



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:56 pm GMT

PDB ID : 1ND9
Title : Solution Structure of the N-terminal Subdomain of Translation Initiation Factor IF2
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Deposited on : 2002-12-09

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

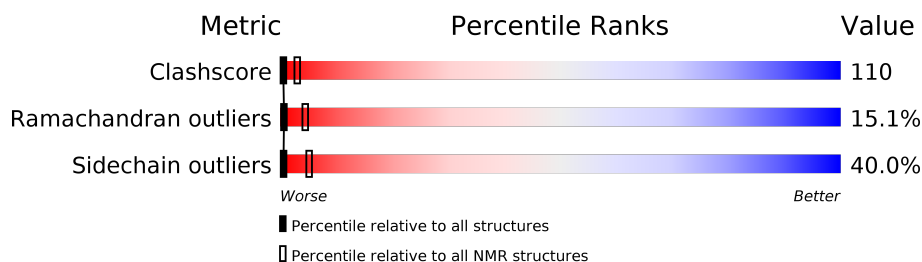
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

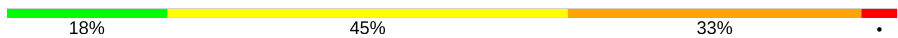
The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	49	

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models).

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:2-A:50 (49)	0.41	3

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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 7
2	5, 8
3	6, 9
Single-model clusters	10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 761 atoms, of which 382 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translation initiation factor IF-2.

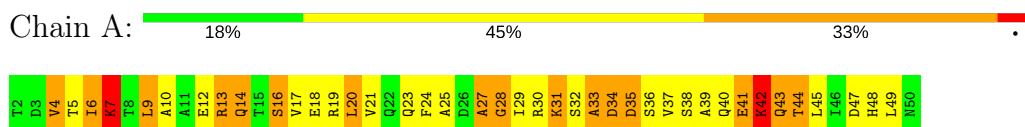
Mol	Chain	Residues	Atoms					Trace
1	A	49	Total	C	H	N	O	0
			761	229	382	69	81	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Translation initiation factor IF-2

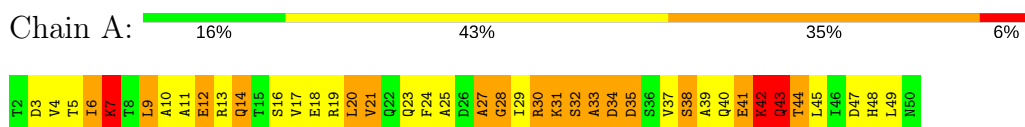


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

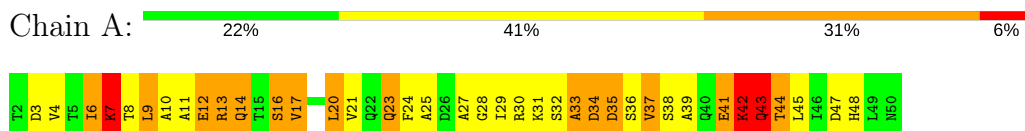
4.2.1 Score per residue for model 1

- Molecule 1: Translation initiation factor IF-2



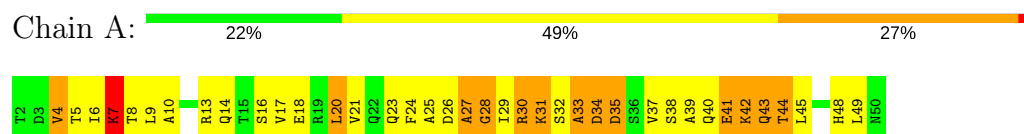
4.2.2 Score per residue for model 2

- Molecule 1: Translation initiation factor IF-2



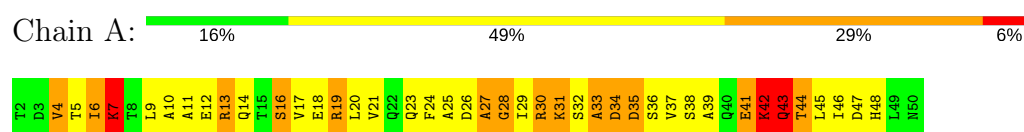
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Translation initiation factor IF-2



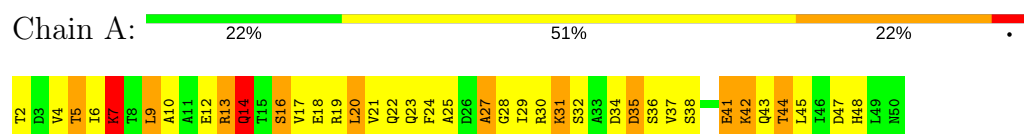
4.2.4 Score per residue for model 4

- Molecule 1: Translation initiation factor IF-2



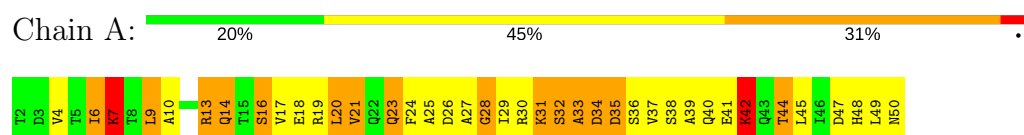
4.2.5 Score per residue for model 5

- Molecule 1: Translation initiation factor IF-2



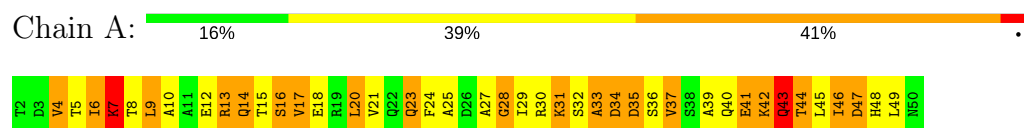
4.2.6 Score per residue for model 6

- Molecule 1: Translation initiation factor IF-2



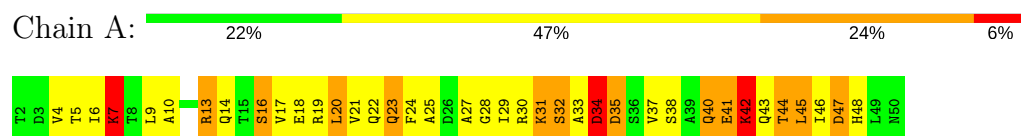
4.2.7 Score per residue for model 7

- Molecule 1: Translation initiation factor IF-2



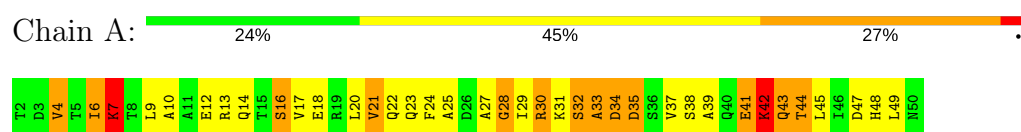
4.2.8 Score per residue for model 8

- Molecule 1: Translation initiation factor IF-2



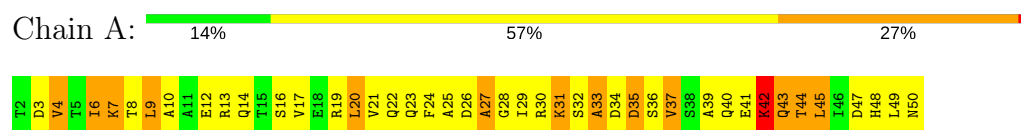
4.2.9 Score per residue for model 9

- Molecule 1: Translation initiation factor IF-2



4.2.10 Score per residue for model 10

- Molecule 1: Translation initiation factor IF-2



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with favorable non-bond energy, structures with the least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 5624
Number of chemical shift lists	1
Total number of shifts	1234
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1234
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	379	382	378	84±5
All	All	3790	3820	3780	835

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 110.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:GLU:O	1:A:21:VAL:HG22	1.05	1.50	7	1
1:A:27:ALA:HB2	1:A:48:HIS:CE1	1.01	1.91	10	10
1:A:21:VAL:HG22	1:A:37:VAL:HG23	0.93	1.40	6	3
1:A:41:GLU:O	1:A:43:GLN:N	0.92	2.03	2	9
1:A:9:LEU:HD21	1:A:39:ALA:HB2	0.91	1.39	4	3
1:A:6:ILE:HD13	1:A:7:LYS:N	0.89	1.82	9	3
1:A:18:GLU:O	1:A:21:VAL:HG12	0.89	1.67	5	3
1:A:21:VAL:HG13	1:A:37:VAL:HG21	0.89	1.45	2	3
1:A:6:ILE:HD13	1:A:21:VAL:HG21	0.85	1.44	10	3
1:A:13:ARG:HB2	1:A:17:VAL:HG12	0.84	1.49	8	10
1:A:21:VAL:HG22	1:A:37:VAL:CG2	0.84	2.01	9	3
1:A:21:VAL:HG12	1:A:37:VAL:HG11	0.84	1.48	7	1
1:A:6:ILE:CG1	1:A:21:VAL:HG21	0.83	2.01	9	3
1:A:27:ALA:HB2	1:A:48:HIS:NE2	0.81	1.90	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PHE:CZ	1:A:44:THR:HB	0.81	2.10	6	5
1:A:17:VAL:O	1:A:20:LEU:HG	0.80	1.75	8	7
1:A:20:LEU:HD12	1:A:21:VAL:N	0.80	1.90	10	7
1:A:28:GLY:O	1:A:29:ILE:HD13	0.80	1.77	4	4
1:A:20:LEU:HD21	1:A:38:SER:O	0.79	1.77	1	6
1:A:9:LEU:HD11	1:A:39:ALA:HB2	0.77	1.54	1	2
1:A:17:VAL:HA	1:A:20:LEU:HD23	0.76	1.54	2	7
1:A:6:ILE:HB	1:A:37:VAL:HB	0.75	1.58	4	7
1:A:21:VAL:HG13	1:A:32:SER:CB	0.74	2.11	4	2
1:A:10:ALA:HB1	1:A:18:GLU:CG	0.74	2.12	4	4
1:A:20:LEU:HD12	1:A:20:LEU:C	0.74	2.04	2	3
1:A:21:VAL:CG1	1:A:37:VAL:HG11	0.74	2.12	7	1
1:A:20:LEU:C	1:A:20:LEU:HD12	0.73	2.03	8	4
1:A:17:VAL:O	1:A:21:VAL:HG23	0.73	1.84	2	5
1:A:28:GLY:C	1:A:29:ILE:HD12	0.73	2.04	7	2
1:A:10:ALA:HB1	1:A:18:GLU:CB	0.72	2.14	4	6
1:A:49:LEU:HD23	1:A:50:ASN:N	0.72	2.00	10	1
1:A:21:VAL:HG12	1:A:31:LYS:C	0.71	2.06	10	3
1:A:6:ILE:HG13	1:A:21:VAL:HG21	0.71	1.61	9	4
1:A:24:PHE:CZ	1:A:44:THR:CB	0.71	2.74	6	5
1:A:21:VAL:HG13	1:A:37:VAL:CG2	0.71	2.16	10	2
1:A:21:VAL:HG13	1:A:32:SER:HB3	0.71	1.61	4	2
1:A:20:LEU:O	1:A:24:PHE:HB2	0.71	1.86	9	10
1:A:17:VAL:HA	1:A:20:LEU:CD2	0.70	2.15	6	7
1:A:19:ARG:HB3	1:A:45:LEU:HD11	0.70	1.62	8	1
1:A:4:VAL:O	1:A:37:VAL:O	0.70	2.10	10	5
1:A:6:ILE:HD13	1:A:21:VAL:CG2	0.70	2.17	10	3
1:A:17:VAL:HA	1:A:20:LEU:CD1	0.70	2.16	7	3
1:A:17:VAL:HA	1:A:20:LEU:HD12	0.69	1.63	4	2
1:A:10:ALA:HB1	1:A:18:GLU:HG3	0.69	1.64	3	4
1:A:6:ILE:HD12	1:A:10:ALA:HB2	0.68	1.65	7	2
1:A:17:VAL:HA	1:A:20:LEU:HG	0.68	1.65	9	4
1:A:21:VAL:HG12	1:A:37:VAL:CG1	0.68	2.18	7	1
1:A:6:ILE:CD1	1:A:21:VAL:HG21	0.67	2.19	2	3
1:A:20:LEU:HD22	1:A:41:GLU:HB2	0.67	1.66	2	2
1:A:21:VAL:HB	1:A:37:VAL:HG23	0.67	1.64	4	2
1:A:18:GLU:O	1:A:21:VAL:HG23	0.67	1.89	9	2
1:A:20:LEU:HD22	1:A:41:GLU:H	0.67	1.49	2	1
1:A:9:LEU:HD22	1:A:17:VAL:HG11	0.67	1.65	1	2
1:A:17:VAL:HA	1:A:20:LEU:CG	0.66	2.20	9	10
1:A:45:LEU:O	1:A:49:LEU:HD13	0.66	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ILE:HG12	1:A:21:VAL:HG21	0.66	1.66	6	3
1:A:16:SER:O	1:A:20:LEU:HG	0.66	1.90	9	3
1:A:29:ILE:HG22	1:A:30:ARG:H	0.65	1.52	9	7
1:A:20:LEU:HD13	1:A:41:GLU:HB3	0.65	1.68	1	2
1:A:10:ALA:HB1	1:A:18:GLU:HA	0.65	1.68	8	1
1:A:21:VAL:HG22	1:A:37:VAL:HG11	0.65	1.67	2	3
1:A:6:ILE:HG13	1:A:21:VAL:HG11	0.65	1.68	4	2
1:A:21:VAL:HG11	1:A:32:SER:O	0.64	1.92	8	1
1:A:37:VAL:HG22	1:A:38:SER:N	0.64	2.07	3	5
1:A:20:LEU:O	1:A:24:PHE:CD1	0.64	2.50	6	4
1:A:31:LYS:HA	1:A:37:VAL:HG22	0.64	1.70	5	2
1:A:25:ALA:HB2	1:A:31:LYS:HA	0.64	1.69	4	4
1:A:10:ALA:HB1	1:A:18:GLU:HB2	0.64	1.70	9	5
1:A:21:VAL:CB	1:A:37:VAL:HG21	0.64	2.23	7	1
1:A:24:PHE:HE2	1:A:41:GLU:O	0.64	1.76	1	2
1:A:6:ILE:CB	1:A:37:VAL:HB	0.63	2.22	4	6
1:A:21:VAL:HG22	1:A:31:LYS:C	0.62	2.14	4	1
1:A:7:LYS:HA	1:A:10:ALA:HB3	0.62	1.72	6	6
1:A:9:LEU:HD12	1:A:17:VAL:HG11	0.62	1.72	10	3
1:A:21:VAL:CG2	1:A:37:VAL:HG23	0.62	2.24	1	2
1:A:4:VAL:HB	1:A:9:LEU:HD22	0.61	1.70	4	4
1:A:20:LEU:HD21	1:A:42:LYS:HA	0.61	1.70	4	1
1:A:44:THR:O	1:A:47:ASP:N	0.61	2.34	5	5
1:A:30:ARG:CB	1:A:36:SER:O	0.61	2.49	2	5
1:A:24:PHE:CD2	1:A:29:ILE:HD13	0.61	2.30	8	2
1:A:13:ARG:CB	1:A:17:VAL:HG12	0.61	2.25	8	6
1:A:21:VAL:HG12	1:A:37:VAL:HG21	0.60	1.72	7	1
1:A:30:ARG:O	1:A:37:VAL:HG22	0.60	1.97	8	2
1:A:6:ILE:HD13	1:A:37:VAL:HG21	0.60	1.74	3	1
1:A:6:ILE:HD12	1:A:7:LYS:N	0.60	2.12	10	3
1:A:6:ILE:N	1:A:37:VAL:HG12	0.60	2.12	6	5
1:A:44:THR:O	1:A:47:ASP:CB	0.60	2.50	5	5
1:A:45:LEU:HA	1:A:48:HIS:CE1	0.59	2.33	10	1
1:A:21:VAL:HG12	1:A:30:ARG:O	0.59	1.96	1	1
1:A:9:LEU:HB3	1:A:17:VAL:HG21	0.59	1.73	2	1
1:A:6:ILE:HG22	1:A:35:ASP:N	0.58	2.13	4	5
1:A:24:PHE:CE2	1:A:41:GLU:O	0.58	2.56	1	4
1:A:4:VAL:CG1	1:A:9:LEU:HD23	0.58	2.28	2	2
1:A:27:ALA:HB2	1:A:48:HIS:ND1	0.58	2.13	10	1
1:A:29:ILE:N	1:A:29:ILE:HD12	0.58	2.13	9	3
1:A:23:GLN:O	1:A:48:HIS:NE2	0.58	2.36	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ILE:CG2	1:A:37:VAL:HB	0.58	2.29	8	2
1:A:30:ARG:C	1:A:37:VAL:HG23	0.58	2.19	2	2
1:A:23:GLN:CG	1:A:45:LEU:HD13	0.58	2.29	10	1
1:A:30:ARG:O	1:A:37:VAL:HG13	0.58	1.99	5	2
1:A:44:THR:OG1	1:A:48:HIS:CE1	0.58	2.57	1	3
1:A:4:VAL:HG11	1:A:9:LEU:HD23	0.58	1.76	2	2
1:A:29:ILE:HG21	1:A:38:SER:HB2	0.57	1.74	9	3
1:A:28:GLY:C	1:A:29:ILE:HD13	0.57	2.18	6	3
1:A:21:VAL:CG1	1:A:37:VAL:HG21	0.57	2.25	2	2
1:A:28:GLY:N	1:A:29:ILE:HD12	0.57	2.13	9	1
1:A:20:LEU:HD13	1:A:42:LYS:N	0.57	2.14	7	3
1:A:18:GLU:O	1:A:21:VAL:CG1	0.57	2.51	3	2
1:A:27:ALA:HB2	1:A:48:HIS:HE2	0.57	1.58	2	2
1:A:37:VAL:HG12	1:A:38:SER:N	0.57	2.14	5	2
1:A:31:LYS:CA	1:A:37:VAL:HG22	0.57	2.30	8	2
1:A:6:ILE:CG1	1:A:21:VAL:HG11	0.57	2.29	10	3
1:A:6:ILE:HD13	1:A:37:VAL:CG2	0.57	2.30	3	1
1:A:6:ILE:CG1	1:A:37:VAL:HB	0.57	2.30	8	1
1:A:21:VAL:HG11	1:A:32:SER:HA	0.57	1.77	2	1
1:A:6:ILE:HG12	1:A:32:SER:HA	0.57	1.77	2	2
1:A:6:ILE:HD12	1:A:7:LYS:H	0.57	1.59	10	3
1:A:32:SER:O	1:A:33:ALA:HB3	0.56	2.00	10	8
1:A:37:VAL:HG13	1:A:38:SER:N	0.56	2.15	2	1
1:A:6:ILE:O	1:A:7:LYS:CB	0.56	2.53	9	10
1:A:19:ARG:CB	1:A:45:LEU:HD11	0.56	2.30	8	1
1:A:17:VAL:HG22	1:A:37:VAL:HG21	0.56	1.77	9	2
1:A:24:PHE:CD2	1:A:44:THR:OG1	0.56	2.58	4	2
1:A:28:GLY:H	1:A:29:ILE:HD12	0.56	1.61	9	1
1:A:6:ILE:C	1:A:6:ILE:HD12	0.56	2.21	8	1
1:A:21:VAL:HG23	1:A:32:SER:HB3	0.56	1.76	7	1
1:A:17:VAL:CA	1:A:20:LEU:HG	0.56	2.31	9	2
1:A:29:ILE:CG2	1:A:30:ARG:N	0.56	2.69	10	2
1:A:24:PHE:CG	1:A:29:ILE:HD12	0.56	2.36	2	1
1:A:6:ILE:HG23	1:A:35:ASP:N	0.55	2.15	2	3
1:A:24:PHE:CZ	1:A:41:GLU:O	0.55	2.59	6	4
1:A:17:VAL:CG2	1:A:37:VAL:HG21	0.55	2.32	6	3
1:A:24:PHE:CE1	1:A:44:THR:HB	0.55	2.37	10	1
1:A:21:VAL:HG23	1:A:32:SER:CB	0.55	2.32	7	1
1:A:27:ALA:HB3	1:A:29:ILE:CD1	0.55	2.32	9	2
1:A:23:GLN:HB3	1:A:48:HIS:CD2	0.55	2.36	9	4
1:A:6:ILE:HG12	1:A:21:VAL:HG11	0.55	1.76	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PHE:CZ	1:A:45:LEU:N	0.54	2.76	10	5
1:A:29:ILE:HG22	1:A:30:ARG:N	0.54	2.17	7	3
1:A:24:PHE:HA	1:A:27:ALA:CB	0.54	2.31	8	6
1:A:6:ILE:CD1	1:A:7:LYS:N	0.54	2.67	6	5
1:A:24:PHE:CD1	1:A:29:ILE:HG13	0.54	2.37	3	3
1:A:24:PHE:CD1	1:A:27:ALA:HB3	0.54	2.37	1	2
1:A:21:VAL:HG21	1:A:32:SER:O	0.54	2.03	5	1
1:A:32:SER:O	1:A:33:ALA:CB	0.54	2.56	10	8
1:A:21:VAL:HA	1:A:37:VAL:HG21	0.54	1.78	7	1
1:A:6:ILE:CD1	1:A:21:VAL:HG11	0.54	2.33	4	3
1:A:20:LEU:N	1:A:45:LEU:HD22	0.53	2.18	10	1
1:A:24:PHE:N	1:A:24:PHE:CD1	0.53	2.75	6	1
1:A:9:LEU:CD1	1:A:17:VAL:HG11	0.53	2.33	5	2
1:A:18:GLU:O	1:A:21:VAL:CG2	0.53	2.42	7	1
1:A:24:PHE:CE2	1:A:44:THR:CB	0.53	2.92	4	7
1:A:37:VAL:CG1	1:A:38:SER:N	0.53	2.71	8	2
1:A:24:PHE:HB3	1:A:29:ILE:HB	0.53	1.81	4	8
1:A:24:PHE:O	1:A:27:ALA:N	0.53	2.42	5	8
1:A:20:LEU:C	1:A:20:LEU:CD1	0.53	2.77	8	4
1:A:21:VAL:HG22	1:A:32:SER:N	0.53	2.19	3	1
1:A:24:PHE:HA	1:A:27:ALA:HB3	0.52	1.81	1	7
1:A:7:LYS:HB2	1:A:34:ASP:HA	0.52	1.79	8	4
1:A:20:LEU:HD22	1:A:41:GLU:N	0.52	2.18	2	2
1:A:21:VAL:HG13	1:A:37:VAL:HA	0.52	1.81	9	1
1:A:45:LEU:C	1:A:45:LEU:HD12	0.52	2.25	10	1
1:A:24:PHE:CD1	1:A:29:ILE:CG1	0.52	2.93	1	3
1:A:24:PHE:CD1	1:A:29:ILE:CD1	0.51	2.93	2	1
1:A:20:LEU:CD1	1:A:42:LYS:N	0.51	2.74	9	2
1:A:37:VAL:CG2	1:A:38:SER:N	0.51	2.73	3	5
1:A:7:LYS:H	1:A:10:ALA:HB2	0.51	1.63	8	2
1:A:29:ILE:HG21	1:A:41:GLU:OE1	0.51	2.05	3	1
1:A:5:THR:HB	1:A:35:ASP:O	0.51	2.05	8	1
1:A:21:VAL:HB	1:A:32:SER:CB	0.51	2.35	9	1
1:A:24:PHE:CE2	1:A:44:THR:HB	0.51	2.40	2	7
1:A:7:LYS:CB	1:A:34:ASP:HA	0.51	2.36	8	2
1:A:10:ALA:HB1	1:A:18:GLU:CA	0.51	2.36	8	1
1:A:24:PHE:CE2	1:A:41:GLU:HB3	0.51	2.41	6	7
1:A:6:ILE:HG13	1:A:21:VAL:CG1	0.51	2.35	4	1
1:A:6:ILE:HD12	1:A:33:ALA:H	0.51	1.66	1	2
1:A:20:LEU:CA	1:A:45:LEU:HD22	0.51	2.36	10	1
1:A:24:PHE:CE2	1:A:44:THR:OG1	0.50	2.64	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:CD2	1:A:38:SER:O	0.50	2.59	3	4
1:A:42:LYS:O	1:A:44:THR:N	0.50	2.44	2	5
1:A:24:PHE:CD2	1:A:41:GLU:HB3	0.50	2.41	2	1
1:A:24:PHE:CE2	1:A:41:GLU:HG3	0.50	2.42	9	1
1:A:21:VAL:HB	1:A:37:VAL:CG2	0.50	2.35	4	2
1:A:20:LEU:CD1	1:A:20:LEU:C	0.50	2.80	1	3
1:A:20:LEU:HD11	1:A:37:VAL:CG1	0.50	2.36	5	2
1:A:24:PHE:CE1	1:A:45:LEU:N	0.50	2.80	6	3
1:A:21:VAL:HG12	1:A:37:VAL:CG2	0.50	2.36	7	1
1:A:6:ILE:HD12	1:A:34:ASP:H	0.49	1.67	9	1
1:A:20:LEU:O	1:A:24:PHE:CB	0.49	2.59	9	3
1:A:13:ARG:HB3	1:A:16:SER:CB	0.49	2.36	7	2
1:A:20:LEU:HA	1:A:44:THR:HG21	0.49	1.83	7	2
1:A:20:LEU:O	1:A:24:PHE:CG	0.49	2.66	6	1
1:A:20:LEU:HA	1:A:45:LEU:HD22	0.49	1.83	10	1
1:A:6:ILE:HD13	1:A:21:VAL:HG11	0.49	1.85	2	2
1:A:20:LEU:HD22	1:A:41:GLU:CB	0.49	2.38	8	2
1:A:30:ARG:O	1:A:37:VAL:HG23	0.49	2.08	10	1
1:A:21:VAL:CA	1:A:37:VAL:HG21	0.49	2.37	7	1
1:A:37:VAL:HG22	1:A:38:SER:H	0.49	1.67	4	2
1:A:19:ARG:CG	1:A:45:LEU:HD11	0.49	2.38	5	1
1:A:23:GLN:C	1:A:48:HIS:NE2	0.49	2.67	7	10
1:A:31:LYS:O	1:A:31:LYS:HG2	0.49	2.08	8	1
1:A:21:VAL:CG1	1:A:32:SER:CB	0.49	2.87	4	3
1:A:30:ARG:O	1:A:37:VAL:HA	0.49	2.07	5	1
1:A:6:ILE:CG2	1:A:35:ASP:N	0.48	2.76	9	4
1:A:24:PHE:HD1	1:A:29:ILE:HD13	0.48	1.68	7	1
1:A:24:PHE:HB3	1:A:29:ILE:CG1	0.48	2.37	5	2
1:A:21:VAL:CG2	1:A:37:VAL:CG2	0.48	2.89	1	3
1:A:20:LEU:HD11	1:A:38:SER:O	0.48	2.08	2	1
1:A:44:THR:CG2	1:A:45:LEU:N	0.48	2.76	7	5
1:A:34:ASP:O	1:A:35:ASP:HB2	0.48	2.07	4	5
1:A:9:LEU:HD23	1:A:37:VAL:HG13	0.48	1.86	4	1
1:A:45:LEU:C	1:A:45:LEU:HD13	0.48	2.29	6	1
1:A:21:VAL:CG1	1:A:32:SER:CA	0.48	2.91	2	1
1:A:9:LEU:O	1:A:12:GLU:HB2	0.48	2.08	5	2
1:A:30:ARG:HB2	1:A:37:VAL:HA	0.48	1.85	2	1
1:A:4:VAL:HG11	1:A:9:LEU:CD2	0.48	2.38	10	1
1:A:32:SER:N	1:A:37:VAL:CG2	0.48	2.77	8	1
1:A:6:ILE:HD13	1:A:6:ILE:C	0.48	2.28	9	1
1:A:37:VAL:HG13	1:A:38:SER:O	0.47	2.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ALA:HB1	1:A:31:LYS:HG3	0.47	1.85	6	1
1:A:6:ILE:HD13	1:A:21:VAL:CB	0.47	2.38	10	1
1:A:9:LEU:CD2	1:A:39:ALA:HB2	0.47	2.40	7	1
1:A:20:LEU:HD22	1:A:45:LEU:HB2	0.47	1.87	9	1
1:A:24:PHE:HE2	1:A:44:THR:HG1	0.47	1.50	9	1
1:A:21:VAL:CG2	1:A:32:SER:HB3	0.47	2.38	7	1
1:A:24:PHE:O	1:A:25:ALA:C	0.47	2.53	1	10
1:A:32:SER:CB	1:A:35:ASP:HB3	0.47	2.39	5	2
1:A:7:LYS:CA	1:A:10:ALA:HB3	0.47	2.39	6	1
1:A:46:ILE:HG23	1:A:47:ASP:N	0.47	2.25	7	2
1:A:29:ILE:CG2	1:A:37:VAL:HG22	0.47	2.40	10	1
1:A:24:PHE:CE2	1:A:45:LEU:N	0.47	2.82	10	1
1:A:9:LEU:HD23	1:A:39:ALA:CB	0.47	2.40	7	1
1:A:6:ILE:HG13	1:A:21:VAL:CB	0.47	2.39	4	1
1:A:4:VAL:HB	1:A:9:LEU:HD13	0.46	1.87	7	1
1:A:20:LEU:HD13	1:A:41:GLU:CB	0.46	2.40	4	3
1:A:5:THR:O	1:A:9:LEU:HB2	0.46	2.11	5	1
1:A:17:VAL:CA	1:A:20:LEU:HD23	0.46	2.33	2	1
1:A:6:ILE:HB	1:A:37:VAL:CB	0.46	2.39	5	1
1:A:46:ILE:CG2	1:A:47:ASP:N	0.46	2.79	7	3
1:A:23:GLN:HB3	1:A:48:HIS:CE1	0.46	2.45	8	2
1:A:14:GLN:O	1:A:15:THR:CB	0.46	2.63	7	1
1:A:19:ARG:HB3	1:A:45:LEU:CD1	0.46	2.41	5	1
1:A:24:PHE:CD1	1:A:29:ILE:HD13	0.46	2.45	7	1
1:A:6:ILE:HD13	1:A:7:LYS:CA	0.46	2.41	6	2
1:A:20:LEU:HD22	1:A:42:LYS:N	0.46	2.26	1	2
1:A:31:LYS:HA	1:A:37:VAL:CG2	0.46	2.41	8	1
1:A:30:ARG:HB3	1:A:36:SER:O	0.46	2.11	7	1
1:A:20:LEU:HD21	1:A:39:ALA:HA	0.45	1.87	2	1
1:A:32:SER:H	1:A:37:VAL:CG2	0.45	2.25	8	2
1:A:21:VAL:CG2	1:A:32:SER:CB	0.45	2.94	7	1
1:A:25:ALA:HB1	1:A:31:LYS:HD3	0.45	1.87	9	1
1:A:21:VAL:HG13	1:A:37:VAL:CB	0.45	2.41	2	1
1:A:24:PHE:CD1	1:A:27:ALA:CB	0.45	2.98	1	1
1:A:20:LEU:HD12	1:A:21:VAL:CA	0.45	2.42	10	1
1:A:6:ILE:HG12	1:A:37:VAL:CG2	0.45	2.41	8	1
1:A:10:ALA:CB	1:A:18:GLU:HB2	0.45	2.39	9	2
1:A:24:PHE:N	1:A:24:PHE:HD1	0.45	2.08	6	1
1:A:9:LEU:CD2	1:A:39:ALA:CB	0.45	2.94	7	1
1:A:6:ILE:C	1:A:6:ILE:CD1	0.45	2.84	8	1
1:A:21:VAL:CG1	1:A:32:SER:HA	0.45	2.40	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PHE:CE2	1:A:41:GLU:CG	0.45	3.00	5	2
1:A:7:LYS:HB2	1:A:34:ASP:CA	0.45	2.42	8	2
1:A:41:GLU:C	1:A:43:GLN:N	0.45	2.71	3	2
1:A:13:ARG:HB3	1:A:16:SER:HB2	0.45	1.88	5	4
1:A:4:VAL:CB	1:A:9:LEU:HD22	0.45	2.42	4	1
1:A:24:PHE:HZ	1:A:44:THR:CB	0.45	2.23	10	1
1:A:24:PHE:CE2	1:A:44:THR:CA	0.45	3.00	7	1
1:A:29:ILE:HG21	1:A:38:SER:CB	0.44	2.41	9	2
1:A:13:ARG:O	1:A:14:GLN:CB	0.44	2.65	5	7
1:A:29:ILE:CG2	1:A:30:ARG:H	0.44	2.25	7	1
1:A:21:VAL:CG2	1:A:37:VAL:HG11	0.44	2.42	2	1
1:A:33:ALA:O	1:A:34:ASP:CB	0.44	2.65	8	1
1:A:29:ILE:HG21	1:A:38:SER:OG	0.44	2.12	8	1
1:A:34:ASP:O	1:A:35:ASP:CB	0.44	2.65	9	2
1:A:20:LEU:CD2	1:A:45:LEU:HB2	0.44	2.43	9	1
1:A:27:ALA:CB	1:A:29:ILE:CD1	0.44	2.95	8	1
1:A:21:VAL:CB	1:A:37:VAL:HG23	0.44	2.39	4	1
1:A:21:VAL:CG2	1:A:31:LYS:C	0.43	2.86	3	1
1:A:6:ILE:HG22	1:A:35:ASP:H	0.43	1.72	4	1
1:A:19:ARG:O	1:A:22:GLN:CG	0.43	2.66	5	1
1:A:21:VAL:HA	1:A:37:VAL:CG2	0.43	2.43	7	1
1:A:4:VAL:HG22	1:A:5:THR:N	0.43	2.29	8	1
1:A:42:LYS:C	1:A:44:THR:N	0.43	2.72	2	3
1:A:30:ARG:O	1:A:37:VAL:CG2	0.43	2.66	2	1
1:A:6:ILE:HG13	1:A:32:SER:HA	0.43	1.90	1	1
1:A:25:ALA:CB	1:A:31:LYS:CG	0.43	2.97	6	3
1:A:21:VAL:HG13	1:A:37:VAL:HG11	0.43	1.89	2	1
1:A:21:VAL:HG13	1:A:37:VAL:HG23	0.43	1.89	1	1
1:A:20:LEU:HD23	1:A:44:THR:HG21	0.43	1.90	7	1
1:A:23:GLN:CG	1:A:48:HIS:CG	0.43	3.02	8	2
1:A:6:ILE:CB	1:A:21:VAL:HG11	0.43	2.44	10	1
1:A:29:ILE:HG23	1:A:30:ARG:H	0.43	1.73	10	1
1:A:25:ALA:HB2	1:A:31:LYS:CB	0.43	2.43	8	1
1:A:6:ILE:O	1:A:7:LYS:HB2	0.43	2.13	6	2
1:A:41:GLU:O	1:A:42:LYS:C	0.43	2.56	4	5
1:A:13:ARG:CG	1:A:17:VAL:HG12	0.42	2.44	4	1
1:A:30:ARG:HB2	1:A:36:SER:O	0.42	2.13	2	1
1:A:13:ARG:HG3	1:A:17:VAL:HG12	0.42	1.91	4	1
1:A:20:LEU:HD13	1:A:41:GLU:HB2	0.42	1.90	2	1
1:A:24:PHE:HD1	1:A:27:ALA:HB3	0.42	1.75	1	2
1:A:23:GLN:CG	1:A:48:HIS:CD2	0.42	3.03	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PHE:CZ	1:A:44:THR:OG1	0.42	2.72	10	1
1:A:24:PHE:CD2	1:A:44:THR:CB	0.42	3.02	2	2
1:A:24:PHE:CZ	1:A:41:GLU:OE1	0.42	2.73	4	3
1:A:21:VAL:HG21	1:A:32:SER:HA	0.42	1.91	3	1
1:A:6:ILE:N	1:A:37:VAL:CG1	0.42	2.83	6	1
1:A:44:THR:O	1:A:47:ASP:HB3	0.42	2.14	10	1
1:A:20:LEU:CD2	1:A:42:LYS:HA	0.42	2.44	9	1
1:A:23:GLN:OE1	1:A:48:HIS:CD2	0.42	2.73	5	1
1:A:4:VAL:HG11	1:A:9:LEU:HD11	0.42	1.92	7	1
1:A:10:ALA:CB	1:A:18:GLU:CB	0.42	2.96	9	1
1:A:9:LEU:HD12	1:A:17:VAL:HG21	0.42	1.90	2	1
1:A:24:PHE:CE1	1:A:41:GLU:OE2	0.42	2.73	1	2
1:A:24:PHE:HB3	1:A:29:ILE:CG2	0.42	2.45	10	1
1:A:6:ILE:HD12	1:A:33:ALA:N	0.41	2.29	1	1
1:A:24:PHE:O	1:A:28:GLY:N	0.41	2.54	1	1
1:A:20:LEU:CD2	1:A:44:THR:CG2	0.41	2.98	7	1
1:A:24:PHE:CE2	1:A:41:GLU:OE1	0.41	2.73	2	1
1:A:6:ILE:CG1	1:A:7:LYS:N	0.41	2.82	7	2
1:A:13:ARG:CG	1:A:16:SER:CB	0.41	2.98	8	1
1:A:20:LEU:HD23	1:A:44:THR:CG2	0.41	2.46	7	1
1:A:21:VAL:CG2	1:A:32:SER:N	0.41	2.83	3	1
1:A:23:GLN:HG3	1:A:48:HIS:CD2	0.41	2.50	6	1
1:A:7:LYS:HA	1:A:10:ALA:CB	0.41	2.44	10	1
1:A:24:PHE:CE2	1:A:44:THR:N	0.41	2.89	2	2
1:A:20:LEU:HD22	1:A:41:GLU:CA	0.41	2.46	1	1
1:A:17:VAL:O	1:A:18:GLU:C	0.41	2.58	5	1
1:A:24:PHE:O	1:A:27:ALA:HB3	0.41	2.16	5	1
1:A:9:LEU:CD1	1:A:39:ALA:HB2	0.41	2.45	10	1
1:A:20:LEU:CD1	1:A:21:VAL:N	0.41	2.78	2	1
1:A:13:ARG:NH2	1:A:40:GLN:CG	0.41	2.84	8	1
1:A:23:GLN:HG3	1:A:45:LEU:HD21	0.41	1.91	9	1
1:A:25:ALA:CB	1:A:31:LYS:CD	0.41	2.99	9	1
1:A:6:ILE:O	1:A:7:LYS:HB3	0.41	2.16	5	2
1:A:24:PHE:CD1	1:A:48:HIS:CE1	0.41	3.09	6	1
1:A:13:ARG:HB2	1:A:17:VAL:CG1	0.41	2.46	2	1
1:A:11:ALA:O	1:A:12:GLU:C	0.41	2.59	1	3
1:A:6:ILE:HB	1:A:37:VAL:CG2	0.41	2.46	5	1
1:A:23:GLN:HB2	1:A:45:LEU:HD23	0.41	1.93	6	1
1:A:31:LYS:N	1:A:31:LYS:CD	0.40	2.84	2	1
1:A:24:PHE:CD1	1:A:24:PHE:N	0.40	2.89	5	1
1:A:7:LYS:H	1:A:10:ALA:CB	0.40	2.28	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:SER:O	1:A:19:ARG:HB2	0.40	2.15	4	1
1:A:4:VAL:HG22	1:A:5:THR:H	0.40	1.75	8	1
1:A:45:LEU:O	1:A:49:LEU:CB	0.40	2.69	3	1
1:A:30:ARG:C	1:A:37:VAL:HG22	0.40	2.36	8	1
1:A:9:LEU:HD22	1:A:17:VAL:HG21	0.40	1.92	6	1
1:A:5:THR:HA	1:A:35:ASP:O	0.40	2.15	8	1
1:A:20:LEU:CD1	1:A:42:LYS:H	0.40	2.28	7	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	47/49 (96%)	32±2 (68±4%)	8±1 (17±2%)	7±1 (15±2%)	1	4
All	All	470/490 (96%)	321 (68%)	78 (17%)	71 (15%)	1	4

All 10 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	35	ASP	10
1	A	7	LYS	10
1	A	28	GLY	10
1	A	42	LYS	10
1	A	34	ASP	9
1	A	33	ALA	8
1	A	43	GLN	5
1	A	27	ALA	5
1	A	14	GLN	3
1	A	12	GLU	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	42/42 (100%)	25±3 (60±7%)	17±3 (40±7%)	0	5
All	All	420/420 (100%)	252 (60%)	168 (40%)	0	5

All 36 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	16	SER	10
1	A	44	THR	10
1	A	7	LYS	9
1	A	31	LYS	8
1	A	41	GLU	8
1	A	20	LEU	8
1	A	42	LYS	8
1	A	6	ILE	7
1	A	9	LEU	7
1	A	4	VAL	7
1	A	40	GLN	6
1	A	14	GLN	6
1	A	13	ARG	6
1	A	43	GLN	6
1	A	5	THR	5
1	A	47	ASP	4
1	A	8	THR	4
1	A	32	SER	4
1	A	19	ARG	4
1	A	30	ARG	4
1	A	26	ASP	4
1	A	23	GLN	4
1	A	21	VAL	3
1	A	49	LEU	3
1	A	12	GLU	3
1	A	37	VAL	3
1	A	3	ASP	3
1	A	22	GLN	3
1	A	17	VAL	2
1	A	34	ASP	2
1	A	45	LEU	2
1	A	50	ASN	1
1	A	2	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	36	SER	1
1	A	46	ILE	1
1	A	38	SER	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 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5624

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	1234
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1234
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 1234 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	37	SER	N	124.5	-1.0	1
UNMAPPED	51	LYS	N	119.9	-1.0	1
UNMAPPED	59	THR	HB	4.16	-1.0	4
UNMAPPED	119	ALA	HB2	1.5	-1.0	1
UNMAPPED	30	LYS	HB3	1.55	-1.0	2
UNMAPPED	28	ILE	HG23	0.6	-1.0	1
UNMAPPED	79	SER	CA	58.4	-1.0	1
UNMAPPED	7	THR	HB	4.27	-1.0	1
UNMAPPED	19	LEU	HD11	0.82	-1.0	1
UNMAPPED	39	GLN	HA	4.09	-1.0	1
UNMAPPED	58	LEU	HA	4.27	-1.0	1
UNMAPPED	19	LEU	CB	42.4	-1.0	1
UNMAPPED	3	VAL	CA	61.0	-1.0	1
UNMAPPED	93	ARG	HG2	1.55	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	86	LYS	H	8.22	-1.0	1
UNMAPPED	77	SER	C	173.9	-1.0	1
UNMAPPED	57	LYS	HE2	2.95	-1.0	1
UNMAPPED	19	LEU	N	122.0	-1.0	1
UNMAPPED	68	LEU	HD23	0.86	-1.0	2
UNMAPPED	82	ILE	HA	4.08	-1.0	1
UNMAPPED	67	THR	H	8.15	-1.0	1
UNMAPPED	149	ARG	H	7.93	-1.0	1
UNMAPPED	74	GLY	CA	45.4	-1.0	1
UNMAPPED	3	VAL	HG23	0.98	-1.0	1
UNMAPPED	153	GLU	CB	30.3	-1.0	1
UNMAPPED	149	ARG	C	177.2	-1.0	1
UNMAPPED	74	GLY	HA3	3.94	-1.0	1
UNMAPPED	36	VAL	H	8.57	-1.0	1
UNMAPPED	84	VAL	HG13	0.88	-1.0	1
UNMAPPED	47	HIS	HB3	3.36	-1.0	2
UNMAPPED	48	LEU	H	8.41	-1.0	1
UNMAPPED	21	GLN	C	177.0	-1.0	1
UNMAPPED	80	VAL	HG23	0.88	-1.0	4
UNMAPPED	5	ILE	HB	2.13	-1.0	1
UNMAPPED	91	VAL	HA	4.0	-1.0	1
UNMAPPED	70	ILE	H	8.01	-1.0	1
UNMAPPED	100	ARG	C	178.2	-1.0	1
UNMAPPED	80	VAL	HG22	0.88	-1.0	4
UNMAPPED	10	ALA	HB2	1.52	-1.0	1
UNMAPPED	32	ALA	HB3	1.32	-1.0	1
UNMAPPED	42	GLN	NE2	115.9	-1.0	1
UNMAPPED	150	GLU	HB2	1.99	-1.0	1
UNMAPPED	32	ALA	N	120.8	-1.0	1
UNMAPPED	74	GLY	C	174.1	-1.0	1
UNMAPPED	44	LEU	CD1	23.4	-1.0	1
UNMAPPED	50	GLN	C	176.2	-1.0	1
UNMAPPED	51	LYS	HA	4.1	-1.0	1
UNMAPPED	13	GLN	HB2	2.16	-1.0	1
UNMAPPED	53	SER	HB2	3.85	-1.0	1
UNMAPPED	32	ALA	CB	19.5	-1.0	1
UNMAPPED	92	LYS	C	175.3	-1.0	1
UNMAPPED	76	LYS	C	175.8	-1.0	1
UNMAPPED	23	PHE	HD1	7.08	-1.0	1
UNMAPPED	152	ALA	C	177.8	-1.0	1
UNMAPPED	85	ARG	HD2	3.14	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	10	ALA	C	181.4	-1.0	1
UNMAPPED	39	GLN	N	118.0	-1.0	1
UNMAPPED	80	VAL	CG2	20.8	-1.0	4
UNMAPPED	83	GLU	CA	56.6	-1.0	1
UNMAPPED	31	SER	HB2	3.8	-1.0	2
UNMAPPED	20	VAL	H	8.8	-1.0	1
UNMAPPED	51	LYS	HB3	1.68	-1.0	1
UNMAPPED	94	ASP	H	8.44	-1.0	1
UNMAPPED	35	SER	H	8.55	-1.0	1
UNMAPPED	21	GLN	CA	58.7	-1.0	1
UNMAPPED	45	ILE	HD11	0.71	-1.0	1
UNMAPPED	149	ARG	CB	30.4	-1.0	1
UNMAPPED	36	VAL	HG21	0.9	-1.0	1
UNMAPPED	16	VAL	HG13	0.88	-1.0	1
UNMAPPED	8	LEU	CB	41.5	-1.0	1
UNMAPPED	8	LEU	HB2	1.44	-1.0	2
UNMAPPED	120	GLU	H	8.15	-1.0	1
UNMAPPED	13	GLN	HG2	2.26	-1.0	1
UNMAPPED	40	GLU	CA	59.5	-1.0	1
UNMAPPED	95	PRO	CA	64.6	-1.0	1
UNMAPPED	121	GLU	HG3	2.27	-1.0	1
UNMAPPED	45	ILE	HB	1.86	-1.0	1
UNMAPPED	31	SER	C	174.1	-1.0	1
UNMAPPED	85	ARG	C	175.6	-1.0	1
UNMAPPED	121	GLU	H	8.32	-1.0	1
UNMAPPED	50	GLN	HG2	2.33	-1.0	2
UNMAPPED	24	ALA	CB	17.3	-1.0	1
UNMAPPED	25	ASP	HA	4.24	-1.0	1
UNMAPPED	13	GLN	HA	3.89	-1.0	1
UNMAPPED	81	GLN	HB2	1.91	-1.0	2
UNMAPPED	46	ASP	HA	4.38	-1.0	1
UNMAPPED	101	LEU	HD22	0.88	-1.0	4
UNMAPPED	52	ASN	CA	53.4	-1.0	1
UNMAPPED	78	LYS	HB2	1.74	-1.0	1
UNMAPPED	41	LYS	HA	3.77	-1.0	1
UNMAPPED	122	SER	N	115.9	-1.0	1
UNMAPPED	59	THR	HG23	1.16	-1.0	1
UNMAPPED	58	LEU	HG	1.38	-1.0	1
UNMAPPED	22	GLN	HG3	2.64	-1.0	2
UNMAPPED	19	LEU	HG	1.72	-1.0	1
UNMAPPED	80	VAL	HA	4.09	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	57	LYS	C	176.0	-1.0	1
UNMAPPED	48	LEU	C	178.7	-1.0	1
UNMAPPED	41	LYS	HE2	2.86	-1.0	1
UNMAPPED	20	VAL	HG22	0.95	-1.0	1
UNMAPPED	27	GLY	C	173.4	-1.0	1
UNMAPPED	72	GLY	HA3	3.99	-1.0	1
UNMAPPED	3	VAL	HG12	0.93	-1.0	1
UNMAPPED	97	GLU	CB	30.1	-1.0	1
UNMAPPED	47	HIS	CB	30.4	-1.0	1
UNMAPPED	60	LEU	HB3	1.55	-1.0	1
UNMAPPED	42	GLN	C	176.7	-1.0	1
UNMAPPED	47	HIS	HD2	6.69	-1.0	1
UNMAPPED	121	GLU	N	120.0	-1.0	1
UNMAPPED	100	ARG	HD2	2.94	-1.0	1
UNMAPPED	92	LYS	N	125.4	-1.0	1
UNMAPPED	55	PRO	HD2	3.64	-1.0	2
UNMAPPED	12	ARG	H	7.99	-1.0	1
UNMAPPED	147	ALA	C	177.8	-1.0	1
UNMAPPED	92	LYS	HD2	1.75	-1.0	4
UNMAPPED	79	SER	HB2	3.84	-1.0	1
UNMAPPED	21	GLN	H	7.54	-1.0	1
UNMAPPED	38	ALA	N	123.9	-1.0	1
UNMAPPED	149	ARG	HB3	1.86	-1.0	1
UNMAPPED	56	ASP	H	8.34	-1.0	1
UNMAPPED	18	ARG	H	7.77	-1.0	1
UNMAPPED	92	LYS	CB	33.1	-1.0	1
UNMAPPED	80	VAL	HG11	0.88	-1.0	4
UNMAPPED	14	THR	HG23	1.22	-1.0	1
UNMAPPED	4	THR	HB	4.66	-1.0	1
UNMAPPED	23	PHE	C	177.6	-1.0	1
UNMAPPED	40	GLU	H	7.87	-1.0	1
UNMAPPED	52	ASN	HB2	2.73	-1.0	2
UNMAPPED	57	LYS	HD2	1.68	-1.0	4
UNMAPPED	27	GLY	HA3	4.13	-1.0	2
UNMAPPED	76	LYS	HB3	1.81	-1.0	2
UNMAPPED	3	VAL	CG2	20.6	-1.0	1
UNMAPPED	15	SER	HA	4.58	-1.0	1
UNMAPPED	17	GLU	C	178.9	-1.0	1
UNMAPPED	57	LYS	HG3	1.43	-1.0	4
UNMAPPED	22	GLN	CB	28.2	-1.0	1
UNMAPPED	26	ALA	H	7.27	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	103	ALA	H	7.91	-1.0	1
UNMAPPED	76	LYS	HB2	1.73	-1.0	2
UNMAPPED	44	LEU	HD12	0.1	-1.0	1
UNMAPPED	95	PRO	HB2	2.32	-1.0	1
UNMAPPED	22	GLN	CD	178.0	-1.0	1
UNMAPPED	99	GLU	HG2	2.4	-1.0	1
UNMAPPED	38	ALA	HB3	1.46	-1.0	1
UNMAPPED	9	ALA	CB	17.6	-1.0	1
UNMAPPED	86	LYS	N	122.5	-1.0	1
UNMAPPED	153	GLU	CA	56.9	-1.0	1
UNMAPPED	96	GLN	CB	28.2	-1.0	1
UNMAPPED	5	ILE	HD13	0.37	-1.0	1
UNMAPPED	24	ALA	C	182.0	-1.0	1
UNMAPPED	104	GLU	N	119.1	-1.0	1
UNMAPPED	72	GLY	H	8.42	-1.0	1
UNMAPPED	24	ALA	HB3	1.55	-1.0	1
UNMAPPED	83	GLU	HB3	1.91	-1.0	1
UNMAPPED	23	PHE	HB3	3.27	-1.0	2
UNMAPPED	104	GLU	CB	32.8	-1.0	1
UNMAPPED	122	SER	HB3	4.0	-1.0	1
UNMAPPED	90	PHE	HE1	7.26	-1.0	1
UNMAPPED	91	VAL	HG11	0.83	-1.0	4
UNMAPPED	147	ALA	HB3	1.42	-1.0	1
UNMAPPED	23	PHE	CA	64.5	-1.0	1
UNMAPPED	61	GLN	HG3	2.35	-1.0	1
UNMAPPED	151	ALA	CA	53.5	-1.0	1
UNMAPPED	19	LEU	H	8.18	-1.0	1
UNMAPPED	36	VAL	CG1	21.6	-1.0	1
UNMAPPED	12	ARG	CA	56.3	-1.0	1
UNMAPPED	46	ASP	CA	57.5	-1.0	1
UNMAPPED	79	SER	CB	63.8	-1.0	1
UNMAPPED	17	GLU	HG2	2.21	-1.0	2
UNMAPPED	41	LYS	C	176.7	-1.0	1
UNMAPPED	42	GLN	HE21	6.75	-1.0	1
UNMAPPED	12	ARG	HA	4.17	-1.0	1
UNMAPPED	7	THR	HG22	1.21	-1.0	1
UNMAPPED	67	THR	CB	69.8	-1.0	1
UNMAPPED	45	ILE	CB	37.7	-1.0	1
UNMAPPED	27	GLY	N	106.4	-1.0	1
UNMAPPED	153	GLU	N	118.7	-1.0	1
UNMAPPED	56	ASP	HA	4.51	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	35	SER	HB3	3.7	-1.0	1
UNMAPPED	48	LEU	N	119.1	-1.0	1
UNMAPPED	95	PRO	HD3	3.84	-1.0	1
UNMAPPED	83	GLU	C	175.6	-1.0	1
UNMAPPED	68	LEU	HD22	0.86	-1.0	2
UNMAPPED	68	LEU	HA	4.29	-1.0	1
UNMAPPED	124	LYS	HG2	1.38	-1.0	1
UNMAPPED	54	GLY	CA	44.9	-1.0	1
UNMAPPED	81	GLN	CB	29.6	-1.0	1
UNMAPPED	48	LEU	CB	41.5	-1.0	1
UNMAPPED	48	LEU	HD22	0.76	-1.0	1
UNMAPPED	28	ILE	HD12	0.97	-1.0	1
UNMAPPED	61	GLN	CA	56.1	-1.0	1
UNMAPPED	153	GLU	HA	4.19	-1.0	1
UNMAPPED	81	GLN	N	124.2	-1.0	1
UNMAPPED	70	ILE	CB	38.7	-1.0	1
UNMAPPED	91	VAL	HG12	0.83	-1.0	4
UNMAPPED	8	LEU	HD21	0.96	-1.0	1
UNMAPPED	81	GLN	HG3	2.3	-1.0	1
UNMAPPED	78	LYS	H	8.31	-1.0	1
UNMAPPED	40	GLU	C	177.8	-1.0	1
UNMAPPED	70	ILE	HD11	0.82	-1.0	1
UNMAPPED	20	VAL	CG2	23.1	-1.0	1
UNMAPPED	81	GLN	HG2	2.3	-1.0	1
UNMAPPED	29	ARG	N	129.3	-1.0	1
UNMAPPED	155	ASP	HB2	2.38	-1.0	2
UNMAPPED	150	GLU	C	176.8	-1.0	1
UNMAPPED	5	ILE	HG22	0.86	-1.0	1
UNMAPPED	51	LYS	CA	57.1	-1.0	1
UNMAPPED	56	ASP	C	177.5	-1.0	1
UNMAPPED	11	GLU	H	8.24	-1.0	1
UNMAPPED	45	ILE	HG12	1.13	-1.0	2
UNMAPPED	94	ASP	N	124.0	-1.0	1
UNMAPPED	73	THR	C	174.8	-1.0	1
UNMAPPED	19	LEU	HD23	0.95	-1.0	1
UNMAPPED	25	ASP	H	8.5	-1.0	1
UNMAPPED	45	ILE	HG13	1.54	-1.0	2
UNMAPPED	14	THR	CB	71.7	-1.0	1
UNMAPPED	41	LYS	HE3	2.86	-1.0	1
UNMAPPED	46	ASP	H	8.77	-1.0	1
UNMAPPED	41	LYS	CA	60.5	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	2	ASP	C	175.1	-1.0	1
UNMAPPED	102	ALA	C	179.4	-1.0	1
UNMAPPED	38	ALA	HB1	1.46	-1.0	1
UNMAPPED	14	THR	N	113.6	-1.0	1
UNMAPPED	8	LEU	H	8.67	-1.0	1
UNMAPPED	22	GLN	NE2	107.9	-1.0	1
UNMAPPED	156	LYS	HB3	1.78	-1.0	2
UNMAPPED	34	ASP	HB2	2.77	-1.0	2
UNMAPPED	3	VAL	HG22	0.98	-1.0	1
UNMAPPED	154	LYS	HE3	2.96	-1.0	1
UNMAPPED	90	PHE	HZ	7.22	-1.0	1
UNMAPPED	6	LYS	HE2	2.92	-1.0	1
UNMAPPED	93	ARG	CB	31.3	-1.0	1
UNMAPPED	103	ALA	HA	4.19	-1.0	1
UNMAPPED	32	ALA	C	176.4	-1.0	1
UNMAPPED	34	ASP	N	120.2	-1.0	1
UNMAPPED	24	ALA	H	7.96	-1.0	1
UNMAPPED	41	LYS	CB	32.6	-1.0	1
UNMAPPED	89	THR	HG23	1.15	-1.0	1
UNMAPPED	41	LYS	HB3	1.99	-1.0	2
UNMAPPED	51	LYS	C	176.3	-1.0	1
UNMAPPED	61	GLN	H	8.13	-1.0	1
UNMAPPED	10	ALA	N	118.8	-1.0	1
UNMAPPED	68	LEU	HD12	0.83	-1.0	2
UNMAPPED	41	LYS	N	119.3	-1.0	1
UNMAPPED	73	THR	HA	4.34	-1.0	1
UNMAPPED	152	ALA	CB	19.1	-1.0	1
UNMAPPED	93	ARG	HB2	1.7	-1.0	1
UNMAPPED	23	PHE	HE2	6.99	-1.0	1
UNMAPPED	10	ALA	HB1	1.52	-1.0	1
UNMAPPED	32	ALA	HB2	1.32	-1.0	1
UNMAPPED	71	PRO	HG2	1.93	-1.0	1
UNMAPPED	10	ALA	CB	17.7	-1.0	1
UNMAPPED	82	ILE	H	8.13	-1.0	1
UNMAPPED	16	VAL	H	8.87	-1.0	1
UNMAPPED	93	ARG	HB3	1.7	-1.0	1
UNMAPPED	57	LYS	CB	32.6	-1.0	1
UNMAPPED	153	GLU	HG3	2.28	-1.0	1
UNMAPPED	68	LEU	HD13	0.83	-1.0	2
UNMAPPED	150	GLU	CB	30.0	-1.0	1
UNMAPPED	98	ALA	CA	55.0	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	53	SER	HB3	3.85	-1.0	1
UNMAPPED	19	LEU	HB2	1.41	-1.0	2
UNMAPPED	69	ASN	CB	30.7	-1.0	1
UNMAPPED	102	ALA	HB2	1.47	-1.0	1
UNMAPPED	47	HIS	H	8.11	-1.0	1
UNMAPPED	30	LYS	CE	42.5	-1.0	1
UNMAPPED	84	VAL	HG21	0.88	-1.0	1
UNMAPPED	84	VAL	HB	2.03	-1.0	1
UNMAPPED	55	PRO	CD	51.7	-1.0	1
UNMAPPED	68	LEU	HD11	0.83	-1.0	2
UNMAPPED	18	ARG	HB3	1.85	-1.0	1
UNMAPPED	21	GLN	HE21	6.79	-1.0	1
UNMAPPED	29	ARG	HA	4.11	-1.0	1
UNMAPPED	21	GLN	CB	28.4	-1.0	1
UNMAPPED	59	THR	CB	69.3	-1.0	1
UNMAPPED	56	ASP	CB	41.1	-1.0	1
UNMAPPED	40	GLU	N	121.6	-1.0	1
UNMAPPED	16	VAL	HG12	0.88	-1.0	1
UNMAPPED	8	LEU	CA	57.3	-1.0	1
UNMAPPED	51	LYS	HG3	1.3	-1.0	4
UNMAPPED	13	GLN	HG3	2.26	-1.0	1
UNMAPPED	40	GLU	CB	30.4	-1.0	1
UNMAPPED	154	LYS	H	7.93	-1.0	1
UNMAPPED	103	ALA	N	122.0	-1.0	1
UNMAPPED	124	LYS	HB2	1.87	-1.0	1
UNMAPPED	44	LEU	HD23	0.1	-1.0	1
UNMAPPED	28	ILE	HG12	1.05	-1.0	2
UNMAPPED	123	ALA	C	180.0	-1.0	1
UNMAPPED	156	LYS	HA	4.09	-1.0	1
UNMAPPED	15	SER	HB2	3.97	-1.0	2
UNMAPPED	22	GLN	H	8.42	-1.0	1
UNMAPPED	26	ALA	CB	18.4	-1.0	1
UNMAPPED	81	GLN	HB3	2.01	-1.0	2
UNMAPPED	124	LYS	HE2	2.95	-1.0	1
UNMAPPED	23	PHE	HZ	6.78	-1.0	1
UNMAPPED	101	LEU	HD23	0.88	-1.0	4
UNMAPPED	73	THR	N	112.5	-1.0	1
UNMAPPED	77	SER	CB	63.8	-1.0	1
UNMAPPED	26	ALA	N	120.1	-1.0	1
UNMAPPED	119	ALA	HB3	1.5	-1.0	1
UNMAPPED	42	GLN	CB	27.8	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	9	ALA	H	8.59	-1.0	1
UNMAPPED	5	ILE	C	176.6	-1.0	1
UNMAPPED	5	ILE	CG2	18.3	-1.0	1
UNMAPPED	94	ASP	HB3	2.85	-1.0	2
UNMAPPED	58	LEU	HD23	0.86	-1.0	1
UNMAPPED	96	GLN	H	8.45	-1.0	1
UNMAPPED	100	ARG	HG2	2.38	-1.0	1
UNMAPPED	39	GLN	HG2	2.37	-1.0	1
UNMAPPED	155	ASP	H	8.18	-1.0	1
UNMAPPED	44	LEU	H	7.75	-1.0	1
UNMAPPED	20	VAL	HG21	0.95	-1.0	1
UNMAPPED	3	VAL	HG13	0.93	-1.0	1
UNMAPPED	8	LEU	C	177.4	-1.0	1
UNMAPPED	123	ALA	H	7.94	-1.0	1
UNMAPPED	89	THR	CA	61.8	-1.0	1
UNMAPPED	77	SER	CA	58.4	-1.0	1
UNMAPPED	80	VAL	HG13	0.88	-1.0	4
UNMAPPED	39	GLN	H	8.44	-1.0	1
UNMAPPED	90	PHE	HB2	2.95	-1.0	2
UNMAPPED	28	ILE	CG1	27.5	-1.0	1
UNMAPPED	154	LYS	HD2	1.65	-1.0	1
UNMAPPED	33	ASP	HB2	2.38	-1.0	2
UNMAPPED	20	VAL	N	118.4	-1.0	1
UNMAPPED	60	LEU	HA	4.22	-1.0	1
UNMAPPED	79	SER	HB3	3.84	-1.0	1
UNMAPPED	3	VAL	HA	4.36	-1.0	1
UNMAPPED	76	LYS	CA	56.3	-1.0	1
UNMAPPED	49	ASN	H	8.11	-1.0	1
UNMAPPED	54	GLY	HA2	4.09	-1.0	1
UNMAPPED	82	ILE	HG22	1.13	-1.0	1
UNMAPPED	124	LYS	HE3	2.95	-1.0	1
UNMAPPED	55	PRO	HA	4.37	-1.0	1
UNMAPPED	148	LYS	H	7.99	-1.0	1
UNMAPPED	91	VAL	CA	62.1	-1.0	1
UNMAPPED	14	THR	HG22	1.22	-1.0	1
UNMAPPED	95	PRO	HA	4.32	-1.0	1
UNMAPPED	82	ILE	N	122.7	-1.0	1
UNMAPPED	82	ILE	HG23	1.13	-1.0	1
UNMAPPED	57	LYS	HD3	1.68	-1.0	4
UNMAPPED	100	ARG	HA	4.08	-1.0	1
UNMAPPED	81	GLN	H	8.34	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	6	LYS	HB3	1.79	-1.0	1
UNMAPPED	57	LYS	HG2	1.43	-1.0	4
UNMAPPED	6	LYS	HG2	1.38	-1.0	4
UNMAPPED	22	GLN	CA	59.6	-1.0	1
UNMAPPED	151	ALA	H	7.9	-1.0	1
UNMAPPED	100	ARG	CB	29.2	-1.0	1
UNMAPPED	98	ALA	HA	4.17	-1.0	1
UNMAPPED	69	ASN	HB3	2.05	-1.0	1
UNMAPPED	44	LEU	HD13	0.1	-1.0	1
UNMAPPED	6	LYS	HE3	2.92	-1.0	1
UNMAPPED	17	GLU	HB2	1.88	-1.0	2
UNMAPPED	69	ASN	CA	57.3	-1.0	1
UNMAPPED	45	ILE	CG2	17.8	-1.0	1
UNMAPPED	31	SER	H	8.9	-1.0	1
UNMAPPED	101	LEU	CA	58.8	-1.0	1
UNMAPPED	102	ALA	HB3	1.47	-1.0	1
UNMAPPED	90	PHE	H	8.28	-1.0	1
UNMAPPED	20	VAL	HG11	0.88	-1.0	1
UNMAPPED	85	ARG	HD3	3.14	-1.0	1
UNMAPPED	9	ALA	HB1	1.38	-1.0	1
UNMAPPED	92	LYS	CA	56.3	-1.0	1
UNMAPPED	119	ALA	HA	4.2	-1.0	1
UNMAPPED	23	PHE	N	117.5	-1.0	1
UNMAPPED	76	LYS	HE2	2.95	-1.0	1
UNMAPPED	70	ILE	C	174.0	-1.0	1
UNMAPPED	154	LYS	HB3	1.8	-1.0	1
UNMAPPED	26	ALA	HB3	1.11	-1.0	1
UNMAPPED	147	ALA	HB2	1.42	-1.0	1
UNMAPPED	46	ASP	N	120.4	-1.0	1
UNMAPPED	60	LEU	HB2	1.55	-1.0	1
UNMAPPED	25	ASP	CB	40.5	-1.0	1
UNMAPPED	51	LYS	HD2	1.54	-1.0	4
UNMAPPED	14	THR	H	8.3	-1.0	1
UNMAPPED	31	SER	HA	4.65	-1.0	1
UNMAPPED	153	GLU	C	176.2	-1.0	1
UNMAPPED	46	ASP	CB	40.3	-1.0	1
UNMAPPED	155	ASP	CA	54.5	-1.0	1
UNMAPPED	84	VAL	HG23	0.88	-1.0	1
UNMAPPED	95	PRO	HG2	1.97	-1.0	1
UNMAPPED	27	GLY	CA	45.4	-1.0	1
UNMAPPED	148	LYS	HG2	1.78	-1.0	4

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	7	THR	HG23	1.21	-1.0	1
UNMAPPED	72	GLY	N	109.3	-1.0	1
UNMAPPED	123	ALA	HB3	1.5	-1.0	1
UNMAPPED	48	LEU	HB2	1.34	-1.0	2
UNMAPPED	48	LEU	HD13	0.64	-1.0	1
UNMAPPED	90	PHE	HD1	7.17	-1.0	1
UNMAPPED	119	ALA	CA	55.1	-1.0	1
UNMAPPED	67	THR	HG21	1.16	-1.0	1
UNMAPPED	97	GLU	HB3	1.94	-1.0	1
UNMAPPED	93	ARG	H	8.32	-1.0	1
UNMAPPED	71	PRO	HA	4.39	-1.0	1
UNMAPPED	68	LEU	HD21	0.86	-1.0	2
UNMAPPED	90	PHE	HD2	7.17	-1.0	1
UNMAPPED	103	ALA	HB2	1.47	-1.0	1
UNMAPPED	21	GLN	CD	179.7	-1.0	1
UNMAPPED	13	GLN	CB	26.4	-1.0	1
UNMAPPED	28	ILE	HD13	0.97	-1.0	1
UNMAPPED	45	ILE	HG23	0.86	-1.0	1
UNMAPPED	70	ILE	CA	59.0	-1.0	1
UNMAPPED	91	VAL	HG13	0.83	-1.0	4
UNMAPPED	29	ARG	CA	56.0	-1.0	1
UNMAPPED	10	ALA	H	7.16	-1.0	1
UNMAPPED	31	SER	HB3	3.89	-1.0	2
UNMAPPED	75	GLY	HA2	3.91	-1.0	1
UNMAPPED	16	VAL	CB	31.9	-1.0	1
UNMAPPED	20	VAL	CG1	21.6	-1.0	1
UNMAPPED	29	ARG	CB	30.1	-1.0	1
UNMAPPED	151	ALA	HB1	1.41	-1.0	1
UNMAPPED	156	LYS	HE3	2.94	-1.0	1
UNMAPPED	37	SER	CB	66.2	-1.0	1
UNMAPPED	100	ARG	N	120.7	-1.0	1
UNMAPPED	43	THR	HG22	1.26	-1.0	1
UNMAPPED	5	ILE	HG23	0.86	-1.0	1
UNMAPPED	51	LYS	CB	28.8	-1.0	1
UNMAPPED	69	ASN	H	7.81	-1.0	1
UNMAPPED	28	ILE	HG21	0.6	-1.0	1
UNMAPPED	121	GLU	HA	4.07	-1.0	1
UNMAPPED	156	LYS	CA	57.8	-1.0	1
UNMAPPED	71	PRO	C	176.8	-1.0	1
UNMAPPED	80	VAL	HG12	0.88	-1.0	4
UNMAPPED	96	GLN	HB2	1.91	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	ILE	CA	62.7	-1.0	1
UNMAPPED	101	LEU	HD13	0.81	-1.0	4
UNMAPPED	121	GLU	HB2	2.07	-1.0	1
UNMAPPED	19	LEU	HD22	0.95	-1.0	1
UNMAPPED	6	LYS	HD3	1.63	-1.0	4
UNMAPPED	93	ARG	N	123.1	-1.0	1
UNMAPPED	14	THR	CA	59.6	-1.0	1
UNMAPPED	155	ASP	C	174.4	-1.0	1
UNMAPPED	148	LYS	HD3	2.61	-1.0	4
UNMAPPED	34	ASP	C	175.7	-1.0	1
UNMAPPED	5	ILE	HD11	0.37	-1.0	1
UNMAPPED	92	LYS	HA	4.19	-1.0	1
UNMAPPED	53	SER	C	173.8	-1.0	1
UNMAPPED	120	GLU	N	120.4	-1.0	1
UNMAPPED	83	GLU	HB2	1.91	-1.0	1
UNMAPPED	76	LYS	HG2	1.39	-1.0	1
UNMAPPED	6	LYS	CB	32.8	-1.0	1
UNMAPPED	50	GLN	HB2	2.06	-1.0	1
UNMAPPED	70	ILE	HD13	0.82	-1.0	1
UNMAPPED	84	VAL	HA	4.0	-1.0	1
UNMAPPED	71	PRO	HB2	2.25	-1.0	1
UNMAPPED	4	THR	H	8.22	-1.0	1
UNMAPPED	6	LYS	N	117.9	-1.0	1
UNMAPPED	151	ALA	HB3	1.41	-1.0	1
UNMAPPED	7	THR	C	176.2	-1.0	1
UNMAPPED	28	ILE	CA	60.3	-1.0	1
UNMAPPED	37	SER	C	174.7	-1.0	1
UNMAPPED	41	LYS	HB2	1.76	-1.0	2
UNMAPPED	49	ASN	HB3	2.84	-1.0	1
UNMAPPED	78	LYS	C	175.8	-1.0	1
UNMAPPED	119	ALA	HB1	1.5	-1.0	1
UNMAPPED	8	LEU	HG	1.44	-1.0	1
UNMAPPED	155	ASP	CB	41.3	-1.0	1
UNMAPPED	152	ALA	CA	53.2	-1.0	1
UNMAPPED	121	GLU	HG2	2.27	-1.0	1
UNMAPPED	120	GLU	HA	4.05	-1.0	1
UNMAPPED	42	GLN	H	7.88	-1.0	1
UNMAPPED	32	ALA	HB1	1.32	-1.0	1
UNMAPPED	12	ARG	HD3	3.2	-1.0	1
UNMAPPED	8	LEU	HA	4.13	-1.0	1
UNMAPPED	70	ILE	HG21	0.9	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	THR	C	172.0	-1.0	1
UNMAPPED	48	LEU	CD2	23.2	-1.0	1
UNMAPPED	147	ALA	H	7.87	-1.0	1
UNMAPPED	150	GLU	CA	57.8	-1.0	1
UNMAPPED	60	LEU	HD23	0.83	-1.0	1
UNMAPPED	55	PRO	CA	63.5	-1.0	1
UNMAPPED	19	LEU	HB3	1.92	-1.0	2
UNMAPPED	38	ALA	C	180.3	-1.0	1
UNMAPPED	26	ALA	HB1	1.11	-1.0	1
UNMAPPED	98	ALA	HB2	1.49	-1.0	1
UNMAPPED	30	LYS	N	126.3	-1.0	1
UNMAPPED	151	ALA	HA	4.19	-1.0	1
UNMAPPED	67	THR	HG23	1.16	-1.0	1
UNMAPPED	55	PRO	CG	27.8	-1.0	1
UNMAPPED	39	GLN	CB	28.7	-1.0	1
UNMAPPED	85	ARG	HG2	1.57	-1.0	1
UNMAPPED	18	ARG	HB2	1.85	-1.0	1
UNMAPPED	150	GLU	HG2	2.21	-1.0	2
UNMAPPED	21	GLN	HE22	7.59	-1.0	1
UNMAPPED	50	GLN	CA	57.3	-1.0	1
UNMAPPED	57	LYS	CA	57.2	-1.0	1
UNMAPPED	156	LYS	HE2	2.94	-1.0	1
UNMAPPED	73	THR	HG21	1.17	-1.0	1
UNMAPPED	49	ASN	CB	38.5	-1.0	1
UNMAPPED	56	ASP	CA	54.5	-1.0	1
UNMAPPED	54	GLY	N	110.5	-1.0	1
UNMAPPED	21	GLN	N	121.3	-1.0	1
UNMAPPED	74	GLY	H	8.49	-1.0	1
UNMAPPED	28	ILE	H	8.44	-1.0	1
UNMAPPED	154	LYS	HE2	2.96	-1.0	1
UNMAPPED	70	ILE	HG12	1.11	-1.0	2
UNMAPPED	6	LYS	HG3	1.38	-1.0	4
UNMAPPED	41	LYS	HG2	1.66	-1.0	1
UNMAPPED	80	VAL	HG21	0.88	-1.0	4
UNMAPPED	91	VAL	H	7.99	-1.0	1
UNMAPPED	124	LYS	HB3	1.87	-1.0	1
UNMAPPED	11	GLU	CB	30.2	-1.0	1
UNMAPPED	44	LEU	HD22	0.1	-1.0	1
UNMAPPED	24	ALA	N	123.1	-1.0	1
UNMAPPED	15	SER	HB3	4.33	-1.0	2
UNMAPPED	153	GLU	H	8.01	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	102	ALA	CA	54.5	-1.0	1
UNMAPPED	11	GLU	N	120.6	-1.0	1
UNMAPPED	52	ASN	HD21	6.78	-1.0	1
UNMAPPED	100	ARG	HG3	2.38	-1.0	1
UNMAPPED	50	GLN	HB3	2.06	-1.0	1
UNMAPPED	95	PRO	CB	32.2	-1.0	1
UNMAPPED	43	THR	CB	68.4	-1.0	1
UNMAPPED	14	THR	HB	3.76	-1.0	1
UNMAPPED	55	PRO	HG3	2.06	-1.0	1
UNMAPPED	78	LYS	N	123.9	-1.0	1
UNMAPPED	119	ALA	C	180.2	-1.0	1
UNMAPPED	21	GLN	HG3	2.41	-1.0	1
UNMAPPED	77	SER	H	8.25	-1.0	1
UNMAPPED	43	THR	N	117.3	-1.0	1
UNMAPPED	41	LYS	HG3	1.66	-1.0	1
UNMAPPED	18	ARG	HA	4.07	-1.0	1
UNMAPPED	33	ASP	HA	4.75	-1.0	1
UNMAPPED	28	ILE	HB	1.71	-1.0	1
UNMAPPED	39	GLN	HG3	2.37	-1.0	1
UNMAPPED	152	ALA	HB1	1.41	-1.0	1
UNMAPPED	78	LYS	CA	56.3	-1.0	1
UNMAPPED	70	ILE	CG1	27.7	-1.0	1
UNMAPPED	156	LYS	HG3	1.34	-1.0	1
UNMAPPED	68	LEU	CA	55.3	-1.0	1
UNMAPPED	30	LYS	HD3	1.74	-1.0	2
UNMAPPED	28	ILE	CB	40.5	-1.0	1
UNMAPPED	47	HIS	N	121.1	-1.0	1
UNMAPPED	90	PHE	N	122.8	-1.0	1
UNMAPPED	67	THR	HB	4.34	-1.0	1
UNMAPPED	20	VAL	CA	68.2	-1.0	1
UNMAPPED	23	PHE	HA	3.88	-1.0	1
UNMAPPED	90	PHE	HB3	3.06	-1.0	2
UNMAPPED	4	THR	C	174.6	-1.0	1
UNMAPPED	33	ASP	HB3	2.82	-1.0	2
UNMAPPED	86	LYS	CB	32.8	-1.0	1
UNMAPPED	50	GLN	H	7.69	-1.0	1
UNMAPPED	21	GLN	NE2	114.0	-1.0	1
UNMAPPED	120	GLU	C	178.7	-1.0	1
UNMAPPED	122	SER	C	176.0	-1.0	1
UNMAPPED	58	LEU	HB3	1.69	-1.0	2
UNMAPPED	38	ALA	CB	18.1	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	54	GLY	HA3	4.09	-1.0	1
UNMAPPED	53	SER	N	117.9	-1.0	1
UNMAPPED	73	THR	H	8.02	-1.0	1
UNMAPPED	101	LEU	C	173.8	-1.0	1
UNMAPPED	154	LYS	HA	4.26	-1.0	1
UNMAPPED	103	ALA	CB	18.4	-1.0	1
UNMAPPED	68	LEU	H	8.16	-1.0	1
UNMAPPED	37	SER	HA	4.69	-1.0	1
UNMAPPED	20	VAL	HA	3.57	-1.0	1
UNMAPPED	6	LYS	HB2	1.79	-1.0	1
UNMAPPED	82	ILE	HD12	0.83	-1.0	1
UNMAPPED	13	GLN	H	7.91	-1.0	1
UNMAPPED	35	SER	HA	4.84	-1.0	1
UNMAPPED	78	LYS	CB	33.0	-1.0	1
UNMAPPED	102	ALA	H	8.01	-1.0	1
UNMAPPED	42	GLN	HG2	2.38	-1.0	1
UNMAPPED	70	ILE	HB	1.82	-1.0	1
UNMAPPED	80	VAL	N	121.8	-1.0	1
UNMAPPED	28	ILE	C	173.6	-1.0	1
UNMAPPED	25	ASP	C	176.0	-1.0	1
UNMAPPED	153	GLU	HB2	1.96	-1.0	1
UNMAPPED	124	LYS	HA	4.11	-1.0	1
UNMAPPED	9	ALA	N	121.6	-1.0	1
UNMAPPED	150	GLU	HB3	1.99	-1.0	1
UNMAPPED	60	LEU	N	123.4	-1.0	1
UNMAPPED	17	GLU	CA	60.5	-1.0	1
UNMAPPED	37	SER	H	9.43	-1.0	1
UNMAPPED	95	PRO	HD2	3.84	-1.0	1
UNMAPPED	85	ARG	CB	30.7	-1.0	1
UNMAPPED	24	ALA	HB1	1.55	-1.0	1
UNMAPPED	51	LYS	H	7.85	-1.0	1
UNMAPPED	61	GLN	HB2	2.08	-1.0	1
UNMAPPED	101	LEU	HG	1.44	-1.0	1
UNMAPPED	76	LYS	HE3	2.95	-1.0	1
UNMAPPED	4	THR	HG21	1.2	-1.0	1
UNMAPPED	85	ARG	N	124.4	-1.0	1
UNMAPPED	55	PRO	HG2	2.06	-1.0	1
UNMAPPED	147	ALA	HB1	1.42	-1.0	1
UNMAPPED	98	ALA	C	179.8	-1.0	1
UNMAPPED	100	ARG	HB2	2.08	-1.0	1
UNMAPPED	7	THR	CG2	22.3	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	51	LYS	HD3	1.54	-1.0	4
UNMAPPED	18	ARG	HD3	3.22	-1.0	2
UNMAPPED	29	ARG	HG2	1.41	-1.0	1
UNMAPPED	18	ARG	CA	58.3	-1.0	1
UNMAPPED	95	PRO	HG3	1.97	-1.0	1
UNMAPPED	30	LYS	HE2	2.21	-1.0	2
UNMAPPED	101	LEU	HB3	1.82	-1.0	1
UNMAPPED	82	ILE	CA	61.1	-1.0	1
UNMAPPED	67	THR	N	116.1	-1.0	1
UNMAPPED	36	VAL	HA	4.28	-1.0	1
UNMAPPED	73	THR	CA	62.0	-1.0	1
UNMAPPED	48	LEU	HB3	1.79	-1.0	2
UNMAPPED	31	SER	CA	56.4	-1.0	1
UNMAPPED	82	ILE	CB	38.8	-1.0	1
UNMAPPED	4	THR	CB	71.4	-1.0	1
UNMAPPED	98	ALA	HB3	1.49	-1.0	1
UNMAPPED	19	LEU	CD2	28.8	-1.0	1
UNMAPPED	12	ARG	C	174.1	-1.0	1
UNMAPPED	31	SER	CB	65.7	-1.0	1
UNMAPPED	55	PRO	HB3	2.35	-1.0	2
UNMAPPED	58	LEU	HD22	0.86	-1.0	1
UNMAPPED	15	SER	CA	56.7	-1.0	1
UNMAPPED	13	GLN	CA	56.6	-1.0	1
UNMAPPED	36	VAL	HG13	0.55	-1.0	1
UNMAPPED	45	ILE	HG22	0.86	-1.0	1
UNMAPPED	85	ARG	HB3	1.93	-1.0	2
UNMAPPED	153	GLU	HG2	2.28	-1.0	1
UNMAPPED	147	ALA	N	121.8	-1.0	1
UNMAPPED	149	ARG	HD3	3.2	-1.0	1
UNMAPPED	47	HIS	HE1	7.46	-1.0	1
UNMAPPED	97	GLU	C	178.5	-1.0	1
UNMAPPED	147	ALA	CB	19.1	-1.0	1
UNMAPPED	17	GLU	H	8.8	-1.0	1
UNMAPPED	7	THR	HA	4.0	-1.0	1
UNMAPPED	22	GLN	C	178.8	-1.0	1
UNMAPPED	19	LEU	HD12	0.82	-1.0	1
UNMAPPED	150	GLU	HA	4.11	-1.0	1
UNMAPPED	91	VAL	HB	1.92	-1.0	1
UNMAPPED	23	PHE	H	8.57	-1.0	1
UNMAPPED	6	LYS	HA	3.86	-1.0	1
UNMAPPED	83	GLU	HA	4.27	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	150	GLU	H	8.21	-1.0	1
UNMAPPED	3	VAL	N	121.0	-1.0	1
UNMAPPED	5	ILE	CB	35.6	-1.0	1
UNMAPPED	44	LEU	N	122.8	-1.0	1
UNMAPPED	152	ALA	HA	4.23	-1.0	1
UNMAPPED	19	LEU	HD21	0.95	-1.0	1
UNMAPPED	6	LYS	HD2	1.63	-1.0	4
UNMAPPED	103	ALA	C	179.0	-1.0	1
UNMAPPED	19	LEU	CA	57.7	-1.0	1
UNMAPPED	52	ASN	HA	4.69	-1.0	1
UNMAPPED	155	ASP	N	121.0	-1.0	1
UNMAPPED	148	LYS	HB2	1.39	-1.0	1
UNMAPPED	26	ALA	C	175.6	-1.0	1
UNMAPPED	5	ILE	HD12	0.37	-1.0	1
UNMAPPED	86	LYS	HA	4.22	-1.0	1
UNMAPPED	82	ILE	HB	1.78	-1.0	1
UNMAPPED	16	VAL	HG21	1.05	-1.0	1
UNMAPPED	123	ALA	HB1	1.5	-1.0	1
UNMAPPED	76	LYS	HG3	1.39	-1.0	1
UNMAPPED	6	LYS	CA	60.6	-1.0	1
UNMAPPED	38	ALA	HB2	1.46	-1.0	1
UNMAPPED	60	LEU	HD12	0.83	-1.0	1
UNMAPPED	149	ARG	HG3	1.58	-1.0	1
UNMAPPED	70	ILE	HD12	0.82	-1.0	1
UNMAPPED	8	LEU	HD13	0.96	-1.0	1
UNMAPPED	98	ALA	H	7.97	-1.0	1
UNMAPPED	5	ILE	HA	3.67	-1.0	1
UNMAPPED	45	ILE	N	119.5	-1.0	1
UNMAPPED	89	THR	N	115.2	-1.0	1
UNMAPPED	34	ASP	CB	44.1	-1.0	1
UNMAPPED	91	VAL	HG23	0.83	-1.0	4
UNMAPPED	152	ALA	HB2	1.41	-1.0	1
UNMAPPED	49	ASN	HB2	2.84	-1.0	1
UNMAPPED	148	LYS	HG3	1.78	-1.0	4
UNMAPPED	43	THR	H	8.21	-1.0	1
UNMAPPED	30	LYS	C	174.0	-1.0	1
UNMAPPED	104	GLU	H	7.75	-1.0	1
UNMAPPED	51	LYS	HG2	1.3	-1.0	4
UNMAPPED	60	LEU	HD11	0.83	-1.0	1
UNMAPPED	12	ARG	HD2	3.2	-1.0	1
UNMAPPED	5	ILE	HG13	1.57	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	29	ARG	HD3	3.09	-1.0	1
UNMAPPED	32	ALA	CA	55.1	-1.0	1
UNMAPPED	19	LEU	C	178.8	-1.0	1
UNMAPPED	48	LEU	CD1	26.0	-1.0	1
UNMAPPED	23	PHE	HD2	7.08	-1.0	1
UNMAPPED	149	ARG	HG2	1.58	-1.0	1
UNMAPPED	77	SER	N	116.8	-1.0	1
UNMAPPED	60	LEU	HD22	0.83	-1.0	1
UNMAPPED	40	GLU	HA	3.89	-1.0	1
UNMAPPED	40	GLU	HG3	2.39	-1.0	1
UNMAPPED	70	ILE	CD1	13.1	-1.0	1
UNMAPPED	26	ALA	HB2	1.11	-1.0	1
UNMAPPED	79	SER	C	173.9	-1.0	1
UNMAPPED	80	VAL	CG1	20.8	-1.0	4
UNMAPPED	83	GLU	N	125.4	-1.0	1
UNMAPPED	60	LEU	HD21	0.83	-1.0	1
UNMAPPED	67	THR	HG22	1.16	-1.0	1
UNMAPPED	50	GLN	N	119.1	-1.0	1
UNMAPPED	39	GLN	CA	57.5	-1.0	1
UNMAPPED	85	ARG	HG3	1.57	-1.0	1
UNMAPPED	21	GLN	HA	4.05	-1.0	1
UNMAPPED	43	THR	HG23	1.26	-1.0	1
UNMAPPED	150	GLU	HG3	2.37	-1.0	2
UNMAPPED	12	ARG	HG2	2.15	-1.0	1
UNMAPPED	50	GLN	CB	28.8	-1.0	1
UNMAPPED	99	GLU	HA	4.11	-1.0	1
UNMAPPED	36	VAL	HG22	0.9	-1.0	1
UNMAPPED	71	PRO	HB3	2.25	-1.0	1
UNMAPPED	82	ILE	HG13	1.41	-1.0	1
UNMAPPED	101	LEU	HD21	0.88	-1.0	4
UNMAPPED	5	ILE	CD1	11.5	-1.0	1
UNMAPPED	94	ASP	CB	41.7	-1.0	1
UNMAPPED	122	SER	HA	4.17	-1.0	1
UNMAPPED	29	ARG	C	174.4	-1.0	1
UNMAPPED	71	PRO	CA	63.6	-1.0	1
UNMAPPED	93	ARG	HA	4.28	-1.0	1
UNMAPPED	68	LEU	CB	42.5	-1.0	1
UNMAPPED	70	ILE	HG13	1.43	-1.0	2
UNMAPPED	16	VAL	CG1	21.5	-1.0	1
UNMAPPED	45	ILE	HA	3.38	-1.0	1
UNMAPPED	48	LEU	HG	1.79	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	96	GLN	HG3	2.38	-1.0	1
UNMAPPED	68	LEU	N	125.0	-1.0	1
UNMAPPED	33	ASP	C	175.3	-1.0	1
UNMAPPED	102	ALA	CB	18.2	-1.0	1
UNMAPPED	52	ASN	HD22	6.78	-1.0	1
UNMAPPED	53	SER	CA	58.5	-1.0	1
UNMAPPED	73	THR	CB	69.9	-1.0	1
UNMAPPED	52	ASN	CB	39.1	-1.0	1
UNMAPPED	43	THR	CA	67.2	-1.0	1
UNMAPPED	60	LEU	H	7.99	-1.0	1
UNMAPPED	148	LYS	HB3	1.39	-1.0	1
UNMAPPED	99	GLU	HB2	2.15	-1.0	1
UNMAPPED	42	GLN	CD	179.8	-1.0	1
UNMAPPED	58	LEU	CA	56.0	-1.0	1
UNMAPPED	21	GLN	HG2	2.41	-1.0	1
UNMAPPED	44	LEU	CA	58.8	-1.0	1
UNMAPPED	58	LEU	HD21	0.86	-1.0	1
UNMAPPED	78	LYS	HE2	2.93	-1.0	1
UNMAPPED	121	GLU	C	178.8	-1.0	1
UNMAPPED	41	LYS	HD3	1.38	-1.0	1
UNMAPPED	85	ARG	H	8.32	-1.0	1
UNMAPPED	47	HIS	CA	60.4	-1.0	1
UNMAPPED	44	LEU	CG	26.4	-1.0	1
UNMAPPED	30	LYS	HD2	1.15	-1.0	2
UNMAPPED	30	LYS	H	8.41	-1.0	1
UNMAPPED	57	LYS	N	121.0	-1.0	1
UNMAPPED	45	ILE	C	178.0	-1.0	1
UNMAPPED	69	ASN	HB2	2.05	-1.0	1
UNMAPPED	101	LEU	CB	38.8	-1.0	1
UNMAPPED	94	ASP	HA	4.81	-1.0	1
UNMAPPED	84	VAL	CA	62.7	-1.0	1
UNMAPPED	16	VAL	HB	1.98	-1.0	1
UNMAPPED	60	LEU	HG	1.37	-1.0	1
UNMAPPED	76	LYS	HD3	1.65	-1.0	1
UNMAPPED	58	LEU	HD13	0.86	-1.0	1
UNMAPPED	58	LEU	HB2	1.57	-1.0	2
UNMAPPED	38	ALA	CA	55.7	-1.0	1
UNMAPPED	15	SER	C	174.8	-1.0	1
UNMAPPED	46	ASP	HB2	2.62	-1.0	2
UNMAPPED	80	VAL	C	175.2	-1.0	1
UNMAPPED	3	VAL	CG1	21.7	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	4	THR	HA	4.82	-1.0	1
UNMAPPED	92	LYS	HE2	2.95	-1.0	1
UNMAPPED	84	VAL	H	8.2	-1.0	1
UNMAPPED	156	LYS	HG2	1.34	-1.0	1
UNMAPPED	20	VAL	HB	2.18	-1.0	1
UNMAPPED	67	THR	C	173.6	-1.0	1
UNMAPPED	82	ILE	HD13	0.83	-1.0	1
UNMAPPED	43	THR	HG21	1.26	-1.0	1
UNMAPPED	22	GLN	CG	34.3	-1.0	1
UNMAPPED	42	GLN	HG3	2.38	-1.0	1
UNMAPPED	53	SER	H	8.01	-1.0	1
UNMAPPED	91	VAL	C	174.7	-1.0	1
UNMAPPED	82	ILE	HG12	1.41	-1.0	1
UNMAPPED	6	LYS	C	179.1	-1.0	1
UNMAPPED	94	ASP	HB2	2.73	-1.0	2
UNMAPPED	17	GLU	N	117.2	-1.0	1
UNMAPPED	58	LEU	HD12	0.86	-1.0	1
UNMAPPED	69	ASN	C	177.2	-1.0	1
UNMAPPED	96	GLN	HG2	2.38	-1.0	1
UNMAPPED	99	GLU	CB	30.2	-1.0	1
UNMAPPED	96	GLN	CA	59.4	-1.0	1
UNMAPPED	17	GLU	CB	29.0	-1.0	1
UNMAPPED	124	LYS	CA	59.1	-1.0	1
UNMAPPED	58	LEU	HD11	0.86	-1.0	1
UNMAPPED	85	ARG	CA	56.2	-1.0	1
UNMAPPED	154	LYS	HG3	1.38	-1.0	1
UNMAPPED	61	GLN	HB3	2.08	-1.0	1
UNMAPPED	23	PHE	CB	37.0	-1.0	1
UNMAPPED	85	ARG	HA	4.28	-1.0	1
UNMAPPED	75	GLY	HA3	3.91	-1.0	1
UNMAPPED	36	VAL	C	174.3	-1.0	1
UNMAPPED	36	VAL	CG2	23.2	-1.0	1
UNMAPPED	12	ARG	N	115.8	-1.0	1
UNMAPPED	11	GLU	HA	3.98	-1.0	1
UNMAPPED	9	ALA	HA	3.7	-1.0	1
UNMAPPED	100	ARG	HB3	2.08	-1.0	1
UNMAPPED	72	GLY	CA	45.4	-1.0	1
UNMAPPED	25	ASP	N	122.5	-1.0	1
UNMAPPED	151	ALA	N	122.7	-1.0	1
UNMAPPED	18	ARG	HD2	3.17	-1.0	2
UNMAPPED	99	GLU	CA	59.5	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	67	THR	CA	61.8	-1.0	1
UNMAPPED	29	ARG	HG3	1.41	-1.0	1
UNMAPPED	97	GLU	HA	4.14	-1.0	1
UNMAPPED	30	LYS	HE3	2.32	-1.0	2
UNMAPPED	101	LEU	HB2	1.82	-1.0	1
UNMAPPED	99	GLU	H	8.27	-1.0	1
UNMAPPED	7	THR	HG21	1.21	-1.0	1
UNMAPPED	22	GLN	HB3	2.38	-1.0	2
UNMAPPED	104	GLU	HA	4.18	-1.0	1
UNMAPPED	124	LYS	C	178.5	-1.0	1
UNMAPPED	45	ILE	H	8.01	-1.0	1
UNMAPPED	24	ALA	HA	3.93	-1.0	1
UNMAPPED	39	GLN	C	177.6	-1.0	1
UNMAPPED	121	GLU	CB	29.4	-1.0	1
UNMAPPED	48	LEU	CG	26.8	-1.0	1
UNMAPPED	4	THR	CA	60.4	-1.0	1
UNMAPPED	93	ARG	HD3	3.08	-1.0	1
UNMAPPED	48	LEU	HD21	0.76	-1.0	1
UNMAPPED	57	LYS	HB3	1.63	-1.0	1
UNMAPPED	34	ASP	H	7.32	-1.0	1
UNMAPPED	73	THR	HG22	1.17	-1.0	1
UNMAPPED	81	GLN	CA	55.7	-1.0	1
UNMAPPED	78	LYS	HA	4.27	-1.0	1
UNMAPPED	122	SER	CA	61.7	-1.0	1
UNMAPPED	8	LEU	HD22	0.96	-1.0	1
UNMAPPED	77	SER	HB3	3.82	-1.0	1
UNMAPPED	68	LEU	HB2	1.55	-1.0	1
UNMAPPED	36	VAL	HG12	0.55	-1.0	1
UNMAPPED	61	GLN	N	120.3	-1.0	1
UNMAPPED	22	GLN	HA	4.04	-1.0	1
UNMAPPED	49	ASN	HA	4.56	-1.0	1
UNMAPPED	11	GLU	HG3	2.38	-1.0	1
UNMAPPED	85	ARG	HB2	1.74	-1.0	2
UNMAPPED	151	ALA	C	177.8	-1.0	1
UNMAPPED	76	LYS	HA	4.32	-1.0	1
UNMAPPED	89	THR	HG21	1.15	-1.0	1
UNMAPPED	154	LYS	CB	33.3	-1.0	1
UNMAPPED	12	ARG	HB3	1.43	-1.0	1
UNMAPPED	11	GLU	HG2	2.38	-1.0	1
UNMAPPED	35	SER	C	172.0	-1.0	1
UNMAPPED	102	ALA	HB1	1.47	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	90	PHE	HA	4.62	-1.0	1
UNMAPPED	124	LYS	H	7.77	-1.0	1
UNMAPPED	32	ALA	HA	3.72	-1.0	1
UNMAPPED	3	VAL	C	174.3	-1.0	1
UNMAPPED	5	ILE	HG21	0.86	-1.0	1
UNMAPPED	19	LEU	HD13	0.82	-1.0	1
UNMAPPED	40	GLU	HB2	1.69	-1.0	2
UNMAPPED	41	LYS	H	8.43	-1.0	1
UNMAPPED	43	THR	CG2	21.7	-1.0	1
UNMAPPED	156	LYS	H	7.64	-1.0	1
UNMAPPED	94	ASP	CA	52.4	-1.0	1
UNMAPPED	84	VAL	C	175.6	-1.0	1
UNMAPPED	82	ILE	HD11	0.83	-1.0	1
UNMAPPED	100	ARG	CA	59.2	-1.0	1
UNMAPPED	57	LYS	HA	4.14	-1.0	1
UNMAPPED	81	GLN	C	175.1	-1.0	1
UNMAPPED	44	LEU	HB2	0.96	-1.0	2
UNMAPPED	71	PRO	HD2	3.65	-1.0	1
UNMAPPED	52	ASN	C	174.6	-1.0	1
UNMAPPED	3	VAL	HG21	0.98	-1.0	1
UNMAPPED	27	GLY	H	7.27	-1.0	1
UNMAPPED	39	GLN	HB3	2.06	-1.0	1
UNMAPPED	44	LEU	HA	3.64	-1.0	1
UNMAPPED	16	VAL	HG22	1.05	-1.0	1
UNMAPPED	79	SER	HA	4.47	-1.0	1
UNMAPPED	45	ILE	CA	65.3	-1.0	1
UNMAPPED	84	VAL	HG11	0.88	-1.0	1
UNMAPPED	73	THR	HG23	1.17	-1.0	1
UNMAPPED	44	LEU	HG	1.04	-1.0	1
UNMAPPED	8	LEU	HD12	0.96	-1.0	1
UNMAPPED	93	ARG	CA	55.8	-1.0	1
UNMAPPED	37	SER	HB2	3.89	-1.0	2
UNMAPPED	34	ASP	CA	55.1	-1.0	1
UNMAPPED	91	VAL	HG22	0.83	-1.0	4
UNMAPPED	18	ARG	C	177.6	-1.0	1
UNMAPPED	122	SER	H	8.36	-1.0	1
UNMAPPED	23	PHE	HE1	6.99	-1.0	1
UNMAPPED	93	ARG	HG3	1.55	-1.0	1
UNMAPPED	10	ALA	CA	55.0	-1.0	1
UNMAPPED	52	ASN	H	8.08	-1.0	1
UNMAPPED	29	ARG	H	8.64	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	ILE	HG12	1.11	-1.0	2
UNMAPPED	29	ARG	HD2	3.09	-1.0	1
UNMAPPED	70	ILE	HG23	0.9	-1.0	1
UNMAPPED	7	THR	CA	66.1	-1.0	1
UNMAPPED	92	LYS	HB2	1.67	-1.0	1
UNMAPPED	82	ILE	CD1	17.3	-1.0	1
UNMAPPED	57	LYS	H	8.21	-1.0	1
UNMAPPED	98	ALA	CB	17.7	-1.0	1
UNMAPPED	13	GLN	C	174.0	-1.0	1
UNMAPPED	148	LYS	C	176.1	-1.0	1
UNMAPPED	40	GLU	HG2	2.39	-1.0	1
UNMAPPED	22	GLN	N	121.0	-1.0	1
UNMAPPED	61	GLN	HA	4.19	-1.0	1
UNMAPPED	30	LYS	HA	4.73	-1.0	1
UNMAPPED	30	LYS	CB	37.1	-1.0	1
UNMAPPED	72	GLY	C	174.0	-1.0	1
UNMAPPED	84	VAL	HG22	0.88	-1.0	1
UNMAPPED	18	ARG	HG2	1.56	-1.0	1
UNMAPPED	86	LYS	HB2	1.7	-1.0	1
UNMAPPED	101	LEU	H	8.01	-1.0	1
UNMAPPED	3	VAL	H	8.31	-1.0	1
UNMAPPED	21	GLN	CG	33.4	-1.0	1
UNMAPPED	12	ARG	HG3	2.15	-1.0	1
UNMAPPED	45	ILE	HD13	0.71	-1.0	1
UNMAPPED	17	GLU	HB3	2.0	-1.0	2
UNMAPPED	36	VAL	HG23	0.9	-1.0	1
UNMAPPED	16	VAL	HG11	0.88	-1.0	1
UNMAPPED	8	LEU	N	125.3	-1.0	1
UNMAPPED	98	ALA	N	121.7	-1.0	1
UNMAPPED	60	LEU	CB	42.3	-1.0	1
UNMAPPED	59	THR	CA	63.0	-1.0	1
UNMAPPED	56	ASP	HB3	2.64	-1.0	1
UNMAPPED	49	ASN	N	117.5	-1.0	1
UNMAPPED	149	ARG	CA	58.1	-1.0	1
UNMAPPED	99	GLU	HG3	2.4	-1.0	1
UNMAPPED	90	PHE	C	174.5	-1.0	1
UNMAPPED	152	ALA	H	7.86	-1.0	1
UNMAPPED	36	VAL	CA	60.9	-1.0	1
UNMAPPED	42	GLN	N	117.7	-1.0	1
UNMAPPED	84	VAL	CB	32.7	-1.0	1
UNMAPPED	59	THR	H	7.93	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	16	VAL	CG2	24.1	-1.0	1
UNMAPPED	103	ALA	CA	54.2	-1.0	1
UNMAPPED	30	LYS	HG2	0.28	-1.0	2
UNMAPPED	84	VAL	N	122.5	-1.0	1
UNMAPPED	120	GLU	CA	59.2	-1.0	1
UNMAPPED	26	ALA	CA	51.5	-1.0	1
UNMAPPED	42	GLN	CA	58.3	-1.0	1
UNMAPPED	53	SER	CB	64.1	-1.0	1
UNMAPPED	59	THR	HG21	1.16	-1.0	1
UNMAPPED	93	ARG	C	174.9	-1.0	1
UNMAPPED	19	LEU	HA	4.33	-1.0	1
UNMAPPED	99	GLU	HB3	2.15	-1.0	1
UNMAPPED	42	GLN	CG	33.1	-1.0	1
UNMAPPED	31	SER	N	116.2	-1.0	1
UNMAPPED	5	ILE	CG1	27.7	-1.0	1
UNMAPPED	44	LEU	CB	41.0	-1.0	1
UNMAPPED	83	GLU	HG2	2.16	-1.0	1
UNMAPPED	78	LYS	HE3	2.93	-1.0	1
UNMAPPED	7	THR	H	8.05	-1.0	1
UNMAPPED	41	LYS	HD2	1.38	-1.0	1
UNMAPPED	17	GLU	HA	3.87	-1.0	1
UNMAPPED	152	ALA	HB3	1.41	-1.0	1
UNMAPPED	60	LEU	HD13	0.83	-1.0	1
UNMAPPED	100	ARG	H	8.18	-1.0	1
UNMAPPED	91	VAL	N	122.6	-1.0	1
UNMAPPED	28	ILE	CG2	18.1	-1.0	1
UNMAPPED	89	THR	CB	69.4	-1.0	1
UNMAPPED	86	LYS	CA	56.5	-1.0	1
UNMAPPED	83	GLU	H	8.39	-1.0	1
UNMAPPED	58	LEU	CB	42.1	-1.0	1
UNMAPPED	79	SER	N	116.8	-1.0	1
UNMAPPED	35	SER	CA	57.9	-1.0	1
UNMAPPED	3	VAL	HB	2.14	-1.0	1
UNMAPPED	80	VAL	HB	2.02	-1.0	1
UNMAPPED	76	LYS	N	121.1	-1.0	1
UNMAPPED	58	LEU	N	121.4	-1.0	1
UNMAPPED	16	VAL	HA	3.37	-1.0	1
UNMAPPED	2	ASP	CA	54.6	-1.0	1
UNMAPPED	76	LYS	HD2	1.65	-1.0	1
UNMAPPED	149	ARG	HB2	1.86	-1.0	1
UNMAPPED	8	LEU	CD1	26.9	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	THR	HG21	1.22	-1.0	1
UNMAPPED	76	LYS	CB	33.1	-1.0	1
UNMAPPED	148	LYS	N	118.6	-1.0	1
UNMAPPED	121	GLU	HB3	2.07	-1.0	1
UNMAPPED	90	PHE	CB	40.0	-1.0	1
UNMAPPED	46	ASP	HB3	2.79	-1.0	2
UNMAPPED	103	ALA	HB1	1.47	-1.0	1
UNMAPPED	91	VAL	CB	33.2	-1.0	1
UNMAPPED	99	GLU	N	120.5	-1.0	1
UNMAPPED	75	GLY	CA	45.4	-1.0	1
UNMAPPED	25	ASP	HB3	2.88	-1.0	2
UNMAPPED	92	LYS	HE3	2.95	-1.0	1
UNMAPPED	93	ARG	HD2	3.08	-1.0	1
UNMAPPED	89	THR	HA	4.27	-1.0	1
UNMAPPED	104	GLU	CA	58.3	-1.0	1
UNMAPPED	45	ILE	CG1	29.3	-1.0	1
UNMAPPED	80	VAL	CB	32.8	-1.0	1
UNMAPPED	154	LYS	HB2	1.8	-1.0	1
UNMAPPED	96	GLN	N	117.9	-1.0	1
UNMAPPED	20	VAL	HG12	0.88	-1.0	1
UNMAPPED	123	ALA	CB	18.2	-1.0	1
UNMAPPED	46	ASP	C	178.2	-1.0	1
UNMAPPED	9	ALA	HB2	1.38	-1.0	1
UNMAPPED	2	ASP	CB	41.5	-1.0	1
UNMAPPED	124	LYS	CB	32.8	-1.0	1
UNMAPPED	33	ASP	CA	54.1	-1.0	1
UNMAPPED	123	ALA	CA	55.0	-1.0	1
UNMAPPED	123	ALA	N	124.2	-1.0	1
UNMAPPED	102	ALA	HA	4.19	-1.0	1
UNMAPPED	101	LEU	HA	4.41	-1.0	1
UNMAPPED	4	THR	HG23	1.2	-1.0	1
UNMAPPED	25	ASP	CA	57.1	-1.0	1
UNMAPPED	50	GLN	HA	4.11	-1.0	1
UNMAPPED	89	THR	HB	4.27	-1.0	4
UNMAPPED	55	PRO	HB2	1.91	-1.0	2
UNMAPPED	29	ARG	HB3	1.69	-1.0	1
UNMAPPED	124	LYS	HD3	1.59	-1.0	1
UNMAPPED	44	LEU	C	176.6	-1.0	1
UNMAPPED	21	GLN	HB2	2.24	-1.0	1
UNMAPPED	96	GLN	HB3	2.11	-1.0	1
UNMAPPED	26	ALA	HA	3.49	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	2	ASP	HB2	2.48	-1.0	2
UNMAPPED	42	GLN	HA	3.81	-1.0	1
UNMAPPED	47	HIS	C	177.5	-1.0	1
UNMAPPED	86	LYS	HB3	1.7	-1.0	1
UNMAPPED	4	THR	HG22	1.2	-1.0	1
UNMAPPED	154	LYS	C	175.7	-1.0	1
UNMAPPED	22	GLN	HB2	1.69	-1.0	2
UNMAPPED	79	SER	H	8.25	-1.0	1
UNMAPPED	82	ILE	C	175.3	-1.0	1
UNMAPPED	61	GLN	HG2	2.35	-1.0	1
UNMAPPED	156	LYS	CB	33.8	-1.0	1
UNMAPPED	53	SER	HA	4.45	-1.0	1
UNMAPPED	75	GLY	H	8.24	-1.0	1
UNMAPPED	149	ARG	HA	4.15	-1.0	1
UNMAPPED	98	ALA	HB1	1.49	-1.0	1
UNMAPPED	124	LYS	HD2	1.59	-1.0	1
UNMAPPED	153	GLU	HB3	1.96	-1.0	1
UNMAPPED	11	GLU	HB2	2.13	-1.0	1
UNMAPPED	78	LYS	HD2	1.69	-1.0	4
UNMAPPED	5	ILE	H	8.42	-1.0	1
UNMAPPED	70	ILE	N	122.6	-1.0	1
UNMAPPED	122	SER	CB	62.7	-1.0	1
UNMAPPED	22	GLN	HE22	7.16	-1.0	1
UNMAPPED	68	LEU	HB3	1.55	-1.0	1
UNMAPPED	36	VAL	HG11	0.55	-1.0	1
UNMAPPED	42	GLN	HB3	2.14	-1.0	1
UNMAPPED	60	LEU	C	177.0	-1.0	1
UNMAPPED	148	LYS	HD2	2.61	-1.0	4
UNMAPPED	12	ARG	CB	29.7	-1.0	1
UNMAPPED	151	ALA	CB	19.0	-1.0	1
UNMAPPED	12	ARG	HB2	1.43	-1.0	1
UNMAPPED	16	VAL	CA	67.3	-1.0	1
UNMAPPED	59	THR	HA	4.15	-1.0	1
UNMAPPED	89	THR	HG22	1.15	-1.0	1
UNMAPPED	28	ILE	HG22	0.6	-1.0	1
UNMAPPED	37	SER	CA	56.8	-1.0	1
UNMAPPED	33	ASP	H	7.76	-1.0	1
UNMAPPED	47	HIS	HB2	3.25	-1.0	2
UNMAPPED	86	LYS	HG3	1.37	-1.0	1
UNMAPPED	40	GLU	HB3	2.51	-1.0	2
UNMAPPED	21	GLN	HB3	2.24	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	86	LYS	HG2	1.37	-1.0	1
UNMAPPED	71	PRO	CB	32.3	-1.0	1
UNMAPPED	3	VAL	CB	33.7	-1.0	1
UNMAPPED	5	ILE	N	122.4	-1.0	1
UNMAPPED	68	LEU	C	175.6	-1.0	1
UNMAPPED	57	LYS	HE3	2.95	-1.0	1
UNMAPPED	19	LEU	CG	27.3	-1.0	1
UNMAPPED	43	THR	HB	4.33	-1.0	1
UNMAPPED	90	PHE	HE2	7.26	-1.0	1
UNMAPPED	39	GLN	HB2	2.06	-1.0	1
UNMAPPED	9	ALA	C	178.2	-1.0	1
UNMAPPED	74	GLY	HA2	3.94	-1.0	1
UNMAPPED	16	VAL	HG23	1.05	-1.0	1
UNMAPPED	74	GLY	N	111.2	-1.0	1
UNMAPPED	28	ILE	N	123.1	-1.0	1
UNMAPPED	84	VAL	HG12	0.88	-1.0	1
UNMAPPED	54	GLY	H	8.16	-1.0	1
UNMAPPED	97	GLU	CA	58.8	-1.0	1
UNMAPPED	8	LEU	HD11	0.96	-1.0	1
UNMAPPED	15	SER	H	8.38	-1.0	1
UNMAPPED	37	SER	HB3	4.38	-1.0	2
UNMAPPED	34	ASP	HB3	2.86	-1.0	2
UNMAPPED	49	ASN	C	176.1	-1.0	1
UNMAPPED	91	VAL	HG21	0.83	-1.0	4
UNMAPPED	152	ALA	N	121.4	-1.0	1
UNMAPPED	42	GLN	HE22	7.83	-1.0	1
UNMAPPED	71	PRO	HG3	1.93	-1.0	1
UNMAPPED	10	ALA	HB3	1.52	-1.0	1
UNMAPPED	38	ALA	H	9.02	-1.0	1
UNMAPPED	148	LYS	CA	56.8	-1.0	1
UNMAPPED	7	THR	N	117.1	-1.0	1
UNMAPPED	44	LEU	CD2	23.4	-1.0	1
UNMAPPED	150	GLU	N	120.1	-1.0	1
UNMAPPED	13	GLN	HB3	2.16	-1.0	1
UNMAPPED	120	GLU	CB	24.8	-1.0	1
UNMAPPED	70	ILE	HG22	0.9	-1.0	1
UNMAPPED	7	THR	CB	68.1	-1.0	1
UNMAPPED	69	ASN	N	125.7	-1.0	1
UNMAPPED	76	LYS	H	8.11	-1.0	1
UNMAPPED	89	THR	C	173.1	-1.0	1
UNMAPPED	82	ILE	HG21	1.13	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	48	LEU	HD12	0.64	-1.0	1
UNMAPPED	55	PRO	CB	32.1	-1.0	1
UNMAPPED	51	LYS	HE3	2.92	-1.0	1
UNMAPPED	89	THR	H	8.03	-1.0	1
UNMAPPED	30	LYS	CA	52.8	-1.0	1
UNMAPPED	83	GLU	CB	30.6	-1.0	1
UNMAPPED	18	ARG	HG3	1.56	-1.0	1
UNMAPPED	81	GLN	HA	4.32	-1.0	1
UNMAPPED	58	LEU	H	8.11	-1.0	1
UNMAPPED	51	LYS	HB2	1.68	-1.0	1
UNMAPPED	51	LYS	HE2	2.92	-1.0	1
UNMAPPED	43	THR	HA	3.97	-1.0	1
UNMAPPED	4	THR	CG2	22.0	-1.0	1
UNMAPPED	59	THR	N	114.9	-1.0	1
UNMAPPED	45	ILE	HD12	0.71	-1.0	1
UNMAPPED	49	ASN	CA	54.5	-1.0	1
UNMAPPED	28	ILE	CD1	14.0	-1.0	1
UNMAPPED	147	ALA	HA	4.21	-1.0	1
UNMAPPED	8	LEU	HB3	1.82	-1.0	2
UNMAPPED	100	ARG	HD3	2.94	-1.0	1
UNMAPPED	36	VAL	N	120.4	-1.0	1
UNMAPPED	56	ASP	HB2	2.64	-1.0	1
UNMAPPED	119	ALA	CB	17.9	-1.0	1
UNMAPPED	77	SER	HA	4.4	-1.0	1
UNMAPPED	151	ALA	HB2	1.41	-1.0	1
UNMAPPED	97	GLU	HB2	1.94	-1.0	1
UNMAPPED	69	ASN	HA	4.11	-1.0	1
UNMAPPED	36	VAL	CB	35.0	-1.0	1
UNMAPPED	44	LEU	HD21	0.1	-1.0	1
UNMAPPED	50	GLN	HG3	2.42	-1.0	2
UNMAPPED	24	ALA	CA	55.7	-1.0	1
UNMAPPED	28	ILE	HG13	1.44	-1.0	2
UNMAPPED	34	ASP	HA	4.69	-1.0	1
UNMAPPED	58	LEU	C	177.5	-1.0	1
UNMAPPED	155	ASP	HB3	2.72	-1.0	2
UNMAPPED	48	LEU	HA	3.82	-1.0	1
UNMAPPED	11	GLU	CA	59.4	-1.0	1
UNMAPPED	123	ALA	HA	4.2	-1.0	1
UNMAPPED	30	LYS	HG3	0.73	-1.0	2
UNMAPPED	78	LYS	HB3	1.74	-1.0	1
UNMAPPED	10	ALA	HA	4.18	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	102	ALA	N	122.3	-1.0	1
UNMAPPED	67	THR	HA	4.29	-1.0	1
UNMAPPED	59	THR	HG22	1.16	-1.0	1
UNMAPPED	52	ASN	N	117.9	-1.0	1
UNMAPPED	22	GLN	HG2	2.27	-1.0	2
UNMAPPED	14	THR	HA	4.74	-1.0	1
UNMAPPED	28	ILE	HA	4.18	-1.0	1
UNMAPPED	149	ARG	HD2	3.2	-1.0	1
UNMAPPED	15	SER	N	118.1	-1.0	1
UNMAPPED	16	VAL	C	176.5	-1.0	1
UNMAPPED	83	GLU	HG3	2.16	-1.0	1
UNMAPPED	20	VAL	HG23	0.95	-1.0	1
UNMAPPED	32	ALA	H	8.46	-1.0	1
UNMAPPED	72	GLY	HA2	3.99	-1.0	1
UNMAPPED	3	VAL	HG11	0.93	-1.0	1
UNMAPPED	57	LYS	HB2	1.63	-1.0	1
UNMAPPED	6	LYS	H	8.07	-1.0	1
UNMAPPED	90	PHE	CA	57.6	-1.0	1
UNMAPPED	103	ALA	HB3	1.47	-1.0	1
UNMAPPED	70	ILE	CG2	17.3	-1.0	1
UNMAPPED	99	GLU	C	178.3	-1.0	1
UNMAPPED	43	THR	C	176.1	-1.0	1
UNMAPPED	35	SER	N	114.4	-1.0	1
UNMAPPED	55	PRO	HD3	3.84	-1.0	2
UNMAPPED	20	VAL	CB	32.0	-1.0	1
UNMAPPED	54	GLY	C	174.6	-1.0	1
UNMAPPED	92	LYS	HD3	1.75	-1.0	4
UNMAPPED	35	SER	CB	65.1	-1.0	1
UNMAPPED	45	ILE	CD1	13.8	-1.0	1
UNMAPPED	101	LEU	N	122.8	-1.0	1
UNMAPPED	11	GLU	C	178.0	-1.0	1
UNMAPPED	61	GLN	C	174.4	-1.0	1
UNMAPPED	78	LYS	HD3	1.69	-1.0	4
UNMAPPED	96	GLN	HA	4.08	-1.0	1
UNMAPPED	8	LEU	CD2	26.9	-1.0	1
UNMAPPED	75	GLY	N	108.6	-1.0	1
UNMAPPED	52	ASN	HB3	2.85	-1.0	2
UNMAPPED	4	THR	N	115.0	-1.0	1
UNMAPPED	27	GLY	HA2	3.65	-1.0	2
UNMAPPED	25	ASP	HB2	2.67	-1.0	2
UNMAPPED	77	SER	HB2	3.82	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	THR	CG2	19.0	-1.0	1
UNMAPPED	78	LYS	HG3	1.41	-1.0	4
UNMAPPED	71	PRO	HD3	3.65	-1.0	1
UNMAPPED	124	LYS	N	119.2	-1.0	1
UNMAPPED	92	LYS	HB3	1.67	-1.0	1
UNMAPPED	61	GLN	CB	30.1	-1.0	1
UNMAPPED	44	LEU	HD11	0.1	-1.0	1
UNMAPPED	95	PRO	HB3	2.32	-1.0	1
UNMAPPED	59	THR	C	174.5	-1.0	1
UNMAPPED	8	LEU	HD23	0.96	-1.0	1
UNMAPPED	9	ALA	CA	55.9	-1.0	1
UNMAPPED	121	GLU	CA	59.3	-1.0	1
UNMAPPED	70	ILE	HA	4.41	-1.0	1
UNMAPPED	80	VAL	CA	62.3	-1.0	1
UNMAPPED	148	LYS	CB	30.2	-1.0	1
UNMAPPED	148	LYS	HA	4.17	-1.0	1
UNMAPPED	60	LEU	CA	55.8	-1.0	1
UNMAPPED	20	VAL	HG13	0.88	-1.0	1
UNMAPPED	33	ASP	N	112.9	-1.0	1
UNMAPPED	149	ARG	N	121.0	-1.0	1
UNMAPPED	9	ALA	HB3	1.38	-1.0	1
UNMAPPED	24	ALA	HB2	1.55	-1.0	1
UNMAPPED	148	LYS	HE3	3.2	-1.0	4
UNMAPPED	23	PHE	HB2	2.85	-1.0	2
UNMAPPED	33	ASP	CB	41.7	-1.0	1
UNMAPPED	44	LEU	HB3	1.85	-1.0	2
UNMAPPED	122	SER	HB2	4.0	-1.0	1
UNMAPPED	47	HIS	HA	4.23	-1.0	1
UNMAPPED	2	ASP	HB3	2.63	-1.0	2
UNMAPPED	95	PRO	C	177.5	-1.0	1
UNMAPPED	30	LYS	HB2	1.33	-1.0	2
UNMAPPED	101	LEU	HD12	0.81	-1.0	4
UNMAPPED	154	LYS	CA	56.7	-1.0	1
UNMAPPED	29	ARG	HB2	1.69	-1.0	1
UNMAPPED	78	LYS	HG2	1.41	-1.0	4
UNMAPPED	17	GLU	HG3	2.35	-1.0	2
UNMAPPED	18	ARG	N	120.0	-1.0	1
UNMAPPED	96	GLN	C	178.4	-1.0	1
UNMAPPED	92	LYS	H	8.24	-1.0	1
UNMAPPED	20	VAL	C	178.8	-1.0	1
UNMAPPED	18	ARG	CB	29.5	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	80	VAL	H	8.09	-1.0	1
UNMAPPED	48	LEU	HD11	0.64	-1.0	1
UNMAPPED	154	LYS	HG2	1.38	-1.0	1
UNMAPPED	2	ASP	HA	4.81	-1.0	1
UNMAPPED	35	SER	HB2	3.7	-1.0	1
UNMAPPED	36	VAL	HB	1.79	-1.0	1
UNMAPPED	154	LYS	HD3	1.65	-1.0	1
UNMAPPED	19	LEU	CD1	24.6	-1.0	1
UNMAPPED	101	LEU	HD11	0.81	-1.0	4
UNMAPPED	124	LYS	HG3	1.38	-1.0	1
UNMAPPED	156	LYS	HB2	1.68	-1.0	2
UNMAPPED	75	GLY	C	176.0	-1.0	1
UNMAPPED	48	LEU	CA	57.2	-1.0	1
UNMAPPED	15	SER	CB	65.2	-1.0	1
UNMAPPED	13	GLN	N	117.7	-1.0	1
UNMAPPED	48	LEU	HD23	0.76	-1.0	1
UNMAPPED	28	ILE	HD11	0.97	-1.0	1
UNMAPPED	45	ILE	HG21	0.86	-1.0	1
UNMAPPED	11	GLU	HB3	2.13	-1.0	1
UNMAPPED	92	LYS	HG3	1.37	-1.0	4
UNMAPPED	148	LYS	HE2	3.2	-1.0	4
UNMAPPED	123	ALA	HB2	1.5	-1.0	1
UNMAPPED	22	GLN	HE21	6.33	-1.0	1
UNMAPPED	155	ASP	HA	4.56	-1.0	1
UNMAPPED	94	ASP	C	174.5	-1.0	1
UNMAPPED	42	GLN	HB2	2.14	-1.0	1
UNMAPPED	16	VAL	N	122.7	-1.0	1
UNMAPPED	92	LYS	HG2	1.37	-1.0	4
UNMAPPED	38	ALA	HA	4.05	-1.0	1
UNMAPPED	154	LYS	N	120.4	-1.0	1
UNMAPPED	147	ALA	CA	53.1	-1.0	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	112	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	107	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	108	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	104	0.00 ± 0.00	None needed (< 0.5 ppm)

7.1.3 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 590. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/245 (0%)	0/98 (0%)	0/98 (0%)	0/49 (0%)
Sidechain	0/328 (0%)	0/188 (0%)	0/122 (0%)	0/18 (0%)
Aromatic	0/17 (0%)	0/9 (0%)	0/6 (0%)	0/2 (0%)
Overall	0/590 (0%)	0/295 (0%)	0/226 (0%)	0/69 (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 590. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/245 (0%)	0/98 (0%)	0/98 (0%)	0/49 (0%)
Sidechain	0/328 (0%)	0/188 (0%)	0/122 (0%)	0/18 (0%)
Aromatic	0/17 (0%)	0/9 (0%)	0/6 (0%)	0/2 (0%)
Overall	0/590 (0%)	0/295 (0%)	0/226 (0%)	0/69 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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