Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1JRU
Title	:	NMR STRUCTURE OF THE UBX DOMAIN FROM P47 (ENERGY MINIMISED AVERAGE)
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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:

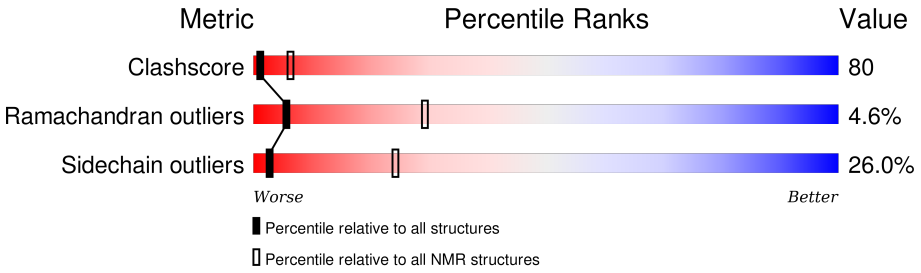
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 is 74%.

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	89	21% 56% 21%

2 Ensemble composition and analysis

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 1414 atoms, of which 719 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called p47 protein.

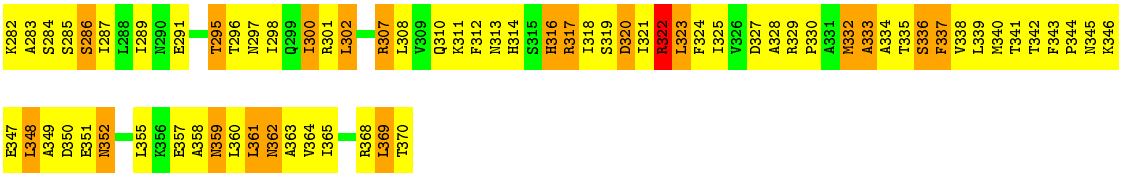
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1414	435	719	126	132	2	0

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: p47 protein

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing.*

Of the ? calculated structures, 1 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.853
X-PLOR	refinement	3.853

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 5155, BMRB entry 5874, BMRB entry 5876
Number of chemical shift lists	3
Total number of shifts	3998
Number of shifts mapped to atoms	1821
Number of unparsed shifts	0
Number of shifts with mapping errors	2177
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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	5
All	All	0	5

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	317	ARG	Sidechain
1	A	322	ARG	Sidechain
1	A	368	ARG	Sidechain
1	A	307	ARG	Sidechain
1	A	301	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	695	719	716	113
All	All	695	719	716	113

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 80.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:302:LEU:HD12	1:A:369:LEU:HD23	0.97	1.33
1:A:314:HIS:CD2	1:A:361:LEU:HD11	0.81	2.11
1:A:295:THR:HG22	1:A:313:ASN:HA	0.76	1.55
1:A:332:MET:SD	1:A:369:LEU:HD21	0.75	2.22
1:A:339:LEU:HD12	1:A:340:MET:N	0.72	1.99
1:A:302:LEU:CD1	1:A:369:LEU:HD23	0.72	2.12
1:A:287:ILE:HG22	1:A:311:LYS:O	0.67	1.90
1:A:339:LEU:HD11	1:A:365:ILE:CG2	0.67	2.19
1:A:362:ASN:O	1:A:363:ALA:HB3	0.66	1.89
1:A:348:LEU:HD23	1:A:349:ALA:N	0.66	2.06
1:A:329:ARG:N	1:A:330:PRO:CD	0.61	2.63
1:A:300:ILE:HD11	1:A:369:LEU:CD2	0.61	2.26
1:A:343:PHE:CB	1:A:344:PRO:CD	0.60	2.80
1:A:300:ILE:HG23	1:A:308:LEU:HB3	0.60	1.72
1:A:339:LEU:HD23	1:A:348:LEU:CD1	0.60	2.27
1:A:346:LYS:CD	1:A:360:LEU:HD21	0.58	2.28
1:A:329:ARG:O	1:A:329:ARG:CG	0.57	2.52
1:A:284:SER:OG	1:A:323:LEU:HD12	0.56	2.00
1:A:343:PHE:CB	1:A:344:PRO:HD3	0.56	2.30
1:A:318:ILE:O	1:A:321:ILE:HG22	0.56	2.00
1:A:348:LEU:C	1:A:348:LEU:HD23	0.56	2.20
1:A:312:PHE:CD1	1:A:316:HIS:NE2	0.56	2.74
1:A:339:LEU:CD2	1:A:348:LEU:HD12	0.55	2.31
1:A:337:PHE:C	1:A:337:PHE:CD1	0.55	2.78
1:A:300:ILE:HD11	1:A:369:LEU:HD22	0.55	1.79
1:A:316:HIS:O	1:A:355:LEU:N	0.54	2.40
1:A:329:ARG:O	1:A:329:ARG:HG3	0.54	2.02
1:A:284:SER:O	1:A:286:SER:N	0.54	2.36
1:A:332:MET:O	1:A:333:ALA:C	0.54	2.46
1:A:289:ILE:CG1	1:A:295:THR:OG1	0.54	2.56
1:A:339:LEU:HD11	1:A:365:ILE:HG22	0.54	1.79
1:A:337:PHE:CB	1:A:369:LEU:CD1	0.54	2.86
1:A:337:PHE:HB2	1:A:369:LEU:CD1	0.54	2.32
1:A:364:VAL:O	1:A:364:VAL:HG13	0.54	2.02
1:A:346:LYS:CD	1:A:360:LEU:CD2	0.53	2.87
1:A:287:ILE:CG2	1:A:311:LYS:O	0.53	2.55
1:A:332:MET:O	1:A:334:ALA:N	0.53	2.42
1:A:344:PRO:CD	1:A:362:ASN:OD1	0.53	2.57
1:A:362:ASN:O	1:A:363:ALA:CB	0.52	2.57
1:A:329:ARG:N	1:A:330:PRO:HD3	0.52	2.19
1:A:359:ASN:ND2	1:A:359:ASN:O	0.52	2.42
1:A:285:SER:OG	1:A:286:SER:N	0.52	2.41
1:A:300:ILE:CD1	1:A:369:LEU:HD22	0.52	2.34

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:316:HIS:CE1	1:A:317:ARG:O	0.52	2.62
1:A:314:HIS:O	1:A:355:LEU:N	0.52	2.42
1:A:328:ALA:C	1:A:330:PRO:CD	0.51	2.79
1:A:313:ASN:OD1	1:A:313:ASN:N	0.51	2.43
1:A:339:LEU:CD2	1:A:348:LEU:CD1	0.50	2.89
1:A:360:LEU:O	1:A:362:ASN:N	0.50	2.45
1:A:360:LEU:O	1:A:362:ASN:ND2	0.50	2.45
1:A:298:ILE:N	1:A:310:GLN:O	0.50	2.44
1:A:346:LYS:HD3	1:A:360:LEU:HD21	0.50	1.84
1:A:344:PRO:CG	1:A:362:ASN:OD1	0.49	2.60
1:A:329:ARG:HD2	1:A:333:ALA:N	0.49	2.22
1:A:358:ALA:O	1:A:359:ASN:CB	0.49	2.61
1:A:337:PHE:C	1:A:338:VAL:CG1	0.48	2.82
1:A:337:PHE:CD1	1:A:337:PHE:O	0.48	2.66
1:A:325:ILE:O	1:A:329:ARG:HB2	0.48	2.07
1:A:289:ILE:O	1:A:289:ILE:CG2	0.48	2.61
1:A:318:ILE:HG12	1:A:355:LEU:HD13	0.48	1.85
1:A:337:PHE:CB	1:A:369:LEU:HD12	0.48	2.38
1:A:295:THR:C	1:A:314:HIS:NE2	0.48	2.67
1:A:289:ILE:HG13	1:A:295:THR:OG1	0.47	2.09
1:A:283:ALA:HB1	1:A:323:LEU:O	0.47	2.09
1:A:358:ALA:O	1:A:359:ASN:OD1	0.47	2.32
1:A:336:SER:O	1:A:370:THR:O	0.47	2.33
1:A:312:PHE:HB3	1:A:316:HIS:CD2	0.47	2.44
1:A:295:THR:HA	1:A:314:HIS:NE2	0.47	2.24
1:A:346:LYS:HD3	1:A:360:LEU:CD2	0.47	2.40
1:A:347:GLU:O	1:A:348:LEU:O	0.46	2.32
1:A:289:ILE:HG23	1:A:289:ILE:O	0.46	2.11
1:A:316:HIS:NE2	1:A:355:LEU:HD22	0.46	2.25
1:A:318:ILE:HG12	1:A:355:LEU:CD1	0.46	2.41
1:A:329:ARG:NE	1:A:332:MET:HB3	0.46	2.26
1:A:341:THR:CG2	1:A:344:PRO:HG2	0.46	2.40
1:A:316:HIS:CD2	1:A:355:LEU:HD22	0.45	2.45
1:A:282:LYS:O	1:A:282:LYS:CG	0.45	2.65
1:A:343:PHE:HB3	1:A:344:PRO:HD3	0.45	1.88
1:A:320:ASP:O	1:A:323:LEU:HG	0.45	2.11
1:A:296:THR:N	1:A:314:HIS:NE2	0.45	2.64
1:A:337:PHE:C	1:A:338:VAL:HG13	0.44	2.31
1:A:283:ALA:O	1:A:284:SER:C	0.44	2.55
1:A:289:ILE:HG13	1:A:295:THR:CB	0.44	2.42
1:A:312:PHE:CG	1:A:316:HIS:NE2	0.44	2.86
1:A:347:GLU:O	1:A:348:LEU:C	0.44	2.54

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:348:LEU:CD2	1:A:349:ALA:N	0.44	2.80
1:A:339:LEU:C	1:A:339:LEU:HD12	0.44	2.32
1:A:349:ALA:HB3	1:A:360:LEU:CD1	0.44	2.42
1:A:342:THR:O	1:A:343:PHE:C	0.44	2.56
1:A:328:ALA:C	1:A:330:PRO:HD3	0.43	2.33
1:A:295:THR:HA	1:A:314:HIS:CE1	0.43	2.48
1:A:295:THR:CA	1:A:314:HIS:NE2	0.43	2.82
1:A:344:PRO:HG3	1:A:362:ASN:OD1	0.43	2.13
1:A:329:ARG:CD	1:A:332:MET:HB3	0.43	2.44
1:A:339:LEU:HD12	1:A:340:MET:H	0.43	1.72
1:A:340:MET:HG2	1:A:341:THR:N	0.43	2.29
1:A:324:PHE:CD1	1:A:324:PHE:C	0.43	2.92
1:A:339:LEU:HD11	1:A:365:ILE:HG21	0.43	1.87
1:A:291:GLU:HG2	1:A:291:GLU:O	0.43	2.12
1:A:350:ASP:OD1	1:A:355:LEU:CD1	0.42	2.68
1:A:284:SER:HB2	1:A:287:ILE:HD11	0.42	1.91
1:A:321:ILE:CG2	1:A:322:ARG:N	0.42	2.82
1:A:312:PHE:HB3	1:A:316:HIS:NE2	0.42	2.30
1:A:325:ILE:O	1:A:329:ARG:CB	0.42	2.68
1:A:316:HIS:O	1:A:355:LEU:HB2	0.41	2.15
1:A:329:ARG:O	1:A:329:ARG:CD	0.41	2.69
1:A:302:LEU:HD12	1:A:369:LEU:CD2	0.41	2.24
1:A:283:ALA:HA	1:A:323:LEU:HB2	0.41	1.91
1:A:351:GLU:O	1:A:352:ASN:CB	0.41	2.66
1:A:298:ILE:HG23	1:A:365:ILE:HB	0.41	1.92
1:A:297:ASN:N	1:A:363:ALA:O	0.41	2.47
1:A:346:LYS:HD2	1:A:360:LEU:CD2	0.41	2.45
1:A:282:LYS:O	1:A:283:ALA:C	0.40	2.58

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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	87/89 (98%)	67 (77%)	16 (18%)	4 (5%)	5 29
All	All	87/89 (98%)	67 (77%)	16 (18%)	4 (5%)	5 29

All 4 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	352	ASN
1	A	348	LEU
1	A	361	LEU
1	A	333	ALA

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	77/77 (100%)	57 (74%)	20 (26%)	3 24
All	All	77/77 (100%)	57 (74%)	20 (26%)	3 24

All 20 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	359	ASN
1	A	332	MET
1	A	345	ASN
1	A	286	SER
1	A	335	THR
1	A	295	THR
1	A	362	ASN
1	A	323	LEU
1	A	300	ILE
1	A	319	SER
1	A	316	HIS
1	A	337	PHE
1	A	302	LEU
1	A	307	ARG
1	A	322	ARG
1	A	320	ASP
1	A	336	SER
1	A	327	ASP
1	A	369	LEU
1	A	357	GLU

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 74% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5155

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	867
Number of shifts mapped to atoms	867
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	88	0.49 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	86	0.87 ± 0.16	Should be applied
$^{13}C'$	0	—	—
^{15}N	86	-0.01 ± 0.30	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 66%, i.e. 730 atoms were assigned a chemical shift out of a possible 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	348/439 (79%)	174/175 (99%)	88/178 (49%)	86/86 (100%)
Sidechain	361/619 (58%)	275/359 (77%)	86/227 (38%)	0/33 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	21/50 (42%)	21/28 (75%)	0/20 (0%)	0/2 (0%)
Overall	730/1108 (66%)	470/562 (84%)	174/425 (41%)	86/121 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 66%, i.e. 730 atoms were assigned a chemical shift out of a possible 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	348/439 (79%)	174/175 (99%)	88/178 (49%)	86/86 (100%)
Sidechain	361/619 (58%)	275/359 (77%)	86/227 (38%)	0/33 (0%)
Aromatic	21/50 (42%)	21/28 (75%)	0/20 (0%)	0/2 (0%)
Overall	730/1108 (66%)	470/562 (84%)	174/425 (41%)	86/121 (71%)

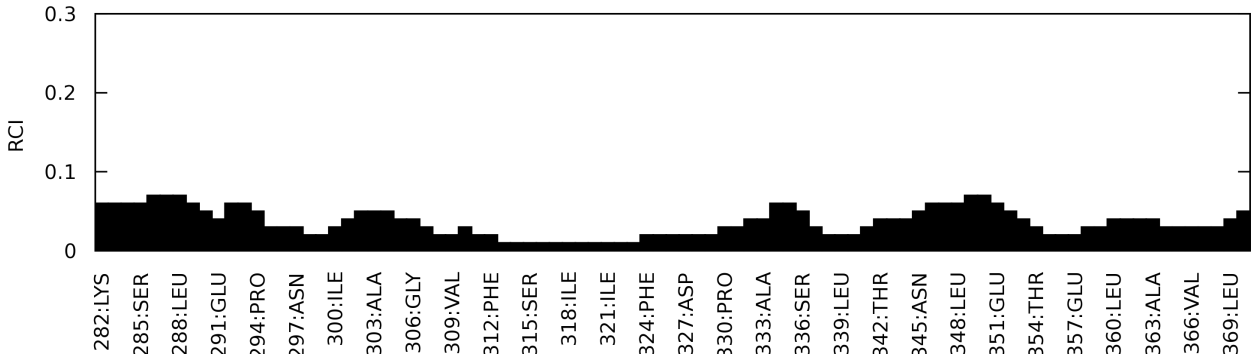
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5874

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 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	1181
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1181
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- Chain not found in structure. All 1181 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	54	SER	HB2	3.866	0.05	1
UNMAPPED	30	ALA	HB3	1.48	0.05	1
UNMAPPED	27	LEU	N	120.609	0.05	1
UNMAPPED	64	GLY	H	8.392	0.05	1
UNMAPPED	159	ALA	HB1	1.346	0.05	1
UNMAPPED	100	GLU	HA	4.283	0.05	1
UNMAPPED	27	LEU	CB	38.769	0.05	1
UNMAPPED	65	THR	H	8.055	0.05	1
UNMAPPED	60	SER	HB2	3.884	0.05	1
UNMAPPED	36	ILE	HD12	0.883	0.05	1
UNMAPPED	49	ASP	H	8.354	0.05	1
UNMAPPED	131	ALA	HA	4.354	0.05	1
UNMAPPED	17	GLY	H	8.694	0.05	1
UNMAPPED	20	GLU	HG2	2.181	0.05	1
UNMAPPED	100	GLU	HG2	2.281	0.05	1
UNMAPPED	72	VAL	CB	31.965	0.05	1
UNMAPPED	25	PHE	HD1	6.577	0.05	1
UNMAPPED	92	GLN	N	119.359	0.05	1
UNMAPPED	64	GLY	HA3	4.005	0.05	1
UNMAPPED	67	PRO	CB	31.506	0.05	1
UNMAPPED	1	MET	C	176.16	0.05	1
UNMAPPED	36	ILE	HA	4.224	0.05	1
UNMAPPED	95	TYR	CA	57.094	0.05	1
UNMAPPED	29	SER	HB2	3.545	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	26	PHE	C	178.17	0.05	1
UNMAPPED	142	GLY	N	108.762	0.05	1
UNMAPPED	42	TYR	HD1	7.218	0.05	1
UNMAPPED	25	PHE	CB	37.775	0.05	1
UNMAPPED	150	PHE	HA	4.511	0.05	1
UNMAPPED	63	ARG	CB	30.359	0.05	1
UNMAPPED	134	VAL	H	8.083	0.05	1
UNMAPPED	159	ALA	N	123.385	0.05	1
UNMAPPED	2	ALA	HB3	1.383	0.05	1
UNMAPPED	155	TYR	H	8.037	0.05	1
UNMAPPED	135	GLU	H	8.464	0.05	1
UNMAPPED	2	ALA	N	122.961	0.05	1
UNMAPPED	67	PRO	CA	62.632	0.05	1
UNMAPPED	55	GLN	HA	4.35	0.05	1
UNMAPPED	8	ALA	CA	55.053	0.05	1
UNMAPPED	10	ARG	HD2	3.29	0.05	1
UNMAPPED	68	SER	CA	57.75	0.05	1
UNMAPPED	46	GLY	HA3	3.667	0.05	1
UNMAPPED	53	ILE	H	8.122	0.05	1
UNMAPPED	134	VAL	HG23	0.919	0.05	1
UNMAPPED	50	ILE	HG13	1.437	0.05	1
UNMAPPED	12	PHE	CA	61.19	0.05	1
UNMAPPED	20	GLU	N	123.173	0.05	1
UNMAPPED	125	GLY	HA2	3.994	0.05	1
UNMAPPED	115	PRO	HD3	3.926	0.05	1
UNMAPPED	6	GLN	H	7.998	0.05	1
UNMAPPED	139	LYS	HG3	1.413	0.05	1
UNMAPPED	122	LEU	N	121.69	0.05	1
UNMAPPED	38	LEU	HB3	1.921	0.05	1
UNMAPPED	38	LEU	HD12	0.091	0.05	1
UNMAPPED	32	TRP	HB3	3.267	0.05	1
UNMAPPED	26	PHE	HB2	2.592	0.05	1
UNMAPPED	35	GLN	NE2	112.469	0.05	1
UNMAPPED	39	ALA	C	180.423	0.05	1
UNMAPPED	141	PRO	HA	4.425	0.05	1
UNMAPPED	99	SER	HB2	3.884	0.05	1
UNMAPPED	148	ARG	HA	4.573	0.05	1
UNMAPPED	3	GLU	CB	28.83	0.05	1
UNMAPPED	51	VAL	CA	62.369	0.05	1
UNMAPPED	53	ILE	HG12	1.175	0.05	1
UNMAPPED	135	GLU	CB	29.748	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	61	VAL	HA	4.167	0.05	1
UNMAPPED	167	TYR	HB2	2.972	0.05	1
UNMAPPED	8	ALA	C	178.449	0.05	1
UNMAPPED	4	GLU	C	176.712	0.05	1
UNMAPPED	37	ALA	N	123.809	0.05	1
UNMAPPED	91	GLY	HA2	3.954	0.05	1
UNMAPPED	56	ALA	CB	18.815	0.05	1
UNMAPPED	107	VAL	HA	4.172	0.05	1
UNMAPPED	119	VAL	H	7.93	0.05	1
UNMAPPED	102	SER	HB3	3.886	0.05	1
UNMAPPED	130	GLY	N	109.822	0.05	1
UNMAPPED	45	GLY	C	174.394	0.05	1
UNMAPPED	37	ALA	CB	18.586	0.05	1
UNMAPPED	138	THR	HG22	1.179	0.05	1
UNMAPPED	45	GLY	CA	45.266	0.05	1
UNMAPPED	139	LYS	HB2	1.809	0.05	1
UNMAPPED	30	ALA	H	7.06	0.05	1
UNMAPPED	116	ASN	HD22	7.636	0.05	1
UNMAPPED	15	VAL	HG11	0.913	0.05	1
UNMAPPED	12	PHE	HZ	7.055	0.05	1
UNMAPPED	17	GLY	HA3	4.137	0.05	1
UNMAPPED	70	ASN	HA	4.674	0.05	1
UNMAPPED	26	PHE	CB	38.692	0.05	1
UNMAPPED	19	GLU	C	174.017	0.05	1
UNMAPPED	35	GLN	C	179.206	0.05	1
UNMAPPED	73	THR	CA	61.485	0.05	1
UNMAPPED	115	PRO	HB2	1.941	0.05	1
UNMAPPED	115	PRO	HD2	3.786	0.05	1
UNMAPPED	122	LEU	H	8.123	0.05	1
UNMAPPED	129	HIS	HA	4.69	0.05	1
UNMAPPED	106	ILE	HG13	1.441	0.05	1
UNMAPPED	9	LEU	CA	58.034	0.05	1
UNMAPPED	32	TRP	NE1	129.799	0.05	1
UNMAPPED	24	ARG	HG3	1.64	0.05	1
UNMAPPED	100	GLU	N	122.537	0.05	1
UNMAPPED	14	ALA	HA	4.091	0.05	1
UNMAPPED	28	GLU	CA	59.027	0.05	1
UNMAPPED	80	HIS	HA	4.59	0.05	1
UNMAPPED	10	ARG	C	179.208	0.05	1
UNMAPPED	42	TYR	CB	37.163	0.05	1
UNMAPPED	20	GLU	HB2	2.066	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	121	ASP	HA	4.563	0.05	1
UNMAPPED	106	ILE	HA	4.179	0.05	1
UNMAPPED	43	GLU	N	120.418	0.05	1
UNMAPPED	69	ASP	N	122.113	0.05	1
UNMAPPED	70	ASN	N	119.358	0.05	1
UNMAPPED	115	PRO	HA	4.379	0.05	1
UNMAPPED	136	ARG	HG3	1.631	0.05	1
UNMAPPED	125	GLY	HA3	3.897	0.05	1
UNMAPPED	4	GLU	HA	4.165	0.05	1
UNMAPPED	5	ARG	HG3	0.924	0.05	1
UNMAPPED	29	SER	CB	61.857	0.05	1
UNMAPPED	106	ILE	HG22	0.921	0.05	1
UNMAPPED	13	VAL	CB	31.888	0.05	1
UNMAPPED	49	ASP	HB2	2.655	0.05	1
UNMAPPED	61	VAL	H	8.023	0.05	1
UNMAPPED	29	SER	N	115.099	0.05	1
UNMAPPED	127	LYS	H	8.271	0.05	1
UNMAPPED	129	HIS	HB2	3.174	0.05	1
UNMAPPED	121	ASP	HB3	2.672	0.05	1
UNMAPPED	9	LEU	C	177.451	0.05	1
UNMAPPED	51	VAL	HB	2.086	0.05	1
UNMAPPED	66	ALA	HA	4.627	0.05	1
UNMAPPED	35	GLN	HA	4.021	0.05	1
UNMAPPED	60	SER	HA	4.454	0.05	1
UNMAPPED	4	GLU	H	8.414	0.05	1
UNMAPPED	5	ARG	HB2	1.451	0.05	1
UNMAPPED	98	GLY	N	108.551	0.05	1
UNMAPPED	132	VAL	HG13	0.92	0.05	1
UNMAPPED	24	ARG	CB	29.213	0.05	1
UNMAPPED	50	ILE	CA	60.862	0.05	1
UNMAPPED	13	VAL	HG13	1.018	0.05	1
UNMAPPED	32	TRP	HE1	10.236	0.05	1
UNMAPPED	97	GLY	N	107.703	0.05	1
UNMAPPED	143	GLU	HA	4.289	0.05	1
UNMAPPED	65	THR	CB	68.967	0.05	1
UNMAPPED	157	LEU	HB3	1.598	0.05	1
UNMAPPED	46	GLY	CA	44.972	0.05	1
UNMAPPED	90	GLU	H	8.451	0.05	1
UNMAPPED	41	PHE	HB2	2.312	0.05	1
UNMAPPED	147	PRO	HA	4.404	0.05	1
UNMAPPED	27	LEU	H	8.045	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	ALA	HB1	1.541	0.05	1
UNMAPPED	19	GLU	HG3	2.563	0.05	1
UNMAPPED	126	ALA	N	123.544	0.05	1
UNMAPPED	35	GLN	H	8.097	0.05	1
UNMAPPED	129	HIS	CA	54.866	0.05	1
UNMAPPED	49	ASP	CB	39.839	0.05	1
UNMAPPED	123	PHE	HB3	3.208	0.05	1
UNMAPPED	105	GLN	CA	55.161	0.05	1
UNMAPPED	151	ALA	CA	55.03	0.05	1
UNMAPPED	15	VAL	HG23	1.028	0.05	1
UNMAPPED	27	LEU	HD12	0.523	0.05	1
UNMAPPED	25	PHE	CA	60.731	0.05	1
UNMAPPED	160	ALA	HA	4.531	0.05	1
UNMAPPED	21	ASP	HB2	2.684	0.05	1
UNMAPPED	137	VAL	CB	32.194	0.05	1
UNMAPPED	3	GLU	HB3	2.09	0.05	1
UNMAPPED	21	ASP	H	8.939	0.05	1
UNMAPPED	97	GLY	HA2	3.918	0.05	1
UNMAPPED	40	SER	N	114.061	0.05	1
UNMAPPED	169	ALA	HA	4.216	0.05	1
UNMAPPED	107	VAL	CA	61.485	0.05	1
UNMAPPED	120	ASP	H	8.256	0.05	1
UNMAPPED	15	VAL	CB	32.347	0.05	1
UNMAPPED	129	HIS	CB	28.525	0.05	1
UNMAPPED	63	ARG	HB3	1.795	0.05	1
UNMAPPED	43	GLU	HB2	2.186	0.05	1
UNMAPPED	40	SER	CB	62.392	0.05	1
UNMAPPED	134	VAL	CB	32.347	0.05	1
UNMAPPED	124	LYS	HG2	1.366	0.05	1
UNMAPPED	75	PHE	HB3	3.124	0.05	1
UNMAPPED	32	TRP	CB	23.632	0.05	1
UNMAPPED	48	GLU	N	120.418	0.05	1
UNMAPPED	26	PHE	HZ	7.166	0.05	1
UNMAPPED	121	ASP	H	8.243	0.05	1
UNMAPPED	90	GLU	HG2	2.33	0.05	1
UNMAPPED	32	TRP	N	110.67	0.05	1
UNMAPPED	48	GLU	CB	30.206	0.05	1
UNMAPPED	4	GLU	CA	58.34	0.05	1
UNMAPPED	55	GLN	HB2	1.977	0.05	1
UNMAPPED	53	ILE	CB	38.081	0.05	1
UNMAPPED	41	PHE	CA	60.634	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	52	THR	HG21	1.141	0.05	1
UNMAPPED	95	TYR	HB2	2.894	0.05	1
UNMAPPED	63	ARG	CA	55.554	0.05	1
UNMAPPED	6	GLN	HB3	2.181	0.05	1
UNMAPPED	53	ILE	N	122.749	0.05	1
UNMAPPED	30	ALA	HB2	1.48	0.05	1
UNMAPPED	106	ILE	HD11	0.856	0.05	1
UNMAPPED	53	ILE	HD12	0.841	0.05	1
UNMAPPED	77	ASP	H	8.186	0.05	1
UNMAPPED	148	ARG	H	8.451	0.05	1
UNMAPPED	71	ARG	HB3	1.805	0.05	1
UNMAPPED	63	ARG	HA	4.376	0.05	1
UNMAPPED	95	TYR	HE1	6.792	0.05	1
UNMAPPED	31	GLY	HA3	4.012	0.05	1
UNMAPPED	137	VAL	N	121.69	0.05	1
UNMAPPED	106	ILE	CA	60.404	0.05	1
UNMAPPED	130	GLY	CA	44.611	0.05	1
UNMAPPED	56	ALA	CA	51.885	0.05	1
UNMAPPED	8	ALA	HA	4.326	0.05	1
UNMAPPED	50	ILE	HG23	0.856	0.05	1
UNMAPPED	151	ALA	H	8.183	0.05	1
UNMAPPED	118	LEU	H	8.134	0.05	1
UNMAPPED	60	SER	H	8.332	0.05	1
UNMAPPED	25	PHE	HD2	6.577	0.05	1
UNMAPPED	92	GLN	HG3	2.311	0.05	1
UNMAPPED	64	GLY	HA2	4.005	0.05	1
UNMAPPED	106	ILE	HG23	0.921	0.05	1
UNMAPPED	54	SER	HA	4.437	0.05	1
UNMAPPED	36	ILE	HB	1.918	0.05	1
UNMAPPED	38	LEU	C	177.189	0.05	1
UNMAPPED	132	VAL	HB	2.04	0.05	1
UNMAPPED	7	ASP	C	177.451	0.05	1
UNMAPPED	132	VAL	CA	61.419	0.05	1
UNMAPPED	94	PHE	HB2	2.92	0.05	1
UNMAPPED	72	VAL	HG21	0.895	0.05	1
UNMAPPED	107	VAL	H	8.245	0.05	1
UNMAPPED	117	GLU	HB3	2.03	0.05	1
UNMAPPED	132	VAL	HG11	0.92	0.05	1
UNMAPPED	119	VAL	CB	32.118	0.05	1
UNMAPPED	48	GLU	HG3	2.326	0.05	1
UNMAPPED	37	ALA	H	8.48	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	50	ILE	HD11	0.856	0.05	1
UNMAPPED	2	ALA	HB2	1.383	0.05	1
UNMAPPED	22	ARG	HD2	3.431	0.05	1
UNMAPPED	30	ALA	HA	4.48	0.05	1
UNMAPPED	75	PHE	H	8.305	0.05	1
UNMAPPED	30	ALA	CB	20.039	0.05	1
UNMAPPED	102	SER	HA	4.422	0.05	1
UNMAPPED	16	THR	CB	71.184	0.05	1
UNMAPPED	28	GLU	HB2	1.831	0.05	1
UNMAPPED	40	SER	HB2	4.077	0.05	1
UNMAPPED	73	THR	HA	4.296	0.05	1
UNMAPPED	100	GLU	HB3	2.056	0.05	1
UNMAPPED	157	LEU	HA	4.27	0.05	1
UNMAPPED	16	THR	N	106.219	0.05	1
UNMAPPED	159	ALA	H	8.024	0.05	1
UNMAPPED	18	ALA	HB3	1.339	0.05	1
UNMAPPED	100	GLU	HB2	1.957	0.05	1
UNMAPPED	107	VAL	HG21	0.919	0.05	1
UNMAPPED	92	GLN	HE21	6.823	0.05	1
UNMAPPED	38	LEU	HB2	1.358	0.05	1
UNMAPPED	45	GLY	HA2	3.901	0.05	1
UNMAPPED	32	TRP	HB2	3.108	0.05	1
UNMAPPED	164	GLU	HB2	1.64	0.05	1
UNMAPPED	75	PHE	CB	38.845	0.05	1
UNMAPPED	43	GLU	H	8.028	0.05	1
UNMAPPED	117	GLU	N	120.559	0.05	1
UNMAPPED	106	ILE	H	8.244	0.05	1
UNMAPPED	158	GLY	H	8.443	0.05	1
UNMAPPED	99	SER	HB3	3.884	0.05	1
UNMAPPED	36	ILE	C	177.748	0.05	1
UNMAPPED	12	PHE	HA	3.73	0.05	1
UNMAPPED	57	THR	HG22	1.246	0.05	1
UNMAPPED	20	GLU	C	175.514	0.05	1
UNMAPPED	55	GLN	HG2	2.37	0.05	1
UNMAPPED	29	SER	H	7.446	0.05	1
UNMAPPED	144	THR	HG22	1.212	0.05	1
UNMAPPED	151	ALA	HB1	1.483	0.05	1
UNMAPPED	13	VAL	H	8.647	0.05	1
UNMAPPED	40	SER	HA	4.288	0.05	1
UNMAPPED	56	ALA	HB2	1.377	0.05	1
UNMAPPED	132	VAL	H	8.082	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	34	LEU	HD21	1.147	0.05	1
UNMAPPED	165	SER	N	116.604	0.05	1
UNMAPPED	48	GLU	HB3	1.957	0.05	1
UNMAPPED	124	LYS	HB2	1.763	0.05	1
UNMAPPED	59	SER	HA	4.444	0.05	1
UNMAPPED	47	ASP	N	119.57	0.05	1
UNMAPPED	98	GLY	H	8.255	0.05	1
UNMAPPED	122	LEU	HB2	1.326	0.05	1
UNMAPPED	1	MET	CA	55.435	0.05	1
UNMAPPED	134	VAL	HG13	0.919	0.05	1
UNMAPPED	2	ALA	H	8.219	0.05	1
UNMAPPED	105	GLN	HA	4.321	0.05	1
UNMAPPED	73	THR	N	118.087	0.05	1
UNMAPPED	17	GLY	HA2	3.81	0.05	1
UNMAPPED	42	TYR	C	177.309	0.05	1
UNMAPPED	26	PHE	CA	62.402	0.05	1
UNMAPPED	170	GLY	CA	44.611	0.05	1
UNMAPPED	127	LYS	HA	4.295	0.05	1
UNMAPPED	24	ARG	H	8.426	0.05	1
UNMAPPED	62	SER	HA	4.298	0.05	1
UNMAPPED	44	ASP	C	176.391	0.05	1
UNMAPPED	37	ALA	C	179.166	0.05	1
UNMAPPED	9	LEU	HD23	0.952	0.05	1
UNMAPPED	65	THR	HA	4.334	0.05	1
UNMAPPED	131	ALA	CA	51.819	0.05	1
UNMAPPED	106	ILE	HG12	1.137	0.05	1
UNMAPPED	92	GLN	HE22	7.573	0.05	1
UNMAPPED	125	GLY	H	8.034	0.05	1
UNMAPPED	28	GLU	N	120.46	0.05	1
UNMAPPED	155	TYR	HA	4.512	0.05	1
UNMAPPED	71	ARG	HG3	1.612	0.05	1
UNMAPPED	24	ARG	HG2	1.64	0.05	1
UNMAPPED	117	GLU	HG3	2.274	0.05	1
UNMAPPED	18	ALA	C	175.714	0.05	1
UNMAPPED	25	PHE	HZ	7.48	0.05	1
UNMAPPED	43	GLU	CA	57.127	0.05	1
UNMAPPED	35	GLN	CB	29.518	0.05	1
UNMAPPED	22	ARG	C	176.992	0.05	1
UNMAPPED	31	GLY	CA	47.2	0.05	1
UNMAPPED	68	SER	HA	4.433	0.05	1
UNMAPPED	20	GLU	HB3	2.066	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	66	ALA	CA	49.919	0.05	1
UNMAPPED	168	VAL	CA	61.255	0.05	1
UNMAPPED	33	ASP	HB2	2.51	0.05	1
UNMAPPED	35	GLN	N	115.544	0.05	1
UNMAPPED	166	ALA	HB1	1.308	0.05	1
UNMAPPED	131	ALA	N	123.809	0.05	1
UNMAPPED	132	VAL	HG21	0.919	0.05	1
UNMAPPED	133	ALA	HA	4.359	0.05	1
UNMAPPED	72	VAL	HB	2.079	0.05	1
UNMAPPED	5	ARG	HG2	0.924	0.05	1
UNMAPPED	29	SER	CA	60.535	0.05	1
UNMAPPED	126	ALA	HB1	1.398	0.05	1
UNMAPPED	13	VAL	CA	66.465	0.05	1
UNMAPPED	96	ALA	HB1	1.86	0.05	1
UNMAPPED	15	VAL	H	7.926	0.05	1
UNMAPPED	64	GLY	CA	44.677	0.05	1
UNMAPPED	94	PHE	N	120.206	0.05	1
UNMAPPED	40	SER	H	8.364	0.05	1
UNMAPPED	75	PHE	CA	57.684	0.05	1
UNMAPPED	144	THR	N	114.908	0.05	1
UNMAPPED	32	TRP	H	8.813	0.05	1
UNMAPPED	133	ALA	HB2	1.354	0.05	1
UNMAPPED	145	SER	H	8.226	0.05	1
UNMAPPED	116	ASN	CA	53.13	0.05	1
UNMAPPED	98	GLY	CA	44.677	0.05	1
UNMAPPED	35	GLN	HE22	7.637	0.05	1
UNMAPPED	48	GLU	H	8.352	0.05	1
UNMAPPED	63	ARG	HB2	1.795	0.05	1
UNMAPPED	169	ALA	H	8.244	0.05	1
UNMAPPED	5	ARG	HB3	1.451	0.05	1
UNMAPPED	138	THR	CB	68.967	0.05	1
UNMAPPED	52	THR	CB	68.661	0.05	1
UNMAPPED	46	GLY	N	108.127	0.05	1
UNMAPPED	57	THR	CA	59.093	0.05	1
UNMAPPED	77	ASP	N	120.842	0.05	1
UNMAPPED	13	VAL	HA	3.484	0.05	1
UNMAPPED	23	ALA	HB3	1.115	0.05	1
UNMAPPED	166	ALA	CA	52.016	0.05	1
UNMAPPED	65	THR	CA	60.928	0.05	1
UNMAPPED	123	PHE	CB	38.387	0.05	1
UNMAPPED	170	GLY	HA2	3.948	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	43	GLU	HG2	2.483	0.05	1
UNMAPPED	41	PHE	HB3	2.806	0.05	1
UNMAPPED	29	SER	C	173.216	0.05	1
UNMAPPED	74	SER	HB3	3.857	0.05	1
UNMAPPED	108	GLY	N	113.001	0.05	1
UNMAPPED	123	PHE	N	118.723	0.05	1
UNMAPPED	19	GLU	HG2	2.548	0.05	1
UNMAPPED	74	SER	CA	57.782	0.05	1
UNMAPPED	76	ARG	HB3	1.767	0.05	1
UNMAPPED	49	ASP	CA	53.785	0.05	1
UNMAPPED	139	LYS	CA	55.325	0.05	1
UNMAPPED	151	ALA	CB	19.045	0.05	1
UNMAPPED	15	VAL	HG22	1.028	0.05	1
UNMAPPED	7	ASP	CB	39.61	0.05	1
UNMAPPED	148	ARG	CB	29.671	0.05	1
UNMAPPED	142	GLY	CA	44.513	0.05	1
UNMAPPED	18	ALA	HB1	1.339	0.05	1
UNMAPPED	107	VAL	N	124.657	0.05	1
UNMAPPED	118	LEU	N	122.325	0.05	1
UNMAPPED	7	ASP	N	119.782	0.05	1
UNMAPPED	105	GLN	H	8.448	0.05	1
UNMAPPED	44	ASP	N	118.299	0.05	1
UNMAPPED	107	VAL	CB	32.347	0.05	1
UNMAPPED	61	VAL	N	121.054	0.05	1
UNMAPPED	108	GLY	HA2	4.013	0.05	1
UNMAPPED	75	PHE	HB2	3.04	0.05	1
UNMAPPED	32	TRP	CA	59.322	0.05	1
UNMAPPED	60	SER	CB	62.851	0.05	1
UNMAPPED	6	GLN	C	175.594	0.05	1
UNMAPPED	32	TRP	HD1	7.055	0.05	1
UNMAPPED	137	VAL	HB	2.072	0.05	1
UNMAPPED	16	THR	H	7.529	0.05	1
UNMAPPED	41	PHE	N	123.809	0.05	1
UNMAPPED	90	GLU	HG3	2.331	0.05	1
UNMAPPED	166	ALA	HB2	1.308	0.05	1
UNMAPPED	60	SER	N	117.663	0.05	1
UNMAPPED	168	VAL	H	7.902	0.05	1
UNMAPPED	65	THR	HG22	1.189	0.05	1
UNMAPPED	133	ALA	H	8.356	0.05	1
UNMAPPED	16	THR	HG23	-0.154	0.05	1
UNMAPPED	145	SER	CB	63.157	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	57	THR	H	8.139	0.05	1
UNMAPPED	48	GLU	HA	4.18	0.05	1
UNMAPPED	108	GLY	CA	43.726	0.05	1
UNMAPPED	125	GLY	CA	44.709	0.05	1
UNMAPPED	150	PHE	HB2	2.849	0.05	1
UNMAPPED	106	ILE	HD12	0.856	0.05	1
UNMAPPED	53	ILE	HD13	0.841	0.05	1
UNMAPPED	119	VAL	HG23	0.926	0.05	1
UNMAPPED	30	ALA	C	177.549	0.05	1
UNMAPPED	35	GLN	HG2	2.493	0.05	1
UNMAPPED	96	ALA	H	8.274	0.05	1
UNMAPPED	28	GLU	HG3	2.321	0.05	1
UNMAPPED	31	GLY	HA2	3.879	0.05	1
UNMAPPED	126	ALA	H	8.049	0.05	1
UNMAPPED	102	SER	CA	57.979	0.05	1
UNMAPPED	106	ILE	CB	38.004	0.05	1
UNMAPPED	50	ILE	HG22	0.856	0.05	1
UNMAPPED	53	ILE	HG13	1.466	0.05	1
UNMAPPED	164	GLU	CA	53.844	0.05	1
UNMAPPED	122	LEU	HB3	1.52	0.05	1
UNMAPPED	2	ALA	HA	3.955	0.05	1
UNMAPPED	92	GLN	HG2	2.311	0.05	1
UNMAPPED	53	ILE	HG21	0.893	0.05	1
UNMAPPED	19	GLU	H	8.634	0.05	1
UNMAPPED	164	GLU	HB3	1.751	0.05	1
UNMAPPED	4	GLU	HG2	2.371	0.05	1
UNMAPPED	99	SER	CA	57.946	0.05	1
UNMAPPED	132	VAL	CB	32.271	0.05	1
UNMAPPED	94	PHE	HB3	3.019	0.05	1
UNMAPPED	151	ALA	HB2	1.483	0.05	1
UNMAPPED	147	PRO	CA	62.337	0.05	1
UNMAPPED	25	PHE	N	118.914	0.05	1
UNMAPPED	48	GLU	HG2	2.326	0.05	1
UNMAPPED	151	ALA	HB3	1.483	0.05	1
UNMAPPED	31	GLY	C	171.759	0.05	1
UNMAPPED	59	SER	HB2	3.875	0.05	1
UNMAPPED	22	ARG	HD3	3.431	0.05	1
UNMAPPED	59	SER	CA	57.946	0.05	1
UNMAPPED	30	ALA	CA	50.476	0.05	1
UNMAPPED	2	ALA	CB	19.518	0.05	1
UNMAPPED	34	LEU	HB3	1.607	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	28	GLU	HB3	1.966	0.05	1
UNMAPPED	55	GLN	HG3	2.37	0.05	1
UNMAPPED	40	SER	HB3	4.169	0.05	1
UNMAPPED	39	ALA	HA	4.216	0.05	1
UNMAPPED	167	TYR	HB3	2.971	0.05	1
UNMAPPED	36	ILE	N	122.06	0.05	1
UNMAPPED	131	ALA	CB	18.968	0.05	1
UNMAPPED	120	ASP	N	123.173	0.05	1
UNMAPPED	20	GLU	CB	29.213	0.05	1
UNMAPPED	27	LEU	HG	0.787	0.05	1
UNMAPPED	36	ILE	CB	37.316	0.05	1
UNMAPPED	12	PHE	HB2	3.009	0.05	1
UNMAPPED	56	ALA	HB3	1.377	0.05	1
UNMAPPED	41	PHE	HD1	5.873	0.05	1
UNMAPPED	45	GLY	HA3	3.901	0.05	1
UNMAPPED	170	GLY	H	8.256	0.05	1
UNMAPPED	104	GLN	HG3	2.318	0.05	1
UNMAPPED	172	ARG	H	8.205	0.05	1
UNMAPPED	3	GLU	HA	4.012	0.05	1
UNMAPPED	56	ALA	HA	4.345	0.05	1
UNMAPPED	166	ALA	HB3	1.308	0.05	1
UNMAPPED	27	LEU	HB3	0.693	0.05	1
UNMAPPED	80	HIS	HB3	3.29	0.05	1
UNMAPPED	3	GLU	N	119.994	0.05	1
UNMAPPED	57	THR	HG23	1.246	0.05	1
UNMAPPED	73	THR	HG21	1.178	0.05	1
UNMAPPED	34	LEU	CB	41.827	0.05	1
UNMAPPED	15	VAL	HB	1.918	0.05	1
UNMAPPED	144	THR	HG23	1.212	0.05	1
UNMAPPED	95	TYR	H	8.086	0.05	1
UNMAPPED	145	SER	N	118.001	0.05	1
UNMAPPED	34	LEU	HD11	1.011	0.05	1
UNMAPPED	18	ALA	HA	4.284	0.05	1
UNMAPPED	105	GLN	CB	32.271	0.05	1
UNMAPPED	124	LYS	HB3	1.824	0.05	1
UNMAPPED	11	GLU	CB	28.219	0.05	1
UNMAPPED	32	TRP	HZ2	6.961	0.05	1
UNMAPPED	94	PHE	H	8.15	0.05	1
UNMAPPED	22	ARG	HA	4.244	0.05	1
UNMAPPED	135	GLU	HB2	1.924	0.05	1
UNMAPPED	105	GLN	HB2	1.958	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	41	PHE	HE1	6.462	0.05	1
UNMAPPED	134	VAL	HG12	0.919	0.05	1
UNMAPPED	11	GLU	N	120.457	0.05	1
UNMAPPED	116	ASN	ND2	113.034	0.05	1
UNMAPPED	38	LEU	CA	57.16	0.05	1
UNMAPPED	169	ALA	CB	18.892	0.05	1
UNMAPPED	107	VAL	HB	2.047	0.05	1
UNMAPPED	145	SER	CA	57.422	0.05	1
UNMAPPED	138	THR	H	8.296	0.05	1
UNMAPPED	52	THR	H	8.213	0.05	1
UNMAPPED	32	TRP	HA	3.574	0.05	1
UNMAPPED	58	PRO	HB2	1.852	0.05	1
UNMAPPED	25	PHE	HA	4.088	0.05	1
UNMAPPED	90	GLU	HA	4.192	0.05	1
UNMAPPED	68	SER	HB2	3.829	0.05	1
UNMAPPED	9	LEU	HD22	0.952	0.05	1
UNMAPPED	33	ASP	HA	4.806	0.05	1
UNMAPPED	148	ARG	HG2	1.685	0.05	1
UNMAPPED	8	ALA	HB3	1.829	0.05	1
UNMAPPED	6	GLN	CA	58.417	0.05	1
UNMAPPED	144	THR	CA	61.288	0.05	1
UNMAPPED	138	THR	HG21	1.179	0.05	1
UNMAPPED	134	VAL	HG11	0.919	0.05	1
UNMAPPED	104	GLN	H	8.172	0.05	1
UNMAPPED	119	VAL	HG12	0.927	0.05	1
UNMAPPED	117	GLU	HG2	2.274	0.05	1
UNMAPPED	139	LYS	N	124.233	0.05	1
UNMAPPED	42	TYR	HB3	3.225	0.05	1
UNMAPPED	44	ASP	HB3	2.928	0.05	1
UNMAPPED	35	GLN	CA	58.929	0.05	1
UNMAPPED	66	ALA	HB1	1.369	0.05	1
UNMAPPED	35	GLN	HB2	2.086	0.05	1
UNMAPPED	19	GLU	HB2	2.062	0.05	1
UNMAPPED	42	TYR	N	116.604	0.05	1
UNMAPPED	13	VAL	HG21	1.098	0.05	1
UNMAPPED	135	GLU	HG2	2.258	0.05	1
UNMAPPED	33	ASP	HB3	3.121	0.05	1
UNMAPPED	7	ASP	H	8.322	0.05	1
UNMAPPED	62	SER	HB2	3.877	0.05	1
UNMAPPED	14	ALA	C	179.268	0.05	1
UNMAPPED	73	THR	HB	4.168	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	61	VAL	HG12	0.925	0.05	1
UNMAPPED	75	PHE	N	122.537	0.05	1
UNMAPPED	137	VAL	HG12	0.92	0.05	1
UNMAPPED	60	SER	HB3	3.885	0.05	1
UNMAPPED	41	PHE	HZ	6.989	0.05	1
UNMAPPED	117	GLU	HB2	2.03	0.05	1
UNMAPPED	10	ARG	CA	58.438	0.05	1
UNMAPPED	139	LYS	HB3	1.809	0.05	1
UNMAPPED	165	SER	H	8.295	0.05	1
UNMAPPED	25	PHE	HB2	3.129	0.05	1
UNMAPPED	136	ARG	CB	33.112	0.05	1
UNMAPPED	98	GLY	HA2	4.004	0.05	1
UNMAPPED	51	VAL	HG23	0.922	0.05	1
UNMAPPED	34	LEU	HD22	1.147	0.05	1
UNMAPPED	124	LYS	HG3	1.423	0.05	1
UNMAPPED	35	GLN	HE21	6.907	0.05	1
UNMAPPED	170	GLY	N	108.127	0.05	1
UNMAPPED	22	ARG	HG3	1.896	0.05	1
UNMAPPED	51	VAL	HG22	0.922	0.05	1
UNMAPPED	66	ALA	CB	17.974	0.05	1
UNMAPPED	131	ALA	HB1	1.362	0.05	1
UNMAPPED	115	PRO	CA	63.516	0.05	1
UNMAPPED	157	LEU	CA	54.768	0.05	1
UNMAPPED	24	ARG	N	116.204	0.05	1
UNMAPPED	9	LEU	HA	3.947	0.05	1
UNMAPPED	140	SER	HB3	3.851	0.05	1
UNMAPPED	104	GLN	HG2	2.318	0.05	1
UNMAPPED	23	ALA	HB2	1.115	0.05	1
UNMAPPED	139	LYS	HD2	1.73	0.05	1
UNMAPPED	157	LEU	HB2	1.598	0.05	1
UNMAPPED	14	ALA	CA	54.703	0.05	1
UNMAPPED	6	GLN	HA	4.057	0.05	1
UNMAPPED	43	GLU	HG3	2.483	0.05	1
UNMAPPED	28	GLU	H	8.531	0.05	1
UNMAPPED	123	PHE	HA	4.558	0.05	1
UNMAPPED	96	ALA	CB	18.968	0.05	1
UNMAPPED	135	GLU	HB3	2.022	0.05	1
UNMAPPED	126	ALA	CB	18.739	0.05	1
UNMAPPED	38	LEU	HG	1.679	0.05	1
UNMAPPED	118	LEU	HB3	1.598	0.05	1
UNMAPPED	168	VAL	HG12	0.877	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	96	ALA	N	126.352	0.05	1
UNMAPPED	169	ALA	N	127.835	0.05	1
UNMAPPED	160	ALA	CA	49.788	0.05	1
UNMAPPED	17	GLY	N	112.789	0.05	1
UNMAPPED	45	GLY	H	8.016	0.05	1
UNMAPPED	15	VAL	HG21	1.028	0.05	1
UNMAPPED	46	GLY	C	173.116	0.05	1
UNMAPPED	19	GLU	CB	29.671	0.05	1
UNMAPPED	21	ASP	CA	56.734	0.05	1
UNMAPPED	25	PHE	C	177.83	0.05	1
UNMAPPED	58	PRO	CA	62.861	0.05	1
UNMAPPED	22	ARG	CA	57.52	0.05	1
UNMAPPED	19	GLU	N	117.875	0.05	1
UNMAPPED	15	VAL	N	114.061	0.05	1
UNMAPPED	77	ASP	HA	4.557	0.05	1
UNMAPPED	168	VAL	CB	32.5	0.05	1
UNMAPPED	131	ALA	H	8.193	0.05	1
UNMAPPED	80	HIS	HB2	3.139	0.05	1
UNMAPPED	7	ASP	HA	4.493	0.05	1
UNMAPPED	1	MET	HB2	1.993	0.05	1
UNMAPPED	166	ALA	H	8.207	0.05	1
UNMAPPED	147	PRO	CB	31.659	0.05	1
UNMAPPED	36	ILE	HG23	0.992	0.05	1
UNMAPPED	15	VAL	HA	3.852	0.05	1
UNMAPPED	139	LYS	HA	4.358	0.05	1
UNMAPPED	137	VAL	HG11	0.92	0.05	1
UNMAPPED	116	ASN	HB3	2.826	0.05	1
UNMAPPED	13	VAL	C	177.571	0.05	1
UNMAPPED	159	ALA	CB	19.427	0.05	1
UNMAPPED	27	LEU	HD21	0.52	0.05	1
UNMAPPED	68	SER	CB	63.233	0.05	1
UNMAPPED	119	VAL	HA	4.052	0.05	1
UNMAPPED	20	GLU	H	8.976	0.05	1
UNMAPPED	91	GLY	N	108.974	0.05	1
UNMAPPED	57	THR	HA	4.595	0.05	1
UNMAPPED	12	PHE	HD1	6.668	0.05	1
UNMAPPED	68	SER	N	115.12	0.05	1
UNMAPPED	150	PHE	HB3	2.949	0.05	1
UNMAPPED	27	LEU	CA	57.815	0.05	1
UNMAPPED	106	ILE	HD13	0.856	0.05	1
UNMAPPED	92	GLN	HB3	2.067	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	119	VAL	HG22	0.926	0.05	1
UNMAPPED	135	GLU	HA	4.297	0.05	1
UNMAPPED	36	ILE	HD11	0.883	0.05	1
UNMAPPED	28	GLU	HG2	2.317	0.05	1
UNMAPPED	148	ARG	HG3	1.685	0.05	1
UNMAPPED	138	THR	N	118.935	0.05	1
UNMAPPED	28	GLU	HA	3.356	0.05	1
UNMAPPED	164	GLU	CB	29.595	0.05	1
UNMAPPED	165	SER	HB3	3.859	0.05	1
UNMAPPED	50	ILE	HG21	0.856	0.05	1
UNMAPPED	36	ILE	H	8.122	0.05	1
UNMAPPED	137	VAL	HG22	0.924	0.05	1
UNMAPPED	57	THR	HB	4.175	0.05	1
UNMAPPED	55	GLN	N	121.902	0.05	1
UNMAPPED	142	GLY	HA3	3.948	0.05	1
UNMAPPED	106	ILE	HG21	0.921	0.05	1
UNMAPPED	53	ILE	HG22	0.893	0.05	1
UNMAPPED	53	ILE	HB	1.869	0.05	1
UNMAPPED	100	GLU	CA	56.341	0.05	1
UNMAPPED	4	GLU	HG3	2.461	0.05	1
UNMAPPED	44	ASP	H	8.024	0.05	1
UNMAPPED	95	TYR	CB	38.692	0.05	1
UNMAPPED	4	GLU	HB3	2.101	0.05	1
UNMAPPED	119	VAL	N	119.782	0.05	1
UNMAPPED	100	GLU	CB	29.136	0.05	1
UNMAPPED	59	SER	N	115.756	0.05	1
UNMAPPED	150	PHE	CA	57.324	0.05	1
UNMAPPED	11	GLU	H	8.455	0.05	1
UNMAPPED	50	ILE	HD13	0.856	0.05	1
UNMAPPED	51	VAL	HA	4.114	0.05	1
UNMAPPED	27	LEU	C	177.81	0.05	1
UNMAPPED	59	SER	HB3	3.914	0.05	1
UNMAPPED	8	ALA	N	123.173	0.05	1
UNMAPPED	2	ALA	CA	58.875	0.05	1
UNMAPPED	34	LEU	HB2	1.603	0.05	1
UNMAPPED	41	PHE	H	8.143	0.05	1
UNMAPPED	118	LEU	HB2	1.598	0.05	1
UNMAPPED	12	PHE	CB	39.457	0.05	1
UNMAPPED	8	ALA	CB	18.204	0.05	1
UNMAPPED	39	ALA	HB1	1.561	0.05	1
UNMAPPED	108	GLY	HA3	4.013	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	66	ALA	N	128.047	0.05	1
UNMAPPED	12	PHE	N	120.19	0.05	1
UNMAPPED	38	LEU	HD11	0.091	0.05	1
UNMAPPED	78	LEU	H	8.024	0.05	1
UNMAPPED	32	TRP	C	174.354	0.05	1
UNMAPPED	21	ASP	C	178.03	0.05	1
UNMAPPED	12	PHE	HB3	3.317	0.05	1
UNMAPPED	43	GLU	CB	28.601	0.05	1
UNMAPPED	25	PHE	HE2	6.938	0.05	1
UNMAPPED	104	GLN	HA	4.319	0.05	1
UNMAPPED	104	GLN	CB	32.729	0.05	1
UNMAPPED	15	VAL	C	176.952	0.05	1
UNMAPPED	155	TYR	HB3	2.91	0.05	1
UNMAPPED	44	ASP	HB2	2.823	0.05	1
UNMAPPED	104	GLN	N	119.57	0.05	1
UNMAPPED	27	LEU	HB2	-0.434	0.05	1
UNMAPPED	139	LYS	CB	32.806	0.05	1
UNMAPPED	36	ILE	HG12	1.158	0.05	1
UNMAPPED	51	VAL	CB	31.888	0.05	1
UNMAPPED	49	ASP	HA	4.602	0.05	1
UNMAPPED	52	THR	HG23	1.141	0.05	1
UNMAPPED	69	ASP	HA	4.626	0.05	1
UNMAPPED	35	GLN	HB3	2.366	0.05	1
UNMAPPED	61	VAL	HB	2.096	0.05	1
UNMAPPED	72	VAL	HG11	0.895	0.05	1
UNMAPPED	143	GLU	H	8.157	0.05	1
UNMAPPED	164	GLU	HA	4.27	0.05	1
UNMAPPED	129	HIS	H	8.477	0.05	1
UNMAPPED	37	ALA	HB3	1.367	0.05	1
UNMAPPED	34	LEU	HD23	1.147	0.05	1
UNMAPPED	165	SER	CB	62.851	0.05	1
UNMAPPED	136	ARG	H	7.975	0.05	1
UNMAPPED	144	THR	CB	68.814	0.05	1
UNMAPPED	119	VAL	HG13	0.927	0.05	1
UNMAPPED	15	VAL	HG12	0.913	0.05	1
UNMAPPED	138	THR	HA	4.346	0.05	1
UNMAPPED	33	ASP	C	174.953	0.05	1
UNMAPPED	158	GLY	CA	44.611	0.05	1
UNMAPPED	105	GLN	HB3	2.064	0.05	1
UNMAPPED	154	GLY	HA3	3.88	0.05	1
UNMAPPED	16	THR	HA	4.15	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	10	ARG	HB3	2.037	0.05	1
UNMAPPED	157	LEU	CB	41.75	0.05	1
UNMAPPED	73	THR	CB	68.89	0.05	1
UNMAPPED	92	GLN	H	8.11	0.05	1
UNMAPPED	147	PRO	HB2	2.166	0.05	1
UNMAPPED	6	GLN	N	119.359	0.05	1
UNMAPPED	116	ASN	HB2	2.72	0.05	1
UNMAPPED	9	LEU	CB	41.903	0.05	1
UNMAPPED	68	SER	HB3	3.906	0.05	1
UNMAPPED	9	LEU	HD21	0.952	0.05	1
UNMAPPED	168	VAL	N	123.809	0.05	1
UNMAPPED	160	ALA	H	8.304	0.05	1
UNMAPPED	23	ALA	HA	3.221	0.05	1
UNMAPPED	99	SER	HA	4.444	0.05	1
UNMAPPED	8	ALA	HB2	1.829	0.05	1
UNMAPPED	142	GLY	H	8.417	0.05	1
UNMAPPED	9	LEU	N	118.935	0.05	1
UNMAPPED	28	GLU	CB	28.372	0.05	1
UNMAPPED	96	ALA	HA	4.273	0.05	1
UNMAPPED	67	PRO	HA	4.354	0.05	1
UNMAPPED	38	LEU	HD21	0.768	0.05	1
UNMAPPED	42	TYR	CA	60.052	0.05	1
UNMAPPED	126	ALA	HA	4.309	0.05	1
UNMAPPED	42	TYR	HB2	2.815	0.05	1
UNMAPPED	66	ALA	HB2	1.369	0.05	1
UNMAPPED	19	GLU	HB3	2.36	0.05	1
UNMAPPED	71	ARG	HA	4.566	0.05	1
UNMAPPED	106	ILE	HB	1.823	0.05	1
UNMAPPED	53	ILE	HA	4.341	0.05	1
UNMAPPED	168	VAL	HG23	0.876	0.05	1
UNMAPPED	115	PRO	HG2	2.029	0.05	1
UNMAPPED	62	SER	HB3	3.924	0.05	1
UNMAPPED	92	GLN	HA	4.263	0.05	1
UNMAPPED	126	ALA	HB3	1.398	0.05	1
UNMAPPED	43	GLU	C	176.411	0.05	1
UNMAPPED	137	VAL	HG13	0.92	0.05	1
UNMAPPED	103	GLY	N	110.67	0.05	1
UNMAPPED	96	ALA	HB3	1.86	0.05	1
UNMAPPED	23	ALA	C	177.73	0.05	1
UNMAPPED	25	PHE	HB3	3.129	0.05	1
UNMAPPED	98	GLY	HA3	4.004	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	10	ARG	HE	7.372	0.05	1
UNMAPPED	121	ASP	N	120.63	0.05	1
UNMAPPED	34	LEU	H	8.814	0.05	1
UNMAPPED	22	ARG	HG2	1.896	0.05	1
UNMAPPED	129	HIS	N	118.723	0.05	1
UNMAPPED	67	PRO	HB2	1.948	0.05	1
UNMAPPED	5	ARG	CA	59.028	0.05	1
UNMAPPED	17	GLY	C	173.099	0.05	1
UNMAPPED	68	SER	H	8.345	0.05	1
UNMAPPED	148	ARG	N	122.537	0.05	1
UNMAPPED	52	THR	N	117.621	0.05	1
UNMAPPED	62	SER	CA	57.782	0.05	1
UNMAPPED	156	ARG	N	122.043	0.05	1
UNMAPPED	124	LYS	CA	55.129	0.05	1
UNMAPPED	6	GLN	HE22	7.447	0.05	1
UNMAPPED	100	GLU	H	8.61	0.05	1
UNMAPPED	137	VAL	HG23	0.924	0.05	1
UNMAPPED	150	PHE	CB	38.234	0.05	1
UNMAPPED	159	ALA	HA	4.33	0.05	1
UNMAPPED	74	SER	HA	4.379	0.05	1
UNMAPPED	47	ASP	CB	39.61	0.05	1
UNMAPPED	80	HIS	N	121.69	0.05	1
UNMAPPED	160	ALA	N	124.657	0.05	1
UNMAPPED	27	LEU	HD11	0.523	0.05	1
UNMAPPED	70	ASN	H	8.34	0.05	1
UNMAPPED	11	GLU	HA	4.19	0.05	1
UNMAPPED	168	VAL	HG13	0.877	0.05	1
UNMAPPED	24	ARG	HA	3.402	0.05	1
UNMAPPED	26	PHE	HA	3.64	0.05	1
UNMAPPED	160	ALA	CB	17.974	0.05	1
UNMAPPED	151	ALA	N	123.173	0.05	1
UNMAPPED	61	VAL	HG21	0.925	0.05	1
UNMAPPED	29	SER	HA	4.002	0.05	1
UNMAPPED	79	ILE	HB	1.797	0.05	1
UNMAPPED	9	LEU	HB2	1.815	0.05	1
UNMAPPED	90	GLU	N	121.266	0.05	1
UNMAPPED	22	ARG	N	122.095	0.05	1
UNMAPPED	140	SER	CA	55.784	0.05	1
UNMAPPED	15	VAL	CA	64.368	0.05	1
UNMAPPED	44	ASP	CB	39.61	0.05	1
UNMAPPED	58	PRO	CB	31.583	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	136	ARG	HA	4.357	0.05	1
UNMAPPED	46	GLY	HA2	3.504	0.05	1
UNMAPPED	39	ALA	N	120.418	0.05	1
UNMAPPED	144	THR	HB	4.263	0.05	1
UNMAPPED	103	GLY	HA2	3.966	0.05	1
UNMAPPED	134	VAL	CA	61.649	0.05	1
UNMAPPED	6	GLN	HG2	2.411	0.05	1
UNMAPPED	76	ARG	HA	4.192	0.05	1
UNMAPPED	73	THR	HG22	1.178	0.05	1
UNMAPPED	1	MET	HB3	1.993	0.05	1
UNMAPPED	140	SER	H	8.488	0.05	1
UNMAPPED	116	ASN	H	8.33	0.05	1
UNMAPPED	36	ILE	HG22	0.992	0.05	1
UNMAPPED	41	PHE	CB	38.616	0.05	1
UNMAPPED	138	THR	HB	4.159	0.05	1
UNMAPPED	34	LEU	HA	3.953	0.05	1
UNMAPPED	12	PHE	H	8.867	0.05	1
UNMAPPED	8	ALA	H	8.061	0.05	1
UNMAPPED	92	GLN	HB2	1.972	0.05	1
UNMAPPED	53	ILE	CA	60.895	0.05	1
UNMAPPED	27	LEU	HD22	0.52	0.05	1
UNMAPPED	23	ALA	H	8.317	0.05	1
UNMAPPED	30	ALA	HB1	1.48	0.05	1
UNMAPPED	34	LEU	HG	1.936	0.05	1
UNMAPPED	108	GLY	H	8.269	0.05	1
UNMAPPED	62	SER	H	8.256	0.05	1
UNMAPPED	124	LYS	H	8.024	0.05	1
UNMAPPED	70	ASN	HB3	2.764	0.05	1
UNMAPPED	53	ILE	HD11	0.841	0.05	1
UNMAPPED	119	VAL	HG21	0.926	0.05	1
UNMAPPED	139	LYS	H	8.365	0.05	1
UNMAPPED	116	ASN	HA	4.622	0.05	1
UNMAPPED	56	ALA	N	124.657	0.05	1
UNMAPPED	74	SER	H	8.304	0.05	1
UNMAPPED	106	ILE	N	122.749	0.05	1
UNMAPPED	165	SER	HB2	3.859	0.05	1
UNMAPPED	146	LYS	N	122.011	0.05	1
UNMAPPED	136	ARG	N	126.988	0.05	1
UNMAPPED	45	GLY	N	109.017	0.05	1
UNMAPPED	51	VAL	H	8.061	0.05	1
UNMAPPED	10	ARG	HG2	1.675	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	50	ILE	N	120.206	0.05	1
UNMAPPED	132	VAL	HA	4.089	0.05	1
UNMAPPED	20	GLU	HA	3.677	0.05	1
UNMAPPED	72	VAL	HG22	0.895	0.05	1
UNMAPPED	53	ILE	HG23	0.893	0.05	1
UNMAPPED	148	ARG	HB2	1.804	0.05	1
UNMAPPED	143	GLU	CB	29.901	0.05	1
UNMAPPED	119	VAL	CA	62.14	0.05	1
UNMAPPED	50	ILE	CB	37.928	0.05	1
UNMAPPED	132	VAL	N	119.528	0.05	1
UNMAPPED	63	ARG	N	123.385	0.05	1
UNMAPPED	2	ALA	HB1	1.383	0.05	1
UNMAPPED	143	GLU	N	120.63	0.05	1
UNMAPPED	42	TYR	HA	4.22	0.05	1
UNMAPPED	139	LYS	HG2	1.413	0.05	1
UNMAPPED	92	GLN	NE2	112.399	0.05	1
UNMAPPED	16	THR	CA	62.435	0.05	1
UNMAPPED	50	ILE	HD12	0.856	0.05	1
UNMAPPED	136	ARG	HB2	1.758	0.05	1
UNMAPPED	71	ARG	N	121.054	0.05	1
UNMAPPED	105	GLN	HG2	2.315	0.05	1
UNMAPPED	130	GLY	HA2	3.949	0.05	1
UNMAPPED	102	SER	HB2	3.886	0.05	1
UNMAPPED	134	VAL	HG21	0.919	0.05	1
UNMAPPED	6	GLN	NE2	111.687	0.05	1
UNMAPPED	61	VAL	HG13	0.925	0.05	1
UNMAPPED	39	ALA	HB2	1.561	0.05	1
UNMAPPED	50	ILE	HA	4.12	0.05	1
UNMAPPED	107	VAL	HG22	0.919	0.05	1
UNMAPPED	131	ALA	HB2	1.362	0.05	1
UNMAPPED	146	LYS	H	8.283	0.05	1
UNMAPPED	9	LEU	H	8.284	0.05	1
UNMAPPED	131	ALA	HB3	1.362	0.05	1
UNMAPPED	27	LEU	HA	3.238	0.05	1
UNMAPPED	37	ALA	HA	4.012	0.05	1
UNMAPPED	25	PHE	HE1	6.938	0.05	1
UNMAPPED	158	GLY	HA2	3.884	0.05	1
UNMAPPED	104	GLN	CA	55.456	0.05	1
UNMAPPED	117	GLU	CA	56.275	0.05	1
UNMAPPED	73	THR	H	8.146	0.05	1
UNMAPPED	133	ALA	CA	51.754	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	137	VAL	HA	4.181	0.05	1
UNMAPPED	52	THR	CA	61.747	0.05	1
UNMAPPED	148	ARG	CA	53.261	0.05	1
UNMAPPED	41	PHE	HA	3.262	0.05	1
UNMAPPED	103	GLY	H	8.468	0.05	1
UNMAPPED	133	ALA	CB	18.815	0.05	1
UNMAPPED	67	PRO	HB3	2.312	0.05	1
UNMAPPED	7	ASP	HB2	2.776	0.05	1
UNMAPPED	36	ILE	HG13	1.475	0.05	1
UNMAPPED	107	VAL	HG11	0.919	0.05	1
UNMAPPED	57	THR	HG21	1.246	0.05	1
UNMAPPED	52	THR	HG22	1.141	0.05	1
UNMAPPED	56	ALA	HB1	1.377	0.05	1
UNMAPPED	73	THR	HG23	1.178	0.05	1
UNMAPPED	34	LEU	N	128.212	0.05	1
UNMAPPED	144	THR	HG21	1.212	0.05	1
UNMAPPED	79	ILE	N	119.782	0.05	1
UNMAPPED	133	ALA	N	128.047	0.05	1
UNMAPPED	97	GLY	CA	44.775	0.05	1
UNMAPPED	21	ASP	HA	4.36	0.05	1
UNMAPPED	47	ASP	HB3	2.814	0.05	1
UNMAPPED	34	LEU	HD13	1.011	0.05	1
UNMAPPED	155	TYR	N	119.994	0.05	1
UNMAPPED	77	ASP	HB2	2.628	0.05	1
UNMAPPED	165	SER	CA	57.979	0.05	1
UNMAPPED	1	MET	CB	28.831	0.05	1
UNMAPPED	15	VAL	HG13	0.913	0.05	1
UNMAPPED	140	SER	CB	62.698	0.05	1
UNMAPPED	26	PHE	N	118.708	0.05	1
UNMAPPED	16	THR	HB	3.317	0.05	1
UNMAPPED	10	ARG	HB2	2.009	0.05	1
UNMAPPED	124	LYS	N	122.113	0.05	1
UNMAPPED	42	TYR	HE1	6.719	0.05	1
UNMAPPED	54	SER	H	8.3	0.05	1
UNMAPPED	158	GLY	N	110.458	0.05	1
UNMAPPED	57	THR	CB	68.737	0.05	1
UNMAPPED	156	ARG	H	8.02	0.05	1
UNMAPPED	65	THR	HB	4.2	0.05	1
UNMAPPED	46	GLY	H	8.167	0.05	1
UNMAPPED	119	VAL	HB	2.086	0.05	1
UNMAPPED	135	GLU	N	124.657	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	31	GLY	H	7.808	0.05	1
UNMAPPED	78	LEU	N	121.69	0.05	1
UNMAPPED	72	VAL	HG13	0.895	0.05	1
UNMAPPED	142	GLY	HA2	3.949	0.05	1
UNMAPPED	8	ALA	HB1	1.829	0.05	1
UNMAPPED	57	THR	N	115.756	0.05	1
UNMAPPED	168	VAL	HA	3.983	0.05	1
UNMAPPED	38	LEU	HD22	0.768	0.05	1
UNMAPPED	167	TYR	H	8.05	0.05	1
UNMAPPED	168	VAL	HB	1.954	0.05	1
UNMAPPED	66	ALA	HB3	1.369	0.05	1
UNMAPPED	132	VAL	HG22	0.919	0.05	1
UNMAPPED	13	VAL	HG23	1.098	0.05	1
UNMAPPED	126	ALA	HB2	1.398	0.05	1
UNMAPPED	72	VAL	HA	4.08	0.05	1
UNMAPPED	140	SER	HB2	3.851	0.05	1
UNMAPPED	168	VAL	HG22	0.876	0.05	1
UNMAPPED	115	PRO	HG3	2.029	0.05	1
UNMAPPED	139	LYS	HD3	1.73	0.05	1
UNMAPPED	19	GLU	HA	4.299	0.05	1
UNMAPPED	13	VAL	N	121.902	0.05	1
UNMAPPED	103	GLY	CA	44.677	0.05	1
UNMAPPED	39	ALA	H	7.773	0.05	1
UNMAPPED	10	ARG	HA	3.987	0.05	1
UNMAPPED	166	ALA	N	125.504	0.05	1
UNMAPPED	51	VAL	HG21	0.922	0.05	1
UNMAPPED	76	ARG	N	121.69	0.05	1
UNMAPPED	96	ALA	HB2	1.86	0.05	1
UNMAPPED	135	GLU	CA	55.882	0.05	1
UNMAPPED	11	GLU	HG3	2.41	0.05	1
UNMAPPED	47	ASP	H	8.137	0.05	1
UNMAPPED	107	VAL	HG12	0.919	0.05	1
UNMAPPED	116	ASN	N	116.486	0.05	1
UNMAPPED	120	ASP	HA	4.582	0.05	1
UNMAPPED	134	VAL	HB	2.031	0.05	1
UNMAPPED	94	PHE	HA	4.577	0.05	1
UNMAPPED	137	VAL	H	8.208	0.05	1
UNMAPPED	90	GLU	HB3	2.072	0.05	1
UNMAPPED	32	TRP	HH2	7.164	0.05	1
UNMAPPED	5	ARG	N	120.206	0.05	1
UNMAPPED	116	ASN	CB	37.928	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	128	GLU	HA	4.214	0.05	1
UNMAPPED	138	THR	CA	61.026	0.05	1
UNMAPPED	166	ALA	CB	18.815	0.05	1
UNMAPPED	6	GLN	HE21	6.906	0.05	1
UNMAPPED	32	TRP	HE3	7.415	0.05	1
UNMAPPED	38	LEU	H	8.707	0.05	1
UNMAPPED	5	ARG	CB	29.213	0.05	1
UNMAPPED	13	VAL	HG11	1.018	0.05	1
UNMAPPED	13	VAL	HB	2.208	0.05	1
UNMAPPED	118	LEU	HA	4.33	0.05	1
UNMAPPED	43	GLU	HA	4.203	0.05	1
UNMAPPED	23	ALA	CB	19.962	0.05	1
UNMAPPED	58	PRO	HA	4.363	0.05	1
UNMAPPED	24	ARG	HB2	1.83	0.05	1
UNMAPPED	62	SER	CB	62.851	0.05	1
UNMAPPED	23	ALA	N	121.266	0.05	1
UNMAPPED	124	LYS	CB	32.271	0.05	1
UNMAPPED	33	ASP	CA	52.704	0.05	1
UNMAPPED	14	ALA	HB3	1.541	0.05	1
UNMAPPED	123	PHE	CA	57.652	0.05	1
UNMAPPED	74	SER	N	118.299	0.05	1
UNMAPPED	118	LEU	CB	41.521	0.05	1
UNMAPPED	14	ALA	N	124.021	0.05	1
UNMAPPED	96	ALA	CA	51.819	0.05	1
UNMAPPED	49	ASP	N	120.206	0.05	1
UNMAPPED	74	SER	CB	63.157	0.05	1
UNMAPPED	38	LEU	HA	3.72	0.05	1
UNMAPPED	130	GLY	H	8.411	0.05	1
UNMAPPED	52	THR	HA	4.333	0.05	1
UNMAPPED	7	ASP	CA	56.123	0.05	1
UNMAPPED	22	ARG	HB2	2.069	0.05	1
UNMAPPED	127	LYS	CB	32.424	0.05	1
UNMAPPED	9	LEU	HB3	2.052	0.05	1
UNMAPPED	128	GLU	HB2	1.899	0.05	1
UNMAPPED	61	VAL	CA	61.845	0.05	1
UNMAPPED	50	ILE	H	7.873	0.05	1
UNMAPPED	56	ALA	H	8.215	0.05	1
UNMAPPED	167	TYR	HA	4.513	0.05	1
UNMAPPED	134	VAL	N	119.994	0.05	1
UNMAPPED	10	ARG	H	8.11	0.05	1
UNMAPPED	37	ALA	HB1	1.367	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	103	GLY	HA3	3.968	0.05	1
UNMAPPED	167	TYR	CB	38.157	0.05	1
UNMAPPED	11	GLU	HB2	2.072	0.05	1
UNMAPPED	120	ASP	HB3	2.653	0.05	1
UNMAPPED	60	SER	CA	58.012	0.05	1
UNMAPPED	26	PHE	HE1	7.459	0.05	1
UNMAPPED	65	THR	HG21	1.189	0.05	1
UNMAPPED	36	ILE	HG21	0.992	0.05	1
UNMAPPED	104	GLN	HB3	2.087	0.05	1
UNMAPPED	51	VAL	HG13	0.921	0.05	1
UNMAPPED	61	VAL	HG22	0.925	0.05	1
UNMAPPED	143	GLU	HB3	2.087	0.05	1
UNMAPPED	37	ALA	HB2	1.367	0.05	1
UNMAPPED	159	ALA	HB2	1.346	0.05	1
UNMAPPED	27	LEU	HD23	0.52	0.05	1
UNMAPPED	54	SER	HB3	3.866	0.05	1
UNMAPPED	122	LEU	HA	4.13	0.05	1
UNMAPPED	61	VAL	HG23	0.925	0.05	1
UNMAPPED	69	ASP	H	8.279	0.05	1
UNMAPPED	117	GLU	HA	4.249	0.05	1
UNMAPPED	33	ASP	H	6.867	0.05	1
UNMAPPED	65	THR	N	113.637	0.05	1
UNMAPPED	118	LEU	CA	54.932	0.05	1
UNMAPPED	14	ALA	H	8.269	0.05	1
UNMAPPED	102	SER	CB	62.927	0.05	1
UNMAPPED	36	ILE	HD13	0.883	0.05	1
UNMAPPED	117	GLU	H	8.084	0.05	1
UNMAPPED	80	HIS	H	8.415	0.05	1
UNMAPPED	140	SER	HA	4.381	0.05	1
UNMAPPED	116	ASN	HD21	6.945	0.05	1
UNMAPPED	20	GLU	HG3	2.365	0.05	1
UNMAPPED	100	GLU	HG3	2.281	0.05	1
UNMAPPED	72	VAL	CA	62.271	0.05	1
UNMAPPED	107	VAL	HG13	0.919	0.05	1
UNMAPPED	18	ALA	HB2	1.339	0.05	1
UNMAPPED	69	ASP	HB3	2.68	0.05	1
UNMAPPED	10	ARG	HG3	1.851	0.05	1
UNMAPPED	105	GLN	N	121.902	0.05	1
UNMAPPED	95	TYR	HA	4.517	0.05	1
UNMAPPED	99	SER	CB	63.08	0.05	1
UNMAPPED	29	SER	HB3	3.59	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	72	VAL	HG23	0.895	0.05	1
UNMAPPED	22	ARG	H	7.315	0.05	1
UNMAPPED	148	ARG	HB3	1.804	0.05	1
UNMAPPED	143	GLU	CA	55.948	0.05	1
UNMAPPED	24	ARG	C	176.213	0.05	1
UNMAPPED	104	GLN	HB2	1.952	0.05	1
UNMAPPED	18	ALA	H	7.951	0.05	1
UNMAPPED	99	SER	N	115.544	0.05	1
UNMAPPED	95	TYR	N	121.69	0.05	1
UNMAPPED	3	GLU	C	177.411	0.05	1
UNMAPPED	127	LYS	HB2	1.747	0.05	1
UNMAPPED	59	SER	CB	62.851	0.05	1
UNMAPPED	30	ALA	N	121.266	0.05	1
UNMAPPED	132	VAL	HG12	0.92	0.05	1
UNMAPPED	34	LEU	C	176.65	0.05	1
UNMAPPED	165	SER	HA	4.384	0.05	1
UNMAPPED	18	ALA	N	122.113	0.05	1
UNMAPPED	2	ALA	C	179.203	0.05	1
UNMAPPED	130	GLY	HA3	3.949	0.05	1
UNMAPPED	99	SER	H	8.266	0.05	1
UNMAPPED	28	GLU	C	180.164	0.05	1
UNMAPPED	134	VAL	HG22	0.919	0.05	1
UNMAPPED	50	ILE	HG12	1.171	0.05	1
UNMAPPED	133	ALA	HB3	1.354	0.05	1
UNMAPPED	31	GLY	N	110.458	0.05	1
UNMAPPED	39	ALA	HB3	1.561	0.05	1
UNMAPPED	50	ILE	HB	1.88	0.05	1
UNMAPPED	107	VAL	HG23	0.919	0.05	1
UNMAPPED	36	ILE	CA	63.877	0.05	1
UNMAPPED	119	VAL	HG11	0.927	0.05	1
UNMAPPED	39	ALA	CB	17.592	0.05	1
UNMAPPED	20	GLU	CA	60.371	0.05	1
UNMAPPED	38	LEU	HD13	0.091	0.05	1
UNMAPPED	144	THR	H	8.246	0.05	1
UNMAPPED	26	PHE	HB3	2.894	0.05	1
UNMAPPED	18	ALA	CA	51.361	0.05	1
UNMAPPED	64	GLY	N	109.61	0.05	1
UNMAPPED	141	PRO	HB2	1.975	0.05	1
UNMAPPED	117	GLU	CB	29.748	0.05	1
UNMAPPED	74	SER	HB2	3.857	0.05	1
UNMAPPED	63	ARG	H	8.402	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	40	SER	C	175.013	0.05	1
UNMAPPED	127	LYS	N	119.782	0.05	1
UNMAPPED	3	GLU	CA	58.34	0.05	1
UNMAPPED	39	ALA	CA	54.866	0.05	1
UNMAPPED	34	LEU	CA	58.012	0.05	1
UNMAPPED	7	ASP	HB3	2.871	0.05	1
UNMAPPED	51	VAL	N	123.597	0.05	1
UNMAPPED	166	ALA	HA	4.286	0.05	1
UNMAPPED	18	ALA	CB	19.656	0.05	1
UNMAPPED	91	GLY	HA3	3.954	0.05	1
UNMAPPED	43	GLU	HB3	2.186	0.05	1
UNMAPPED	25	PHE	H	7.44	0.05	1
UNMAPPED	144	THR	HA	4.371	0.05	1
UNMAPPED	37	ALA	CA	54.899	0.05	1
UNMAPPED	138	THR	HG23	1.179	0.05	1
UNMAPPED	34	LEU	HD12	1.011	0.05	1
UNMAPPED	44	ASP	CA	53.621	0.05	1
UNMAPPED	77	ASP	HB3	2.763	0.05	1
UNMAPPED	76	ARG	H	8.097	0.05	1
UNMAPPED	12	PHE	HE1	6.525	0.05	1
UNMAPPED	11	GLU	CA	58.438	0.05	1
UNMAPPED	61	VAL	HG11	0.925	0.05	1
UNMAPPED	38	LEU	N	118.299	0.05	1
UNMAPPED	169	ALA	CA	52.081	0.05	1
UNMAPPED	71	ARG	H	8.242	0.05	1
UNMAPPED	38	LEU	CB	41.598	0.05	1
UNMAPPED	5	ARG	H	7.931	0.05	1
UNMAPPED	54	SER	N	119.147	0.05	1
UNMAPPED	97	GLY	H	7.849	0.05	1
UNMAPPED	159	ALA	CA	51.328	0.05	1
UNMAPPED	47	ASP	HB2	2.661	0.05	1
UNMAPPED	48	GLU	HB2	1.89	0.05	1
UNMAPPED	6	GLN	CB	27.76	0.05	1
UNMAPPED	16	THR	C	176.513	0.05	1
UNMAPPED	47	ASP	HA	4.615	0.05	1
UNMAPPED	72	VAL	HG12	0.895	0.05	1
UNMAPPED	137	VAL	CA	61.681	0.05	1
UNMAPPED	170	GLY	HA3	3.948	0.05	1
UNMAPPED	38	LEU	HD23	0.768	0.05	1
UNMAPPED	59	SER	H	8.438	0.05	1
UNMAPPED	3	GLU	H	8.442	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	132	VAL	HG23	0.919	0.05	1
UNMAPPED	115	PRO	HB3	2.31	0.05	1
UNMAPPED	13	VAL	HG22	1.098	0.05	1
UNMAPPED	136	ARG	HG2	1.631	0.05	1
UNMAPPED	11	GLU	C	176.952	0.05	1
UNMAPPED	168	VAL	HG21	0.876	0.05	1
UNMAPPED	167	TYR	CA	57.488	0.05	1
UNMAPPED	143	GLU	HG3	2.285	0.05	1
UNMAPPED	49	ASP	HB3	2.737	0.05	1
UNMAPPED	10	ARG	N	117.875	0.05	1
UNMAPPED	41	PHE	C	176.73	0.05	1
UNMAPPED	172	ARG	N	120.773	0.05	1
UNMAPPED	12	PHE	C	179.627	0.05	1
UNMAPPED	136	ARG	CA	56.963	0.05	1
UNMAPPED	10	ARG	CB	28.983	0.05	1
UNMAPPED	11	GLU	HG2	2.437	0.05	1
UNMAPPED	129	HIS	HB3	3.286	0.05	1
UNMAPPED	44	ASP	HA	4.714	0.05	1
UNMAPPED	134	VAL	HA	4.076	0.05	1
UNMAPPED	136	ARG	HB3	1.824	0.05	1
UNMAPPED	90	GLU	HB2	2.011	0.05	1
UNMAPPED	47	ASP	CA	53.447	0.05	1
UNMAPPED	127	LYS	HB3	1.747	0.05	1
UNMAPPED	26	PHE	H	7.82	0.05	1
UNMAPPED	95	TYR	HD1	7.08	0.05	1
UNMAPPED	158	GLY	HA3	3.949	0.05	1
UNMAPPED	141	PRO	CA	63.123	0.05	1
UNMAPPED	24	ARG	CA	59.65	0.05	1
UNMAPPED	79	ILE	H	7.931	0.05	1
UNMAPPED	55	GLN	H	8.281	0.05	1
UNMAPPED	13	VAL	HG12	1.018	0.05	1
UNMAPPED	23	ALA	HB1	1.115	0.05	1
UNMAPPED	115	PRO	CB	31.43	0.05	1
UNMAPPED	23	ALA	CA	54.211	0.05	1
UNMAPPED	33	ASP	N	118.511	0.05	1
UNMAPPED	147	PRO	HB3	2.265	0.05	1
UNMAPPED	24	ARG	HB3	1.914	0.05	1
UNMAPPED	91	GLY	H	8.386	0.05	1
UNMAPPED	26	PHE	HD1	7.597	0.05	1
UNMAPPED	123	PHE	H	8.114	0.05	1
UNMAPPED	33	ASP	CB	41.674	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	ALA	HB2	1.541	0.05	1
UNMAPPED	65	THR	HG23	1.189	0.05	1
UNMAPPED	14	ALA	CB	17.898	0.05	1
UNMAPPED	137	VAL	HG21	0.924	0.05	1
UNMAPPED	141	PRO	HB3	2.304	0.05	1
UNMAPPED	5	ARG	C	177.211	0.05	1
UNMAPPED	123	PHE	HB2	3.042	0.05	1
UNMAPPED	42	TYR	H	8.06	0.05	1
UNMAPPED	17	GLY	CA	45.004	0.05	1
UNMAPPED	51	VAL	HG12	0.921	0.05	1
UNMAPPED	126	ALA	CA	52.147	0.05	1
UNMAPPED	27	LEU	HD13	0.523	0.05	1
UNMAPPED	168	VAL	HG11	0.877	0.05	1
UNMAPPED	52	THR	HB	4.154	0.05	1
UNMAPPED	21	ASP	HB3	2.684	0.05	1
UNMAPPED	167	TYR	N	119.57	0.05	1
UNMAPPED	140	SER	N	119.147	0.05	1
UNMAPPED	22	ARG	HB3	2.171	0.05	1
UNMAPPED	127	LYS	CA	56.013	0.05	1
UNMAPPED	21	ASP	N	116.392	0.05	1
UNMAPPED	97	GLY	HA3	3.918	0.05	1
UNMAPPED	128	GLU	HB3	1.968	0.05	1
UNMAPPED	133	ALA	HB1	1.354	0.05	1
UNMAPPED	22	ARG	CB	29.595	0.05	1
UNMAPPED	19	GLU	CA	55.751	0.05	1
UNMAPPED	61	VAL	CB	32.118	0.05	1
UNMAPPED	169	ALA	HB3	1.398	0.05	1
UNMAPPED	21	ASP	CB	38.922	0.05	1
UNMAPPED	16	THR	HG22	-0.154	0.05	1
UNMAPPED	40	SER	CA	60.993	0.05	1
UNMAPPED	124	LYS	HA	4.201	0.05	1
UNMAPPED	10	ARG	NE	110.882	0.05	1
UNMAPPED	169	ALA	HB2	1.398	0.05	1
UNMAPPED	58	PRO	HB3	2.24	0.05	1
UNMAPPED	16	THR	HG21	-0.154	0.05	1
UNMAPPED	143	GLU	HB2	1.991	0.05	1
UNMAPPED	141	PRO	CB	31.43	0.05	1
UNMAPPED	11	GLU	HB3	2.244	0.05	1
UNMAPPED	48	GLU	CA	55.97	0.05	1
UNMAPPED	5	ARG	HA	4.064	0.05	1
UNMAPPED	51	VAL	HG11	0.921	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	125	GLY	N	108.762	0.05	1
UNMAPPED	4	GLU	CB	28.525	0.05	1
UNMAPPED	55	GLN	HB3	2.139	0.05	1
UNMAPPED	95	TYR	HB3	3.0	0.05	1
UNMAPPED	135	GLU	HG3	2.258	0.05	1
UNMAPPED	4	GLU	N	119.57	0.05	1
UNMAPPED	169	ALA	HB1	1.398	0.05	1
UNMAPPED	159	ALA	HB3	1.346	0.05	1
UNMAPPED	66	ALA	H	8.4	0.05	1

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	125	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	111	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	46	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	134	0.00 ± 0.00	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/439 (0%)	0/175 (0%)	0/178 (0%)	0/86 (0%)
Sidechain	0/619 (0%)	0/359 (0%)	0/227 (0%)	0/33 (0%)
Aromatic	0/50 (0%)	0/28 (0%)	0/20 (0%)	0/2 (0%)
Overall	0/1108 (0%)	0/562 (0%)	0/425 (0%)	0/121 (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 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/439 (0%)	0/175 (0%)	0/178 (0%)	0/86 (0%)
Sidechain	0/619 (0%)	0/359 (0%)	0/227 (0%)	0/33 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/50 (0%)	0/28 (0%)	0/20 (0%)	0/2 (0%)
Overall	0/1108 (0%)	0/562 (0%)	0/425 (0%)	0/121 (0%)

7.2.4 Statistically unusual chemical shifts

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

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
???	UNMAPPED	10	ARG	NE	110.88	92.63 – 76.73	16.5
???	UNMAPPED	27	LEU	HB2	-0.43	3.32 – -0.08	-6.0
???	UNMAPPED	16	THR	HG21	-0.15	2.29 – -0.01	-5.6
???	UNMAPPED	16	THR	HG22	-0.15	2.29 – -0.01	-5.6
???	UNMAPPED	16	THR	HG23	-0.15	2.29 – -0.01	-5.6

7.2.5 Random Coil Index (RCI) plots

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.

7.3 Chemical shift list 3

File name: BMRB entry 5876

Chemical shift list name: *assigned_chem_shift_list_1*

7.3.1 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	1950
Number of shifts mapped to atoms	954
Number of unparsed shifts	0
Number of shifts with mapping errors	996
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

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

- Residue not found in structure. All 996 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	68	HIS	HB2	1.775	0.05	1
A	8	GLN	HB3	2.016	0.05	1
A	10	VAL	HB	1.857	0.05	1
A	22	SER	CB	67.864	0.05	1
A	74	VAL	HB	1.444	0.05	1
A	80	PHE	HA	4.445	0.05	1
A	33	ASP	CB	42.805	0.05	1
A	40	LEU	HD11	0.628	0.05	1
A	70	ASP	HB3	2.65	0.05	1
A	52	LEU	CB	41.843	0.05	1
A	26	GLY	CA	45.28	0.05	1
A	90	LEU	CB	42.985	0.05	1
A	75	LYS	HG3	1.279	0.05	1
A	36	ASN	HB2	3.022	0.05	1
A	73	PHE	CA	59.542	0.05	1
A	67	ASP	N	125.299	0.05	1
A	19	THR	HG22	1.162	0.05	1
A	110	GLU	CB	30.24	0.05	1
A	41	GLU	HG2	2.178	0.05	1
A	97	VAL	HB	1.9	0.05	1
A	8	GLN	H	8.175	0.05	1
A	20	GLY	CA	45.349	0.05	1
A	17	TRP	CA	56.009	0.05	1
A	76	PRO	HB2	0.413	0.05	1
A	81	LYS	HB2	1.525	0.05	1
A	71	GLU	HB3	2.34	0.05	1
A	63	LEU	HD11	0.627	0.05	1
A	88	GLN	N	119.692	0.05	1
A	21	PHE	H	8.507	0.05	1
A	38	GLN	N	118.1	0.05	1
A	84	THR	C	173.651	0.05	1
A	73	PHE	HD1	5.649	0.05	1
A	47	GLU	CA	53.931	0.05	1
A	85	GLY	HA2	3.792	0.05	1
A	22	SER	H	9.928	0.05	1
A	50	ALA	CB	18.614	0.05	1
A	47	GLU	HG2	1.899	0.05	1
A	19	THR	C	173.826	0.05	1
A	32	GLN	NE2	109.315	0.05	1
A	73	PHE	HE2	6.945	0.05	1
A	59	GLY	HA2	3.603	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	12	VAL	HB	1.653	0.05	1
A	29	ARG	HB2	-0.239	0.05	1
A	57	HIS	C	173.805	0.05	1
A	28	LEU	N	120.201	0.05	1
A	100	THR	CA	62.234	0.05	1
A	39	PHE	H	8.362	0.05	1
A	26	GLY	N	107.166	0.05	1
A	34	PRO	HD2	3.904	0.05	1
A	71	GLU	HG2	2.209	0.05	1
A	35	SER	CA	61.558	0.05	1
A	96	GLN	CA	56.277	0.05	1
A	93	THR	HA	4.256	0.05	1
A	36	ASN	N	118.949	0.05	1
A	48	VAL	N	122.18	0.05	1
A	21	PHE	HE2	6.756	0.05	1
A	42	SER	HB2	3.431	0.05	1
A	55	LEU	HD23	0.79	0.05	1
A	62	ASN	HB3	2.457	0.05	1
A	54	ARG	N	116.292	0.05	1
A	81	LYS	C	174.128	0.05	1
A	43	ILE	HG23	0.614	0.05	1
A	15	LYS	HG2	0.876	0.05	1
A	43	ILE	HD11	0.356	0.05	1
A	16	LEU	CB	42.898	0.05	1
A	10	VAL	HG23	0.79	0.05	1
A	88	GLN	HB2	1.849	0.05	1
A	11	HIS	HB3	3.084	0.05	1
A	11	HIS	CB	30.785	0.05	1
A	50	ALA	H	8.96	0.05	1
A	80	PHE	HB2	2.933	0.05	1
A	10	VAL	CB	35.37	0.05	1
A	17	TRP	HE3	6.934	0.05	1
A	57	HIS	CA	56.35	0.05	1
A	63	LEU	HB2	1.008	0.05	1
A	98	LEU	HD12	0.753	0.05	1
A	47	GLU	HB2	1.62	0.05	1
A	24	ASP	H	10.036	0.05	1
A	46	GLY	H	7.897	0.05	1
A	88	GLN	H	8.082	0.05	1
A	21	PHE	HA	6.158	0.05	1
A	21	PHE	CA	54.463	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	76	PRO	HG2	0.778	0.05	1
A	75	LYS	CB	34.555	0.05	1
A	13	VAL	HG23	0.79	0.05	1
A	9	ASP	H	8.062	0.05	1
A	43	ILE	HG13	1.224	0.05	1
A	67	ASP	C	174.107	0.05	1
A	60	GLN	HE21	6.705	0.05	1
A	99	ASN	CB	39.381	0.05	1
A	57	HIS	HB2	3.208	0.05	1
A	52	LEU	HG	2.178	0.05	1
A	69	ARG	C	180.93	0.05	1
A	90	LEU	HA	4.162	0.05	1
A	35	SER	N	115.007	0.05	1
A	28	LEU	HD12	-0.084	0.05	1
A	96	GLN	N	120.627	0.05	1
A	52	LEU	N	114.987	0.05	1
A	34	PRO	CD	51.832	0.05	1
A	36	ASN	CA	56.758	0.05	1
A	92	SER	N	115.758	0.05	1
A	42	SER	HA	3.827	0.05	1
A	48	VAL	CA	60.917	0.05	1
A	60	GLN	N	119.476	0.05	1
A	48	VAL	HG12	0.814	0.05	1
A	43	ILE	N	119.403	0.05	1
A	11	HIS	H	8.889	0.05	1
A	81	LYS	N	124.07	0.05	1
A	61	VAL	HG11	0.574	0.05	1
A	100	THR	HA	4.263	0.05	1
A	67	ASP	CB	41.35	0.05	1
A	53	ARG	C	175.683	0.05	1
A	102	SER	HB2	3.811	0.05	1
A	44	ARG	C	176.871	0.05	1
A	16	LEU	HD23	0.805	0.05	1
A	88	GLN	CB	30.212	0.05	1
A	66	GLU	C	173.222	0.05	1
A	33	ASP	C	175.108	0.05	1
A	25	ASN	CA	53.637	0.05	1
A	68	HIS	HA	4.75	0.05	1
A	50	ALA	N	128.816	0.05	1
A	44	ARG	NE	117.211	0.05	1
A	89	LYS	HB2	1.661	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	44	ARG	HD2	3.015	0.05	1
A	43	ILE	CG2	18.467	0.05	1
A	14	LEU	HD12	0.728	0.05	1
A	95	PRO	CB	32.497	0.05	1
A	43	ILE	HB	1.906	0.05	1
A	28	LEU	CB	41.98	0.05	1
A	53	ARG	CA	60.137	0.05	1
A	102	SER	N	119.221	0.05	1
A	50	ALA	HB3	1.348	0.05	1
A	22	SER	HB3	3.641	0.05	1
A	94	ALA	HB3	1.244	0.05	1
A	54	ARG	C	177.391	0.05	1
A	93	THR	CB	70.295	0.05	1
A	84	THR	HA	4.172	0.05	1
A	66	GLU	H	9.131	0.05	1
A	89	LYS	H	8.288	0.05	1
A	54	ARG	HE	7.025	0.05	1
A	14	LEU	HD23	0.728	0.05	1
A	96	GLN	HB2	1.893	0.05	1
A	52	LEU	CA	56.263	0.05	1
A	52	LEU	HB2	1.279	0.05	1
A	31	TYR	N	126.23	0.05	1
A	70	ASP	CA	53.932	0.05	1
A	23	LEU	CB	43.724	0.05	1
A	74	VAL	HG22	0.61	0.05	1
A	60	GLN	HB2	1.787	0.05	1
A	30	SER	HB3	3.882	0.05	1
A	54	ARG	HG3	1.527	0.05	1
A	18	LYS	N	121.17	0.05	1
A	21	PHE	HB2	2.96	0.05	1
A	67	ASP	HB3	2.836	0.05	1
A	60	GLN	HG2	2.147	0.05	1
A	69	ARG	HB3	1.782	0.05	1
A	101	SER	H	8.212	0.05	1
A	76	PRO	C	175.661	0.05	1
A	96	GLN	H	8.378	0.05	1
A	16	LEU	N	122.207	0.05	1
A	105	GLN	HB2	2.0	0.05	1
A	34	PRO	HB3	2.402	0.05	1
A	68	HIS	CB	29.481	0.05	1
A	16	LEU	HD13	0.805	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	63	LEU	HD22	0.627	0.05	1
A	59	GLY	H	7.543	0.05	1
A	10	VAL	N	120.491	0.05	1
A	82	ALA	CA	52.746	0.05	1
A	19	THR	N	100.489	0.05	1
A	28	LEU	H	7.115	0.05	1
A	76	PRO	HD3	3.801	0.05	1
A	51	GLU	C	176.935	0.05	1
A	104	ALA	HB1	1.284	0.05	1
A	50	ALA	CA	56.263	0.05	1
A	87	GLY	C	172.984	0.05	1
A	105	GLN	H	7.984	0.05	1
A	111	ALA	HB3	1.4	0.05	1
A	79	ALA	C	176.05	0.05	1
A	68	HIS	C	175.489	0.05	1
A	18	LYS	HE2	3.455	0.05	1
A	10	VAL	HG13	0.79	0.05	1
A	92	SER	C	173.697	0.05	1
A	58	GLY	N	107.009	0.05	1
A	38	GLN	HA	4.013	0.05	1
A	6	SER	C	173.878	0.05	1
A	24	ASP	HB3	2.712	0.05	1
A	35	SER	HB2	3.827	0.05	1
A	23	LEU	HD12	0.913	0.05	1
A	83	PHE	HB2	2.982	0.05	1
A	12	VAL	HG22	0.783	0.05	1
A	23	LEU	HD21	0.913	0.05	1
A	96	GLN	CB	30.316	0.05	1
A	20	GLY	H	6.985	0.05	1
A	44	ARG	N	122.028	0.05	1
A	65	MET	HB3	1.782	0.05	1
A	45	ARG	N	115.942	0.05	1
A	97	VAL	C	174.647	0.05	1
A	68	HIS	H	8.56	0.05	1
A	81	LYS	CB	34.054	0.05	1
A	98	LEU	HD23	0.753	0.05	1
A	51	GLU	HA	3.992	0.05	1
A	110	GLU	HB2	1.893	0.05	1
A	65	MET	HE3	1.95	0.05	1
A	33	ASP	HB3	2.829	0.05	1
A	78	GLY	H	8.251	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	16	LEU	CA	54.096	0.05	1
A	26	GLY	HA3	4.08	0.05	1
A	47	GLU	HA	4.347	0.05	1
A	15	LYS	HD2	1.482	0.05	1
A	90	LEU	HB2	1.835	0.05	1
A	7	GLY	N	110.908	0.05	1
A	8	GLN	CA	55.69	0.05	1
A	87	GLY	N	109.871	0.05	1
A	103	PRO	C	177.087	0.05	1
A	61	VAL	HG21	0.574	0.05	1
A	31	TYR	C	174.399	0.05	1
A	91	GLY	C	173.061	0.05	1
A	98	LEU	N	125.744	0.05	1
A	87	GLY	HA3	3.828	0.05	1
A	101	SER	HB3	3.763	0.05	1
A	48	VAL	HG22	0.814	0.05	1
A	18	LYS	HB3	1.776	0.05	1
A	47	GLU	H	7.898	0.05	1
A	18	LYS	C	178.341	0.05	1
A	11	HIS	HA	5.439	0.05	1
A	101	SER	C	172.962	0.05	1
A	32	GLN	CA	56.541	0.05	1
A	60	GLN	C	174.379	0.05	1
A	52	LEU	HD13	0.721	0.05	1
A	31	TYR	CB	38.026	0.05	1
A	34	PRO	CA	65.386	0.05	1
A	86	GLU	HB2	1.835	0.05	1
A	23	LEU	N	120.478	0.05	1
A	45	ARG	HB2	1.658	0.05	1
A	48	VAL	HA	3.758	0.05	1
A	15	LYS	CB	34.086	0.05	1
A	84	THR	HG21	1.043	0.05	1
A	30	SER	HA	4.099	0.05	1
A	5	HIS	HB3	3.084	0.05	1
A	71	GLU	C	174.236	0.05	1
A	45	ARG	H	7.464	0.05	1
A	8	GLN	HE22	7.551	0.05	1
A	8	GLN	HG2	2.216	0.05	1
A	56	ALA	C	176.676	0.05	1
A	27	ASP	H	7.988	0.05	1
A	28	LEU	HD23	0.226	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	40	LEU	HB3	1.713	0.05	1
A	94	ALA	HA	4.48	0.05	1
A	40	LEU	HA	3.789	0.05	1
A	6	SER	HA	4.402	0.05	1
A	102	SER	CB	63.875	0.05	1
A	40	LEU	HD23	1.031	0.05	1
A	13	VAL	HG11	0.79	0.05	1
A	38	GLN	H	8.394	0.05	1
A	104	ALA	HA	4.14	0.05	1
A	5	HIS	HB2	3.084	0.05	1
A	41	GLU	CB	29.313	0.05	1
A	71	GLU	H	8.629	0.05	1
A	95	PRO	CA	63.338	0.05	1
A	40	LEU	N	116.907	0.05	1
A	53	ARG	CB	30.123	0.05	1
A	27	ASP	C	173.826	0.05	1
A	21	PHE	HD1	6.671	0.05	1
A	106	GLN	HB3	2.248	0.05	1
A	75	LYS	HB3	1.465	0.05	1
A	17	TRP	HB3	3.732	0.05	1
A	72	ASP	HA	4.782	0.05	1
A	78	GLY	HA3	3.766	0.05	1
A	86	GLU	HA	4.169	0.05	1
A	101	SER	HA	4.452	0.05	1
A	51	GLU	H	9.226	0.05	1
A	77	LYS	H	8.33	0.05	1
A	23	LEU	CA	52.811	0.05	1
A	14	LEU	HB3	1.858	0.05	1
A	45	ARG	CB	31.653	0.05	1
A	27	ASP	CB	42.917	0.05	1
A	65	MET	HA	5.377	0.05	1
A	44	ARG	HB3	1.844	0.05	1
A	99	ASN	C	174.323	0.05	1
A	63	LEU	H	8.446	0.05	1
A	31	TYR	HD2	7.105	0.05	1
A	22	SER	HA	4.633	0.05	1
A	8	GLN	HA	4.355	0.05	1
A	57	HIS	HD2	7.157	0.05	1
A	25	ASN	HA	5.005	0.05	1
A	98	LEU	C	175.678	0.05	1
A	52	LEU	HD21	0.876	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	7	GLY	HA2	3.89	0.05	1
A	53	ARG	H	7.555	0.05	1
A	9	ASP	HB3	2.469	0.05	1
A	15	LYS	HE3	2.849	0.05	1
A	17	TRP	HZ3	6.596	0.05	1
A	38	GLN	HG3	2.433	0.05	1
A	21	PHE	HZ	6.33	0.05	1
A	54	ARG	HB3	1.744	0.05	1
A	98	LEU	CB	43.249	0.05	1
A	28	LEU	HD21	0.226	0.05	1
A	63	LEU	HA	4.942	0.05	1
A	49	PRO	CA	63.085	0.05	1
A	62	ASN	H	8.733	0.05	1
A	10	VAL	HA	4.199	0.05	1
A	68	HIS	HB3	1.775	0.05	1
A	64	ASP	C	173.135	0.05	1
A	74	VAL	HA	3.474	0.05	1
A	45	ARG	C	175.251	0.05	1
A	40	LEU	HD12	0.628	0.05	1
A	54	ARG	HA	3.975	0.05	1
A	70	ASP	HB2	2.57	0.05	1
A	97	VAL	CB	33.287	0.05	1
A	49	PRO	HD3	2.934	0.05	1
A	90	LEU	CA	56.069	0.05	1
A	75	LYS	HG2	1.279	0.05	1
A	41	GLU	HB3	1.968	0.05	1
A	15	LYS	HD3	1.715	0.05	1
A	69	ARG	HE	7.587	0.05	1
A	19	THR	HG23	1.162	0.05	1
A	110	GLU	CA	56.14	0.05	1
A	5	HIS	HA	4.633	0.05	1
A	41	GLU	HG3	2.178	0.05	1
A	98	LEU	HB3	1.489	0.05	1
A	70	ASP	H	8.553	0.05	1
A	23	LEU	HG	1.596	0.05	1
A	87	GLY	H	8.456	0.05	1
A	17	TRP	CB	31.647	0.05	1
A	76	PRO	HB3	1.216	0.05	1
A	24	ASP	CA	57.716	0.05	1
A	37	ALA	HB1	1.534	0.05	1
A	64	ASP	H	8.756	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	94	ALA	HB2	1.244	0.05	1
A	92	SER	H	8.292	0.05	1
A	49	PRO	C	175.683	0.05	1
A	60	GLN	H	8.449	0.05	1
A	75	LYS	H	7.846	0.05	1
A	95	PRO	HB3	2.154	0.05	1
A	98	LEU	HA	4.257	0.05	1
A	88	GLN	HA	4.198	0.05	1
A	85	GLY	HA3	3.792	0.05	1
A	61	VAL	HG22	0.574	0.05	1
A	104	ALA	CA	54.382	0.05	1
A	47	GLU	HG3	1.899	0.05	1
A	82	ALA	HB1	1.199	0.05	1
A	49	PRO	HD2	2.934	0.05	1
A	55	LEU	HD11	0.604	0.05	1
A	12	VAL	HA	4.511	0.05	1
A	5	HIS	CA	55.796	0.05	1
A	41	GLU	N	121.165	0.05	1
A	40	LEU	HD22	1.031	0.05	1
A	100	THR	CB	70.086	0.05	1
A	92	SER	HA	4.401	0.05	1
A	48	VAL	H	8.398	0.05	1
A	34	PRO	HD3	4.12	0.05	1
A	75	LYS	CA	54.624	0.05	1
A	52	LEU	HA	4.261	0.05	1
A	70	ASP	HA	4.695	0.05	1
A	38	GLN	HG2	2.433	0.05	1
A	14	LEU	CB	44.642	0.05	1
A	34	PRO	CB	32.618	0.05	1
A	35	SER	CB	63.183	0.05	1
A	15	LYS	C	173.426	0.05	1
A	78	GLY	CA	45.477	0.05	1
A	72	ASP	HB3	2.533	0.05	1
A	38	GLN	C	177.41	0.05	1
A	48	VAL	HB	1.744	0.05	1
A	92	SER	CB	64.376	0.05	1
A	11	HIS	HD2	7.112	0.05	1
A	60	GLN	CB	30.852	0.05	1
A	46	GLY	HA3	3.951	0.05	1
A	21	PHE	HE1	6.756	0.05	1
A	43	ILE	CB	36.521	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	42	SER	HB3	3.758	0.05	1
A	111	ALA	CA	52.156	0.05	1
A	84	THR	HG22	1.043	0.05	1
A	43	ILE	HG22	0.614	0.05	1
A	56	ALA	HB3	1.1	0.05	1
A	24	ASP	N	124.874	0.05	1
A	80	PHE	CB	40.285	0.05	1
A	5	HIS	C	173.478	0.05	1
A	79	ALA	HB2	1.189	0.05	1
A	18	LYS	H	8.758	0.05	1
A	103	PRO	HA	4.234	0.05	1
A	61	VAL	HB	1.736	0.05	1
A	98	LEU	HD11	0.753	0.05	1
A	25	ASN	HB3	2.898	0.05	1
A	15	LYS	HB2	2.224	0.05	1
A	21	PHE	CB	43.724	0.05	1
A	66	GLU	CA	54.968	0.05	1
A	14	LEU	H	8.999	0.05	1
A	41	GLU	CA	59.42	0.05	1
A	77	LYS	N	122.015	0.05	1
A	53	ARG	NE	118.749	0.05	1
A	13	VAL	HG22	0.79	0.05	1
A	42	SER	CA	62.541	0.05	1
A	16	LEU	HB3	1.795	0.05	1
A	17	TRP	HA	5.191	0.05	1
A	43	ILE	H	7.437	0.05	1
A	57	HIS	HB3	3.208	0.05	1
A	31	TYR	HB3	3.262	0.05	1
A	30	SER	CB	70.159	0.05	1
A	79	ALA	HB1	1.189	0.05	1
A	28	LEU	HD13	-0.084	0.05	1
A	23	LEU	HB3	1.596	0.05	1
A	57	HIS	N	117.178	0.05	1
A	69	ARG	NE	117.488	0.05	1
A	51	GLU	HB2	1.906	0.05	1
A	51	GLU	CA	59.89	0.05	1
A	48	VAL	HG13	0.814	0.05	1
A	62	ASN	ND2	112.441	0.05	1
A	39	PHE	C	176.504	0.05	1
A	18	LYS	CB	33.995	0.05	1
A	67	ASP	CA	54.795	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	54	ARG	HD3	2.798	0.05	1
A	46	GLY	C	172.984	0.05	1
A	102	SER	HB3	3.811	0.05	1
A	20	GLY	N	113.583	0.05	1
A	17	TRP	N	121.383	0.05	1
A	94	ALA	C	178.043	0.05	1
A	29	ARG	C	175.441	0.05	1
A	39	PHE	HB3	3.386	0.05	1
A	88	GLN	CA	56.277	0.05	1
A	58	GLY	HA2	3.532	0.05	1
A	56	ALA	HA	4.137	0.05	1
A	29	ARG	HG2	1.031	0.05	1
A	95	PRO	HA	4.299	0.05	1
A	53	ARG	HA	3.727	0.05	1
A	40	LEU	C	178.015	0.05	1
A	20	GLY	HA3	3.517	0.05	1
A	66	GLU	N	123.661	0.05	1
A	36	ASN	C	174.625	0.05	1
A	55	LEU	HB2	1.564	0.05	1
A	44	ARG	HD3	3.015	0.05	1
A	30	SER	H	8.133	0.05	1
A	82	ALA	HA	4.101	0.05	1
A	14	LEU	HD11	0.728	0.05	1
A	100	THR	N	114.217	0.05	1
A	106	GLN	C	179.332	0.05	1
A	50	ALA	HB2	1.348	0.05	1
A	42	SER	N	115.378	0.05	1
A	46	GLY	CA	46.592	0.05	1
A	79	ALA	CA	52.642	0.05	1
A	34	PRO	HA	4.323	0.05	1
A	99	ASN	HB2	2.654	0.05	1
A	101	SER	N	117.916	0.05	1
A	38	GLN	HB2	2.123	0.05	1
A	96	GLN	HB3	1.893	0.05	1
A	77	LYS	HA	4.139	0.05	1
A	39	PHE	N	122.864	0.05	1
A	74	VAL	HG23	0.61	0.05	1
A	51	GLU	N	115.667	0.05	1
A	102	SER	H	8.365	0.05	1
A	30	SER	HB2	3.572	0.05	1
A	21	PHE	HB3	3.362	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	67	ASP	HB2	2.267	0.05	1
A	60	GLN	HG3	2.426	0.05	1
A	17	TRP	C	176.939	0.05	1
A	69	ARG	HB2	1.782	0.05	1
A	19	THR	H	7.65	0.05	1
A	54	ARG	NE	116.314	0.05	1
A	37	ALA	HB2	1.534	0.05	1
A	57	HIS	H	8.021	0.05	1
A	105	GLN	HB3	2.27	0.05	1
A	16	LEU	HD12	0.805	0.05	1
A	56	ALA	N	118.256	0.05	1
A	47	GLU	C	174.258	0.05	1
A	82	ALA	CB	20.243	0.05	1
A	93	THR	HG21	1.087	0.05	1
A	25	ASN	N	113.166	0.05	1
A	17	TRP	HD1	6.596	0.05	1
A	104	ALA	CB	19.459	0.05	1
A	104	ALA	HB2	1.284	0.05	1
A	63	LEU	C	174.128	0.05	1
A	8	GLN	C	174.017	0.05	1
A	82	ALA	HB2	1.199	0.05	1
A	73	PHE	HA	2.364	0.05	1
A	55	LEU	HD12	0.604	0.05	1
A	6	SER	CB	64.605	0.05	1
A	18	LYS	HE3	3.455	0.05	1
A	69	ARG	N	116.118	0.05	1
A	44	ARG	H	8.128	0.05	1
A	48	VAL	HG23	0.814	0.05	1
A	40	LEU	HD21	1.031	0.05	1
A	39	PHE	HD2	6.77	0.05	1
A	32	GLN	HG3	2.359	0.05	1
A	46	GLY	N	108.614	0.05	1
A	35	SER	HB3	3.827	0.05	1
A	12	VAL	C	172.158	0.05	1
A	82	ALA	C	176.072	0.05	1
A	83	PHE	HB3	2.982	0.05	1
A	12	VAL	HG23	0.783	0.05	1
A	23	LEU	HD22	0.913	0.05	1
A	28	LEU	HB2	-0.642	0.05	1
A	62	ASN	HD22	7.112	0.05	1
A	65	MET	HB2	1.782	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	92	SER	CA	58.665	0.05	1
A	32	GLN	C	174.798	0.05	1
A	60	GLN	CA	55.745	0.05	1
A	81	LYS	CA	56.277	0.05	1
A	69	ARG	HA	3.452	0.05	1
A	36	ASN	HA	5.036	0.05	1
A	18	LYS	HD3	1.534	0.05	1
A	34	PRO	C	177.778	0.05	1
A	26	GLY	HA2	4.08	0.05	1
A	107	ALA	CB	19.341	0.05	1
A	93	THR	C	172.833	0.05	1
A	30	SER	C	172.207	0.05	1
A	61	VAL	HA	4.267	0.05	1
A	71	GLU	HA	4.695	0.05	1
A	71	GLU	CA	55.935	0.05	1
A	8	GLN	CB	30.075	0.05	1
A	63	LEU	N	126.641	0.05	1
A	85	GLY	C	172.941	0.05	1
A	53	ARG	N	118.772	0.05	1
A	25	ASN	HD21	6.866	0.05	1
A	100	THR	HG21	1.087	0.05	1
A	74	VAL	C	172.293	0.05	1
A	12	VAL	HG13	0.783	0.05	1
A	94	ALA	H	8.182	0.05	1
A	101	SER	HB2	3.763	0.05	1
A	13	VAL	HG21	0.79	0.05	1
A	37	ALA	CA	54.28	0.05	1
A	18	LYS	HB2	1.776	0.05	1
A	42	SER	CB	64.743	0.05	1
A	92	SER	HB3	3.77	0.05	1
A	32	GLN	CB	29.602	0.05	1
A	52	LEU	HD12	0.721	0.05	1
A	30	SER	CA	61.806	0.05	1
A	31	TYR	CA	60.613	0.05	1
A	86	GLU	HB3	1.951	0.05	1
A	33	ASP	HA	4.812	0.05	1
A	65	MET	N	120.543	0.05	1
A	39	PHE	CB	39.177	0.05	1
A	29	ARG	HD3	2.209	0.05	1
A	51	GLU	CB	31.307	0.05	1
A	61	VAL	HG13	0.574	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	18	LYS	CA	61.99	0.05	1
A	27	ASP	N	116.163	0.05	1
A	41	GLU	HA	4.001	0.05	1
A	89	LYS	HA	4.198	0.05	1
A	14	LEU	HG	1.303	0.05	1
A	74	VAL	CA	60.826	0.05	1
A	9	ASP	CA	54.622	0.05	1
A	16	LEU	HD21	0.805	0.05	1
A	99	ASN	HA	4.691	0.05	1
A	103	PRO	HB3	2.255	0.05	1
A	56	ALA	CB	20.254	0.05	1
A	39	PHE	HE1	6.378	0.05	1
A	71	GLU	N	121.173	0.05	1
A	94	ALA	CB	18.582	0.05	1
A	82	ALA	N	125.461	0.05	1
A	62	ASN	CA	52.637	0.05	1
A	28	LEU	CD1	23.645	0.05	1
A	42	SER	H	7.864	0.05	1
A	16	LEU	H	7.954	0.05	1
A	32	GLN	N	113.761	0.05	1
A	32	GLN	HE21	6.493	0.05	1
A	53	ARG	HB2	1.744	0.05	1
A	13	VAL	HG12	0.79	0.05	1
A	36	ASN	HD21	7.328	0.05	1
A	91	GLY	HA3	4.168	0.05	1
A	32	GLN	H	8.11	0.05	1
A	33	ASP	H	6.837	0.05	1
A	10	VAL	H	8.388	0.05	1
A	6	SER	N	117.541	0.05	1
A	58	GLY	CA	45.815	0.05	1
A	37	ALA	N	123.622	0.05	1
A	90	LEU	H	8.25	0.05	1
A	21	PHE	HD2	6.671	0.05	1
A	106	GLN	HB2	2.248	0.05	1
A	79	ALA	CB	20.14	0.05	1
A	31	TYR	HE1	6.795	0.05	1
A	14	LEU	HB2	1.15	0.05	1
A	64	ASP	CA	53.327	0.05	1
A	45	ARG	CA	56.667	0.05	1
A	36	ASN	ND2	118.134	0.05	1
A	76	PRO	CA	63.118	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	27	ASP	CA	54.34	0.05	1
A	59	GLY	CA	44.655	0.05	1
A	23	LEU	HA	5.374	0.05	1
A	93	THR	HB	4.125	0.05	1
A	65	MET	CB	35.969	0.05	1
A	49	PRO	HB2	1.303	0.05	1
A	31	TYR	HD1	7.105	0.05	1
A	7	GLY	C	172.749	0.05	1
A	68	HIS	HD2	5.773	0.05	1
A	19	THR	HB	4.516	0.05	1
A	16	LEU	HD11	0.805	0.05	1
A	105	GLN	CA	58.015	0.05	1
A	9	ASP	HA	4.776	0.05	1
A	63	LEU	HD21	0.627	0.05	1
A	67	ASP	H	8.719	0.05	1
A	52	LEU	HD22	0.876	0.05	1
A	93	THR	HG22	1.087	0.05	1
A	8	GLN	N	119.173	0.05	1
A	87	GLY	CA	45.892	0.05	1
A	15	LYS	HE2	2.849	0.05	1
A	89	LYS	N	122.617	0.05	1
A	6	SER	CA	58.311	0.05	1
A	7	GLY	H	8.5	0.05	1
A	54	ARG	HB2	1.744	0.05	1
A	98	LEU	CA	55.437	0.05	1
A	61	VAL	CA	62.187	0.05	1
A	27	ASP	HB3	2.464	0.05	1
A	39	PHE	HA	3.82	0.05	1
A	81	LYS	HA	4.088	0.05	1
A	40	LEU	HD13	0.628	0.05	1
A	14	LEU	N	131.038	0.05	1
A	62	ASN	HD21	6.864	0.05	1
A	97	VAL	CA	62.82	0.05	1
A	41	GLU	HB2	1.968	0.05	1
A	72	ASP	N	121.282	0.05	1
A	106	GLN	CB	30.939	0.05	1
A	25	ASN	ND2	114.972	0.05	1
A	75	LYS	N	126.565	0.05	1
A	73	PHE	HB3	2.178	0.05	1
A	65	MET	HE1	1.95	0.05	1
A	98	LEU	HB2	1.489	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	14	LEU	HA	4.948	0.05	1
A	91	GLY	H	8.386	0.05	1
A	66	GLU	HA	4.391	0.05	1
A	24	ASP	CB	40.209	0.05	1
A	63	LEU	HD13	0.627	0.05	1
A	107	ALA	CA	54.499	0.05	1
A	105	GLN	N	119.132	0.05	1
A	95	PRO	HB2	1.762	0.05	1
A	77	LYS	HB2	1.651	0.05	1
A	9	ASP	C	175.649	0.05	1
A	94	ALA	N	127.81	0.05	1
A	55	LEU	CA	56.868	0.05	1
A	84	THR	CA	62.092	0.05	1
A	85	GLY	N	110.218	0.05	1
A	61	VAL	HG23	0.574	0.05	1
A	25	ASN	HD22	7.78	0.05	1
A	100	THR	HG22	1.087	0.05	1
A	44	ARG	HE	7.168	0.05	1
A	80	PHE	C	174.236	0.05	1
A	5	HIS	CB	30.178	0.05	1
A	65	MET	H	8.651	0.05	1
A	57	HIS	HA	4.323	0.05	1
A	100	THR	C	173.474	0.05	1
A	9	ASP	N	121.592	0.05	1
A	52	LEU	HD11	0.721	0.05	1
A	104	ALA	C	178.166	0.05	1
A	94	ALA	HB1	1.244	0.05	1
A	14	LEU	CA	54.004	0.05	1
A	42	SER	C	174.841	0.05	1
A	55	LEU	HD22	0.79	0.05	1
A	86	GLU	CA	57.211	0.05	1
A	72	ASP	HB2	2.34	0.05	1
A	46	GLY	HA2	3.703	0.05	1
A	111	ALA	CB	19.107	0.05	1
A	84	THR	HG23	1.043	0.05	1
A	12	VAL	H	8.384	0.05	1
A	43	ILE	HG21	0.614	0.05	1
A	74	VAL	CB	33.984	0.05	1
A	56	ALA	HB2	1.1	0.05	1
A	80	PHE	CA	58.353	0.05	1
A	43	ILE	HD13	0.356	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	79	ALA	HB3	1.189	0.05	1
A	89	LYS	C	175.424	0.05	1
A	61	VAL	CG1	24.79	0.05	1
A	38	GLN	CA	60.062	0.05	1
A	79	ALA	HA	4.095	0.05	1
A	94	ALA	CA	51.396	0.05	1
A	17	TRP	HE1	10.359	0.05	1
A	111	ALA	C	178.965	0.05	1
A	53	ARG	HD2	3.054	0.05	1
A	84	THR	N	115.617	0.05	1
A	47	GLU	N	119.484	0.05	1
A	69	ARG	HD3	3.173	0.05	1
A	25	ASN	HB2	2.712	0.05	1
A	15	LYS	HB3	2.224	0.05	1
A	86	GLU	C	176.072	0.05	1
A	36	ASN	HD22	7.328	0.05	1
A	66	GLU	CB	33.934	0.05	1
A	89	LYS	CB	33.535	0.05	1
A	64	ASP	HB2	2.402	0.05	1
A	12	VAL	CB	36.49	0.05	1
A	40	LEU	CA	57.951	0.05	1
A	23	LEU	H	9.165	0.05	1
A	16	LEU	HB2	1.532	0.05	1
A	45	ARG	HE	7.388	0.05	1
A	96	GLN	HA	4.212	0.05	1
A	24	ASP	HA	4.122	0.05	1
A	49	PRO	HA	4.075	0.05	1
A	69	ARG	HG2	1.558	0.05	1
A	101	SER	CB	64.578	0.05	1
A	31	TYR	HB2	2.767	0.05	1
A	74	VAL	H	5.492	0.05	1
A	44	ARG	CD	43.779	0.05	1
A	23	LEU	HB2	1.219	0.05	1
A	41	GLU	C	177.67	0.05	1
A	51	GLU	HB3	2.215	0.05	1
A	47	GLU	HB3	1.62	0.05	1
A	43	ILE	C	179.32	0.05	1
A	54	ARG	HD2	2.705	0.05	1
A	31	TYR	H	8.092	0.05	1
A	22	SER	C	170.89	0.05	1
A	83	PHE	CA	58.25	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	15	LYS	H	9.566	0.05	1
A	105	GLN	CB	29.654	0.05	1
A	39	PHE	HB2	3.201	0.05	1
A	32	GLN	HB2	1.844	0.05	1
A	58	GLY	HA3	4.199	0.05	1
A	29	ARG	HG3	1.161	0.05	1
A	13	VAL	CA	61.351	0.05	1
A	26	GLY	C	172.12	0.05	1
A	20	GLY	HA2	2.085	0.05	1
A	55	LEU	HB3	1.72	0.05	1
A	6	SER	HB3	3.765	0.05	1
A	21	PHE	N	115.139	0.05	1
A	63	LEU	HG	1.279	0.05	1
A	69	ARG	CB	30.271	0.05	1
A	50	ALA	HB1	1.348	0.05	1
A	73	PHE	C	173.178	0.05	1
A	8	GLN	HB2	1.848	0.05	1
A	22	SER	CA	57.736	0.05	1
A	81	LYS	H	8.023	0.05	1
A	31	TYR	HA	4.502	0.05	1
A	99	ASN	HB3	2.755	0.05	1
A	33	ASP	CA	51.801	0.05	1
A	72	ASP	C	174.215	0.05	1
A	32	GLN	HE22	7.448	0.05	1
A	38	GLN	HB3	2.123	0.05	1
A	14	LEU	HD21	0.728	0.05	1
A	65	MET	CE	19.618	0.05	1
A	18	LYS	HA	4.446	0.05	1
A	36	ASN	HB3	3.022	0.05	1
A	106	GLN	CA	57.211	0.05	1
A	19	THR	HG21	1.162	0.05	1
A	24	ASP	C	176.784	0.05	1
A	81	LYS	HB3	1.525	0.05	1
A	37	ALA	HB3	1.534	0.05	1
A	71	GLU	HB2	2.34	0.05	1
A	10	VAL	HG12	0.79	0.05	1
A	37	ALA	HA	4.137	0.05	1
A	77	LYS	CB	33.743	0.05	1
A	55	LEU	CB	42.533	0.05	1
A	69	ARG	H	8.17	0.05	1
A	63	LEU	CB	45.038	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	47	GLU	CB	32.593	0.05	1
A	40	LEU	CB	42.072	0.05	1
A	13	VAL	N	126.899	0.05	1
A	66	GLU	HG2	1.928	0.05	1
A	77	LYS	C	176.072	0.05	1
A	104	ALA	HB3	1.284	0.05	1
A	29	ARG	HA	3.884	0.05	1
A	111	ALA	HB1	1.4	0.05	1
A	96	GLN	C	174.798	0.05	1
A	82	ALA	HB3	1.199	0.05	1
A	59	GLY	HA3	4.219	0.05	1
A	55	LEU	HD13	0.604	0.05	1
A	50	ALA	C	178.749	0.05	1
A	29	ARG	HB3	0.603	0.05	1
A	110	GLU	HA	4.212	0.05	1
A	10	VAL	HG11	0.79	0.05	1
A	17	TRP	HH2	7.064	0.05	1
A	23	LEU	HD11	0.913	0.05	1
A	11	HIS	C	172.784	0.05	1
A	102	SER	CA	56.843	0.05	1
A	39	PHE	HD1	6.77	0.05	1
A	111	ALA	HA	4.22	0.05	1
A	32	GLN	HG2	2.359	0.05	1
A	22	SER	N	114.805	0.05	1
A	60	GLN	HA	4.254	0.05	1
A	33	ASP	N	121.149	0.05	1
A	43	ILE	CD1	12.14	0.05	1
A	32	GLN	HA	4.199	0.05	1
A	23	LEU	HD23	0.913	0.05	1
A	78	GLY	C	172.358	0.05	1
A	28	LEU	HB3	0.814	0.05	1
A	71	GLU	HG3	2.209	0.05	1
A	35	SER	C	176.158	0.05	1
A	98	LEU	H	8.249	0.05	1
A	70	ASP	N	115.274	0.05	1
A	86	GLU	CB	30.939	0.05	1
A	27	ASP	HA	4.387	0.05	1
A	37	ALA	H	7.9	0.05	1
A	26	GLY	H	8.671	0.05	1
A	18	LYS	HD2	1.534	0.05	1
A	64	ASP	HA	4.995	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	62	ASN	HB2	2.284	0.05	1
A	98	LEU	HD21	0.753	0.05	1
A	55	LEU	H	7.705	0.05	1
A	15	LYS	HG3	0.876	0.05	1
A	56	ALA	HB1	1.1	0.05	1
A	10	VAL	HG22	0.79	0.05	1
A	88	GLN	HB3	1.943	0.05	1
A	11	HIS	HB2	3.084	0.05	1
A	11	HIS	CA	54.519	0.05	1
A	38	GLN	CB	28.763	0.05	1
A	80	PHE	HB3	2.933	0.05	1
A	10	VAL	CA	61.98	0.05	1
A	41	GLU	H	8.329	0.05	1
A	66	GLU	HB3	1.618	0.05	1
A	54	ARG	H	7.786	0.05	1
A	71	GLU	CB	34.096	0.05	1
A	58	GLY	H	8.482	0.05	1
A	19	THR	CA	61.256	0.05	1
A	63	LEU	HB3	1.627	0.05	1
A	98	LEU	HD13	0.753	0.05	1
A	17	TRP	H	8.766	0.05	1
A	16	LEU	HA	4.574	0.05	1
A	76	PRO	HG3	0.822	0.05	1
A	30	SER	N	115.909	0.05	1
A	12	VAL	HG12	0.783	0.05	1
A	37	ALA	CB	18.892	0.05	1
A	13	VAL	H	8.957	0.05	1
A	43	ILE	HG12	1.038	0.05	1
A	25	ASN	H	6.929	0.05	1
A	92	SER	HB2	3.77	0.05	1
A	58	GLY	C	173.783	0.05	1
A	101	SER	CA	58.718	0.05	1
A	44	ARG	CA	60.39	0.05	1
A	36	ASN	CB	39.577	0.05	1
A	39	PHE	CA	61.992	0.05	1
A	29	ARG	HD2	2.209	0.05	1
A	15	LYS	HA	4.846	0.05	1
A	48	VAL	HG11	0.814	0.05	1
A	61	VAL	HG12	0.574	0.05	1
A	10	VAL	C	173.2	0.05	1
A	102	SER	HA	4.614	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	35	SER	H	8.646	0.05	1
A	11	HIS	N	126.534	0.05	1
A	72	ASP	H	8.477	0.05	1
A	16	LEU	HD22	0.805	0.05	1
A	57	HIS	CB	28.026	0.05	1
A	56	ALA	CA	52.223	0.05	1
A	39	PHE	HE2	6.378	0.05	1
A	7	GLY	CA	46.055	0.05	1
A	21	PHE	C	171.257	0.05	1
A	62	ASN	CB	40.029	0.05	1
A	13	VAL	CB	33.392	0.05	1
A	25	ASN	CB	38.401	0.05	1
A	48	VAL	HG21	0.814	0.05	1
A	52	LEU	C	176.892	0.05	1
A	13	VAL	HG13	0.79	0.05	1
A	91	GLY	HA2	3.811	0.05	1
A	70	ASP	C	174.906	0.05	1
A	43	ILE	CA	63.459	0.05	1
A	67	ASP	HA	4.391	0.05	1
A	59	GLY	C	171.289	0.05	1
A	69	ARG	CA	61.013	0.05	1
A	14	LEU	HD13	0.728	0.05	1
A	43	ILE	HA	3.765	0.05	1
A	36	ASN	H	8.108	0.05	1
A	22	SER	HB2	3.269	0.05	1
A	31	TYR	HE2	6.795	0.05	1
A	45	ARG	HA	4.215	0.05	1
A	93	THR	CA	62.196	0.05	1
A	14	LEU	HD22	0.728	0.05	1
A	52	LEU	HB3	1.62	0.05	1
A	70	ASP	CB	40.806	0.05	1
A	75	LYS	HA	3.889	0.05	1
A	64	ASP	CB	44.088	0.05	1
A	74	VAL	HG21	0.61	0.05	1
A	60	GLN	HB3	1.787	0.05	1
A	23	LEU	C	176.46	0.05	1
A	72	ASP	CB	42.648	0.05	1
A	54	ARG	HG2	1.527	0.05	1
A	76	PRO	CB	33.639	0.05	1
A	29	ARG	CB	29.681	0.05	1
A	49	PRO	HB3	2.216	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	13	VAL	HA	4.523	0.05	1
A	34	PRO	HB2	2.03	0.05	1
A	68	HIS	CA	54.364	0.05	1
A	19	THR	HA	4.695	0.05	1
A	53	ARG	HE	7.062	0.05	1
A	73	PHE	H	7.929	0.05	1
A	25	ASN	C	174.107	0.05	1
A	65	MET	C	174.755	0.05	1
A	13	VAL	C	173.374	0.05	1
A	52	LEU	HD23	0.876	0.05	1
A	12	VAL	N	126.812	0.05	1
A	93	THR	HG23	1.087	0.05	1
A	63	LEU	CA	54.277	0.05	1
A	100	THR	H	8.086	0.05	1
A	76	PRO	HD2	2.973	0.05	1
A	111	ALA	HB2	1.4	0.05	1
A	62	ASN	HA	4.757	0.05	1
A	88	GLN	C	174.884	0.05	1
A	55	LEU	HA	4.013	0.05	1
A	24	ASP	HB2	2.712	0.05	1
A	23	LEU	HD13	0.913	0.05	1
A	84	THR	H	8.042	0.05	1
A	27	ASP	HB2	2.278	0.05	1
A	12	VAL	HG21	0.783	0.05	1
A	9	ASP	CB	42.133	0.05	1
A	53	ARG	HB3	1.744	0.05	1
A	16	LEU	HG	1.062	0.05	1
A	29	ARG	H	8.882	0.05	1
A	10	VAL	HG21	0.79	0.05	1
A	65	MET	CA	54.882	0.05	1
A	14	LEU	C	172.749	0.05	1
A	61	VAL	C	173.956	0.05	1
A	90	LEU	C	176.719	0.05	1
A	73	PHE	HB2	1.992	0.05	1
A	73	PHE	CB	40.84	0.05	1
A	98	LEU	HD22	0.753	0.05	1
A	110	GLU	HB3	1.893	0.05	1
A	65	MET	HE2	1.95	0.05	1
A	33	ASP	HB2	2.519	0.05	1
A	97	VAL	HA	3.98	0.05	1
A	74	VAL	N	126.501	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	68	HIS	N	127.698	0.05	1
A	63	LEU	HD12	0.627	0.05	1
A	85	GLY	H	7.696	0.05	1
A	16	LEU	C	173.739	0.05	1
A	90	LEU	HB3	1.943	0.05	1
A	28	LEU	HG	0.567	0.05	1
A	28	LEU	HA	2.96	0.05	1
A	77	LYS	HB3	1.651	0.05	1
A	63	LEU	HD23	0.627	0.05	1
A	19	THR	CB	69.7	0.05	1
A	73	PHE	HD2	5.649	0.05	1
A	105	GLN	HA	4.28	0.05	1
A	62	ASN	N	126.704	0.05	1
A	61	VAL	H	8.164	0.05	1
A	84	THR	CB	70.295	0.05	1
A	100	THR	HG23	1.087	0.05	1
A	29	ARG	HE	6.014	0.05	1
A	12	VAL	HG11	0.783	0.05	1
A	73	PHE	HE1	6.945	0.05	1
A	37	ALA	C	179.419	0.05	1
A	87	GLY	HA2	3.828	0.05	1
A	17	TRP	HB2	3.038	0.05	1
A	75	LYS	C	173.297	0.05	1
A	55	LEU	C	176.18	0.05	1
A	12	VAL	CA	60.902	0.05	1
A	66	GLU	HB2	1.618	0.05	1
A	35	SER	HA	4.285	0.05	1
A	44	ARG	CB	30.53	0.05	1
A	40	LEU	H	7.973	0.05	1
A	106	GLN	HA	4.227	0.05	1
A	55	LEU	HD21	0.79	0.05	1
A	90	LEU	N	123.725	0.05	1
A	45	ARG	NE	116.801	0.05	1
A	64	ASP	N	127.484	0.05	1
A	45	ARG	HB3	1.844	0.05	1
A	15	LYS	CA	56.109	0.05	1
A	9	ASP	HB2	2.469	0.05	1
A	59	GLY	N	108.012	0.05	1
A	29	ARG	N	128.584	0.05	1
A	44	ARG	HA	3.889	0.05	1
A	43	ILE	HD12	0.356	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	8	GLN	HE21	6.765	0.05	1
A	8	GLN	HG3	2.216	0.05	1
A	40	LEU	HB2	1.434	0.05	1
A	62	ASN	C	171.3	0.05	1
A	103	PRO	CA	65.047	0.05	1
A	53	ARG	HD3	3.054	0.05	1
A	85	GLY	CA	45.789	0.05	1
A	91	GLY	CA	45.685	0.05	1
A	17	TRP	NE1	129.922	0.05	1
A	69	ARG	HD2	3.046	0.05	1
A	83	PHE	HA	4.578	0.05	1
A	89	LYS	CA	56.38	0.05	1
A	64	ASP	HB3	2.712	0.05	1
A	50	ALA	HA	3.775	0.05	1
A	61	VAL	N	121.573	0.05	1
A	60	GLN	NE2	111.302	0.05	1
A	75	LYS	HB2	1.465	0.05	1
A	60	GLN	HE22	7.546	0.05	1
A	78	GLY	HA2	3.766	0.05	1
A	99	ASN	CA	53.679	0.05	1
A	103	PRO	HB2	1.878	0.05	1
A	89	LYS	HB3	1.661	0.05	1
A	69	ARG	HG3	1.558	0.05	1
A	28	LEU	HD11	-0.084	0.05	1
A	78	GLY	N	109.579	0.05	1
A	15	LYS	N	127.611	0.05	1
A	72	ASP	CA	54.536	0.05	1
A	100	THR	HB	4.205	0.05	1
A	44	ARG	HB2	1.844	0.05	1
A	73	PHE	N	120.67	0.05	1
A	28	LEU	C	175.165	0.05	1
A	29	ARG	CA	54.463	0.05	1
A	52	LEU	H	7.207	0.05	1
A	82	ALA	H	8.078	0.05	1
A	49	PRO	CB	34.886	0.05	1
A	105	GLN	C	176.033	0.05	1
A	13	VAL	HB	1.968	0.05	1
A	83	PHE	CB	40.181	0.05	1
A	28	LEU	HD22	0.226	0.05	1
A	32	GLN	HB3	2.209	0.05	1
A	6	SER	H	8.374	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	7	GLY	HA3	3.89	0.05	1
A	91	GLY	N	109.934	0.05	1
A	95	PRO	C	175.661	0.05	1
A	29	ARG	NE	115.348	0.05	1
A	17	TRP	HZ2	6.415	0.05	1
A	83	PHE	C	174.841	0.05	1
A	20	GLY	C	115.139	0.05	1
A	56	ALA	H	7.161	0.05	1
A	6	SER	HB2	3.765	0.05	1
A	77	LYS	CA	56.796	0.05	1
A	66	GLU	HG3	2.27	0.05	1
A	28	LEU	CA	56.207	0.05	1

7.3.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	192	-0.57 ± 0.13	Should be applied
$^{13}C_{\beta}$	177	-0.44 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	187	1.21 ± 0.21	Should be applied
^{15}N	170	0.46 ± 0.34	None needed (< 0.5 ppm)

7.3.3 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 74%, i.e. 817 atoms were assigned a chemical shift out of a possible 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	431/439 (98%)	173/175 (99%)	174/178 (98%)	84/86 (98%)
Sidechain	365/619 (59%)	279/359 (78%)	86/227 (38%)	0/33 (0%)
Aromatic	21/50 (42%)	21/28 (75%)	0/20 (0%)	0/2 (0%)
Overall	817/1108 (74%)	473/562 (84%)	260/425 (61%)	84/121 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 817 atoms were assigned a chemical shift out of a possible 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	431/439 (98%)	173/175 (99%)	174/178 (98%)	84/86 (98%)
Sidechain	365/619 (59%)	279/359 (78%)	86/227 (38%)	0/33 (0%)
Aromatic	21/50 (42%)	21/28 (75%)	0/20 (0%)	0/2 (0%)
Overall	817/1108 (74%)	473/562 (84%)	260/425 (61%)	84/121 (69%)

7.3.4 Statistically unusual chemical shifts (i)

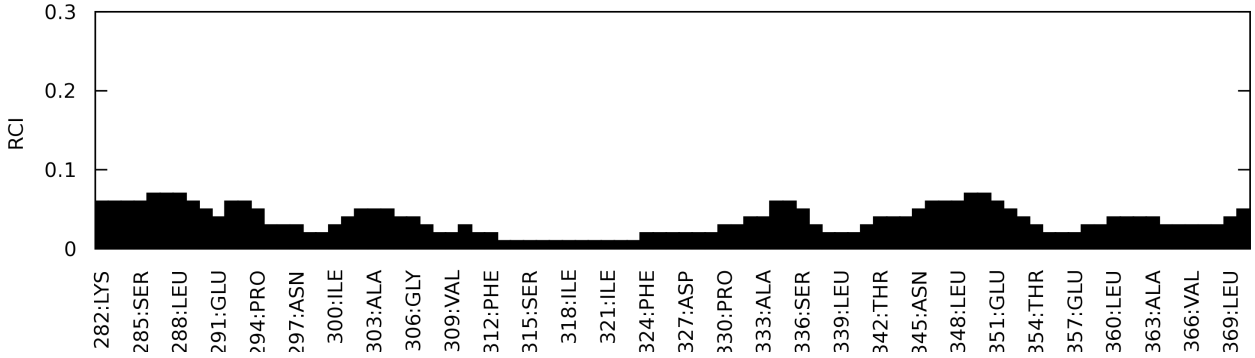
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	20	GLY	C	115.14	183.33 – 164.53	-31.3
1	A	53	ARG	NE	118.75	92.63 – 76.73	21.4
1	A	69	ARG	NE	117.49	92.63 – 76.73	20.6
1	A	44	ARG	NE	117.21	92.63 – 76.73	20.5
1	A	45	ARG	NE	116.80	92.63 – 76.73	20.2
1	A	54	ARG	NE	116.31	92.63 – 76.73	19.9
1	A	29	ARG	NE	115.35	92.63 – 76.73	19.3
1	A	317	ARG	HD2	1.20	4.27 – 1.97	-8.4
1	A	317	ARG	HD3	1.20	4.36 – 1.86	-7.6
1	A	29	ARG	HB2	-0.24	3.15 – 0.45	-7.6
1	A	322	ARG	HD2	1.43	4.27 – 1.97	-7.3
1	A	322	ARG	HD3	1.43	4.36 – 1.86	-6.7
1	A	28	LEU	HB2	-0.64	3.32 – -0.08	-6.7

7.3.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:


RCI
0.3
0.2
0.1
0
282:LYS
285:SER
288:LEU
291:GLU
294:PRO
297:ASN
300:ILE
303:ALA
306:GLY
309:VAL
312:PHE
315:SER
318:ILE
321:ILE
324:PHE
327:ASP
330:PRO
333:ALA
336:SER
339:LEU
342:THR
345:ASN
348:LEU
351:GLU
354:THR
357:GLU
360:LEU
363:ALA
366:VAL
369:LEU