Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 04:17 PM BST

PDB ID	:	1Q1O
Title	:	Solution Structure of the PB1 Domain of Cdc24p (Long Form)
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Deposited on	:	2003-07-22

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

The following versions of software and data (see references (1)) were used in the production of this report:

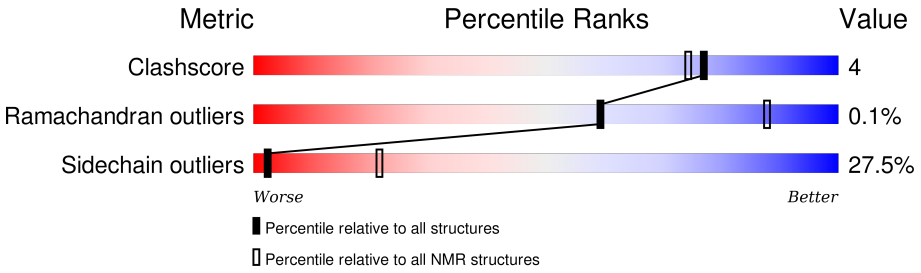
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal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

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	98	47% 24% 29%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:761-A:768, A:779-A:799, A:814-A:854 (70)	0.25	15

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 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1555 atoms, of which 765 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cell division control protein 24.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1555	498	765	130	160	2	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	757	GLY	-	CLONING ARTIFACT	UNP P11433
A	758	PRO	-	CLONING ARTIFACT	UNP P11433
A	759	LEU	-	CLONING ARTIFACT	UNP P11433
A	760	GLY	-	CLONING ARTIFACT	UNP P11433

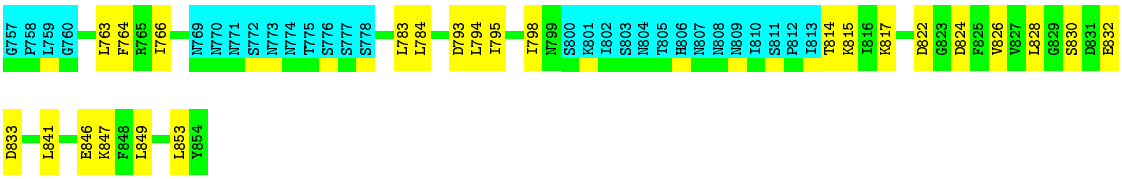
4 Residue-property plots

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: Cell division control protein 24

Chain A:



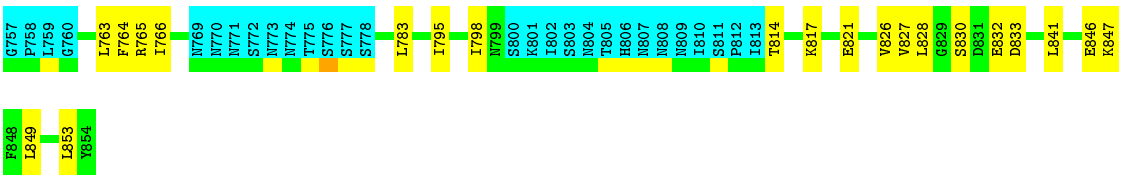
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Cell division control protein 24

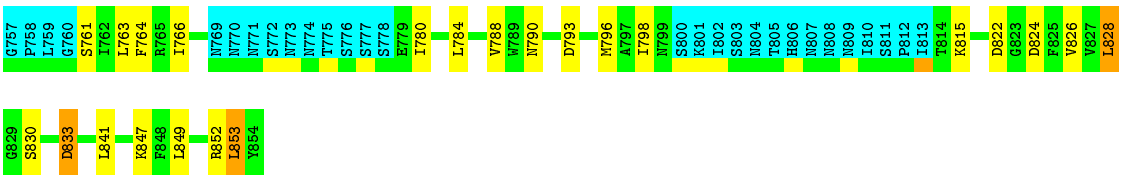
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: Cell division control protein 24

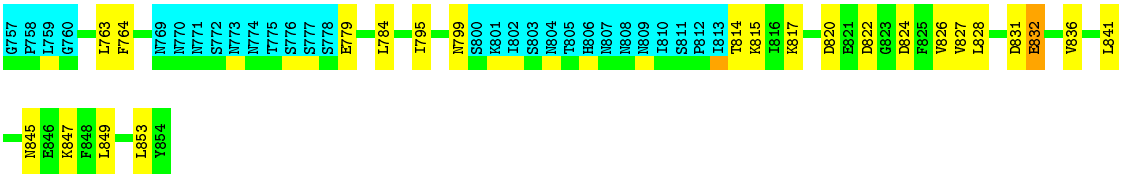
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Cell division control protein 24

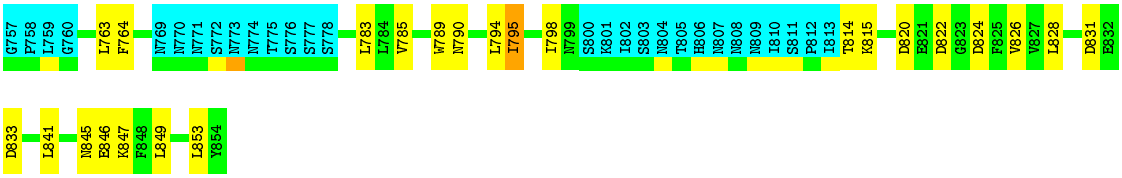
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Cell division control protein 24

Chain A:



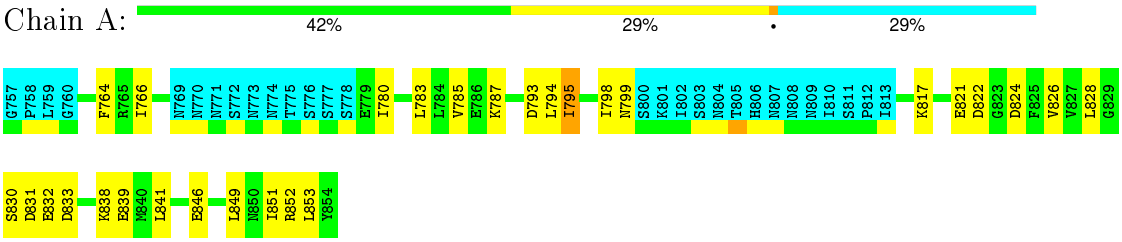
4.2.5 Score per residue for model 5

- Molecule 1: Cell division control protein 24

Chain A:

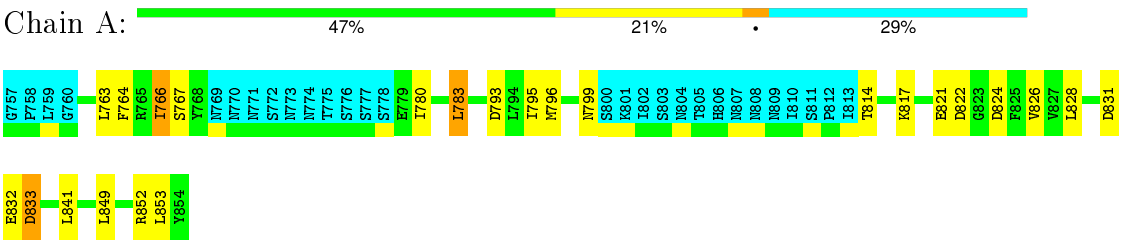
4.2.6 Score per residue for model 6

- Molecule 1: Cell division control protein 24



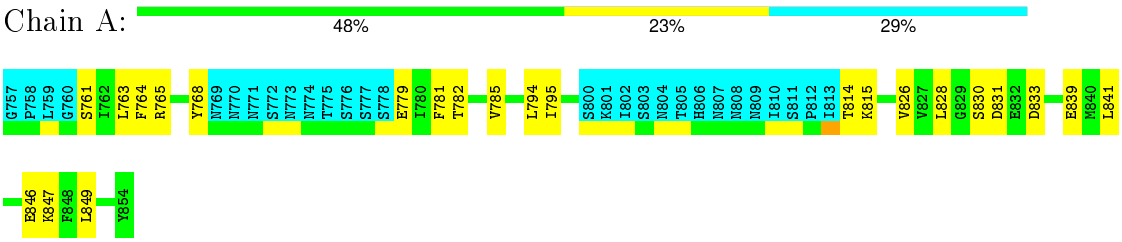
4.2.7 Score per residue for model 7

- Molecule 1: Cell division control protein 24



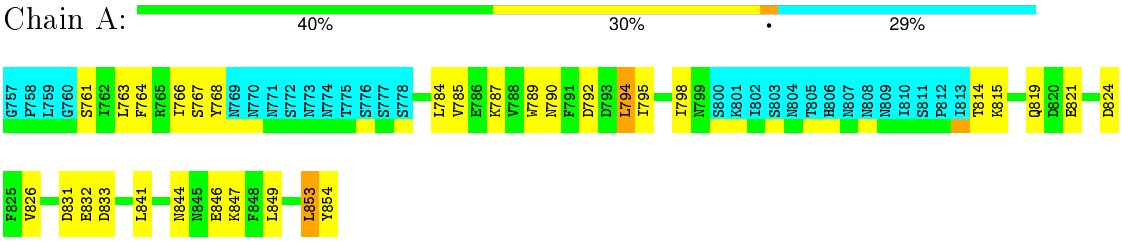
4.2.8 Score per residue for model 8

- Molecule 1: Cell division control protein 24



4.2.9 Score per residue for model 9

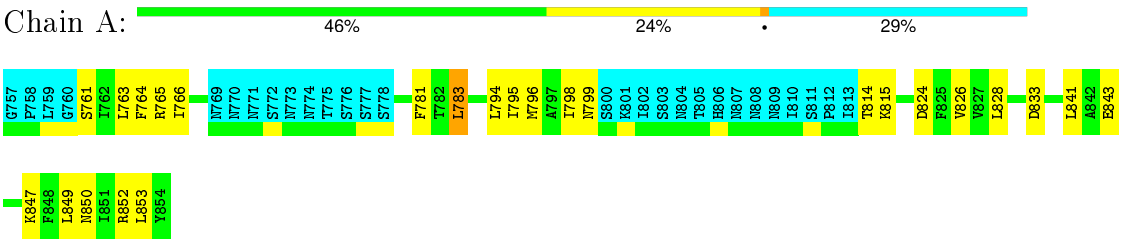
- Molecule 1: Cell division control protein 24



4.2.10 Score per residue for model 10

- Molecule 1: Cell division control protein 24

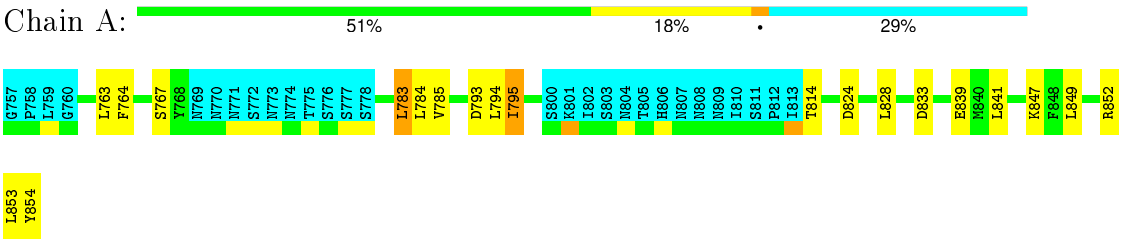
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Cell division control protein 24

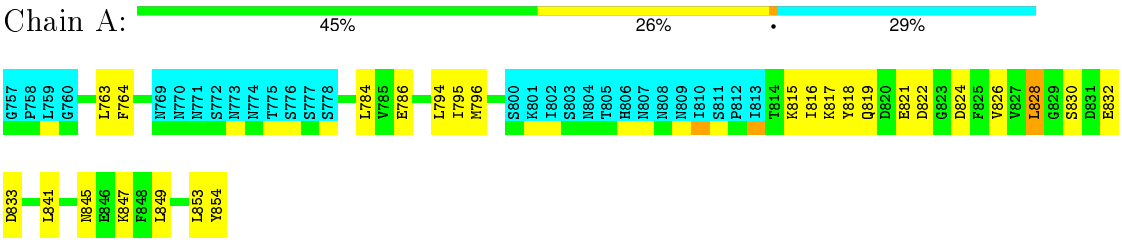
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: Cell division control protein 24

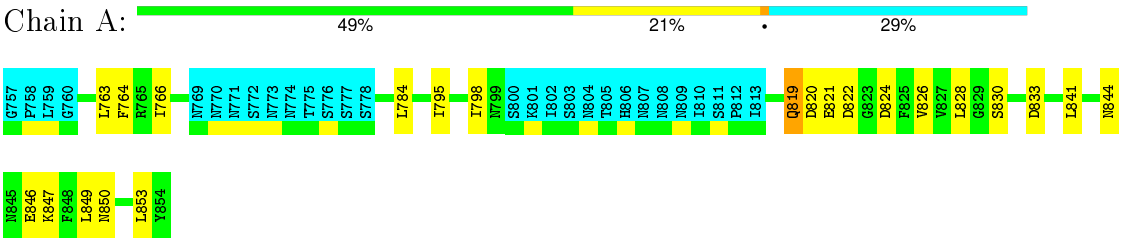
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Cell division control protein 24

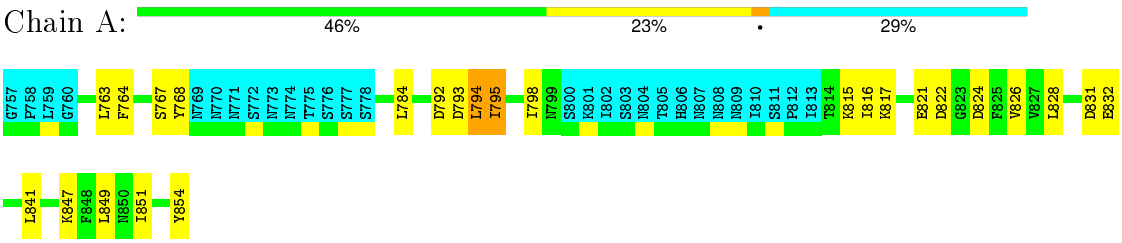
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Cell division control protein 24

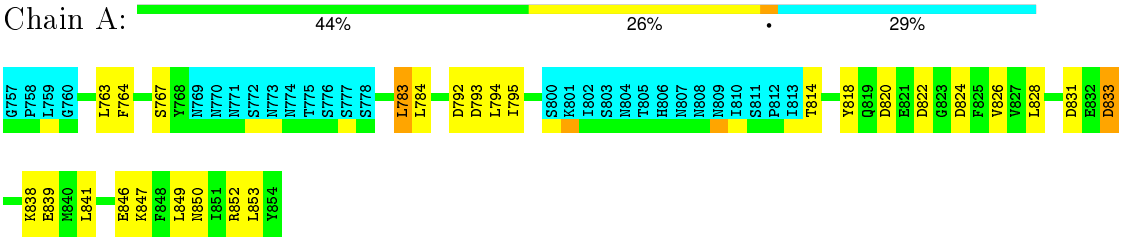
Chain A:



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Cell division control protein 24

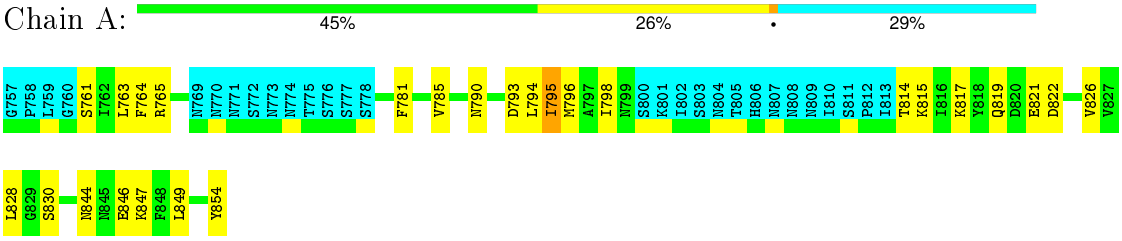
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Cell division control protein 24

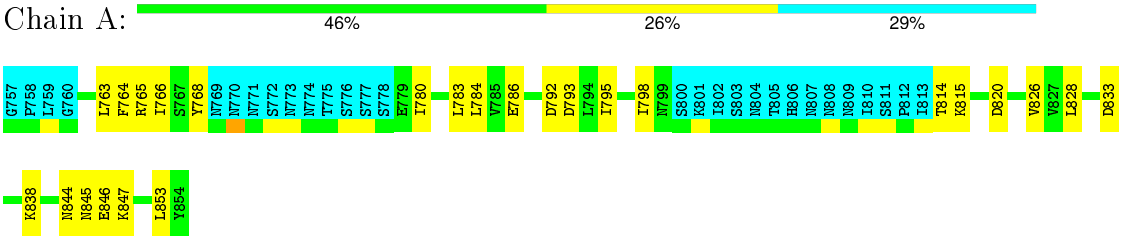
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Cell division control protein 24

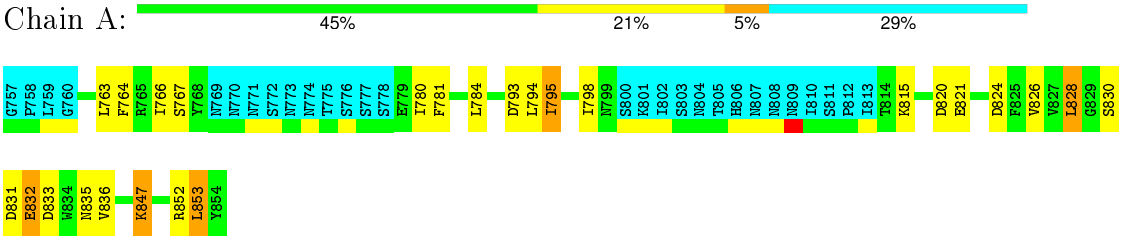
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Cell division control protein 24

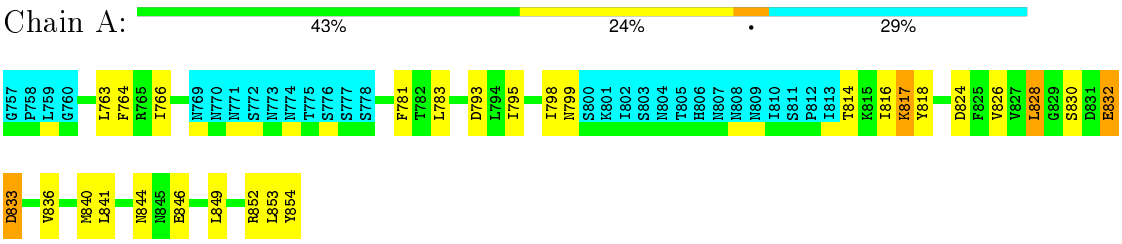
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Cell division control protein 24

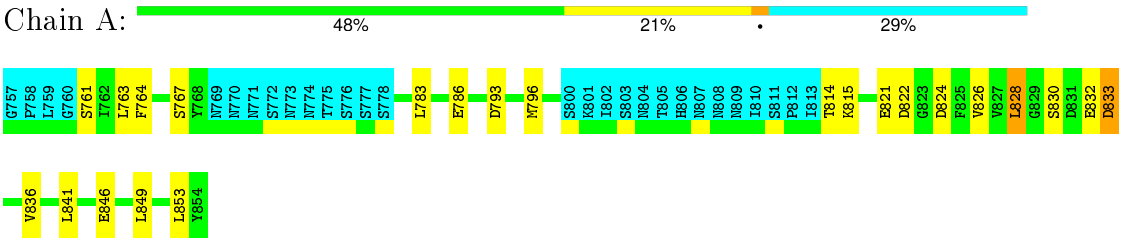
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Cell division control protein 24

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	refinement	
ARIA	structure solution	
CNS	structure solution	

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

Chemical shift file(s)	BMRB entry 5875
Number of chemical shift lists	1
Total number of shifts	598
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	598
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality

6.1 Standard geometry

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

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

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	589	575	575	4±1
All	All	11780	11500	11500	85

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:795:ILE:HA	1:A:798:ILE:HD12	0.67	1.66	18	9
1:A:785:VAL:HG11	1:A:794:LEU:HD12	0.67	1.66	8	5
1:A:841:LEU:HD21	1:A:849:LEU:HD13	0.66	1.66	1	16
1:A:828:LEU:HD12	1:A:833:ASP:HB3	0.65	1.68	11	10
1:A:818:TYR:HB2	1:A:849:LEU:HD21	0.61	1.73	19	2
1:A:766:ILE:HD13	1:A:798:ILE:HG23	0.59	1.75	13	3
1:A:817:LYS:HE3	1:A:827:VAL:HG22	0.53	1.80	1	2
1:A:763:LEU:HD21	1:A:782:THR:HG22	0.52	1.81	8	1
1:A:794:LEU:HD21	1:A:816:ILE:HD11	0.50	1.82	14	1
1:A:766:ILE:HD12	1:A:781:PHE:HB2	0.48	1.85	19	3
1:A:766:ILE:HD11	1:A:783:LEU:HD23	0.48	1.86	7	1
1:A:832:GLU:O	1:A:836:VAL:HG23	0.46	2.11	3	5
1:A:819:GLN:O	1:A:849:LEU:HD11	0.46	2.11	9	4
1:A:817:LYS:HG3	1:A:854:TYR:OH	0.46	2.11	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:766:ILE:O	1:A:780:ILE:HA	0.45	2.12	6	5
1:A:765:ARG:HA	1:A:781:PHE:O	0.43	2.14	8	3
1:A:787:LYS:HG2	1:A:838:LYS:HD2	0.42	1.90	6	1
1:A:853:LEU:HG	1:A:854:TYR:N	0.42	2.29	11	1
1:A:853:LEU:HD13	1:A:854:TYR:N	0.42	2.30	9	1
1:A:817:LYS:O	1:A:851:ILE:HA	0.42	2.15	6	2
1:A:817:LYS:NZ	1:A:827:VAL:HG22	0.42	2.30	5	1
1:A:785:VAL:HG13	1:A:789:TRP:CE3	0.41	2.50	9	2
1:A:841:LEU:HA	1:A:846:GLU:HB2	0.41	1.91	4	1
1:A:768:TYR:HB3	1:A:779:GLU:HB2	0.41	1.92	8	1
1:A:818:TYR:CD1	1:A:828:LEU:HB2	0.40	2.51	12	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	69/98 (70%)	65±2 (94±2%)	4±2 (6±2%)	0±0 (0±0%)	59	88
All	All	1380/1960 (70%)	1292 (94%)	86 (6%)	2 (0%)	59	88

All 2 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	788	VAL	1
1	A	847	LYS	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	65/91 (71%)	47±3 (73±4%)	18±3 (27±4%)	2 21
All	All	1300/1820 (71%)	943 (73%)	357 (27%)	2 21

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

Mol	Chain	Res	Type	Models (Total)
1	A	764	PHE	20
1	A	826	VAL	19
1	A	763	LEU	18
1	A	847	LYS	16
1	A	828	LEU	15
1	A	824	ASP	15
1	A	814	THR	14
1	A	833	ASP	13
1	A	795	ILE	13
1	A	793	ASP	12
1	A	853	LEU	12
1	A	815	LYS	12
1	A	822	ASP	12
1	A	830	SER	11
1	A	784	LEU	11
1	A	846	GLU	10
1	A	821	GLU	10
1	A	783	LEU	10
1	A	832	GLU	9
1	A	831	ASP	9
1	A	794	LEU	8
1	A	852	ARG	8
1	A	767	SER	7
1	A	761	SER	7
1	A	844	ASN	6
1	A	796	MET	6
1	A	820	ASP	6
1	A	845	ASN	5
1	A	799	ASN	5
1	A	790	ASN	4
1	A	792	ASP	4
1	A	786	GLU	4
1	A	839	GLU	4
1	A	850	ASN	3
1	A	816	ILE	2
1	A	766	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	843	GLU	2
1	A	817	LYS	2
1	A	768	TYR	2
1	A	765	ARG	2
1	A	838	LYS	2
1	A	787	LYS	1
1	A	779	GLU	1
1	A	840	MET	1
1	A	835	ASN	1
1	A	819	GLN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: BMRB entry 5875

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	598
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	598
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- Chain not found in structure. All 598 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	13	LYS	H	8.264	0.02	1
UNMAPPED	4	LYS	HG2	1.49	0.02	2
UNMAPPED	49	THR	N	102.8466	0.2	1
UNMAPPED	13	LYS	CG	24.5222	0.2	1
UNMAPPED	49	THR	CB	70.077	0.2	1
UNMAPPED	35	ASN	HB2	2.764	0.02	2
UNMAPPED	13	LYS	HG2	1.4454	0.02	2
UNMAPPED	44	THR	N	116.602	0.2	1
UNMAPPED	3	TYR	HE1	6.884	0.02	1
UNMAPPED	4	LYS	CA	54.751	0.2	1
UNMAPPED	50	LYS	HG2	1.427	0.02	2
UNMAPPED	35	ASN	ND2	113.178	0.2	1
UNMAPPED	5	VAL	H	9.271	0.02	1
UNMAPPED	4	LYS	CG	25.4398	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	41	GLY	N	107.0975	0.2	1
UNMAPPED	8	ASN	HD22	7.35	0.02	2
UNMAPPED	33	PHE	N	120.4218	0.2	1
UNMAPPED	2	GLN	H	8.2137	0.02	1
UNMAPPED	17	THR	HA	5.4605	0.02	1
UNMAPPED	43	TRP	HZ3	6.061	0.02	1
UNMAPPED	38	GLY	CA	46.5288	0.2	1
UNMAPPED	33	PHE	CB	39.0248	0.2	1
UNMAPPED	22	ASP	HA	4.8046	0.02	1
UNMAPPED	55	THR	CB	70.8313	0.2	1
UNMAPPED	39	VAL	H	7.818	0.02	1
UNMAPPED	20	ALA	HA	4.87	0.02	1
UNMAPPED	45	TYR	CA	57.161	0.2	1
UNMAPPED	4	LYS	HB2	1.9772	0.02	1
UNMAPPED	36	ASP	CA	56.491	0.2	1
UNMAPPED	13	LYS	CE	42.3544	0.2	1
UNMAPPED	30	VAL	CB	30.8499	0.2	1
UNMAPPED	21	VAL	CG2	19.71	0.2	2
UNMAPPED	20	ALA	HB3	1.466	0.02	1
UNMAPPED	18	THR	HA	5.0148	0.02	1
UNMAPPED	30	VAL	N	121.5242	0.2	1
UNMAPPED	18	THR	CB	71.0378	0.2	1
UNMAPPED	44	THR	CB	70.5025	0.2	1
UNMAPPED	33	PHE	HE1	6.957	0.2	1
UNMAPPED	32	GLN	CA	58.7702	0.2	1
UNMAPPED	32	GLN	CG	33.4732	0.2	1
UNMAPPED	43	TRP	HB2	3.2525	0.02	2
UNMAPPED	42	GLU	N	122.1924	0.2	1
UNMAPPED	17	THR	N	115.6911	0.2	1
UNMAPPED	13	LYS	HE2	2.934	0.02	2
UNMAPPED	7	LEU	HD22	0.76	0.02	2
UNMAPPED	24	ALA	CB	18.0378	0.2	1
UNMAPPED	39	VAL	CG2	20.94	0.2	2
UNMAPPED	17	THR	CB	71.7139	0.2	1
UNMAPPED	46	ASP	HA	4.5859	0.02	1
UNMAPPED	53	THR	N	117.0785	0.2	1
UNMAPPED	32	GLN	HG2	2.45	0.02	2
UNMAPPED	53	THR	CB	70.3964	0.2	1
UNMAPPED	41	GLY	HA3	4.139	0.02	2
UNMAPPED	34	PHE	HB2	3.416	0.02	2
UNMAPPED	50	LYS	HG3	1.28	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	34	PHE	HB3	3.46	0.02	2
UNMAPPED	12	LEU	N	122.3313	0.2	1
UNMAPPED	51	THR	CG2	21.2009	0.2	1
UNMAPPED	33	PHE	CD1	132.56	0.2	2
UNMAPPED	12	LEU	CB	44.7693	0.2	1
UNMAPPED	48	ALA	HA	4.11	0.02	1
UNMAPPED	50	LYS	CE	42.87	0.2	1
UNMAPPED	5	VAL	CG2	21.45	0.2	2
UNMAPPED	4	LYS	HD2	1.694	0.02	2
UNMAPPED	4	LYS	CD	29.0839	0.2	1
UNMAPPED	8	ASN	CB	39.3208	0.2	1
UNMAPPED	12	LEU	HD11	0.131	0.02	2
UNMAPPED	49	THR	HA	4.3981	0.02	1
UNMAPPED	28	LYS	HB2	1.8295	0.02	2
UNMAPPED	56	GLU	HB3	2.064	0.02	2
UNMAPPED	26	ALA	H	7.64	0.02	1
UNMAPPED	21	VAL	HG12	1.02	0.02	2
UNMAPPED	53	THR	HG21	1.0949	0.02	1
UNMAPPED	5	VAL	HB	2.096	0.02	1
UNMAPPED	5	VAL	HG13	0.8493	0.02	2
UNMAPPED	40	ASP	HB3	2.6075	0.02	2
UNMAPPED	54	VAL	HG23	-0.5566	0.02	2
UNMAPPED	7	LEU	HG	1.553	0.02	1
UNMAPPED	24	ALA	HB3	1.281	0.02	1
UNMAPPED	37	ASN	HD22	6.734	0.02	2
UNMAPPED	19	GLU	HG3	2.265	0.02	2
UNMAPPED	10	LYS	HE2	3.0053	0.02	2
UNMAPPED	41	GLY	CA	45.006	0.2	1
UNMAPPED	29	VAL	HB	2.1099	0.02	1
UNMAPPED	46	ASP	CA	51.9086	0.2	1
UNMAPPED	5	VAL	CB	32.9465	0.2	1
UNMAPPED	5	VAL	HG23	0.4014	0.02	2
UNMAPPED	56	GLU	H	7.9692	0.02	1
UNMAPPED	12	LEU	HB2	1.15	0.02	1
UNMAPPED	2	GLN	CB	30.4319	0.2	1
UNMAPPED	21	VAL	N	114.9366	0.2	1
UNMAPPED	7	LEU	CA	53.7996	0.2	1
UNMAPPED	10	LYS	HG2	1.507	0.02	2
UNMAPPED	28	LYS	HG3	1.289	0.02	2
UNMAPPED	47	ASP	HA	4.15	0.02	1
UNMAPPED	10	LYS	CE	42.165	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	33	PHE	H	7.8383	0.02	1
UNMAPPED	2	GLN	N	122.4064	0.2	1
UNMAPPED	15	GLU	H	8.5285	0.02	1
UNMAPPED	32	GLN	HE21	6.835	0.02	2
UNMAPPED	37	ASN	ND2	114.0	0.2	1
UNMAPPED	30	VAL	HG11	0.84	0.02	2
UNMAPPED	39	VAL	CB	32.5607	0.2	1
UNMAPPED	35	ASN	HB3	2.864	0.02	2
UNMAPPED	4	LYS	HG3	1.553	0.02	2
UNMAPPED	20	ALA	CA	51.2749	0.2	1
UNMAPPED	31	LYS	HD2	0.96	0.02	2
UNMAPPED	42	GLU	HG3	2.236	0.02	2
UNMAPPED	31	LYS	HG3	0.938	0.02	2
UNMAPPED	55	THR	N	122.1127	0.2	1
UNMAPPED	7	LEU	CD2	24.4535	0.2	2
UNMAPPED	54	VAL	CG2	18.531	0.2	2
UNMAPPED	48	ALA	CA	55.0867	0.2	1
UNMAPPED	46	ASP	H	7.6426	0.02	1
UNMAPPED	34	PHE	HE1	6.91	0.2	1
UNMAPPED	43	TRP	NE1	128.0	0.2	1
UNMAPPED	11	THR	CG2	22.2084	0.2	1
UNMAPPED	51	THR	CA	61.8523	0.2	1
UNMAPPED	43	TRP	HZ2	7.298	0.02	1
UNMAPPED	24	ALA	H	8.1328	0.02	1
UNMAPPED	42	GLU	HG2	2.327	0.02	2
UNMAPPED	16	THR	CB	72.3807	0.2	1
UNMAPPED	39	VAL	HG21	1.014	0.02	2
UNMAPPED	31	LYS	CG	28.24	0.2	1
UNMAPPED	44	THR	HB	4.3009	0.02	1
UNMAPPED	32	GLN	HB3	2.0943	0.02	2
UNMAPPED	39	VAL	HG23	1.014	0.02	2
UNMAPPED	52	PHE	CD1	132.4	0.2	1
UNMAPPED	6	ILE	N	128.6638	0.2	1
UNMAPPED	35	ASN	H	8.3303	0.02	1
UNMAPPED	31	LYS	CD	29.84	0.2	1
UNMAPPED	1	MET	HG2	2.4302	0.02	2
UNMAPPED	38	GLY	HA2	4.174	0.02	2
UNMAPPED	12	LEU	H	7.0855	0.02	1
UNMAPPED	18	THR	CA	60.3163	0.2	1
UNMAPPED	32	GLN	CB	28.1442	0.2	1
UNMAPPED	11	THR	HG21	1.1731	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	39	VAL	HA	3.929	0.02	1
UNMAPPED	8	ASN	H	9.102	0.02	1
UNMAPPED	33	PHE	HZ	6.8727	0.02	1
UNMAPPED	10	LYS	HB2	1.8873	0.02	2
UNMAPPED	47	ASP	N	124.6094	0.2	1
UNMAPPED	2	GLN	HE21	6.866	0.02	2
UNMAPPED	26	ALA	CB	18.4377	0.2	1
UNMAPPED	1	MET	CA	54.6325	0.2	1
UNMAPPED	26	ALA	N	123.5422	0.2	1
UNMAPPED	18	THR	HG23	1.0071	0.02	1
UNMAPPED	6	ILE	HD13	0.877	0.02	1
UNMAPPED	52	PHE	HE1	7.06	0.2	1
UNMAPPED	2	GLN	HG3	2.1043	0.02	2
UNMAPPED	12	LEU	CG	26.1302	0.2	1
UNMAPPED	49	THR	CG2	21.3263	0.2	1
UNMAPPED	3	TYR	CB	42.0135	0.2	1
UNMAPPED	50	LYS	HB3	2.085	0.02	2
UNMAPPED	56	GLU	N	129.5426	0.2	1
UNMAPPED	50	LYS	N	123.3235	0.2	1
UNMAPPED	51	THR	HG22	1.0698	0.02	1
UNMAPPED	56	GLU	CB	32.3133	0.2	1
UNMAPPED	8	ASN	CA	51.8525	0.2	1
UNMAPPED	49	THR	HB	4.412	0.02	1
UNMAPPED	27	GLU	H	7.6667	0.02	1
UNMAPPED	2	GLN	NE2	111.69	0.2	1
UNMAPPED	29	VAL	HG22	1.048	0.02	2
UNMAPPED	54	VAL	HB	1.72	0.02	1
UNMAPPED	55	THR	HB	4.09	0.02	1
UNMAPPED	15	GLU	CB	33.4709	0.2	1
UNMAPPED	12	LEU	HG	1.16	0.02	1
UNMAPPED	22	ASP	H	7.3339	0.02	1
UNMAPPED	21	VAL	HG11	1.02	0.02	2
UNMAPPED	7	LEU	HD11	0.766	0.02	2
UNMAPPED	55	THR	HA	5.0876	0.02	1
UNMAPPED	11	THR	CB	69.5289	0.2	1
UNMAPPED	13	LYS	CD	29.0987	0.2	1
UNMAPPED	8	ASN	HA	5.2868	0.02	1
UNMAPPED	11	THR	N	108.17	0.2	1
UNMAPPED	52	PHE	HZ	7.0	0.02	1
UNMAPPED	10	LYS	HD2	1.7062	0.02	2
UNMAPPED	33	PHE	CZ	128.85	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	16	THR	CG2	22.0305	0.2	1
UNMAPPED	37	ASN	HD21	6.36	0.02	2
UNMAPPED	49	THR	HG23	1.0825	0.02	1
UNMAPPED	25	THR	HG23	1.2758	0.02	1
UNMAPPED	19	GLU	HG2	2.061	0.02	2
UNMAPPED	37	ASN	N	114.184	0.2	1
UNMAPPED	46	ASP	N	128.2256	0.2	1
UNMAPPED	6	ILE	CA	60.4361	0.2	1
UNMAPPED	28	LYS	CG	24.8569	0.2	1
UNMAPPED	11	THR	HB	4.416	0.02	1
UNMAPPED	12	LEU	CD2	24.63	0.2	2
UNMAPPED	46	ASP	CB	43.0939	0.2	1
UNMAPPED	17	THR	CG2	21.5865	0.2	1
UNMAPPED	13	LYS	HB3	1.925	0.02	2
UNMAPPED	6	ILE	CG1	27.6495	0.2	1
UNMAPPED	5	VAL	HG22	0.4014	0.02	2
UNMAPPED	1	MET	HG3	2.1593	0.02	2
UNMAPPED	19	GLU	CG	35.7593	0.2	1
UNMAPPED	7	LEU	HB3	1.034	0.02	2
UNMAPPED	7	LEU	CB	40.6369	0.2	1
UNMAPPED	28	LYS	HG2	1.2833	0.02	2
UNMAPPED	10	LYS	N	120.6371	0.2	1
UNMAPPED	25	THR	HB	4.024	0.02	1
UNMAPPED	16	THR	H	9.0531	0.02	1
UNMAPPED	48	ALA	H	8.3268	0.02	1
UNMAPPED	10	LYS	CB	32.6304	0.2	1
UNMAPPED	25	THR	N	115.7892	0.2	1
UNMAPPED	1	MET	HE1	2.11	0.02	1
UNMAPPED	44	THR	HA	4.7181	0.02	1
UNMAPPED	20	ALA	N	126.3437	0.2	1
UNMAPPED	39	VAL	CA	64.2326	0.2	1
UNMAPPED	20	ALA	CB	23.6474	0.2	1
UNMAPPED	31	LYS	HD3	1.171	0.02	2
UNMAPPED	35	ASN	HD21	7.564	0.02	2
UNMAPPED	14	GLY	CA	46.6008	0.2	1
UNMAPPED	31	LYS	HG2	0.976	0.02	2
UNMAPPED	6	ILE	HB	2.11	0.02	1
UNMAPPED	48	ALA	N	119.5493	0.2	1
UNMAPPED	7	LEU	CD1	25.1	0.2	2
UNMAPPED	14	GLY	HA2	4.6004	0.02	2
UNMAPPED	19	GLU	H	7.9231	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	9	GLY	CA	44.717	0.2	1
UNMAPPED	34	PHE	HZ	6.87	0.02	1
UNMAPPED	54	VAL	HG21	-0.5566	0.02	2
UNMAPPED	51	THR	N	110.6459	0.2	1
UNMAPPED	15	GLU	HG2	2.252	0.02	2
UNMAPPED	39	VAL	HB	2.2008	0.02	1
UNMAPPED	10	LYS	HG3	1.564	0.02	2
UNMAPPED	1	MET	HA	4.1617	0.02	1
UNMAPPED	31	LYS	CB	32.593	0.2	1
UNMAPPED	32	GLN	HB2	2.171	0.02	2
UNMAPPED	31	LYS	N	118.5449	0.2	1
UNMAPPED	27	GLU	CG	34.2	0.2	1
UNMAPPED	13	LYS	CA	54.0333	0.2	1
UNMAPPED	36	ASP	HB2	2.6208	0.02	2
UNMAPPED	34	PHE	CA	58.1859	0.2	1
UNMAPPED	9	GLY	HA3	3.8266	0.02	2
UNMAPPED	26	ALA	HB1	0.955	0.02	1
UNMAPPED	21	VAL	HG22	1.006	0.02	2
UNMAPPED	17	THR	HG22	1.1855	0.02	1
UNMAPPED	28	LYS	HE2	2.8686	0.02	2
UNMAPPED	10	LYS	HA	4.1467	0.02	1
UNMAPPED	20	ALA	HB1	1.466	0.02	1
UNMAPPED	38	GLY	HA3	3.9612	0.02	2
UNMAPPED	11	THR	HG22	1.1731	0.02	1
UNMAPPED	27	GLU	N	115.2124	0.2	1
UNMAPPED	40	ASP	CB	41.0099	0.2	1
UNMAPPED	28	LYS	HD2	1.581	0.02	2
UNMAPPED	47	ASP	CA	56.3057	0.2	1
UNMAPPED	27	GLU	CB	28.7118	0.2	1
UNMAPPED	40	ASP	N	118.5166	0.2	1
UNMAPPED	42	GLU	CB	29.8783	0.2	1
UNMAPPED	43	TRP	N	127.741	0.2	1
UNMAPPED	5	VAL	CG1	20.68	0.2	2
UNMAPPED	33	PHE	HA	4.27	0.02	1
UNMAPPED	24	ALA	N	120.169	0.2	1
UNMAPPED	38	GLY	H	7.955	0.02	1
UNMAPPED	22	ASP	CB	41.8333	0.2	1
UNMAPPED	52	PHE	HB2	3.17	0.02	2
UNMAPPED	11	THR	H	8.928	0.02	1
UNMAPPED	1	MET	CG	30.7102	0.2	1
UNMAPPED	45	TYR	H	8.8528	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	18	THR	HG22	1.0071	0.02	1
UNMAPPED	6	ILE	HD12	0.877	0.02	1
UNMAPPED	31	LYS	HB2	1.586	0.02	2
UNMAPPED	6	ILE	H	9.4648	0.02	1
UNMAPPED	19	GLU	HB2	1.936	0.02	2
UNMAPPED	43	TRP	HH2	6.501	0.02	1
UNMAPPED	50	LYS	CA	56.48	0.2	1
UNMAPPED	3	TYR	CA	57.6536	0.2	1
UNMAPPED	50	LYS	HB2	1.991	0.02	2
UNMAPPED	56	GLU	CG	36.69	0.2	1
UNMAPPED	50	LYS	CG	24.5176	0.2	1
UNMAPPED	12	LEU	HD13	0.131	0.02	2
UNMAPPED	44	THR	HG22	1.3086	0.02	1
UNMAPPED	52	PHE	CA	56.8768	0.2	1
UNMAPPED	21	VAL	H	8.4761	0.02	1
UNMAPPED	29	VAL	HG23	1.048	0.02	2
UNMAPPED	3	TYR	HA	5.1474	0.02	1
UNMAPPED	7	LEU	HD12	0.766	0.02	2
UNMAPPED	3	TYR	H	9.0682	0.02	1
UNMAPPED	41	GLY	H	7.6131	0.02	1
UNMAPPED	5	VAL	HG11	0.8493	0.02	2
UNMAPPED	55	THR	HG21	1.2781	0.02	1
UNMAPPED	23	ALA	HB2	0.898	0.02	1
UNMAPPED	7	LEU	HA	4.7	0.02	1
UNMAPPED	30	VAL	HG21	0.42	0.02	2
UNMAPPED	24	ALA	HB1	1.281	0.02	1
UNMAPPED	20	ALA	H	9.3006	0.02	1
UNMAPPED	49	THR	HG22	1.0825	0.02	1
UNMAPPED	25	THR	HG22	1.2758	0.02	1
UNMAPPED	35	ASN	HA	4.433	0.02	1
UNMAPPED	55	THR	CG2	21.6276	0.2	1
UNMAPPED	11	THR	HA	4.485	0.02	1
UNMAPPED	5	VAL	N	123.9405	0.2	1
UNMAPPED	22	ASP	N	114.7224	0.2	1
UNMAPPED	19	GLU	CB	31.0611	0.2	1
UNMAPPED	53	THR	HB	3.8709	0.02	1
UNMAPPED	29	VAL	CG2	22.48	0.2	2
UNMAPPED	5	VAL	HG21	0.4014	0.02	2
UNMAPPED	18	THR	HG21	1.0071	0.02	1
UNMAPPED	19	GLU	N	127.0458	0.2	1
UNMAPPED	6	ILE	HG22	0.967	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	10	LYS	CG	25.5373	0.2	1
UNMAPPED	31	LYS	H	8.1288	0.02	1
UNMAPPED	45	TYR	HB2	2.9913	0.02	2
UNMAPPED	32	GLN	HA	3.9033	0.02	1
UNMAPPED	52	PHE	CE1	131.4	0.2	1
UNMAPPED	16	THR	HG22	0.9257	0.02	1
UNMAPPED	41	GLY	HA2	4.053	0.02	2
UNMAPPED	22	ASP	HB2	3.0087	0.02	2
UNMAPPED	30	VAL	HG13	0.84	0.02	2
UNMAPPED	34	PHE	HA	3.965	0.02	1
UNMAPPED	44	THR	CA	62.0905	0.2	1
UNMAPPED	6	ILE	HG12	1.564	0.02	2
UNMAPPED	42	GLU	HB2	2.148	0.02	2
UNMAPPED	4	LYS	CB	35.3469	0.2	1
UNMAPPED	9	GLY	N	108.8629	0.2	1
UNMAPPED	50	LYS	HD3	1.47	0.02	2
UNMAPPED	40	ASP	H	8.0676	0.02	1
UNMAPPED	51	THR	HB	3.7957	0.02	1
UNMAPPED	29	VAL	HG13	0.877	0.02	2
UNMAPPED	8	ASN	HD21	6.84	0.02	2
UNMAPPED	33	PHE	CA	61.3986	0.2	1
UNMAPPED	12	LEU	HD21	0.119	0.02	2
UNMAPPED	17	THR	HB	4.0611	0.02	1
UNMAPPED	16	THR	N	116.3954	0.2	1
UNMAPPED	52	PHE	HD1	7.53	0.02	1
UNMAPPED	31	LYS	CE	41.1221	0.2	1
UNMAPPED	45	TYR	CB	41.792	0.2	1
UNMAPPED	34	PHE	N	119.8191	0.2	1
UNMAPPED	36	ASP	N	117.7265	0.2	1
UNMAPPED	45	TYR	N	124.0573	0.2	1
UNMAPPED	27	GLU	HG2	1.3155	0.02	2
UNMAPPED	9	GLY	HA2	4.8061	0.02	2
UNMAPPED	26	ALA	HB2	0.955	0.02	1
UNMAPPED	6	ILE	CB	38.3201	0.2	1
UNMAPPED	33	PHE	HD1	6.977	0.02	1
UNMAPPED	17	THR	HG23	1.1855	0.02	1
UNMAPPED	18	THR	HB	3.7825	0.02	1
UNMAPPED	30	VAL	CA	66.6542	0.2	1
UNMAPPED	21	VAL	CG1	20.66	0.2	2
UNMAPPED	32	GLN	N	117.8373	0.2	1
UNMAPPED	11	THR	HG23	1.1731	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	13	LYS	HA	5.1176	0.02	1
UNMAPPED	50	LYS	HE2	2.98	0.02	2
UNMAPPED	36	ASP	HA	4.4288	0.02	1
UNMAPPED	51	THR	H	7.3062	0.02	1
UNMAPPED	7	LEU	HD21	0.76	0.02	2
UNMAPPED	50	LYS	HE3	3.11	0.02	2
UNMAPPED	39	VAL	CG1	21.32	0.2	2
UNMAPPED	1	MET	CE	16.35	0.2	1
UNMAPPED	2	GLN	HA	4.8907	0.02	1
UNMAPPED	28	LYS	HA	3.6453	0.02	1
UNMAPPED	16	THR	HA	5.3919	0.02	1
UNMAPPED	45	TYR	HD1	6.31	0.02	1
UNMAPPED	29	VAL	CA	65.9955	0.2	1
UNMAPPED	52	PHE	HB3	3.24	0.02	2
UNMAPPED	36	ASP	CB	40.4741	0.2	1
UNMAPPED	4	LYS	HA	5.3461	0.02	1
UNMAPPED	18	THR	HG1	4.622	0.02	1
UNMAPPED	6	ILE	HD11	0.877	0.02	1
UNMAPPED	23	ALA	HA	3.037	0.02	1
UNMAPPED	35	ASN	N	116.4094	0.2	1
UNMAPPED	11	THR	HG1	4.785	0.02	1
UNMAPPED	35	ASN	CB	39.8472	0.2	1
UNMAPPED	12	LEU	CA	54.4617	0.2	1
UNMAPPED	34	PHE	HD1	6.84	0.02	1
UNMAPPED	39	VAL	HG11	0.938	0.02	2
UNMAPPED	51	THR	HG21	1.0698	0.02	1
UNMAPPED	52	PHE	N	129.0896	0.2	1
UNMAPPED	46	ASP	HB2	2.6198	0.02	2
UNMAPPED	12	LEU	HD12	0.131	0.02	2
UNMAPPED	39	VAL	HG12	0.938	0.02	2
UNMAPPED	44	THR	HG23	1.3086	0.02	1
UNMAPPED	50	LYS	CD	28.67	0.2	1
UNMAPPED	43	TRP	H	8.8487	0.02	1
UNMAPPED	32	GLN	H	8.0803	0.02	1
UNMAPPED	51	THR	HG23	1.0698	0.02	1
UNMAPPED	45	TYR	CE1	117.45	0.2	1
UNMAPPED	12	LEU	HA	5.0068	0.02	1
UNMAPPED	53	THR	HG22	1.0949	0.02	1
UNMAPPED	7	LEU	HD13	0.766	0.02	2
UNMAPPED	29	VAL	H	8.4383	0.02	1
UNMAPPED	44	THR	H	8.8459	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	48	ALA	HB1	1.502	0.02	1
UNMAPPED	55	THR	HG22	1.2781	0.02	1
UNMAPPED	30	VAL	HG22	0.42	0.02	2
UNMAPPED	49	THR	HG21	1.0825	0.02	1
UNMAPPED	29	VAL	HA	3.664	0.02	1
UNMAPPED	5	VAL	CA	61.1945	0.2	1
UNMAPPED	28	LYS	CA	59.5916	0.2	1
UNMAPPED	52	PHE	HA	5.913	0.02	1
UNMAPPED	4	LYS	H	8.6725	0.02	1
UNMAPPED	54	VAL	HG13	0.531	0.02	2
UNMAPPED	40	ASP	HA	4.6761	0.02	1
UNMAPPED	54	VAL	HG12	0.531	0.02	2
UNMAPPED	24	ALA	HA	3.991	0.02	1
UNMAPPED	54	VAL	HG11	0.531	0.02	2
UNMAPPED	2	GLN	CA	55.8717	0.2	1
UNMAPPED	1	MET	HB3	2.2144	0.02	2
UNMAPPED	8	ASN	HB3	2.5652	0.02	2
UNMAPPED	43	TRP	HA	5.2975	0.02	1
UNMAPPED	13	LYS	HD2	1.729	0.02	1
UNMAPPED	42	GLU	H	8.7412	0.02	1
UNMAPPED	7	LEU	H	8.5222	0.02	1
UNMAPPED	16	THR	HG21	0.9257	0.02	1
UNMAPPED	23	ALA	H	8.1183	0.02	1
UNMAPPED	33	PHE	HB3	3.036	0.02	2
UNMAPPED	30	VAL	HG12	0.84	0.02	2
UNMAPPED	54	VAL	CA	61.04	0.2	1
UNMAPPED	36	ASP	H	8.7485	0.02	1
UNMAPPED	54	VAL	CB	32.5379	0.2	1
UNMAPPED	55	THR	CA	60.9894	0.2	1
UNMAPPED	31	LYS	HA	3.6676	0.02	1
UNMAPPED	37	ASN	HA	4.7864	0.02	1
UNMAPPED	6	ILE	HG13	1.3124	0.02	2
UNMAPPED	48	ALA	CB	18.4487	0.2	1
UNMAPPED	42	GLU	HB3	2.003	0.02	2
UNMAPPED	28	LYS	H	7.1864	0.02	1
UNMAPPED	4	LYS	CE	41.8662	0.2	1
UNMAPPED	54	VAL	CG1	21.2558	0.2	2
UNMAPPED	54	VAL	N	128.8547	0.2	1
UNMAPPED	50	LYS	HD2	1.78	0.02	2
UNMAPPED	33	PHE	CE1	130.64	0.2	2
UNMAPPED	51	THR	HA	5.6016	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	29	VAL	HG12	0.877	0.02	2
UNMAPPED	51	THR	CB	72.5259	0.2	1
UNMAPPED	12	LEU	HD22	0.119	0.02	2
UNMAPPED	16	THR	CA	60.6303	0.2	1
UNMAPPED	42	GLU	HA	4.5663	0.02	1
UNMAPPED	21	VAL	HG23	1.006	0.02	2
UNMAPPED	21	VAL	CB	32.045	0.2	1
UNMAPPED	10	LYS	H	9.312	0.02	1
UNMAPPED	27	GLU	HA	2.9529	0.02	1
UNMAPPED	27	GLU	HG3	1.097	0.02	2
UNMAPPED	37	ASN	HB2	2.443	0.02	2
UNMAPPED	26	ALA	HB3	0.955	0.02	1
UNMAPPED	13	LYS	HB2	1.7814	0.02	2
UNMAPPED	18	THR	N	117.5122	0.2	1
UNMAPPED	9	GLY	H	7.9571	0.02	1
UNMAPPED	33	PHE	HB2	3.177	0.02	2
UNMAPPED	50	LYS	HA	4.197	0.02	1
UNMAPPED	47	ASP	HB3	2.5303	0.02	2
UNMAPPED	3	TYR	CE1	117.8	0.2	1
UNMAPPED	2	GLN	HE22	7.8407	0.02	2
UNMAPPED	43	TRP	CB	30.5899	0.2	1
UNMAPPED	1	MET	CB	32.4489	0.2	1
UNMAPPED	29	VAL	N	119.1251	0.2	1
UNMAPPED	30	VAL	CG1	22.542	0.2	2
UNMAPPED	26	ALA	CA	55.31	0.2	1
UNMAPPED	16	THR	HB	3.879	0.02	1
UNMAPPED	29	VAL	CB	31.7429	0.2	1
UNMAPPED	23	ALA	CA	54.7281	0.2	1
UNMAPPED	23	ALA	HB3	0.898	0.02	1
UNMAPPED	15	GLU	HB2	2.1396	0.02	2
UNMAPPED	34	PHE	H	8.6363	0.02	1
UNMAPPED	55	THR	HG23	1.2781	0.02	1
UNMAPPED	37	ASN	H	7.72	0.02	1
UNMAPPED	21	VAL	HA	4.0986	0.02	1
UNMAPPED	25	THR	H	8.4462	0.02	1
UNMAPPED	2	GLN	HG2	2.3329	0.02	2
UNMAPPED	56	GLU	CA	57.845	0.2	1
UNMAPPED	8	ASN	N	124.7681	0.2	1
UNMAPPED	23	ALA	N	121.6519	0.2	1
UNMAPPED	44	THR	CG2	22.0369	0.2	1
UNMAPPED	3	TYR	HD1	7.02	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	46	ASP	HB3	2.2655	0.02	2
UNMAPPED	54	VAL	HA	4.1887	0.02	1
UNMAPPED	47	ASP	H	8.5817	0.02	1
UNMAPPED	18	THR	CG2	19.0174	0.2	1
UNMAPPED	15	GLU	CG	36.0648	0.2	1
UNMAPPED	29	VAL	HG21	1.048	0.02	2
UNMAPPED	15	GLU	HA	5.4956	0.02	1
UNMAPPED	15	GLU	CA	55.6912	0.2	1
UNMAPPED	53	THR	HG23	1.0949	0.02	1
UNMAPPED	31	LYS	HE3	1.847	0.02	2
UNMAPPED	11	THR	CA	61.0945	0.2	1
UNMAPPED	48	ALA	HB2	1.502	0.02	1
UNMAPPED	23	ALA	CB	17.5438	0.2	1
UNMAPPED	55	THR	H	8.4126	0.02	1
UNMAPPED	49	THR	H	7.0003	0.02	1
UNMAPPED	25	THR	CG2	21.5729	0.2	1
UNMAPPED	30	VAL	HG23	0.42	0.02	2
UNMAPPED	14	GLY	H	8.6539	0.02	1
UNMAPPED	26	ALA	HA	3.59	0.02	1
UNMAPPED	28	LYS	N	116.8282	0.2	1
UNMAPPED	43	TRP	HE1	10.11	0.02	1
UNMAPPED	28	LYS	CB	32.5466	0.2	1
UNMAPPED	12	LEU	CD1	26.4967	0.2	2
UNMAPPED	25	THR	CA	67.036	0.2	1
UNMAPPED	28	LYS	CD	29.3618	0.2	1
UNMAPPED	6	ILE	CG2	17.3127	0.2	1
UNMAPPED	52	PHE	H	10.2436	0.02	1
UNMAPPED	7	LEU	CG	27.6816	0.2	1
UNMAPPED	3	TYR	HB3	2.639	0.02	2
UNMAPPED	37	ASN	CB	39.57	0.2	1
UNMAPPED	53	THR	CG2	21.2014	0.2	1
UNMAPPED	54	VAL	H	8.8604	0.02	1
UNMAPPED	30	VAL	HB	1.857	0.02	1
UNMAPPED	10	LYS	CA	59.3335	0.2	1
UNMAPPED	8	ASN	HB2	2.994	0.02	2
UNMAPPED	25	THR	HA	3.7059	0.02	1
UNMAPPED	13	LYS	HD3	1.836	0.02	1
UNMAPPED	16	THR	HG1	2.695	0.02	1
UNMAPPED	1	MET	HE2	2.11	0.02	1
UNMAPPED	37	ASN	CA	54.5283	0.2	1
UNMAPPED	8	ASN	ND2	111.22	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	GLY	N	108.452	0.2	1
UNMAPPED	27	GLU	HB2	1.587	0.02	2
UNMAPPED	35	ASN	HD22	6.854	0.02	2
UNMAPPED	43	TRP	HE3	7.021	0.02	1
UNMAPPED	6	ILE	HA	4.43	0.02	1
UNMAPPED	4	LYS	N	122.1187	0.2	1
UNMAPPED	50	LYS	H	7.8543	0.02	1
UNMAPPED	56	GLU	HB2	2.202	0.02	2
UNMAPPED	54	VAL	HG22	-0.5566	0.02	2
UNMAPPED	56	GLU	HG2	2.406	0.02	1
UNMAPPED	29	VAL	HG11	0.877	0.02	2
UNMAPPED	12	LEU	HD23	0.119	0.02	2
UNMAPPED	38	GLY	N	106.737	0.2	1
UNMAPPED	31	LYS	CA	61.746	0.2	1
UNMAPPED	39	VAL	HG22	1.014	0.02	2
UNMAPPED	13	LYS	CB	36.4188	0.2	1
UNMAPPED	34	PHE	CB	36.6219	0.2	1
UNMAPPED	34	PHE	CD1	129.4	0.2	1
UNMAPPED	13	LYS	N	120.3738	0.2	1
UNMAPPED	37	ASN	HB3	1.748	0.02	2
UNMAPPED	7	LEU	N	126.09	0.2	1
UNMAPPED	21	VAL	HG21	1.006	0.02	2
UNMAPPED	20	ALA	HB2	1.466	0.02	1
UNMAPPED	17	THR	HG21	1.1855	0.02	1
UNMAPPED	25	THR	CB	67.7	0.2	1
UNMAPPED	27	GLU	CA	59.0941	0.2	1
UNMAPPED	40	ASP	CA	54.6088	0.2	1
UNMAPPED	45	TYR	HA	4.942	0.02	1
UNMAPPED	42	GLU	CG	35.7186	0.2	1
UNMAPPED	7	LEU	HB2	1.4367	0.02	2
UNMAPPED	13	LYS	HE3	3.033	0.02	2
UNMAPPED	47	ASP	HB2	2.8403	0.02	2
UNMAPPED	47	ASP	CB	42.1665	0.2	1
UNMAPPED	7	LEU	HD23	0.76	0.02	2
UNMAPPED	24	ALA	CA	54.7899	0.2	1
UNMAPPED	42	GLU	CA	55.6336	0.2	1
UNMAPPED	43	TRP	CA	55.5955	0.2	1
UNMAPPED	17	THR	CA	60.7031	0.2	1
UNMAPPED	21	VAL	CA	63.8046	0.2	1
UNMAPPED	22	ASP	CA	52.522	0.2	1
UNMAPPED	32	GLN	HG3	2.354	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	2	GLN	HB2	1.9799	0.02	2
UNMAPPED	35	ASN	CA	56.773	0.2	1
UNMAPPED	53	THR	CA	62.6793	0.2	1
UNMAPPED	15	GLU	HB3	2.0859	0.02	2
UNMAPPED	2	GLN	HB3	1.9028	0.02	2
UNMAPPED	30	VAL	H	7.9981	0.02	1
UNMAPPED	10	LYS	CD	29.005	0.2	1
UNMAPPED	3	TYR	N	123.7074	0.2	1
UNMAPPED	18	THR	H	8.8949	0.02	1
UNMAPPED	1	MET	HB2	2.068	0.02	2
UNMAPPED	50	LYS	CB	29.1832	0.2	1
UNMAPPED	51	THR	HG1	4.421	0.02	1
UNMAPPED	39	VAL	HG13	0.938	0.02	2
UNMAPPED	6	ILE	CD1	12.38	0.2	1
UNMAPPED	52	PHE	CB	43.0099	0.2	1
UNMAPPED	43	TRP	HD1	7.112	0.02	1
UNMAPPED	4	LYS	HE2	2.922	0.02	2
UNMAPPED	44	THR	HG21	1.3086	0.02	1
UNMAPPED	15	GLU	N	119.3863	0.2	1
UNMAPPED	17	THR	H	9.2726	0.02	1
UNMAPPED	21	VAL	HG13	1.02	0.02	2
UNMAPPED	45	TYR	HB3	2.6108	0.02	2
UNMAPPED	5	VAL	HA	4.9758	0.02	1
UNMAPPED	5	VAL	HG12	0.8493	0.02	2
UNMAPPED	31	LYS	HE2	1.165	0.02	2
UNMAPPED	40	ASP	HB2	2.8064	0.02	2
UNMAPPED	23	ALA	HB1	0.898	0.02	1
UNMAPPED	48	ALA	HB3	1.502	0.02	1
UNMAPPED	30	VAL	CG2	22.98	0.2	2
UNMAPPED	53	THR	H	9.1022	0.02	1
UNMAPPED	24	ALA	HB2	1.281	0.02	1
UNMAPPED	19	GLU	HA	5.2654	0.02	1
UNMAPPED	21	VAL	HB	2.195	0.02	1
UNMAPPED	25	THR	HG21	1.2758	0.02	1
UNMAPPED	28	LYS	CE	42.0126	0.2	1
UNMAPPED	6	ILE	HG23	0.967	0.02	1
UNMAPPED	32	GLN	HE22	7.973	0.02	2
UNMAPPED	3	TYR	CD1	133.5	0.2	1
UNMAPPED	53	THR	HA	4.9828	0.02	1
UNMAPPED	16	THR	HG23	0.9257	0.02	1
UNMAPPED	56	GLU	HA	4.239	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	19	GLU	CA	54.5657	0.2	1
UNMAPPED	29	VAL	CG1	20.95	0.2	2
UNMAPPED	6	ILE	HG21	0.967	0.02	1
UNMAPPED	3	TYR	HB2	3.0297	0.02	2
UNMAPPED	2	GLN	CG	34.928	0.2	1
UNMAPPED	1	MET	HE3	2.11	0.02	1
UNMAPPED	30	VAL	HA	3.2967	0.02	1
UNMAPPED	39	VAL	N	118.4043	0.2	1
UNMAPPED	49	THR	CA	60.4545	0.2	1
UNMAPPED	32	GLN	NE2	114.299	0.2	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	56	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	52	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	55	0.00 ± 0.00	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 907. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/350 (0%)	0/140 (0%)	0/140 (0%)	0/70 (0%)
Sidechain	0/464 (0%)	0/267 (0%)	0/179 (0%)	0/18 (0%)
Aromatic	0/93 (0%)	0/49 (0%)	0/42 (0%)	0/2 (0%)
Overall	0/907 (0%)	0/456 (0%)	0/361 (0%)	0/90 (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 1213. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/486 (0%)	0/194 (0%)	0/196 (0%)	0/96 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	0/626 (0%)	0/363 (0%)	0/235 (0%)	0/28 (0%)
Aromatic	0/101 (0%)	0/53 (0%)	0/44 (0%)	0/4 (0%)
Overall	0/1213 (0%)	0/610 (0%)	0/475 (0%)	0/128 (0%)

7.1.4 Statistically unusual chemical shifts (i)

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

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
???	UNMAPPED	31	LYS	HE2	1.17	3.87 – 1.97	-9.2
???	UNMAPPED	31	LYS	HE3	1.85	3.86 – 1.96	-5.6
???	UNMAPPED	27	GLU	HG3	1.10	3.31 – 1.21	-5.5

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.