



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 10, 2019 – 09:50 AM EDT

PDB ID : 6PPF  
EMDB ID: : EMD-20435  
Title : Bacterial 45SRbgA ribosomal particle class B  
Authors : Ortega, J.; Seffouh, A.; Jain, N.; Jahagirdar, D.; Basu, K.; Razi, A.; Ni, X.;  
Guarne, A.; Britton, R.A.  
Deposited on : 2019-07-06  
Resolution : 3.40 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

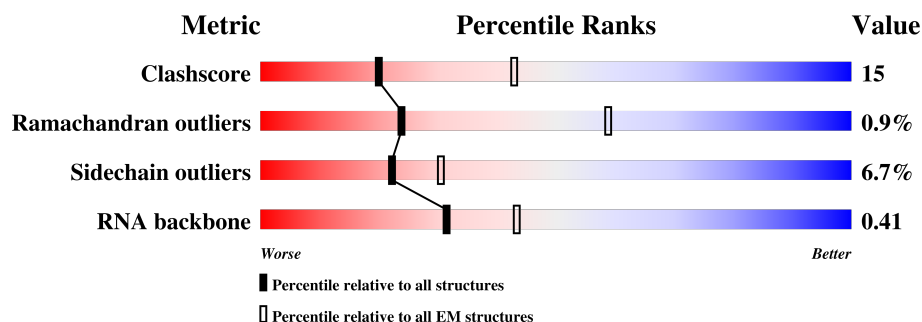
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	2927	45% 31% 8% • 16%
2	B	119	36% 43% 15% 6%
3	C	277	51% 26% • 20%
4	D	209	47% 25% 7% • 20%
5	E	207	56% 35% • 6%
6	J	145	66% 27% • • •
7	K	122	66% 34% •
8	L	145	56% 28% • 12%

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Mol	Chain	Length	Quality of chain
9	N	120	 86% 13% .
10	O	120	 51% 32% . 13%
11	P	115	 61% 27% . 10%
12	Q	118	 58% 33% 7% ..
13	R	102	 48% 41% . . 6%
14	S	113	 74% 21% . .
15	T	95	 53% 38% . 7%
16	U	103	 68% 21% 6% 5%
17	V	94	 32% 40% 5% 22%
18	Z	59	 73% 25% .
19	b	59	 81% 10% 8%
20	Y	66	 79% 18% . .
21	d	44	 100%

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 71835 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2471	Total	C	N	O	P	0	0
			53094	23688	9835	17100	2471		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2395	1068	435	780	112		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	221	Total	C	N	O	S	0	0
			1684	1047	326	307	4		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	167	Total	C	N	O	S	0	0
			1265	802	220	240	3		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	194	Total	C	N	O	S	0	0
			1484	937	270	275	2		

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	141	Total	C	N	O	S	0	0
			1119	708	205	201	5		

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	128	Total	C	N	O	S	0	0
			952	594	179	177	2		

- Molecule 9 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 10 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	O	104	Total	C	N	O	0	0
			791	492	157	142		

- Molecule 11 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	P	103	Total	C	N	O	0	0
			846	540	162	144		

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 13 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	R	96	Total	C	N	O	0	0
			758	485	134	139		

- Molecule 14 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 15 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	88	Total	C	N	O	S	0	0
			707	441	131	132	3		

- Molecule 16 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	98	Total	C	N	O	S	0	0
			739	464	138	134	3		

- Molecule 17 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	73	Total	C	N	O	S	0	0
			555	344	106	105			

- Molecule 18 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 19 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 20 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 21 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

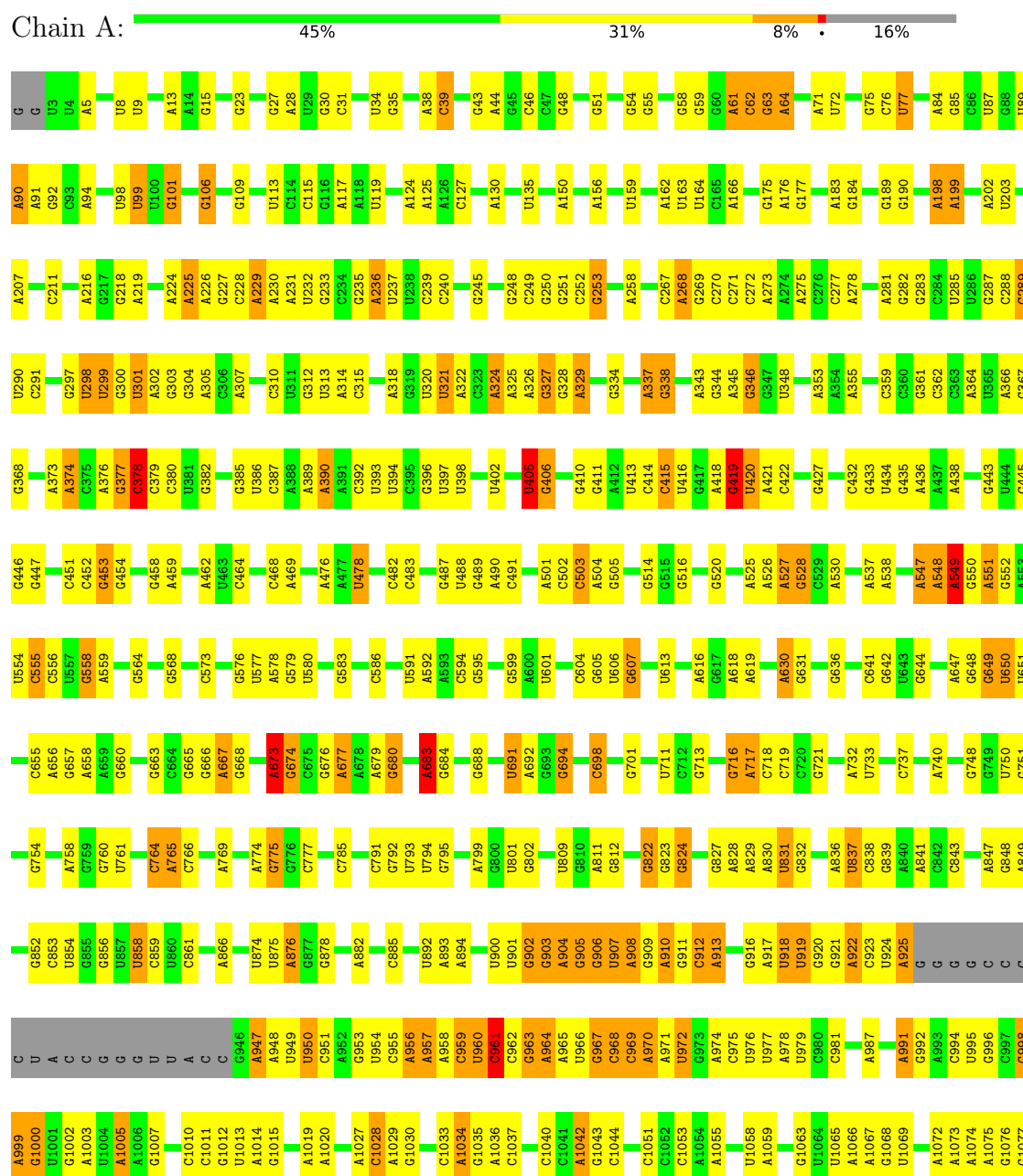
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	A	13	Total	O	0
			13	13	

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

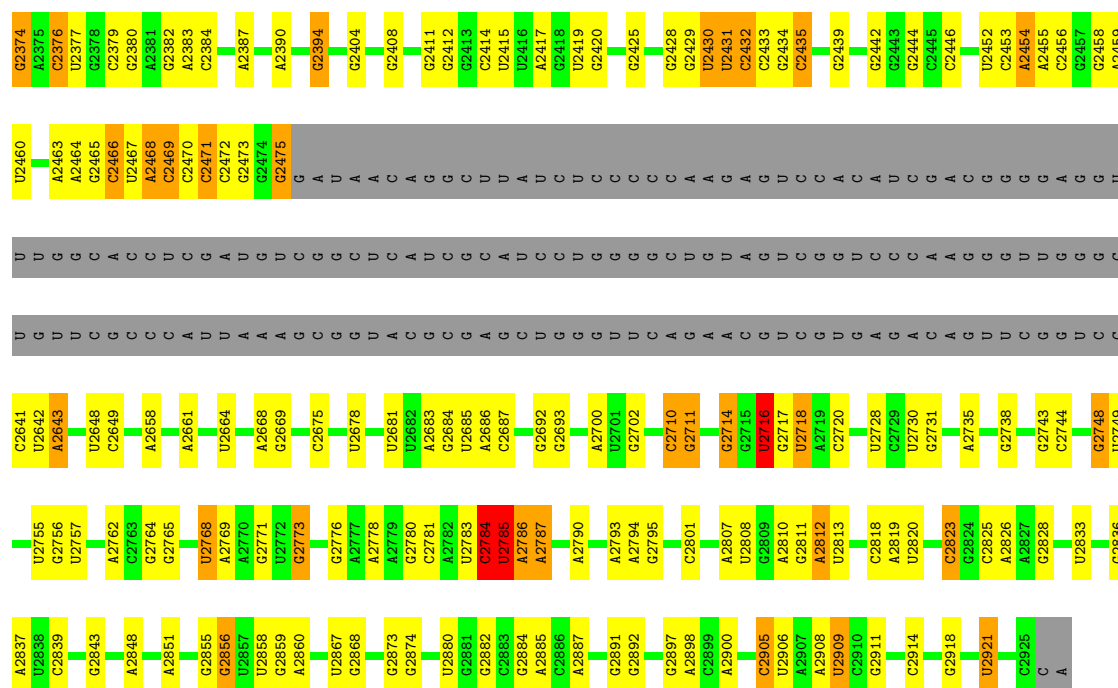
#### • Molecule 1: 23S rRNA





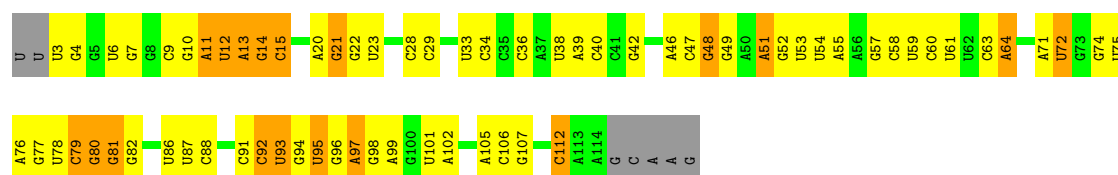
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM



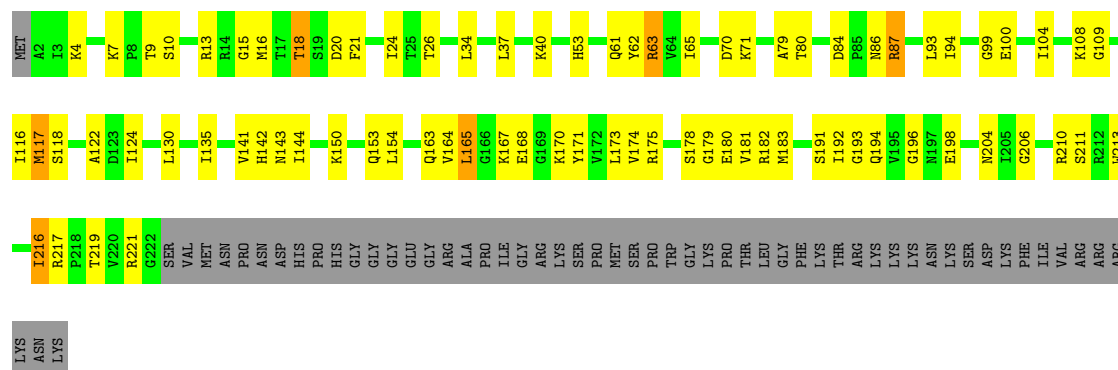
### • Molecule 2: 5S rRNA

Chain B: 36% 43% 15% 6%



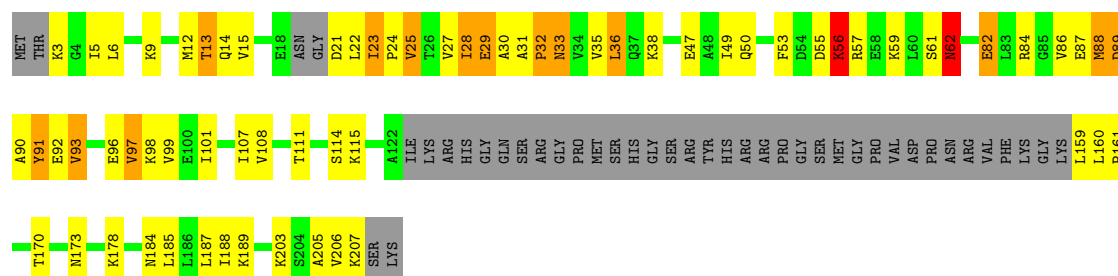
### • Molecule 3: 50S ribosomal protein L2

Chain C: 51% 26% 20%



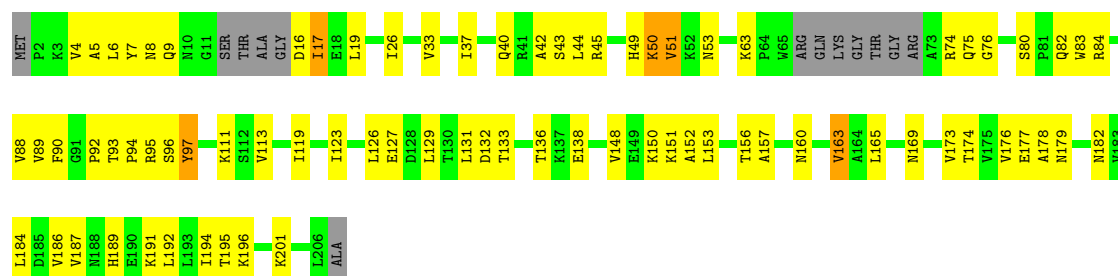
### • Molecule 4: 50S ribosomal protein L3

Chain D: 47% 25% 7% 20%



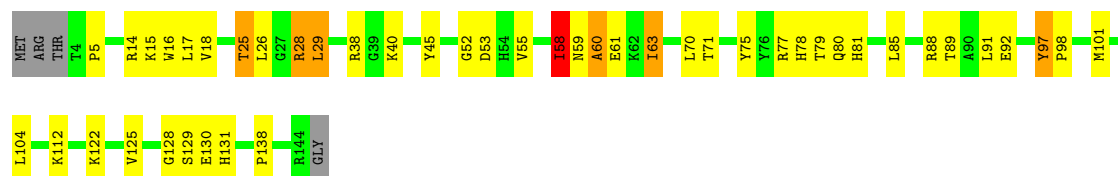
• Molecule 5: 50S ribosomal protein L4

Chain E: 56% 35% 6%



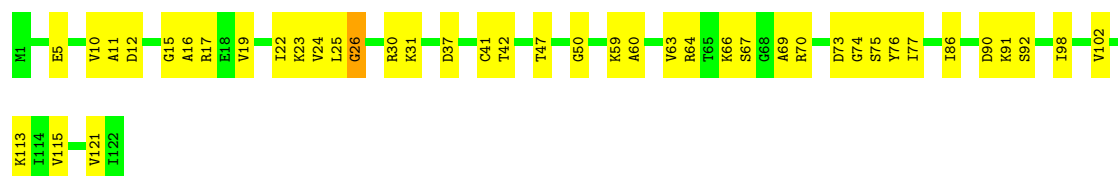
• Molecule 6: 50S ribosomal protein L13

Chain J: 66% 27% 6%



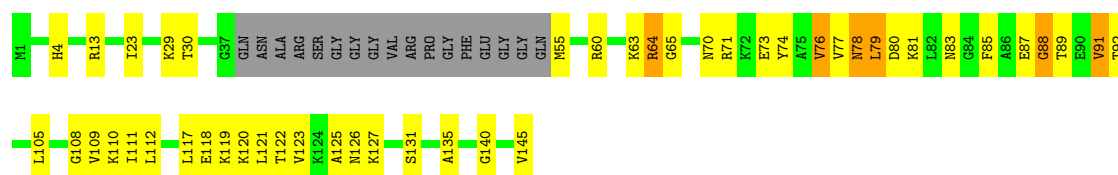
• Molecule 7: 50S ribosomal protein L14

Chain K: 66% 34% 6%




• Molecule 8: 50S ribosomal protein L15

Chain L: 56% 28% 12%



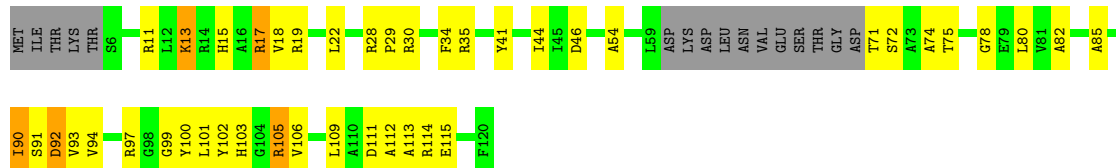
- Molecule 9: 50S ribosomal protein L17

Chain N:  86% 13%



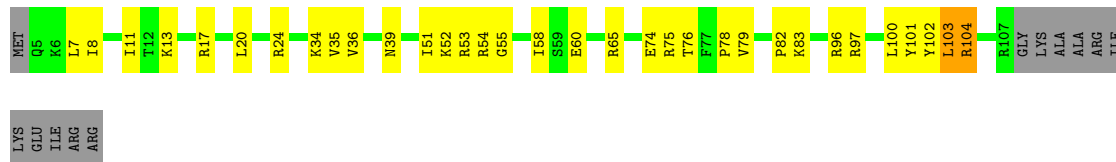
- Molecule 10: 50S ribosomal protein L18

Chain O:  51% 32% 13%




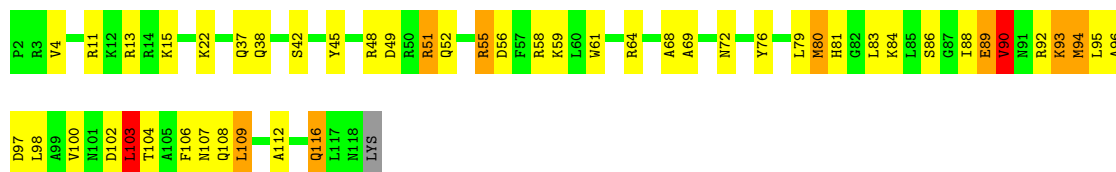
- Molecule 11: 50S ribosomal protein L19

Chain P:  61% 27% 10%



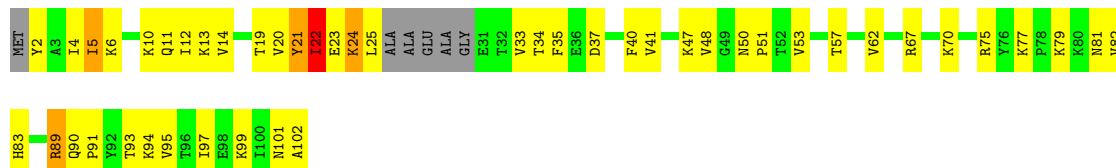
- Molecule 12: 50S ribosomal protein L20

Chain Q:  58% 33% 7%



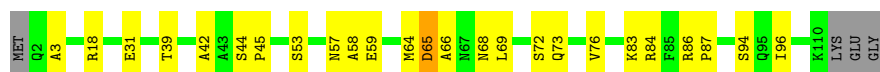
- Molecule 13: 50S ribosomal protein L21

Chain R:  48% 41% 6%



- Molecule 14: 50S ribosomal protein L22

Chain S:  74% 21% 5%



- Molecule 15: 50S ribosomal protein L23

Chain T: 53% 38% 7%



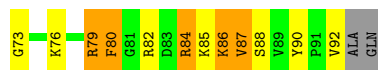
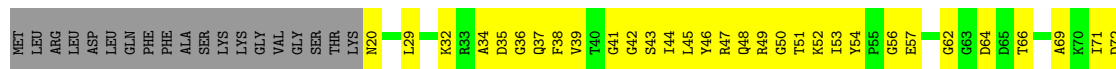
- Molecule 16: 50S ribosomal protein L24

Chain U: 68% 21% 6% 5%



- Molecule 17: 50S ribosomal protein L27

Chain V: 32% 40% 5% 22%



- Molecule 18: 50S ribosomal protein L30

Chain Z: 73% 25%



- Molecule 19: 50S ribosomal protein L32

Chain b: 81% 10% 8%



- Molecule 20: 50S ribosomal protein L29

Chain Y: 79% 18% 2%



- Molecule 21: 50S ribosomal protein L34

Chain d:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	546297	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	A	0.77	0/59472	1.00	137/92759 (0.1%)
10	O	0.24	0/799	0.67	3/1070 (0.3%)
11	P	0.35	0/859	0.52	0/1152
12	Q	0.39	0/952	0.63	2/1266 (0.2%)
13	R	0.39	0/768	0.67	2/1029 (0.2%)
14	S	0.34	0/851	0.50	0/1146
15	T	0.36	0/713	0.46	0/951
16	U	0.34	0/748	0.51	0/1000
17	V	0.20	0/563	0.33	0/753
18	Z	0.33	0/457	0.54	0/613
19	b	0.34	0/433	0.45	0/574
2	B	0.33	0/2678	0.94	3/4174 (0.1%)
20	Y	0.31	0/531	0.47	0/707
21	d	0.39	0/370	0.49	0/483
3	C	0.33	0/1709	0.53	2/2296 (0.1%)
4	D	0.35	0/1276	0.64	3/1709 (0.2%)
5	E	0.32	0/1501	0.60	4/2025 (0.2%)
6	J	0.36	0/1142	0.60	2/1537 (0.1%)
7	K	0.33	0/927	0.54	0/1245
8	L	0.29	0/961	0.78	7/1281 (0.5%)
9	N	0.40	0/960	0.54	0/1284
All	All	0.69	0/78670	0.94	165/119054 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	Q	0	1
4	D	0	1
All	All	0	2



There are no bond length outliers.

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Q	103	LEU	CB-CA-C	15.54	139.72	110.20
1	A	1433	U	C2-N1-C1'	12.62	132.85	117.70
10	O	90	ILE	CB-CA-C	-12.23	87.14	111.60
8	L	85	PHE	CB-CA-C	-12.23	85.95	110.40
1	A	961	C	N1-C2-O2	11.32	125.69	118.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	56	LYS	Peptide
12	Q	103	LEU	Peptide

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	53094	0	26707	695	0
2	B	2395	0	1212	52	0
3	C	1684	0	1754	81	0
4	D	1265	0	1332	102	0
5	E	1484	0	1565	80	0
6	J	1119	0	1159	47	0
7	K	920	0	977	54	0
8	L	952	0	1002	104	0
9	N	953	0	983	12	0
10	O	791	0	824	39	0
11	P	846	0	902	54	0
12	Q	940	0	1005	123	0
13	R	758	0	801	97	0
14	S	842	0	899	27	0
15	T	707	0	751	35	0
16	U	739	0	790	41	0
17	V	555	0	540	81	0
18	Z	455	0	491	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	b	426	0	445	0	0
20	Y	530	0	568	20	0
21	d	367	0	410	0	0
22	A	13	0	0	0	0
All	All	71835	0	45117	1512	0

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 15.

The worst 5 of 1512 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:61:TRP:CZ2	12:Q:94:MET:HB2	1.27	1.60
12:Q:95:LEU:HD22	13:R:11:GLN:CB	1.28	1.57
1:A:901:U:H2'	1:A:902:G:C8	1.36	1.56
1:A:2465:G:H2'	1:A:2466:C:C5'	1.38	1.52
12:Q:95:LEU:CD2	13:R:11:GLN:HB3	1.30	1.52

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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 EM 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	
3	C	219/277 (79%)	199 (91%)	20 (9%)	0	100	100
4	D	161/209 (77%)	138 (86%)	20 (12%)	3 (2%)	9	42
5	E	188/207 (91%)	159 (85%)	28 (15%)	1 (0%)	31	69
6	J	139/145 (96%)	122 (88%)	14 (10%)	3 (2%)	7	39
7	K	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	21	60
8	L	124/145 (86%)	115 (93%)	6 (5%)	3 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	N	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
10	O	100/120 (83%)	92 (92%)	7 (7%)	1 (1%)	17	56
11	P	101/115 (88%)	92 (91%)	9 (9%)	0	100	100
12	Q	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	19	58
13	R	92/102 (90%)	77 (84%)	15 (16%)	0	100	100
14	S	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
15	T	86/95 (90%)	79 (92%)	7 (8%)	0	100	100
16	U	94/103 (91%)	82 (87%)	9 (10%)	3 (3%)	4	31
17	V	71/94 (76%)	62 (87%)	8 (11%)	1 (1%)	12	48
18	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
19	b	52/59 (88%)	47 (90%)	4 (8%)	1 (2%)	9	42
20	Y	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
21	d	42/44 (96%)	42 (100%)	0	0	100	100
All	All	2047/2313 (88%)	1844 (90%)	185 (9%)	18 (1%)	24	58

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	O	102	TYR
4	D	93	VAL
6	J	59	ASN
7	K	26	GLY
12	Q	90	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	
3	C	177/225 (79%)	168 (95%)	9 (5%)	26	61
4	D	135/170 (79%)	115 (85%)	20 (15%)	3	17
5	E	162/170 (95%)	148 (91%)	14 (9%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	120/123 (98%)	113 (94%)	7 (6%)	22	58
7	K	101/101 (100%)	100 (99%)	1 (1%)	78	89
8	L	98/109 (90%)	92 (94%)	6 (6%)	20	56
9	N	99/100 (99%)	99 (100%)	0	100	100
10	O	78/93 (84%)	71 (91%)	7 (9%)	10	39
11	P	91/100 (91%)	87 (96%)	4 (4%)	31	66
12	Q	96/97 (99%)	83 (86%)	13 (14%)	4	20
13	R	82/84 (98%)	75 (92%)	7 (8%)	12	42
14	S	90/93 (97%)	87 (97%)	3 (3%)	41	73
15	T	79/85 (93%)	74 (94%)	5 (6%)	20	55
16	U	82/87 (94%)	78 (95%)	4 (5%)	27	63
17	V	54/74 (73%)	44 (82%)	10 (18%)	2	8
18	Z	52/53 (98%)	52 (100%)	0	100	100
19	b	48/53 (91%)	43 (90%)	5 (10%)	8	32
20	Y	56/57 (98%)	55 (98%)	1 (2%)	62	83
21	d	39/39 (100%)	39 (100%)	0	100	100
All	All	1739/1913 (91%)	1623 (93%)	116 (7%)	22	53

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	L	76	VAL
11	P	35	VAL
17	V	84	ARG
8	L	89	THR
10	O	17	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
8	L	126	ASN
10	O	49	ASN
17	V	20	ASN
10	O	15	HIS
10	O	103	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2458/2927 (83%)	792 (32%)	50 (2%)
2	B	111/119 (93%)	45 (40%)	3 (2%)
All	All	2569/3046 (84%)	837 (32%)	53 (2%)

5 of 837 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	13	A
1	A	15	G
1	A	23	G

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	908	A
1	A	1250	G
1	A	2785	U
1	A	962	C
1	A	1103	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.