Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 12:23 AM EDT

PDB ID	:	1WKI
Title	:	solution structure of ribosomal protein L16 from thermus thermophilus HB8
Authors	:	Nishimura, M.; Yoshida, T.; Shirouzu, M.; Terada, T.; Kuramitsu, S.; Yokoyama, S.; Ohkubo, T.; Kobayashi, Y.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-05-31

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

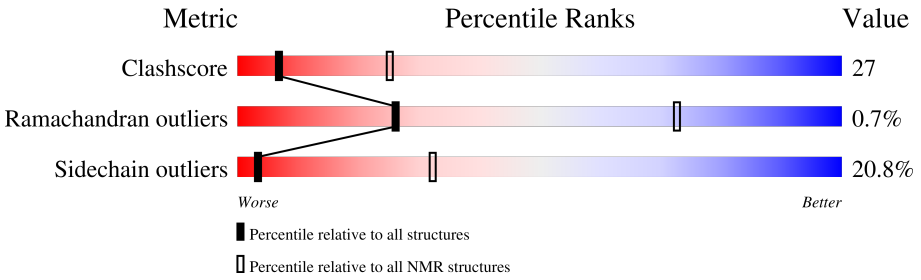
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	141	26% 28% • 43%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 16 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:31-A:70, A:94-A:133 (80)	0.21	16

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 8, 9, 10, 12, 18, 23, 27, 28
2	3, 5, 6, 13, 16, 17, 19, 21, 25, 26
3	20, 24, 30
4	14, 15, 22
5	7, 11, 29

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2303 atoms, of which 1181 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LSU ribosomal protein L16P.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	141	2303	715	1181	212	188	7	0

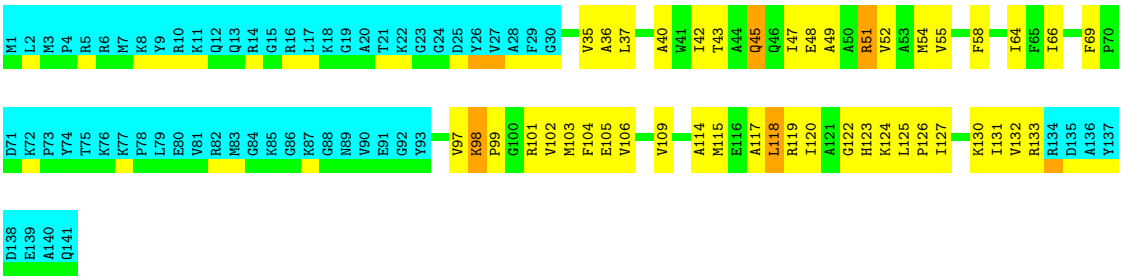
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: LSU ribosomal protein L16P

Chain A: 26% 28% • 43%



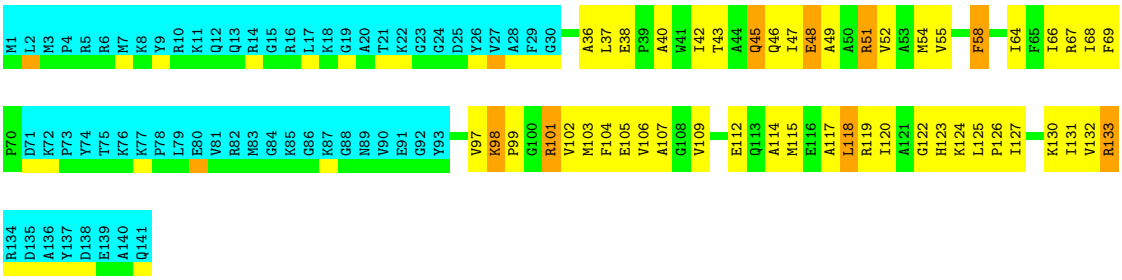
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: LSU ribosomal protein L16P

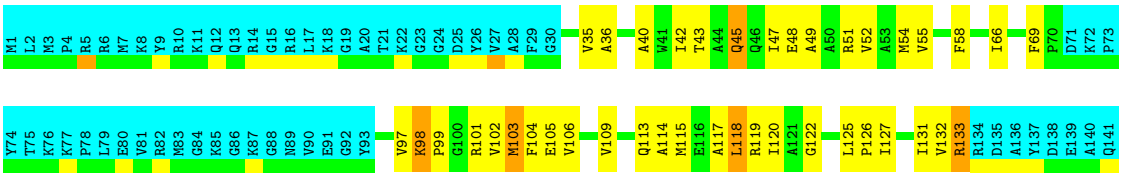
Chain A: 22% 29% 6% 43%



4.2.2 Score per residue for model 2

• Molecule 1: LSU ribosomal protein L16P

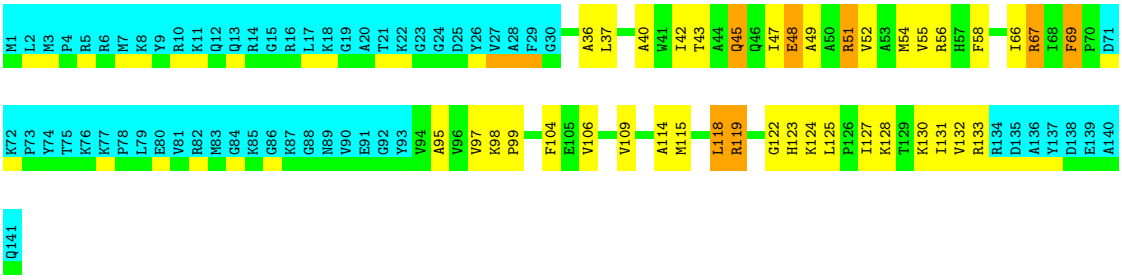
Chain A: 28% 25% • 43%



4.2.3 Score per residue for model 3

• Molecule 1: LSU ribosomal protein L16P

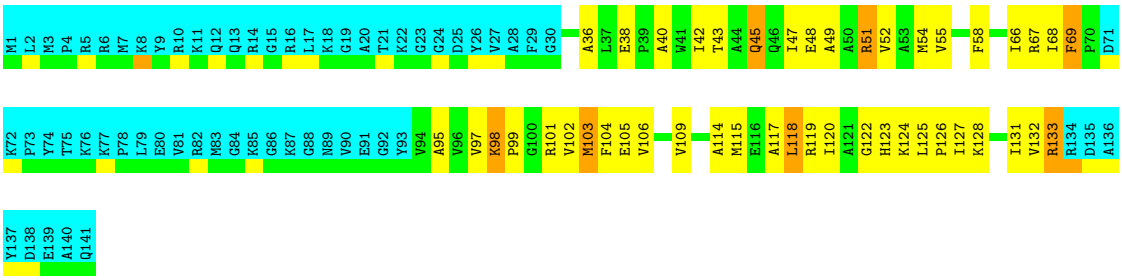
Chain A: 29% 23% 5% 43%



4.2.4 Score per residue for model 4

• Molecule 1: LSU ribosomal protein L16P

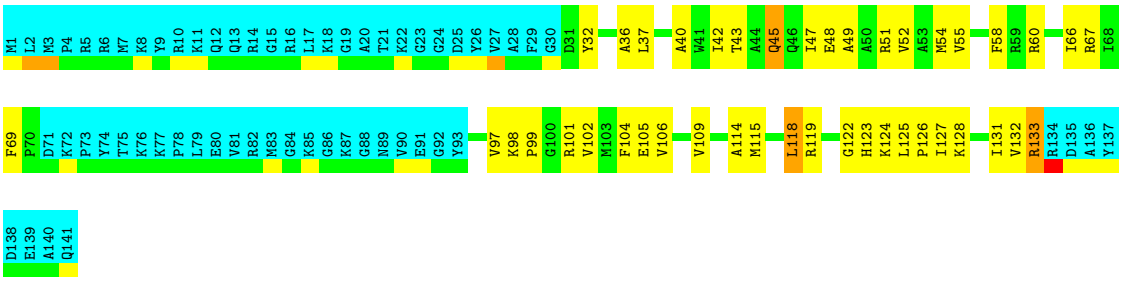
Chain A: 25% 27% 5% 43%



4.2.5 Score per residue for model 5

• Molecule 1: LSU ribosomal protein L16P

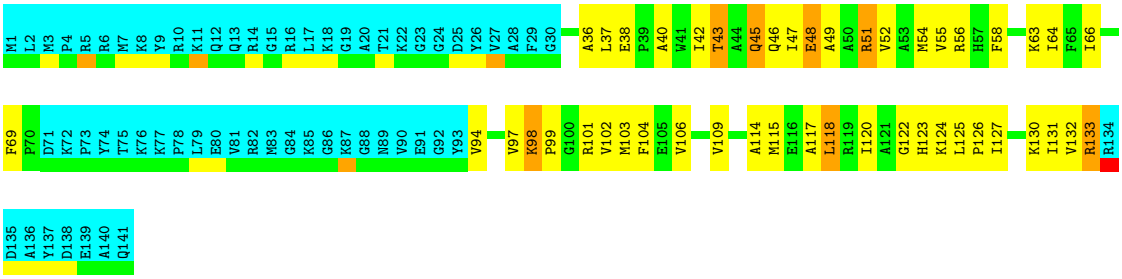
Chain A: 27% 28% • 43%



4.2.6 Score per residue for model 6

- Molecule 1: LSU ribosomal protein L16P

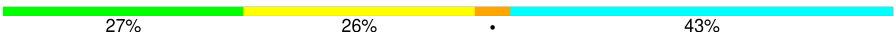
Chain A:

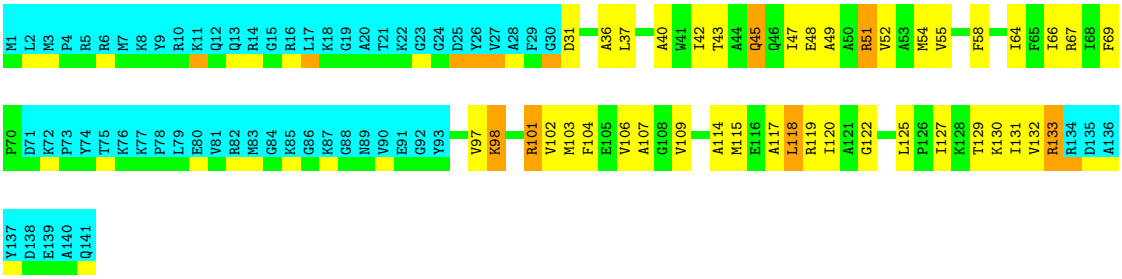


4.2.7 Score per residue for model 7

- Molecule 1: LSU ribosomal protein L16P

Chain A:

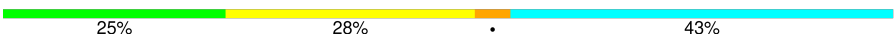


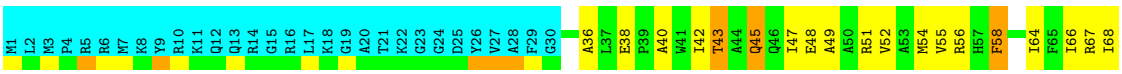


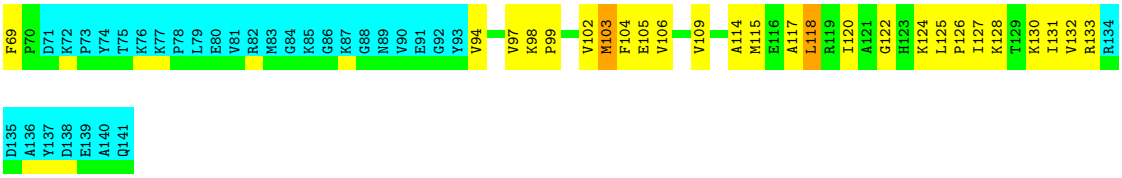
4.2.8 Score per residue for model 8

- Molecule 1: LSU ribosomal protein L16P

Chain A:



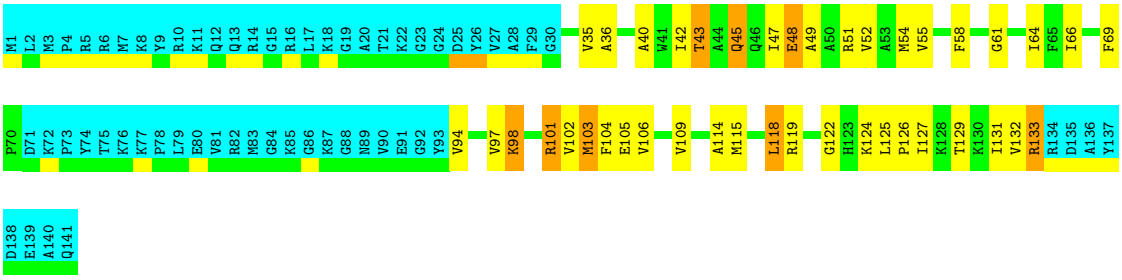




4.2.9 Score per residue for model 9

- Molecule 1: LSU ribosomal protein L16P

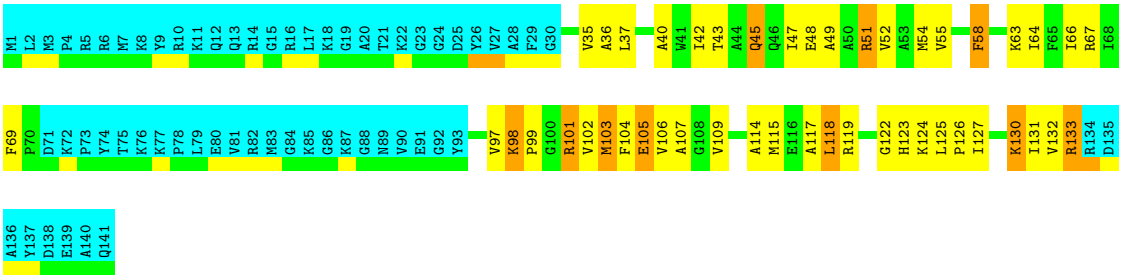
Chain A: 28% 23% 6% 43%



4.2.10 Score per residue for model 10

- Molecule 1: LSU ribosomal protein L16P

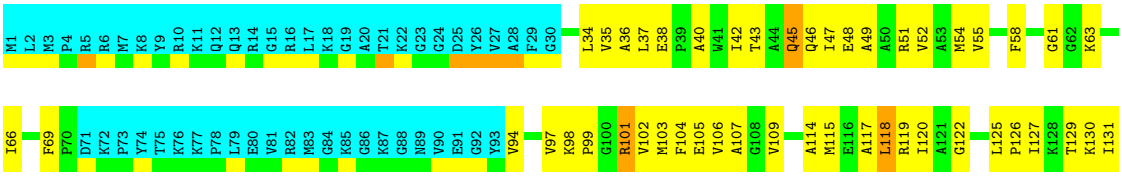
Chain A: 24% 26% 7% 43%



4.2.11 Score per residue for model 11

- Molecule 1: LSU ribosomal protein L16P

Chain A: 22% 32% • 43%



V132 R133 R134 D135 A136 Y137 D138 E139 A140 Q141

4.2.12 Score per residue for model 12

- Molecule 1: LSU ribosomal protein L16P

Chain A: 23% 28% 5% 43%

M1 L2 M3 P4 R5 R6 M7 K8 Y9 R10 K11 Q12 Q13 R14 G15 R16 L17 K18 G19 A20 T21 K22 G23 G24 D25 Y26 V27 A28 F29 G30 D31 L34 V35 A36 L37 E38 P39 A40 W41 I42 T43 A44 Q45 Q46 I47 E48 A49 A50 R51 V52 A53 M54 V55 F58 I64 F65 I66

R67 I68 F69 P70 D71 K72 P73 Y74 T75 K76 K77 P78 L79 E80 V81 R82 M83 G84 K85 G86 K87 G88 N89 V90 E91 G92 Y93 V97 K98 P99 G100 R101 V102 M103 F104 E105 V106 A107 G108 V109 A114 M115 L118 R119 G122 H123 K124 L125 P126 I127 K130 I131 V132 R133 R134

D135 A136 Y137 D138 E139 A140 Q141

4.2.13 Score per residue for model 13

- Molecule 1: LSU ribosomal protein L16P

Chain A: 20% 30% 6% 43%

M1 L2 M3 P4 R5 R6 M7 K8 Y9 R10 K11 Q12 Q13 R14 G15 R16 L17 K18 G19 A20 T21 K22 G23 G24 D25 Y26 V27 A28 F29 G30 G33 L34 V35 A36 L37 E38 P39 A40 W41 I42 T43 A44 Q45 Q46 I47 E48 A49 A50 R51 V52 A53 M54 V55 F58 K63 I64 F65

I66 R67 I68 F69 P70 D71 K72 P73 Y74 T75 K76 K77 P78 L79 E80 V81 R82 M83 G84 K85 G86 K87 G88 N89 V90 E91 G92 Y93 V96 V97 K98 P99 G100 R101 V102 M103 F104 E105 V106 V109 E112 Q113 A114 M115 E116 A117 L118 R119 I120 H123 K124 L125 P126 I127 K130

I131 V132 R133 R134 D135 A136 Y137 D138 E139 A140 Q141

4.2.14 Score per residue for model 14

- Molecule 1: LSU ribosomal protein L16P

Chain A: 23% 30% • 43%

M1 L2 M3 P4 R5 R6 M7 K8 Y9 R10 K11 Q12 Q13 R14 G15 R16 L17 K18 G19 A20 T21 K22 G23 G24 D25 Y26 V27 A28 F29 G30 D31 Y32 V35 A36 L37 E38 P39 A40 W41 I42 T43 A44 Q45 Q46 I47 E48 A49 A50 R51 V52 A53 M54 V55 F58 R59 I64 F65

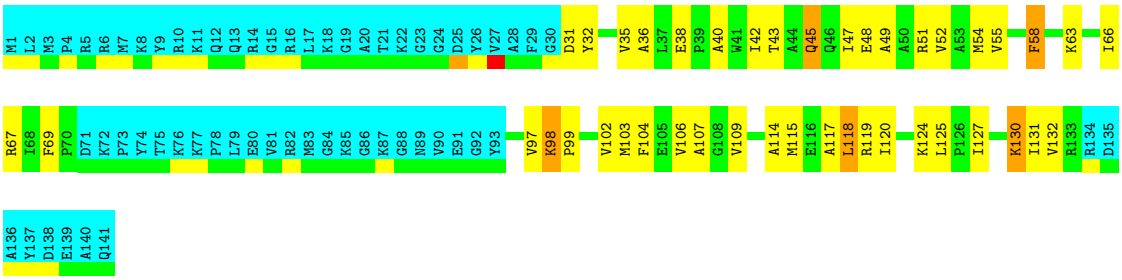
I66 F69 P70 D71 K72 P73 Y74 T75 K76 K77 P78 L79 E80 V81 R82 M83 G84 K85 G86 K87 G88 N89 V90 E91 G92 Y93 V96 V97 K98 R101 V102 M103 F104 E105 V106 V109 E112 Q113 A114 M115 E116 A117 L118 R119 I120 A121 G122 H123 K124 L125 P126 I127 K130 I131

V132 R133 R134 D135 A136 Y137 D138 E139 A140 Q141

4.2.15 Score per residue for model 15

- Molecule 1: LSU ribosomal protein L16P

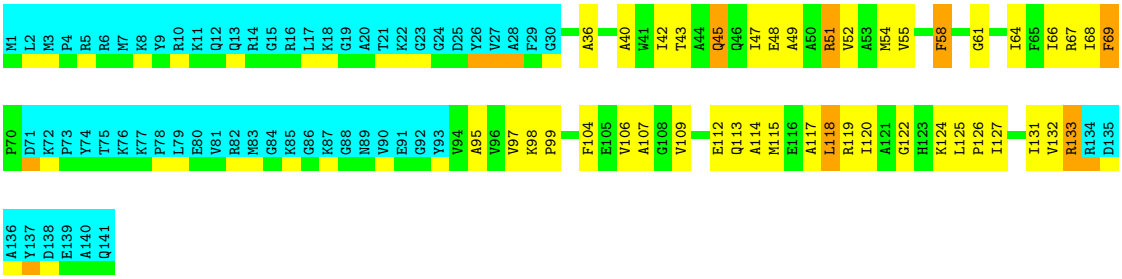
Chain A: 27% 26% • 43%



4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: LSU ribosomal protein L16P

Chain A: 26% 26% • 43%



4.2.17 Score per residue for model 17

- Molecule 1: LSU ribosomal protein L16P

Chain A: 23% 30% • 43%

4.2.18 Score per residue for model 18

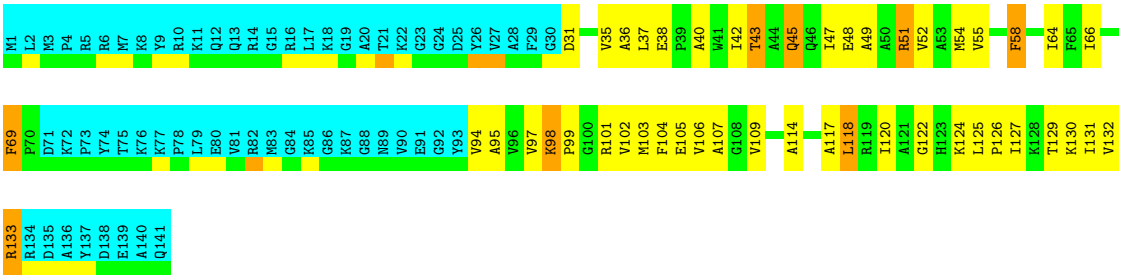
- Molecule 1: LSU ribosomal protein L16P

Chain A: 25% 28% • 43%

4.2.19 Score per residue for model 19

- Molecule 1: LSU ribosomal protein L16P

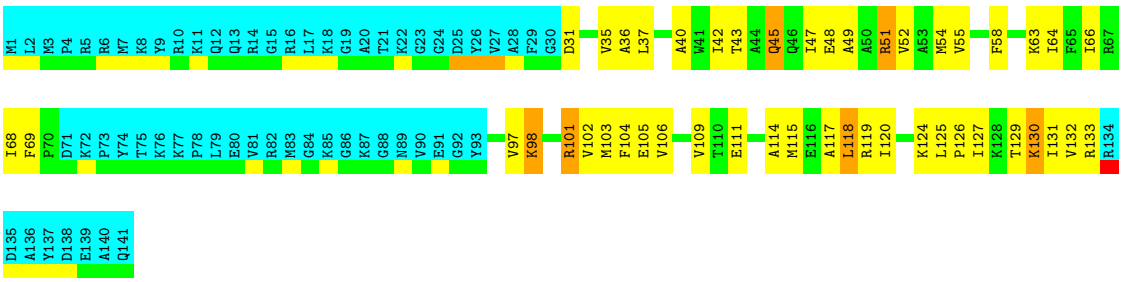
Chain A: 23% 28% 6% 43%



4.2.20 Score per residue for model 20

- Molecule 1: LSU ribosomal protein L16P

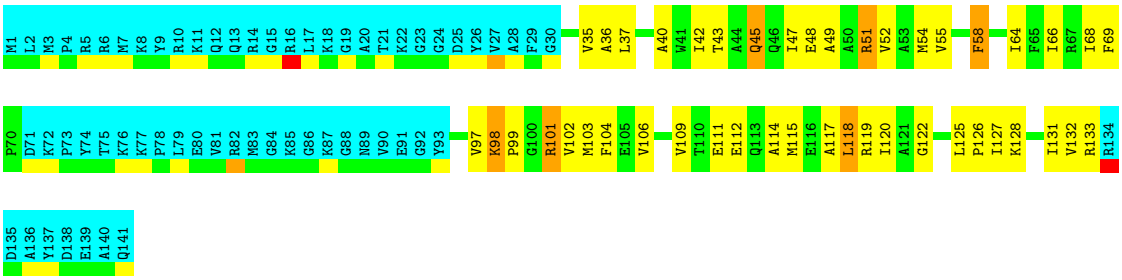
Chain A: 24% 28% • 43%



4.2.21 Score per residue for model 21

• Molecule 1: LSU ribosomal protein L16P

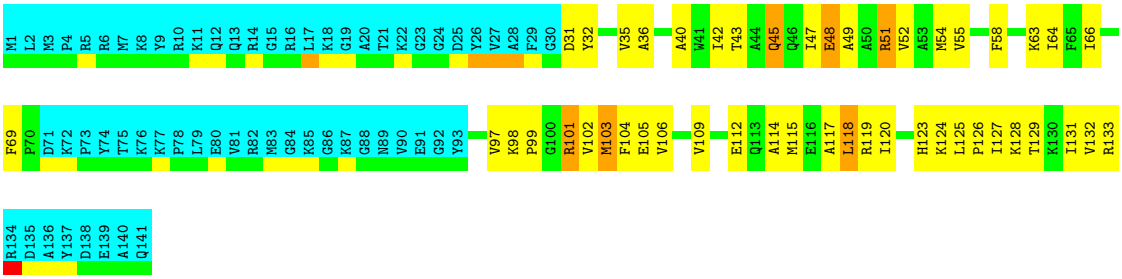
Chain A: 26% 27% • 43%



4.2.22 Score per residue for model 22

• Molecule 1: LSU ribosomal protein L16P

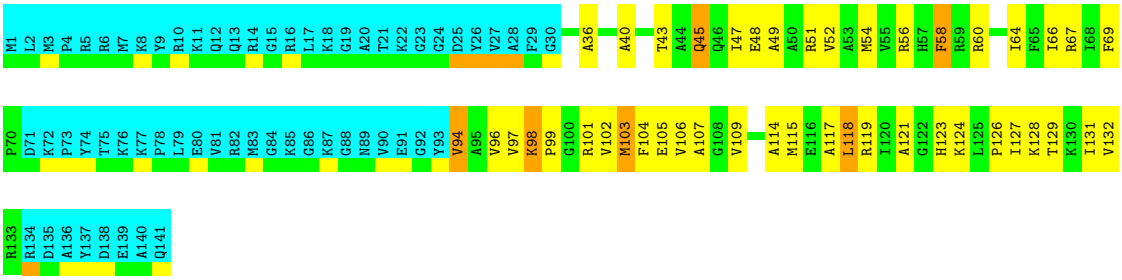
Chain A: 23% 29% • 43%



4.2.23 Score per residue for model 23

• Molecule 1: LSU ribosomal protein L16P

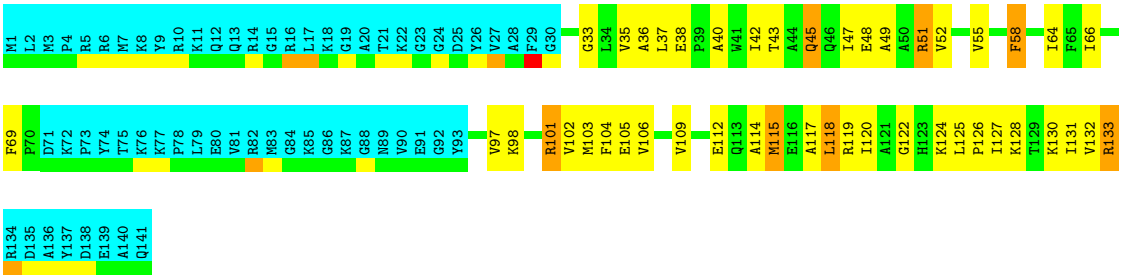
Chain A: 26% 27% • 43%



4.2.24 Score per residue for model 24

• Molecule 1: LSU ribosomal protein L16P

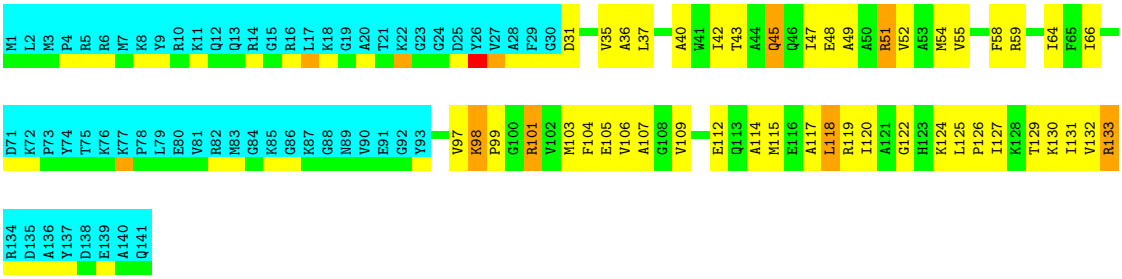
Chain A: 25% 27% 5% 43%



4.2.25 Score per residue for model 25

• Molecule 1: LSU ribosomal protein L16P

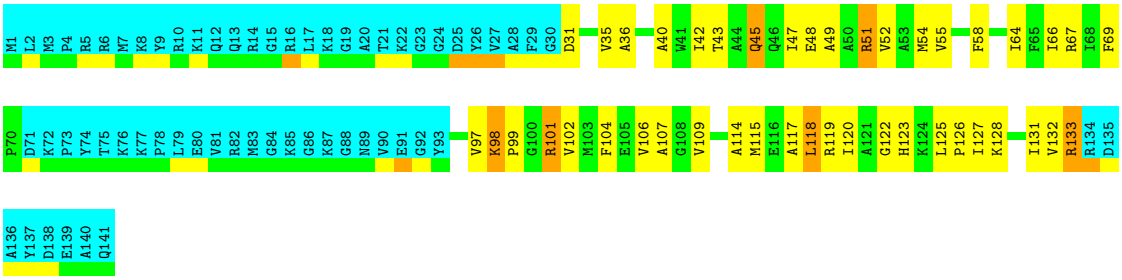
Chain A: 24% 28% • 43%



4.2.26 Score per residue for model 26

• Molecule 1: LSU ribosomal protein L16P

Chain A: 26% 26% • 43%



4.2.27 Score per residue for model 27

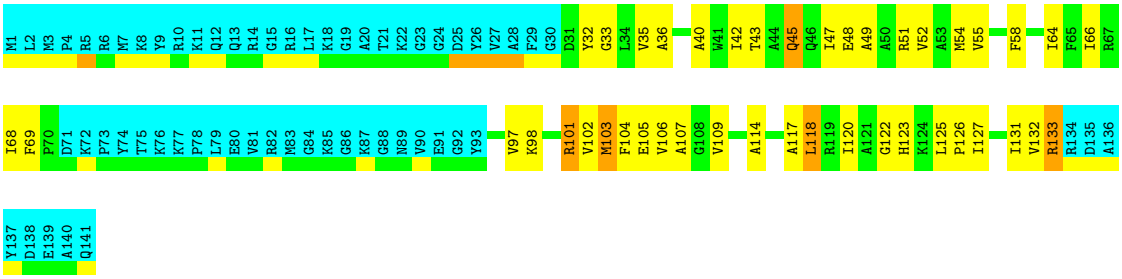
- Molecule 1: LSU ribosomal protein L16P

Chain A: 24% 28% 5% 43%

4.2.28 Score per residue for model 28

- Molecule 1: LSU ribosomal protein L16P

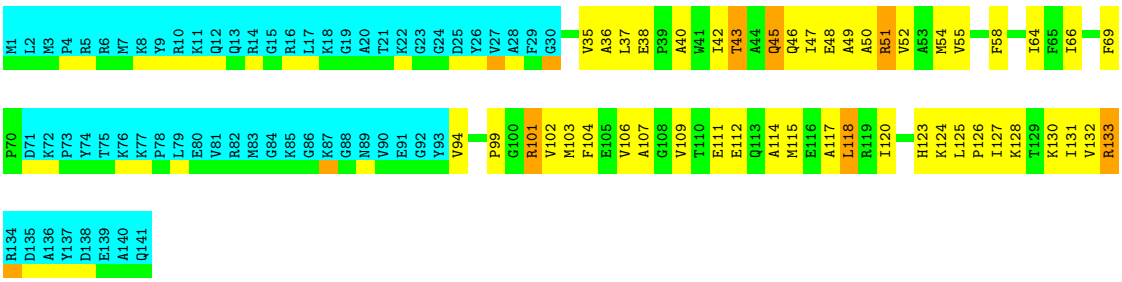
Chain A: 27% 26% • 43%



4.2.29 Score per residue for model 29

- Molecule 1: LSU ribosomal protein L16P

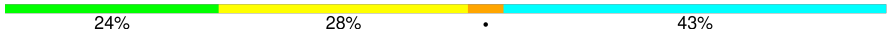
Chain A: 23% 29% • 43%

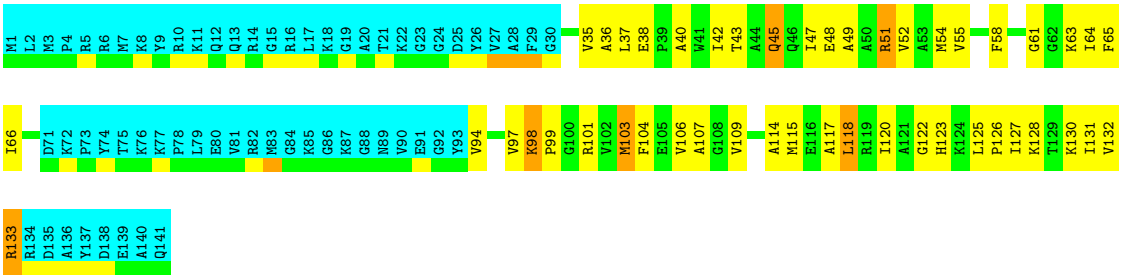


4.2.30 Score per residue for model 30

- Molecule 1: LSU ribosomal protein L16P

Chain A:





5 Refinement protocol and experimental data overview (i)

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

Of the 700 calculated structures, 30 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
CNS	refinement	1.1
CNS	structure solution	1.1

No chemical shift data was provided.

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	630	675	673	36±4
All	All	18900	20250	20190	1072

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:VAL:HG23	1:A:114:ALA:HB2	0.94	1.36	28	30
1:A:47:ILE:HG23	1:A:66:ILE:HG21	0.87	1.43	14	29
1:A:58:PHE:CD1	1:A:109:VAL:HG11	0.83	2.09	7	30
1:A:42:ILE:HD12	1:A:125:LEU:HD22	0.82	1.49	30	29
1:A:48:GLU:O	1:A:52:VAL:HG23	0.79	1.78	23	30
1:A:51:ARG:O	1:A:55:VAL:HG23	0.77	1.79	1	29
1:A:102:VAL:HG12	1:A:105:GLU:OE2	0.76	1.81	2	12
1:A:40:ALA:HB2	1:A:127:ILE:HG23	0.72	1.60	15	30
1:A:51:ARG:HG2	1:A:64:ILE:HD12	0.72	1.61	23	14
1:A:118:LEU:HD23	1:A:131:ILE:HG23	0.72	1.62	29	30
1:A:42:ILE:HD12	1:A:125:LEU:CD2	0.71	2.16	2	29
1:A:40:ALA:HB2	1:A:127:ILE:CG2	0.70	2.16	22	30
1:A:106:VAL:HG13	1:A:118:LEU:HD11	0.69	1.65	19	30
1:A:42:ILE:CD1	1:A:125:LEU:HD22	0.69	2.18	6	29

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ALA:HB2	1:A:103:MET:CE	0.68	2.18	25	25
1:A:46:GLN:OE1	1:A:125:LEU:HD23	0.68	1.89	6	1
1:A:118:LEU:CB	1:A:131:ILE:HD12	0.67	2.19	11	30
1:A:35:VAL:HG11	1:A:130:LYS:HE3	0.67	1.64	15	2
1:A:66:ILE:HD12	1:A:104:PHE:CE2	0.67	2.25	8	24
1:A:40:ALA:HB1	1:A:126:PRO:HG2	0.66	1.67	22	27
1:A:117:ALA:HA	1:A:120:ILE:HD12	0.66	1.67	28	24
1:A:119:ARG:HG3	1:A:131:ILE:HD11	0.65	1.67	20	7
1:A:54:MET:CE	1:A:64:ILE:HD13	0.64	2.22	9	1
1:A:66:ILE:HD12	1:A:104:PHE:CD2	0.63	2.28	27	23
1:A:109:VAL:CG2	1:A:114:ALA:HB2	0.62	2.23	24	11
1:A:42:ILE:HG21	1:A:68:ILE:HD12	0.62	1.71	16	4
1:A:37:LEU:HD21	1:A:130:LYS:HG2	0.61	1.72	6	14
1:A:118:LEU:HB3	1:A:131:ILE:HD12	0.61	1.70	22	30
1:A:47:ILE:CG2	1:A:66:ILE:HG21	0.59	2.24	9	18
1:A:36:ALA:HB2	1:A:103:MET:SD	0.58	2.37	15	16
1:A:122:GLY:HA2	1:A:125:LEU:HD12	0.57	1.76	5	23
1:A:36:ALA:HB2	1:A:103:MET:HE1	0.57	1.75	25	1
1:A:102:VAL:HG12	1:A:105:GLU:OE1	0.56	2.00	1	1
1:A:45:GLN:O	1:A:49:ALA:CB	0.56	2.53	6	30
1:A:45:GLN:O	1:A:49:ALA:HB3	0.56	2.01	29	30
1:A:45:GLN:O	1:A:49:ALA:N	0.55	2.38	21	30
1:A:51:ARG:CG	1:A:64:ILE:HD12	0.55	2.32	28	3
1:A:69:PHE:O	1:A:95:ALA:HB2	0.55	2.02	4	4
1:A:35:VAL:HG23	1:A:101:ARG:N	0.52	2.19	10	20
1:A:68:ILE:HD13	1:A:103:MET:HB3	0.52	1.81	1	4
1:A:54:MET:HE1	1:A:104:PHE:CD2	0.51	2.39	15	15
1:A:54:MET:HE3	1:A:64:ILE:HD13	0.51	1.81	9	1
1:A:37:LEU:HD11	1:A:130:LYS:HG2	0.51	1.82	12	1
1:A:54:MET:SD	1:A:121:ALA:HB2	0.50	2.46	14	2
1:A:66:ILE:HG22	1:A:68:ILE:HG12	0.50	1.82	13	3
1:A:118:LEU:HB2	1:A:131:ILE:HD12	0.50	1.84	11	13
1:A:51:ARG:HD3	1:A:64:ILE:HD12	0.48	1.85	18	2
1:A:54:MET:CE	1:A:104:PHE:CD2	0.47	2.97	4	28
1:A:54:MET:HE3	1:A:64:ILE:CD1	0.47	2.40	9	1
1:A:115:MET:HA	1:A:131:ILE:HG21	0.47	1.86	13	2
1:A:37:LEU:HD12	1:A:128:LYS:HG2	0.47	1.85	5	1
1:A:54:MET:HE3	1:A:104:PHE:CD2	0.47	2.45	27	2
1:A:97:VAL:HG12	1:A:98:LYS:N	0.47	2.24	2	29
1:A:40:ALA:HB2	1:A:127:ILE:HG21	0.47	1.84	7	10
1:A:58:PHE:CG	1:A:109:VAL:HG11	0.47	2.45	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ALA:O	1:A:99:PRO:HA	0.46	2.09	30	23
1:A:58:PHE:CE1	1:A:117:ALA:CB	0.46	2.98	10	10
1:A:51:ARG:HD3	1:A:66:ILE:HD11	0.46	1.87	5	1
1:A:106:VAL:CG1	1:A:118:LEU:HD11	0.46	2.39	19	1
1:A:34:LEU:HD23	1:A:118:LEU:HB3	0.46	1.88	13	4
1:A:58:PHE:CZ	1:A:117:ALA:CB	0.46	2.99	16	5
1:A:97:VAL:CG1	1:A:101:ARG:CB	0.46	2.94	26	4
1:A:35:VAL:HG11	1:A:130:LYS:CE	0.46	2.38	15	1
1:A:43:THR:HG23	1:A:94:VAL:CG1	0.46	2.40	19	6
1:A:54:MET:HE1	1:A:64:ILE:HG21	0.45	1.88	9	1
1:A:97:VAL:CG1	1:A:101:ARG:HB3	0.45	2.42	12	5
1:A:66:ILE:CD1	1:A:104:PHE:CD2	0.45	3.00	16	9
1:A:32:TYR:CD2	1:A:114:ALA:CB	0.45	3.00	14	3
1:A:127:ILE:HD12	1:A:127:ILE:O	0.45	2.10	16	12
1:A:37:LEU:HD21	1:A:130:LYS:CD	0.45	2.41	17	1
1:A:42:ILE:HG23	1:A:46:GLN:OE1	0.44	2.13	1	1
1:A:64:ILE:HG23	1:A:106:VAL:CG1	0.44	2.43	29	2
1:A:34:LEU:HD23	1:A:131:ILE:HD13	0.44	1.90	17	1
1:A:127:ILE:C	1:A:127:ILE:HD12	0.44	2.33	14	19
1:A:33:GLY:O	1:A:132:VAL:HG22	0.44	2.13	13	2
1:A:37:LEU:HD12	1:A:128:LYS:HG3	0.43	1.89	18	1
1:A:66:ILE:HD13	1:A:66:ILE:N	0.43	2.28	13	1
1:A:32:TYR:CE1	1:A:133:ARG:HG3	0.43	2.49	5	2
1:A:132:VAL:O	1:A:132:VAL:HG23	0.43	2.12	17	4
1:A:118:LEU:HD23	1:A:131:ILE:CG2	0.43	2.41	15	9
1:A:54:MET:CB	1:A:64:ILE:HD11	0.43	2.44	16	5
1:A:51:ARG:HG3	1:A:64:ILE:HD12	0.43	1.90	8	1
1:A:34:LEU:HD13	1:A:34:LEU:C	0.43	2.35	17	1
1:A:106:VAL:HG13	1:A:118:LEU:CD1	0.42	2.44	13	4
1:A:119:ARG:HD3	1:A:131:ILE:HD11	0.42	1.89	18	1
1:A:42:ILE:HG21	1:A:68:ILE:CD1	0.42	2.42	16	1
1:A:127:ILE:CD1	1:A:129:THR:CG2	0.42	2.98	18	8
1:A:61:GLY:O	1:A:109:VAL:HG12	0.42	2.13	17	2
1:A:54:MET:O	1:A:58:PHE:CD2	0.42	2.73	10	14
1:A:51:ARG:HG3	1:A:66:ILE:HD11	0.42	1.92	13	1
1:A:34:LEU:HD11	1:A:129:THR:CB	0.41	2.46	11	1
1:A:54:MET:O	1:A:58:PHE:CE2	0.41	2.74	8	2
1:A:119:ARG:NH2	1:A:131:ILE:CG1	0.41	2.84	13	1
1:A:41:TRP:CD1	1:A:96:VAL:HG22	0.41	2.49	13	1
1:A:46:GLN:O	1:A:50:ALA:HB3	0.41	2.15	29	1
1:A:118:LEU:CD2	1:A:131:ILE:HG23	0.41	2.42	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:GLN:NE2	1:A:125:LEU:HD23	0.40	2.30	11	1
1:A:33:GLY:N	1:A:132:VAL:O	0.40	2.54	24	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	80/141 (57%)	75±2 (94±2%)	4±2 (5±2%)	1±1 (1±1%)	26	73
All	All	2400/4230 (57%)	2259 (94%)	125 (5%)	16 (1%)	26	73

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	58	PHE	12
1	A	61	GLY	4

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	63/111 (57%)	50±2 (79±4%)	13±2 (21±4%)	3	32
All	All	1890/3330 (57%)	1497 (79%)	393 (21%)	3	32

All 28 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	43	THR	30

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Mol	Chain	Res	Type	Models (Total)
1	A	45	GLN	30
1	A	118	LEU	30
1	A	69	PHE	28
1	A	115	MET	27
1	A	124	LYS	23
1	A	101	ARG	21
1	A	133	ARG	21
1	A	51	ARG	20
1	A	98	LYS	18
1	A	119	ARG	17
1	A	123	HIS	16
1	A	38	GLU	15
1	A	67	ARG	14
1	A	103	MET	12
1	A	128	LYS	11
1	A	112	GLU	10
1	A	48	GLU	8
1	A	63	LYS	8
1	A	31	ASP	7
1	A	130	LYS	6
1	A	105	GLU	5
1	A	56	ARG	4
1	A	111	GLU	4
1	A	59	ARG	3
1	A	113	GLN	2
1	A	60	ARG	2
1	A	94	VAL	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 monosaccharides 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 (i)

No chemical shift data were provided