



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:44 PM BST

PDB ID : 2JPO
Title : NMR structure of Antheraea polyphemus pheromone-binding protein 1 at pH 4.5
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Deposited on : 2007-05-20

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

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

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

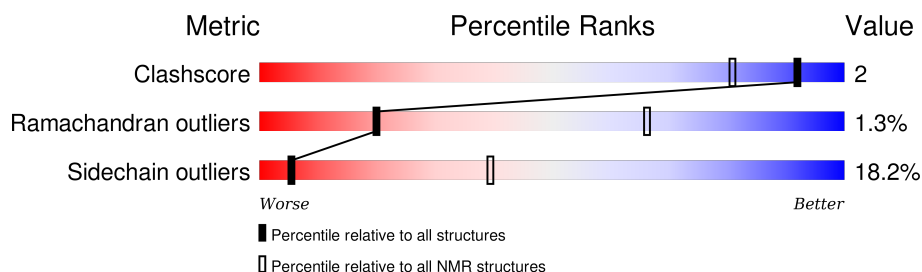
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	142	 81% 13% • 5%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:142 (135)	0.35	4

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 4, 5, 8, 11, 18, 19
2	7, 9, 13, 14
3	2, 6, 15
4	16, 17, 20
5	1, 12
Single-model clusters	10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2167 atoms, of which 1070 are hydrogens and 0 are deuteriums.

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

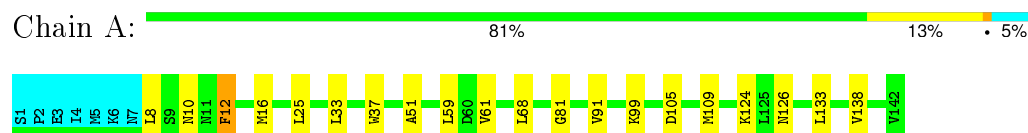
Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2167	686	1070	183	214	14	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Pheromone-binding protein

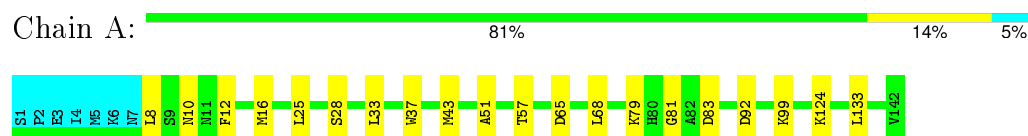


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

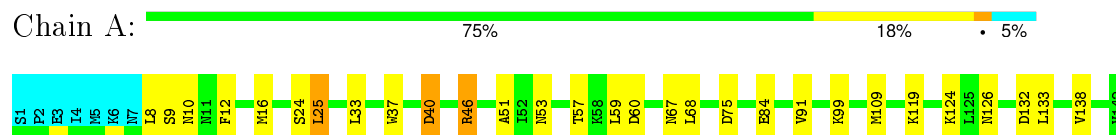
4.2.1 Score per residue for model 1

- Molecule 1: Pheromone-binding protein



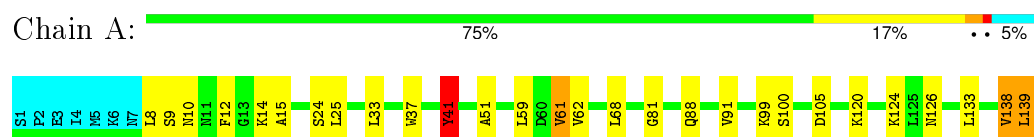
4.2.2 Score per residue for model 2

- Molecule 1: Pheromone-binding protein



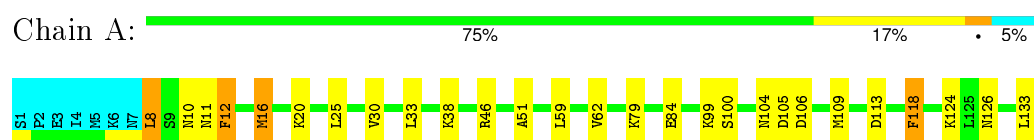
4.2.3 Score per residue for model 3

- Molecule 1: Pheromone-binding protein



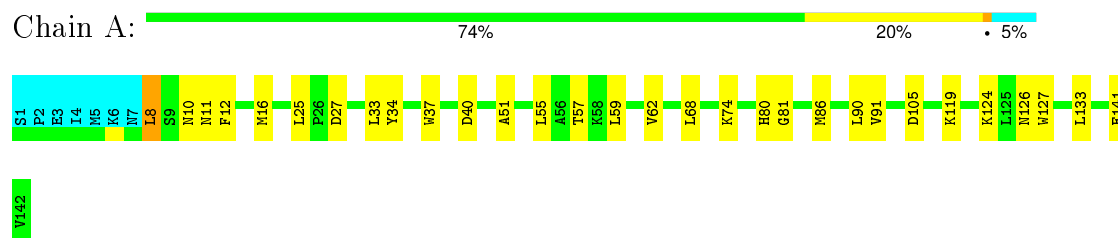
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Pheromone-binding protein



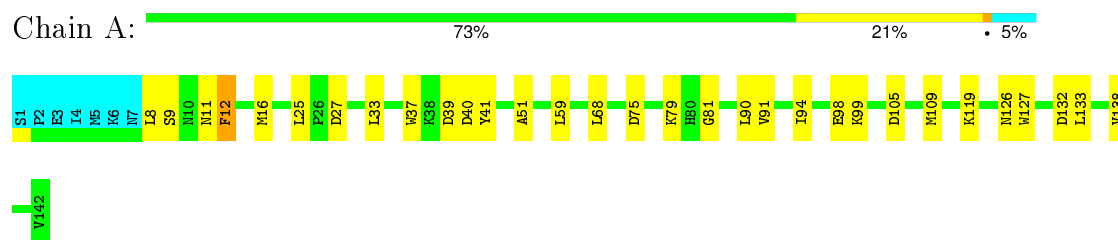
4.2.5 Score per residue for model 5

- Molecule 1: Pheromone-binding protein



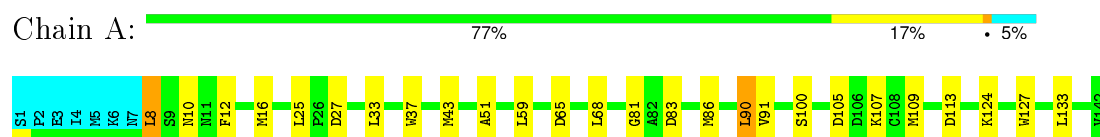
4.2.6 Score per residue for model 6

- Molecule 1: Pheromone-binding protein



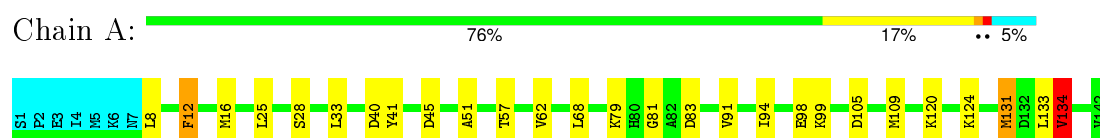
4.2.7 Score per residue for model 7

- Molecule 1: Pheromone-binding protein



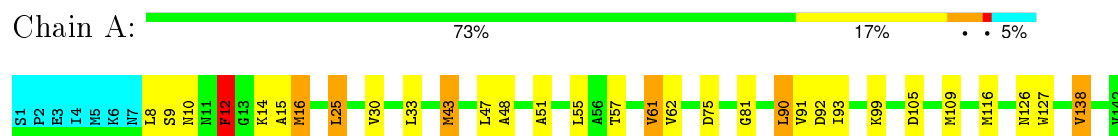
4.2.8 Score per residue for model 8

- Molecule 1: Pheromone-binding protein



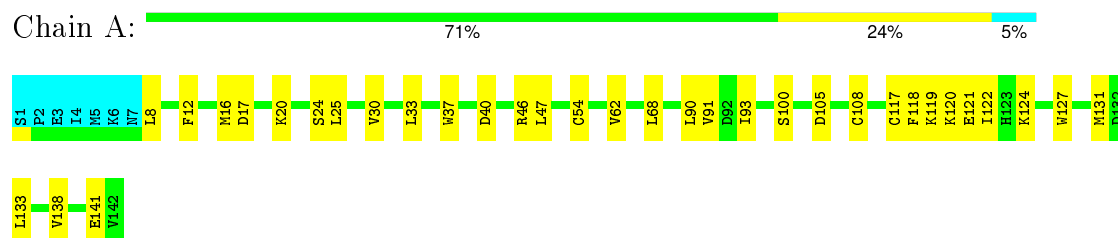
4.2.9 Score per residue for model 9

- Molecule 1: Pheromone-binding protein



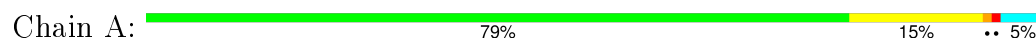
4.2.10 Score per residue for model 10

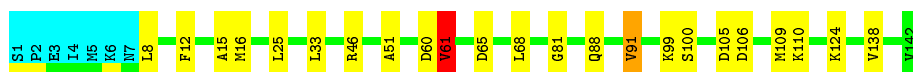
- Molecule 1: Pheromone-binding protein



4.2.11 Score per residue for model 11

- Molecule 1: Pheromone-binding protein





4.2.12 Score per residue for model 12

- Molecule 1: Pheromone-binding protein

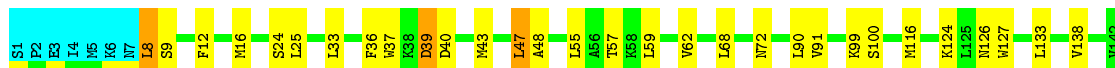
Chain A: 76% 19% 5%



4.2.13 Score per residue for model 13

- Molecule 1: Pheromone-binding protein

Chain A: 74% 19% 5%



4.2.14 Score per residue for model 14

- Molecule 1: Pheromone-binding protein

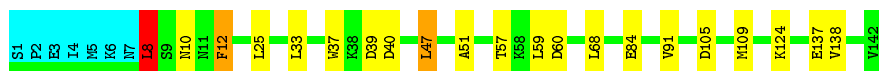
Chain A: 73% 19% 5%



4.2.15 Score per residue for model 15

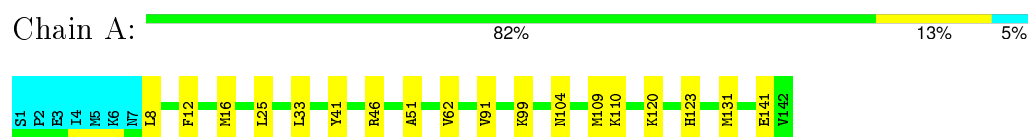
- Molecule 1: Pheromone-binding protein

Chain A: 80% 13% 5%



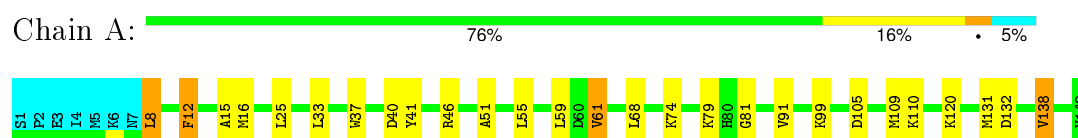
4.2.16 Score per residue for model 16

- Molecule 1: Pheromone-binding protein



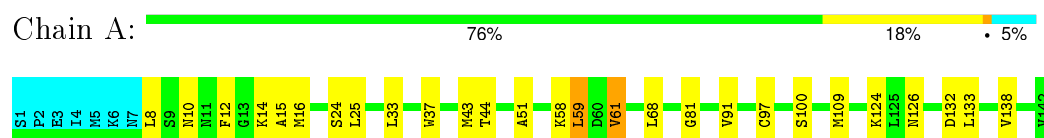
4.2.17 Score per residue for model 17

- Molecule 1: Pheromone-binding protein



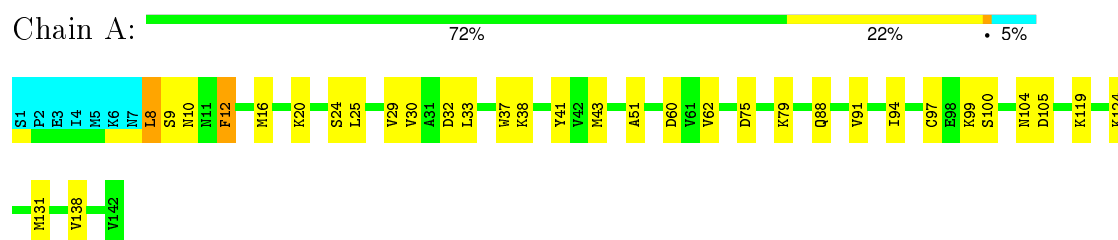
4.2.18 Score per residue for model 18

- Molecule 1: Pheromone-binding protein



4.2.19 Score per residue for model 19

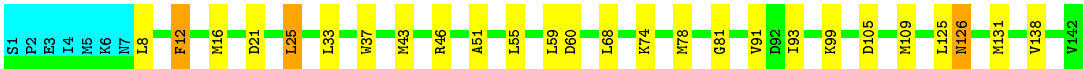
- Molecule 1: Pheromone-binding protein



4.2.20 Score per residue for model 20

- Molecule 1: Pheromone-binding protein





5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *TARGET FUNCTION*.

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

Software name	Classification	Version
OPALP	refinement	1.2
CARA	structure solution	1.8
ATNOS/CANDID	structure solution	1.2
DYANA	structure solution	1.0.3
MOLMOL	structure solution	2.2K

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 16079, BMRB entry 16078, BMRB entry 1608
Number of chemical shift lists	
Total number of shifts	
Number of shifts mapped to atoms	
Number of unparsed shifts	
Number of shifts with mapping errors	
Number of shifts with mapping warnings	
Assignment completeness (well-defined parts)	

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

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.54±0.01	0±0/1061 (0.0±0.0%)	1.05±0.03	1±1/1435 (0.1±0.1%)
All	All	0.54	0/21220 (0.0%)	1.05	24/28700 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.9
All	All	0	17

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	LEU	CB-CG-CD1	7.02	122.93	111.00	15	2
1	A	108	CYS	CA-CB-SG	6.43	125.58	114.00	10	1
1	A	138	VAL	CA-CB-CG2	6.08	120.02	110.90	14	2
1	A	138	VAL	CA-CB-CG1	6.06	120.00	110.90	12	9
1	A	90	LEU	CB-CG-CD1	6.01	121.22	111.00	7	2
1	A	46	ARG	NE-CZ-NH2	-5.60	117.50	120.30	2	1
1	A	8	LEU	CB-CA-C	5.52	120.69	110.20	3	1
1	A	68	LEU	CB-CG-CD1	5.48	120.32	111.00	17	2
1	A	41	TYR	CB-CG-CD1	-5.43	117.74	121.00	3	1
1	A	61	VAL	CG1-CB-CG2	-5.14	102.68	110.90	11	1
1	A	62	VAL	CA-CB-CG1	5.05	118.48	110.90	3	1
1	A	134	VAL	CA-CB-CG2	5.04	118.47	110.90	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	12	PHE	Sidechain	7
1	A	41	TYR	Sidechain	4
1	A	46	ARG	Sidechain	1
1	A	39	ASP	Peptide	1
1	A	34	TYR	Sidechain	1
1	A	106	ASP	Peptide	1
1	A	118	PHE	Sidechain	1
1	A	36	PHE	Sidechain	1

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	1042	1013	1008	4±2
All	All	20840	20260	20160	79

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:CD1	1:A:51:ALA:HB2	0.72	2.14	7	17
1:A:25:LEU:HD12	1:A:51:ALA:HB2	0.68	1.65	1	16
1:A:15:ALA:HB2	1:A:61:VAL:CG1	0.66	2.21	18	6
1:A:43:MET:SD	1:A:48:ALA:HB1	0.59	2.37	13	1
1:A:15:ALA:HB2	1:A:61:VAL:HG13	0.53	1.81	18	1
1:A:25:LEU:HD11	1:A:51:ALA:HB2	0.53	1.79	9	3
1:A:93:ILE:HD11	1:A:125:LEU:HD11	0.53	1.81	20	1
1:A:90:LEU:HD11	1:A:127:TRP:CH2	0.52	2.39	6	7
1:A:93:ILE:HG23	1:A:121:GLU:HB2	0.49	1.84	10	1
1:A:8:LEU:HD21	1:A:12:PHE:CD2	0.48	2.44	17	2
1:A:15:ALA:HB2	1:A:61:VAL:HG12	0.48	1.86	3	2
1:A:88:GLN:HA	1:A:91:VAL:HG23	0.47	1.86	11	1
1:A:131:MET:HA	1:A:134:VAL:CG2	0.46	2.40	8	1
1:A:59:LEU:HD22	1:A:68:LEU:HG	0.46	1.87	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:H	1:A:47:LEU:HD22	0.45	1.72	9	1
1:A:41:TYR:CD1	1:A:41:TYR:C	0.45	2.89	3	1
1:A:16:MET:CE	1:A:30:VAL:HG22	0.45	2.42	9	3
1:A:20:LYS:CD	1:A:30:VAL:HG21	0.45	2.42	4	3
1:A:125:LEU:C	1:A:126:ASN:HD22	0.43	2.16	20	1
1:A:90:LEU:HD11	1:A:127:TRP:CZ2	0.43	2.49	6	1
1:A:59:LEU:HD21	1:A:139:LEU:HB3	0.43	1.91	3	1
1:A:12:PHE:HA	1:A:62:VAL:HG23	0.42	1.90	9	1
1:A:8:LEU:HD13	1:A:80:HIS:CE1	0.42	2.50	5	1
1:A:43:MET:SD	1:A:48:ALA:HB3	0.41	2.55	9	1
1:A:36:PHE:CD1	1:A:43:MET:HG3	0.41	2.51	13	1
1:A:93:ILE:HG22	1:A:118:PHE:HA	0.41	1.91	10	1
1:A:59:LEU:HD22	1:A:59:LEU:H	0.41	1.76	18	1
1:A:118:PHE:CD1	1:A:122:ILE:HD11	0.40	2.51	10	1
1:A:14:LYS:HE3	1:A:61:VAL:HG22	0.40	1.90	9	1

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	134/142 (94%)	120±2 (89±1%)	13±2 (9±2%)	2±1 (1±1%)	20	66
All	All	2680/2840 (94%)	2392 (89%)	254 (9%)	34 (1%)	20	66

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	81	GLY	13
1	A	105	ASP	6
1	A	8	LEU	5
1	A	40	ASP	5
1	A	43	MET	1
1	A	104	ASN	1
1	A	39	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	123	HIS	1
1	A	38	LYS	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	116/123 (94%)	95±3 (82±3%)	21±3 (18±3%)	5	39
All	All	2320/2460 (94%)	1898 (82%)	422 (18%)	5	39

All 80 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	12	PHE	20
1	A	33	LEU	20
1	A	16	MET	18
1	A	8	LEU	18
1	A	91	VAL	17
1	A	37	TRP	15
1	A	124	LYS	14
1	A	99	LYS	14
1	A	109	MET	13
1	A	68	LEU	13
1	A	133	LEU	12
1	A	10	ASN	11
1	A	126	ASN	11
1	A	100	SER	9
1	A	105	ASP	9
1	A	59	LEU	9
1	A	138	VAL	8
1	A	57	THR	8
1	A	62	VAL	8
1	A	79	LYS	7
1	A	24	SER	7
1	A	9	SER	6
1	A	61	VAL	6

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Mol	Chain	Res	Type	Models (Total)
1	A	25	LEU	6
1	A	60	ASP	6
1	A	46	ARG	6
1	A	55	LEU	6
1	A	131	MET	6
1	A	120	LYS	5
1	A	132	ASP	5
1	A	43	MET	5
1	A	119	LYS	5
1	A	75	ASP	5
1	A	40	ASP	4
1	A	110	LYS	4
1	A	74	LYS	4
1	A	84	GLU	3
1	A	113	ASP	3
1	A	98	GLU	3
1	A	141	GLU	3
1	A	104	ASN	3
1	A	65	ASP	3
1	A	83	ASP	3
1	A	11	ASN	3
1	A	47	LEU	3
1	A	27	ASP	3
1	A	94	ILE	3
1	A	137	GLU	3
1	A	97	CYS	3
1	A	107	LYS	2
1	A	116	MET	2
1	A	54	CYS	2
1	A	41	TYR	2
1	A	86	MET	2
1	A	88	GLN	2
1	A	106	ASP	2
1	A	39	ASP	2
1	A	14	LYS	2
1	A	28	SER	2
1	A	92	ASP	2
1	A	58	LYS	2
1	A	93	ILE	1
1	A	139	LEU	1
1	A	17	ASP	1
1	A	118	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	89	GLN	1
1	A	38	LYS	1
1	A	134	VAL	1
1	A	78	MET	1
1	A	32	ASP	1
1	A	53	ASN	1
1	A	44	THR	1
1	A	142	VAL	1
1	A	29	VAL	1
1	A	18	GLN	1
1	A	67	ASN	1
1	A	117	CYS	1
1	A	45	ASP	1
1	A	21	ASP	1
1	A	72	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 94% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 15256

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	1767
Number of shifts mapped to atoms	1767
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 \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	142	-0.24 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	135	0.48 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	139	0.19 ± 0.11	None needed (< 0.5 ppm)
^{15}N	135	0.56 ± 0.15	Should be applied

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 94%, i.e. 1502 atoms were assigned a chemical shift out of a possible 1596. 23 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	663/665 (100%)	265/265 (100%)	268/270 (99%)	130/130 (100%)
Sidechain	754/815 (93%)	466/473 (99%)	275/315 (87%)	13/27 (48%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	85/116 (73%)	44/60 (73%)	40/44 (91%)	1/12 (8%)
Overall	1502/1596 (94%)	775/798 (97%)	583/629 (93%)	144/169 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 1583 atoms were assigned a chemical shift out of a possible 1685. 23 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	693/698 (99%)	277/278 (100%)	281/284 (99%)	135/136 (99%)
Sidechain	805/871 (92%)	499/507 (98%)	292/335 (87%)	14/29 (48%)
Aromatic	85/116 (73%)	44/60 (73%)	40/44 (91%)	1/12 (8%)
Overall	1583/1685 (94%)	820/845 (97%)	613/663 (92%)	150/177 (85%)

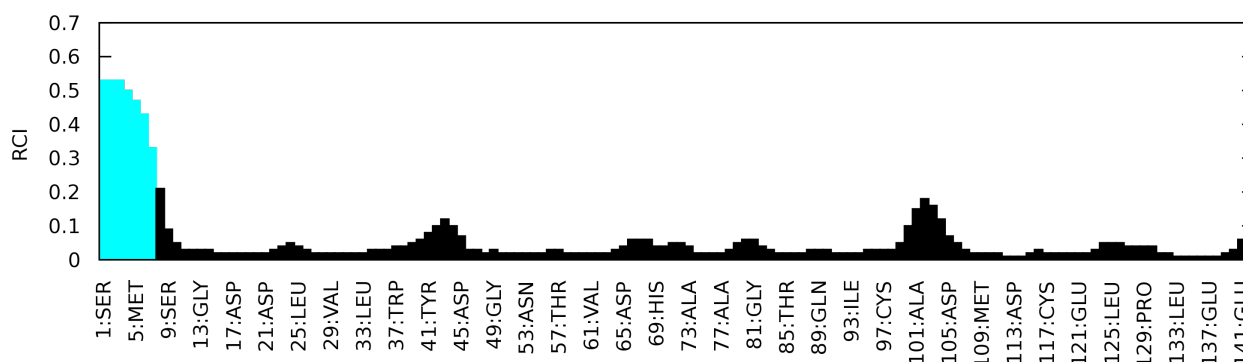
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 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:



7.2 Chemical shift list 2

File name: BMRB entry 16071

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	643
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	643
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 643 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	7	GLY	C	174.534	0.3	1
UNMAPPED	66	ASN	N	115.4	0.3	1
UNMAPPED	55	GLY	N	109.36	0.3	1
UNMAPPED	66	ASN	CB	40.812	0.3	1
UNMAPPED	102	VAL	CA	65.909	0.3	1
UNMAPPED	115	ASP	H	7.536	0.02	1
UNMAPPED	36	GLY	N	113.686	0.3	1
UNMAPPED	54	PHE	CB	40.454	0.3	1
UNMAPPED	3	GLY	H	8.321	0.02	1
UNMAPPED	14	LYS	CB	32.17	0.3	1
UNMAPPED	33	ALA	CA	51.893	0.3	1
UNMAPPED	25	VAL	N	123.056	0.3	1
UNMAPPED	134	GLU	CB	29.611	0.3	1
UNMAPPED	49	ARG	C	174.653	0.3	1
UNMAPPED	69	ARG	N	119.184	0.3	1
UNMAPPED	126	MET	C	178.555	0.3	1
UNMAPPED	52	ILE	CA	58.683	0.3	1
UNMAPPED	95	ILE	CB	36.224	0.3	1
UNMAPPED	69	ARG	CB	30.368	0.3	1
UNMAPPED	37	GLY	N	108.739	0.3	1
UNMAPPED	50	PRO	C	175.696	0.3	1
UNMAPPED	40	GLY	N	109.553	0.3	1
UNMAPPED	74	VAL	H	8.476	0.02	1
UNMAPPED	64	ARG	CA	59.587	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	130	GLN	CA	58.212	0.3	1
UNMAPPED	89	VAL	C	176.661	0.3	1
UNMAPPED	20	THR	N	115.678	0.3	1
UNMAPPED	5	GLY	H	8.596	0.02	1
UNMAPPED	111	PHE	H	8.787	0.02	1
UNMAPPED	112	THR	C	175.455	0.3	1
UNMAPPED	71	PRO	C	175.089	0.3	1
UNMAPPED	16	SER	H	8.482	0.02	1
UNMAPPED	49	ARG	CA	54.354	0.3	1
UNMAPPED	28	ALA	C	177.726	0.3	1
UNMAPPED	143	ARG	CA	55.47	0.3	1
UNMAPPED	24	HIS	C	175.38	0.3	1
UNMAPPED	108	GLY	N	108.091	0.3	1
UNMAPPED	88	PHE	CA	60.37	0.3	1
UNMAPPED	47	MET	CB	36.369	0.3	1
UNMAPPED	115	ASP	C	177.617	0.3	1
UNMAPPED	60	ASP	N	119.045	0.3	1
UNMAPPED	104	THR	C	177.155	0.3	1
UNMAPPED	30	ALA	H	8.237	0.02	1
UNMAPPED	133	LYS	H	7.873	0.02	1
UNMAPPED	89	VAL	CA	67.341	0.3	1
UNMAPPED	51	MET	CB	30.031	0.3	1
UNMAPPED	60	ASP	CB	40.349	0.3	1
UNMAPPED	87	ASN	CA	55.659	0.3	1
UNMAPPED	51	MET	N	122.17	0.3	1
UNMAPPED	63	TYR	C	177.055	0.3	1
UNMAPPED	129	THR	CA	66.641	0.3	1
UNMAPPED	95	ILE	C	177.933	0.3	1
UNMAPPED	27	GLY	C	173.998	0.3	1
UNMAPPED	41	TYR	C	175.736	0.3	1
UNMAPPED	24	HIS	CA	55.751	0.3	1
UNMAPPED	121	ARG	CA	58.015	0.3	1
UNMAPPED	67	MET	H	7.895	0.02	1
UNMAPPED	22	LEU	CB	41.885	0.3	1
UNMAPPED	101	THR	C	176.495	0.3	1
UNMAPPED	130	GLN	C	177.419	0.3	1
UNMAPPED	31	ALA	H	8.261	0.02	1
UNMAPPED	12	TRP	CB	28.79	0.3	1
UNMAPPED	46	ALA	CB	18.028	0.3	1
UNMAPPED	141	GLY	H	7.863	0.02	1
UNMAPPED	138	TYR	C	177.195	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	128	VAL	CA	67.341	0.3	1
UNMAPPED	11	GLN	H	8.367	0.02	1
UNMAPPED	109	GLU	CA	55.109	0.3	1
UNMAPPED	35	VAL	C	176.675	0.3	1
UNMAPPED	140	ASP	H	8.251	0.02	1
UNMAPPED	129	THR	C	176.694	0.3	1
UNMAPPED	127	CYS	N	119.731	0.3	1
UNMAPPED	26	ALA	H	8.459	0.02	1
UNMAPPED	91	ASP	CA	56.742	0.3	1
UNMAPPED	133	LYS	C	179.779	0.3	1
UNMAPPED	61	ARG	H	8.031	0.02	1
UNMAPPED	62	TYR	CB	37.85	0.3	1
UNMAPPED	100	HIS	H	8.52	0.02	1
UNMAPPED	70	TYR	N	121.708	0.3	1
UNMAPPED	107	LYS	CA	55.773	0.3	1
UNMAPPED	119	MET	CB	33.701	0.3	1
UNMAPPED	10	ASN	CA	52.74	0.3	1
UNMAPPED	106	THR	H	7.835	0.02	1
UNMAPPED	24	HIS	H	8.276	0.02	1
UNMAPPED	58	TRP	CB	28.202	0.3	1
UNMAPPED	50	PRO	CA	61.903	0.3	1
UNMAPPED	66	ASN	H	7.562	0.02	1
UNMAPPED	3	GLY	N	109.35	0.3	1
UNMAPPED	83	SER	CA	58.41	0.3	1
UNMAPPED	17	LYS	CB	32.316	0.3	1
UNMAPPED	54	PHE	H	10.382	0.02	1
UNMAPPED	139	TYR	CB	37.802	0.3	1
UNMAPPED	113	GLU	N	120.166	0.3	1
UNMAPPED	99	GLN	H	8.556	0.02	1
UNMAPPED	27	GLY	N	108.976	0.3	1
UNMAPPED	120	GLU	CA	60.275	0.3	1
UNMAPPED	134	GLU	CA	57.443	0.3	1
UNMAPPED	87	ASN	H	8.588	0.02	1
UNMAPPED	113	GLU	CB	28.793	0.3	1
UNMAPPED	90	HIS	N	118.047	0.3	1
UNMAPPED	6	GLY	CA	44.795	0.3	1
UNMAPPED	134	GLU	H	8.441	0.02	1
UNMAPPED	59	GLU	CB	29.307	0.3	1
UNMAPPED	95	ILE	H	8.805	0.02	1
UNMAPPED	144	SER	H	8.01	0.02	1
UNMAPPED	91	ASP	H	7.427	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	108	GLY	H	7.922	0.02	1
UNMAPPED	131	TYR	N	120.443	0.3	1
UNMAPPED	35	VAL	H	8.32	0.02	1
UNMAPPED	105	THR	C	178.065	0.3	1
UNMAPPED	117	LYS	N	119.296	0.3	1
UNMAPPED	52	ILE	CB	38.503	0.3	1
UNMAPPED	14	LYS	C	178.724	0.3	1
UNMAPPED	103	THR	C	176.773	0.3	1
UNMAPPED	8	THR	CB	69.153	0.3	1
UNMAPPED	53	HIS	CB	30.462	0.3	1
UNMAPPED	144	SER	CA	59.552	0.3	1
UNMAPPED	73	GLN	N	114.512	0.3	1
UNMAPPED	63	TYR	CA	62.63	0.3	1
UNMAPPED	34	VAL	CA	61.707	0.3	1
UNMAPPED	53	HIS	N	123.378	0.3	1
UNMAPPED	38	LEU	C	177.983	0.3	1
UNMAPPED	125	GLN	CA	58.715	0.3	1
UNMAPPED	33	ALA	CB	19.152	0.3	1
UNMAPPED	144	SER	N	122.986	0.3	1
UNMAPPED	55	GLY	C	173.298	0.3	1
UNMAPPED	62	TYR	C	179.585	0.3	1
UNMAPPED	30	ALA	CA	52.069	0.3	1
UNMAPPED	75	TYR	N	121.837	0.3	1
UNMAPPED	30	ALA	CB	18.87	0.3	1
UNMAPPED	77	ARG	N	120.875	0.3	1
UNMAPPED	51	MET	H	8.719	0.02	1
UNMAPPED	64	ARG	N	117.514	0.3	1
UNMAPPED	137	ALA	C	179.014	0.3	1
UNMAPPED	109	GLU	C	174.901	0.3	1
UNMAPPED	112	THR	CB	71.675	0.3	1
UNMAPPED	98	LYS	H	8.149	0.02	1
UNMAPPED	64	ARG	CB	29.365	0.3	1
UNMAPPED	13	ASN	N	120.188	0.3	1
UNMAPPED	22	LEU	H	8.29	0.02	1
UNMAPPED	15	PRO	CA	62.615	0.3	1
UNMAPPED	110	ASN	C	173.583	0.3	1
UNMAPPED	141	GLY	N	108.188	0.3	1
UNMAPPED	31	ALA	CB	18.887	0.3	1
UNMAPPED	142	ARG	CA	55.788	0.3	1
UNMAPPED	12	TRP	H	8.084	0.02	1
UNMAPPED	46	ALA	H	8.756	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	31	ALA	N	123.565	0.3	1
UNMAPPED	105	THR	N	118.61	0.3	1
UNMAPPED	11	GLN	N	120.447	0.3	1
UNMAPPED	11	GLN	CB	28.702	0.3	1
UNMAPPED	93	VAL	N	125.192	0.3	1
UNMAPPED	26	ALA	CB	18.872	0.3	1
UNMAPPED	136	GLN	CA	57.67	0.3	1
UNMAPPED	4	GLN	C	176.761	0.3	1
UNMAPPED	26	ALA	N	128.384	0.3	1
UNMAPPED	76	TYR	CA	55.556	0.3	1
UNMAPPED	23	LYS	CB	32.546	0.3	1
UNMAPPED	62	TYR	H	8.262	0.02	1
UNMAPPED	2	SER	C	174.733	0.3	1
UNMAPPED	19	LYS	C	176.864	0.3	1
UNMAPPED	24	HIS	N	121.561	0.3	1
UNMAPPED	142	ARG	CB	30.192	0.3	1
UNMAPPED	84	ASN	CA	51.783	0.3	1
UNMAPPED	13	ASN	CB	38.371	0.3	1
UNMAPPED	94	ASN	CB	38.621	0.3	1
UNMAPPED	56	ASN	H	7.254	0.02	1
UNMAPPED	24	HIS	CB	30.754	0.3	1
UNMAPPED	58	TRP	H	8.561	0.02	1
UNMAPPED	20	THR	H	8.198	0.02	1
UNMAPPED	94	ASN	N	116.547	0.3	1
UNMAPPED	111	PHE	N	122.005	0.3	1
UNMAPPED	16	SER	N	117.221	0.3	1
UNMAPPED	97	ILE	CA	66.163	0.3	1
UNMAPPED	140	ASP	C	177.3	0.3	1
UNMAPPED	99	GLN	N	117.383	0.3	1
UNMAPPED	4	GLN	CA	55.628	0.3	1
UNMAPPED	17	LYS	H	8.378	0.02	1
UNMAPPED	7	GLY	H	8.407	0.02	1
UNMAPPED	99	GLN	CB	27.689	0.3	1
UNMAPPED	124	GLU	CB	28.607	0.3	1
UNMAPPED	110	ASN	H	8.565	0.02	1
UNMAPPED	113	GLU	H	9.211	0.02	1
UNMAPPED	19	LYS	CA	55.899	0.3	1
UNMAPPED	91	ASP	N	118.269	0.3	1
UNMAPPED	34	VAL	C	176.395	0.3	1
UNMAPPED	59	GLU	H	8.132	0.02	1
UNMAPPED	43	LEU	CB	43.407	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	91	ASP	CB	41.2	0.3	1
UNMAPPED	43	LEU	N	121.434	0.3	1
UNMAPPED	76	TYR	H	8.52	0.02	1
UNMAPPED	35	VAL	CB	32.174	0.3	1
UNMAPPED	117	LYS	H	7.698	0.02	1
UNMAPPED	62	TYR	CA	61.739	0.3	1
UNMAPPED	97	ILE	C	178.836	0.3	1
UNMAPPED	35	VAL	N	125.041	0.3	1
UNMAPPED	52	ILE	H	6.584	0.02	1
UNMAPPED	42	MET	CA	53.209	0.3	1
UNMAPPED	58	TRP	CA	61.452	0.3	1
UNMAPPED	8	THR	H	8.168	0.02	1
UNMAPPED	50	PRO	CB	32.139	0.3	1
UNMAPPED	53	HIS	H	8.108	0.02	1
UNMAPPED	137	ALA	CA	53.679	0.3	1
UNMAPPED	126	MET	CA	59.543	0.3	1
UNMAPPED	120	GLU	C	178.737	0.3	1
UNMAPPED	37	GLY	C	174.382	0.3	1
UNMAPPED	132	GLN	C	178.553	0.3	1
UNMAPPED	27	GLY	CA	44.739	0.3	1
UNMAPPED	41	TYR	CA	57.919	0.3	1
UNMAPPED	4	GLN	H	8.362	0.02	1
UNMAPPED	90	HIS	CA	59.574	0.3	1
UNMAPPED	15	PRO	C	176.966	0.3	1
UNMAPPED	33	ALA	H	8.101	0.02	1
UNMAPPED	131	TYR	C	178.197	0.3	1
UNMAPPED	119	MET	CA	59.574	0.3	1
UNMAPPED	19	LYS	H	8.583	0.02	1
UNMAPPED	65	GLU	H	7.925	0.02	1
UNMAPPED	42	MET	C	172.943	0.3	1
UNMAPPED	58	TRP	C	179.171	0.3	1
UNMAPPED	98	LYS	N	123.637	0.3	1
UNMAPPED	16	SER	C	174.163	0.3	1
UNMAPPED	129	THR	H	8.128	0.02	1
UNMAPPED	44	GLY	C	172.828	0.3	1
UNMAPPED	86	ASN	CB	37.211	0.3	1
UNMAPPED	98	LYS	CB	31.967	0.3	1
UNMAPPED	64	ARG	H	7.888	0.02	1
UNMAPPED	70	TYR	H	7.46	0.02	1
UNMAPPED	29	ALA	H	8.327	0.02	1
UNMAPPED	30	ALA	C	177.613	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	73	GLN	CA	53.686	0.3	1
UNMAPPED	8	THR	CA	61.568	0.3	1
UNMAPPED	34	VAL	N	119.892	0.3	1
UNMAPPED	76	TYR	C	173.579	0.3	1
UNMAPPED	107	LYS	C	176.733	0.3	1
UNMAPPED	47	MET	N	121.601	0.3	1
UNMAPPED	130	GLN	N	122.87	0.3	1
UNMAPPED	125	GLN	N	115.483	0.3	1
UNMAPPED	54	PHE	N	125.431	0.3	1
UNMAPPED	123	VAL	CA	65.909	0.3	1
UNMAPPED	125	GLN	CB	27.601	0.3	1
UNMAPPED	14	LYS	N	122.799	0.3	1
UNMAPPED	45	SER	CA	58.142	0.3	1
UNMAPPED	134	GLU	N	118.533	0.3	1
UNMAPPED	52	ILE	C	173.116	0.3	1
UNMAPPED	114	THR	H	7.972	0.02	1
UNMAPPED	95	ILE	N	119.2	0.3	1
UNMAPPED	122	VAL	N	119.325	0.3	1
UNMAPPED	131	TYR	H	8.623	0.02	1
UNMAPPED	141	GLY	C	174.426	0.3	1
UNMAPPED	56	ASN	N	114.524	0.3	1
UNMAPPED	138	TYR	CB	38.349	0.3	1
UNMAPPED	86	ASN	H	8.424	0.02	1
UNMAPPED	94	ASN	H	7.602	0.02	1
UNMAPPED	11	GLN	CA	55.786	0.3	1
UNMAPPED	56	ASN	CB	41.25	0.3	1
UNMAPPED	138	TYR	N	119.383	0.3	1
UNMAPPED	20	THR	CB	69.28	0.3	1
UNMAPPED	142	ARG	N	120.249	0.3	1
UNMAPPED	139	TYR	H	8.057	0.02	1
UNMAPPED	105	THR	CA	65.017	0.3	1
UNMAPPED	93	VAL	C	177.247	0.3	1
UNMAPPED	64	ARG	C	179.123	0.3	1
UNMAPPED	71	PRO	CA	63.108	0.3	1
UNMAPPED	65	GLU	C	177.613	0.3	1
UNMAPPED	126	MET	CB	34.11	0.3	1
UNMAPPED	71	PRO	CB	31.842	0.3	1
UNMAPPED	61	ARG	C	177.615	0.3	1
UNMAPPED	110	ASN	CB	40.9	0.3	1
UNMAPPED	110	ASN	N	119.655	0.3	1
UNMAPPED	43	LEU	H	8.066	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	114	THR	CA	66.386	0.3	1
UNMAPPED	38	LEU	CA	54.418	0.3	1
UNMAPPED	47	MET	C	175.646	0.3	1
UNMAPPED	130	GLN	H	8.731	0.02	1
UNMAPPED	142	ARG	C	176.219	0.3	1
UNMAPPED	74	VAL	CA	58.179	0.3	1
UNMAPPED	94	ASN	CA	56.296	0.3	1
UNMAPPED	111	PHE	CA	56.041	0.3	1
UNMAPPED	5	GLY	CA	44.926	0.3	1
UNMAPPED	87	ASN	C	177.358	0.3	1
UNMAPPED	25	VAL	C	175.558	0.3	1
UNMAPPED	16	SER	CA	57.697	0.3	1
UNMAPPED	139	TYR	CA	59.325	0.3	1
UNMAPPED	72	ASN	H	8.645	0.02	1
UNMAPPED	4	GLN	N	120.242	0.3	1
UNMAPPED	12	TRP	N	121.244	0.3	1
UNMAPPED	46	ALA	N	125.806	0.3	1
UNMAPPED	116	VAL	CB	31.023	0.3	1
UNMAPPED	4	GLN	CB	29.026	0.3	1
UNMAPPED	143	ARG	H	8.255	0.02	1
UNMAPPED	92	CYS	C	177.524	0.3	1
UNMAPPED	101	THR	CA	66.386	0.3	1
UNMAPPED	93	VAL	H	9.31	0.02	1
UNMAPPED	144	SER	C	178.645	0.3	1
UNMAPPED	19	LYS	CB	32.448	0.3	1
UNMAPPED	65	GLU	CB	29.888	0.3	1
UNMAPPED	89	VAL	H	8.891	0.02	1
UNMAPPED	114	THR	CB	68.324	0.3	1
UNMAPPED	103	THR	N	115.582	0.3	1
UNMAPPED	43	LEU	CA	52.795	0.3	1
UNMAPPED	65	GLU	N	116.104	0.3	1
UNMAPPED	96	THR	CA	68.041	0.3	1
UNMAPPED	103	THR	H	8.22	0.02	1
UNMAPPED	45	SER	C	174.968	0.3	1
UNMAPPED	35	VAL	CA	62.057	0.3	1
UNMAPPED	136	GLN	N	120.975	0.3	1
UNMAPPED	70	TYR	CB	34.306	0.3	1
UNMAPPED	29	ALA	CB	18.87	0.3	1
UNMAPPED	67	MET	CA	58.747	0.3	1
UNMAPPED	137	ALA	N	120.921	0.3	1
UNMAPPED	57	ASP	C	177.895	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	55	GLY	H	8.933	0.02	1
UNMAPPED	96	THR	CB	67.71	0.3	1
UNMAPPED	47	MET	H	8.805	0.02	1
UNMAPPED	28	ALA	CA	52.116	0.3	1
UNMAPPED	41	TYR	N	118.254	0.3	1
UNMAPPED	77	ARG	C	178.159	0.3	1
UNMAPPED	36	GLY	H	8.611	0.02	1
UNMAPPED	43	LEU	C	178.225	0.3	1
UNMAPPED	68	TYR	CA	58.805	0.3	1
UNMAPPED	51	MET	C	175.034	0.3	1
UNMAPPED	125	GLN	H	7.083	0.02	1
UNMAPPED	98	LYS	C	179.059	0.3	1
UNMAPPED	109	GLU	H	7.452	0.02	1
UNMAPPED	140	ASP	CA	54.835	0.3	1
UNMAPPED	67	MET	C	176.382	0.3	1
UNMAPPED	104	THR	N	114.887	0.3	1
UNMAPPED	57	ASP	CA	57.442	0.3	1
UNMAPPED	108	GLY	C	174.242	0.3	1
UNMAPPED	61	ARG	CA	59.32	0.3	1
UNMAPPED	100	HIS	CB	31.852	0.3	1
UNMAPPED	104	THR	CB	68.505	0.3	1
UNMAPPED	131	TYR	CB	40.928	0.3	1
UNMAPPED	72	ASN	C	172.843	0.3	1
UNMAPPED	138	TYR	H	7.947	0.02	1
UNMAPPED	69	ARG	C	176.776	0.3	1
UNMAPPED	85	GLN	C	176.89	0.3	1
UNMAPPED	11	GLN	C	175.763	0.3	1
UNMAPPED	18	PRO	CA	62.598	0.3	1
UNMAPPED	129	THR	N	118.389	0.3	1
UNMAPPED	47	MET	CA	53.463	0.3	1
UNMAPPED	142	ARG	H	7.843	0.02	1
UNMAPPED	36	GLY	CA	44.933	0.3	1
UNMAPPED	26	ALA	C	178.234	0.3	1
UNMAPPED	14	LYS	CA	53.718	0.3	1
UNMAPPED	25	VAL	CA	61.545	0.3	1
UNMAPPED	22	LEU	N	123.328	0.3	1
UNMAPPED	33	ALA	N	123.832	0.3	1
UNMAPPED	6	GLY	H	8.381	0.02	1
UNMAPPED	75	TYR	CB	41.752	0.3	1
UNMAPPED	69	ARG	CA	55.882	0.3	1
UNMAPPED	37	GLY	CA	44.91	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	85	GLN	CA	58.62	0.3	1
UNMAPPED	39	GLY	CA	45.888	0.3	1
UNMAPPED	40	GLY	CA	44.742	0.3	1
UNMAPPED	125	GLN	C	179.238	0.3	1
UNMAPPED	130	GLN	CB	28.024	0.3	1
UNMAPPED	112	THR	N	116.237	0.3	1
UNMAPPED	84	ASN	CB	40.731	0.3	1
UNMAPPED	68	TYR	C	175.926	0.3	1
UNMAPPED	36	GLY	C	174.708	0.3	1
UNMAPPED	99	GLN	C	178.646	0.3	1
UNMAPPED	116	VAL	C	177.419	0.3	1
UNMAPPED	34	VAL	H	8.166	0.02	1
UNMAPPED	139	TYR	N	119.886	0.3	1
UNMAPPED	72	ASN	CB	38.056	0.3	1
UNMAPPED	102	VAL	C	178.553	0.3	1
UNMAPPED	72	ASN	N	116.465	0.3	1
UNMAPPED	143	ARG	CB	30.577	0.3	1
UNMAPPED	8	THR	C	174.831	0.3	1
UNMAPPED	110	ASN	CA	52.317	0.3	1
UNMAPPED	93	VAL	CB	31.577	0.3	1
UNMAPPED	21	ASN	C	175.013	0.3	1
UNMAPPED	89	VAL	CB	31.819	0.3	1
UNMAPPED	116	VAL	CA	67.436	0.3	1
UNMAPPED	132	GLN	H	8.255	0.02	1
UNMAPPED	89	VAL	N	120.641	0.3	1
UNMAPPED	51	MET	CA	53.686	0.3	1
UNMAPPED	40	GLY	H	8.414	0.02	1
UNMAPPED	139	TYR	C	176.932	0.3	1
UNMAPPED	122	VAL	H	8.275	0.02	1
UNMAPPED	53	HIS	C	175.423	0.3	1
UNMAPPED	23	LYS	H	8.312	0.02	1
UNMAPPED	119	MET	C	177.801	0.3	1
UNMAPPED	121	ARG	N	117.009	0.3	1
UNMAPPED	121	ARG	CB	29.562	0.3	1
UNMAPPED	12	TRP	CA	56.729	0.3	1
UNMAPPED	137	ALA	H	7.609	0.02	1
UNMAPPED	135	SER	C	175.736	0.3	1
UNMAPPED	109	GLU	N	120.435	0.3	1
UNMAPPED	84	ASN	C	174.01	0.3	1
UNMAPPED	109	GLU	CB	31.001	0.3	1
UNMAPPED	65	GLU	CA	57.41	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	114	THR	C	175.666	0.3	1
UNMAPPED	126	MET	H	8.133	0.02	1
UNMAPPED	104	THR	H	8.059	0.02	1
UNMAPPED	21	ASN	CB	38.392	0.3	1
UNMAPPED	120	GLU	H	8.587	0.02	1
UNMAPPED	135	SER	CA	60.731	0.3	1
UNMAPPED	107	LYS	CB	32.193	0.3	1
UNMAPPED	40	GLY	C	173.96	0.3	1
UNMAPPED	133	LYS	CB	32.14	0.3	1
UNMAPPED	127	CYS	C	176.905	0.3	1
UNMAPPED	74	VAL	C	174.112	0.3	1
UNMAPPED	94	ASN	C	178.51	0.3	1
UNMAPPED	120	GLU	CB	28.863	0.3	1
UNMAPPED	17	LYS	CA	53.764	0.3	1
UNMAPPED	6	GLY	N	109.132	0.3	1
UNMAPPED	120	GLU	N	119.139	0.3	1
UNMAPPED	128	VAL	H	8.514	0.02	1
UNMAPPED	75	TYR	H	8.483	0.02	1
UNMAPPED	56	ASN	C	174.323	0.3	1
UNMAPPED	57	ASP	N	123.558	0.3	1
UNMAPPED	59	GLU	CA	59.563	0.3	1
UNMAPPED	90	HIS	C	177.726	0.3	1
UNMAPPED	127	CYS	CA	59.606	0.3	1
UNMAPPED	131	TYR	CA	61.638	0.3	1
UNMAPPED	127	CYS	CB	41.528	0.3	1
UNMAPPED	117	LYS	CA	58.715	0.3	1
UNMAPPED	135	SER	H	8.423	0.02	1
UNMAPPED	118	MET	H	8.182	0.02	1
UNMAPPED	17	LYS	C	174.391	0.3	1
UNMAPPED	63	TYR	CB	38.013	0.3	1
UNMAPPED	32	GLY	N	108.224	0.3	1
UNMAPPED	18	PRO	CB	31.724	0.3	1
UNMAPPED	44	GLY	CA	44.487	0.3	1
UNMAPPED	34	VAL	CB	32.414	0.3	1
UNMAPPED	53	HIS	CA	54.418	0.3	1
UNMAPPED	13	ASN	C	174.343	0.3	1
UNMAPPED	63	TYR	N	120.771	0.3	1
UNMAPPED	41	TYR	H	7.871	0.02	1
UNMAPPED	27	GLY	H	8.419	0.02	1
UNMAPPED	68	TYR	H	7.597	0.02	1
UNMAPPED	25	VAL	CB	32.433	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	119	MET	H	8.708	0.02	1
UNMAPPED	132	GLN	CA	58.64	0.3	1
UNMAPPED	31	ALA	C	178.272	0.3	1
UNMAPPED	85	GLN	N	120.218	0.3	1
UNMAPPED	77	ARG	CA	53.038	0.3	1
UNMAPPED	39	GLY	N	110.233	0.3	1
UNMAPPED	75	TYR	CA	56.63	0.3	1
UNMAPPED	132	GLN	CB	27.085	0.3	1
UNMAPPED	96	THR	H	8.168	0.02	1
UNMAPPED	112	THR	CA	59.988	0.3	1
UNMAPPED	122	VAL	CB	31.842	0.3	1
UNMAPPED	13	ASN	CA	52.388	0.3	1
UNMAPPED	103	THR	CA	65.113	0.3	1
UNMAPPED	7	GLY	CA	44.732	0.3	1
UNMAPPED	23	LYS	N	122.041	0.3	1
UNMAPPED	117	LYS	C	180.056	0.3	1
UNMAPPED	73	GLN	H	7.296	0.02	1
UNMAPPED	15	PRO	CB	31.867	0.3	1
UNMAPPED	44	GLY	H	9.439	0.02	1
UNMAPPED	115	ASP	CA	57.633	0.3	1
UNMAPPED	141	GLY	CA	45.197	0.3	1
UNMAPPED	31	ALA	CA	52.266	0.3	1
UNMAPPED	72	ASN	CA	51.556	0.3	1
UNMAPPED	75	TYR	C	174.708	0.3	1
UNMAPPED	7	GLY	N	109.076	0.3	1
UNMAPPED	124	GLU	H	8.011	0.02	1
UNMAPPED	29	ALA	C	177.664	0.3	1
UNMAPPED	45	SER	H	8.347	0.02	1
UNMAPPED	93	VAL	CA	65.686	0.3	1
UNMAPPED	77	ARG	H	7.943	0.02	1
UNMAPPED	118	MET	C	178.21	0.3	1
UNMAPPED	26	ALA	CA	52.238	0.3	1
UNMAPPED	32	GLY	C	173.706	0.3	1
UNMAPPED	123	VAL	C	177.617	0.3	1
UNMAPPED	66	ASN	C	175.482	0.3	1
UNMAPPED	76	TYR	N	111.224	0.3	1
UNMAPPED	13	ASN	H	8.081	0.02	1
UNMAPPED	100	HIS	CA	59.415	0.3	1
UNMAPPED	107	LYS	H	7.465	0.02	1
UNMAPPED	86	ASN	CA	56.041	0.3	1
UNMAPPED	39	GLY	C	174.848	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	106	THR	C	175.165	0.3	1
UNMAPPED	49	ARG	H	8.704	0.02	1
UNMAPPED	97	ILE	CB	36.44	0.3	1
UNMAPPED	105	THR	H	8.288	0.02	1
UNMAPPED	118	MET	N	118.639	0.3	1
UNMAPPED	97	ILE	N	121.32	0.3	1
UNMAPPED	99	GLN	CA	57.652	0.3	1
UNMAPPED	111	PHE	C	176.694	0.3	1
UNMAPPED	5	GLY	C	174.797	0.3	1
UNMAPPED	124	GLU	CA	60.784	0.3	1
UNMAPPED	118	MET	CB	32.397	0.3	1
UNMAPPED	102	VAL	H	8.104	0.02	1
UNMAPPED	10	ASN	C	175.226	0.3	1
UNMAPPED	48	SER	C	174.431	0.3	1
UNMAPPED	19	LYS	N	122.438	0.3	1
UNMAPPED	86	ASN	C	177.714	0.3	1
UNMAPPED	103	THR	CB	68.843	0.3	1
UNMAPPED	132	GLN	N	119.893	0.3	1
UNMAPPED	38	LEU	H	8.244	0.02	1
UNMAPPED	28	ALA	H	8.169	0.02	1
UNMAPPED	92	CYS	CA	58.2	0.3	1
UNMAPPED	62	TYR	N	121.052	0.3	1
UNMAPPED	135	SER	N	115.424	0.3	1
UNMAPPED	21	ASN	CA	52.248	0.3	1
UNMAPPED	42	MET	CB	33.962	0.3	1
UNMAPPED	135	SER	CB	62.09	0.3	1
UNMAPPED	29	ALA	N	123.442	0.3	1
UNMAPPED	58	TRP	N	120.539	0.3	1
UNMAPPED	32	GLY	H	8.322	0.02	1
UNMAPPED	42	MET	N	121.73	0.3	1
UNMAPPED	121	ARG	H	7.282	0.02	1
UNMAPPED	63	TYR	H	9.034	0.02	1
UNMAPPED	6	GLY	C	174.776	0.3	1
UNMAPPED	48	SER	CA	58.174	0.3	1
UNMAPPED	41	TYR	CB	39.777	0.3	1
UNMAPPED	17	LYS	N	124.531	0.3	1
UNMAPPED	121	ARG	C	179.331	0.3	1
UNMAPPED	90	HIS	CB	29.846	0.3	1
UNMAPPED	25	VAL	H	8.032	0.02	1
UNMAPPED	117	LYS	CB	31.558	0.3	1
UNMAPPED	12	TRP	C	175.902	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	101	THR	H	8.533	0.02	1
UNMAPPED	133	LYS	CA	58.94	0.3	1
UNMAPPED	124	GLU	C	177.525	0.3	1
UNMAPPED	59	GLU	N	120.76	0.3	1
UNMAPPED	119	MET	N	118.433	0.3	1
UNMAPPED	39	GLY	H	8.586	0.02	1
UNMAPPED	137	ALA	CB	18.023	0.3	1
UNMAPPED	92	CYS	H	8.16	0.02	1
UNMAPPED	98	LYS	CA	59.765	0.3	1
UNMAPPED	102	VAL	N	123.523	0.3	1
UNMAPPED	52	ILE	N	124.643	0.3	1
UNMAPPED	143	ARG	C	175.507	0.3	1
UNMAPPED	102	VAL	CB	31.31	0.3	1
UNMAPPED	8	THR	N	113.67	0.3	1
UNMAPPED	32	GLY	CA	44.742	0.3	1
UNMAPPED	44	GLY	N	115.484	0.3	1
UNMAPPED	88	PHE	C	177.499	0.3	1
UNMAPPED	66	ASN	CA	54.467	0.3	1
UNMAPPED	73	GLN	CB	32.967	0.3	1
UNMAPPED	55	GLY	CA	45.251	0.3	1
UNMAPPED	129	THR	CB	67.71	0.3	1
UNMAPPED	23	LYS	C	176.228	0.3	1
UNMAPPED	100	HIS	C	178.737	0.3	1
UNMAPPED	48	SER	H	8.47	0.02	1
UNMAPPED	54	PHE	CA	59.145	0.3	1
UNMAPPED	123	VAL	CB	30.61	0.3	1
UNMAPPED	45	SER	N	114.006	0.3	1
UNMAPPED	20	THR	C	173.904	0.3	1
UNMAPPED	123	VAL	N	121.597	0.3	1
UNMAPPED	18	PRO	C	176.864	0.3	1
UNMAPPED	45	SER	CB	63.456	0.3	1
UNMAPPED	30	ALA	N	123.582	0.3	1
UNMAPPED	144	SER	CB	64.403	0.3	1
UNMAPPED	95	ILE	CA	61.675	0.3	1
UNMAPPED	57	ASP	H	9.03	0.02	1
UNMAPPED	123	VAL	H	9.172	0.02	1
UNMAPPED	106	THR	N	116.693	0.3	1
UNMAPPED	134	GLU	C	179.238	0.3	1
UNMAPPED	122	VAL	CA	65.208	0.3	1
UNMAPPED	126	MET	N	119.47	0.3	1
UNMAPPED	23	LYS	CA	55.905	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	56	ASN	CA	52.063	0.3	1
UNMAPPED	138	TYR	CA	59.507	0.3	1
UNMAPPED	54	PHE	C	177.167	0.3	1
UNMAPPED	106	THR	CB	68.537	0.3	1
UNMAPPED	59	GLU	C	177.714	0.3	1
UNMAPPED	60	ASP	C	179.079	0.3	1
UNMAPPED	115	ASP	N	120.142	0.3	1
UNMAPPED	20	THR	CA	61.176	0.3	1
UNMAPPED	22	LEU	C	177.245	0.3	1
UNMAPPED	113	GLU	C	179.291	0.3	1
UNMAPPED	49	ARG	CB	29.26	0.3	1
UNMAPPED	97	ILE	H	8.477	0.02	1
UNMAPPED	115	ASP	CB	41.59	0.3	1
UNMAPPED	105	THR	CB	68.57	0.3	1
UNMAPPED	49	ARG	N	127.082	0.3	1
UNMAPPED	91	ASP	C	175.913	0.3	1
UNMAPPED	136	GLN	H	7.607	0.02	1
UNMAPPED	106	THR	CA	64.444	0.3	1
UNMAPPED	128	VAL	N	123.916	0.3	1
UNMAPPED	143	ARG	N	122.741	0.3	1
UNMAPPED	14	LYS	H	8.023	0.02	1
UNMAPPED	128	VAL	CB	31.334	0.3	1
UNMAPPED	108	GLY	CA	45.028	0.3	1
UNMAPPED	127	CYS	H	9.235	0.02	1
UNMAPPED	37	GLY	H	8.31	0.02	1
UNMAPPED	85	GLN	H	8.666	0.02	1
UNMAPPED	114	THR	N	116.891	0.3	1
UNMAPPED	38	LEU	N	122.033	0.3	1
UNMAPPED	28	ALA	N	124.115	0.3	1
UNMAPPED	69	ARG	H	7.519	0.02	1
UNMAPPED	60	ASP	CA	58.142	0.3	1
UNMAPPED	87	ASN	CB	37.771	0.3	1
UNMAPPED	38	LEU	CB	42.013	0.3	1
UNMAPPED	28	ALA	CB	19.119	0.3	1
UNMAPPED	96	THR	N	118.293	0.3	1
UNMAPPED	100	HIS	N	120.435	0.3	1
UNMAPPED	74	VAL	CB	33.235	0.3	1
UNMAPPED	87	ASN	N	118.438	0.3	1
UNMAPPED	86	ASN	N	117.362	0.3	1
UNMAPPED	42	MET	H	9.138	0.02	1
UNMAPPED	74	VAL	N	112.994	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	22	LEU	CA	54.806	0.3	1
UNMAPPED	111	PHE	CB	39.758	0.3	1
UNMAPPED	33	ALA	C	177.613	0.3	1
UNMAPPED	5	GLY	N	110.918	0.3	1
UNMAPPED	16	SER	CB	63.483	0.3	1
UNMAPPED	46	ALA	CA	52.51	0.3	1
UNMAPPED	70	TYR	C	172.801	0.3	1
UNMAPPED	136	GLN	C	177.191	0.3	1
UNMAPPED	124	GLU	N	120.964	0.3	1
UNMAPPED	101	THR	N	115.465	0.3	1
UNMAPPED	90	HIS	H	8.372	0.02	1
UNMAPPED	101	THR	CB	68.42	0.3	1
UNMAPPED	116	VAL	H	8.262	0.02	1
UNMAPPED	92	CYS	N	119.182	0.3	1
UNMAPPED	60	ASP	H	7.921	0.02	1
UNMAPPED	3	GLY	C	174.302	0.3	1
UNMAPPED	116	VAL	N	119.915	0.3	1
UNMAPPED	92	CYS	CB	40.586	0.3	1
UNMAPPED	46	ALA	C	177.539	0.3	1
UNMAPPED	29	ALA	CA	52.03	0.3	1
UNMAPPED	10	ASN	CB	38.305	0.3	1
UNMAPPED	136	GLN	CB	28.152	0.3	1
UNMAPPED	67	MET	N	118.641	0.3	1
UNMAPPED	70	TYR	CA	52.254	0.3	1
UNMAPPED	118	MET	CA	59.31	0.3	1
UNMAPPED	107	LYS	N	119.828	0.3	1
UNMAPPED	48	SER	N	116.486	0.3	1
UNMAPPED	122	VAL	C	177.037	0.3	1
UNMAPPED	133	LYS	N	119.653	0.3	1
UNMAPPED	128	VAL	C	178.078	0.3	1
UNMAPPED	48	SER	CB	62.692	0.3	1
UNMAPPED	83	SER	CB	63.71	0.3	1
UNMAPPED	68	TYR	N	116.831	0.3	1
UNMAPPED	96	THR	C	177.702	0.3	1
UNMAPPED	3	GLY	CA	44.893	0.3	1
UNMAPPED	68	TYR	CB	35.559	0.3	1
UNMAPPED	113	GLU	CA	59.606	0.3	1
UNMAPPED	140	ASP	CB	40.505	0.3	1
UNMAPPED	104	THR	CA	64.954	0.3	1
UNMAPPED	140	ASP	N	121.166	0.3	1
UNMAPPED	57	ASP	CB	40.64	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	112	THR	H	9.61	0.02	1
UNMAPPED	61	ARG	N	119.929	0.3	1
UNMAPPED	73	GLN	C	174.987	0.3	1
UNMAPPED	61	ARG	CB	29.403	0.3	1

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	136	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	117	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	136	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	127	0.00 \pm 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 1596. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/665 (0%)	0/265 (0%)	0/270 (0%)	0/130 (0%)
Sidechain	0/815 (0%)	0/473 (0%)	0/315 (0%)	0/27 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1596 (0%)	0/798 (0%)	0/629 (0%)	0/169 (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 1685. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/698 (0%)	0/278 (0%)	0/284 (0%)	0/136 (0%)
Sidechain	0/871 (0%)	0/507 (0%)	0/335 (0%)	0/29 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1685 (0%)	0/845 (0%)	0/663 (0%)	0/177 (0%)

7.2.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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 16075

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	518
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	518
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 518 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	47	PRO	CA	61.881	0.3	1
UNMAPPED	139	ARG	C	176.214	0.3	1
UNMAPPED	33	GLY	C	174.716	0.3	1
UNMAPPED	20	LYS	H	8.317	0.02	1
UNMAPPED	29	GLY	H	8.324	0.02	1
UNMAPPED	39	VAL	CA	59.893	0.3	1
UNMAPPED	65	TYR	C	175.922	0.3	1
UNMAPPED	115	MET	N	118.7	0.3	1
UNMAPPED	48	MET	C	175.036	0.3	1
UNMAPPED	114	LYS	C	180.059	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	36	GLY	N	110.236	0.3	1
UNMAPPED	19	LEU	N	123.355	0.3	1
UNMAPPED	100	THR	N	115.63	0.3	1
UNMAPPED	41	GLY	N	115.643	0.3	1
UNMAPPED	3	GLY	H	8.404	0.02	1
UNMAPPED	86	VAL	N	120.455	0.3	1
UNMAPPED	11	LYS	N	122.826	0.3	1
UNMAPPED	70	GLN	CA	53.653	0.3	1
UNMAPPED	131	GLU	N	118.773	0.3	1
UNMAPPED	33	GLY	CA	44.908	0.3	1
UNMAPPED	37	GLY	N	109.942	0.3	1
UNMAPPED	66	ARG	CA	55.864	0.3	1
UNMAPPED	14	LYS	C	174.325	0.3	1
UNMAPPED	84	ASN	CA	55.594	0.3	1
UNMAPPED	29	GLY	CA	44.691	0.3	1
UNMAPPED	132	SER	H	8.472	0.02	1
UNMAPPED	72	TYR	H	8.488	0.02	1
UNMAPPED	74	ARG	H	7.983	0.02	1
UNMAPPED	2	GLY	N	110.576	0.3	1
UNMAPPED	98	THR	N	115.483	0.3	1
UNMAPPED	124	CYS	H	9.231	0.02	1
UNMAPPED	63	ASN	C	175.481	0.3	1
UNMAPPED	119	VAL	H	8.291	0.02	1
UNMAPPED	17	THR	N	115.71	0.3	1
UNMAPPED	21	HIS	C	175.325	0.3	1
UNMAPPED	12	PRO	CA	62.627	0.3	1
UNMAPPED	30	ALA	H	8.09	0.02	1
UNMAPPED	29	GLY	C	173.745	0.3	1
UNMAPPED	60	TYR	H	9.034	0.02	1
UNMAPPED	130	LYS	H	7.833	0.02	1
UNMAPPED	107	ASN	C	173.592	0.3	1
UNMAPPED	102	THR	H	8.282	0.02	1
UNMAPPED	140	ARG	N	122.693	0.3	1
UNMAPPED	38	TYR	C	175.555	0.3	1
UNMAPPED	95	LYS	N	123.647	0.3	1
UNMAPPED	132	SER	CA	60.818	0.3	1
UNMAPPED	101	THR	C	177.151	0.3	1
UNMAPPED	85	PHE	CA	60.485	0.3	1
UNMAPPED	58	ARG	H	8.043	0.02	1
UNMAPPED	59	TYR	H	8.265	0.02	1
UNMAPPED	74	ARG	CA	52.849	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	93	THR	C	177.725	0.3	1
UNMAPPED	124	CYS	CA	59.585	0.3	1
UNMAPPED	120	VAL	N	121.72	0.3	1
UNMAPPED	52	GLY	N	109.348	0.3	1
UNMAPPED	26	ALA	H	8.33	0.02	1
UNMAPPED	64	MET	C	176.351	0.3	1
UNMAPPED	112	ASP	N	120.187	0.3	1
UNMAPPED	61	ARG	H	7.892	0.02	1
UNMAPPED	43	ALA	CA	52.534	0.3	1
UNMAPPED	10	ASN	CA	52.378	0.3	1
UNMAPPED	55	TRP	N	120.565	0.3	1
UNMAPPED	126	THR	CA	66.652	0.3	1
UNMAPPED	7	ASN	C	175.205	0.3	1
UNMAPPED	19	LEU	H	8.294	0.02	1
UNMAPPED	135	TYR	N	119.516	0.3	1
UNMAPPED	45	SER	N	116.445	0.3	1
UNMAPPED	3	GLY	N	109.097	0.3	1
UNMAPPED	50	HIS	C	175.355	0.3	1
UNMAPPED	64	MET	CA	58.675	0.3	1
UNMAPPED	56	GLU	H	8.134	0.02	1
UNMAPPED	41	GLY	H	9.361	0.02	1
UNMAPPED	14	LYS	N	124.554	0.3	1
UNMAPPED	83	ASN	H	8.416	0.02	1
UNMAPPED	34	GLY	C	174.389	0.3	1
UNMAPPED	134	ALA	CA	53.751	0.3	1
UNMAPPED	45	SER	CA	58.262	0.3	1
UNMAPPED	67	TYR	C	172.761	0.3	1
UNMAPPED	27	ALA	H	8.242	0.02	1
UNMAPPED	126	THR	C	176.772	0.3	1
UNMAPPED	51	PHE	H	10.381	0.02	1
UNMAPPED	94	ILE	H	8.469	0.02	1
UNMAPPED	21	HIS	CA	55.805	0.3	1
UNMAPPED	118	ARG	H	7.293	0.02	1
UNMAPPED	66	ARG	N	119.194	0.3	1
UNMAPPED	12	PRO	C	176.965	0.3	1
UNMAPPED	50	HIS	CA	54.36	0.3	1
UNMAPPED	43	ALA	C	177.443	0.3	1
UNMAPPED	103	THR	C	175.178	0.3	1
UNMAPPED	46	ARG	CA	54.327	0.3	1
UNMAPPED	106	GLU	CA	55.141	0.3	1
UNMAPPED	82	GLN	C	176.877	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	141	SER	H	8.008	0.02	1
UNMAPPED	138	GLY	C	174.438	0.3	1
UNMAPPED	116	MET	N	118.47	0.3	1
UNMAPPED	86	VAL	CA	67.318	0.3	1
UNMAPPED	49	ILE	N	124.649	0.3	1
UNMAPPED	70	GLN	N	114.616	0.3	1
UNMAPPED	31	VAL	N	119.946	0.3	1
UNMAPPED	33	GLY	N	113.618	0.3	1
UNMAPPED	27	ALA	CA	51.974	0.3	1
UNMAPPED	109	THR	C	175.466	0.3	1
UNMAPPED	66	ARG	C	176.826	0.3	1
UNMAPPED	135	TYR	C	177.349	0.3	1
UNMAPPED	93	THR	CA	68.098	0.3	1
UNMAPPED	84	ASN	N	118.511	0.3	1
UNMAPPED	82	GLN	CA	58.935	0.3	1
UNMAPPED	138	GLY	CA	45.16	0.3	1
UNMAPPED	117	GLU	N	119.114	0.3	1
UNMAPPED	138	GLY	H	7.852	0.02	1
UNMAPPED	102	THR	N	118.614	0.3	1
UNMAPPED	32	VAL	N	125.091	0.3	1
UNMAPPED	46	ARG	H	8.712	0.02	1
UNMAPPED	2	GLY	CA	44.793	0.3	1
UNMAPPED	27	ALA	C	177.634	0.3	1
UNMAPPED	7	ASN	CA	52.752	0.3	1
UNMAPPED	48	MET	CA	53.661	0.3	1
UNMAPPED	53	ASN	CA	52.078	0.3	1
UNMAPPED	114	LYS	CA	58.716	0.3	1
UNMAPPED	120	VAL	H	9.166	0.02	1
UNMAPPED	52	GLY	H	8.944	0.02	1
UNMAPPED	26	ALA	N	123.457	0.3	1
UNMAPPED	96	GLN	H	8.557	0.02	1
UNMAPPED	2	GLY	C	174.758	0.3	1
UNMAPPED	123	MET	H	8.173	0.02	1
UNMAPPED	135	TYR	H	7.964	0.02	1
UNMAPPED	56	GLU	N	120.752	0.3	1
UNMAPPED	98	THR	H	8.521	0.02	1
UNMAPPED	46	ARG	C	174.613	0.3	1
UNMAPPED	104	LYS	N	119.833	0.3	1
UNMAPPED	48	MET	H	8.728	0.02	1
UNMAPPED	53	ASN	H	7.257	0.02	1
UNMAPPED	108	PHE	N	122.098	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	GLN	N	122.123	0.3	1
UNMAPPED	88	ASP	N	118.38	0.3	1
UNMAPPED	94	ILE	N	121.286	0.3	1
UNMAPPED	86	VAL	C	176.683	0.3	1
UNMAPPED	92	ILE	C	178.003	0.3	1
UNMAPPED	100	THR	C	176.771	0.3	1
UNMAPPED	126	THR	N	118.436	0.3	1
UNMAPPED	117	GLU	CA	60.219	0.3	1
UNMAPPED	138	GLY	N	108.09	0.3	1
UNMAPPED	135	TYR	CA	59.719	0.3	1
UNMAPPED	13	SER	C	174.157	0.3	1
UNMAPPED	4	GLY	H	8.338	0.02	1
UNMAPPED	140	ARG	H	8.239	0.02	1
UNMAPPED	37	GLY	C	173.877	0.3	1
UNMAPPED	137	ASP	C	177.35	0.3	1
UNMAPPED	15	PRO	CA	62.513	0.3	1
UNMAPPED	38	TYR	CA	57.787	0.3	1
UNMAPPED	132	SER	C	175.842	0.3	1
UNMAPPED	44	MET	C	175.523	0.3	1
UNMAPPED	15	PRO	C	176.862	0.3	1
UNMAPPED	35	LEU	CA	54.357	0.3	1
UNMAPPED	90	VAL	N	125.066	0.3	1
UNMAPPED	129	GLN	C	178.5	0.3	1
UNMAPPED	74	ARG	C	178.119	0.3	1
UNMAPPED	128	TYR	H	8.621	0.02	1
UNMAPPED	110	GLU	C	179.289	0.3	1
UNMAPPED	89	CYS	CA	58.123	0.3	1
UNMAPPED	91	ASN	CA	56.34	0.3	1
UNMAPPED	84	ASN	H	8.578	0.02	1
UNMAPPED	53	ASN	C	174.351	0.3	1
UNMAPPED	22	VAL	N	123.068	0.3	1
UNMAPPED	30	ALA	C	177.623	0.3	1
UNMAPPED	69	ASN	H	8.633	0.02	1
UNMAPPED	106	GLU	N	120.48	0.3	1
UNMAPPED	73	TYR	C	173.592	0.3	1
UNMAPPED	98	THR	C	176.498	0.3	1
UNMAPPED	92	ILE	H	8.765	0.02	1
UNMAPPED	63	ASN	H	7.568	0.02	1
UNMAPPED	129	GLN	H	8.241	0.02	1
UNMAPPED	129	GLN	CA	58.662	0.3	1
UNMAPPED	116	MET	CA	59.542	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	4	GLY	CA	44.806	0.3	1
UNMAPPED	65	TYR	CA	58.798	0.3	1
UNMAPPED	25	ALA	CA	52.141	0.3	1
UNMAPPED	111	THR	CA	66.464	0.3	1
UNMAPPED	35	LEU	H	8.274	0.02	1
UNMAPPED	99	VAL	H	8.101	0.02	1
UNMAPPED	30	ALA	CA	51.891	0.3	1
UNMAPPED	130	LYS	CA	58.892	0.3	1
UNMAPPED	51	PHE	N	125.436	0.3	1
UNMAPPED	141	SER	C	178.605	0.3	1
UNMAPPED	113	VAL	N	119.964	0.3	1
UNMAPPED	69	ASN	CA	51.459	0.3	1
UNMAPPED	121	GLU	N	120.934	0.3	1
UNMAPPED	110	GLU	H	9.212	0.02	1
UNMAPPED	61	ARG	C	179.116	0.3	1
UNMAPPED	84	ASN	C	177.318	0.3	1
UNMAPPED	43	ALA	N	125.738	0.3	1
UNMAPPED	14	LYS	H	8.383	0.02	1
UNMAPPED	136	TYR	C	177.072	0.3	1
UNMAPPED	105	GLY	C	174.247	0.3	1
UNMAPPED	116	MET	C	177.809	0.3	1
UNMAPPED	11	LYS	C	178.581	0.3	1
UNMAPPED	136	TYR	N	119.711	0.3	1
UNMAPPED	87	HIS	CA	59.612	0.3	1
UNMAPPED	53	ASN	N	114.549	0.3	1
UNMAPPED	65	TYR	H	7.592	0.02	1
UNMAPPED	49	ILE	H	6.585	0.02	1
UNMAPPED	24	GLY	H	8.43	0.02	1
UNMAPPED	62	GLU	CA	57.447	0.3	1
UNMAPPED	33	GLY	H	8.6	0.02	1
UNMAPPED	9	TRP	H	8.089	0.02	1
UNMAPPED	1	GLN	H	8.199	0.02	1
UNMAPPED	133	GLN	N	121.032	0.3	1
UNMAPPED	44	MET	CA	53.411	0.3	1
UNMAPPED	58	ARG	C	177.592	0.3	1
UNMAPPED	25	ALA	H	8.169	0.02	1
UNMAPPED	105	GLY	CA	45.03	0.3	1
UNMAPPED	126	THR	H	8.155	0.02	1
UNMAPPED	133	GLN	CA	57.76	0.3	1
UNMAPPED	67	TYR	H	7.473	0.02	1
UNMAPPED	91	ASN	C	178.465	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	34	GLY	H	8.3	0.02	1
UNMAPPED	39	VAL	C	172.945	0.3	1
UNMAPPED	141	SER	N	122.973	0.3	1
UNMAPPED	51	PHE	C	177.138	0.3	1
UNMAPPED	97	HIS	N	120.475	0.3	1
UNMAPPED	101	THR	CA	64.91	0.3	1
UNMAPPED	83	ASN	CA	56.124	0.3	1
UNMAPPED	128	TYR	N	120.45	0.3	1
UNMAPPED	85	PHE	C	177.807	0.3	1
UNMAPPED	133	GLN	H	7.586	0.02	1
UNMAPPED	61	ARG	CA	59.596	0.3	1
UNMAPPED	103	THR	N	116.732	0.3	1
UNMAPPED	60	TYR	CA	62.667	0.3	1
UNMAPPED	124	CYS	C	176.878	0.3	1
UNMAPPED	54	ASP	N	123.538	0.3	1
UNMAPPED	25	ALA	C	177.737	0.3	1
UNMAPPED	22	VAL	H	8.045	0.02	1
UNMAPPED	111	THR	C	175.66	0.3	1
UNMAPPED	8	GLN	C	175.754	0.3	1
UNMAPPED	5	THR	H	8.175	0.02	1
UNMAPPED	122	GLN	N	115.538	0.3	1
UNMAPPED	63	ASN	N	115.402	0.3	1
UNMAPPED	57	ASP	C	179.032	0.3	1
UNMAPPED	130	LYS	C	179.783	0.3	1
UNMAPPED	115	MET	H	8.189	0.02	1
UNMAPPED	109	THR	N	116.258	0.3	1
UNMAPPED	92	ILE	N	119.161	0.3	1
UNMAPPED	58	ARG	N	120.002	0.3	1
UNMAPPED	139	ARG	N	120.215	0.3	1
UNMAPPED	106	GLU	C	174.901	0.3	1
UNMAPPED	35	LEU	N	121.983	0.3	1
UNMAPPED	127	GLN	H	8.76	0.02	1
UNMAPPED	99	VAL	N	123.514	0.3	1
UNMAPPED	8	GLN	CA	55.818	0.3	1
UNMAPPED	108	PHE	H	8.788	0.02	1
UNMAPPED	11	LYS	CA	53.738	0.3	1
UNMAPPED	89	CYS	N	119.332	0.3	1
UNMAPPED	57	ASP	CA	58.175	0.3	1
UNMAPPED	87	HIS	C	177.663	0.3	1
UNMAPPED	93	THR	H	8.173	0.02	1
UNMAPPED	113	VAL	H	8.267	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	104	LYS	H	7.471	0.02	1
UNMAPPED	22	VAL	CA	61.562	0.3	1
UNMAPPED	131	GLU	C	179.22	0.3	1
UNMAPPED	110	GLU	N	120.191	0.3	1
UNMAPPED	19	LEU	CA	54.794	0.3	1
UNMAPPED	100	THR	CA	65.09	0.3	1
UNMAPPED	64	MET	H	7.899	0.02	1
UNMAPPED	36	GLY	CA	45.932	0.3	1
UNMAPPED	26	ALA	C	177.637	0.3	1
UNMAPPED	14	LYS	CA	53.749	0.3	1
UNMAPPED	41	GLY	CA	44.663	0.3	1
UNMAPPED	111	THR	N	116.924	0.3	1
UNMAPPED	136	TYR	H	8.066	0.02	1
UNMAPPED	119	VAL	N	119.393	0.3	1
UNMAPPED	131	GLU	CA	57.47	0.3	1
UNMAPPED	42	SER	C	174.966	0.3	1
UNMAPPED	37	GLY	CA	44.662	0.3	1
UNMAPPED	8	GLN	H	8.378	0.02	1
UNMAPPED	123	MET	C	178.472	0.3	1
UNMAPPED	125	VAL	CA	67.27	0.3	1
UNMAPPED	51	PHE	CA	59.177	0.3	1
UNMAPPED	121	GLU	C	177.525	0.3	1
UNMAPPED	113	VAL	CA	67.418	0.3	1
UNMAPPED	83	ASN	C	177.811	0.3	1
UNMAPPED	19	LEU	C	177.244	0.3	1
UNMAPPED	36	GLY	C	174.845	0.3	1
UNMAPPED	56	GLU	C	177.715	0.3	1
UNMAPPED	29	GLY	N	108.23	0.3	1
UNMAPPED	50	HIS	H	8.118	0.02	1
UNMAPPED	32	VAL	H	8.329	0.02	1
UNMAPPED	59	TYR	N	121.058	0.3	1
UNMAPPED	100	THR	H	8.225	0.02	1
UNMAPPED	97	HIS	H	8.526	0.02	1
UNMAPPED	108	PHE	C	176.681	0.3	1
UNMAPPED	98	THR	CA	66.374	0.3	1
UNMAPPED	86	VAL	H	8.934	0.02	1
UNMAPPED	131	GLU	H	8.432	0.02	1
UNMAPPED	4	GLY	C	174.526	0.3	1
UNMAPPED	137	ASP	H	8.262	0.02	1
UNMAPPED	44	MET	N	121.473	0.3	1
UNMAPPED	118	ARG	C	179.322	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	95	LYS	C	179.061	0.3	1
UNMAPPED	82	GLN	H	8.677	0.02	1
UNMAPPED	72	TYR	CA	56.695	0.3	1
UNMAPPED	55	TRP	H	8.566	0.02	1
UNMAPPED	132	SER	N	115.548	0.3	1
UNMAPPED	42	SER	CA	58.07	0.3	1
UNMAPPED	71	VAL	H	8.531	0.02	1
UNMAPPED	121	GLU	H	8.015	0.02	1
UNMAPPED	42	SER	N	113.766	0.3	1
UNMAPPED	141	SER	CA	59.522	0.3	1
UNMAPPED	5	THR	CA	61.563	0.3	1
UNMAPPED	74	ARG	N	120.691	0.3	1
UNMAPPED	139	ARG	H	7.825	0.02	1
UNMAPPED	40	LEU	CA	52.785	0.3	1
UNMAPPED	109	THR	H	9.601	0.02	1
UNMAPPED	69	ASN	C	172.779	0.3	1
UNMAPPED	124	CYS	N	119.496	0.3	1
UNMAPPED	23	ALA	C	178.219	0.3	1
UNMAPPED	120	VAL	CA	65.96	0.3	1
UNMAPPED	133	GLN	C	177.255	0.3	1
UNMAPPED	16	LYS	H	8.584	0.02	1
UNMAPPED	114	LYS	H	7.693	0.02	1
UNMAPPED	52	GLY	CA	45.27	0.3	1
UNMAPPED	54	ASP	CA	57.448	0.3	1
UNMAPPED	73	TYR	H	8.53	0.02	1
UNMAPPED	89	CYS	H	8.198	0.02	1
UNMAPPED	10	ASN	N	120.265	0.3	1
UNMAPPED	62	GLU	C	177.61	0.3	1
UNMAPPED	96	GLN	CA	57.62	0.3	1
UNMAPPED	40	LEU	C	177.895	0.3	1
UNMAPPED	66	ARG	H	7.521	0.02	1
UNMAPPED	92	ILE	CA	61.625	0.3	1
UNMAPPED	58	ARG	CA	59.419	0.3	1
UNMAPPED	120	VAL	C	177.606	0.3	1
UNMAPPED	64	MET	N	118.693	0.3	1
UNMAPPED	65	TYR	N	116.838	0.3	1
UNMAPPED	13	SER	CA	57.637	0.3	1
UNMAPPED	117	GLU	H	8.58	0.02	1
UNMAPPED	70	GLN	H	7.314	0.02	1
UNMAPPED	88	ASP	C	175.93	0.3	1
UNMAPPED	31	VAL	H	8.168	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	57	ASP	N	119.06	0.3	1
UNMAPPED	21	HIS	N	121.512	0.3	1
UNMAPPED	72	TYR	C	174.809	0.3	1
UNMAPPED	50	HIS	N	123.328	0.3	1
UNMAPPED	122	GLN	H	7.113	0.02	1
UNMAPPED	110	GLU	CA	59.729	0.3	1
UNMAPPED	89	CYS	C	177.533	0.3	1
UNMAPPED	46	ARG	N	127.152	0.3	1
UNMAPPED	24	GLY	C	174.02	0.3	1
UNMAPPED	17	THR	C	173.892	0.3	1
UNMAPPED	38	TYR	H	7.811	0.02	1
UNMAPPED	140	ARG	CA	55.494	0.3	1
UNMAPPED	102	THR	C	178.042	0.3	1
UNMAPPED	119	VAL	CA	65.264	0.3	1
UNMAPPED	13	SER	H	8.483	0.02	1
UNMAPPED	107	ASN	H	8.571	0.02	1
UNMAPPED	59	TYR	C	179.592	0.3	1
UNMAPPED	49	ILE	CA	58.686	0.3	1
UNMAPPED	27	ALA	N	123.59	0.3	1
UNMAPPED	62	GLU	H	7.934	0.02	1
UNMAPPED	125	VAL	N	123.771	0.3	1
UNMAPPED	31	VAL	CA	61.736	0.3	1
UNMAPPED	136	TYR	CA	59.406	0.3	1
UNMAPPED	18	ASN	CA	52.549	0.3	1
UNMAPPED	91	ASN	H	7.582	0.02	1
UNMAPPED	44	MET	H	8.818	0.02	1
UNMAPPED	93	THR	N	118.416	0.3	1
UNMAPPED	82	GLN	N	120.321	0.3	1
UNMAPPED	137	ASP	N	121.078	0.3	1
UNMAPPED	140	ARG	C	175.503	0.3	1
UNMAPPED	20	LYS	CA	55.912	0.3	1
UNMAPPED	102	THR	CA	65.033	0.3	1
UNMAPPED	32	VAL	CA	61.99	0.3	1
UNMAPPED	54	ASP	C	177.895	0.3	1
UNMAPPED	123	MET	N	119.82	0.3	1
UNMAPPED	59	TYR	CA	61.737	0.3	1
UNMAPPED	71	VAL	N	113.15	0.3	1
UNMAPPED	112	ASP	C	177.623	0.3	1
UNMAPPED	22	VAL	C	175.557	0.3	1
UNMAPPED	80	SER	CA	58.442	0.3	1
UNMAPPED	31	VAL	C	176.406	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	128	TYR	C	178.183	0.3	1
UNMAPPED	116	MET	H	8.709	0.02	1
UNMAPPED	111	THR	H	7.971	0.02	1
UNMAPPED	114	LYS	N	119.337	0.3	1
UNMAPPED	45	SER	H	8.467	0.02	1
UNMAPPED	48	MET	N	122.23	0.3	1
UNMAPPED	88	ASP	CA	56.734	0.3	1
UNMAPPED	45	SER	C	174.431	0.3	1
UNMAPPED	112	ASP	CA	57.586	0.3	1
UNMAPPED	26	ALA	CA	52.076	0.3	1
UNMAPPED	16	LYS	N	122.458	0.3	1
UNMAPPED	28	ALA	CA	52.255	0.3	1
UNMAPPED	115	MET	C	178.189	0.3	1
UNMAPPED	125	VAL	C	178.003	0.3	1
UNMAPPED	5	THR	N	113.704	0.3	1
UNMAPPED	68	PRO	C	175.084	0.3	1
UNMAPPED	137	ASP	CA	54.938	0.3	1
UNMAPPED	104	LYS	CA	55.776	0.3	1
UNMAPPED	40	LEU	N	124.224	0.3	1
UNMAPPED	47	PRO	C	175.668	0.3	1
UNMAPPED	99	VAL	C	178.564	0.3	1
UNMAPPED	118	ARG	N	117.018	0.3	1
UNMAPPED	56	GLU	CA	59.525	0.3	1
UNMAPPED	23	ALA	N	128.388	0.3	1
UNMAPPED	87	HIS	H	8.307	0.02	1
UNMAPPED	127	GLN	N	122.759	0.3	1
UNMAPPED	24	GLY	CA	44.775	0.3	1
UNMAPPED	10	ASN	C	174.346	0.3	1
UNMAPPED	108	PHE	CA	56.053	0.3	1
UNMAPPED	1	GLN	CA	54.619	0.3	1
UNMAPPED	11	LYS	H	8.027	0.02	1
UNMAPPED	119	VAL	C	177.048	0.3	1
UNMAPPED	9	TRP	CA	56.766	0.3	1
UNMAPPED	28	ALA	H	8.264	0.02	1
UNMAPPED	94	ILE	CA	66.08	0.3	1
UNMAPPED	96	GLN	N	117.291	0.3	1
UNMAPPED	118	ARG	CA	58.01	0.3	1
UNMAPPED	49	ILE	C	173.121	0.3	1
UNMAPPED	21	HIS	H	8.278	0.02	1
UNMAPPED	105	GLY	H	7.923	0.02	1
UNMAPPED	60	TYR	C	177.013	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	127	GLN	CA	58.202	0.3	1
UNMAPPED	106	GLU	H	7.463	0.02	1
UNMAPPED	34	GLY	CA	44.892	0.3	1
UNMAPPED	67	TYR	CA	52.242	0.3	1
UNMAPPED	34	GLY	N	108.735	0.3	1
UNMAPPED	1	GLN	C	176.518	0.3	1
UNMAPPED	32	VAL	C	176.672	0.3	1
UNMAPPED	9	TRP	C	175.883	0.3	1
UNMAPPED	38	TYR	N	118.315	0.3	1
UNMAPPED	90	VAL	CA	65.691	0.3	1
UNMAPPED	101	THR	H	8.06	0.02	1
UNMAPPED	107	ASN	N	119.703	0.3	1
UNMAPPED	42	SER	H	8.326	0.02	1
UNMAPPED	125	VAL	H	8.522	0.02	1
UNMAPPED	73	TYR	N	111.063	0.3	1
UNMAPPED	91	ASN	N	116.422	0.3	1
UNMAPPED	10	ASN	H	8.081	0.02	1
UNMAPPED	52	GLY	C	173.275	0.3	1
UNMAPPED	28	ALA	C	178.278	0.3	1
UNMAPPED	4	GLY	N	108.993	0.3	1
UNMAPPED	104	LYS	C	176.695	0.3	1
UNMAPPED	115	MET	CA	59.262	0.3	1
UNMAPPED	129	GLN	N	119.888	0.3	1
UNMAPPED	2	GLY	H	8.52	0.02	1
UNMAPPED	36	GLY	H	8.57	0.02	1
UNMAPPED	25	ALA	N	124.151	0.3	1
UNMAPPED	68	PRO	CA	63.138	0.3	1
UNMAPPED	90	VAL	H	9.286	0.02	1
UNMAPPED	134	ALA	H	7.595	0.02	1
UNMAPPED	30	ALA	N	123.859	0.3	1
UNMAPPED	57	ASP	H	7.914	0.02	1
UNMAPPED	41	GLY	C	172.851	0.3	1
UNMAPPED	130	LYS	N	119.46	0.3	1
UNMAPPED	20	LYS	N	122.046	0.3	1
UNMAPPED	69	ASN	N	116.54	0.3	1
UNMAPPED	16	LYS	C	176.853	0.3	1
UNMAPPED	123	MET	CA	59.762	0.3	1
UNMAPPED	117	GLU	C	178.747	0.3	1
UNMAPPED	71	VAL	CA	58.207	0.3	1
UNMAPPED	121	GLU	CA	60.776	0.3	1
UNMAPPED	94	ILE	C	178.786	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	113	VAL	C	177.442	0.3	1
UNMAPPED	40	LEU	H	7.971	0.02	1
UNMAPPED	87	HIS	N	118.054	0.3	1
UNMAPPED	81	ASN	C	173.97	0.3	1
UNMAPPED	43	ALA	H	8.755	0.02	1
UNMAPPED	37	GLY	H	8.443	0.02	1
UNMAPPED	17	THR	CA	61.155	0.3	1
UNMAPPED	62	GLU	N	116.106	0.3	1
UNMAPPED	16	LYS	CA	55.908	0.3	1
UNMAPPED	28	ALA	N	123.562	0.3	1
UNMAPPED	103	THR	H	7.84	0.02	1
UNMAPPED	13	SER	N	117.237	0.3	1
UNMAPPED	90	VAL	C	177.25	0.3	1
UNMAPPED	105	GLY	N	108.076	0.3	1
UNMAPPED	18	ASN	C	175.006	0.3	1
UNMAPPED	72	TYR	N	121.633	0.3	1
UNMAPPED	95	LYS	CA	59.865	0.3	1
UNMAPPED	134	ALA	C	179.128	0.3	1
UNMAPPED	70	GLN	C	174.903	0.3	1
UNMAPPED	20	LYS	C	176.211	0.3	1
UNMAPPED	97	HIS	CA	59.475	0.3	1
UNMAPPED	101	THR	N	114.889	0.3	1
UNMAPPED	122	GLN	C	179.235	0.3	1
UNMAPPED	83	ASN	N	117.085	0.3	1
UNMAPPED	24	GLY	N	108.991	0.3	1
UNMAPPED	17	THR	H	8.202	0.02	1
UNMAPPED	128	TYR	CA	61.507	0.3	1
UNMAPPED	9	TRP	N	121.269	0.3	1
UNMAPPED	60	TYR	N	120.742	0.3	1
UNMAPPED	103	THR	CA	64.434	0.3	1
UNMAPPED	3	GLY	C	174.764	0.3	1
UNMAPPED	23	ALA	CA	52.233	0.3	1
UNMAPPED	97	HIS	C	178.707	0.3	1
UNMAPPED	127	GLN	C	177.455	0.3	1
UNMAPPED	55	TRP	CA	61.418	0.3	1
UNMAPPED	122	GLN	CA	58.716	0.3	1
UNMAPPED	63	ASN	CA	54.519	0.3	1
UNMAPPED	67	TYR	N	121.771	0.3	1
UNMAPPED	95	LYS	H	8.137	0.02	1
UNMAPPED	35	LEU	C	177.997	0.3	1
UNMAPPED	88	ASP	H	7.504	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	96	GLN	C	178.651	0.3	1
UNMAPPED	109	THR	CA	59.972	0.3	1
UNMAPPED	139	ARG	CA	55.725	0.3	1
UNMAPPED	3	GLY	CA	44.806	0.3	1
UNMAPPED	71	VAL	C	174.066	0.3	1
UNMAPPED	107	ASN	CA	52.342	0.3	1
UNMAPPED	112	ASP	H	7.534	0.02	1
UNMAPPED	99	VAL	CA	65.95	0.3	1
UNMAPPED	134	ALA	N	120.791	0.3	1
UNMAPPED	23	ALA	H	8.465	0.02	1
UNMAPPED	8	GLN	N	120.542	0.3	1
UNMAPPED	61	ARG	N	117.568	0.3	1
UNMAPPED	73	TYR	CA	55.457	0.3	1
UNMAPPED	55	TRP	C	179.115	0.3	1
UNMAPPED	81	ASN	CA	52.256	0.3	1
UNMAPPED	54	ASP	H	9.038	0.02	1

7.3.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	135	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	133	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	125	0.00 \pm 0.00	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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1596. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/665 (0%)	0/265 (0%)	0/270 (0%)	0/130 (0%)
Sidechain	0/815 (0%)	0/473 (0%)	0/315 (0%)	0/27 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1596 (0%)	0/798 (0%)	0/629 (0%)	0/169 (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 1685. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/698 (0%)	0/278 (0%)	0/284 (0%)	0/136 (0%)
Sidechain	0/871 (0%)	0/507 (0%)	0/335 (0%)	0/29 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1685 (0%)	0/845 (0%)	0/663 (0%)	0/177 (0%)

7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.

7.4 Chemical shift list 4

File name: BMRB entry 16076

Chemical shift list name: *assigned_chem_shift_list_1*

7.4.1 Bookkeeping [i](#)

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	522
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	522
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 522 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	47	PRO	CA	61.99	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	139	ARG	C	176.205	0.3	1
UNMAPPED	33	GLY	C	174.735	0.3	1
UNMAPPED	20	LYS	H	8.307	0.02	1
UNMAPPED	29	GLY	H	8.321	0.02	1
UNMAPPED	65	TYR	C	175.889	0.3	1
UNMAPPED	115	MET	N	118.651	0.3	1
UNMAPPED	48	MET	C	174.997	0.3	1
UNMAPPED	114	LYS	C	180.042	0.3	1
UNMAPPED	36	GLY	N	110.217	0.3	1
UNMAPPED	19	LEU	N	123.32	0.3	1
UNMAPPED	100	THR	N	115.553	0.3	1
UNMAPPED	41	GLY	N	115.48	0.3	1
UNMAPPED	3	GLY	H	8.384	0.02	1
UNMAPPED	15	PRO	CA	62.643	0.3	1
UNMAPPED	86	VAL	N	120.611	0.3	1
UNMAPPED	11	LYS	N	121.498	0.3	1
UNMAPPED	70	GLN	CA	53.789	0.3	1
UNMAPPED	131	GLU	N	118.562	0.3	1
UNMAPPED	33	GLY	CA	44.956	0.3	1
UNMAPPED	37	GLY	N	109.543	0.3	1
UNMAPPED	66	ARG	CA	55.869	0.3	1
UNMAPPED	14	LYS	C	174.355	0.3	1
UNMAPPED	84	ASN	CA	55.716	0.3	1
UNMAPPED	29	GLY	CA	44.786	0.3	1
UNMAPPED	132	SER	H	8.425	0.02	1
UNMAPPED	72	TYR	H	8.484	0.02	1
UNMAPPED	74	ARG	H	7.951	0.02	1
UNMAPPED	2	GLY	N	110.584	0.3	1
UNMAPPED	98	THR	N	115.461	0.3	1
UNMAPPED	124	CYS	H	9.236	0.02	1
UNMAPPED	63	ASN	C	175.469	0.3	1
UNMAPPED	119	VAL	H	8.273	0.02	1
UNMAPPED	17	THR	N	115.569	0.3	1
UNMAPPED	21	HIS	C	175.308	0.3	1
UNMAPPED	30	ALA	H	8.101	0.02	1
UNMAPPED	29	GLY	C	173.689	0.3	1
UNMAPPED	60	TYR	H	9.032	0.02	1
UNMAPPED	130	LYS	H	7.873	0.02	1
UNMAPPED	107	ASN	C	173.577	0.3	1
UNMAPPED	102	THR	H	8.288	0.02	1
UNMAPPED	140	ARG	N	122.74	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	38	TYR	C	175.72	0.3	1
UNMAPPED	95	LYS	N	123.761	0.3	1
UNMAPPED	132	SER	CA	60.796	0.3	1
UNMAPPED	101	THR	C	177.138	0.3	1
UNMAPPED	85	PHE	CA	60.445	0.3	1
UNMAPPED	58	ARG	H	8.037	0.02	1
UNMAPPED	12	LEU	N	122.218	0.3	1
UNMAPPED	59	TYR	H	8.263	0.02	1
UNMAPPED	74	ARG	CA	53.112	0.3	1
UNMAPPED	93	THR	C	177.676	0.3	1
UNMAPPED	124	CYS	CA	59.733	0.3	1
UNMAPPED	120	VAL	N	121.593	0.3	1
UNMAPPED	52	GLY	N	109.359	0.3	1
UNMAPPED	26	ALA	H	8.327	0.02	1
UNMAPPED	64	MET	C	176.316	0.3	1
UNMAPPED	112	ASP	N	120.137	0.3	1
UNMAPPED	61	ARG	H	7.889	0.02	1
UNMAPPED	43	ALA	CA	52.539	0.3	1
UNMAPPED	10	ASN	CA	52.927	0.3	1
UNMAPPED	55	TRP	N	120.558	0.3	1
UNMAPPED	126	THR	CA	66.668	0.3	1
UNMAPPED	7	ASN	C	175.273	0.3	1
UNMAPPED	19	LEU	H	8.284	0.02	1
UNMAPPED	135	TYR	N	119.382	0.3	1
UNMAPPED	45	SER	N	116.482	0.3	1
UNMAPPED	3	GLY	N	109.222	0.3	1
UNMAPPED	39	MET	CA	53.242	0.3	1
UNMAPPED	50	HIS	C	175.289	0.3	1
UNMAPPED	64	MET	CA	58.687	0.3	1
UNMAPPED	56	GLU	H	8.137	0.02	1
UNMAPPED	41	GLY	H	9.435	0.02	1
UNMAPPED	14	LYS	N	124.662	0.3	1
UNMAPPED	83	ASN	H	8.425	0.02	1
UNMAPPED	34	GLY	C	174.35	0.3	1
UNMAPPED	134	ALA	CA	53.711	0.3	1
UNMAPPED	45	SER	CA	58.208	0.3	1
UNMAPPED	67	TYR	C	172.791	0.3	1
UNMAPPED	27	ALA	H	8.237	0.02	1
UNMAPPED	126	THR	C	176.692	0.3	1
UNMAPPED	51	PHE	H	10.377	0.02	1
UNMAPPED	94	ILE	H	8.481	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	21	HIS	CA	55.896	0.3	1
UNMAPPED	118	ARG	H	7.287	0.02	1
UNMAPPED	66	ARG	N	119.167	0.3	1
UNMAPPED	50	HIS	CA	54.386	0.3	1
UNMAPPED	43	ALA	C	177.508	0.3	1
UNMAPPED	103	THR	C	175.14	0.3	1
UNMAPPED	46	ARG	CA	54.412	0.3	1
UNMAPPED	106	GLU	CA	55.244	0.3	1
UNMAPPED	82	GLN	C	176.862	0.3	1
UNMAPPED	141	SER	H	8.01	0.02	1
UNMAPPED	138	GLY	C	174.431	0.3	1
UNMAPPED	116	MET	N	118.45	0.3	1
UNMAPPED	86	VAL	CA	67.35	0.3	1
UNMAPPED	49	ILE	N	124.646	0.3	1
UNMAPPED	70	GLN	N	114.502	0.3	1
UNMAPPED	31	VAL	N	119.904	0.3	1
UNMAPPED	33	GLY	N	113.686	0.3	1
UNMAPPED	27	ALA	CA	52.111	0.3	1
UNMAPPED	109	THR	C	175.456	0.3	1
UNMAPPED	18	ASN	N	121.856	0.3	1
UNMAPPED	66	ARG	C	176.785	0.3	1
UNMAPPED	135	TYR	C	177.164	0.3	1
UNMAPPED	93	THR	CA	68.146	0.3	1
UNMAPPED	84	ASN	N	118.482	0.3	1
UNMAPPED	82	GLN	CA	58.796	0.3	1
UNMAPPED	138	GLY	CA	45.25	0.3	1
UNMAPPED	117	GLU	N	119.118	0.3	1
UNMAPPED	138	GLY	H	7.862	0.02	1
UNMAPPED	102	THR	N	118.607	0.3	1
UNMAPPED	32	VAL	N	125.034	0.3	1
UNMAPPED	46	ARG	H	8.706	0.02	1
UNMAPPED	2	GLY	CA	44.901	0.3	1
UNMAPPED	12	LEU	H	8.156	0.02	1
UNMAPPED	27	ALA	C	177.605	0.3	1
UNMAPPED	7	ASN	CA	52.849	0.3	1
UNMAPPED	48	MET	CA	53.709	0.3	1
UNMAPPED	53	ASN	CA	52.137	0.3	1
UNMAPPED	114	LYS	CA	58.796	0.3	1
UNMAPPED	120	VAL	H	9.172	0.02	1
UNMAPPED	52	GLY	H	8.948	0.02	1
UNMAPPED	26	ALA	N	123.452	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	96	GLN	H	8.556	0.02	1
UNMAPPED	2	GLY	C	174.743	0.3	1
UNMAPPED	123	MET	H	8.129	0.02	1
UNMAPPED	135	TYR	H	7.945	0.02	1
UNMAPPED	56	GLU	N	120.796	0.3	1
UNMAPPED	98	THR	H	8.533	0.02	1
UNMAPPED	46	ARG	C	174.643	0.3	1
UNMAPPED	104	LYS	N	119.843	0.3	1
UNMAPPED	48	MET	H	8.725	0.02	1
UNMAPPED	53	ASN	H	7.256	0.02	1
UNMAPPED	108	PHE	N	121.994	0.3	1
UNMAPPED	137	ASP	CA	54.903	0.3	1
UNMAPPED	88	ASP	N	118.318	0.3	1
UNMAPPED	94	ILE	N	121.317	0.3	1
UNMAPPED	86	VAL	C	176.678	0.3	1
UNMAPPED	92	ILE	C	177.965	0.3	1
UNMAPPED	100	THR	C	176.757	0.3	1
UNMAPPED	126	THR	N	118.374	0.3	1
UNMAPPED	117	GLU	CA	60.334	0.3	1
UNMAPPED	138	GLY	N	108.176	0.3	1
UNMAPPED	135	TYR	CA	59.579	0.3	1
UNMAPPED	13	SER	C	173.944	0.3	1
UNMAPPED	39	MET	N	121.729	0.3	1
UNMAPPED	4	GLY	H	8.411	0.02	1
UNMAPPED	140	ARG	H	8.253	0.02	1
UNMAPPED	37	GLY	C	173.944	0.3	1
UNMAPPED	137	ASP	C	177.243	0.3	1
UNMAPPED	5	THR	H	8.178	0.02	1
UNMAPPED	38	TYR	CA	57.968	0.3	1
UNMAPPED	132	SER	C	175.64	0.3	1
UNMAPPED	44	MET	C	175.593	0.3	1
UNMAPPED	15	PRO	C	176.869	0.3	1
UNMAPPED	35	LEU	CA	54.525	0.3	1
UNMAPPED	90	VAL	N	125.178	0.3	1
UNMAPPED	129	GLN	C	178.556	0.3	1
UNMAPPED	74	ARG	C	178.149	0.3	1
UNMAPPED	128	TYR	H	8.625	0.02	1
UNMAPPED	110	GLU	C	179.24	0.3	1
UNMAPPED	89	CYS	CA	58.334	0.3	1
UNMAPPED	91	ASN	CA	56.38	0.3	1
UNMAPPED	84	ASN	H	8.593	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	53	ASN	C	174.325	0.3	1
UNMAPPED	22	VAL	N	123.062	0.3	1
UNMAPPED	30	ALA	C	177.559	0.3	1
UNMAPPED	69	ASN	H	8.648	0.02	1
UNMAPPED	106	GLU	N	120.439	0.3	1
UNMAPPED	73	TYR	C	173.576	0.3	1
UNMAPPED	98	THR	C	176.494	0.3	1
UNMAPPED	92	ILE	H	8.805	0.02	1
UNMAPPED	63	ASN	H	7.563	0.02	1
UNMAPPED	129	GLN	H	8.253	0.02	1
UNMAPPED	129	GLN	CA	58.69	0.3	1
UNMAPPED	116	MET	CA	59.682	0.3	1
UNMAPPED	4	GLY	CA	44.801	0.3	1
UNMAPPED	65	TYR	CA	58.9	0.3	1
UNMAPPED	25	ALA	CA	52.182	0.3	1
UNMAPPED	111	THR	CA	66.527	0.3	1
UNMAPPED	35	LEU	H	8.242	0.02	1
UNMAPPED	99	VAL	H	8.105	0.02	1
UNMAPPED	30	ALA	CA	51.955	0.3	1
UNMAPPED	39	MET	C	172.942	0.3	1
UNMAPPED	130	LYS	CA	59.0	0.3	1
UNMAPPED	51	PHE	N	125.395	0.3	1
UNMAPPED	141	SER	C	178.635	0.3	1
UNMAPPED	113	VAL	N	119.923	0.3	1
UNMAPPED	69	ASN	CA	51.612	0.3	1
UNMAPPED	121	GLU	N	120.957	0.3	1
UNMAPPED	110	GLU	H	9.212	0.02	1
UNMAPPED	61	ARG	C	179.119	0.3	1
UNMAPPED	84	ASN	C	177.348	0.3	1
UNMAPPED	43	ALA	N	125.799	0.3	1
UNMAPPED	14	LYS	H	8.307	0.02	1
UNMAPPED	136	TYR	C	176.887	0.3	1
UNMAPPED	105	GLY	C	174.234	0.3	1
UNMAPPED	116	MET	C	177.813	0.3	1
UNMAPPED	11	LYS	C	176.56	0.3	1
UNMAPPED	136	TYR	N	119.886	0.3	1
UNMAPPED	87	HIS	CA	59.522	0.3	1
UNMAPPED	53	ASN	N	114.522	0.3	1
UNMAPPED	65	TYR	H	7.597	0.02	1
UNMAPPED	49	ILE	H	6.583	0.02	1
UNMAPPED	24	GLY	H	8.425	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	62	GLU	CA	57.497	0.3	1
UNMAPPED	33	GLY	H	8.612	0.02	1
UNMAPPED	9	TRP	H	8.098	0.02	1
UNMAPPED	133	GLN	N	120.976	0.3	1
UNMAPPED	44	MET	CA	53.523	0.3	1
UNMAPPED	58	ARG	C	177.597	0.3	1
UNMAPPED	25	ALA	H	8.167	0.02	1
UNMAPPED	105	GLY	CA	45.135	0.3	1
UNMAPPED	126	THR	H	8.128	0.02	1
UNMAPPED	133	GLN	CA	57.737	0.3	1
UNMAPPED	67	TYR	H	7.46	0.02	1
UNMAPPED	91	ASN	C	178.478	0.3	1
UNMAPPED	34	GLY	H	8.308	0.02	1
UNMAPPED	39	MET	H	9.139	0.02	1
UNMAPPED	141	SER	N	123.0	0.3	1
UNMAPPED	51	PHE	C	177.085	0.3	1
UNMAPPED	97	HIS	N	120.416	0.3	1
UNMAPPED	101	THR	CA	65.015	0.3	1
UNMAPPED	83	ASN	CA	56.131	0.3	1
UNMAPPED	128	TYR	N	120.47	0.3	1
UNMAPPED	85	PHE	C	177.506	0.3	1
UNMAPPED	133	GLN	H	7.606	0.02	1
UNMAPPED	61	ARG	CA	59.623	0.3	1
UNMAPPED	103	THR	N	116.677	0.3	1
UNMAPPED	60	TYR	CA	62.74	0.3	1
UNMAPPED	124	CYS	C	176.901	0.3	1
UNMAPPED	54	ASP	N	123.49	0.3	1
UNMAPPED	25	ALA	C	177.707	0.3	1
UNMAPPED	22	VAL	H	8.04	0.02	1
UNMAPPED	111	THR	C	175.64	0.3	1
UNMAPPED	8	GLN	C	175.919	0.3	1
UNMAPPED	122	GLN	N	115.478	0.3	1
UNMAPPED	63	ASN	N	115.424	0.3	1
UNMAPPED	57	ASP	C	179.038	0.3	1
UNMAPPED	130	LYS	C	179.778	0.3	1
UNMAPPED	115	MET	H	8.181	0.02	1
UNMAPPED	109	THR	N	116.218	0.3	1
UNMAPPED	92	ILE	N	119.19	0.3	1
UNMAPPED	58	ARG	N	119.975	0.3	1
UNMAPPED	139	ARG	N	120.252	0.3	1
UNMAPPED	106	GLU	C	174.891	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	35	LEU	N	122.02	0.3	1
UNMAPPED	127	GLN	H	8.732	0.02	1
UNMAPPED	99	VAL	N	123.51	0.3	1
UNMAPPED	8	GLN	CA	56.011	0.3	1
UNMAPPED	108	PHE	H	8.789	0.02	1
UNMAPPED	11	LYS	CA	56.326	0.3	1
UNMAPPED	89	CYS	N	119.164	0.3	1
UNMAPPED	57	ASP	CA	58.219	0.3	1
UNMAPPED	87	HIS	C	177.598	0.3	1
UNMAPPED	93	THR	H	8.169	0.02	1
UNMAPPED	113	VAL	H	8.268	0.02	1
UNMAPPED	104	LYS	H	7.468	0.02	1
UNMAPPED	12	LEU	C	177.331	0.3	1
UNMAPPED	22	VAL	CA	61.627	0.3	1
UNMAPPED	131	GLU	C	179.214	0.3	1
UNMAPPED	110	GLU	N	120.174	0.3	1
UNMAPPED	19	LEU	CA	54.881	0.3	1
UNMAPPED	100	THR	CA	65.138	0.3	1
UNMAPPED	64	MET	H	7.892	0.02	1
UNMAPPED	36	GLY	CA	45.873	0.3	1
UNMAPPED	26	ALA	C	177.623	0.3	1
UNMAPPED	14	LYS	CA	53.844	0.3	1
UNMAPPED	41	GLY	CA	44.558	0.3	1
UNMAPPED	111	THR	N	116.886	0.3	1
UNMAPPED	136	TYR	H	8.058	0.02	1
UNMAPPED	119	VAL	N	119.326	0.3	1
UNMAPPED	131	GLU	CA	57.489	0.3	1
UNMAPPED	42	SER	C	174.946	0.3	1
UNMAPPED	37	GLY	CA	44.792	0.3	1
UNMAPPED	8	GLN	H	8.384	0.02	1
UNMAPPED	123	MET	C	178.544	0.3	1
UNMAPPED	125	VAL	CA	67.388	0.3	1
UNMAPPED	51	PHE	CA	59.232	0.3	1
UNMAPPED	121	GLU	C	177.519	0.3	1
UNMAPPED	113	VAL	CA	67.484	0.3	1
UNMAPPED	83	ASN	C	177.703	0.3	1
UNMAPPED	19	LEU	C	177.214	0.3	1
UNMAPPED	36	GLY	C	174.807	0.3	1
UNMAPPED	56	GLU	C	177.699	0.3	1
UNMAPPED	29	GLY	N	108.224	0.3	1
UNMAPPED	50	HIS	H	8.123	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	32	VAL	H	8.321	0.02	1
UNMAPPED	59	TYR	N	121.098	0.3	1
UNMAPPED	100	THR	H	8.22	0.02	1
UNMAPPED	97	HIS	H	8.52	0.02	1
UNMAPPED	108	PHE	C	176.678	0.3	1
UNMAPPED	98	THR	CA	66.445	0.3	1
UNMAPPED	86	VAL	H	8.903	0.02	1
UNMAPPED	131	GLU	H	8.44	0.02	1
UNMAPPED	4	GLY	C	174.527	0.3	1
UNMAPPED	137	ASP	H	8.25	0.02	1
UNMAPPED	44	MET	N	121.603	0.3	1
UNMAPPED	118	ARG	C	179.319	0.3	1
UNMAPPED	95	LYS	C	179.03	0.3	1
UNMAPPED	82	GLN	H	8.672	0.02	1
UNMAPPED	72	TYR	CA	56.717	0.3	1
UNMAPPED	55	TRP	H	8.563	0.02	1
UNMAPPED	132	SER	N	115.426	0.3	1
UNMAPPED	42	SER	CA	58.17	0.3	1
UNMAPPED	71	VAL	H	8.48	0.02	1
UNMAPPED	121	GLU	H	8.011	0.02	1
UNMAPPED	42	SER	N	113.999	0.3	1
UNMAPPED	141	SER	CA	59.611	0.3	1
UNMAPPED	5	THR	CA	61.617	0.3	1
UNMAPPED	12	LEU	CA	54.671	0.3	1
UNMAPPED	74	ARG	N	120.885	0.3	1
UNMAPPED	139	ARG	H	7.844	0.02	1
UNMAPPED	40	LEU	CA	52.784	0.3	1
UNMAPPED	109	THR	H	9.613	0.02	1
UNMAPPED	69	ASN	C	172.853	0.3	1
UNMAPPED	124	CYS	N	119.706	0.3	1
UNMAPPED	23	ALA	C	178.202	0.3	1
UNMAPPED	120	VAL	CA	66.015	0.3	1
UNMAPPED	133	GLN	C	177.164	0.3	1
UNMAPPED	16	LYS	H	8.568	0.02	1
UNMAPPED	114	LYS	H	7.699	0.02	1
UNMAPPED	52	GLY	CA	45.354	0.3	1
UNMAPPED	54	ASP	CA	57.541	0.3	1
UNMAPPED	73	TYR	H	8.52	0.02	1
UNMAPPED	89	CYS	H	8.164	0.02	1
UNMAPPED	10	ASN	N	120.111	0.3	1
UNMAPPED	62	GLU	C	177.572	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	96	GLN	CA	57.734	0.3	1
UNMAPPED	40	LEU	C	178.143	0.3	1
UNMAPPED	66	ARG	H	7.522	0.02	1
UNMAPPED	92	ILE	CA	61.736	0.3	1
UNMAPPED	58	ARG	CA	59.369	0.3	1
UNMAPPED	120	VAL	C	177.571	0.3	1
UNMAPPED	64	MET	N	118.62	0.3	1
UNMAPPED	65	TYR	N	116.821	0.3	1
UNMAPPED	13	SER	CA	57.825	0.3	1
UNMAPPED	117	GLU	H	8.587	0.02	1
UNMAPPED	70	GLN	H	7.299	0.02	1
UNMAPPED	88	ASP	C	175.85	0.3	1
UNMAPPED	31	VAL	H	8.167	0.02	1
UNMAPPED	57	ASP	N	119.066	0.3	1
UNMAPPED	18	ASN	H	8.572	0.02	1
UNMAPPED	21	HIS	N	121.437	0.3	1
UNMAPPED	72	TYR	C	174.707	0.3	1
UNMAPPED	50	HIS	N	123.257	0.3	1
UNMAPPED	122	GLN	H	7.085	0.02	1
UNMAPPED	110	GLU	CA	59.724	0.3	1
UNMAPPED	89	CYS	C	177.519	0.3	1
UNMAPPED	46	ARG	N	127.086	0.3	1
UNMAPPED	24	GLY	C	173.98	0.3	1
UNMAPPED	17	THR	C	173.961	0.3	1
UNMAPPED	38	TYR	H	7.87	0.02	1
UNMAPPED	140	ARG	CA	55.559	0.3	1
UNMAPPED	102	THR	C	178.005	0.3	1
UNMAPPED	119	VAL	CA	65.361	0.3	1
UNMAPPED	13	SER	H	8.194	0.02	1
UNMAPPED	107	ASN	H	8.563	0.02	1
UNMAPPED	59	TYR	C	179.569	0.3	1
UNMAPPED	49	ILE	CA	58.811	0.3	1
UNMAPPED	27	ALA	N	123.596	0.3	1
UNMAPPED	62	GLU	H	7.924	0.02	1
UNMAPPED	125	VAL	N	123.899	0.3	1
UNMAPPED	31	VAL	CA	61.767	0.3	1
UNMAPPED	136	TYR	CA	59.377	0.3	1
UNMAPPED	18	ASN	CA	52.62	0.3	1
UNMAPPED	91	ASN	H	7.602	0.02	1
UNMAPPED	44	MET	H	8.805	0.02	1
UNMAPPED	93	THR	N	118.249	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	82	GLN	N	120.198	0.3	1
UNMAPPED	137	ASP	N	121.202	0.3	1
UNMAPPED	140	ARG	C	175.471	0.3	1
UNMAPPED	20	LYS	CA	55.994	0.3	1
UNMAPPED	102	THR	CA	65.144	0.3	1
UNMAPPED	32	VAL	CA	62.099	0.3	1
UNMAPPED	54	ASP	C	177.902	0.3	1
UNMAPPED	123	MET	N	119.602	0.3	1
UNMAPPED	59	TYR	CA	61.792	0.3	1
UNMAPPED	71	VAL	N	113.008	0.3	1
UNMAPPED	112	ASP	C	177.624	0.3	1
UNMAPPED	22	VAL	C	175.543	0.3	1
UNMAPPED	80	SER	CA	58.497	0.3	1
UNMAPPED	31	VAL	C	176.363	0.3	1
UNMAPPED	128	TYR	C	178.018	0.3	1
UNMAPPED	116	MET	H	8.709	0.02	1
UNMAPPED	111	THR	H	7.97	0.02	1
UNMAPPED	114	LYS	N	119.301	0.3	1
UNMAPPED	45	SER	H	8.469	0.02	1
UNMAPPED	48	MET	N	122.177	0.3	1
UNMAPPED	88	ASP	CA	56.783	0.3	1
UNMAPPED	45	SER	C	174.426	0.3	1
UNMAPPED	112	ASP	CA	57.645	0.3	1
UNMAPPED	26	ALA	CA	52.083	0.3	1
UNMAPPED	16	LYS	N	122.346	0.3	1
UNMAPPED	28	ALA	CA	52.342	0.3	1
UNMAPPED	115	MET	C	178.189	0.3	1
UNMAPPED	125	VAL	C	178.044	0.3	1
UNMAPPED	5	THR	N	113.664	0.3	1
UNMAPPED	68	PRO	C	175.025	0.3	1
UNMAPPED	104	LYS	CA	55.792	0.3	1
UNMAPPED	40	LEU	N	121.435	0.3	1
UNMAPPED	47	PRO	C	175.656	0.3	1
UNMAPPED	99	VAL	C	178.557	0.3	1
UNMAPPED	118	ARG	N	117.007	0.3	1
UNMAPPED	56	GLU	CA	59.605	0.3	1
UNMAPPED	23	ALA	N	128.376	0.3	1
UNMAPPED	87	HIS	H	8.381	0.02	1
UNMAPPED	127	GLN	N	122.857	0.3	1
UNMAPPED	24	GLY	CA	44.786	0.3	1
UNMAPPED	10	ASN	C	175.062	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	108	PHE	CA	56.084	0.3	1
UNMAPPED	1	GLN	CA	55.625	0.3	1
UNMAPPED	11	LYS	H	8.069	0.02	1
UNMAPPED	119	VAL	C	177.006	0.3	1
UNMAPPED	9	TRP	CA	56.976	0.3	1
UNMAPPED	28	ALA	H	8.268	0.02	1
UNMAPPED	94	ILE	CA	66.201	0.3	1
UNMAPPED	96	GLN	N	117.396	0.3	1
UNMAPPED	118	ARG	CA	58.076	0.3	1
UNMAPPED	49	ILE	C	173.107	0.3	1
UNMAPPED	21	HIS	H	8.287	0.02	1
UNMAPPED	105	GLY	H	7.925	0.02	1
UNMAPPED	60	TYR	C	176.976	0.3	1
UNMAPPED	127	GLN	CA	58.308	0.3	1
UNMAPPED	106	GLU	H	7.457	0.02	1
UNMAPPED	34	GLY	CA	44.911	0.3	1
UNMAPPED	67	TYR	CA	52.322	0.3	1
UNMAPPED	34	GLY	N	108.731	0.3	1
UNMAPPED	1	GLN	C	176.532	0.3	1
UNMAPPED	32	VAL	C	176.647	0.3	1
UNMAPPED	9	TRP	C	176.117	0.3	1
UNMAPPED	38	TYR	N	118.246	0.3	1
UNMAPPED	90	VAL	CA	65.743	0.3	1
UNMAPPED	101	THR	H	8.055	0.02	1
UNMAPPED	107	ASN	N	119.665	0.3	1
UNMAPPED	42	SER	H	8.347	0.02	1
UNMAPPED	125	VAL	H	8.51	0.02	1
UNMAPPED	73	TYR	N	111.235	0.3	1
UNMAPPED	91	ASN	N	116.544	0.3	1
UNMAPPED	10	ASN	H	8.119	0.02	1
UNMAPPED	52	GLY	C	173.221	0.3	1
UNMAPPED	28	ALA	C	178.257	0.3	1
UNMAPPED	4	GLY	N	109.137	0.3	1
UNMAPPED	104	LYS	C	176.704	0.3	1
UNMAPPED	115	MET	CA	59.397	0.3	1
UNMAPPED	129	GLN	N	119.889	0.3	1
UNMAPPED	2	GLY	H	8.521	0.02	1
UNMAPPED	36	GLY	H	8.583	0.02	1
UNMAPPED	25	ALA	N	124.124	0.3	1
UNMAPPED	68	PRO	CA	63.154	0.3	1
UNMAPPED	90	VAL	H	9.303	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	134	ALA	H	7.607	0.02	1
UNMAPPED	30	ALA	N	123.834	0.3	1
UNMAPPED	57	ASP	H	7.917	0.02	1
UNMAPPED	41	GLY	C	172.788	0.3	1
UNMAPPED	130	LYS	N	119.649	0.3	1
UNMAPPED	20	LYS	N	122.014	0.3	1
UNMAPPED	69	ASN	N	116.48	0.3	1
UNMAPPED	16	LYS	C	176.817	0.3	1
UNMAPPED	123	MET	CA	59.592	0.3	1
UNMAPPED	117	GLU	C	178.728	0.3	1
UNMAPPED	71	VAL	CA	58.266	0.3	1
UNMAPPED	121	GLU	CA	60.857	0.3	1
UNMAPPED	94	ILE	C	178.82	0.3	1
UNMAPPED	113	VAL	C	177.387	0.3	1
UNMAPPED	40	LEU	H	8.068	0.02	1
UNMAPPED	87	HIS	N	117.907	0.3	1
UNMAPPED	81	ASN	C	174.0	0.3	1
UNMAPPED	43	ALA	H	8.753	0.02	1
UNMAPPED	37	GLY	H	8.417	0.02	1
UNMAPPED	17	THR	CA	61.222	0.3	1
UNMAPPED	62	GLU	N	116.096	0.3	1
UNMAPPED	16	LYS	CA	55.97	0.3	1
UNMAPPED	28	ALA	N	123.563	0.3	1
UNMAPPED	103	THR	H	7.833	0.02	1
UNMAPPED	13	SER	N	117.169	0.3	1
UNMAPPED	90	VAL	C	177.243	0.3	1
UNMAPPED	105	GLY	N	108.097	0.3	1
UNMAPPED	18	ASN	C	174.998	0.3	1
UNMAPPED	72	TYR	N	121.827	0.3	1
UNMAPPED	95	LYS	CA	59.835	0.3	1
UNMAPPED	134	ALA	C	178.964	0.3	1
UNMAPPED	70	GLN	C	174.996	0.3	1
UNMAPPED	20	LYS	C	176.215	0.3	1
UNMAPPED	97	HIS	CA	59.502	0.3	1
UNMAPPED	101	THR	N	114.882	0.3	1
UNMAPPED	122	GLN	C	179.174	0.3	1
UNMAPPED	83	ASN	N	117.395	0.3	1
UNMAPPED	24	GLY	N	108.962	0.3	1
UNMAPPED	17	THR	H	8.183	0.02	1
UNMAPPED	128	TYR	CA	61.627	0.3	1
UNMAPPED	9	TRP	N	121.328	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	60	TYR	N	120.754	0.3	1
UNMAPPED	103	THR	CA	64.448	0.3	1
UNMAPPED	3	GLY	C	174.756	0.3	1
UNMAPPED	23	ALA	CA	52.293	0.3	1
UNMAPPED	97	HIS	C	178.754	0.3	1
UNMAPPED	127	GLN	C	177.421	0.3	1
UNMAPPED	55	TRP	CA	61.496	0.3	1
UNMAPPED	122	GLN	CA	58.793	0.3	1
UNMAPPED	63	ASN	CA	54.554	0.3	1
UNMAPPED	67	TYR	N	121.714	0.3	1
UNMAPPED	95	LYS	H	8.15	0.02	1
UNMAPPED	35	LEU	C	177.94	0.3	1
UNMAPPED	88	ASP	H	7.431	0.02	1
UNMAPPED	96	GLN	C	178.649	0.3	1
UNMAPPED	109	THR	CA	60.02	0.3	1
UNMAPPED	139	ARG	CA	55.787	0.3	1
UNMAPPED	3	GLY	CA	44.946	0.3	1
UNMAPPED	71	VAL	C	174.122	0.3	1
UNMAPPED	107	ASN	CA	52.42	0.3	1
UNMAPPED	112	ASP	H	7.537	0.02	1
UNMAPPED	99	VAL	CA	65.964	0.3	1
UNMAPPED	134	ALA	N	120.917	0.3	1
UNMAPPED	23	ALA	H	8.463	0.02	1
UNMAPPED	8	GLN	N	120.572	0.3	1
UNMAPPED	61	ARG	N	117.536	0.3	1
UNMAPPED	73	TYR	CA	55.556	0.3	1
UNMAPPED	55	TRP	C	179.122	0.3	1
UNMAPPED	81	ASN	CA	51.957	0.3	1
UNMAPPED	54	ASP	H	9.029	0.02	1

7.4.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	135	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	133	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	127	0.00 \pm 0.00	None needed (< 0.5 ppm)

7.4.3 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 1596. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/665 (0%)	0/265 (0%)	0/270 (0%)	0/130 (0%)
Sidechain	0/815 (0%)	0/473 (0%)	0/315 (0%)	0/27 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1596 (0%)	0/798 (0%)	0/629 (0%)	0/169 (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 1685. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/698 (0%)	0/278 (0%)	0/284 (0%)	0/136 (0%)
Sidechain	0/871 (0%)	0/507 (0%)	0/335 (0%)	0/29 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1685 (0%)	0/845 (0%)	0/663 (0%)	0/177 (0%)

7.4.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.

7.5 Chemical shift list 5

File name: BMRB entry 16077

Chemical shift list name: *assigned_chem_shift_list_1*

7.5.1 Bookkeeping [i](#)

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	522
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	522
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 522 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	47	PRO	CA	61.99	0.3	1
UNMAPPED	139	ARG	C	176.366	0.3	1
UNMAPPED	33	GLY	C	174.725	0.3	1
UNMAPPED	20	LYS	H	8.3	0.02	1
UNMAPPED	29	GLY	H	8.32	0.02	1
UNMAPPED	65	TYR	C	175.933	0.3	1
UNMAPPED	115	MET	N	118.671	0.3	1
UNMAPPED	48	MET	C	175.077	0.3	1
UNMAPPED	114	LYS	C	180.056	0.3	1
UNMAPPED	36	GLY	N	110.221	0.3	1
UNMAPPED	19	LEU	N	123.178	0.3	1
UNMAPPED	100	THR	N	115.532	0.3	1
UNMAPPED	41	GLY	N	115.456	0.3	1
UNMAPPED	3	GLY	H	8.395	0.02	1
UNMAPPED	86	VAL	N	120.606	0.3	1
UNMAPPED	11	LYS	N	122.734	0.3	1
UNMAPPED	70	GLN	CA	53.73	0.3	1
UNMAPPED	131	GLU	N	118.618	0.3	1
UNMAPPED	33	GLY	CA	44.954	0.3	1
UNMAPPED	37	GLY	N	109.575	0.3	1
UNMAPPED	66	ARG	CA	55.958	0.3	1
UNMAPPED	14	LYS	C	176.453	0.3	1
UNMAPPED	84	ASN	CA	55.705	0.3	1
UNMAPPED	15	LEU	H	8.208	0.02	1
UNMAPPED	29	GLY	CA	44.777	0.3	1
UNMAPPED	132	SER	H	8.444	0.02	1
UNMAPPED	72	TYR	H	8.482	0.02	1
UNMAPPED	74	ARG	H	7.947	0.02	1
UNMAPPED	2	GLY	N	110.556	0.3	1
UNMAPPED	98	THR	N	115.439	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	124	CYS	H	9.238	0.02	1
UNMAPPED	63	ASN	C	175.537	0.3	1
UNMAPPED	119	VAL	H	8.275	0.02	1
UNMAPPED	17	THR	N	115.559	0.3	1
UNMAPPED	21	HIS	C	175.276	0.3	1
UNMAPPED	12	PRO	CA	62.807	0.3	1
UNMAPPED	30	ALA	H	8.099	0.02	1
UNMAPPED	29	GLY	C	173.74	0.3	1
UNMAPPED	60	TYR	H	9.033	0.02	1
UNMAPPED	130	LYS	H	7.867	0.02	1
UNMAPPED	107	ASN	C	173.587	0.3	1
UNMAPPED	102	THR	H	8.287	0.02	1
UNMAPPED	140	ARG	N	122.008	0.3	1
UNMAPPED	38	TYR	C	175.749	0.3	1
UNMAPPED	95	LYS	N	123.717	0.3	1
UNMAPPED	132	SER	CA	60.852	0.3	1
UNMAPPED	101	THR	C	177.147	0.3	1
UNMAPPED	85	PHE	CA	60.472	0.3	1
UNMAPPED	58	ARG	H	8.04	0.02	1
UNMAPPED	59	TYR	H	8.265	0.02	1
UNMAPPED	74	ARG	CA	53.138	0.3	1
UNMAPPED	93	THR	C	177.693	0.3	1
UNMAPPED	124	CYS	CA	59.707	0.3	1
UNMAPPED	120	VAL	N	121.569	0.3	1
UNMAPPED	52	GLY	N	109.318	0.3	1
UNMAPPED	26	ALA	H	8.322	0.02	1
UNMAPPED	64	MET	C	176.401	0.3	1
UNMAPPED	112	ASP	N	120.114	0.3	1
UNMAPPED	61	ARG	H	7.891	0.02	1
UNMAPPED	43	ALA	CA	52.545	0.3	1
UNMAPPED	10	ASN	CA	52.447	0.3	1
UNMAPPED	55	TRP	N	120.576	0.3	1
UNMAPPED	126	THR	CA	66.675	0.3	1
UNMAPPED	7	ASN	C	175.232	0.3	1
UNMAPPED	19	LEU	H	8.256	0.02	1
UNMAPPED	135	TYR	N	119.455	0.3	1
UNMAPPED	45	SER	N	116.458	0.3	1
UNMAPPED	3	GLY	N	109.074	0.3	1
UNMAPPED	39	MET	CA	53.245	0.3	1
UNMAPPED	50	HIS	C	175.275	0.3	1
UNMAPPED	64	MET	CA	58.723	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	56	GLU	H	8.135	0.02	1
UNMAPPED	41	GLY	H	9.43	0.02	1
UNMAPPED	43	ALA	N	125.795	0.3	1
UNMAPPED	83	ASN	H	8.425	0.02	1
UNMAPPED	34	GLY	C	174.41	0.3	1
UNMAPPED	134	ALA	CA	53.79	0.3	1
UNMAPPED	45	SER	CA	58.261	0.3	1
UNMAPPED	67	TYR	C	172.831	0.3	1
UNMAPPED	27	ALA	H	8.236	0.02	1
UNMAPPED	126	THR	C	176.773	0.3	1
UNMAPPED	51	PHE	H	10.374	0.02	1
UNMAPPED	94	ILE	H	8.479	0.02	1
UNMAPPED	21	HIS	CA	55.901	0.3	1
UNMAPPED	118	ARG	H	7.282	0.02	1
UNMAPPED	66	ARG	N	119.126	0.3	1
UNMAPPED	12	PRO	C	177.041	0.3	1
UNMAPPED	50	HIS	CA	54.417	0.3	1
UNMAPPED	43	ALA	C	177.535	0.3	1
UNMAPPED	103	THR	C	175.183	0.3	1
UNMAPPED	46	ARG	CA	54.398	0.3	1
UNMAPPED	106	GLU	CA	55.17	0.3	1
UNMAPPED	82	GLN	C	176.937	0.3	1
UNMAPPED	141	SER	H	8.425	0.02	1
UNMAPPED	138	GLY	C	174.607	0.3	1
UNMAPPED	116	MET	N	118.461	0.3	1
UNMAPPED	86	VAL	CA	67.37	0.3	1
UNMAPPED	49	ILE	N	124.636	0.3	1
UNMAPPED	70	GLN	N	114.477	0.3	1
UNMAPPED	31	VAL	N	119.886	0.3	1
UNMAPPED	33	GLY	N	113.662	0.3	1
UNMAPPED	27	ALA	CA	52.104	0.3	1
UNMAPPED	109	THR	C	175.473	0.3	1
UNMAPPED	18	ASN	N	121.611	0.3	1
UNMAPPED	66	ARG	C	176.852	0.3	1
UNMAPPED	135	TYR	C	177.33	0.3	1
UNMAPPED	93	THR	CA	68.145	0.3	1
UNMAPPED	84	ASN	N	118.486	0.3	1
UNMAPPED	82	GLN	CA	58.678	0.3	1
UNMAPPED	138	GLY	CA	45.254	0.3	1
UNMAPPED	117	GLU	N	119.136	0.3	1
UNMAPPED	138	GLY	H	7.891	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	102	THR	N	118.578	0.3	1
UNMAPPED	32	VAL	N	125.021	0.3	1
UNMAPPED	46	ARG	H	8.704	0.02	1
UNMAPPED	2	GLY	CA	44.891	0.3	1
UNMAPPED	27	ALA	C	177.64	0.3	1
UNMAPPED	7	ASN	CA	52.785	0.3	1
UNMAPPED	48	MET	CA	53.649	0.3	1
UNMAPPED	53	ASN	CA	52.13	0.3	1
UNMAPPED	114	LYS	CA	58.783	0.3	1
UNMAPPED	120	VAL	H	9.172	0.02	1
UNMAPPED	52	GLY	H	8.946	0.02	1
UNMAPPED	26	ALA	N	123.436	0.3	1
UNMAPPED	96	GLN	H	8.557	0.02	1
UNMAPPED	2	GLY	C	174.804	0.3	1
UNMAPPED	123	MET	H	8.131	0.02	1
UNMAPPED	135	TYR	H	7.959	0.02	1
UNMAPPED	56	GLU	N	120.797	0.3	1
UNMAPPED	98	THR	H	8.53	0.02	1
UNMAPPED	46	ARG	C	174.683	0.3	1
UNMAPPED	104	LYS	N	119.836	0.3	1
UNMAPPED	48	MET	H	8.727	0.02	1
UNMAPPED	53	ASN	H	7.259	0.02	1
UNMAPPED	108	PHE	N	121.964	0.3	1
UNMAPPED	1	GLN	N	120.087	0.3	1
UNMAPPED	88	ASP	N	118.313	0.3	1
UNMAPPED	94	ILE	N	121.288	0.3	1
UNMAPPED	86	VAL	C	176.674	0.3	1
UNMAPPED	92	ILE	C	177.982	0.3	1
UNMAPPED	100	THR	C	176.767	0.3	1
UNMAPPED	126	THR	N	118.399	0.3	1
UNMAPPED	117	GLU	CA	60.315	0.3	1
UNMAPPED	138	GLY	N	108.188	0.3	1
UNMAPPED	135	TYR	CA	59.619	0.3	1
UNMAPPED	13	SER	C	174.804	0.3	1
UNMAPPED	39	MET	N	121.705	0.3	1
UNMAPPED	4	GLY	H	8.396	0.02	1
UNMAPPED	140	ARG	H	8.196	0.02	1
UNMAPPED	37	GLY	C	174.0	0.3	1
UNMAPPED	137	ASP	C	177.448	0.3	1
UNMAPPED	5	THR	H	8.173	0.02	1
UNMAPPED	38	TYR	CA	58.012	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	132	SER	C	175.736	0.3	1
UNMAPPED	44	MET	C	175.644	0.3	1
UNMAPPED	35	LEU	CA	54.515	0.3	1
UNMAPPED	90	VAL	N	125.161	0.3	1
UNMAPPED	129	GLN	C	178.559	0.3	1
UNMAPPED	15	LEU	C	177.331	0.3	1
UNMAPPED	74	ARG	C	178.189	0.3	1
UNMAPPED	128	TYR	H	8.631	0.02	1
UNMAPPED	110	GLU	C	179.295	0.3	1
UNMAPPED	89	CYS	CA	58.24	0.3	1
UNMAPPED	91	ASN	CA	56.369	0.3	1
UNMAPPED	84	ASN	H	8.596	0.02	1
UNMAPPED	53	ASN	C	174.403	0.3	1
UNMAPPED	22	VAL	N	123.006	0.3	1
UNMAPPED	30	ALA	C	177.611	0.3	1
UNMAPPED	69	ASN	H	8.644	0.02	1
UNMAPPED	106	GLU	N	120.46	0.3	1
UNMAPPED	73	TYR	C	173.587	0.3	1
UNMAPPED	98	THR	C	176.511	0.3	1
UNMAPPED	92	ILE	H	8.797	0.02	1
UNMAPPED	63	ASN	H	7.561	0.02	1
UNMAPPED	129	GLN	CA	58.695	0.3	1
UNMAPPED	116	MET	CA	59.63	0.3	1
UNMAPPED	4	GLY	CA	44.809	0.3	1
UNMAPPED	65	TYR	CA	58.896	0.3	1
UNMAPPED	25	ALA	CA	52.217	0.3	1
UNMAPPED	111	THR	CA	66.498	0.3	1
UNMAPPED	35	LEU	H	8.243	0.02	1
UNMAPPED	99	VAL	H	8.106	0.02	1
UNMAPPED	30	ALA	CA	51.92	0.3	1
UNMAPPED	39	MET	C	172.952	0.3	1
UNMAPPED	130	LYS	CA	59.034	0.3	1
UNMAPPED	51	PHE	N	125.389	0.3	1
UNMAPPED	141	SER	C	173.674	0.3	1
UNMAPPED	113	VAL	N	119.86	0.3	1
UNMAPPED	69	ASN	CA	51.619	0.3	1
UNMAPPED	121	GLU	N	120.949	0.3	1
UNMAPPED	110	GLU	H	9.21	0.02	1
UNMAPPED	61	ARG	C	179.123	0.3	1
UNMAPPED	84	ASN	C	177.388	0.3	1
UNMAPPED	129	GLN	H	8.253	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	136	TYR	C	177.076	0.3	1
UNMAPPED	105	GLY	C	174.254	0.3	1
UNMAPPED	116	MET	C	177.811	0.3	1
UNMAPPED	11	LYS	C	178.558	0.3	1
UNMAPPED	136	TYR	N	119.84	0.3	1
UNMAPPED	87	HIS	CA	59.477	0.3	1
UNMAPPED	53	ASN	N	114.532	0.3	1
UNMAPPED	65	TYR	H	7.595	0.02	1
UNMAPPED	49	ILE	H	6.585	0.02	1
UNMAPPED	24	GLY	H	8.42	0.02	1
UNMAPPED	62	GLU	CA	57.445	0.3	1
UNMAPPED	33	GLY	H	8.609	0.02	1
UNMAPPED	9	TRP	H	8.083	0.02	1
UNMAPPED	1	GLN	H	8.323	0.02	1
UNMAPPED	133	GLN	N	120.987	0.3	1
UNMAPPED	44	MET	CA	53.533	0.3	1
UNMAPPED	58	ARG	C	177.588	0.3	1
UNMAPPED	25	ALA	H	8.166	0.02	1
UNMAPPED	15	LEU	CA	54.802	0.3	1
UNMAPPED	105	GLY	CA	45.153	0.3	1
UNMAPPED	126	THR	H	8.133	0.02	1
UNMAPPED	133	GLN	CA	57.758	0.3	1
UNMAPPED	67	TYR	H	7.456	0.02	1
UNMAPPED	91	ASN	C	178.546	0.3	1
UNMAPPED	34	GLY	H	8.302	0.02	1
UNMAPPED	39	MET	H	9.134	0.02	1
UNMAPPED	141	SER	N	117.787	0.3	1
UNMAPPED	51	PHE	C	177.102	0.3	1
UNMAPPED	97	HIS	N	120.404	0.3	1
UNMAPPED	101	THR	CA	65.002	0.3	1
UNMAPPED	83	ASN	CA	56.113	0.3	1
UNMAPPED	128	TYR	N	120.495	0.3	1
UNMAPPED	85	PHE	C	177.546	0.3	1
UNMAPPED	133	GLN	H	7.611	0.02	1
UNMAPPED	61	ARG	CA	59.664	0.3	1
UNMAPPED	103	THR	N	116.708	0.3	1
UNMAPPED	60	TYR	CA	62.74	0.3	1
UNMAPPED	124	CYS	C	176.963	0.3	1
UNMAPPED	54	ASP	N	123.434	0.3	1
UNMAPPED	25	ALA	C	177.758	0.3	1
UNMAPPED	22	VAL	H	8.037	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	111	THR	C	175.723	0.3	1
UNMAPPED	8	GLN	C	175.789	0.3	1
UNMAPPED	122	GLN	N	115.479	0.3	1
UNMAPPED	63	ASN	N	115.414	0.3	1
UNMAPPED	57	ASP	C	179.074	0.3	1
UNMAPPED	130	LYS	C	179.859	0.3	1
UNMAPPED	115	MET	H	8.182	0.02	1
UNMAPPED	109	THR	N	116.245	0.3	1
UNMAPPED	92	ILE	N	119.146	0.3	1
UNMAPPED	58	ARG	N	119.923	0.3	1
UNMAPPED	139	ARG	N	120.095	0.3	1
UNMAPPED	106	GLU	C	174.908	0.3	1
UNMAPPED	35	LEU	N	121.991	0.3	1
UNMAPPED	127	GLN	H	8.739	0.02	1
UNMAPPED	99	VAL	N	123.479	0.3	1
UNMAPPED	8	GLN	CA	55.821	0.3	1
UNMAPPED	108	PHE	H	8.788	0.02	1
UNMAPPED	11	LYS	CA	53.898	0.3	1
UNMAPPED	89	CYS	N	119.2	0.3	1
UNMAPPED	57	ASP	CA	58.146	0.3	1
UNMAPPED	87	HIS	C	177.552	0.3	1
UNMAPPED	93	THR	H	8.162	0.02	1
UNMAPPED	113	VAL	H	8.266	0.02	1
UNMAPPED	104	LYS	H	7.47	0.02	1
UNMAPPED	22	VAL	CA	61.566	0.3	1
UNMAPPED	131	GLU	C	179.306	0.3	1
UNMAPPED	110	GLU	N	120.188	0.3	1
UNMAPPED	19	LEU	CA	54.833	0.3	1
UNMAPPED	100	THR	CA	65.101	0.3	1
UNMAPPED	64	MET	H	7.891	0.02	1
UNMAPPED	36	GLY	CA	45.9	0.3	1
UNMAPPED	26	ALA	C	177.693	0.3	1
UNMAPPED	14	LYS	CA	56.027	0.3	1
UNMAPPED	41	GLY	CA	44.572	0.3	1
UNMAPPED	111	THR	N	116.869	0.3	1
UNMAPPED	136	TYR	H	8.075	0.02	1
UNMAPPED	119	VAL	N	119.339	0.3	1
UNMAPPED	131	GLU	CA	57.488	0.3	1
UNMAPPED	42	SER	C	175.0	0.3	1
UNMAPPED	37	GLY	CA	44.756	0.3	1
UNMAPPED	8	GLN	H	8.379	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	123	MET	C	178.573	0.3	1
UNMAPPED	125	VAL	CA	67.375	0.3	1
UNMAPPED	51	PHE	CA	59.261	0.3	1
UNMAPPED	121	GLU	C	177.539	0.3	1
UNMAPPED	113	VAL	CA	67.503	0.3	1
UNMAPPED	83	ASN	C	177.763	0.3	1
UNMAPPED	19	LEU	C	177.238	0.3	1
UNMAPPED	36	GLY	C	174.843	0.3	1
UNMAPPED	56	GLU	C	177.732	0.3	1
UNMAPPED	29	GLY	N	108.209	0.3	1
UNMAPPED	50	HIS	H	8.129	0.02	1
UNMAPPED	32	VAL	H	8.319	0.02	1
UNMAPPED	59	TYR	N	121.062	0.3	1
UNMAPPED	100	THR	H	8.215	0.02	1
UNMAPPED	97	HIS	H	8.521	0.02	1
UNMAPPED	108	PHE	C	176.675	0.3	1
UNMAPPED	98	THR	CA	66.463	0.3	1
UNMAPPED	86	VAL	H	8.907	0.02	1
UNMAPPED	131	GLU	H	8.454	0.02	1
UNMAPPED	4	GLY	C	174.551	0.3	1
UNMAPPED	137	ASP	H	8.278	0.02	1
UNMAPPED	44	MET	N	121.584	0.3	1
UNMAPPED	118	ARG	C	179.359	0.3	1
UNMAPPED	95	LYS	C	179.072	0.3	1
UNMAPPED	15	LEU	N	123.179	0.3	1
UNMAPPED	82	GLN	H	8.667	0.02	1
UNMAPPED	72	TYR	CA	56.665	0.3	1
UNMAPPED	55	TRP	H	8.563	0.02	1
UNMAPPED	132	SER	N	115.517	0.3	1
UNMAPPED	42	SER	CA	58.185	0.3	1
UNMAPPED	71	VAL	H	8.484	0.02	1
UNMAPPED	121	GLU	H	8.011	0.02	1
UNMAPPED	42	SER	N	113.97	0.3	1
UNMAPPED	141	SER	CA	57.943	0.3	1
UNMAPPED	5	THR	CA	61.661	0.3	1
UNMAPPED	74	ARG	N	120.848	0.3	1
UNMAPPED	139	ARG	H	7.83	0.02	1
UNMAPPED	40	LEU	CA	52.745	0.3	1
UNMAPPED	109	THR	H	9.61	0.02	1
UNMAPPED	69	ASN	C	172.84	0.3	1
UNMAPPED	124	CYS	N	119.682	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	23	ALA	C	178.231	0.3	1
UNMAPPED	120	VAL	CA	66.023	0.3	1
UNMAPPED	133	GLN	C	177.246	0.3	1
UNMAPPED	16	LYS	H	8.407	0.02	1
UNMAPPED	114	LYS	H	7.698	0.02	1
UNMAPPED	52	GLY	CA	45.317	0.3	1
UNMAPPED	54	ASP	CA	57.489	0.3	1
UNMAPPED	73	TYR	H	8.516	0.02	1
UNMAPPED	89	CYS	H	8.161	0.02	1
UNMAPPED	10	ASN	N	120.173	0.3	1
UNMAPPED	62	GLU	C	177.631	0.3	1
UNMAPPED	96	GLN	CA	57.715	0.3	1
UNMAPPED	40	LEU	C	178.181	0.3	1
UNMAPPED	66	ARG	H	7.52	0.02	1
UNMAPPED	92	ILE	CA	61.724	0.3	1
UNMAPPED	58	ARG	CA	59.338	0.3	1
UNMAPPED	120	VAL	C	177.631	0.3	1
UNMAPPED	64	MET	N	118.658	0.3	1
UNMAPPED	65	TYR	N	116.849	0.3	1
UNMAPPED	13	SER	CA	57.952	0.3	1
UNMAPPED	117	GLU	H	8.587	0.02	1
UNMAPPED	70	GLN	H	7.297	0.02	1
UNMAPPED	88	ASP	C	175.89	0.3	1
UNMAPPED	31	VAL	H	8.166	0.02	1
UNMAPPED	57	ASP	N	119.088	0.3	1
UNMAPPED	18	ASN	H	8.541	0.02	1
UNMAPPED	21	HIS	N	121.577	0.3	1
UNMAPPED	72	TYR	C	174.725	0.3	1
UNMAPPED	50	HIS	N	123.192	0.3	1
UNMAPPED	122	GLN	H	7.086	0.02	1
UNMAPPED	110	GLU	CA	59.717	0.3	1
UNMAPPED	89	CYS	C	177.535	0.3	1
UNMAPPED	46	ARG	N	127.061	0.3	1
UNMAPPED	24	GLY	C	174.032	0.3	1
UNMAPPED	17	THR	C	174.055	0.3	1
UNMAPPED	38	TYR	H	7.871	0.02	1
UNMAPPED	140	ARG	CA	55.748	0.3	1
UNMAPPED	102	THR	C	178.06	0.3	1
UNMAPPED	119	VAL	CA	65.371	0.3	1
UNMAPPED	13	SER	H	8.473	0.02	1
UNMAPPED	107	ASN	H	8.565	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	59	TYR	C	179.594	0.3	1
UNMAPPED	49	ILE	CA	58.8	0.3	1
UNMAPPED	27	ALA	N	123.558	0.3	1
UNMAPPED	62	GLU	H	7.925	0.02	1
UNMAPPED	125	VAL	N	123.912	0.3	1
UNMAPPED	31	VAL	CA	61.751	0.3	1
UNMAPPED	136	TYR	CA	59.499	0.3	1
UNMAPPED	18	ASN	CA	52.551	0.3	1
UNMAPPED	91	ASN	H	7.601	0.02	1
UNMAPPED	44	MET	H	8.804	0.02	1
UNMAPPED	93	THR	N	118.272	0.3	1
UNMAPPED	82	GLN	N	120.221	0.3	1
UNMAPPED	137	ASP	N	121.221	0.3	1
UNMAPPED	140	ARG	C	176.393	0.3	1
UNMAPPED	20	LYS	CA	55.94	0.3	1
UNMAPPED	102	THR	CA	65.116	0.3	1
UNMAPPED	32	VAL	CA	62.063	0.3	1
UNMAPPED	54	ASP	C	177.94	0.3	1
UNMAPPED	123	MET	N	119.707	0.3	1
UNMAPPED	59	TYR	CA	61.836	0.3	1
UNMAPPED	71	VAL	N	112.956	0.3	1
UNMAPPED	112	ASP	C	177.614	0.3	1
UNMAPPED	22	VAL	C	175.578	0.3	1
UNMAPPED	80	SER	CA	58.445	0.3	1
UNMAPPED	31	VAL	C	176.403	0.3	1
UNMAPPED	128	TYR	C	178.192	0.3	1
UNMAPPED	116	MET	H	8.707	0.02	1
UNMAPPED	111	THR	H	7.971	0.02	1
UNMAPPED	114	LYS	N	119.31	0.3	1
UNMAPPED	45	SER	H	8.467	0.02	1
UNMAPPED	48	MET	N	122.186	0.3	1
UNMAPPED	88	ASP	CA	56.795	0.3	1
UNMAPPED	45	SER	C	174.437	0.3	1
UNMAPPED	112	ASP	CA	57.656	0.3	1
UNMAPPED	26	ALA	CA	52.258	0.3	1
UNMAPPED	16	LYS	N	123.042	0.3	1
UNMAPPED	28	ALA	CA	52.29	0.3	1
UNMAPPED	115	MET	C	178.231	0.3	1
UNMAPPED	125	VAL	C	178.089	0.3	1
UNMAPPED	5	THR	N	113.628	0.3	1
UNMAPPED	68	PRO	C	175.079	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	137	ASP	CA	55.011	0.3	1
UNMAPPED	104	LYS	CA	55.829	0.3	1
UNMAPPED	40	LEU	N	121.46	0.3	1
UNMAPPED	47	PRO	C	175.723	0.3	1
UNMAPPED	99	VAL	C	178.573	0.3	1
UNMAPPED	118	ARG	N	117.009	0.3	1
UNMAPPED	56	GLU	CA	59.598	0.3	1
UNMAPPED	21	HIS	H	8.281	0.02	1
UNMAPPED	87	HIS	H	8.381	0.02	1
UNMAPPED	127	GLN	N	122.878	0.3	1
UNMAPPED	24	GLY	CA	44.835	0.3	1
UNMAPPED	10	ASN	C	174.41	0.3	1
UNMAPPED	108	PHE	CA	56.088	0.3	1
UNMAPPED	1	GLN	CA	55.601	0.3	1
UNMAPPED	11	LYS	H	8.017	0.02	1
UNMAPPED	119	VAL	C	177.068	0.3	1
UNMAPPED	9	TRP	CA	56.764	0.3	1
UNMAPPED	28	ALA	H	8.264	0.02	1
UNMAPPED	94	ILE	CA	66.166	0.3	1
UNMAPPED	96	GLN	N	117.371	0.3	1
UNMAPPED	118	ARG	CA	58.078	0.3	1
UNMAPPED	49	ILE	C	173.207	0.3	1
UNMAPPED	23	ALA	N	128.319	0.3	1
UNMAPPED	105	GLY	H	7.924	0.02	1
UNMAPPED	60	TYR	C	177.042	0.3	1
UNMAPPED	127	GLN	CA	58.323	0.3	1
UNMAPPED	106	GLU	H	7.454	0.02	1
UNMAPPED	34	GLY	CA	44.945	0.3	1
UNMAPPED	67	TYR	CA	52.319	0.3	1
UNMAPPED	34	GLY	N	108.729	0.3	1
UNMAPPED	1	GLN	C	176.576	0.3	1
UNMAPPED	32	VAL	C	176.675	0.3	1
UNMAPPED	9	TRP	C	175.92	0.3	1
UNMAPPED	38	TYR	N	118.248	0.3	1
UNMAPPED	90	VAL	CA	65.774	0.3	1
UNMAPPED	101	THR	H	8.057	0.02	1
UNMAPPED	107	ASN	N	119.667	0.3	1
UNMAPPED	42	SER	H	8.347	0.02	1
UNMAPPED	125	VAL	H	8.512	0.02	1
UNMAPPED	73	TYR	N	111.213	0.3	1
UNMAPPED	91	ASN	N	116.546	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	10	ASN	H	8.079	0.02	1
UNMAPPED	52	GLY	C	173.3	0.3	1
UNMAPPED	28	ALA	C	178.271	0.3	1
UNMAPPED	4	GLY	N	109.165	0.3	1
UNMAPPED	104	LYS	C	176.754	0.3	1
UNMAPPED	115	MET	CA	59.364	0.3	1
UNMAPPED	129	GLN	N	119.911	0.3	1
UNMAPPED	2	GLY	H	8.518	0.02	1
UNMAPPED	36	GLY	H	8.582	0.02	1
UNMAPPED	25	ALA	N	124.113	0.3	1
UNMAPPED	68	PRO	CA	63.143	0.3	1
UNMAPPED	90	VAL	H	9.299	0.02	1
UNMAPPED	134	ALA	H	7.604	0.02	1
UNMAPPED	30	ALA	N	123.817	0.3	1
UNMAPPED	57	ASP	H	7.912	0.02	1
UNMAPPED	41	GLY	C	172.834	0.3	1
UNMAPPED	130	LYS	N	119.611	0.3	1
UNMAPPED	20	LYS	N	121.958	0.3	1
UNMAPPED	69	ASN	N	116.477	0.3	1
UNMAPPED	16	LYS	C	176.645	0.3	1
UNMAPPED	123	MET	CA	59.603	0.3	1
UNMAPPED	117	GLU	C	178.743	0.3	1
UNMAPPED	71	VAL	CA	58.249	0.3	1
UNMAPPED	121	GLU	CA	60.849	0.3	1
UNMAPPED	94	ILE	C	178.848	0.3	1
UNMAPPED	113	VAL	C	177.443	0.3	1
UNMAPPED	40	LEU	H	8.066	0.02	1
UNMAPPED	87	HIS	N	117.862	0.3	1
UNMAPPED	81	ASN	C	174.04	0.3	1
UNMAPPED	43	ALA	H	8.754	0.02	1
UNMAPPED	37	GLY	H	8.418	0.02	1
UNMAPPED	17	THR	CA	61.342	0.3	1
UNMAPPED	62	GLU	N	116.104	0.3	1
UNMAPPED	16	LYS	CA	55.896	0.3	1
UNMAPPED	28	ALA	N	123.518	0.3	1
UNMAPPED	103	THR	H	7.835	0.02	1
UNMAPPED	13	SER	N	116.76	0.3	1
UNMAPPED	90	VAL	C	177.238	0.3	1
UNMAPPED	105	GLY	N	108.075	0.3	1
UNMAPPED	18	ASN	C	175.026	0.3	1
UNMAPPED	72	TYR	N	121.828	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	95	LYS	CA	59.89	0.3	1
UNMAPPED	134	ALA	C	179.124	0.3	1
UNMAPPED	70	GLN	C	175.014	0.3	1
UNMAPPED	20	LYS	C	176.235	0.3	1
UNMAPPED	97	HIS	CA	59.5	0.3	1
UNMAPPED	101	THR	N	114.905	0.3	1
UNMAPPED	122	GLN	C	179.215	0.3	1
UNMAPPED	83	ASN	N	117.375	0.3	1
UNMAPPED	24	GLY	N	108.92	0.3	1
UNMAPPED	17	THR	H	8.141	0.02	1
UNMAPPED	128	TYR	CA	61.635	0.3	1
UNMAPPED	9	TRP	N	121.207	0.3	1
UNMAPPED	60	TYR	N	120.753	0.3	1
UNMAPPED	103	THR	CA	64.434	0.3	1
UNMAPPED	3	GLY	C	174.809	0.3	1
UNMAPPED	23	ALA	CA	52.348	0.3	1
UNMAPPED	97	HIS	C	178.757	0.3	1
UNMAPPED	127	GLN	C	177.443	0.3	1
UNMAPPED	55	TRP	CA	61.511	0.3	1
UNMAPPED	122	GLN	CA	58.766	0.3	1
UNMAPPED	63	ASN	CA	54.61	0.3	1
UNMAPPED	67	TYR	N	121.736	0.3	1
UNMAPPED	95	LYS	H	8.15	0.02	1
UNMAPPED	35	LEU	C	177.982	0.3	1
UNMAPPED	88	ASP	H	7.444	0.02	1
UNMAPPED	96	GLN	C	178.665	0.3	1
UNMAPPED	109	THR	CA	59.981	0.3	1
UNMAPPED	139	ARG	CA	55.793	0.3	1
UNMAPPED	3	GLY	CA	44.809	0.3	1
UNMAPPED	71	VAL	C	174.149	0.3	1
UNMAPPED	107	ASN	CA	52.409	0.3	1
UNMAPPED	112	ASP	H	7.536	0.02	1
UNMAPPED	99	VAL	CA	65.96	0.3	1
UNMAPPED	134	ALA	N	120.854	0.3	1
UNMAPPED	23	ALA	H	8.46	0.02	1
UNMAPPED	8	GLN	N	120.521	0.3	1
UNMAPPED	61	ARG	N	117.56	0.3	1
UNMAPPED	73	TYR	CA	55.52	0.3	1
UNMAPPED	55	TRP	C	179.188	0.3	1
UNMAPPED	81	ASN	CA	51.86	0.3	1
UNMAPPED	54	ASP	H	9.034	0.02	1

7.5.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	135	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	133	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	127	0.00 \pm 0.00	None needed (< 0.5 ppm)

7.5.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1596. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/665 (0%)	0/265 (0%)	0/270 (0%)	0/130 (0%)
Sidechain	0/815 (0%)	0/473 (0%)	0/315 (0%)	0/27 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1596 (0%)	0/798 (0%)	0/629 (0%)	0/169 (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 1685. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/698 (0%)	0/278 (0%)	0/284 (0%)	0/136 (0%)
Sidechain	0/871 (0%)	0/507 (0%)	0/335 (0%)	0/29 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1685 (0%)	0/845 (0%)	0/663 (0%)	0/177 (0%)

7.5.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.5.5 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.

7.6 Chemical shift list 6

File name: BMRB entry 16078

Chemical shift list name: *assigned_chem_shift_list_1*

7.6.1 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	524
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	524
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 524 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	36	LEU	H	8.221	0.02	1
UNMAPPED	51	HIS	C	175.277	0.3	1
UNMAPPED	83	GLN	N	120.174	0.3	1
UNMAPPED	16	PRO	CA	62.543	0.3	1
UNMAPPED	72	VAL	N	112.983	0.3	1
UNMAPPED	55	ASP	C	177.894	0.3	1
UNMAPPED	130	GLN	C	178.549	0.3	1
UNMAPPED	29	ALA	H	8.456	0.02	1
UNMAPPED	75	ARG	H	7.944	0.02	1
UNMAPPED	3	GLY	H	8.595	0.02	1
UNMAPPED	2	GLN	H	8.363	0.02	1
UNMAPPED	48	PRO	CA	61.908	0.3	1
UNMAPPED	42	GLY	C	172.809	0.3	1
UNMAPPED	105	LYS	CA	55.77	0.3	1
UNMAPPED	51	HIS	CA	54.332	0.3	1
UNMAPPED	38	GLY	CA	44.667	0.3	1
UNMAPPED	37	GLY	N	110.217	0.3	1
UNMAPPED	142	SER	H	8.012	0.02	1
UNMAPPED	84	ASN	CA	56.095	0.3	1
UNMAPPED	47	ARG	C	174.613	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	130	GLN	CA	58.666	0.3	1
UNMAPPED	25	GLY	H	8.412	0.02	1
UNMAPPED	108	ASN	N	119.652	0.3	1
UNMAPPED	100	VAL	N	123.465	0.3	1
UNMAPPED	5	GLY	H	8.387	0.02	1
UNMAPPED	54	ASN	C	174.333	0.3	1
UNMAPPED	28	VAL	N	119.942	0.3	1
UNMAPPED	129	TYR	C	178.182	0.3	1
UNMAPPED	112	THR	C	175.651	0.3	1
UNMAPPED	46	SER	CA	58.194	0.3	1
UNMAPPED	105	LYS	C	176.683	0.3	1
UNMAPPED	134	GLN	C	177.161	0.3	1
UNMAPPED	88	HIS	H	8.382	0.02	1
UNMAPPED	94	THR	C	177.659	0.3	1
UNMAPPED	132	GLU	H	8.435	0.02	1
UNMAPPED	40	MET	H	9.136	0.02	1
UNMAPPED	85	ASN	H	8.592	0.02	1
UNMAPPED	36	LEU	C	177.894	0.3	1
UNMAPPED	133	SER	H	8.421	0.02	1
UNMAPPED	104	THR	C	175.133	0.3	1
UNMAPPED	54	ASN	CA	52.1	0.3	1
UNMAPPED	113	ASP	C	177.57	0.3	1
UNMAPPED	66	TYR	C	175.852	0.3	1
UNMAPPED	60	TYR	H	8.267	0.02	1
UNMAPPED	94	THR	CA	68.055	0.3	1
UNMAPPED	92	ASN	N	116.517	0.3	1
UNMAPPED	102	THR	H	8.055	0.02	1
UNMAPPED	118	GLU	N	119.119	0.3	1
UNMAPPED	74	TYR	N	111.242	0.3	1
UNMAPPED	6	THR	N	113.632	0.3	1
UNMAPPED	101	THR	C	176.727	0.3	1
UNMAPPED	31	ALA	H	8.12	0.02	1
UNMAPPED	52	PHE	C	177.07	0.3	1
UNMAPPED	70	ASN	N	116.465	0.3	1
UNMAPPED	64	ASN	H	7.562	0.02	1
UNMAPPED	44	ALA	C	177.51	0.3	1
UNMAPPED	131	LYS	H	7.873	0.02	1
UNMAPPED	50	ILE	N	124.628	0.3	1
UNMAPPED	120	VAL	N	119.306	0.3	1
UNMAPPED	28	VAL	C	175.932	0.3	1
UNMAPPED	63	GLU	C	177.593	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	26	ALA	H	8.121	0.02	1
UNMAPPED	40	MET	C	172.934	0.3	1
UNMAPPED	24	ALA	C	178.096	0.3	1
UNMAPPED	116	MET	C	178.195	0.3	1
UNMAPPED	107	GLU	C	174.897	0.3	1
UNMAPPED	36	LEU	N	122.027	0.3	1
UNMAPPED	132	GLU	C	179.229	0.3	1
UNMAPPED	39	TYR	H	7.89	0.02	1
UNMAPPED	127	THR	CA	66.624	0.3	1
UNMAPPED	66	TYR	H	7.597	0.02	1
UNMAPPED	136	TYR	C	177.161	0.3	1
UNMAPPED	63	GLU	CA	57.439	0.3	1
UNMAPPED	3	GLY	N	110.765	0.3	1
UNMAPPED	75	ARG	N	120.895	0.3	1
UNMAPPED	59	ARG	N	119.94	0.3	1
UNMAPPED	106	GLY	N	108.071	0.3	1
UNMAPPED	34	GLY	C	174.705	0.3	1
UNMAPPED	114	VAL	C	177.386	0.3	1
UNMAPPED	2	GLN	N	120.233	0.3	1
UNMAPPED	27	ALA	H	8.338	0.02	1
UNMAPPED	139	GLY	H	7.861	0.02	1
UNMAPPED	95	ILE	H	8.479	0.02	1
UNMAPPED	121	VAL	CA	65.967	0.3	1
UNMAPPED	115	LYS	N	119.284	0.3	1
UNMAPPED	86	PHE	C	177.476	0.3	1
UNMAPPED	12	LYS	H	8.027	0.02	1
UNMAPPED	27	ALA	N	123.787	0.3	1
UNMAPPED	103	THR	C	178.012	0.3	1
UNMAPPED	41	LEU	H	8.075	0.02	1
UNMAPPED	128	GLN	CA	58.258	0.3	1
UNMAPPED	124	MET	CA	59.572	0.3	1
UNMAPPED	65	MET	H	7.889	0.02	1
UNMAPPED	27	ALA	C	177.714	0.3	1
UNMAPPED	107	GLU	H	7.454	0.02	1
UNMAPPED	116	MET	N	118.695	0.3	1
UNMAPPED	50	ILE	CA	58.766	0.3	1
UNMAPPED	47	ARG	N	127.094	0.3	1
UNMAPPED	124	MET	N	119.434	0.3	1
UNMAPPED	24	ALA	H	8.462	0.02	1
UNMAPPED	27	ALA	CA	51.93	0.3	1
UNMAPPED	121	VAL	H	9.174	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	95	ILE	N	121.315	0.3	1
UNMAPPED	39	TYR	C	175.695	0.3	1
UNMAPPED	84	ASN	N	117.395	0.3	1
UNMAPPED	118	GLU	H	8.585	0.02	1
UNMAPPED	74	TYR	H	8.515	0.02	1
UNMAPPED	12	LYS	CA	53.739	0.3	1
UNMAPPED	59	ARG	C	177.541	0.3	1
UNMAPPED	123	GLN	N	115.479	0.3	1
UNMAPPED	28	VAL	CA	61.593	0.3	1
UNMAPPED	102	THR	N	114.875	0.3	1
UNMAPPED	32	VAL	N	119.899	0.3	1
UNMAPPED	31	ALA	N	123.838	0.3	1
UNMAPPED	122	GLU	H	8.013	0.02	1
UNMAPPED	131	LYS	N	119.622	0.3	1
UNMAPPED	136	TYR	CA	59.497	0.3	1
UNMAPPED	109	PHE	CA	56.058	0.3	1
UNMAPPED	33	VAL	H	8.321	0.02	1
UNMAPPED	120	VAL	H	8.273	0.02	1
UNMAPPED	46	SER	C	174.413	0.3	1
UNMAPPED	125	CYS	H	9.233	0.02	1
UNMAPPED	26	ALA	N	123.883	0.3	1
UNMAPPED	42	GLY	CA	44.526	0.3	1
UNMAPPED	6	THR	CA	61.597	0.3	1
UNMAPPED	49	MET	CA	53.616	0.3	1
UNMAPPED	30	GLY	H	8.39	0.02	1
UNMAPPED	68	TYR	C	172.761	0.3	1
UNMAPPED	110	THR	C	175.457	0.3	1
UNMAPPED	70	ASN	CA	51.578	0.3	1
UNMAPPED	58	ASP	CA	58.193	0.3	1
UNMAPPED	66	TYR	N	116.808	0.3	1
UNMAPPED	99	THR	CA	66.378	0.3	1
UNMAPPED	23	VAL	C	175.508	0.3	1
UNMAPPED	17	LYS	H	8.58	0.02	1
UNMAPPED	106	GLY	H	7.923	0.02	1
UNMAPPED	8	ASN	CA	52.782	0.3	1
UNMAPPED	91	VAL	CA	65.771	0.3	1
UNMAPPED	127	THR	H	8.132	0.02	1
UNMAPPED	85	ASN	N	118.486	0.3	1
UNMAPPED	49	MET	C	175.002	0.3	1
UNMAPPED	57	GLU	CA	59.595	0.3	1
UNMAPPED	137	TYR	H	8.056	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	99	THR	C	176.488	0.3	1
UNMAPPED	36	LEU	CA	54.456	0.3	1
UNMAPPED	11	ASN	CA	52.396	0.3	1
UNMAPPED	34	GLY	N	113.691	0.3	1
UNMAPPED	133	SER	CA	60.774	0.3	1
UNMAPPED	4	GLY	H	8.373	0.02	1
UNMAPPED	140	ARG	H	7.842	0.02	1
UNMAPPED	37	GLY	C	174.805	0.3	1
UNMAPPED	57	GLU	C	177.711	0.3	1
UNMAPPED	137	TYR	C	176.9	0.3	1
UNMAPPED	110	THR	H	9.608	0.02	1
UNMAPPED	18	THR	C	173.872	0.3	1
UNMAPPED	13	PRO	CA	62.64	0.3	1
UNMAPPED	35	GLY	CA	44.906	0.3	1
UNMAPPED	9	GLN	CA	55.795	0.3	1
UNMAPPED	123	GLN	H	7.088	0.02	1
UNMAPPED	47	ARG	H	8.703	0.02	1
UNMAPPED	117	MET	CA	59.586	0.3	1
UNMAPPED	11	ASN	C	174.334	0.3	1
UNMAPPED	141	ARG	N	122.737	0.3	1
UNMAPPED	20	LEU	CA	54.787	0.3	1
UNMAPPED	87	VAL	C	176.677	0.3	1
UNMAPPED	112	THR	H	7.971	0.02	1
UNMAPPED	84	ASN	H	8.428	0.02	1
UNMAPPED	62	ARG	C	179.112	0.3	1
UNMAPPED	31	ALA	CA	51.853	0.3	1
UNMAPPED	14	SER	N	117.211	0.3	1
UNMAPPED	134	GLN	N	120.946	0.3	1
UNMAPPED	61	TYR	CA	62.665	0.3	1
UNMAPPED	73	TYR	C	174.705	0.3	1
UNMAPPED	46	SER	N	116.455	0.3	1
UNMAPPED	116	MET	CA	59.31	0.3	1
UNMAPPED	4	GLY	CA	44.837	0.3	1
UNMAPPED	18	THR	CA	61.142	0.3	1
UNMAPPED	53	GLY	C	173.235	0.3	1
UNMAPPED	113	ASP	H	7.533	0.02	1
UNMAPPED	20	LEU	C	177.195	0.3	1
UNMAPPED	132	GLU	CA	57.432	0.3	1
UNMAPPED	33	VAL	N	124.978	0.3	1
UNMAPPED	70	ASN	C	172.808	0.3	1
UNMAPPED	55	ASP	CA	57.399	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	35	GLY	H	8.307	0.02	1
UNMAPPED	90	CYS	CA	58.25	0.3	1
UNMAPPED	62	ARG	CA	59.532	0.3	1
UNMAPPED	92	ASN	C	178.466	0.3	1
UNMAPPED	96	LYS	C	179.025	0.3	1
UNMAPPED	125	CYS	N	119.691	0.3	1
UNMAPPED	56	TRP	H	8.561	0.02	1
UNMAPPED	114	VAL	CA	67.442	0.3	1
UNMAPPED	139	GLY	N	108.171	0.3	1
UNMAPPED	53	GLY	CA	45.264	0.3	1
UNMAPPED	44	ALA	N	125.817	0.3	1
UNMAPPED	86	PHE	CA	60.398	0.3	1
UNMAPPED	84	ASN	C	177.711	0.3	1
UNMAPPED	93	ILE	H	8.804	0.02	1
UNMAPPED	136	TYR	N	119.363	0.3	1
UNMAPPED	138	ASP	C	177.253	0.3	1
UNMAPPED	129	TYR	CA	61.608	0.3	1
UNMAPPED	55	ASP	H	9.034	0.02	1
UNMAPPED	89	ASP	H	7.436	0.02	1
UNMAPPED	24	ALA	N	128.548	0.3	1
UNMAPPED	38	GLY	H	8.416	0.02	1
UNMAPPED	126	VAL	N	123.887	0.3	1
UNMAPPED	50	ILE	C	173.13	0.3	1
UNMAPPED	67	ARG	H	7.522	0.02	1
UNMAPPED	35	GLY	C	174.334	0.3	1
UNMAPPED	29	ALA	C	178.083	0.3	1
UNMAPPED	9	GLN	C	175.748	0.3	1
UNMAPPED	114	VAL	H	8.268	0.02	1
UNMAPPED	53	GLY	H	8.941	0.02	1
UNMAPPED	96	LYS	H	8.152	0.02	1
UNMAPPED	39	TYR	CA	57.965	0.3	1
UNMAPPED	69	PRO	CA	63.13	0.3	1
UNMAPPED	51	HIS	H	8.129	0.02	1
UNMAPPED	5	GLY	CA	44.783	0.3	1
UNMAPPED	66	TYR	CA	58.8	0.3	1
UNMAPPED	46	SER	H	8.468	0.02	1
UNMAPPED	81	SER	CA	58.355	0.3	1
UNMAPPED	34	GLY	H	8.613	0.02	1
UNMAPPED	115	LYS	C	180.041	0.3	1
UNMAPPED	88	HIS	CA	59.49	0.3	1
UNMAPPED	122	GLU	N	120.925	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	142	SER	C	178.605	0.3	1
UNMAPPED	1	GLY	H	8.317	0.02	1
UNMAPPED	129	TYR	H	8.62	0.02	1
UNMAPPED	85	ASN	CA	55.618	0.3	1
UNMAPPED	52	PHE	CA	59.191	0.3	1
UNMAPPED	22	HIS	C	175.224	0.3	1
UNMAPPED	65	MET	C	176.324	0.3	1
UNMAPPED	45	MET	N	121.585	0.3	1
UNMAPPED	103	THR	N	118.577	0.3	1
UNMAPPED	60	TYR	CA	61.73	0.3	1
UNMAPPED	138	ASP	H	8.249	0.02	1
UNMAPPED	14	SER	H	8.48	0.02	1
UNMAPPED	90	CYS	C	177.528	0.3	1
UNMAPPED	88	HIS	C	177.573	0.3	1
UNMAPPED	30	GLY	N	108.834	0.3	1
UNMAPPED	85	ASN	C	177.318	0.3	1
UNMAPPED	25	GLY	N	108.933	0.3	1
UNMAPPED	22	HIS	CA	55.839	0.3	1
UNMAPPED	118	GLU	C	178.702	0.3	1
UNMAPPED	65	MET	CA	58.671	0.3	1
UNMAPPED	64	ASN	CA	54.54	0.3	1
UNMAPPED	68	TYR	CA	52.223	0.3	1
UNMAPPED	139	GLY	CA	45.176	0.3	1
UNMAPPED	113	ASP	N	120.149	0.3	1
UNMAPPED	42	GLY	H	9.433	0.02	1
UNMAPPED	20	LEU	N	123.344	0.3	1
UNMAPPED	23	VAL	CA	61.509	0.3	1
UNMAPPED	21	LYS	H	8.316	0.02	1
UNMAPPED	104	THR	N	116.681	0.3	1
UNMAPPED	8	ASN	C	175.191	0.3	1
UNMAPPED	119	ARG	C	179.312	0.3	1
UNMAPPED	14	SER	CA	57.69	0.3	1
UNMAPPED	44	ALA	H	8.754	0.02	1
UNMAPPED	135	ALA	CA	53.673	0.3	1
UNMAPPED	118	GLU	CA	60.314	0.3	1
UNMAPPED	83	GLN	CA	58.734	0.3	1
UNMAPPED	100	VAL	H	8.104	0.02	1
UNMAPPED	124	MET	H	8.162	0.02	1
UNMAPPED	63	GLU	H	7.925	0.02	1
UNMAPPED	26	ALA	C	177.432	0.3	1
UNMAPPED	55	ASP	N	123.502	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	95	ILE	C	178.833	0.3	1
UNMAPPED	90	CYS	N	119.182	0.3	1
UNMAPPED	137	TYR	CA	59.31	0.3	1
UNMAPPED	136	TYR	H	7.947	0.02	1
UNMAPPED	126	VAL	H	8.509	0.02	1
UNMAPPED	111	GLU	C	179.239	0.3	1
UNMAPPED	51	HIS	N	123.217	0.3	1
UNMAPPED	37	GLY	CA	45.84	0.3	1
UNMAPPED	123	GLN	C	179.216	0.3	1
UNMAPPED	89	ASP	N	118.315	0.3	1
UNMAPPED	67	ARG	N	119.168	0.3	1
UNMAPPED	112	THR	N	116.887	0.3	1
UNMAPPED	108	ASN	CA	52.362	0.3	1
UNMAPPED	130	GLN	N	119.92	0.3	1
UNMAPPED	117	MET	C	177.777	0.3	1
UNMAPPED	100	VAL	CA	65.959	0.3	1
UNMAPPED	106	GLY	C	174.237	0.3	1
UNMAPPED	96	LYS	N	123.653	0.3	1
UNMAPPED	128	GLN	H	8.732	0.02	1
UNMAPPED	12	LYS	C	178.66	0.3	1
UNMAPPED	19	ASN	CA	52.592	0.3	1
UNMAPPED	134	GLN	CA	57.673	0.3	1
UNMAPPED	126	VAL	CA	67.274	0.3	1
UNMAPPED	4	GLY	C	174.648	0.3	1
UNMAPPED	127	THR	N	118.339	0.3	1
UNMAPPED	54	ASN	N	114.498	0.3	1
UNMAPPED	57	GLU	H	8.136	0.02	1
UNMAPPED	100	VAL	C	178.552	0.3	1
UNMAPPED	45	MET	C	175.589	0.3	1
UNMAPPED	138	ASP	N	121.189	0.3	1
UNMAPPED	56	TRP	N	120.6	0.3	1
UNMAPPED	74	TYR	CA	55.501	0.3	1
UNMAPPED	92	ASN	CA	56.317	0.3	1
UNMAPPED	28	VAL	H	8.116	0.02	1
UNMAPPED	111	GLU	CA	59.726	0.3	1
UNMAPPED	141	ARG	H	8.251	0.02	1
UNMAPPED	119	ARG	CA	58.051	0.3	1
UNMAPPED	98	HIS	H	8.521	0.02	1
UNMAPPED	111	GLU	N	120.184	0.3	1
UNMAPPED	88	HIS	N	117.889	0.3	1
UNMAPPED	135	ALA	C	178.952	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	52	PHE	N	125.391	0.3	1
UNMAPPED	109	PHE	H	8.787	0.02	1
UNMAPPED	124	MET	C	178.549	0.3	1
UNMAPPED	122	GLU	CA	60.792	0.3	1
UNMAPPED	97	GLN	H	8.56	0.02	1
UNMAPPED	45	MET	CA	53.476	0.3	1
UNMAPPED	120	VAL	CA	65.266	0.3	1
UNMAPPED	74	TYR	C	173.575	0.3	1
UNMAPPED	117	MET	H	8.707	0.02	1
UNMAPPED	75	ARG	C	178.119	0.3	1
UNMAPPED	15	LYS	CA	53.769	0.3	1
UNMAPPED	91	VAL	C	177.224	0.3	1
UNMAPPED	73	TYR	H	8.484	0.02	1
UNMAPPED	91	VAL	N	125.174	0.3	1
UNMAPPED	30	GLY	CA	44.715	0.3	1
UNMAPPED	6	THR	H	8.165	0.02	1
UNMAPPED	61	TYR	H	9.031	0.02	1
UNMAPPED	41	LEU	N	121.383	0.3	1
UNMAPPED	110	THR	CA	59.992	0.3	1
UNMAPPED	70	ASN	H	8.646	0.02	1
UNMAPPED	63	GLU	N	116.085	0.3	1
UNMAPPED	40	MET	N	121.696	0.3	1
UNMAPPED	58	ASP	H	7.914	0.02	1
UNMAPPED	120	VAL	C	177.012	0.3	1
UNMAPPED	64	ASN	N	115.422	0.3	1
UNMAPPED	75	ARG	CA	53.044	0.3	1
UNMAPPED	101	THR	CA	65.132	0.3	1
UNMAPPED	17	LYS	CA	55.962	0.3	1
UNMAPPED	69	PRO	C	175.028	0.3	1
UNMAPPED	106	GLY	CA	45.078	0.3	1
UNMAPPED	56	TRP	C	179.125	0.3	1
UNMAPPED	2	GLN	CA	55.533	0.3	1
UNMAPPED	23	VAL	N	123.141	0.3	1
UNMAPPED	115	LYS	CA	58.723	0.3	1
UNMAPPED	121	VAL	N	121.57	0.3	1
UNMAPPED	110	THR	N	116.21	0.3	1
UNMAPPED	128	GLN	C	177.393	0.3	1
UNMAPPED	142	SER	CA	59.56	0.3	1
UNMAPPED	135	ALA	N	120.897	0.3	1
UNMAPPED	89	ASP	C	175.842	0.3	1
UNMAPPED	43	SER	N	114.014	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	133	SER	C	175.643	0.3	1
UNMAPPED	17	LYS	C	176.797	0.3	1
UNMAPPED	128	GLN	N	122.861	0.3	1
UNMAPPED	48	PRO	C	175.656	0.3	1
UNMAPPED	87	VAL	CA	67.337	0.3	1
UNMAPPED	97	GLN	C	178.65	0.3	1
UNMAPPED	71	GLN	H	7.295	0.02	1
UNMAPPED	140	ARG	CA	55.732	0.3	1
UNMAPPED	102	THR	C	177.134	0.3	1
UNMAPPED	61	TYR	C	176.991	0.3	1
UNMAPPED	47	ARG	CA	54.397	0.3	1
UNMAPPED	31	ALA	C	177.555	0.3	1
UNMAPPED	89	ASP	CA	56.696	0.3	1
UNMAPPED	9	GLN	H	8.373	0.02	1
UNMAPPED	123	GLN	CA	58.71	0.3	1
UNMAPPED	115	LYS	H	7.697	0.02	1
UNMAPPED	64	ASN	C	175.46	0.3	1
UNMAPPED	21	LYS	N	122.041	0.3	1
UNMAPPED	67	ARG	CA	55.903	0.3	1
UNMAPPED	112	THR	CA	66.498	0.3	1
UNMAPPED	12	LYS	N	122.79	0.3	1
UNMAPPED	10	TRP	N	121.268	0.3	1
UNMAPPED	133	SER	N	115.422	0.3	1
UNMAPPED	140	ARG	C	176.206	0.3	1
UNMAPPED	102	THR	CA	64.913	0.3	1
UNMAPPED	96	LYS	CA	59.861	0.3	1
UNMAPPED	32	VAL	CA	61.67	0.3	1
UNMAPPED	1	GLY	C	174.256	0.3	1
UNMAPPED	87	VAL	H	8.904	0.02	1
UNMAPPED	18	THR	N	115.618	0.3	1
UNMAPPED	14	SER	C	174.151	0.3	1
UNMAPPED	116	MET	H	8.182	0.02	1
UNMAPPED	83	GLN	C	176.88	0.3	1
UNMAPPED	131	LYS	CA	58.924	0.3	1
UNMAPPED	25	GLY	C	173.682	0.3	1
UNMAPPED	90	CYS	H	8.164	0.02	1
UNMAPPED	43	SER	C	174.937	0.3	1
UNMAPPED	62	ARG	H	7.89	0.02	1
UNMAPPED	109	PHE	N	121.993	0.3	1
UNMAPPED	82	ASN	CA	51.824	0.3	1
UNMAPPED	97	GLN	N	117.392	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	104	THR	H	7.83	0.02	1
UNMAPPED	26	ALA	CA	51.847	0.3	1
UNMAPPED	138	ASP	CA	54.887	0.3	1
UNMAPPED	56	TRP	CA	61.375	0.3	1
UNMAPPED	2	GLN	C	176.69	0.3	1
UNMAPPED	49	MET	N	122.192	0.3	1
UNMAPPED	127	THR	C	176.69	0.3	1
UNMAPPED	119	ARG	N	116.978	0.3	1
UNMAPPED	32	VAL	H	8.188	0.02	1
UNMAPPED	58	ASP	N	119.043	0.3	1
UNMAPPED	108	ASN	C	173.575	0.3	1
UNMAPPED	93	ILE	CA	61.669	0.3	1
UNMAPPED	99	THR	N	115.451	0.3	1
UNMAPPED	40	MET	CA	53.235	0.3	1
UNMAPPED	5	GLY	C	174.519	0.3	1
UNMAPPED	10	TRP	C	175.852	0.3	1
UNMAPPED	19	ASN	C	174.988	0.3	1
UNMAPPED	15	LYS	N	124.501	0.3	1
UNMAPPED	54	ASN	H	7.26	0.02	1
UNMAPPED	57	GLU	N	120.714	0.3	1
UNMAPPED	43	SER	H	8.343	0.02	1
UNMAPPED	126	VAL	C	178.041	0.3	1
UNMAPPED	94	THR	H	8.166	0.02	1
UNMAPPED	29	ALA	N	128.393	0.3	1
UNMAPPED	83	GLN	H	8.658	0.02	1
UNMAPPED	41	LEU	CA	52.944	0.3	1
UNMAPPED	11	ASN	N	120.247	0.3	1
UNMAPPED	60	TYR	C	179.57	0.3	1
UNMAPPED	67	ARG	C	176.775	0.3	1
UNMAPPED	98	HIS	N	120.41	0.3	1
UNMAPPED	34	GLY	CA	44.911	0.3	1
UNMAPPED	38	GLY	C	173.93	0.3	1
UNMAPPED	17	LYS	N	122.443	0.3	1
UNMAPPED	32	VAL	C	176.337	0.3	1
UNMAPPED	50	ILE	H	6.584	0.02	1
UNMAPPED	139	GLY	C	174.413	0.3	1
UNMAPPED	52	PHE	H	10.372	0.02	1
UNMAPPED	9	GLN	N	120.492	0.3	1
UNMAPPED	1	GLY	CA	44.902	0.3	1
UNMAPPED	35	GLY	N	108.736	0.3	1
UNMAPPED	142	SER	N	122.99	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	111	GLU	H	9.208	0.02	1
UNMAPPED	131	LYS	C	179.777	0.3	1
UNMAPPED	10	TRP	H	8.09	0.02	1
UNMAPPED	73	TYR	N	121.825	0.3	1
UNMAPPED	43	SER	CA	58.079	0.3	1
UNMAPPED	108	ASN	H	8.562	0.02	1
UNMAPPED	87	VAL	N	120.628	0.3	1
UNMAPPED	61	TYR	N	120.752	0.3	1
UNMAPPED	22	HIS	H	8.282	0.02	1
UNMAPPED	72	VAL	CA	58.222	0.3	1
UNMAPPED	4	GLY	N	109.186	0.3	1
UNMAPPED	140	ARG	N	120.25	0.3	1
UNMAPPED	30	GLY	C	173.68	0.3	1
UNMAPPED	132	GLU	N	118.538	0.3	1
UNMAPPED	68	TYR	H	7.454	0.02	1
UNMAPPED	33	VAL	CA	62.001	0.3	1
UNMAPPED	59	ARG	CA	59.262	0.3	1
UNMAPPED	23	VAL	H	8.047	0.02	1
UNMAPPED	95	ILE	CA	66.146	0.3	1
UNMAPPED	21	LYS	CA	55.909	0.3	1
UNMAPPED	105	LYS	N	119.832	0.3	1
UNMAPPED	62	ARG	N	117.57	0.3	1
UNMAPPED	38	GLY	N	109.464	0.3	1
UNMAPPED	98	HIS	C	178.75	0.3	1
UNMAPPED	125	CYS	CA	59.659	0.3	1
UNMAPPED	10	TRP	CA	56.761	0.3	1
UNMAPPED	135	ALA	H	7.608	0.02	1
UNMAPPED	42	GLY	N	115.453	0.3	1
UNMAPPED	114	VAL	N	119.868	0.3	1
UNMAPPED	44	ALA	CA	52.527	0.3	1
UNMAPPED	49	MET	H	8.725	0.02	1
UNMAPPED	53	GLY	N	109.357	0.3	1
UNMAPPED	141	ARG	CA	55.451	0.3	1
UNMAPPED	119	ARG	H	7.286	0.02	1
UNMAPPED	141	ARG	C	175.486	0.3	1
UNMAPPED	109	PHE	C	176.676	0.3	1
UNMAPPED	71	GLN	N	114.497	0.3	1
UNMAPPED	99	THR	H	8.535	0.02	1
UNMAPPED	72	VAL	H	8.475	0.02	1
UNMAPPED	21	LYS	C	176.168	0.3	1
UNMAPPED	41	LEU	C	178.143	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	25	GLY	CA	44.77	0.3	1
UNMAPPED	91	VAL	H	9.301	0.02	1
UNMAPPED	129	TYR	N	120.465	0.3	1
UNMAPPED	97	GLN	CA	57.678	0.3	1
UNMAPPED	24	ALA	CA	52.258	0.3	1
UNMAPPED	37	GLY	H	8.585	0.02	1
UNMAPPED	103	THR	H	8.287	0.02	1
UNMAPPED	16	PRO	C	176.839	0.3	1
UNMAPPED	101	THR	H	8.216	0.02	1
UNMAPPED	15	LYS	H	8.376	0.02	1
UNMAPPED	58	ASP	C	179.046	0.3	1
UNMAPPED	117	MET	N	118.44	0.3	1
UNMAPPED	11	ASN	H	8.082	0.02	1
UNMAPPED	39	TYR	N	118.243	0.3	1
UNMAPPED	94	THR	N	118.262	0.3	1
UNMAPPED	137	TYR	N	119.867	0.3	1
UNMAPPED	5	GLY	N	109.051	0.3	1
UNMAPPED	59	ARG	H	8.028	0.02	1
UNMAPPED	93	ILE	N	119.173	0.3	1
UNMAPPED	18	THR	H	8.195	0.02	1
UNMAPPED	134	GLN	H	7.608	0.02	1
UNMAPPED	121	VAL	C	177.607	0.3	1
UNMAPPED	101	THR	N	115.515	0.3	1
UNMAPPED	107	GLU	CA	55.141	0.3	1
UNMAPPED	122	GLU	C	177.514	0.3	1
UNMAPPED	72	VAL	C	174.114	0.3	1
UNMAPPED	20	LEU	H	8.288	0.02	1
UNMAPPED	71	GLN	C	174.968	0.3	1
UNMAPPED	60	TYR	N	121.063	0.3	1
UNMAPPED	103	THR	CA	65.1	0.3	1
UNMAPPED	3	GLY	C	174.766	0.3	1
UNMAPPED	33	VAL	C	176.599	0.3	1
UNMAPPED	29	ALA	CA	52.24	0.3	1
UNMAPPED	82	ASN	C	173.97	0.3	1
UNMAPPED	98	HIS	CA	59.49	0.3	1
UNMAPPED	92	ASN	H	7.601	0.02	1
UNMAPPED	15	LYS	C	174.434	0.3	1
UNMAPPED	125	CYS	C	176.886	0.3	1
UNMAPPED	13	PRO	C	176.95	0.3	1
UNMAPPED	65	MET	N	118.623	0.3	1
UNMAPPED	22	HIS	N	121.52	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	71	GLN	CA	53.732	0.3	1
UNMAPPED	68	TYR	N	121.709	0.3	1
UNMAPPED	3	GLY	CA	44.921	0.3	1
UNMAPPED	113	ASP	CA	57.67	0.3	1
UNMAPPED	1	GLY	N	109.327	0.3	1
UNMAPPED	130	GLN	H	8.25	0.02	1
UNMAPPED	105	LYS	H	7.465	0.02	1
UNMAPPED	104	THR	CA	64.432	0.3	1
UNMAPPED	45	MET	H	8.801	0.02	1
UNMAPPED	93	ILE	C	177.907	0.3	1
UNMAPPED	73	TYR	CA	56.575	0.3	1
UNMAPPED	107	GLU	N	120.437	0.3	1

7.6.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	136	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	134	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	127	0.00 \pm 0.00	None needed (< 0.5 ppm)

7.6.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1596. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/665 (0%)	0/265 (0%)	0/270 (0%)	0/130 (0%)
Sidechain	0/815 (0%)	0/473 (0%)	0/315 (0%)	0/27 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1596 (0%)	0/798 (0%)	0/629 (0%)	0/169 (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 1685. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/698 (0%)	0/278 (0%)	0/284 (0%)	0/136 (0%)
Sidechain	0/871 (0%)	0/507 (0%)	0/335 (0%)	0/29 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1685 (0%)	0/845 (0%)	0/663 (0%)	0/177 (0%)

7.6.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.

7.7 Chemical shift list 7

File name: BMRB entry 16079

Chemical shift list name: *assigned_chem_shift_list_1*

7.7.1 Bookkeeping [i](#)

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	639
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	639
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 639 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	36	LEU	H	8.219	0.02	1
UNMAPPED	51	HIS	C	175.271	0.3	1
UNMAPPED	83	GLN	N	120.237	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	16	PRO	CA	62.56	0.3	1
UNMAPPED	72	VAL	N	112.959	0.3	1
UNMAPPED	55	ASP	C	177.925	0.3	1
UNMAPPED	72	VAL	CB	33.579	0.3	1
UNMAPPED	130	GLN	C	178.581	0.3	1
UNMAPPED	124	MET	C	178.569	0.3	1
UNMAPPED	75	ARG	H	7.943	0.02	1
UNMAPPED	3	GLY	H	8.532	0.02	1
UNMAPPED	2	GLN	H	8.321	0.02	1
UNMAPPED	48	PRO	CA	61.917	0.3	1
UNMAPPED	42	GLY	C	172.823	0.3	1
UNMAPPED	105	LYS	CA	55.785	0.3	1
UNMAPPED	51	HIS	CA	54.314	0.3	1
UNMAPPED	38	GLY	CA	44.599	0.3	1
UNMAPPED	59	ARG	CB	29.174	0.3	1
UNMAPPED	27	ALA	CB	18.982	0.3	1
UNMAPPED	95	ILE	CB	36.541	0.3	1
UNMAPPED	37	GLY	N	110.148	0.3	1
UNMAPPED	142	SER	H	8.01	0.02	1
UNMAPPED	12	LYS	CB	32.099	0.3	1
UNMAPPED	47	ARG	C	174.623	0.3	1
UNMAPPED	130	GLN	CA	58.768	0.3	1
UNMAPPED	25	GLY	H	8.491	0.02	1
UNMAPPED	108	ASN	N	119.679	0.3	1
UNMAPPED	100	VAL	N	123.452	0.3	1
UNMAPPED	5	GLY	H	8.383	0.02	1
UNMAPPED	54	ASN	C	174.379	0.3	1
UNMAPPED	129	TYR	C	178.2	0.3	1
UNMAPPED	112	THR	C	175.705	0.3	1
UNMAPPED	46	SER	CA	58.198	0.3	1
UNMAPPED	105	LYS	C	176.763	0.3	1
UNMAPPED	19	ASN	CB	38.401	0.3	1
UNMAPPED	18	THR	CB	69.523	0.3	1
UNMAPPED	88	HIS	H	8.377	0.02	1
UNMAPPED	94	THR	C	177.692	0.3	1
UNMAPPED	132	GLU	H	8.434	0.02	1
UNMAPPED	40	MET	H	9.134	0.02	1
UNMAPPED	85	ASN	H	8.589	0.02	1
UNMAPPED	36	LEU	C	177.954	0.3	1
UNMAPPED	133	SER	H	8.426	0.02	1
UNMAPPED	104	THR	C	175.18	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	54	ASN	CA	52.075	0.3	1
UNMAPPED	87	VAL	CB	31.596	0.3	1
UNMAPPED	113	ASP	C	177.613	0.3	1
UNMAPPED	66	TYR	C	175.904	0.3	1
UNMAPPED	60	TYR	H	8.259	0.02	1
UNMAPPED	118	GLU	CB	28.772	0.3	1
UNMAPPED	94	THR	CA	68.179	0.3	1
UNMAPPED	92	ASN	N	116.544	0.3	1
UNMAPPED	102	THR	H	8.053	0.02	1
UNMAPPED	118	GLU	N	119.104	0.3	1
UNMAPPED	74	TYR	N	111.251	0.3	1
UNMAPPED	6	THR	N	113.592	0.3	1
UNMAPPED	92	ASN	CB	38.669	0.3	1
UNMAPPED	101	THR	C	176.776	0.3	1
UNMAPPED	31	ALA	H	8.153	0.02	1
UNMAPPED	52	PHE	C	177.124	0.3	1
UNMAPPED	70	ASN	N	116.489	0.3	1
UNMAPPED	64	ASN	H	7.56	0.02	1
UNMAPPED	44	ALA	C	177.518	0.3	1
UNMAPPED	122	GLU	CB	28.527	0.3	1
UNMAPPED	131	LYS	H	7.866	0.02	1
UNMAPPED	8	ASN	CB	38.267	0.3	1
UNMAPPED	24	VAL	H	8.27	0.02	1
UNMAPPED	50	ILE	N	124.684	0.3	1
UNMAPPED	132	GLU	N	118.576	0.3	1
UNMAPPED	120	VAL	N	119.313	0.3	1
UNMAPPED	63	GLU	C	177.627	0.3	1
UNMAPPED	45	MET	CB	36.369	0.3	1
UNMAPPED	120	VAL	CB	31.988	0.3	1
UNMAPPED	40	MET	C	172.967	0.3	1
UNMAPPED	132	GLU	CB	29.644	0.3	1
UNMAPPED	36	LEU	CB	42.011	0.3	1
UNMAPPED	116	MET	C	178.229	0.3	1
UNMAPPED	107	GLU	C	174.904	0.3	1
UNMAPPED	36	LEU	N	122.023	0.3	1
UNMAPPED	132	GLU	C	179.277	0.3	1
UNMAPPED	39	TYR	H	7.886	0.02	1
UNMAPPED	127	THR	CA	66.655	0.3	1
UNMAPPED	66	TYR	H	7.597	0.02	1
UNMAPPED	136	TYR	C	177.217	0.3	1
UNMAPPED	63	GLU	CA	57.485	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	3	GLY	N	110.613	0.3	1
UNMAPPED	17	LYS	CB	32.51	0.3	1
UNMAPPED	75	ARG	N	120.875	0.3	1
UNMAPPED	13	PRO	CB	31.654	0.3	1
UNMAPPED	2	GLN	CB	28.975	0.3	1
UNMAPPED	106	GLY	N	108.083	0.3	1
UNMAPPED	34	GLY	C	174.721	0.3	1
UNMAPPED	114	VAL	C	177.43	0.3	1
UNMAPPED	90	CYS	CB	40.654	0.3	1
UNMAPPED	2	GLN	N	120.06	0.3	1
UNMAPPED	27	ALA	H	8.412	0.02	1
UNMAPPED	136	TYR	H	7.943	0.02	1
UNMAPPED	95	ILE	H	8.48	0.02	1
UNMAPPED	121	VAL	CA	65.984	0.3	1
UNMAPPED	115	LYS	N	119.282	0.3	1
UNMAPPED	86	PHE	C	177.486	0.3	1
UNMAPPED	12	LYS	H	8.026	0.02	1
UNMAPPED	90	CYS	CA	58.278	0.3	1
UNMAPPED	126	VAL	H	8.511	0.02	1
UNMAPPED	27	ALA	N	128.097	0.3	1
UNMAPPED	139	GLY	C	174.433	0.3	1
UNMAPPED	139	GLY	H	7.86	0.02	1
UNMAPPED	103	THR	C	178.058	0.3	1
UNMAPPED	41	LEU	H	8.081	0.02	1
UNMAPPED	141	ARG	N	122.762	0.3	1
UNMAPPED	128	GLN	CA	58.218	0.3	1
UNMAPPED	124	MET	CA	59.483	0.3	1
UNMAPPED	65	MET	H	7.893	0.02	1
UNMAPPED	140	ARG	CB	30.145	0.3	1
UNMAPPED	107	GLU	H	7.449	0.02	1
UNMAPPED	116	MET	N	118.656	0.3	1
UNMAPPED	50	ILE	CA	58.733	0.3	1
UNMAPPED	114	VAL	CB	30.978	0.3	1
UNMAPPED	47	ARG	N	127.095	0.3	1
UNMAPPED	124	MET	N	119.678	0.3	1
UNMAPPED	51	HIS	CB	30.406	0.3	1
UNMAPPED	123	GLN	CB	27.372	0.3	1
UNMAPPED	47	ARG	CB	29.172	0.3	1
UNMAPPED	27	ALA	CA	51.884	0.3	1
UNMAPPED	121	VAL	H	9.17	0.02	1
UNMAPPED	95	ILE	N	121.287	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	39	TYR	C	175.742	0.3	1
UNMAPPED	84	ASN	N	117.396	0.3	1
UNMAPPED	112	THR	CB	68.64	0.3	1
UNMAPPED	118	GLU	H	8.582	0.02	1
UNMAPPED	74	TYR	H	8.514	0.02	1
UNMAPPED	12	LYS	CA	53.745	0.3	1
UNMAPPED	59	ARG	C	177.61	0.3	1
UNMAPPED	123	GLN	N	115.448	0.3	1
UNMAPPED	102	THR	CB	68.706	0.3	1
UNMAPPED	102	THR	N	114.877	0.3	1
UNMAPPED	32	VAL	N	119.885	0.3	1
UNMAPPED	59	ARG	N	119.938	0.3	1
UNMAPPED	31	ALA	CB	19.149	0.3	1
UNMAPPED	31	ALA	N	123.966	0.3	1
UNMAPPED	122	GLU	H	8.009	0.02	1
UNMAPPED	24	VAL	N	124.755	0.3	1
UNMAPPED	131	LYS	CB	32.079	0.3	1
UNMAPPED	24	VAL	CB	32.382	0.3	1
UNMAPPED	131	LYS	N	119.574	0.3	1
UNMAPPED	136	TYR	CA	59.504	0.3	1
UNMAPPED	109	PHE	CA	56.068	0.3	1
UNMAPPED	82	ASN	CB	39.627	0.3	1
UNMAPPED	33	VAL	H	8.315	0.02	1
UNMAPPED	127	THR	CB	68.038	0.3	1
UNMAPPED	120	VAL	H	8.269	0.02	1
UNMAPPED	46	SER	C	174.432	0.3	1
UNMAPPED	124	MET	CB	33.966	0.3	1
UNMAPPED	56	TRP	CB	28.063	0.3	1
UNMAPPED	42	GLY	CA	44.499	0.3	1
UNMAPPED	6	THR	CA	61.634	0.3	1
UNMAPPED	84	ASN	CA	56.059	0.3	1
UNMAPPED	49	MET	CA	53.629	0.3	1
UNMAPPED	30	GLY	H	8.492	0.02	1
UNMAPPED	39	TYR	CB	39.604	0.3	1
UNMAPPED	68	TYR	C	172.771	0.3	1
UNMAPPED	110	THR	C	175.456	0.3	1
UNMAPPED	66	TYR	CB	35.528	0.3	1
UNMAPPED	70	ASN	CA	51.527	0.3	1
UNMAPPED	58	ASP	CA	58.191	0.3	1
UNMAPPED	66	TYR	N	116.866	0.3	1
UNMAPPED	93	ILE	CB	36.043	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	99	THR	CA	66.385	0.3	1
UNMAPPED	23	VAL	C	175.784	0.3	1
UNMAPPED	17	LYS	H	8.575	0.02	1
UNMAPPED	106	GLY	H	7.925	0.02	1
UNMAPPED	8	ASN	CA	52.709	0.3	1
UNMAPPED	40	MET	N	121.668	0.3	1
UNMAPPED	127	THR	H	8.125	0.02	1
UNMAPPED	85	ASN	N	118.454	0.3	1
UNMAPPED	49	MET	C	175.062	0.3	1
UNMAPPED	57	GLU	CA	59.614	0.3	1
UNMAPPED	137	TYR	H	8.053	0.02	1
UNMAPPED	99	THR	C	176.493	0.3	1
UNMAPPED	36	LEU	CA	54.492	0.3	1
UNMAPPED	141	ARG	CB	30.493	0.3	1
UNMAPPED	11	ASN	CA	52.411	0.3	1
UNMAPPED	141	ARG	CA	55.472	0.3	1
UNMAPPED	41	LEU	CB	43.263	0.3	1
UNMAPPED	34	GLY	N	113.752	0.3	1
UNMAPPED	133	SER	CA	60.728	0.3	1
UNMAPPED	4	GLY	H	8.374	0.02	1
UNMAPPED	140	ARG	H	7.838	0.02	1
UNMAPPED	37	GLY	C	174.799	0.3	1
UNMAPPED	57	GLU	C	177.715	0.3	1
UNMAPPED	137	TYR	C	176.953	0.3	1
UNMAPPED	110	THR	H	9.608	0.02	1
UNMAPPED	13	PRO	CA	62.652	0.3	1
UNMAPPED	35	GLY	CA	44.895	0.3	1
UNMAPPED	9	GLN	CA	55.845	0.3	1
UNMAPPED	123	GLN	H	7.081	0.02	1
UNMAPPED	47	ARG	H	8.698	0.02	1
UNMAPPED	117	MET	CA	59.593	0.3	1
UNMAPPED	11	ASN	C	174.361	0.3	1
UNMAPPED	121	VAL	CB	30.436	0.3	1
UNMAPPED	20	LEU	CA	54.762	0.3	1
UNMAPPED	87	VAL	C	176.723	0.3	1
UNMAPPED	112	THR	H	7.968	0.02	1
UNMAPPED	14	SER	CB	63.604	0.3	1
UNMAPPED	84	ASN	H	8.423	0.02	1
UNMAPPED	62	ARG	C	179.158	0.3	1
UNMAPPED	18	THR	N	115.588	0.3	1
UNMAPPED	14	SER	N	117.196	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	134	GLN	N	120.945	0.3	1
UNMAPPED	61	TYR	CA	62.66	0.3	1
UNMAPPED	73	TYR	C	174.721	0.3	1
UNMAPPED	116	MET	CA	59.327	0.3	1
UNMAPPED	4	GLY	CA	44.736	0.3	1
UNMAPPED	27	ALA	C	177.255	0.3	1
UNMAPPED	53	GLY	C	173.302	0.3	1
UNMAPPED	113	ASP	H	7.53	0.02	1
UNMAPPED	20	LEU	C	177.242	0.3	1
UNMAPPED	132	GLU	CA	57.464	0.3	1
UNMAPPED	29	VAL	C	176.677	0.3	1
UNMAPPED	33	VAL	N	124.908	0.3	1
UNMAPPED	70	ASN	C	172.829	0.3	1
UNMAPPED	55	ASP	CA	57.362	0.3	1
UNMAPPED	35	GLY	H	8.297	0.02	1
UNMAPPED	33	VAL	CB	32.084	0.3	1
UNMAPPED	62	ARG	CA	59.583	0.3	1
UNMAPPED	139	GLY	N	108.169	0.3	1
UNMAPPED	92	ASN	C	178.556	0.3	1
UNMAPPED	21	LYS	CB	32.497	0.3	1
UNMAPPED	96	LYS	C	179.08	0.3	1
UNMAPPED	125	CYS	CB	41.472	0.3	1
UNMAPPED	125	CYS	N	119.705	0.3	1
UNMAPPED	56	TRP	H	8.564	0.02	1
UNMAPPED	114	VAL	CA	67.378	0.3	1
UNMAPPED	44	ALA	CB	18.072	0.3	1
UNMAPPED	53	GLY	CA	45.272	0.3	1
UNMAPPED	44	ALA	N	125.778	0.3	1
UNMAPPED	100	VAL	CB	31.272	0.3	1
UNMAPPED	86	PHE	CA	60.307	0.3	1
UNMAPPED	84	ASN	C	177.744	0.3	1
UNMAPPED	93	ILE	H	8.807	0.02	1
UNMAPPED	136	TYR	N	119.35	0.3	1
UNMAPPED	138	ASP	C	177.312	0.3	1
UNMAPPED	129	TYR	CA	61.652	0.3	1
UNMAPPED	55	ASP	H	9.031	0.02	1
UNMAPPED	89	ASP	H	7.438	0.02	1
UNMAPPED	136	TYR	CB	38.255	0.3	1
UNMAPPED	38	GLY	H	8.41	0.02	1
UNMAPPED	126	VAL	N	123.917	0.3	1
UNMAPPED	50	ILE	C	173.203	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	67	ARG	H	7.518	0.02	1
UNMAPPED	35	GLY	C	174.379	0.3	1
UNMAPPED	124	MET	H	8.131	0.02	1
UNMAPPED	9	GLN	C	175.737	0.3	1
UNMAPPED	114	VAL	H	8.264	0.02	1
UNMAPPED	18	THR	CA	61.124	0.3	1
UNMAPPED	126	VAL	CB	31.118	0.3	1
UNMAPPED	53	GLY	H	8.942	0.02	1
UNMAPPED	96	LYS	H	8.151	0.02	1
UNMAPPED	39	TYR	CA	57.948	0.3	1
UNMAPPED	69	PRO	CA	63.114	0.3	1
UNMAPPED	51	HIS	H	8.128	0.02	1
UNMAPPED	5	GLY	CA	44.775	0.3	1
UNMAPPED	66	TYR	CA	58.78	0.3	1
UNMAPPED	46	SER	H	8.468	0.02	1
UNMAPPED	81	SER	CA	58.372	0.3	1
UNMAPPED	34	GLY	H	8.615	0.02	1
UNMAPPED	115	LYS	C	180.061	0.3	1
UNMAPPED	88	HIS	CA	59.454	0.3	1
UNMAPPED	122	GLU	N	120.961	0.3	1
UNMAPPED	110	THR	CB	71.765	0.3	1
UNMAPPED	142	SER	C	178.615	0.3	1
UNMAPPED	1	GLY	H	8.603	0.02	1
UNMAPPED	129	TYR	H	8.622	0.02	1
UNMAPPED	85	ASN	CA	55.68	0.3	1
UNMAPPED	52	PHE	CA	59.141	0.3	1
UNMAPPED	22	HIS	C	174.996	0.3	1
UNMAPPED	65	MET	C	176.396	0.3	1
UNMAPPED	45	MET	N	121.6	0.3	1
UNMAPPED	103	THR	N	118.598	0.3	1
UNMAPPED	57	GLU	CB	29.387	0.3	1
UNMAPPED	60	TYR	CA	61.733	0.3	1
UNMAPPED	138	ASP	H	8.253	0.02	1
UNMAPPED	103	THR	H	8.285	0.02	1
UNMAPPED	14	SER	H	8.477	0.02	1
UNMAPPED	90	CYS	C	177.544	0.3	1
UNMAPPED	125	CYS	H	9.233	0.02	1
UNMAPPED	88	HIS	C	177.6	0.3	1
UNMAPPED	30	GLY	N	112.8	0.3	1
UNMAPPED	98	HIS	CB	31.67	0.3	1
UNMAPPED	85	ASN	C	177.328	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	25	GLY	N	113.003	0.3	1
UNMAPPED	22	HIS	CA	55.654	0.3	1
UNMAPPED	118	GLU	C	178.733	0.3	1
UNMAPPED	65	MET	CA	58.688	0.3	1
UNMAPPED	15	LYS	H	8.378	0.02	1
UNMAPPED	113	ASP	CB	41.372	0.3	1
UNMAPPED	64	ASN	CA	54.539	0.3	1
UNMAPPED	68	TYR	CA	52.266	0.3	1
UNMAPPED	139	GLY	CA	45.177	0.3	1
UNMAPPED	113	ASP	N	120.136	0.3	1
UNMAPPED	42	GLY	H	9.425	0.02	1
UNMAPPED	20	LEU	N	123.328	0.3	1
UNMAPPED	23	VAL	CA	61.709	0.3	1
UNMAPPED	117	MET	CB	33.473	0.3	1
UNMAPPED	21	LYS	H	8.31	0.02	1
UNMAPPED	104	THR	N	116.689	0.3	1
UNMAPPED	8	ASN	C	175.261	0.3	1
UNMAPPED	119	ARG	C	179.367	0.3	1
UNMAPPED	73	TYR	CB	41.735	0.3	1
UNMAPPED	104	THR	CB	68.706	0.3	1
UNMAPPED	14	SER	CA	57.697	0.3	1
UNMAPPED	44	ALA	H	8.752	0.02	1
UNMAPPED	135	ALA	CA	53.66	0.3	1
UNMAPPED	118	GLU	CA	60.32	0.3	1
UNMAPPED	83	GLN	CA	58.619	0.3	1
UNMAPPED	16	PRO	CB	31.776	0.3	1
UNMAPPED	100	VAL	H	8.099	0.02	1
UNMAPPED	24	VAL	C	176.598	0.3	1
UNMAPPED	61	TYR	CB	37.975	0.3	1
UNMAPPED	26	VAL	H	8.042	0.02	1
UNMAPPED	63	GLU	H	7.924	0.02	1
UNMAPPED	55	ASP	N	123.488	0.3	1
UNMAPPED	95	ILE	C	178.831	0.3	1
UNMAPPED	90	CYS	N	119.189	0.3	1
UNMAPPED	137	TYR	CA	59.353	0.3	1
UNMAPPED	55	ASP	CB	40.682	0.3	1
UNMAPPED	89	ASP	CB	41.05	0.3	1
UNMAPPED	111	GLU	C	179.289	0.3	1
UNMAPPED	51	HIS	N	123.142	0.3	1
UNMAPPED	37	GLY	CA	45.792	0.3	1
UNMAPPED	123	GLN	C	179.223	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	89	ASP	N	118.351	0.3	1
UNMAPPED	67	ARG	CB	30.318	0.3	1
UNMAPPED	130	GLN	CB	26.946	0.3	1
UNMAPPED	67	ARG	N	119.16	0.3	1
UNMAPPED	112	THR	N	116.879	0.3	1
UNMAPPED	84	ASN	CB	37.211	0.3	1
UNMAPPED	108	ASN	CA	52.314	0.3	1
UNMAPPED	130	GLN	N	119.941	0.3	1
UNMAPPED	117	MET	C	177.81	0.3	1
UNMAPPED	96	LYS	CB	31.748	0.3	1
UNMAPPED	100	VAL	CA	65.958	0.3	1
UNMAPPED	106	GLY	C	174.235	0.3	1
UNMAPPED	46	SER	CB	62.782	0.3	1
UNMAPPED	96	LYS	N	123.707	0.3	1
UNMAPPED	128	GLN	H	8.728	0.02	1
UNMAPPED	46	SER	N	116.504	0.3	1
UNMAPPED	19	ASN	CA	52.563	0.3	1
UNMAPPED	134	GLN	CA	57.717	0.3	1
UNMAPPED	129	TYR	CB	41.285	0.3	1
UNMAPPED	126	VAL	CA	67.251	0.3	1
UNMAPPED	4	GLY	C	174.792	0.3	1
UNMAPPED	127	THR	N	118.377	0.3	1
UNMAPPED	54	ASN	N	114.525	0.3	1
UNMAPPED	57	GLU	H	8.129	0.02	1
UNMAPPED	111	GLU	CB	28.772	0.3	1
UNMAPPED	100	VAL	C	178.581	0.3	1
UNMAPPED	29	VAL	CA	61.973	0.3	1
UNMAPPED	138	ASP	CB	40.407	0.3	1
UNMAPPED	45	MET	C	175.64	0.3	1
UNMAPPED	138	ASP	N	121.189	0.3	1
UNMAPPED	56	TRP	N	120.603	0.3	1
UNMAPPED	74	TYR	CA	55.518	0.3	1
UNMAPPED	92	ASN	CA	56.313	0.3	1
UNMAPPED	137	TYR	CB	37.822	0.3	1
UNMAPPED	111	GLU	CA	59.635	0.3	1
UNMAPPED	141	ARG	H	8.253	0.02	1
UNMAPPED	134	GLN	CB	27.896	0.3	1
UNMAPPED	69	PRO	CB	31.712	0.3	1
UNMAPPED	119	ARG	CA	58.069	0.3	1
UNMAPPED	98	HIS	H	8.521	0.02	1
UNMAPPED	111	GLU	N	120.173	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	88	HIS	N	117.833	0.3	1
UNMAPPED	134	GLN	H	7.606	0.02	1
UNMAPPED	135	ALA	C	179.014	0.3	1
UNMAPPED	52	PHE	N	125.407	0.3	1
UNMAPPED	109	PHE	H	8.787	0.02	1
UNMAPPED	122	GLU	CA	60.78	0.3	1
UNMAPPED	97	GLN	H	8.553	0.02	1
UNMAPPED	45	MET	CA	53.505	0.3	1
UNMAPPED	120	VAL	CA	65.289	0.3	1
UNMAPPED	74	TYR	C	173.591	0.3	1
UNMAPPED	117	MET	H	8.704	0.02	1
UNMAPPED	142	SER	CB	64.53	0.3	1
UNMAPPED	75	ARG	C	178.129	0.3	1
UNMAPPED	29	VAL	H	8.182	0.02	1
UNMAPPED	15	LYS	CA	53.84	0.3	1
UNMAPPED	91	VAL	C	177.234	0.3	1
UNMAPPED	73	TYR	H	8.48	0.02	1
UNMAPPED	91	VAL	N	125.151	0.3	1
UNMAPPED	30	GLY	CA	44.704	0.3	1
UNMAPPED	6	THR	H	8.167	0.02	1
UNMAPPED	61	TYR	H	9.031	0.02	1
UNMAPPED	41	LEU	N	121.384	0.3	1
UNMAPPED	110	THR	CA	59.965	0.3	1
UNMAPPED	70	ASN	H	8.649	0.02	1
UNMAPPED	63	GLU	N	116.118	0.3	1
UNMAPPED	91	VAL	CA	65.714	0.3	1
UNMAPPED	58	ASP	H	7.909	0.02	1
UNMAPPED	120	VAL	C	177.051	0.3	1
UNMAPPED	64	ASN	N	115.43	0.3	1
UNMAPPED	63	GLU	CB	29.71	0.3	1
UNMAPPED	75	ARG	CA	53.039	0.3	1
UNMAPPED	101	THR	CA	65.088	0.3	1
UNMAPPED	17	LYS	CA	55.943	0.3	1
UNMAPPED	69	PRO	C	175.075	0.3	1
UNMAPPED	106	GLY	CA	45.072	0.3	1
UNMAPPED	56	TRP	C	179.198	0.3	1
UNMAPPED	2	GLN	CA	55.43	0.3	1
UNMAPPED	23	VAL	N	123.19	0.3	1
UNMAPPED	115	LYS	CA	58.786	0.3	1
UNMAPPED	121	VAL	N	121.56	0.3	1
UNMAPPED	110	THR	N	116.223	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	128	GLN	C	177.43	0.3	1
UNMAPPED	142	SER	CA	59.523	0.3	1
UNMAPPED	135	ALA	N	120.858	0.3	1
UNMAPPED	43	SER	CB	63.641	0.3	1
UNMAPPED	89	ASP	C	175.899	0.3	1
UNMAPPED	43	SER	N	114.007	0.3	1
UNMAPPED	133	SER	C	175.742	0.3	1
UNMAPPED	17	LYS	C	176.867	0.3	1
UNMAPPED	128	GLN	N	122.851	0.3	1
UNMAPPED	48	PRO	C	175.719	0.3	1
UNMAPPED	87	VAL	CA	67.269	0.3	1
UNMAPPED	97	GLN	C	178.647	0.3	1
UNMAPPED	128	GLN	CB	27.894	0.3	1
UNMAPPED	71	GLN	H	7.295	0.02	1
UNMAPPED	140	ARG	CA	55.728	0.3	1
UNMAPPED	102	THR	C	177.155	0.3	1
UNMAPPED	61	TYR	C	177.051	0.3	1
UNMAPPED	50	ILE	CB	38.395	0.3	1
UNMAPPED	47	ARG	CA	54.371	0.3	1
UNMAPPED	31	ALA	C	177.675	0.3	1
UNMAPPED	89	ASP	CA	56.723	0.3	1
UNMAPPED	9	GLN	H	8.371	0.02	1
UNMAPPED	123	GLN	CA	58.785	0.3	1
UNMAPPED	115	LYS	H	7.695	0.02	1
UNMAPPED	64	ASN	C	175.508	0.3	1
UNMAPPED	21	LYS	N	121.977	0.3	1
UNMAPPED	67	ARG	CA	55.944	0.3	1
UNMAPPED	10	TRP	CB	28.659	0.3	1
UNMAPPED	112	THR	CA	66.434	0.3	1
UNMAPPED	103	THR	CB	68.83	0.3	1
UNMAPPED	12	LYS	N	122.777	0.3	1
UNMAPPED	10	TRP	N	121.259	0.3	1
UNMAPPED	107	GLU	CA	55.151	0.3	1
UNMAPPED	133	SER	N	115.424	0.3	1
UNMAPPED	108	ASN	CB	40.872	0.3	1
UNMAPPED	140	ARG	C	176.226	0.3	1
UNMAPPED	102	THR	CA	64.957	0.3	1
UNMAPPED	96	LYS	CA	59.918	0.3	1
UNMAPPED	32	VAL	CA	61.976	0.3	1
UNMAPPED	1	GLY	C	174.335	0.3	1
UNMAPPED	87	VAL	H	8.898	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	31	ALA	CA	51.861	0.3	1
UNMAPPED	14	SER	C	174.184	0.3	1
UNMAPPED	28	ALA	H	8.279	0.02	1
UNMAPPED	116	MET	H	8.178	0.02	1
UNMAPPED	83	GLN	C	176.88	0.3	1
UNMAPPED	24	VAL	CA	61.98	0.3	1
UNMAPPED	131	LYS	CA	58.857	0.3	1
UNMAPPED	25	GLY	C	173.867	0.3	1
UNMAPPED	109	PHE	CB	39.745	0.3	1
UNMAPPED	90	CYS	H	8.159	0.02	1
UNMAPPED	43	SER	C	174.97	0.3	1
UNMAPPED	97	GLN	CB	27.43	0.3	1
UNMAPPED	62	ARG	H	7.891	0.02	1
UNMAPPED	109	PHE	N	122.002	0.3	1
UNMAPPED	82	ASN	CA	51.906	0.3	1
UNMAPPED	29	VAL	N	119.875	0.3	1
UNMAPPED	97	GLN	N	117.404	0.3	1
UNMAPPED	104	THR	H	7.828	0.02	1
UNMAPPED	29	VAL	CB	32.34	0.3	1
UNMAPPED	28	ALA	CA	51.827	0.3	1
UNMAPPED	138	ASP	CA	54.87	0.3	1
UNMAPPED	56	TRP	CA	61.427	0.3	1
UNMAPPED	2	GLN	C	177.064	0.3	1
UNMAPPED	49	MET	N	122.18	0.3	1
UNMAPPED	6	THR	CB	69.506	0.3	1
UNMAPPED	119	ARG	N	116.986	0.3	1
UNMAPPED	49	MET	CB	29.959	0.3	1
UNMAPPED	32	VAL	H	8.161	0.02	1
UNMAPPED	58	ASP	N	119.074	0.3	1
UNMAPPED	119	ARG	CB	29.585	0.3	1
UNMAPPED	70	ASN	CB	37.936	0.3	1
UNMAPPED	99	THR	CB	68.447	0.3	1
UNMAPPED	58	ASP	CB	40.164	0.3	1
UNMAPPED	108	ASN	C	173.591	0.3	1
UNMAPPED	93	ILE	CA	61.713	0.3	1
UNMAPPED	99	THR	N	115.449	0.3	1
UNMAPPED	40	MET	CA	53.266	0.3	1
UNMAPPED	5	GLY	C	174.513	0.3	1
UNMAPPED	10	TRP	C	175.885	0.3	1
UNMAPPED	91	VAL	CB	31.432	0.3	1
UNMAPPED	19	ASN	C	174.983	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	15	LYS	N	124.512	0.3	1
UNMAPPED	54	ASN	H	7.253	0.02	1
UNMAPPED	57	GLU	N	120.784	0.3	1
UNMAPPED	15	LYS	CB	32.327	0.3	1
UNMAPPED	43	SER	H	8.343	0.02	1
UNMAPPED	126	VAL	C	178.085	0.3	1
UNMAPPED	94	THR	H	8.166	0.02	1
UNMAPPED	11	ASN	CB	38.445	0.3	1
UNMAPPED	83	GLN	H	8.67	0.02	1
UNMAPPED	41	LEU	CA	52.797	0.3	1
UNMAPPED	11	ASN	N	120.297	0.3	1
UNMAPPED	60	TYR	C	179.577	0.3	1
UNMAPPED	67	ARG	C	176.848	0.3	1
UNMAPPED	142	SER	N	122.992	0.3	1
UNMAPPED	26	VAL	CA	61.588	0.3	1
UNMAPPED	98	HIS	N	120.407	0.3	1
UNMAPPED	34	GLY	CA	44.956	0.3	1
UNMAPPED	26	VAL	N	119.783	0.3	1
UNMAPPED	38	GLY	C	173.959	0.3	1
UNMAPPED	17	LYS	N	122.412	0.3	1
UNMAPPED	71	GLN	CB	32.749	0.3	1
UNMAPPED	134	GLN	C	177.221	0.3	1
UNMAPPED	32	VAL	C	176.396	0.3	1
UNMAPPED	50	ILE	H	6.584	0.02	1
UNMAPPED	26	VAL	CB	32.485	0.3	1
UNMAPPED	52	PHE	H	10.371	0.02	1
UNMAPPED	9	GLN	N	120.492	0.3	1
UNMAPPED	1	GLY	CA	45.007	0.3	1
UNMAPPED	35	GLY	N	108.665	0.3	1
UNMAPPED	9	GLN	CB	28.501	0.3	1
UNMAPPED	20	LEU	CB	41.813	0.3	1
UNMAPPED	115	LYS	CB	31.409	0.3	1
UNMAPPED	111	GLU	H	9.202	0.02	1
UNMAPPED	131	LYS	C	179.812	0.3	1
UNMAPPED	10	TRP	H	8.089	0.02	1
UNMAPPED	73	TYR	N	121.771	0.3	1
UNMAPPED	43	SER	CA	58.091	0.3	1
UNMAPPED	108	ASN	H	8.56	0.02	1
UNMAPPED	87	VAL	N	120.636	0.3	1
UNMAPPED	28	ALA	C	177.623	0.3	1
UNMAPPED	61	TYR	N	120.767	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	22	HIS	H	8.276	0.02	1
UNMAPPED	65	MET	CB	29.883	0.3	1
UNMAPPED	72	VAL	CA	58.183	0.3	1
UNMAPPED	4	GLY	N	109.092	0.3	1
UNMAPPED	140	ARG	N	120.258	0.3	1
UNMAPPED	30	GLY	C	173.604	0.3	1
UNMAPPED	116	MET	CB	32.325	0.3	1
UNMAPPED	68	TYR	H	7.455	0.02	1
UNMAPPED	48	PRO	CB	31.905	0.3	1
UNMAPPED	33	VAL	CA	62.066	0.3	1
UNMAPPED	105	LYS	CB	32.013	0.3	1
UNMAPPED	62	ARG	CB	29.284	0.3	1
UNMAPPED	59	ARG	CA	59.288	0.3	1
UNMAPPED	23	VAL	H	8.1	0.02	1
UNMAPPED	95	ILE	CA	66.141	0.3	1
UNMAPPED	21	LYS	CA	55.945	0.3	1
UNMAPPED	105	LYS	N	119.847	0.3	1
UNMAPPED	62	ARG	N	117.558	0.3	1
UNMAPPED	38	GLY	N	109.461	0.3	1
UNMAPPED	98	HIS	C	178.765	0.3	1
UNMAPPED	125	CYS	CA	59.782	0.3	1
UNMAPPED	10	TRP	CA	56.782	0.3	1
UNMAPPED	135	ALA	H	7.606	0.02	1
UNMAPPED	42	GLY	N	115.435	0.3	1
UNMAPPED	114	VAL	N	119.863	0.3	1
UNMAPPED	44	ALA	CA	52.487	0.3	1
UNMAPPED	49	MET	H	8.725	0.02	1
UNMAPPED	53	GLY	N	109.338	0.3	1
UNMAPPED	32	VAL	CB	32.337	0.3	1
UNMAPPED	119	ARG	H	7.281	0.02	1
UNMAPPED	141	ARG	C	175.532	0.3	1
UNMAPPED	109	PHE	C	176.684	0.3	1
UNMAPPED	71	GLN	N	114.537	0.3	1
UNMAPPED	99	THR	H	8.533	0.02	1
UNMAPPED	72	VAL	H	8.473	0.02	1
UNMAPPED	21	LYS	C	176.191	0.3	1
UNMAPPED	41	LEU	C	178.2	0.3	1
UNMAPPED	25	GLY	CA	44.668	0.3	1
UNMAPPED	91	VAL	H	9.294	0.02	1
UNMAPPED	26	VAL	C	175.915	0.3	1
UNMAPPED	129	TYR	N	120.434	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	97	GLN	CA	57.657	0.3	1
UNMAPPED	37	GLY	H	8.574	0.02	1
UNMAPPED	28	ALA	N	124.137	0.3	1
UNMAPPED	54	ASN	CB	41.138	0.3	1
UNMAPPED	16	PRO	C	176.861	0.3	1
UNMAPPED	101	THR	H	8.218	0.02	1
UNMAPPED	28	ALA	CB	19.081	0.3	1
UNMAPPED	58	ASP	C	179.107	0.3	1
UNMAPPED	117	MET	N	118.434	0.3	1
UNMAPPED	94	THR	CB	67.8	0.3	1
UNMAPPED	11	ASN	H	8.089	0.02	1
UNMAPPED	39	TYR	N	118.207	0.3	1
UNMAPPED	94	THR	N	118.242	0.3	1
UNMAPPED	137	TYR	N	119.895	0.3	1
UNMAPPED	5	GLY	N	109.025	0.3	1
UNMAPPED	59	ARG	H	8.042	0.02	1
UNMAPPED	93	ILE	N	119.174	0.3	1
UNMAPPED	81	SER	CB	63.8	0.3	1
UNMAPPED	18	THR	H	8.193	0.02	1
UNMAPPED	88	HIS	CB	29.223	0.3	1
UNMAPPED	121	VAL	C	177.613	0.3	1
UNMAPPED	40	MET	CB	33.899	0.3	1
UNMAPPED	101	THR	N	115.55	0.3	1
UNMAPPED	52	PHE	CB	40.389	0.3	1
UNMAPPED	101	THR	CB	68.838	0.3	1
UNMAPPED	122	GLU	C	177.535	0.3	1
UNMAPPED	72	VAL	C	174.158	0.3	1
UNMAPPED	85	ASN	CB	37.74	0.3	1
UNMAPPED	133	SER	CB	62.243	0.3	1
UNMAPPED	20	LEU	H	8.283	0.02	1
UNMAPPED	71	GLN	C	174.996	0.3	1
UNMAPPED	60	TYR	N	121.007	0.3	1
UNMAPPED	103	THR	CA	65.039	0.3	1
UNMAPPED	3	GLY	C	174.792	0.3	1
UNMAPPED	60	TYR	CB	37.832	0.3	1
UNMAPPED	33	VAL	C	176.671	0.3	1
UNMAPPED	127	THR	C	176.763	0.3	1
UNMAPPED	82	ASN	C	173.98	0.3	1
UNMAPPED	98	HIS	CA	59.422	0.3	1
UNMAPPED	92	ASN	H	7.598	0.02	1
UNMAPPED	125	CYS	C	176.946	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	13	PRO	C	176.959	0.3	1
UNMAPPED	22	HIS	CB	30.388	0.3	1
UNMAPPED	65	MET	N	118.618	0.3	1
UNMAPPED	22	HIS	N	121.143	0.3	1
UNMAPPED	64	ASN	CB	40.785	0.3	1
UNMAPPED	71	GLN	CA	53.726	0.3	1
UNMAPPED	68	TYR	N	121.716	0.3	1
UNMAPPED	3	GLY	CA	44.76	0.3	1
UNMAPPED	113	ASP	CA	57.607	0.3	1
UNMAPPED	1	GLY	N	111.231	0.3	1
UNMAPPED	130	GLN	H	8.255	0.02	1
UNMAPPED	68	TYR	CB	34.372	0.3	1
UNMAPPED	105	LYS	H	7.465	0.02	1
UNMAPPED	104	THR	CA	64.415	0.3	1
UNMAPPED	23	VAL	CB	32.382	0.3	1
UNMAPPED	45	MET	H	8.804	0.02	1
UNMAPPED	107	GLU	CB	30.802	0.3	1
UNMAPPED	93	ILE	C	177.925	0.3	1
UNMAPPED	73	TYR	CA	56.666	0.3	1
UNMAPPED	107	GLU	N	120.448	0.3	1
UNMAPPED	135	ALA	CB	18.051	0.3	1

7.7.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, <i>ppm</i>	Suggested action
$^{13}\text{C}_\alpha$	136	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	118	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	131	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	127	0.00 \pm 0.00	None needed (< 0.5 ppm)

7.7.3 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 1596. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/665 (0%)	0/265 (0%)	0/270 (0%)	0/130 (0%)

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	Total	¹H	¹³C	¹⁵N
Sidechain	0/815 (0%)	0/473 (0%)	0/315 (0%)	0/27 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1596 (0%)	0/798 (0%)	0/629 (0%)	0/169 (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 1685. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/698 (0%)	0/278 (0%)	0/284 (0%)	0/136 (0%)
Sidechain	0/871 (0%)	0/507 (0%)	0/335 (0%)	0/29 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1685 (0%)	0/845 (0%)	0/663 (0%)	0/177 (0%)

7.7.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.

7.8 Chemical shift list 8

File name: BMRB entry 16080

Chemical shift list name: *assigned_chem_shift_list_1*

7.8.1 Bookkeeping [i](#)

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	526
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	526
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 526 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	36	LEU	H	8.245	0.02	1
UNMAPPED	51	HIS	C	175.286	0.3	1
UNMAPPED	83	GLN	N	120.325	0.3	1
UNMAPPED	16	PRO	CA	62.582	0.3	1
UNMAPPED	72	VAL	N	113.013	0.3	1
UNMAPPED	55	ASP	C	177.89	0.3	1
UNMAPPED	130	GLN	C	178.558	0.3	1
UNMAPPED	29	ALA	H	8.257	0.02	1
UNMAPPED	75	ARG	H	7.947	0.02	1
UNMAPPED	3	GLY	H	8.6	0.02	1
UNMAPPED	2	GLN	H	8.365	0.02	1
UNMAPPED	48	PRO	CA	61.962	0.3	1
UNMAPPED	42	GLY	C	172.825	0.3	1
UNMAPPED	105	LYS	CA	55.813	0.3	1
UNMAPPED	51	HIS	CA	54.382	0.3	1
UNMAPPED	38	GLY	CA	44.764	0.3	1
UNMAPPED	37	GLY	N	110.174	0.3	1
UNMAPPED	142	SER	H	8.012	0.02	1
UNMAPPED	84	ASN	CA	56.12	0.3	1
UNMAPPED	47	ARG	C	174.633	0.3	1
UNMAPPED	130	GLN	CA	58.773	0.3	1
UNMAPPED	25	GLY	H	8.432	0.02	1
UNMAPPED	108	ASN	N	119.633	0.3	1
UNMAPPED	100	VAL	N	123.511	0.3	1
UNMAPPED	5	GLY	H	8.381	0.02	1
UNMAPPED	54	ASN	C	174.343	0.3	1
UNMAPPED	129	TYR	C	178.191	0.3	1
UNMAPPED	112	THR	C	175.668	0.3	1
UNMAPPED	46	SER	CA	58.28	0.3	1
UNMAPPED	105	LYS	C	176.708	0.3	1
UNMAPPED	134	GLN	C	177.17	0.3	1
UNMAPPED	88	HIS	H	8.377	0.02	1
UNMAPPED	94	THR	C	177.694	0.3	1
UNMAPPED	19	ASN	N	121.547	0.3	1
UNMAPPED	132	GLU	H	8.442	0.02	1
UNMAPPED	40	MET	H	9.135	0.02	1
UNMAPPED	85	ASN	H	8.592	0.02	1
UNMAPPED	36	LEU	C	177.943	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	133	SER	H	8.43	0.02	1
UNMAPPED	104	THR	C	175.168	0.3	1
UNMAPPED	54	ASN	CA	52.164	0.3	1
UNMAPPED	113	ASP	C	177.615	0.3	1
UNMAPPED	66	TYR	C	175.875	0.3	1
UNMAPPED	60	TYR	H	8.266	0.02	1
UNMAPPED	94	THR	CA	68.206	0.3	1
UNMAPPED	92	ASN	N	116.537	0.3	1
UNMAPPED	102	THR	H	8.056	0.02	1
UNMAPPED	118	GLU	N	119.115	0.3	1
UNMAPPED	74	TYR	N	111.261	0.3	1
UNMAPPED	6	THR	N	113.642	0.3	1
UNMAPPED	101	THR	C	176.76	0.3	1
UNMAPPED	31	ALA	H	8.088	0.02	1
UNMAPPED	52	PHE	C	177.105	0.3	1
UNMAPPED	70	ASN	N	116.481	0.3	1
UNMAPPED	64	ASN	H	7.565	0.02	1
UNMAPPED	44	ALA	C	177.509	0.3	1
UNMAPPED	131	LYS	H	7.87	0.02	1
UNMAPPED	50	ILE	N	124.629	0.3	1
UNMAPPED	120	VAL	N	119.299	0.3	1
UNMAPPED	63	GLU	C	177.615	0.3	1
UNMAPPED	26	ALA	H	8.163	0.02	1
UNMAPPED	22	ILE	C	176.058	0.3	1
UNMAPPED	40	MET	C	172.943	0.3	1
UNMAPPED	21	ILE	H	8.211	0.02	1
UNMAPPED	24	ALA	C	178.1	0.3	1
UNMAPPED	116	MET	C	178.204	0.3	1
UNMAPPED	107	GLU	C	174.893	0.3	1
UNMAPPED	36	LEU	N	121.968	0.3	1
UNMAPPED	132	GLU	C	179.278	0.3	1
UNMAPPED	39	TYR	H	7.888	0.02	1
UNMAPPED	127	THR	CA	66.677	0.3	1
UNMAPPED	66	TYR	H	7.598	0.02	1
UNMAPPED	136	TYR	C	177.227	0.3	1
UNMAPPED	63	GLU	CA	57.477	0.3	1
UNMAPPED	3	GLY	N	110.726	0.3	1
UNMAPPED	22	ILE	CA	60.222	0.3	1
UNMAPPED	75	ARG	N	120.845	0.3	1
UNMAPPED	59	ARG	N	119.965	0.3	1
UNMAPPED	106	GLY	N	108.075	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	34	GLY	C	174.723	0.3	1
UNMAPPED	114	VAL	C	177.419	0.3	1
UNMAPPED	2	GLN	N	120.215	0.3	1
UNMAPPED	27	ALA	H	8.328	0.02	1
UNMAPPED	139	GLY	H	7.859	0.02	1
UNMAPPED	95	ILE	H	8.48	0.02	1
UNMAPPED	121	VAL	CA	65.986	0.3	1
UNMAPPED	115	LYS	N	119.263	0.3	1
UNMAPPED	86	PHE	C	177.496	0.3	1
UNMAPPED	12	LYS	H	8.026	0.02	1
UNMAPPED	27	ALA	N	123.362	0.3	1
UNMAPPED	103	THR	C	178.045	0.3	1
UNMAPPED	41	LEU	H	8.067	0.02	1
UNMAPPED	128	GLN	CA	58.315	0.3	1
UNMAPPED	124	MET	CA	59.538	0.3	1
UNMAPPED	19	ASN	H	8.549	0.02	1
UNMAPPED	65	MET	H	7.894	0.02	1
UNMAPPED	107	GLU	H	7.454	0.02	1
UNMAPPED	116	MET	N	118.641	0.3	1
UNMAPPED	50	ILE	CA	58.778	0.3	1
UNMAPPED	47	ARG	N	127.075	0.3	1
UNMAPPED	124	MET	N	119.653	0.3	1
UNMAPPED	24	ALA	H	8.494	0.02	1
UNMAPPED	27	ALA	CA	52.103	0.3	1
UNMAPPED	121	VAL	H	9.171	0.02	1
UNMAPPED	95	ILE	N	121.308	0.3	1
UNMAPPED	39	TYR	C	175.731	0.3	1
UNMAPPED	84	ASN	N	117.359	0.3	1
UNMAPPED	118	GLU	H	8.586	0.02	1
UNMAPPED	74	TYR	H	8.521	0.02	1
UNMAPPED	12	LYS	CA	53.844	0.3	1
UNMAPPED	59	ARG	C	177.572	0.3	1
UNMAPPED	123	GLN	N	115.472	0.3	1
UNMAPPED	102	THR	N	114.886	0.3	1
UNMAPPED	32	VAL	N	119.863	0.3	1
UNMAPPED	31	ALA	N	123.814	0.3	1
UNMAPPED	122	GLU	H	8.012	0.02	1
UNMAPPED	131	LYS	N	119.637	0.3	1
UNMAPPED	136	TYR	CA	59.59	0.3	1
UNMAPPED	109	PHE	CA	56.077	0.3	1
UNMAPPED	33	VAL	H	8.317	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	120	VAL	H	8.275	0.02	1
UNMAPPED	46	SER	C	174.422	0.3	1
UNMAPPED	125	CYS	H	9.237	0.02	1
UNMAPPED	26	ALA	N	124.083	0.3	1
UNMAPPED	42	GLY	CA	44.525	0.3	1
UNMAPPED	6	THR	CA	61.612	0.3	1
UNMAPPED	49	MET	CA	53.694	0.3	1
UNMAPPED	30	GLY	H	8.324	0.02	1
UNMAPPED	68	TYR	C	172.781	0.3	1
UNMAPPED	110	THR	C	175.469	0.3	1
UNMAPPED	70	ASN	CA	51.631	0.3	1
UNMAPPED	58	ASP	CA	58.197	0.3	1
UNMAPPED	66	TYR	N	116.817	0.3	1
UNMAPPED	99	THR	CA	66.433	0.3	1
UNMAPPED	23	VAL	C	175.639	0.3	1
UNMAPPED	17	LYS	H	8.571	0.02	1
UNMAPPED	106	GLY	H	7.92	0.02	1
UNMAPPED	8	ASN	CA	52.755	0.3	1
UNMAPPED	91	VAL	CA	65.783	0.3	1
UNMAPPED	127	THR	H	8.129	0.02	1
UNMAPPED	85	ASN	N	118.472	0.3	1
UNMAPPED	49	MET	C	175.027	0.3	1
UNMAPPED	57	GLU	CA	59.624	0.3	1
UNMAPPED	137	TYR	H	8.057	0.02	1
UNMAPPED	99	THR	C	176.503	0.3	1
UNMAPPED	36	LEU	CA	54.472	0.3	1
UNMAPPED	11	ASN	CA	52.42	0.3	1
UNMAPPED	34	GLY	N	113.641	0.3	1
UNMAPPED	133	SER	CA	60.785	0.3	1
UNMAPPED	4	GLY	H	8.377	0.02	1
UNMAPPED	140	ARG	H	7.837	0.02	1
UNMAPPED	37	GLY	C	174.801	0.3	1
UNMAPPED	57	GLU	C	177.707	0.3	1
UNMAPPED	137	TYR	C	176.955	0.3	1
UNMAPPED	110	THR	H	9.609	0.02	1
UNMAPPED	18	THR	C	173.951	0.3	1
UNMAPPED	13	PRO	CA	62.733	0.3	1
UNMAPPED	35	GLY	CA	44.924	0.3	1
UNMAPPED	9	GLN	CA	55.75	0.3	1
UNMAPPED	123	GLN	H	7.085	0.02	1
UNMAPPED	47	ARG	H	8.698	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	117	MET	CA	59.625	0.3	1
UNMAPPED	11	ASN	C	174.343	0.3	1
UNMAPPED	141	ARG	N	122.755	0.3	1
UNMAPPED	20	LEU	CA	54.821	0.3	1
UNMAPPED	87	VAL	C	176.673	0.3	1
UNMAPPED	112	THR	H	7.97	0.02	1
UNMAPPED	84	ASN	H	8.424	0.02	1
UNMAPPED	62	ARG	C	179.121	0.3	1
UNMAPPED	18	THR	N	115.559	0.3	1
UNMAPPED	14	SER	N	117.211	0.3	1
UNMAPPED	134	GLN	N	120.977	0.3	1
UNMAPPED	61	TYR	CA	62.727	0.3	1
UNMAPPED	73	TYR	C	174.71	0.3	1
UNMAPPED	46	SER	N	116.488	0.3	1
UNMAPPED	116	MET	CA	59.381	0.3	1
UNMAPPED	4	GLY	CA	44.899	0.3	1
UNMAPPED	27	ALA	C	177.694	0.3	1
UNMAPPED	53	GLY	C	173.283	0.3	1
UNMAPPED	113	ASP	H	7.536	0.02	1
UNMAPPED	20	LEU	C	176.791	0.3	1
UNMAPPED	132	GLU	CA	57.51	0.3	1
UNMAPPED	33	VAL	N	125.002	0.3	1
UNMAPPED	70	ASN	C	172.825	0.3	1
UNMAPPED	55	ASP	CA	57.477	0.3	1
UNMAPPED	35	GLY	H	8.299	0.02	1
UNMAPPED	90	CYS	CA	58.325	0.3	1
UNMAPPED	62	ARG	CA	59.611	0.3	1
UNMAPPED	92	ASN	C	178.466	0.3	1
UNMAPPED	96	LYS	C	179.032	0.3	1
UNMAPPED	125	CYS	N	119.708	0.3	1
UNMAPPED	56	TRP	H	8.561	0.02	1
UNMAPPED	114	VAL	CA	67.472	0.3	1
UNMAPPED	139	GLY	N	108.145	0.3	1
UNMAPPED	53	GLY	CA	45.375	0.3	1
UNMAPPED	44	ALA	N	125.79	0.3	1
UNMAPPED	86	PHE	CA	60.417	0.3	1
UNMAPPED	84	ASN	C	177.706	0.3	1
UNMAPPED	93	ILE	H	8.801	0.02	1
UNMAPPED	136	TYR	N	119.37	0.3	1
UNMAPPED	21	ILE	C	175.835	0.3	1
UNMAPPED	138	ASP	C	177.299	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	129	TYR	CA	61.615	0.3	1
UNMAPPED	55	ASP	H	9.032	0.02	1
UNMAPPED	89	ASP	H	7.438	0.02	1
UNMAPPED	24	ALA	N	128.919	0.3	1
UNMAPPED	38	GLY	H	8.413	0.02	1
UNMAPPED	126	VAL	N	123.896	0.3	1
UNMAPPED	50	ILE	C	173.11	0.3	1
UNMAPPED	67	ARG	H	7.519	0.02	1
UNMAPPED	35	GLY	C	174.356	0.3	1
UNMAPPED	29	ALA	C	178.27	0.3	1
UNMAPPED	9	GLN	C	175.757	0.3	1
UNMAPPED	114	VAL	H	8.265	0.02	1
UNMAPPED	18	THR	CA	61.142	0.3	1
UNMAPPED	53	GLY	H	8.944	0.02	1
UNMAPPED	96	LYS	H	8.148	0.02	1
UNMAPPED	39	TYR	CA	57.961	0.3	1
UNMAPPED	69	PRO	CA	63.143	0.3	1
UNMAPPED	51	HIS	H	8.112	0.02	1
UNMAPPED	5	GLY	CA	44.788	0.3	1
UNMAPPED	66	TYR	CA	58.877	0.3	1
UNMAPPED	46	SER	H	8.468	0.02	1
UNMAPPED	81	SER	CA	58.374	0.3	1
UNMAPPED	34	GLY	H	8.608	0.02	1
UNMAPPED	115	LYS	C	180.05	0.3	1
UNMAPPED	88	HIS	CA	59.56	0.3	1
UNMAPPED	122	GLU	N	120.948	0.3	1
UNMAPPED	142	SER	C	178.705	0.3	1
UNMAPPED	1	GLY	H	8.326	0.02	1
UNMAPPED	129	TYR	H	8.627	0.02	1
UNMAPPED	85	ASN	CA	55.721	0.3	1
UNMAPPED	52	PHE	CA	59.264	0.3	1
UNMAPPED	65	MET	C	176.385	0.3	1
UNMAPPED	45	MET	N	121.594	0.3	1
UNMAPPED	103	THR	N	118.598	0.3	1
UNMAPPED	60	TYR	CA	61.823	0.3	1
UNMAPPED	138	ASP	H	8.254	0.02	1
UNMAPPED	14	SER	H	8.48	0.02	1
UNMAPPED	90	CYS	C	177.524	0.3	1
UNMAPPED	88	HIS	C	177.602	0.3	1
UNMAPPED	30	GLY	N	108.202	0.3	1
UNMAPPED	85	ASN	C	177.338	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	25	GLY	N	108.976	0.3	1
UNMAPPED	118	GLU	C	178.741	0.3	1
UNMAPPED	65	MET	CA	58.773	0.3	1
UNMAPPED	64	ASN	CA	54.548	0.3	1
UNMAPPED	68	TYR	CA	52.319	0.3	1
UNMAPPED	139	GLY	CA	45.247	0.3	1
UNMAPPED	113	ASP	N	120.142	0.3	1
UNMAPPED	42	GLY	H	9.429	0.02	1
UNMAPPED	20	LEU	N	123.208	0.3	1
UNMAPPED	23	VAL	CA	61.617	0.3	1
UNMAPPED	104	THR	N	116.678	0.3	1
UNMAPPED	8	ASN	C	175.257	0.3	1
UNMAPPED	119	ARG	C	179.332	0.3	1
UNMAPPED	21	ILE	CA	60.543	0.3	1
UNMAPPED	14	SER	CA	57.7	0.3	1
UNMAPPED	44	ALA	H	8.753	0.02	1
UNMAPPED	135	ALA	CA	53.729	0.3	1
UNMAPPED	118	GLU	CA	60.357	0.3	1
UNMAPPED	83	GLN	CA	58.871	0.3	1
UNMAPPED	100	VAL	H	8.105	0.02	1
UNMAPPED	124	MET	H	8.135	0.02	1
UNMAPPED	22	ILE	H	8.325	0.02	1
UNMAPPED	63	GLU	H	7.926	0.02	1
UNMAPPED	26	ALA	C	177.707	0.3	1
UNMAPPED	55	ASP	N	123.496	0.3	1
UNMAPPED	95	ILE	C	178.848	0.3	1
UNMAPPED	90	CYS	N	119.188	0.3	1
UNMAPPED	137	TYR	CA	59.354	0.3	1
UNMAPPED	136	TYR	H	7.944	0.02	1
UNMAPPED	126	VAL	H	8.514	0.02	1
UNMAPPED	111	GLU	C	179.265	0.3	1
UNMAPPED	51	HIS	N	123.213	0.3	1
UNMAPPED	37	GLY	CA	45.842	0.3	1
UNMAPPED	123	GLN	C	179.199	0.3	1
UNMAPPED	89	ASP	N	118.34	0.3	1
UNMAPPED	67	ARG	N	119.171	0.3	1
UNMAPPED	112	THR	N	116.871	0.3	1
UNMAPPED	108	ASN	CA	52.431	0.3	1
UNMAPPED	130	GLN	N	119.877	0.3	1
UNMAPPED	117	MET	C	177.799	0.3	1
UNMAPPED	100	VAL	CA	66.052	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	106	GLY	C	174.252	0.3	1
UNMAPPED	96	LYS	N	123.72	0.3	1
UNMAPPED	128	GLN	H	8.731	0.02	1
UNMAPPED	12	LYS	C	178.782	0.3	1
UNMAPPED	19	ASN	CA	52.692	0.3	1
UNMAPPED	134	GLN	CA	57.73	0.3	1
UNMAPPED	126	VAL	CA	67.371	0.3	1
UNMAPPED	4	GLY	C	174.819	0.3	1
UNMAPPED	127	THR	N	118.365	0.3	1
UNMAPPED	54	ASN	N	114.504	0.3	1
UNMAPPED	57	GLU	H	8.13	0.02	1
UNMAPPED	100	VAL	C	178.558	0.3	1
UNMAPPED	45	MET	C	175.609	0.3	1
UNMAPPED	138	ASP	N	121.166	0.3	1
UNMAPPED	56	TRP	N	120.567	0.3	1
UNMAPPED	74	TYR	CA	55.529	0.3	1
UNMAPPED	92	ASN	CA	56.42	0.3	1
UNMAPPED	111	GLU	CA	59.718	0.3	1
UNMAPPED	141	ARG	H	8.252	0.02	1
UNMAPPED	119	ARG	CA	58.072	0.3	1
UNMAPPED	98	HIS	H	8.52	0.02	1
UNMAPPED	111	GLU	N	120.154	0.3	1
UNMAPPED	88	HIS	N	117.905	0.3	1
UNMAPPED	135	ALA	C	179.006	0.3	1
UNMAPPED	52	PHE	N	125.408	0.3	1
UNMAPPED	109	PHE	H	8.79	0.02	1
UNMAPPED	124	MET	C	178.558	0.3	1
UNMAPPED	122	GLU	CA	60.869	0.3	1
UNMAPPED	97	GLN	H	8.557	0.02	1
UNMAPPED	45	MET	CA	53.541	0.3	1
UNMAPPED	120	VAL	CA	65.358	0.3	1
UNMAPPED	74	TYR	C	173.584	0.3	1
UNMAPPED	117	MET	H	8.706	0.02	1
UNMAPPED	75	ARG	C	178.139	0.3	1
UNMAPPED	15	LYS	CA	53.825	0.3	1
UNMAPPED	91	VAL	C	177.236	0.3	1
UNMAPPED	73	TYR	H	8.477	0.02	1
UNMAPPED	91	VAL	N	125.178	0.3	1
UNMAPPED	30	GLY	CA	44.786	0.3	1
UNMAPPED	6	THR	H	8.168	0.02	1
UNMAPPED	61	TYR	H	9.031	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	41	LEU	N	121.426	0.3	1
UNMAPPED	110	THR	CA	60.014	0.3	1
UNMAPPED	70	ASN	H	8.649	0.02	1
UNMAPPED	63	GLU	N	116.103	0.3	1
UNMAPPED	40	MET	N	121.669	0.3	1
UNMAPPED	58	ASP	H	7.912	0.02	1
UNMAPPED	120	VAL	C	177.04	0.3	1
UNMAPPED	64	ASN	N	115.431	0.3	1
UNMAPPED	75	ARG	CA	53.14	0.3	1
UNMAPPED	101	THR	CA	65.155	0.3	1
UNMAPPED	17	LYS	CA	56.006	0.3	1
UNMAPPED	22	ILE	N	126.934	0.3	1
UNMAPPED	69	PRO	C	175.079	0.3	1
UNMAPPED	106	GLY	CA	45.138	0.3	1
UNMAPPED	56	TRP	C	179.134	0.3	1
UNMAPPED	2	GLN	CA	55.563	0.3	1
UNMAPPED	23	VAL	N	126.259	0.3	1
UNMAPPED	115	LYS	CA	58.779	0.3	1
UNMAPPED	121	VAL	N	121.577	0.3	1
UNMAPPED	110	THR	N	116.217	0.3	1
UNMAPPED	128	GLN	C	177.419	0.3	1
UNMAPPED	142	SER	CA	59.604	0.3	1
UNMAPPED	135	ALA	N	120.905	0.3	1
UNMAPPED	89	ASP	C	175.848	0.3	1
UNMAPPED	43	SER	N	113.994	0.3	1
UNMAPPED	133	SER	C	175.718	0.3	1
UNMAPPED	17	LYS	C	176.804	0.3	1
UNMAPPED	128	GLN	N	122.854	0.3	1
UNMAPPED	48	PRO	C	175.704	0.3	1
UNMAPPED	87	VAL	CA	67.332	0.3	1
UNMAPPED	97	GLN	C	178.665	0.3	1
UNMAPPED	71	GLN	H	7.298	0.02	1
UNMAPPED	140	ARG	CA	55.777	0.3	1
UNMAPPED	102	THR	C	177.154	0.3	1
UNMAPPED	61	TYR	C	177.013	0.3	1
UNMAPPED	47	ARG	CA	54.422	0.3	1
UNMAPPED	31	ALA	C	177.602	0.3	1
UNMAPPED	89	ASP	CA	56.779	0.3	1
UNMAPPED	9	GLN	H	8.374	0.02	1
UNMAPPED	123	GLN	CA	58.794	0.3	1
UNMAPPED	115	LYS	H	7.697	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	64	ASN	C	175.484	0.3	1
UNMAPPED	67	ARG	CA	55.971	0.3	1
UNMAPPED	112	THR	CA	66.536	0.3	1
UNMAPPED	12	LYS	N	122.752	0.3	1
UNMAPPED	10	TRP	N	121.222	0.3	1
UNMAPPED	133	SER	N	115.424	0.3	1
UNMAPPED	140	ARG	C	176.202	0.3	1
UNMAPPED	102	THR	CA	64.995	0.3	1
UNMAPPED	96	LYS	CA	59.859	0.3	1
UNMAPPED	32	VAL	CA	61.779	0.3	1
UNMAPPED	1	GLY	C	174.289	0.3	1
UNMAPPED	87	VAL	H	8.905	0.02	1
UNMAPPED	31	ALA	CA	51.963	0.3	1
UNMAPPED	14	SER	C	174.147	0.3	1
UNMAPPED	116	MET	H	8.183	0.02	1
UNMAPPED	83	GLN	C	176.905	0.3	1
UNMAPPED	131	LYS	CA	58.937	0.3	1
UNMAPPED	25	GLY	C	174.003	0.3	1
UNMAPPED	90	CYS	H	8.161	0.02	1
UNMAPPED	43	SER	C	174.961	0.3	1
UNMAPPED	62	ARG	H	7.891	0.02	1
UNMAPPED	109	PHE	N	121.985	0.3	1
UNMAPPED	82	ASN	CA	51.817	0.3	1
UNMAPPED	97	GLN	N	117.389	0.3	1
UNMAPPED	104	THR	H	7.83	0.02	1
UNMAPPED	26	ALA	CA	52.193	0.3	1
UNMAPPED	28	ALA	CA	52.051	0.3	1
UNMAPPED	138	ASP	CA	54.911	0.3	1
UNMAPPED	56	TRP	CA	61.44	0.3	1
UNMAPPED	2	GLN	C	176.725	0.3	1
UNMAPPED	49	MET	N	122.169	0.3	1
UNMAPPED	127	THR	C	176.739	0.3	1
UNMAPPED	119	ARG	N	116.993	0.3	1
UNMAPPED	32	VAL	H	8.16	0.02	1
UNMAPPED	58	ASP	N	119.055	0.3	1
UNMAPPED	108	ASN	C	173.571	0.3	1
UNMAPPED	93	ILE	CA	61.717	0.3	1
UNMAPPED	99	THR	N	115.469	0.3	1
UNMAPPED	40	MET	CA	53.268	0.3	1
UNMAPPED	5	GLY	C	174.513	0.3	1
UNMAPPED	10	TRP	C	175.875	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	19	ASN	C	174.697	0.3	1
UNMAPPED	15	LYS	N	124.493	0.3	1
UNMAPPED	54	ASN	H	7.259	0.02	1
UNMAPPED	57	GLU	N	120.805	0.3	1
UNMAPPED	28	ALA	H	8.228	0.02	1
UNMAPPED	43	SER	H	8.344	0.02	1
UNMAPPED	126	VAL	C	178.074	0.3	1
UNMAPPED	94	THR	H	8.169	0.02	1
UNMAPPED	29	ALA	N	123.469	0.3	1
UNMAPPED	83	GLN	H	8.66	0.02	1
UNMAPPED	41	LEU	CA	52.921	0.3	1
UNMAPPED	11	ASN	N	120.242	0.3	1
UNMAPPED	60	TYR	C	179.579	0.3	1
UNMAPPED	67	ARG	C	176.804	0.3	1
UNMAPPED	98	HIS	N	120.369	0.3	1
UNMAPPED	34	GLY	CA	45.003	0.3	1
UNMAPPED	38	GLY	C	173.95	0.3	1
UNMAPPED	17	LYS	N	122.432	0.3	1
UNMAPPED	32	VAL	C	176.398	0.3	1
UNMAPPED	50	ILE	H	6.584	0.02	1
UNMAPPED	139	GLY	C	174.422	0.3	1
UNMAPPED	52	PHE	H	10.372	0.02	1
UNMAPPED	9	GLN	N	120.456	0.3	1
UNMAPPED	1	GLY	CA	44.951	0.3	1
UNMAPPED	35	GLY	N	108.688	0.3	1
UNMAPPED	142	SER	N	122.998	0.3	1
UNMAPPED	111	GLU	H	9.209	0.02	1
UNMAPPED	131	LYS	C	179.788	0.3	1
UNMAPPED	10	TRP	H	8.087	0.02	1
UNMAPPED	73	TYR	N	121.826	0.3	1
UNMAPPED	43	SER	CA	58.2	0.3	1
UNMAPPED	108	ASN	H	8.564	0.02	1
UNMAPPED	87	VAL	N	120.616	0.3	1
UNMAPPED	28	ALA	C	177.629	0.3	1
UNMAPPED	61	TYR	N	120.755	0.3	1
UNMAPPED	72	VAL	CA	58.292	0.3	1
UNMAPPED	4	GLY	N	109.143	0.3	1
UNMAPPED	140	ARG	N	120.239	0.3	1
UNMAPPED	30	GLY	C	173.715	0.3	1
UNMAPPED	132	GLU	N	118.556	0.3	1
UNMAPPED	68	TYR	H	7.457	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	33	VAL	CA	62.141	0.3	1
UNMAPPED	59	ARG	CA	59.281	0.3	1
UNMAPPED	23	VAL	H	8.327	0.02	1
UNMAPPED	95	ILE	CA	66.138	0.3	1
UNMAPPED	105	LYS	N	119.804	0.3	1
UNMAPPED	62	ARG	N	117.555	0.3	1
UNMAPPED	38	GLY	N	109.541	0.3	1
UNMAPPED	98	HIS	C	178.741	0.3	1
UNMAPPED	125	CYS	CA	59.72	0.3	1
UNMAPPED	10	TRP	CA	56.788	0.3	1
UNMAPPED	135	ALA	H	7.606	0.02	1
UNMAPPED	42	GLY	N	115.478	0.3	1
UNMAPPED	114	VAL	N	119.91	0.3	1
UNMAPPED	44	ALA	CA	52.567	0.3	1
UNMAPPED	49	MET	H	8.723	0.02	1
UNMAPPED	53	GLY	N	109.344	0.3	1
UNMAPPED	141	ARG	CA	55.502	0.3	1
UNMAPPED	119	ARG	H	7.283	0.02	1
UNMAPPED	141	ARG	C	175.508	0.3	1
UNMAPPED	109	PHE	C	176.673	0.3	1
UNMAPPED	71	GLN	N	114.509	0.3	1
UNMAPPED	99	THR	H	8.537	0.02	1
UNMAPPED	72	VAL	H	8.483	0.02	1
UNMAPPED	41	LEU	C	178.191	0.3	1
UNMAPPED	25	GLY	CA	44.827	0.3	1
UNMAPPED	91	VAL	H	9.301	0.02	1
UNMAPPED	129	TYR	N	120.421	0.3	1
UNMAPPED	97	GLN	CA	57.706	0.3	1
UNMAPPED	24	ALA	CA	52.297	0.3	1
UNMAPPED	37	GLY	H	8.579	0.02	1
UNMAPPED	28	ALA	N	123.536	0.3	1
UNMAPPED	103	THR	H	8.286	0.02	1
UNMAPPED	16	PRO	C	176.824	0.3	1
UNMAPPED	101	THR	H	8.218	0.02	1
UNMAPPED	15	LYS	H	8.369	0.02	1
UNMAPPED	58	ASP	C	179.056	0.3	1
UNMAPPED	117	MET	N	118.427	0.3	1
UNMAPPED	11	ASN	H	8.081	0.02	1
UNMAPPED	39	TYR	N	118.246	0.3	1
UNMAPPED	94	THR	N	118.234	0.3	1
UNMAPPED	137	TYR	N	119.874	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	GLY	N	109.089	0.3	1
UNMAPPED	59	ARG	H	8.039	0.02	1
UNMAPPED	93	ILE	N	119.168	0.3	1
UNMAPPED	18	THR	H	8.173	0.02	1
UNMAPPED	134	GLN	H	7.606	0.02	1
UNMAPPED	121	VAL	C	177.615	0.3	1
UNMAPPED	101	THR	N	115.538	0.3	1
UNMAPPED	107	GLU	CA	55.179	0.3	1
UNMAPPED	122	GLU	C	177.524	0.3	1
UNMAPPED	72	VAL	C	174.147	0.3	1
UNMAPPED	20	LEU	H	8.216	0.02	1
UNMAPPED	71	GLN	C	174.988	0.3	1
UNMAPPED	60	TYR	N	121.039	0.3	1
UNMAPPED	103	THR	CA	65.154	0.3	1
UNMAPPED	3	GLY	C	174.788	0.3	1
UNMAPPED	33	VAL	C	176.673	0.3	1
UNMAPPED	29	ALA	CA	52.342	0.3	1
UNMAPPED	82	ASN	C	173.99	0.3	1
UNMAPPED	98	HIS	CA	59.49	0.3	1
UNMAPPED	92	ASN	H	7.6	0.02	1
UNMAPPED	15	LYS	C	174.462	0.3	1
UNMAPPED	125	CYS	C	176.922	0.3	1
UNMAPPED	13	PRO	C	176.97	0.3	1
UNMAPPED	65	MET	N	118.624	0.3	1
UNMAPPED	71	GLN	CA	53.803	0.3	1
UNMAPPED	68	TYR	N	121.712	0.3	1
UNMAPPED	3	GLY	CA	45.024	0.3	1
UNMAPPED	113	ASP	CA	57.613	0.3	1
UNMAPPED	1	GLY	N	109.177	0.3	1
UNMAPPED	130	GLN	H	8.258	0.02	1
UNMAPPED	105	LYS	H	7.463	0.02	1
UNMAPPED	104	THR	CA	64.488	0.3	1
UNMAPPED	45	MET	H	8.804	0.02	1
UNMAPPED	93	ILE	C	177.903	0.3	1
UNMAPPED	21	ILE	N	123.3	0.3	1
UNMAPPED	73	TYR	CA	56.716	0.3	1
UNMAPPED	107	GLU	N	120.417	0.3	1

7.8.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	136	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	134	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	128	0.00 \pm 0.00	None needed (< 0.5 ppm)

7.8.3 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 1596. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/665 (0%)	0/265 (0%)	0/270 (0%)	0/130 (0%)
Sidechain	0/815 (0%)	0/473 (0%)	0/315 (0%)	0/27 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1596 (0%)	0/798 (0%)	0/629 (0%)	0/169 (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 1685. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/698 (0%)	0/278 (0%)	0/284 (0%)	0/136 (0%)
Sidechain	0/871 (0%)	0/507 (0%)	0/335 (0%)	0/29 (0%)
Aromatic	0/116 (0%)	0/60 (0%)	0/44 (0%)	0/12 (0%)
Overall	0/1685 (0%)	0/845 (0%)	0/663 (0%)	0/177 (0%)

7.8.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.