMAPPED	131	LEU	HD13	0.86	0.04	2
UNMAPPED	165	MET	CB	31.19	0.2	1
UNMAPPED	70	ILE	HD12	0.74	0.04	1
UNMAPPED	42	ILE	HG21	0.29	0.04	1
UNMAPPED	119	ILE	HG23	0.89	0.04	1
UNMAPPED	32	ARG	HG2	1.88	0.04	2
UNMAPPED	15	LYS	HE2	3.01	0.04	2
UNMAPPED	50	CYS	CB	26.31	0.2	1
UNMAPPED	141	ILE	CG1	28.78	0.2	1
UNMAPPED	92	LEU	HD12	0.73	0.04	2
UNMAPPED	91	LEU	N	119.38	0.2	1
UNMAPPED	105	ARG	HG2	1.39	0.04	2
UNMAPPED	18	SER	HA	4.53	0.04	1
UNMAPPED	113	THR	HG21	1.28	0.04	1
UNMAPPED	165	MET	HA	4.31	0.04	1
UNMAPPED	128	MET	HG3	2.55	0.04	2
UNMAPPED	95	THR	C	174.65	0.2	1
UNMAPPED	42	ILE	CG1	25.07	0.2	1
UNMAPPED	51	MET	CA	60.91	0.2	1
UNMAPPED	136	VAL	CG1	20.84	0.2	1
UNMAPPED	107	ALA	HB3	1.66	0.04	1
UNMAPPED	80	PHE	HB2	2.08	0.04	2
UNMAPPED	52	ARG	CG	28.85	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	91	LEU	CD1	23.72	0.2	1
UNMAPPED	48	GLY	HA2	3.65	0.04	2
UNMAPPED	22	GLU	N	116.66	0.2	1
UNMAPPED	108	PHE	HA	3.06	0.04	1
UNMAPPED	52	ARG	N	117.8	0.2	1
UNMAPPED	23	GLU	CG	37.84	0.2	1
UNMAPPED	148	VAL	HG23	0.96	0.04	2
UNMAPPED	46	ASP	HB2	2.62	0.04	2
UNMAPPED	15	LYS	CA	56.42	0.2	1
UNMAPPED	101	VAL	C	177.2	0.2	1
UNMAPPED	112	ASP	CA	51.95	0.2	1
UNMAPPED	125	ARG	HG3	1.63	0.04	2
UNMAPPED	76	GLY	HA2	4.2	0.04	2
UNMAPPED	104	LEU	CB	42.15	0.2	1
UNMAPPED	99	ILE	CD1	13.22	0.2	1
UNMAPPED	84	VAL	CG2	21.5	0.2	1
UNMAPPED	26	GLU	HA	4.19	0.04	1
UNMAPPED	20	ARG	CA	54.92	0.2	1
UNMAPPED	39	ASP	CB	41.09	0.02	1
UNMAPPED	63	LEU	HD12	0.83	0.04	2
UNMAPPED	13	SER	CA	58.65	0.2	1
UNMAPPED	45	ARG	CG	27.25	0.2	1
UNMAPPED	155	ARG	HB2	1.51	0.04	2
UNMAPPED	132	LEU	N	116.31	0.2	1
UNMAPPED	124	LEU	HB2	1.95	0.04	2
UNMAPPED	50	CYS	H	8.3	0.04	1
UNMAPPED	52	ARG	C	181.04	0.2	1
UNMAPPED	152	GLY	C	174.79	0.2	1
UNMAPPED	44	CYS	CB	26.85	0.2	1
UNMAPPED	61	MET	CG	32.39	0.2	1
UNMAPPED	95	THR	CA	62.08	0.2	1
UNMAPPED	142	GLU	HA	3.88	0.04	1
UNMAPPED	77	HIS	HA	5.14	0.04	1
UNMAPPED	82	ASP	C	178.35	0.2	1
UNMAPPED	145	ILE	HG22	0.87	0.04	1
UNMAPPED	120	SER	HB2	4.45	0.04	2
UNMAPPED	161	PHE	CB	39.56	0.2	1
UNMAPPED	92	LEU	N	118.11	0.2	1
UNMAPPED	94	GLU	N	118.94	0.2	1
UNMAPPED	131	LEU	HG	1.7	0.04	1
UNMAPPED	45	ARG	C	177.77	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	95	THR	HG21	1.24	0.04	1
UNMAPPED	123	GLU	HA	4.16	0.04	1
UNMAPPED	143	GLU	N	118.03	0.2	1
UNMAPPED	31	PHE	HD1	6.534	0.04	3
UNMAPPED	85	GLU	HA	3.92	0.04	1
UNMAPPED	164	MET	HG3	2.39	0.04	2
UNMAPPED	131	LEU	N	118.58	0.2	1
UNMAPPED	70	ILE	HG23	0.9	0.04	1
UNMAPPED	140	ASP	C	178.24	0.2	1
UNMAPPED	104	LEU	HD23	0.87	0.04	2
UNMAPPED	132	LEU	HA	4.36	0.04	1
UNMAPPED	150	LEU	HD13	0.96	0.04	2
UNMAPPED	101	VAL	CA	65.04	0.2	1
UNMAPPED	112	ASP	C	177.01	0.2	1
UNMAPPED	146	ARG	N	118.86	0.2	1
UNMAPPED	132	LEU	HD22	0.8	0.04	2
UNMAPPED	109	ARG	CA	58.54	0.2	1
UNMAPPED	101	VAL	HG21	1.02	0.04	2
UNMAPPED	80	PHE	C	176.38	0.2	1
UNMAPPED	84	VAL	N	120.09	0.2	1
UNMAPPED	129	ARG	H	7.82	0.04	1
UNMAPPED	46	ASP	C	177.42	0.2	1
UNMAPPED	54	MET	CG	32.44	0.2	1
UNMAPPED	22	GLU	HB2	2.05	0.04	2
UNMAPPED	159	GLU	HA	3.72	0.04	1
UNMAPPED	52	ARG	CA	59.74	0.2	1
UNMAPPED	74	LEU	C	177.89	0.2	1
UNMAPPED	156	VAL	HG22	0.81	0.04	2
UNMAPPED	39	ASP	H	8.43	0.04	1
UNMAPPED	111	PHE	C	176.61	0.2	1
UNMAPPED	119	ILE	N	126.63	0.2	1
UNMAPPED	63	LEU	N	119.24	0.2	1
UNMAPPED	96	ALA	HB2	1.42	0.04	1
UNMAPPED	29	GLU	CB	29.59	0.2	1
UNMAPPED	99	ILE	CG2	17.5	0.2	1
UNMAPPED	108	PHE	CA	61.22	0.2	1
UNMAPPED	129	ARG	CG	26.75	0.2	1
UNMAPPED	93	ALA	CA	53.17	0.2	1
UNMAPPED	136	VAL	HA	4.16	0.04	1
UNMAPPED	159	GLU	CG	36.64	0.2	1
UNMAPPED	20	ARG	N	123.72	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	109	ARG	HB2	1.91	0.04	2
UNMAPPED	151	ASN	N	112.52	0.2	1
UNMAPPED	75	GLY	H	7.98	0.04	1
UNMAPPED	58	PRO	HB2	1.94	0.04	2
UNMAPPED	96	ALA	N	125.55	0.2	1
UNMAPPED	21	PRO	CA	66.4	0.2	1
UNMAPPED	106	ASP	H	8.06	0.04	1
UNMAPPED	84	VAL	CG1	24.06	0.2	1
UNMAPPED	115	GLY	HA2	3.8	0.04	2
UNMAPPED	101	VAL	HG13	1.07	0.04	2
UNMAPPED	159	GLU	H	8.11	0.04	1
UNMAPPED	94	GLU	CA	56.88	0.2	1
UNMAPPED	156	VAL	C	175.53	0.2	1
UNMAPPED	63	LEU	CD1	22.93	0.2	1
UNMAPPED	71	ASN	N	119.79	0.2	1
UNMAPPED	19	LEU	CG	26.64	0.2	1
UNMAPPED	143	GLU	CA	58.78	0.2	1
UNMAPPED	84	VAL	HB	1.81	0.04	1
UNMAPPED	69	GLN	CB	28.5	0.2	1
UNMAPPED	131	LEU	HB2	1.75	0.04	2
UNMAPPED	12	LEU	HD23	0.89	0.04	2
UNMAPPED	35	ASP	HA	5.34	0.04	1
UNMAPPED	156	VAL	HG12	1.14	0.04	2
UNMAPPED	114	ASN	CA	51.53	0.2	1
UNMAPPED	146	ARG	C	177.77	0.2	1
UNMAPPED	165	MET	CA	54.48	0.2	1
UNMAPPED	148	VAL	C	176.71	0.2	1
UNMAPPED	107	ALA	HA	4.13	0.04	1
UNMAPPED	72	MET	CA	57.87	0.2	1
UNMAPPED	80	PHE	N	118.45	0.2	1
UNMAPPED	43	ASN	H	8.74	0.04	1
UNMAPPED	31	PHE	HZ	7.381	0.04	1
UNMAPPED	84	VAL	CA	67.46	0.2	1
UNMAPPED	47	LEU	CD1	26.44	0.2	1
UNMAPPED	35	ASP	HB3	1.74	0.04	2
UNMAPPED	104	LEU	CD1	24.0	0.2	1
UNMAPPED	93	ALA	HB3	1.49	0.04	1
UNMAPPED	59	THR	HG22	1.38	0.04	1
UNMAPPED	29	GLU	C	179.06	0.2	1
UNMAPPED	53	THR	CG2	21.75	0.2	1
UNMAPPED	127	ALA	HB2	0.73	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	123	GLU	CA	58.33	0.2	1
UNMAPPED	56	TYR	C	173.56	0.2	1
UNMAPPED	21	PRO	C	179.26	0.2	1
UNMAPPED	108	PHE	HE1	7.0	0.04	3
UNMAPPED	74	LEU	HD12	0.96	0.04	2
UNMAPPED	156	VAL	CG1	21.39	0.2	1
UNMAPPED	95	THR	CG2	21.86	0.2	1
UNMAPPED	83	PHE	H	8.62	0.04	1
UNMAPPED	79	ASP	CB	41.15	0.2	1
UNMAPPED	141	ILE	HD11	0.77	0.04	1
UNMAPPED	163	ARG	C	178.7	0.2	1
UNMAPPED	112	ASP	HA	4.53	0.04	1
UNMAPPED	94	GLU	C	176.9	0.2	1
UNMAPPED	61	MET	CB	31.83	0.2	1
UNMAPPED	86	LEU	H	7.86	0.04	1
UNMAPPED	108	PHE	HB2	2.88	0.04	2
UNMAPPED	131	LEU	HD22	0.96	0.04	2
UNMAPPED	65	GLU	CG	36.57	0.2	1
UNMAPPED	59	THR	C	175.13	0.2	1
UNMAPPED	106	ASP	HB2	2.79	0.04	2
UNMAPPED	99	ILE	HG21	0.95	0.04	1
UNMAPPED	161	PHE	C	176.35	0.2	1
UNMAPPED	24	ILE	HG22	1.09	0.04	1
UNMAPPED	87	MET	N	114.47	0.2	1
UNMAPPED	124	LEU	CD1	26.62	0.2	1
UNMAPPED	77	HIS	HB3	3.08	0.04	2
UNMAPPED	60	GLU	HB3	2.38	0.04	2
UNMAPPED	53	THR	HA	4.18	0.04	1
UNMAPPED	151	ASN	HB2	3.27	0.04	2
UNMAPPED	16	ASP	H	8.28	0.04	1
UNMAPPED	83	PHE	HB2	3.14	0.04	2
UNMAPPED	101	VAL	CG2	21.09	0.2	1
UNMAPPED	142	GLU	H	8.13	0.04	1
UNMAPPED	69	GLN	H	7.9	0.04	1
UNMAPPED	93	ALA	H	7.44	0.04	1
UNMAPPED	60	GLU	N	121.01	0.2	1
UNMAPPED	132	LEU	CB	42.4	0.2	1
UNMAPPED	143	GLU	HB2	2.12	0.04	2
UNMAPPED	153	ASP	C	177.73	0.2	1
UNMAPPED	44	CYS	N	117.54	0.2	1
UNMAPPED	92	LEU	C	177.44	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	137	GLY	CA	45.02	0.2	1
UNMAPPED	51	MET	HE1	1.72	0.04	1
UNMAPPED	47	LEU	CB	41.73	0.2	1
UNMAPPED	110	GLU	CG	36.16	0.2	1
UNMAPPED	154	GLY	N	113.01	0.2	1
UNMAPPED	34	PHE	HA	4.21	0.04	1
UNMAPPED	167	ARG	HB2	1.71	0.04	2
UNMAPPED	38	LYS	N	114.84	0.2	1
UNMAPPED	79	ASP	HB3	2.98	0.04	2
UNMAPPED	42	ILE	HG22	0.29	0.04	1
UNMAPPED	68	GLN	H	7.95	0.04	1
UNMAPPED	84	VAL	HG13	0.29	0.04	2
UNMAPPED	40	GLY	N	112.61	0.2	1
UNMAPPED	72	MET	HG2	2.64	0.04	2
UNMAPPED	33	GLU	N	118.22	0.2	1
UNMAPPED	74	LEU	H	7.61	0.04	1
UNMAPPED	113	THR	HG22	1.28	0.04	1
UNMAPPED	42	ILE	CG2	15.9	0.2	1
UNMAPPED	46	ASP	HA	4.65	0.04	1
UNMAPPED	51	MET	CB	32.85	0.2	1
UNMAPPED	136	VAL	CG2	21.63	0.2	1
UNMAPPED	26	GLU	CB	29.39	0.2	1
UNMAPPED	19	LEU	HG	1.7	0.04	1
UNMAPPED	154	GLY	CA	45.5	0.2	1
UNMAPPED	24	ILE	HG13	1.14	0.04	1
UNMAPPED	68	GLN	HB2	2.23	0.04	2
UNMAPPED	35	ASP	N	122.49	0.2	1
UNMAPPED	33	GLU	C	177.29	0.2	1
UNMAPPED	23	GLU	CB	30.31	0.2	1
UNMAPPED	74	LEU	CG	27.25	0.2	1
UNMAPPED	47	LEU	HD23	1.04	0.04	2
UNMAPPED	12	LEU	CB	42.39	0.2	1
UNMAPPED	162	VAL	CA	66.74	0.2	1
UNMAPPED	77	HIS	CB	31.98	0.2	1
UNMAPPED	53	THR	HG21	1.55	0.04	1
UNMAPPED	104	LEU	C	179.09	0.2	1
UNMAPPED	71	ASN	CB	38.04	0.2	1
UNMAPPED	92	LEU	CD1	23.03	0.2	1
UNMAPPED	104	LEU	HG	1.84	0.04	1
UNMAPPED	104	LEU	CG	27.67	0.2	1
UNMAPPED	19	LEU	H	8.51	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	27	LEU	HD12	0.75	0.04	2
UNMAPPED	42	ILE	C	174.59	0.2	1
UNMAPPED	63	LEU	HD11	0.83	0.04	2
UNMAPPED	78	VAL	N	115.3	0.2	1
UNMAPPED	89	PRO	CD	47.23	0.2	1
UNMAPPED	17	ARG	HG2	1.537	0.04	2
UNMAPPED	68	GLN	CB	28.12	0.2	1
UNMAPPED	43	ASN	C	175.78	0.2	1
UNMAPPED	67	SER	HA	4.19	0.04	1
UNMAPPED	145	ILE	HD13	0.72	0.04	1
UNMAPPED	28	ARG	C	178.75	0.2	1
UNMAPPED	143	GLU	HG2	2.24	0.04	2
UNMAPPED	75	GLY	HA3	3.95	0.04	2
UNMAPPED	44	CYS	CA	62.63	0.2	1
UNMAPPED	164	MET	CA	58.45	0.2	1
UNMAPPED	125	ARG	CG	27.83	0.2	1
UNMAPPED	95	THR	CB	69.99	0.2	1
UNMAPPED	30	ALA	HB2	1.75	0.04	1
UNMAPPED	126	GLU	HB2	2.05	0.04	2
UNMAPPED	78	VAL	HG22	1.13	0.04	2
UNMAPPED	87	MET	H	8.26	0.04	1
UNMAPPED	145	ILE	HG21	0.87	0.04	1
UNMAPPED	39	ASP	C	177.06	0.2	1
UNMAPPED	77	HIS	HD2	6.909	0.04	1
UNMAPPED	24	ILE	CB	36.99	0.2	1
UNMAPPED	100	GLY	HA3	3.99	0.04	2
UNMAPPED	144	ILE	N	119.67	0.2	1
UNMAPPED	34	PHE	HE1	7.45	0.04	3
UNMAPPED	121	THR	HB	4.19	0.04	1
UNMAPPED	55	GLY	C	173.32	0.2	1
UNMAPPED	69	GLN	N	119.11	0.2	1
UNMAPPED	124	LEU	HD11	0.9	0.04	2
UNMAPPED	56	TYR	N	121.71	0.2	1
UNMAPPED	47	LEU	HD12	0.92	0.04	2
UNMAPPED	113	THR	HB	4.19	0.04	1
UNMAPPED	42	ILE	H	9.37	0.04	1
UNMAPPED	95	THR	HA	4.4	0.04	1
UNMAPPED	101	VAL	CB	31.83	0.2	1
UNMAPPED	121	THR	C	175.51	0.2	1
UNMAPPED	89	PRO	HD3	3.53	0.04	2
UNMAPPED	99	ILE	HD13	0.84	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	80	PHE	CB	38.21	0.2	1
UNMAPPED	128	MET	N	115.21	0.2	1
UNMAPPED	109	ARG	CD	42.93	0.2	1
UNMAPPED	12	LEU	H	8.31	0.04	1
UNMAPPED	31	PHE	CA	62.35	0.2	1
UNMAPPED	120	SER	N	124.53	0.2	1
UNMAPPED	73	ASN	HA	4.98	0.04	1
UNMAPPED	16	ASP	C	175.64	0.2	1
UNMAPPED	117	GLY	CA	45.4	0.2	1
UNMAPPED	51	MET	CE	16.73	0.2	1
UNMAPPED	118	GLU	H	7.89	0.04	1
UNMAPPED	54	MET	CB	33.24	0.2	1
UNMAPPED	155	ARG	CA	53.47	0.2	1
UNMAPPED	114	ASN	HB3	2.87	0.04	2
UNMAPPED	153	ASP	N	118.91	0.2	1
UNMAPPED	119	ILE	HD11	0.24	0.04	1
UNMAPPED	152	GLY	H	7.7	0.04	1
UNMAPPED	96	ALA	HB1	1.42	0.04	1
UNMAPPED	51	MET	HB2	2.29	0.04	2
UNMAPPED	25	GLU	HG2	2.4	0.04	2
UNMAPPED	64	ILE	HG21	0.91	0.04	1
UNMAPPED	118	GLU	HB2	1.73	0.04	2
UNMAPPED	93	ALA	CB	19.13	0.2	1
UNMAPPED	66	LEU	HD13	0.86	0.04	2
UNMAPPED	41	TYR	HA	5.66	0.04	1
UNMAPPED	95	THR	H	8.02	0.04	1
UNMAPPED	87	MET	CB	31.85	0.2	1
UNMAPPED	68	GLN	HG2	2.56	0.04	2
UNMAPPED	78	VAL	HG13	0.99	0.04	2
UNMAPPED	141	ILE	N	121.9	0.2	1
UNMAPPED	63	LEU	HB3	1.88	0.04	2
UNMAPPED	24	ILE	H	7.8	0.04	1
UNMAPPED	46	ASP	CB	41.52	0.2	1
UNMAPPED	39	ASP	HB3	2.58	0.04	2
UNMAPPED	111	PHE	HB2	2.78	0.04	2
UNMAPPED	82	ASP	HA	4.35	0.04	1
UNMAPPED	145	ILE	HA	3.63	0.04	1
UNMAPPED	165	MET	H	7.62	0.04	1
UNMAPPED	144	ILE	HD13	0.78	0.04	1
UNMAPPED	65	GLU	H	8.01	0.04	1
UNMAPPED	73	ASN	CA	54.55	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	136	VAL	HG23	0.92	0.04	2
UNMAPPED	164	MET	N	119.2	0.2	1
UNMAPPED	121	THR	HG22	1.23	0.04	1
UNMAPPED	131	LEU	CD1	22.66	0.2	1
UNMAPPED	109	ARG	N	115.63	0.2	1
UNMAPPED	116	ASP	HB2	3.1	0.04	2
UNMAPPED	90	LYS	C	177.96	0.2	1
UNMAPPED	64	ILE	CB	38.05	0.2	1
UNMAPPED	96	ALA	H	8.3	0.04	1
UNMAPPED	101	VAL	H	8.16	0.04	1
UNMAPPED	117	GLY	C	173.18	0.2	1
UNMAPPED	135	GLN	CG	33.5	0.2	1
UNMAPPED	67	SER	H	8.27	0.04	1
UNMAPPED	63	LEU	CD2	25.13	0.2	1
UNMAPPED	19	LEU	HD22	0.74	0.04	2
UNMAPPED	162	VAL	H	8.52	0.04	1
UNMAPPED	38	LYS	CB	29.35	0.2	1
UNMAPPED	135	GLN	C	175.99	0.2	1
UNMAPPED	105	ARG	CA	59.36	0.2	1
UNMAPPED	156	VAL	HG11	1.14	0.04	2
UNMAPPED	128	MET	HB2	2.14	0.04	2
UNMAPPED	149	ASP	CA	52.81	0.2	1
UNMAPPED	130	LYS	CA	58.66	0.2	1
UNMAPPED	18	SER	HB2	3.81	0.04	2
UNMAPPED	137	GLY	H	8.64	0.04	1
UNMAPPED	50	CYS	HB2	2.67	0.04	2
UNMAPPED	64	ILE	HG12	1.78	0.04	1
UNMAPPED	65	GLU	C	179.58	0.2	1
UNMAPPED	150	LEU	H	7.8	0.04	1
UNMAPPED	74	LEU	HD21	0.97	0.04	2
UNMAPPED	135	GLN	HB2	2.05	0.04	2
UNMAPPED	89	PRO	HG2	2.05	0.04	2
UNMAPPED	86	LEU	HD23	0.8	0.04	2
UNMAPPED	117	GLY	N	112.67	0.2	1
UNMAPPED	92	LEU	H	7.86	0.04	1
UNMAPPED	163	ARG	HB2	1.82	0.04	2
UNMAPPED	128	MET	H	8.33	0.04	1
UNMAPPED	47	LEU	HB2	1.96	0.04	2
UNMAPPED	66	LEU	HB2	1.54	0.04	2
UNMAPPED	144	ILE	HG12	1.7	0.04	1
UNMAPPED	127	ALA	HB1	0.73	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	73	ASN	C	176.23	0.2	1
UNMAPPED	66	LEU	C	178.73	0.2	1
UNMAPPED	74	LEU	HD11	0.96	0.04	2
UNMAPPED	160	GLU	HG3	2.33	0.04	2
UNMAPPED	80	PHE	HE1	7.071	0.04	3
UNMAPPED	145	ILE	HG13	1.12	0.04	1
UNMAPPED	125	ARG	HA	3.66	0.04	1
UNMAPPED	23	GLU	N	120.78	0.2	1
UNMAPPED	124	LEU	HD22	0.95	0.04	2
UNMAPPED	159	GLU	C	180.53	0.2	1
UNMAPPED	41	TYR	CD1	133.13	0.2	3
UNMAPPED	12	LEU	HD13	0.84	0.04	2
UNMAPPED	131	LEU	HD21	0.96	0.04	2
UNMAPPED	65	GLU	CB	29.42	0.2	1
UNMAPPED	21	PRO	HA	4.23	0.04	1
UNMAPPED	17	ARG	CA	55.42	0.2	1
UNMAPPED	136	VAL	HG12	0.9	0.04	2
UNMAPPED	99	ILE	HG22	0.95	0.04	1
UNMAPPED	103	GLU	N	119.4	0.2	1
UNMAPPED	145	ILE	N	116.77	0.2	1
UNMAPPED	79	ASP	C	176.47	0.2	1
UNMAPPED	64	ILE	H	8.17	0.04	1
UNMAPPED	96	ALA	CB	19.44	0.2	1
UNMAPPED	67	SER	HB2	3.93	0.04	2
UNMAPPED	130	LYS	C	178.52	0.2	1
UNMAPPED	129	ARG	C	178.91	0.2	1
UNMAPPED	83	PHE	HZ	7.317	0.04	1
UNMAPPED	118	GLU	C	174.24	0.2	1
UNMAPPED	24	ILE	HD13	0.82	0.04	1
UNMAPPED	58	PRO	CA	62.08	0.2	1
UNMAPPED	25	GLU	N	118.26	0.2	1
UNMAPPED	73	ASN	N	114.33	0.2	1
UNMAPPED	108	PHE	H	8.42	0.04	1
UNMAPPED	148	VAL	HG13	0.97	0.04	2
UNMAPPED	27	LEU	HD21	0.77	0.04	2
UNMAPPED	107	ALA	CB	17.64	0.2	1
UNMAPPED	144	ILE	HG22	0.85	0.04	1
UNMAPPED	123	GLU	HB2	2.5	0.04	2
UNMAPPED	110	GLU	CB	28.99	0.2	1
UNMAPPED	42	ILE	HD13	0.33	0.04	1
UNMAPPED	61	MET	HG2	2.65	0.04	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	157	ASP	HB2	3.3	0.04	2
UNMAPPED	144	ILE	CB	38.41	0.2	1
UNMAPPED	81	ASP	N	118.16	0.2	1
UNMAPPED	128	MET	HA	4.22	0.04	1
UNMAPPED	156	VAL	HB	2.23	0.04	1
UNMAPPED	146	ARG	HB2	1.88	0.04	2
UNMAPPED	92	LEU	HG	1.6	0.04	1
UNMAPPED	48	GLY	C	175.51	0.2	1
UNMAPPED	165	MET	N	114.48	0.2	1
UNMAPPED	44	CYS	HB3	2.88	0.04	2
UNMAPPED	92	LEU	CB	41.99	0.2	1
UNMAPPED	119	ILE	CG1	27.73	0.2	1
UNMAPPED	125	ARG	H	8.31	0.04	1
UNMAPPED	16	ASP	HA	4.6	0.04	1
UNMAPPED	50	CYS	N	123.47	0.2	1
UNMAPPED	103	GLU	HB2	2.24	0.04	2
UNMAPPED	63	LEU	HD23	0.86	0.04	2
UNMAPPED	165	MET	HB3	1.55	0.04	2
UNMAPPED	102	LYS	HB3	1.89	0.04	2
UNMAPPED	105	ARG	CG	26.63	0.2	1
UNMAPPED	143	GLU	H	7.59	0.04	1
UNMAPPED	40	GLY	HA3	3.52	0.04	2
UNMAPPED	56	TYR	HB3	2.84	0.04	2
UNMAPPED	156	VAL	H	9.39	0.04	1
UNMAPPED	86	LEU	HB3	1.71	0.04	2
UNMAPPED	85	GLU	HB2	2.12	0.04	2
UNMAPPED	62	GLU	CB	30.04	0.2	1
UNMAPPED	92	LEU	HD22	0.75	0.04	2
UNMAPPED	38	LYS	HB2	1.96	0.04	2
UNMAPPED	162	VAL	HG12	0.36	0.04	2
UNMAPPED	35	ASP	C	179.17	0.2	1
UNMAPPED	125	ARG	HB2	1.98	0.04	2
UNMAPPED	110	GLU	HG2	2.27	0.04	2
UNMAPPED	96	ALA	HA	4.32	0.04	1
UNMAPPED	158	PHE	HE1	7.05	0.04	3
UNMAPPED	165	MET	C	176.94	0.2	1
UNMAPPED	23	GLU	CA	58.79	0.2	1
UNMAPPED	154	GLY	HA3	3.48	0.04	2
UNMAPPED	22	GLU	CB	28.11	0.2	1
UNMAPPED	12	LEU	CA	55.73	0.2	1
UNMAPPED	94	GLU	HG2	2.36	0.04	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	43	ASN	HB2	3.28	0.04	2
UNMAPPED	81	ASP	HB2	2.57	0.04	2
UNMAPPED	69	GLN	HB2	2.24	0.04	2
UNMAPPED	17	ARG	N	119.42	0.2	1
UNMAPPED	53	THR	HG22	1.55	0.04	1
UNMAPPED	49	ASN	H	7.79	0.04	1
UNMAPPED	119	ILE	C	175.56	0.2	1
UNMAPPED	129	ARG	N	119.22	0.2	1
UNMAPPED	92	LEU	CD2	25.29	0.2	1
UNMAPPED	107	ALA	H	8.0	0.04	1
UNMAPPED	145	ILE	CA	64.26	0.2	1
UNMAPPED	62	GLU	C	179.42	0.2	1
UNMAPPED	62	GLU	HB3	2.0	0.04	2
UNMAPPED	159	GLU	HB2	2.02	0.04	2
UNMAPPED	141	ILE	CB	36.94	0.2	1
UNMAPPED	27	LEU	HD11	0.75	0.04	2
UNMAPPED	102	LYS	CB	32.05	0.2	1
UNMAPPED	83	PHE	CA	61.23	0.2	1
UNMAPPED	68	GLN	CA	58.96	0.2	1
UNMAPPED	73	ASN	HB2	2.89	0.04	2
UNMAPPED	65	GLU	HG2	2.37	0.04	2
UNMAPPED	63	LEU	HA	4.12	0.04	1
UNMAPPED	122	SER	CA	61.73	0.2	1
UNMAPPED	158	PHE	CB	38.49	0.2	1
UNMAPPED	91	LEU	H	7.67	0.04	1
UNMAPPED	164	MET	CB	32.41	0.2	1
UNMAPPED	125	ARG	CB	30.01	0.2	1
UNMAPPED	17	ARG	HD2	3.118	0.04	2
UNMAPPED	59	THR	HB	4.73	0.04	1
UNMAPPED	22	GLU	HG2	2.41	0.04	2
UNMAPPED	19	LEU	HD13	0.76	0.04	2
UNMAPPED	64	ILE	N	123.5	0.2	1
UNMAPPED	23	GLU	HA	4.25	0.04	1
UNMAPPED	131	LEU	HA	4.23	0.04	1
UNMAPPED	35	ASP	CA	52.47	0.2	1
UNMAPPED	64	ILE	HD11	0.87	0.04	1
UNMAPPED	150	LEU	CG	26.45	0.2	1
UNMAPPED	41	TYR	H	8.2	0.04	1
UNMAPPED	81	ASP	CA	57.94	0.2	1
UNMAPPED	124	LEU	HA	3.95	0.04	1
UNMAPPED	158	PHE	HB2	2.66	0.04	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	118	GLU	HA	4.91	0.04	1
UNMAPPED	13	SER	H	8.25	0.04	1
UNMAPPED	70	ILE	HD11	0.74	0.04	1
UNMAPPED	25	GLU	H	8.11	0.04	1
UNMAPPED	88	GLY	HA3	3.59	0.04	2
UNMAPPED	62	GLU	H	7.89	0.04	1
UNMAPPED	102	LYS	C	178.11	0.2	1
UNMAPPED	124	LEU	HD12	0.9	0.04	2
UNMAPPED	32	ARG	HG3	1.72	0.04	2
UNMAPPED	99	ILE	HG13	1.2	0.04	2
UNMAPPED	27	LEU	HA	4.45	0.04	1
UNMAPPED	104	LEU	HB2	2.25	0.04	2
UNMAPPED	109	ARG	CG	27.15	0.2	1
UNMAPPED	153	ASP	H	8.0	0.04	1
UNMAPPED	82	ASP	HB2	2.53	0.04	2
UNMAPPED	152	GLY	N	109.37	0.2	1
UNMAPPED	57	MET	H	8.08	0.04	1
UNMAPPED	33	GLU	HG2	1.94	0.04	2
UNMAPPED	128	MET	HG2	2.63	0.04	2
UNMAPPED	90	LYS	H	7.07	0.04	1
UNMAPPED	88	GLY	CA	49.15	0.2	1
UNMAPPED	68	GLN	C	178.34	0.2	1
UNMAPPED	107	ALA	HB2	1.66	0.04	1
UNMAPPED	149	ASP	HB3	2.22	0.04	2
UNMAPPED	141	ILE	HA	3.78	0.04	1
UNMAPPED	55	GLY	HA3	3.63	0.04	2
UNMAPPED	157	ASP	HA	5.11	0.04	1
UNMAPPED	129	ARG	HA	3.99	0.04	1
UNMAPPED	148	VAL	HG22	0.96	0.04	2
UNMAPPED	46	ASP	HB3	2.8	0.04	2
UNMAPPED	75	GLY	CA	46.55	0.2	1
UNMAPPED	64	ILE	HG22	0.91	0.04	1
UNMAPPED	63	LEU	CB	41.3	0.2	1
UNMAPPED	29	GLU	N	118.95	0.2	1
UNMAPPED	133	GLY	HA3	3.83	0.04	2
UNMAPPED	22	GLU	HA	4.2	0.04	1
UNMAPPED	106	ASP	CA	56.97	0.2	1
UNMAPPED	15	LYS	CB	32.92	0.2	1
UNMAPPED	98	MET	CG	32.07	0.2	1
UNMAPPED	108	PHE	CB	39.31	0.2	1
UNMAPPED	58	PRO	HA	4.69	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	103	GLU	CB	28.84	0.2	1
UNMAPPED	48	GLY	H	8.34	0.04	1
UNMAPPED	28	ARG	CB	29.82	0.2	1
UNMAPPED	28	ARG	CG	27.05	0.2	1
UNMAPPED	141	ILE	HG12	1.46	0.04	2
UNMAPPED	28	ARG	HA	3.74	0.04	1
UNMAPPED	76	GLY	HA3	3.7	0.04	2
UNMAPPED	20	ARG	CB	29.79	0.2	1
UNMAPPED	145	ILE	HB	1.93	0.04	1
UNMAPPED	13	SER	CB	64.05	0.2	1
UNMAPPED	25	GLU	CB	28.85	0.2	1
UNMAPPED	73	ASN	CB	40.15	0.2	1
UNMAPPED	70	ILE	N	119.82	0.2	1
UNMAPPED	60	GLU	CG	36.52	0.2	1
UNMAPPED	27	LEU	HD13	0.75	0.04	2
UNMAPPED	124	LEU	HB3	1.51	0.04	2
UNMAPPED	32	ARG	CG	27.74	0.2	1
UNMAPPED	14	ARG	HA	4.06	0.04	1
UNMAPPED	121	THR	HG21	1.23	0.04	1
UNMAPPED	107	ALA	N	123.03	0.2	1
UNMAPPED	153	ASP	CA	53.07	0.2	1
UNMAPPED	135	GLN	CB	28.93	0.2	1
UNMAPPED	103	GLU	C	179.87	0.2	1
UNMAPPED	120	SER	HB3	4.01	0.04	2
UNMAPPED	38	LYS	CE	41.14	0.2	1
UNMAPPED	95	THR	HG22	1.24	0.04	1
UNMAPPED	100	GLY	C	174.14	0.2	1
UNMAPPED	15	LYS	HD2	1.68	0.04	2
UNMAPPED	29	GLU	HG2	2.415	0.04	2
UNMAPPED	166	SER	H	7.5	0.04	1
UNMAPPED	69	GLN	HA	4.12	0.04	1
UNMAPPED	54	MET	HB2	2.4	0.04	2
UNMAPPED	164	MET	HG2	2.29	0.04	2
UNMAPPED	110	GLU	HA	3.87	0.04	1
UNMAPPED	75	GLY	C	175.62	0.2	1
UNMAPPED	72	MET	CG	32.09	0.2	1
UNMAPPED	70	ILE	HG22	0.9	0.04	1
UNMAPPED	33	GLU	CG	35.6	0.2	1
UNMAPPED	104	LEU	HD22	0.87	0.04	2
UNMAPPED	150	LEU	HG	1.75	0.04	1
UNMAPPED	47	LEU	HA	3.81	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	147	ASP	CB	41.47	0.2	1
UNMAPPED	106	ASP	C	178.59	0.2	1
UNMAPPED	150	LEU	HD12	0.96	0.04	2
UNMAPPED	152	GLY	CA	47.1	0.2	1
UNMAPPED	132	LEU	HD23	0.8	0.04	2
UNMAPPED	46	ASP	N	117.7	0.2	1
UNMAPPED	111	PHE	HE1	7.3	0.04	3
UNMAPPED	114	ASN	C	176.66	0.2	1
UNMAPPED	82	ASP	CA	57.41	0.2	1
UNMAPPED	161	PHE	HD1	6.89	0.04	3
UNMAPPED	107	ALA	C	178.32	0.2	1
UNMAPPED	101	VAL	HG22	1.02	0.04	2
UNMAPPED	116	ASP	H	8.0	0.04	1
UNMAPPED	63	LEU	H	8.01	0.04	1
UNMAPPED	62	GLU	N	121.06	0.2	1
UNMAPPED	88	GLY	N	108.31	0.2	1
UNMAPPED	21	PRO	HB2	2.02	0.04	2
UNMAPPED	129	ARG	HD2	2.78	0.04	2
UNMAPPED	103	GLU	H	8.37	0.04	1
UNMAPPED	64	ILE	HB	2.03	0.04	1
UNMAPPED	146	ARG	HA	4.06	0.04	1
UNMAPPED	70	ILE	CG2	17.6	0.2	1
UNMAPPED	78	VAL	HB	2.47	0.04	1
UNMAPPED	111	PHE	CB	39.08	0.2	1
UNMAPPED	74	LEU	N	118.97	0.2	1
UNMAPPED	156	VAL	HG23	0.81	0.04	2
UNMAPPED	143	GLU	HG3	2.37	0.04	2
UNMAPPED	75	GLY	N	107.26	0.2	1
UNMAPPED	79	ASP	N	126.73	0.2	1
UNMAPPED	59	THR	CG2	22.03	0.2	1
UNMAPPED	29	GLU	CA	59.11	0.2	1
UNMAPPED	61	MET	N	116.6	0.2	1
UNMAPPED	17	ARG	CB	30.81	0.2	1
UNMAPPED	83	PHE	HA	4.07	0.04	1
UNMAPPED	157	ASP	CB	41.62	0.2	1
UNMAPPED	53	THR	H	8.16	0.04	1
UNMAPPED	47	LEU	H	8.17	0.04	1
UNMAPPED	132	LEU	HD13	0.8	0.04	2
UNMAPPED	68	GLN	HA	4.15	0.04	1
UNMAPPED	122	SER	HB2	3.9	0.04	2
UNMAPPED	135	GLN	H	8.2	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	131	LEU	C	178.52	0.2	1
UNMAPPED	104	LEU	HD11	0.82	0.04	2
UNMAPPED	102	LYS	N	122.15	0.2	1
UNMAPPED	160	GLU	HA	3.97	0.04	1
UNMAPPED	58	PRO	HB3	2.18	0.04	2
UNMAPPED	113	THR	CG2	22.53	0.2	1
UNMAPPED	119	ILE	HG13	0.39	0.04	2
UNMAPPED	86	LEU	HA	4.12	0.04	1
UNMAPPED	21	PRO	CB	31.8	0.2	1
UNMAPPED	18	SER	H	8.14	0.04	1
UNMAPPED	158	PHE	N	118.46	0.2	1
UNMAPPED	107	ALA	CA	54.64	0.2	1
UNMAPPED	125	ARG	N	118.96	0.2	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	152	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	139	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	144	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	147	0.00 \pm 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 866. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/335 (0%)	0/134 (0%)	0/134 (0%)	0/67 (0%)
Sidechain	0/481 (0%)	0/280 (0%)	0/169 (0%)	0/32 (0%)
Aromatic	0/50 (0%)	0/28 (0%)	0/20 (0%)	0/2 (0%)
Overall	0/866 (0%)	0/442 (0%)	0/323 (0%)	0/101 (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 914. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/360 (0%)	0/144 (0%)	0/144 (0%)	0/72 (0%)
Sidechain	0/504 (0%)	0/293 (0%)	0/179 (0%)	0/32 (0%)
Aromatic	0/50 (0%)	0/28 (0%)	0/20 (0%)	0/2 (0%)
Overall	0/914 (0%)	0/465 (0%)	0/343 (0%)	0/106 (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.