



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:24 pm GMT

PDB ID : 1ILY
Title : Solution Structure of Ribosomal Protein L18 of *Thermus thermophilus*
Authors : Woestenenk, E.A.; Gongadze, G.M.; Shcherbakov, D.V.; Rak, A.V.; Garber, M.B.; Hard, T.; Berglund, H.
Deposited on : 2001-05-09

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

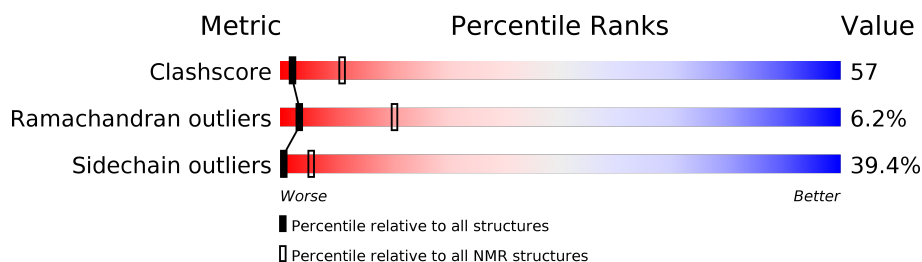
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 75%.

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	90	

2 Ensemble composition and analysis

This entry contains 27 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:23-A:52, A:63-A:111 (79)	0.23	5

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

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

The models can be grouped into 3 clusters and 9 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 7, 10, 12, 15, 16, 25, 26, 27
2	8, 19, 20
3	11, 18
Single-model clusters	2; 9; 13; 14; 17; 21; 22; 23; 24

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1439 atoms, of which 743 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RIBOSOMAL PROTEIN L18.

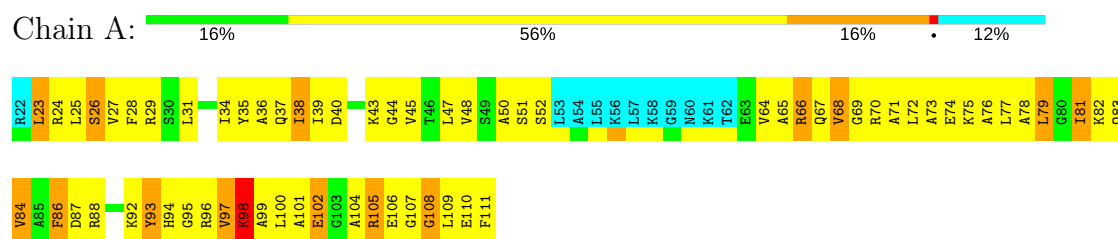
Mol	Chain	Residues	Atoms					Trace
1	A	90	Total	C	H	N	O	0
			1439	442	743	131	123	

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: RIBOSOMAL PROTEIN L18

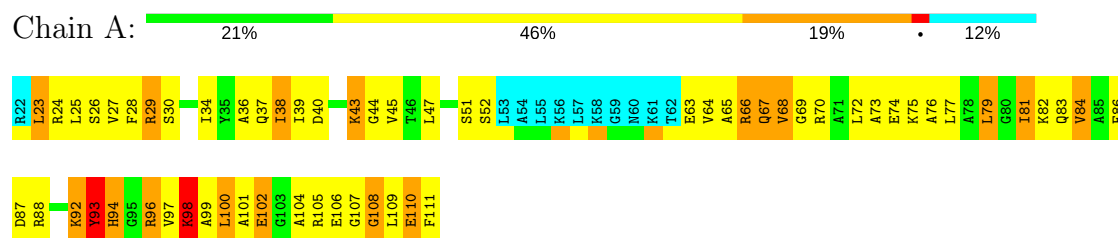


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

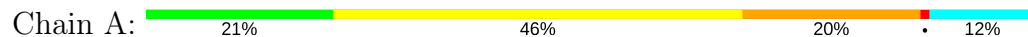
4.2.1 Score per residue for model 1

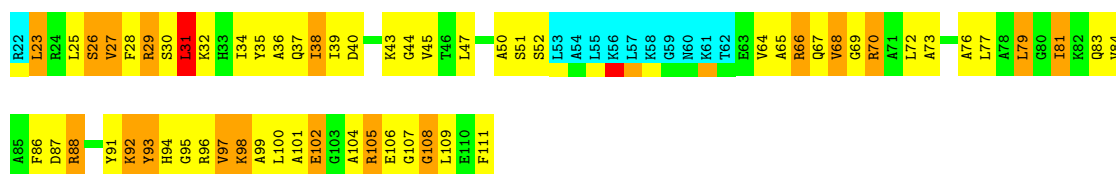
• Molecule 1: RIBOSOMAL PROTEIN L18



4.2.2 Score per residue for model 2

• Molecule 1: RIBOSOMAL PROTEIN L18

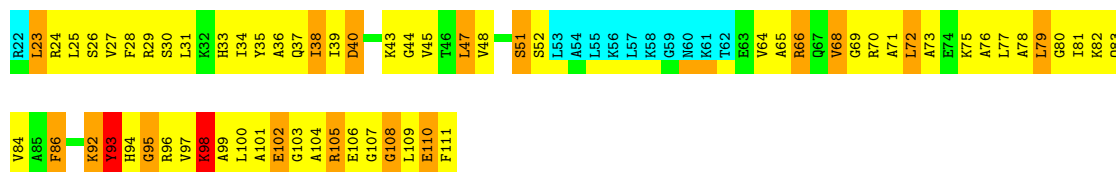




4.2.3 Score per residue for model 3

- Molecule 1: RIBOSOMAL PROTEIN L18

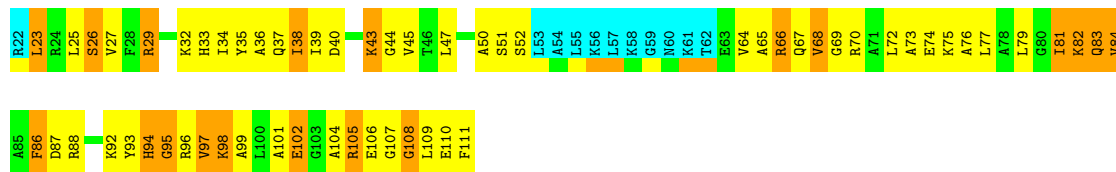
Chain A: 17% 51% 18% 12%



4.2.4 Score per residue for model 4

- Molecule 1: RIBOSOMAL PROTEIN L18

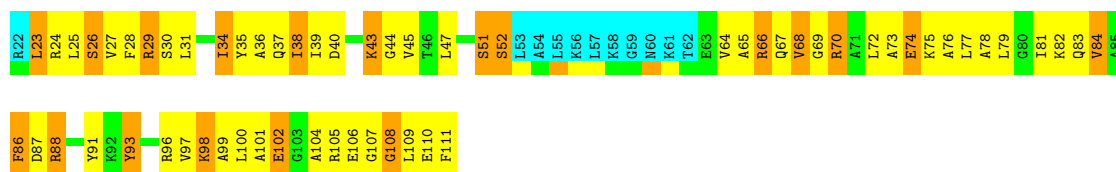
Chain A: 21% 46% 21% 12%



4.2.5 Score per residue for model 5 (medoid)

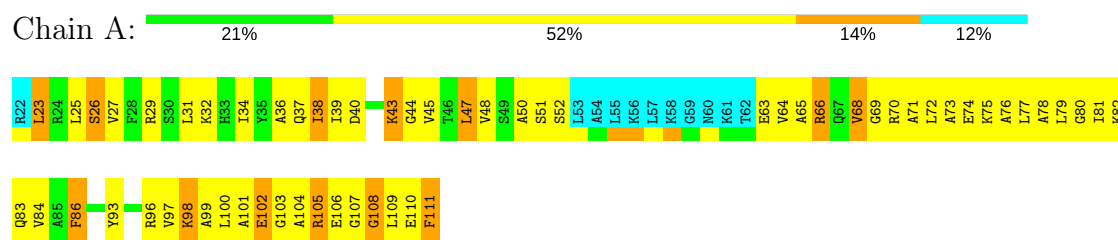
- Molecule 1: RIBOSOMAL PROTEIN L18

Chain A: 20% 47% 21% 12%



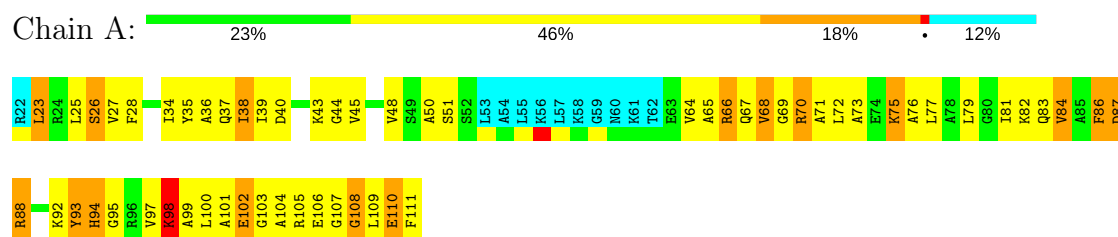
4.2.6 Score per residue for model 6

- Molecule 1: RIBOSOMAL PROTEIN L18



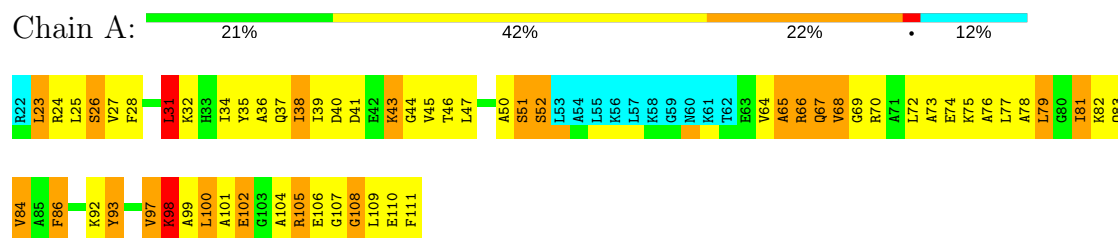
4.2.7 Score per residue for model 7

- Molecule 1: RIBOSOMAL PROTEIN L18



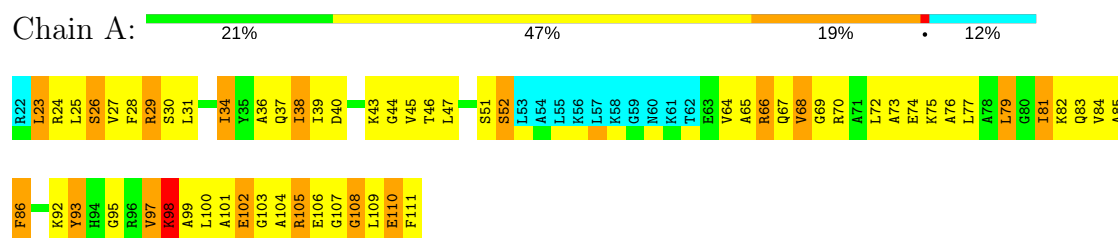
4.2.8 Score per residue for model 8

- Molecule 1: RIBOSOMAL PROTEIN L18



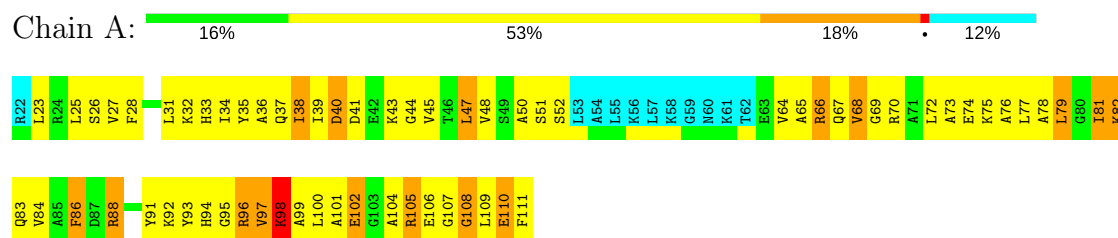
4.2.9 Score per residue for model 9

- Molecule 1: RIBOSOMAL PROTEIN L18



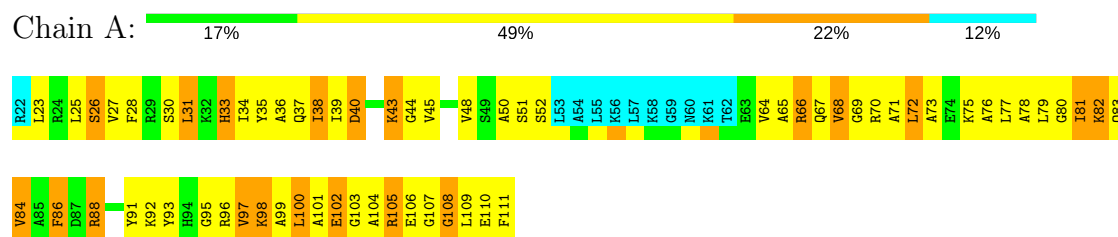
4.2.10 Score per residue for model 10

• Molecule 1: RIBOSOMAL PROTEIN L18



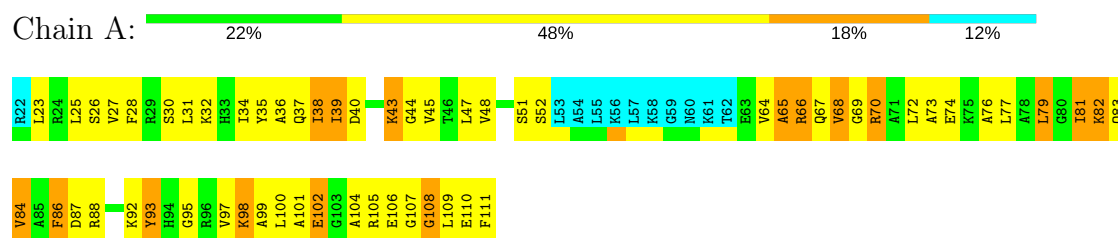
4.2.11 Score per residue for model 11

• Molecule 1: RIBOSOMAL PROTEIN L18



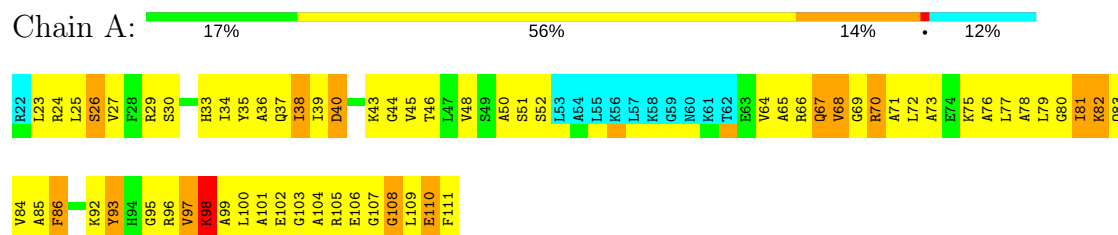
4.2.12 Score per residue for model 12

• Molecule 1: RIBOSOMAL PROTEIN L18



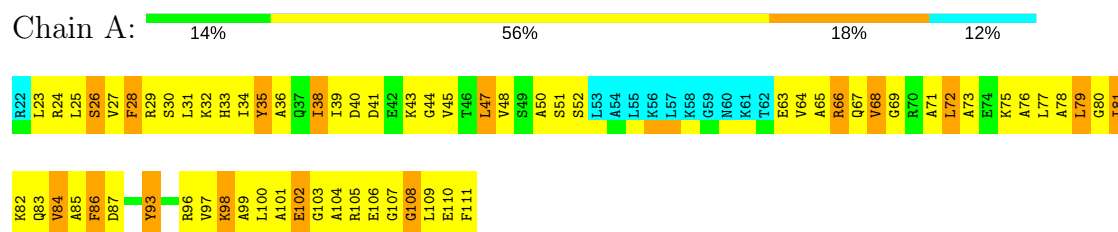
4.2.13 Score per residue for model 13

• Molecule 1: RIBOSOMAL PROTEIN L18



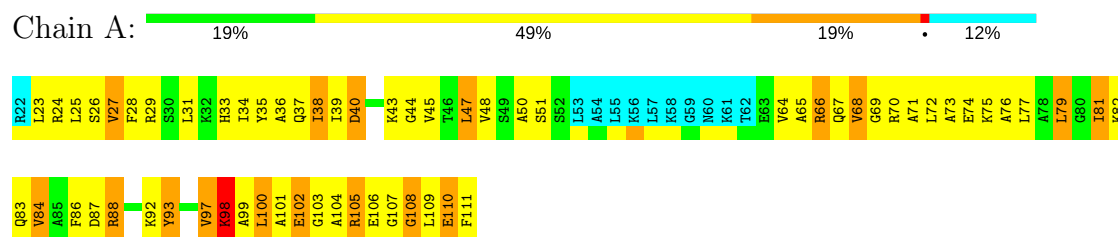
4.2.18 Score per residue for model 18

- Molecule 1: RIBOSOMAL PROTEIN L18



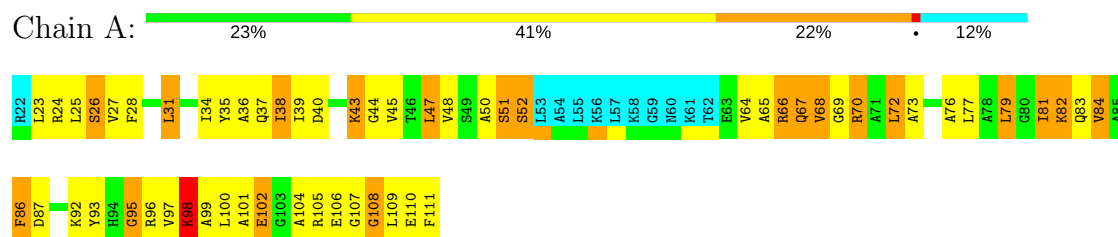
4.2.19 Score per residue for model 19

- Molecule 1: RIBOSOMAL PROTEIN L18



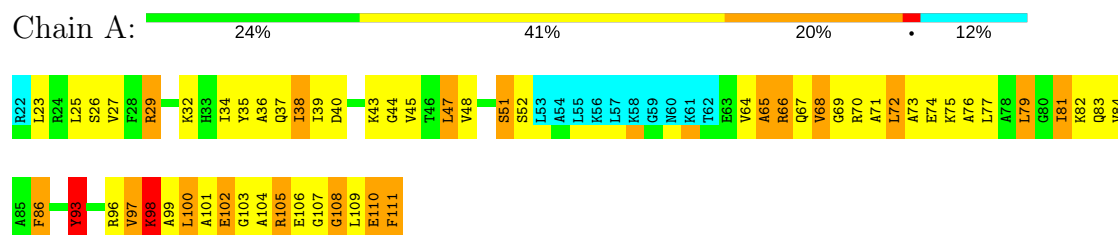
4.2.20 Score per residue for model 20

- Molecule 1: RIBOSOMAL PROTEIN L18



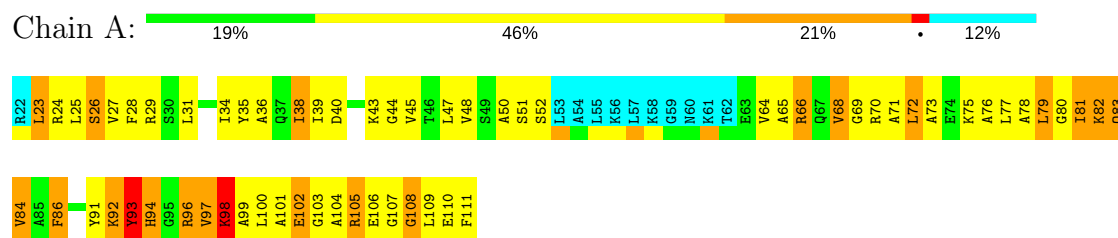
4.2.21 Score per residue for model 21

- Molecule 1: RIBOSOMAL PROTEIN L18



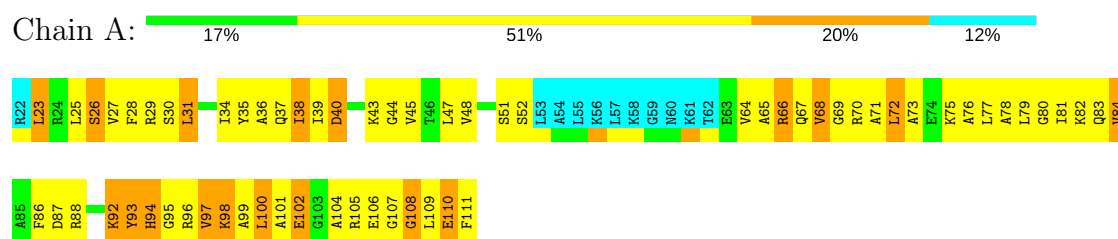
4.2.22 Score per residue for model 22

- Molecule 1: RIBOSOMAL PROTEIN L18



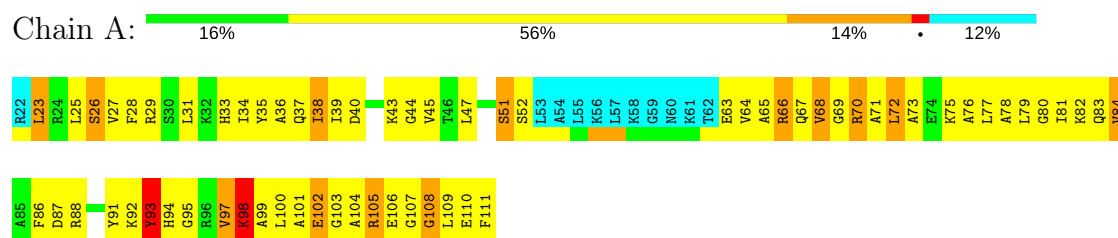
4.2.23 Score per residue for model 23

- Molecule 1: RIBOSOMAL PROTEIN L18



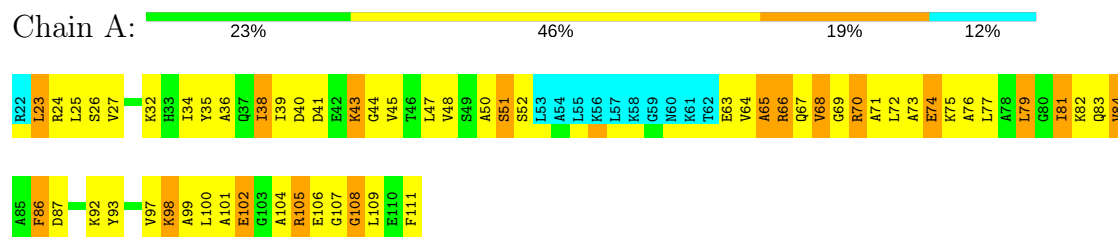
4.2.24 Score per residue for model 24

- Molecule 1: RIBOSOMAL PROTEIN L18



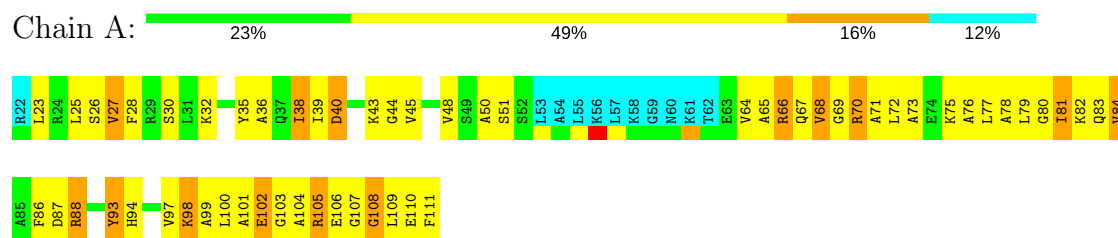
4.2.25 Score per residue for model 25

- Molecule 1: RIBOSOMAL PROTEIN L18



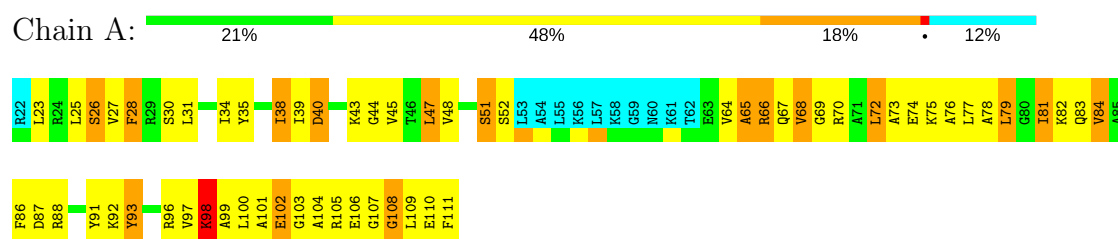
4.2.26 Score per residue for model 26

• Molecule 1: RIBOSOMAL PROTEIN L18



4.2.27 Score per residue for model 27

• Molecule 1: RIBOSOMAL PROTEIN L18



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 27 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
CNS	structure solution	1.0
CNS	refinement	1.0

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 4688
Number of chemical shift lists	1
Total number of shifts	1158
Number of shifts mapped to atoms	945
Number of unparsed shifts	0
Number of shifts with mapping errors	213
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

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	610	635	633	70±5
All	All	16470	17145	17091	1900

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:HD11	1:A:72:LEU:HD21	1.05	1.23	3	13
1:A:65:ALA:O	1:A:68:VAL:HG12	0.98	1.57	17	27
1:A:36:ALA:HB2	1:A:100:LEU:HD11	0.87	1.44	21	7
1:A:36:ALA:HB3	1:A:72:LEU:HD22	0.87	1.45	21	7
1:A:102:GLU:O	1:A:106:GLU:N	0.85	2.09	25	27
1:A:36:ALA:HB3	1:A:72:LEU:HD13	0.85	1.48	14	15
1:A:73:ALA:HB2	1:A:104:ALA:HA	0.84	1.47	16	27
1:A:36:ALA:HB3	1:A:72:LEU:CD1	0.84	2.02	14	15
1:A:105:ARG:HA	1:A:109:LEU:O	0.83	1.73	22	27
1:A:25:LEU:HD23	1:A:26:SER:N	0.83	1.87	26	27
1:A:38:ILE:HD11	1:A:72:LEU:CD2	0.83	2.04	6	15
1:A:94:HIS:CE1	1:A:97:VAL:HG23	0.82	2.08	3	1
1:A:25:LEU:HD22	1:A:86:PHE:CE2	0.80	2.10	24	3
1:A:25:LEU:HD22	1:A:86:PHE:CE1	0.76	2.15	22	23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HD11	1:A:100:LEU:HD13	0.76	1.55	10	20
1:A:38:ILE:HD11	1:A:72:LEU:HD22	0.75	1.59	14	2
1:A:48:VAL:CG1	1:A:72:LEU:HD23	0.75	2.10	13	4
1:A:50:ALA:HB2	1:A:75:LYS:CE	0.75	2.11	10	2
1:A:38:ILE:HD11	1:A:72:LEU:HD11	0.75	1.57	9	2
1:A:34:ILE:HD11	1:A:100:LEU:CD1	0.74	2.12	2	10
1:A:38:ILE:HD12	1:A:109:LEU:CD2	0.74	2.12	18	26
1:A:34:ILE:HD13	1:A:96:ARG:HB3	0.74	1.59	13	10
1:A:34:ILE:HD11	1:A:100:LEU:HD12	0.73	1.61	5	3
1:A:27:VAL:HG12	1:A:88:ARG:HG2	0.73	1.59	14	1
1:A:27:VAL:HG12	1:A:88:ARG:NH1	0.72	2.00	16	1
1:A:27:VAL:CG1	1:A:97:VAL:HG22	0.71	2.15	17	3
1:A:27:VAL:HG11	1:A:97:VAL:HG22	0.71	1.62	17	5
1:A:48:VAL:HG21	1:A:75:LYS:HB2	0.71	1.61	25	8
1:A:48:VAL:HG12	1:A:72:LEU:HD23	0.70	1.63	22	2
1:A:86:PHE:CZ	1:A:88:ARG:CZ	0.69	2.75	19	4
1:A:34:ILE:HD12	1:A:35:TYR:N	0.69	2.01	5	1
1:A:48:VAL:HG21	1:A:75:LYS:CB	0.69	2.17	18	11
1:A:50:ALA:HB3	1:A:72:LEU:HG	0.68	1.63	2	9
1:A:25:LEU:HD22	1:A:86:PHE:CD2	0.68	2.24	24	3
1:A:38:ILE:CD1	1:A:72:LEU:HD21	0.68	2.15	23	13
1:A:23:LEU:HD22	1:A:81:ILE:HG13	0.68	1.65	11	13
1:A:27:VAL:O	1:A:88:ARG:HG2	0.68	1.89	24	3
1:A:86:PHE:CE2	1:A:88:ARG:CZ	0.68	2.77	16	4
1:A:29:ARG:HG2	1:A:34:ILE:HD12	0.68	1.62	22	3
1:A:36:ALA:HB3	1:A:72:LEU:CD2	0.67	2.19	11	7
1:A:71:ALA:O	1:A:75:LYS:HG3	0.66	1.91	13	14
1:A:38:ILE:CG1	1:A:72:LEU:HD21	0.66	2.20	9	2
1:A:48:VAL:HG21	1:A:76:ALA:N	0.66	2.06	7	1
1:A:47:LEU:HD22	1:A:79:LEU:HD13	0.66	1.68	18	2
1:A:67:GLN:O	1:A:70:ARG:HG3	0.66	1.91	19	15
1:A:50:ALA:HB3	1:A:72:LEU:CD2	0.66	2.20	8	4
1:A:82:LYS:O	1:A:110:GLU:N	0.65	2.29	4	24
1:A:77:LEU:HD11	1:A:108:GLY:HA3	0.65	1.68	27	27
1:A:38:ILE:HD11	1:A:72:LEU:CD1	0.65	2.22	27	2
1:A:66:ARG:HA	1:A:99:ALA:O	0.65	1.92	16	27
1:A:23:LEU:HD22	1:A:81:ILE:CG1	0.65	2.21	13	11
1:A:27:VAL:HG11	1:A:97:VAL:HG23	0.64	1.69	1	1
1:A:29:ARG:NH2	1:A:34:ILE:HD12	0.64	2.08	4	1
1:A:43:LYS:O	1:A:45:VAL:HG23	0.64	1.93	14	25
1:A:48:VAL:HG22	1:A:75:LYS:HD3	0.64	1.69	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:VAL:O	1:A:101:ALA:CB	0.64	2.46	14	26
1:A:76:ALA:HB3	1:A:109:LEU:HD11	0.64	1.67	16	27
1:A:38:ILE:HD12	1:A:109:LEU:HD21	0.64	1.69	18	24
1:A:34:ILE:HD13	1:A:96:ARG:CB	0.64	2.22	13	4
1:A:25:LEU:CD1	1:A:111:PHE:CE2	0.63	2.81	14	1
1:A:38:ILE:CD1	1:A:72:LEU:HD11	0.63	2.23	9	1
1:A:95:GLY:C	1:A:98:LYS:HE2	0.63	2.14	23	1
1:A:77:LEU:HD11	1:A:107:GLY:O	0.63	1.93	18	27
1:A:38:ILE:O	1:A:47:LEU:HD12	0.62	1.93	17	2
1:A:65:ALA:HB3	1:A:99:ALA:HB3	0.62	1.72	9	11
1:A:27:VAL:HG21	1:A:100:LEU:CD2	0.62	2.24	24	2
1:A:73:ALA:HA	1:A:109:LEU:HD13	0.62	1.71	9	25
1:A:43:LYS:O	1:A:45:VAL:N	0.62	2.33	12	27
1:A:25:LEU:HG	1:A:38:ILE:HD13	0.62	1.71	6	25
1:A:50:ALA:HB3	1:A:72:LEU:CG	0.61	2.24	13	9
1:A:86:PHE:CD1	1:A:88:ARG:NH2	0.61	2.68	16	1
1:A:37:GLN:HG3	1:A:39:ILE:HD11	0.61	1.72	12	1
1:A:100:LEU:HD23	1:A:101:ALA:N	0.61	2.11	17	17
1:A:84:VAL:HG21	1:A:109:LEU:HD23	0.61	1.71	22	8
1:A:23:LEU:HD13	1:A:81:ILE:HG13	0.61	1.72	27	13
1:A:27:VAL:HG23	1:A:86:PHE:CE2	0.61	2.31	24	1
1:A:35:TYR:N	1:A:35:TYR:CD1	0.61	2.69	18	1
1:A:52:SER:N	1:A:68:VAL:HG21	0.60	2.10	6	15
1:A:23:LEU:N	1:A:23:LEU:HD23	0.60	2.11	14	5
1:A:88:ARG:C	1:A:88:ARG:HD3	0.60	2.17	2	1
1:A:102:GLU:O	1:A:106:GLU:HB3	0.60	1.96	3	27
1:A:34:ILE:HD13	1:A:96:ARG:HD2	0.60	1.72	15	2
1:A:86:PHE:CD1	1:A:111:PHE:CD2	0.60	2.90	15	23
1:A:23:LEU:HD23	1:A:23:LEU:N	0.59	2.13	22	8
1:A:25:LEU:HD23	1:A:26:SER:H	0.59	1.58	17	25
1:A:29:ARG:CZ	1:A:34:ILE:HD12	0.59	2.28	4	1
1:A:88:ARG:CD	1:A:88:ARG:N	0.59	2.65	26	2
1:A:25:LEU:HD12	1:A:111:PHE:CD2	0.59	2.33	14	1
1:A:27:VAL:CG2	1:A:100:LEU:HD13	0.58	2.27	21	14
1:A:94:HIS:CD2	1:A:94:HIS:N	0.58	2.70	22	1
1:A:98:LYS:HG2	1:A:99:ALA:N	0.58	2.13	23	1
1:A:86:PHE:CE2	1:A:88:ARG:NE	0.58	2.71	7	1
1:A:25:LEU:CD1	1:A:111:PHE:CD2	0.57	2.87	14	1
1:A:50:ALA:HB2	1:A:75:LYS:HE2	0.57	1.76	10	2
1:A:36:ALA:CB	1:A:72:LEU:HD22	0.57	2.29	6	1
1:A:98:LYS:N	1:A:98:LYS:HE3	0.57	2.14	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:HD11	1:A:72:LEU:HD13	0.57	1.76	11	3
1:A:93:TYR:CD1	1:A:98:LYS:CE	0.57	2.88	21	6
1:A:23:LEU:HD13	1:A:47:LEU:CD1	0.57	2.30	4	9
1:A:23:LEU:HD23	1:A:47:LEU:CD1	0.57	2.30	16	3
1:A:34:ILE:HG21	1:A:96:ARG:HD2	0.56	1.77	18	1
1:A:27:VAL:HG11	1:A:29:ARG:NH2	0.56	2.15	23	1
1:A:29:ARG:HA	1:A:33:HIS:O	0.56	2.00	14	1
1:A:70:ARG:O	1:A:74:GLU:HB2	0.56	2.01	25	5
1:A:92:LYS:O	1:A:93:TYR:C	0.56	2.44	2	4
1:A:93:TYR:CE1	1:A:98:LYS:HG3	0.56	2.35	21	5
1:A:23:LEU:HD13	1:A:40:ASP:HA	0.56	1.77	25	1
1:A:104:ALA:HB3	1:A:111:PHE:CZ	0.55	2.36	22	20
1:A:73:ALA:HB2	1:A:104:ALA:CA	0.55	2.31	4	24
1:A:27:VAL:CG2	1:A:34:ILE:HD11	0.55	2.31	21	1
1:A:34:ILE:HD13	1:A:96:ARG:CD	0.55	2.32	4	1
1:A:88:ARG:NH2	1:A:91:TYR:CE2	0.55	2.75	2	1
1:A:25:LEU:HD22	1:A:86:PHE:HE1	0.54	1.62	19	10
1:A:93:TYR:CE1	1:A:98:LYS:CE	0.54	2.90	20	7
1:A:109:LEU:N	1:A:109:LEU:HD12	0.54	2.17	24	17
1:A:48:VAL:HG13	1:A:75:LYS:HD2	0.54	1.80	7	1
1:A:27:VAL:HG21	1:A:100:LEU:CD1	0.54	2.32	23	3
1:A:50:ALA:HB2	1:A:75:LYS:HE3	0.54	1.79	10	1
1:A:109:LEU:HD12	1:A:109:LEU:N	0.53	2.18	13	10
1:A:36:ALA:HB3	1:A:72:LEU:HD11	0.53	1.77	20	1
1:A:48:VAL:HG23	1:A:79:LEU:HD21	0.53	1.79	19	4
1:A:23:LEU:O	1:A:84:VAL:HG12	0.53	2.03	12	13
1:A:27:VAL:HG21	1:A:100:LEU:HD22	0.53	1.79	24	3
1:A:29:ARG:CG	1:A:34:ILE:HD12	0.53	2.33	3	1
1:A:31:LEU:HD12	1:A:32:LYS:N	0.53	2.19	8	1
1:A:23:LEU:CD1	1:A:47:LEU:HD13	0.53	2.33	1	3
1:A:104:ALA:HB3	1:A:111:PHE:HZ	0.52	1.64	22	26
1:A:23:LEU:O	1:A:84:VAL:HA	0.52	2.04	5	4
1:A:86:PHE:CE1	1:A:88:ARG:NH2	0.52	2.78	7	3
1:A:50:ALA:HB3	1:A:72:LEU:CD1	0.52	2.34	22	4
1:A:104:ALA:O	1:A:109:LEU:HB2	0.52	2.04	16	19
1:A:66:ARG:O	1:A:69:GLY:N	0.51	2.43	8	27
1:A:34:ILE:O	1:A:34:ILE:HG23	0.51	2.05	4	2
1:A:50:ALA:HB2	1:A:75:LYS:NZ	0.51	2.20	7	3
1:A:97:VAL:O	1:A:101:ALA:HB2	0.51	2.05	21	8
1:A:29:ARG:NE	1:A:96:ARG:CB	0.51	2.74	23	1
1:A:95:GLY:O	1:A:98:LYS:NZ	0.51	2.41	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ALA:O	1:A:72:LEU:HD21	0.51	2.05	22	1
1:A:34:ILE:HG23	1:A:34:ILE:O	0.51	2.06	20	3
1:A:25:LEU:HD13	1:A:111:PHE:CE2	0.51	2.41	17	2
1:A:36:ALA:O	1:A:72:LEU:HD11	0.51	2.05	14	1
1:A:39:ILE:HG22	1:A:40:ASP:N	0.51	2.21	19	26
1:A:94:HIS:CD2	1:A:97:VAL:HG21	0.51	2.41	22	1
1:A:102:GLU:O	1:A:106:GLU:CB	0.51	2.58	13	20
1:A:23:LEU:HD13	1:A:47:LEU:HD13	0.50	1.81	4	2
1:A:72:LEU:HD13	1:A:73:ALA:N	0.50	2.21	9	1
1:A:23:LEU:O	1:A:84:VAL:CG1	0.50	2.60	12	10
1:A:67:GLN:O	1:A:70:ARG:HG2	0.50	2.06	8	3
1:A:27:VAL:CG2	1:A:100:LEU:CD1	0.50	2.90	26	14
1:A:29:ARG:NH2	1:A:34:ILE:CD1	0.50	2.74	4	3
1:A:98:LYS:O	1:A:102:GLU:HG2	0.50	2.06	23	2
1:A:88:ARG:NE	1:A:91:TYR:CD2	0.50	2.80	2	1
1:A:35:TYR:CD2	1:A:51:SER:CB	0.50	2.94	18	2
1:A:73:ALA:HB3	1:A:107:GLY:HA3	0.50	1.83	20	20
1:A:65:ALA:O	1:A:100:LEU:HA	0.49	2.06	23	16
1:A:27:VAL:HG21	1:A:100:LEU:HD13	0.49	1.84	18	16
1:A:23:LEU:CD2	1:A:23:LEU:N	0.49	2.75	7	5
1:A:86:PHE:CG	1:A:88:ARG:NH2	0.49	2.80	16	1
1:A:73:ALA:O	1:A:77:LEU:HB2	0.49	2.06	2	27
1:A:88:ARG:NE	1:A:88:ARG:N	0.49	2.60	19	2
1:A:38:ILE:HD11	1:A:72:LEU:CG	0.49	2.38	4	6
1:A:34:ILE:C	1:A:35:TYR:CD1	0.49	2.86	18	5
1:A:109:LEU:N	1:A:109:LEU:CD1	0.49	2.76	21	17
1:A:23:LEU:N	1:A:23:LEU:CD2	0.49	2.76	22	6
1:A:35:TYR:CE2	1:A:51:SER:CB	0.49	2.96	21	2
1:A:88:ARG:NH2	1:A:91:TYR:CZ	0.49	2.80	2	1
1:A:111:PHE:CD1	1:A:111:PHE:N	0.48	2.81	21	8
1:A:88:ARG:HG2	1:A:91:TYR:CZ	0.48	2.43	24	1
1:A:27:VAL:HG12	1:A:88:ARG:HH11	0.48	1.67	16	1
1:A:111:PHE:N	1:A:111:PHE:CD1	0.48	2.81	6	17
1:A:109:LEU:CD1	1:A:109:LEU:N	0.48	2.76	6	10
1:A:93:TYR:CD1	1:A:98:LYS:HE2	0.48	2.43	21	6
1:A:97:VAL:O	1:A:98:LYS:C	0.48	2.50	23	1
1:A:27:VAL:HG22	1:A:35:TYR:O	0.48	2.08	26	1
1:A:27:VAL:HG21	1:A:29:ARG:NH2	0.48	2.23	22	2
1:A:50:ALA:HB3	1:A:72:LEU:HD12	0.48	1.84	14	1
1:A:50:ALA:HB3	1:A:72:LEU:HB2	0.48	1.84	4	1
1:A:50:ALA:N	1:A:72:LEU:HD21	0.48	2.22	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HG21	1:A:52:SER:OG	0.48	2.08	4	2
1:A:72:LEU:HD13	1:A:72:LEU:C	0.48	2.29	9	1
1:A:92:LYS:O	1:A:94:HIS:N	0.48	2.47	3	3
1:A:29:ARG:CD	1:A:96:ARG:HB2	0.48	2.39	21	1
1:A:69:GLY:HA2	1:A:72:LEU:HD12	0.48	1.84	2	4
1:A:27:VAL:HG11	1:A:29:ARG:HH22	0.48	1.68	23	1
1:A:88:ARG:HB3	1:A:88:ARG:NH1	0.48	2.23	16	1
1:A:93:TYR:CE2	1:A:98:LYS:CD	0.47	2.97	3	1
1:A:23:LEU:HD22	1:A:40:ASP:CG	0.47	2.30	14	2
1:A:23:LEU:HD13	1:A:40:ASP:CA	0.47	2.39	25	1
1:A:70:ARG:O	1:A:74:GLU:CG	0.47	2.62	4	9
1:A:64:VAL:HG13	1:A:67:GLN:HB2	0.47	1.86	15	9
1:A:35:TYR:CG	1:A:51:SER:HB2	0.47	2.44	2	4
1:A:23:LEU:HD22	1:A:40:ASP:HA	0.47	1.86	6	1
1:A:34:ILE:HG21	1:A:52:SER:HB2	0.47	1.86	8	1
1:A:23:LEU:HD23	1:A:23:LEU:H	0.47	1.69	24	1
1:A:91:TYR:CD2	1:A:94:HIS:CE1	0.47	3.03	22	1
1:A:75:LYS:O	1:A:78:ALA:N	0.47	2.47	26	13
1:A:27:VAL:HG21	1:A:29:ARG:HH22	0.47	1.69	5	1
1:A:27:VAL:HG13	1:A:27:VAL:O	0.47	2.08	11	10
1:A:50:ALA:HB3	1:A:72:LEU:HD21	0.47	1.85	8	1
1:A:86:PHE:CZ	1:A:88:ARG:NH1	0.47	2.82	19	3
1:A:86:PHE:CD2	1:A:88:ARG:CZ	0.47	2.98	16	1
1:A:23:LEU:HD12	1:A:81:ILE:CG1	0.47	2.40	4	1
1:A:93:TYR:CE1	1:A:98:LYS:HE3	0.47	2.45	9	5
1:A:52:SER:N	1:A:68:VAL:CG2	0.46	2.78	12	5
1:A:35:TYR:CD2	1:A:51:SER:HB3	0.46	2.44	11	5
1:A:35:TYR:CG	1:A:51:SER:HB3	0.46	2.45	14	5
1:A:29:ARG:HD3	1:A:34:ILE:HA	0.46	1.86	17	1
1:A:88:ARG:NE	1:A:88:ARG:H	0.46	2.08	16	1
1:A:35:TYR:CD1	1:A:51:SER:HB3	0.46	2.46	20	1
1:A:23:LEU:CD1	1:A:47:LEU:CD1	0.46	2.94	1	4
1:A:86:PHE:CD2	1:A:88:ARG:HD3	0.46	2.45	11	3
1:A:86:PHE:CD2	1:A:88:ARG:NE	0.46	2.84	16	2
1:A:88:ARG:NH1	1:A:97:VAL:HG21	0.46	2.26	1	1
1:A:88:ARG:HG3	1:A:91:TYR:HB2	0.46	1.88	10	3
1:A:50:ALA:HB3	1:A:72:LEU:HD23	0.46	1.87	18	2
1:A:47:LEU:H	1:A:47:LEU:HD12	0.46	1.71	10	4
1:A:27:VAL:HG12	1:A:86:PHE:HZ	0.46	1.70	23	1
1:A:93:TYR:CZ	1:A:98:LYS:CE	0.46	2.99	20	1
1:A:100:LEU:HD23	1:A:100:LEU:C	0.46	2.32	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ALA:O	1:A:102:GLU:HG3	0.46	2.11	1	1
1:A:40:ASP:N	1:A:47:LEU:HD11	0.46	2.26	10	1
1:A:97:VAL:O	1:A:101:ALA:HB3	0.46	2.11	24	8
1:A:86:PHE:CE1	1:A:88:ARG:CZ	0.45	3.00	7	1
1:A:87:ASP:N	1:A:88:ARG:NH1	0.45	2.63	7	1
1:A:34:ILE:CD1	1:A:100:LEU:HD13	0.45	2.38	13	1
1:A:29:ARG:HH12	1:A:34:ILE:HD13	0.45	1.71	5	1
1:A:93:TYR:CZ	1:A:98:LYS:HE2	0.45	2.46	7	2
1:A:23:LEU:HD22	1:A:40:ASP:OD1	0.45	2.10	14	6
1:A:86:PHE:CG	1:A:88:ARG:NH1	0.45	2.83	7	1
1:A:94:HIS:CD2	1:A:97:VAL:CG2	0.45	2.99	22	1
1:A:29:ARG:HD3	1:A:97:VAL:HG23	0.45	1.87	13	1
1:A:25:LEU:HB3	1:A:86:PHE:CD1	0.45	2.47	6	6
1:A:81:ILE:CD1	1:A:81:ILE:N	0.45	2.80	10	5
1:A:27:VAL:O	1:A:27:VAL:HG13	0.45	2.10	9	3
1:A:81:ILE:N	1:A:81:ILE:CD1	0.45	2.79	20	7
1:A:28:PHE:HA	1:A:88:ARG:NH2	0.45	2.27	2	1
1:A:38:ILE:HD11	1:A:72:LEU:HD23	0.45	1.85	6	1
1:A:94:HIS:O	1:A:95:GLY:C	0.45	2.55	3	1
1:A:47:LEU:HD12	1:A:47:LEU:H	0.45	1.71	27	1
1:A:84:VAL:HB	1:A:111:PHE:HB3	0.45	1.89	27	5
1:A:77:LEU:CD1	1:A:107:GLY:O	0.45	2.65	18	5
1:A:94:HIS:O	1:A:98:LYS:HE3	0.45	2.12	2	3
1:A:64:VAL:O	1:A:65:ALA:C	0.44	2.55	7	26
1:A:100:LEU:C	1:A:100:LEU:HD23	0.44	2.32	8	2
1:A:34:ILE:O	1:A:35:TYR:CD1	0.44	2.71	22	11
1:A:93:TYR:CZ	1:A:98:LYS:HD3	0.44	2.48	3	2
1:A:34:ILE:HG23	1:A:52:SER:H	0.44	1.72	2	2
1:A:65:ALA:HB3	1:A:99:ALA:CB	0.44	2.41	1	1
1:A:79:LEU:HD12	1:A:81:ILE:HG12	0.44	1.88	25	9
1:A:38:ILE:HG13	1:A:72:LEU:HD21	0.44	1.89	9	1
1:A:71:ALA:O	1:A:75:LYS:CG	0.44	2.65	7	1
1:A:88:ARG:CD	1:A:88:ARG:H	0.44	2.24	19	1
1:A:48:VAL:CG1	1:A:72:LEU:CD1	0.44	2.96	6	1
1:A:35:TYR:CD2	1:A:51:SER:HB2	0.44	2.48	10	5
1:A:94:HIS:ND1	1:A:97:VAL:HG23	0.44	2.27	3	1
1:A:66:ARG:CG	1:A:99:ALA:O	0.44	2.66	17	4
1:A:73:ALA:O	1:A:77:LEU:CB	0.44	2.65	2	1
1:A:71:ALA:O	1:A:75:LYS:HG2	0.44	2.13	7	1
1:A:98:LYS:O	1:A:102:GLU:CG	0.44	2.66	23	6
1:A:24:ARG:HG3	1:A:85:ALA:O	0.44	2.13	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:VAL:O	1:A:67:GLN:N	0.44	2.51	19	17
1:A:25:LEU:HB2	1:A:84:VAL:CG1	0.44	2.42	1	3
1:A:26:SER:OG	1:A:39:ILE:CD1	0.43	2.65	22	1
1:A:35:TYR:CE2	1:A:51:SER:HB3	0.43	2.48	22	3
1:A:88:ARG:HD2	1:A:91:TYR:CG	0.43	2.49	2	1
1:A:76:ALA:O	1:A:79:LEU:HD12	0.43	2.13	22	2
1:A:34:ILE:HG21	1:A:52:SER:HB3	0.43	1.89	22	1
1:A:27:VAL:N	1:A:88:ARG:HD3	0.43	2.28	17	1
1:A:88:ARG:CZ	1:A:88:ARG:HB3	0.43	2.44	19	1
1:A:29:ARG:NH2	1:A:34:ILE:HG13	0.43	2.29	9	1
1:A:93:TYR:CE1	1:A:98:LYS:HE2	0.43	2.48	7	1
1:A:77:LEU:O	1:A:80:GLY:N	0.43	2.52	26	10
1:A:72:LEU:O	1:A:75:LYS:HB2	0.43	2.13	14	5
1:A:88:ARG:CZ	1:A:91:TYR:CZ	0.43	3.01	2	1
1:A:23:LEU:HD13	1:A:81:ILE:CG1	0.43	2.44	20	5
1:A:34:ILE:HG12	1:A:52:SER:HB2	0.43	1.90	9	1
1:A:98:LYS:O	1:A:102:GLU:HG3	0.42	2.14	3	2
1:A:23:LEU:HD12	1:A:81:ILE:HG13	0.42	1.91	4	2
1:A:42:GLU:CG	1:A:43:LYS:N	0.42	2.82	14	1
1:A:29:ARG:NH1	1:A:97:VAL:CG2	0.42	2.82	15	2
1:A:66:ARG:HG2	1:A:99:ALA:O	0.42	2.14	13	2
1:A:95:GLY:N	1:A:98:LYS:NZ	0.42	2.67	20	1
1:A:50:ALA:H	1:A:72:LEU:HD21	0.42	1.74	13	1
1:A:27:VAL:CG2	1:A:35:TYR:O	0.42	2.67	26	3
1:A:27:VAL:O	1:A:27:VAL:CG1	0.42	2.68	27	1
1:A:28:PHE:O	1:A:34:ILE:HA	0.42	2.14	18	1
1:A:25:LEU:CD1	1:A:111:PHE:CE1	0.42	3.02	18	2
1:A:23:LEU:HD21	1:A:40:ASP:OD1	0.42	2.14	13	1
1:A:25:LEU:HB2	1:A:84:VAL:HG11	0.42	1.92	17	1
1:A:106:GLU:CG	1:A:107:GLY:N	0.42	2.82	22	4
1:A:25:LEU:HB3	1:A:86:PHE:CD2	0.42	2.50	17	1
1:A:96:ARG:O	1:A:98:LYS:N	0.42	2.52	13	2
1:A:93:TYR:CZ	1:A:98:LYS:HG3	0.42	2.50	13	1
1:A:29:ARG:HG3	1:A:96:ARG:HG3	0.42	1.92	2	1
1:A:34:ILE:C	1:A:34:ILE:HD12	0.42	2.35	5	1
1:A:95:GLY:N	1:A:98:LYS:HZ3	0.42	2.11	17	1
1:A:93:TYR:CZ	1:A:98:LYS:CD	0.42	3.02	20	1
1:A:94:HIS:O	1:A:96:ARG:N	0.42	2.52	2	1
1:A:96:ARG:O	1:A:97:VAL:C	0.41	2.59	22	2
1:A:52:SER:OG	1:A:68:VAL:HG21	0.41	2.15	17	1
1:A:23:LEU:HD13	1:A:47:LEU:HD11	0.41	1.91	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:PHE:CZ	1:A:88:ARG:NH2	0.41	2.87	19	1
1:A:88:ARG:CZ	1:A:91:TYR:CE2	0.41	3.03	2	1
1:A:29:ARG:HG3	1:A:91:TYR:CE2	0.41	2.50	5	1
1:A:29:ARG:CZ	1:A:97:VAL:CG2	0.41	2.98	18	1
1:A:103:GLY:HA2	1:A:106:GLU:HG2	0.41	1.92	13	13
1:A:29:ARG:NE	1:A:96:ARG:HB2	0.41	2.30	23	2
1:A:34:ILE:CG2	1:A:52:SER:HB2	0.41	2.45	8	1
1:A:23:LEU:HD13	1:A:81:ILE:CD1	0.41	2.44	11	1
1:A:69:GLY:HA2	1:A:72:LEU:CG	0.41	2.45	18	3
1:A:29:ARG:HD3	1:A:96:ARG:HB2	0.41	1.91	21	1
1:A:73:ALA:HA	1:A:109:LEU:CD1	0.41	2.45	25	3
1:A:29:ARG:CZ	1:A:96:ARG:CB	0.41	2.98	5	1
1:A:94:HIS:O	1:A:98:LYS:NZ	0.41	2.51	7	1
1:A:75:LYS:O	1:A:78:ALA:HB3	0.41	2.16	14	2
1:A:65:ALA:CB	1:A:99:ALA:HB3	0.41	2.44	9	1
1:A:50:ALA:CB	1:A:72:LEU:HG	0.41	2.45	13	2
1:A:76:ALA:HA	1:A:79:LEU:CD1	0.41	2.46	21	2
1:A:70:ARG:CD	1:A:71:ALA:N	0.41	2.84	24	2
1:A:27:VAL:HG12	1:A:86:PHE:CE2	0.41	2.51	22	1
1:A:93:TYR:CD1	1:A:98:LYS:HE3	0.41	2.50	1	1
1:A:48:VAL:HG21	1:A:75:LYS:HB3	0.41	1.90	18	2
1:A:27:VAL:CG1	1:A:27:VAL:O	0.41	2.68	23	1
1:A:35:TYR:CE2	1:A:51:SER:OG	0.41	2.72	5	2
1:A:35:TYR:CD1	1:A:51:SER:HB2	0.41	2.50	14	1
1:A:86:PHE:CE2	1:A:88:ARG:HD3	0.41	2.51	5	1
1:A:48:VAL:HG13	1:A:75:LYS:CD	0.41	2.45	7	1
1:A:106:GLU:HG3	1:A:107:GLY:N	0.41	2.30	13	1
1:A:23:LEU:HD23	1:A:47:LEU:HD11	0.41	1.92	16	2
1:A:34:ILE:CD1	1:A:100:LEU:CD1	0.41	2.98	5	1
1:A:29:ARG:CD	1:A:96:ARG:CB	0.41	2.99	15	1
1:A:82:LYS:O	1:A:110:GLU:HB2	0.41	2.16	13	1
1:A:105:ARG:HG2	1:A:111:PHE:CZ	0.41	2.51	14	1
1:A:94:HIS:O	1:A:98:LYS:HD2	0.41	2.16	14	1
1:A:29:ARG:NH1	1:A:31:LEU:N	0.41	2.69	2	1
1:A:77:LEU:CD1	1:A:108:GLY:HA3	0.40	2.44	24	2
1:A:73:ALA:O	1:A:77:LEU:CG	0.40	2.69	20	2
1:A:27:VAL:CG1	1:A:88:ARG:NH1	0.40	2.81	16	1
1:A:29:ARG:NH2	1:A:97:VAL:HA	0.40	2.32	22	1
1:A:29:ARG:NH1	1:A:29:ARG:HB2	0.40	2.31	17	1
1:A:34:ILE:O	1:A:51:SER:CB	0.40	2.69	18	2
1:A:83:GLN:HG3	1:A:110:GLU:HB2	0.40	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:PHE:HA	1:A:91:TYR:CE2	0.40	2.52	27	1
1:A:47:LEU:HD12	1:A:47:LEU:N	0.40	2.32	2	1
1:A:86:PHE:CE2	1:A:88:ARG:CD	0.40	3.04	5	1
1:A:34:ILE:CG2	1:A:96:ARG:NH1	0.40	2.84	5	1
1:A:68:VAL:O	1:A:72:LEU:HD12	0.40	2.16	25	1
1:A:83:GLN:HG2	1:A:110:GLU:HB2	0.40	1.92	22	1
1:A:68:VAL:O	1:A:72:LEU:CD2	0.40	2.70	21	1
1:A:72:LEU:O	1:A:75:LYS:N	0.40	2.54	17	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	78/90 (87%)	63±2 (81±2%)	10±2 (13±3%)	5±1 (6±1%)	3	20
All	All	2106/2430 (87%)	1706 (81%)	269 (13%)	131 (6%)	3	20

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

Mol	Chain	Res	Type	Models (Total)
1	A	108	GLY	27
1	A	44	GLY	27
1	A	98	LYS	23
1	A	93	TYR	15
1	A	97	VAL	14
1	A	31	LEU	12
1	A	95	GLY	6
1	A	65	ALA	6
1	A	52	SER	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	60/69 (87%)	36±2 (61±4%)	24±2 (39±4%)	1	5
All	All	1620/1863 (87%)	982 (61%)	638 (39%)	1	5

All 48 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	38	ILE	27
1	A	81	ILE	27
1	A	79	LEU	27
1	A	68	VAL	27
1	A	84	VAL	27
1	A	83	GLN	27
1	A	98	LYS	27
1	A	66	ARG	26
1	A	102	GLU	26
1	A	93	TYR	22
1	A	28	PHE	21
1	A	37	GLN	20
1	A	86	PHE	19
1	A	92	LYS	19
1	A	26	SER	18
1	A	87	ASP	18
1	A	70	ARG	16
1	A	105	ARG	15
1	A	51	SER	14
1	A	23	LEU	14
1	A	31	LEU	14
1	A	40	ASP	13
1	A	30	SER	13
1	A	110	GLU	12
1	A	24	ARG	11
1	A	72	LEU	11
1	A	29	ARG	11
1	A	32	LYS	11
1	A	47	LEU	11
1	A	88	ARG	11
1	A	82	LYS	10
1	A	43	LYS	10
1	A	94	HIS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	100	LEU	7
1	A	63	GLU	6
1	A	67	GLN	5
1	A	52	SER	5
1	A	27	VAL	5
1	A	111	PHE	4
1	A	33	HIS	4
1	A	46	THR	4
1	A	96	ARG	4
1	A	41	ASP	4
1	A	74	GLU	3
1	A	34	ILE	2
1	A	39	ILE	1
1	A	35	TYR	1
1	A	75	LYS	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 75% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4688

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	1158
Number of shifts mapped to atoms	945
Number of unparsed shifts	0
Number of shifts with mapping errors	213
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.

- Residue not found in structure. All 213 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	18	LYS	HB2	1.887	0.005	2
A	14	ARG	HD2	3.23	0.005	1
A	10	LYS	CG	24.51	0.05	1
A	3	LEU	CD1	23.398	0.05	1
A	6	TYR	CB	38.535	0.05	1
A	6	TYR	HD1	7.169	0.005	1
A	17	ILE	CG2	17.393	0.05	1
A	15	ASN	HB3	2.817	0.005	2
A	6	TYR	HE1	6.914	0.005	1
A	5	ALA	HB1	1.547	0.005	1
A	19	ARG	HG2	1.729	0.005	2
A	7	GLU	HB2	2.095	0.005	1
A	18	LYS	CA	56.364	0.05	1
A	4	THR	HG22	1.297	0.005	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	16	ARG	HG2	1.494	0.005	1
A	17	ILE	HG22	0.972	0.005	1
A	19	ARG	CB	31.069	0.05	1
A	4	THR	CB	70.353	0.05	1
A	4	THR	N	115.663	0.05	1
A	6	TYR	HA	4.484	0.005	1
A	20	THR	HG23	4.347	0.005	1
A	20	THR	CG2	21.498	0.05	1
A	20	THR	CB	70.087	0.05	1
A	17	ILE	CA	61.152	0.05	1
A	8	ARG	N	121.628	0.05	1
A	8	ARG	CB	30.58	0.05	1
A	21	GLY	N	111.76	0.05	1
A	9	ARG	N	121.363	0.05	1
A	19	ARG	HD2	3.286	0.005	2
A	10	LYS	HD2	1.241	0.005	1
A	11	PHE	HE1	7.406	0.005	1
A	13	VAL	HG12	1.039	0.005	2
A	20	THR	HB	4.347	0.005	1
A	16	ARG	CB	30.801	0.05	1
A	8	ARG	HG2	1.765	0.005	2
A	16	ARG	CD	43.261	0.05	1
A	15	ASN	HD21	7.582	0.005	1
A	15	ASN	N	120.417	0.05	1
A	12	ARG	H	8.078	0.005	1
A	13	VAL	H	8.102	0.005	1
A	12	ARG	CD	43.271	0.05	1
A	20	THR	HG21	4.347	0.005	1
A	18	LYS	N	126.502	0.05	1
A	5	ALA	CA	53.652	0.05	1
A	4	THR	HB	4.397	0.005	1
A	13	VAL	CG1	20.635	0.05	2
A	2	ARG	CB	31.083	0.05	1
A	17	ILE	HG23	0.972	0.005	1
A	20	THR	H	8.268	0.005	1
A	4	THR	CA	61.511	0.05	1
A	17	ILE	HD11	0.94	0.005	1
A	17	ILE	HB	1.94	0.005	1
A	21	GLY	HA2	4.123	0.005	1
A	9	ARG	HB2	1.982	0.005	1
A	12	ARG	HG2	1.639	0.005	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	8	ARG	CG	27.347	0.05	1
A	11	PHE	HD1	7.318	0.005	1
A	5	ALA	HB3	1.547	0.005	1
A	13	VAL	CB	32.564	0.05	1
A	19	ARG	HD3	3.218	0.005	2
A	13	VAL	HG13	1.039	0.005	2
A	14	ARG	CD	43.261	0.05	1
A	16	ARG	CA	56.4	0.05	1
A	8	ARG	HA	4.256	0.005	1
A	8	ARG	HG3	1.658	0.005	2
A	17	ILE	HG13	1.275	0.005	2
A	11	PHE	CA	57.852	0.05	1
A	9	ARG	HD2	3.322	0.005	1
A	8	ARG	HD3	3.242	0.005	2
A	9	ARG	HG3	1.72	0.005	2
A	7	GLU	HG2	2.333	0.005	1
A	14	ARG	HG2	1.714	0.005	1
A	21	GLY	H	8.433	0.005	1
A	10	LYS	CA	56.652	0.05	1
A	20	THR	HG22	4.347	0.005	1
A	9	ARG	CA	57.106	0.05	1
A	5	ALA	N	125.85	0.05	1
A	14	ARG	HB3	1.847	0.005	2
A	9	ARG	CG	27.155	0.05	1
A	5	ALA	CB	19.045	0.05	1
A	2	ARG	CG	26.814	0.05	1
A	2	ARG	CA	56.156	0.05	1
A	10	LYS	N	121.566	0.05	1
A	18	LYS	CE	41.948	0.05	1
A	14	ARG	HB2	1.912	0.005	2
A	10	LYS	HB2	1.699	0.005	1
A	8	ARG	HB3	1.851	0.005	2
A	19	ARG	CD	43.137	0.05	1
A	11	PHE	HB2	3.232	0.005	2
A	13	VAL	HA	4.123	0.005	1
A	17	ILE	HA	4.21	0.005	1
A	21	GLY	HA3	4.07	0.005	1
A	12	ARG	HB2	1.837	0.005	1
A	15	ASN	ND2	113.629	0.05	1
A	18	LYS	H	8.352	0.005	1
A	19	ARG	N	124.12	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	13	VAL	CA	62.806	0.05	1
A	14	ARG	CA	56.4	0.05	1
A	7	GLU	CG	36.633	0.05	1
A	14	ARG	CG	27.071	0.05	1
A	17	ILE	HG12	1.546	0.005	2
A	3	LEU	CA	54.984	0.05	1
A	5	ALA	H	8.469	0.005	1
A	12	ARG	N	122.871	0.05	1
A	3	LEU	CG	24.968	0.05	1
A	15	ASN	CB	38.576	0.05	1
A	8	ARG	HD2	3.281	0.005	2
A	13	VAL	HG22	1.005	0.005	2
A	2	ARG	HG2	1.508	0.005	1
A	2	ARG	HA	4.26	0.005	1
A	9	ARG	CB	30.565	0.05	1
A	9	ARG	HA	3.836	0.005	1
A	6	TYR	CA	58.983	0.05	1
A	5	ALA	HA	3.852	0.005	1
A	5	ALA	HB2	1.547	0.005	1
A	10	LYS	HA	4.228	0.005	1
A	18	LYS	CD	29.208	0.05	1
A	4	THR	HG21	1.297	0.005	1
A	18	LYS	CB	33.06	0.05	1
A	8	ARG	HB2	1.955	0.005	2
A	11	PHE	HB3	3.094	0.005	2
A	15	ASN	HA	4.741	0.005	1
A	3	LEU	N	125.146	0.05	1
A	8	ARG	CD	43.271	0.05	1
A	3	LEU	HD11	0.94	0.005	1
A	17	ILE	CB	38.53	0.05	1
A	12	ARG	HA	4.347	0.005	1
A	17	ILE	N	122.659	0.05	1
A	8	ARG	CA	57.313	0.05	1
A	21	GLY	CA	45.317	0.05	1
A	16	ARG	CG	27.071	0.05	1
A	9	ARG	H	8.055	0.005	1
A	3	LEU	CB	42.667	0.05	1
A	18	LYS	HE2	3.078	0.005	1
A	17	ILE	CD1	12.632	0.05	1
A	2	ARG	HD2	3.06	0.005	1
A	10	LYS	CE	41.902	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	6	TYR	N	119.279	0.05	1
A	20	THR	CA	61.877	0.05	1
A	12	ARG	HD2	3.237	0.005	1
A	4	THR	HA	4.4	0.005	1
A	13	VAL	CG2	21.033	0.05	2
A	18	LYS	HG2	1.512	0.005	1
A	10	LYS	HG2	1.347	0.005	2
A	19	ARG	HB2	1.974	0.005	2
A	11	PHE	HZ	7.363	0.005	1
A	18	LYS	CG	24.91	0.05	1
A	15	ASN	H	8.428	0.005	1
A	16	ARG	HD2	3.093	0.005	1
A	18	LYS	HD2	1.757	0.005	1
A	17	ILE	H	8.118	0.005	1
A	17	ILE	HD12	0.94	0.005	1
A	6	TYR	HB2	3.084	0.005	1
A	3	LEU	H	8.448	0.005	1
A	20	THR	N	115.985	0.05	1
A	3	LEU	HD12	0.94	0.005	1
A	3	LEU	HA	4.546	0.005	1
A	3	LEU	HG	1.498	0.005	1
A	14	ARG	HA	4.405	0.005	1
A	7	GLU	HA	4.167	0.005	1
A	7	GLU	CA	57.29	0.05	1
A	12	ARG	CB	30.942	0.05	1
A	3	LEU	HB2	1.728	0.005	2
A	11	PHE	N	120.693	0.05	1
A	11	PHE	CB	39.525	0.05	1
A	18	LYS	HB3	1.825	0.005	2
A	10	LYS	CD	28.973	0.05	1
A	10	LYS	HE2	2.979	0.005	1
A	10	LYS	CB	32.678	0.05	1
A	14	ARG	N	125.034	0.05	1
A	14	ARG	H	8.348	0.005	1
A	7	GLU	H	8.039	0.005	1
A	17	ILE	CG1	27.302	0.05	1
A	9	ARG	CD	43.383	0.05	1
A	15	ASN	HB2	2.88	0.005	2
A	2	ARG	CD	43.235	0.05	1
A	18	LYS	HA	4.436	0.005	1
A	10	LYS	HG3	1.266	0.005	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	19	ARG	HB3	1.891	0.005	2
A	19	ARG	HG3	1.699	0.005	2
A	11	PHE	HA	4.662	0.005	1
A	4	THR	HG23	1.297	0.005	1
A	6	TYR	H	8.074	0.005	1
A	9	ARG	HG2	1.795	0.005	2
A	17	ILE	HG21	0.972	0.005	1
A	19	ARG	CA	55.995	0.05	1
A	19	ARG	CG	27.071	0.05	1
A	17	ILE	HD13	0.94	0.005	1
A	13	VAL	HB	2.14	0.005	1
A	12	ARG	CA	56.398	0.05	1
A	2	ARG	HB2	1.635	0.005	1
A	3	LEU	HD13	0.94	0.005	1
A	19	ARG	H	8.437	0.005	1
A	4	THR	H	8.31	0.005	1
A	11	PHE	H	8.028	0.005	1
A	16	ARG	HA	4.198	0.005	1
A	13	VAL	N	121.857	0.05	1
A	19	ARG	HA	4.527	0.005	1
A	7	GLU	N	122.087	0.05	1
A	10	LYS	H	8.016	0.005	1
A	13	VAL	HG11	1.039	0.005	2
A	14	ARG	CB	30.801	0.05	1
A	7	GLU	CB	30.575	0.05	1
A	4	THR	CG2	21.554	0.05	1
A	12	ARG	CG	26.956	0.05	1
A	16	ARG	HB2	1.709	0.005	1
A	13	VAL	HG23	1.005	0.005	2
A	20	THR	HA	4.477	0.005	1
A	3	LEU	HB3	1.665	0.005	2
A	8	ARG	H	8.263	0.005	1
A	15	ASN	HD22	6.875	0.005	1
A	13	VAL	HG21	1.005	0.005	2
A	15	ASN	CA	53.312	0.05	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
$^{13}\text{C}_\alpha$	110	-0.28 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	99	-0.37 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	102	-0.42 ± 0.47	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 75%, i.e. 731 atoms were assigned a chemical shift out of a possible 981. 1 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	304/393 (77%)	151/157 (96%)	79/158 (50%)	74/78 (95%)
Sidechain	410/521 (79%)	243/304 (80%)	160/187 (86%)	7/30 (23%)
Aromatic	17/67 (25%)	17/35 (49%)	0/28 (0%)	0/4 (0%)
Overall	731/981 (75%)	411/496 (83%)	239/373 (64%)	81/112 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 825 atoms were assigned a chemical shift out of a possible 1133. 2 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	345/448 (77%)	171/179 (96%)	90/180 (50%)	84/89 (94%)
Sidechain	463/618 (75%)	272/361 (75%)	183/220 (83%)	8/37 (22%)
Aromatic	17/67 (25%)	17/35 (49%)	0/28 (0%)	0/4 (0%)
Overall	825/1133 (73%)	460/575 (80%)	273/428 (64%)	92/130 (71%)

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
1	A	20	THR	HG23	4.35	2.29 – -0.01	13.9
1	A	20	THR	HG22	4.35	2.29 – -0.01	13.9
1	A	20	THR	HG21	4.35	2.29 – -0.01	13.9

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

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

Random coil index (RCI) for chain A:

