



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 18, 2017 – 07:26 AM EDT

PDB ID : 5UZ4
EMDB ID: : EMD-8621
Title : The cryo-EM structure of YjeQ bound to the 30S subunit suggests a fidelity checkpoint function for this protein in ribosome assembly
Authors : Razi, A.; Guarne, A.; Ortega, J.
Deposited on : unknown
Resolution : 5.80 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

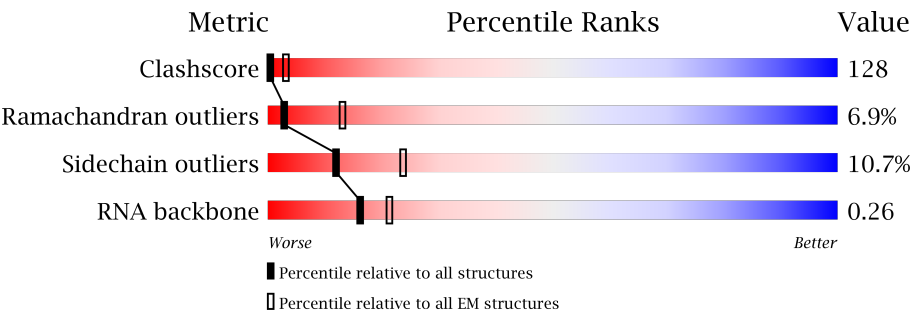
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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.






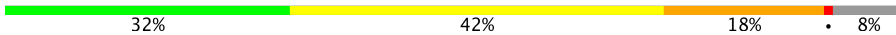
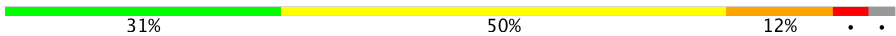
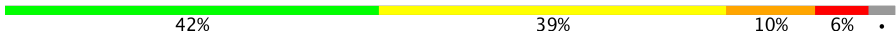
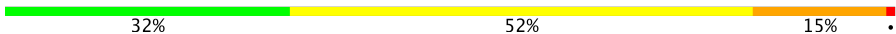
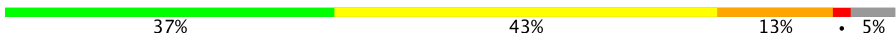
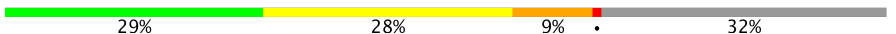

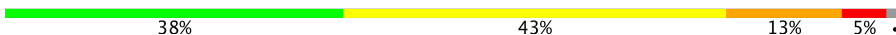

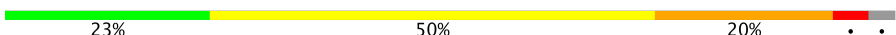
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 ≥ 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	1527	<div><div>39%51%8%</div></div>
2	C	233	<div><div>39%35%11%12%</div></div>
3	D	206	<div><div>38%37%17%8%</div></div>
4	E	167	<div><div>37%37%16%10%</div></div>
5	F	131	<div><div>34%32%7%24%</div></div>
6	G	179	<div><div>49%27%7%17%</div></div>
7	H	130	<div><div>48%32%17%</div></div>
8	I	130	<div><div>42%45%8%</div></div>

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Mol	Chain	Length	Quality of chain
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	S	92	
19	T	87	
20	B	241	
21	Z	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	GGM	Z	402	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 53225 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 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1527	Total	C	N	O	P	0	0
			32767	14614	6014	10613	1526		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	A	G	conflict	GB 1095872043

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	205	Total	C	N	O	S	0	0
			1639	1023	314	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	149	Total	C	N	O	S	0	0
			1160	721	222	213	4		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	129	Total	C	N	O	S	0	0
			975	613	172	184	6		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			951	587	195	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	109	Total	C	N	O	S	0	0
			845	522	169	151	3		

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	98	Total	C	N	O	S	0	0
			759	472	157	127	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	86	Total	C	N	O	S	0	0
			700	431	144	124	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	51	Total	C	N	O	0	0
			414	264	77	73		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	79	Total	C	N	O	S	0	0
			619	393	117	107	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	233	Total	C	N	O	S	2	0
			1830	1154	328	340	8		

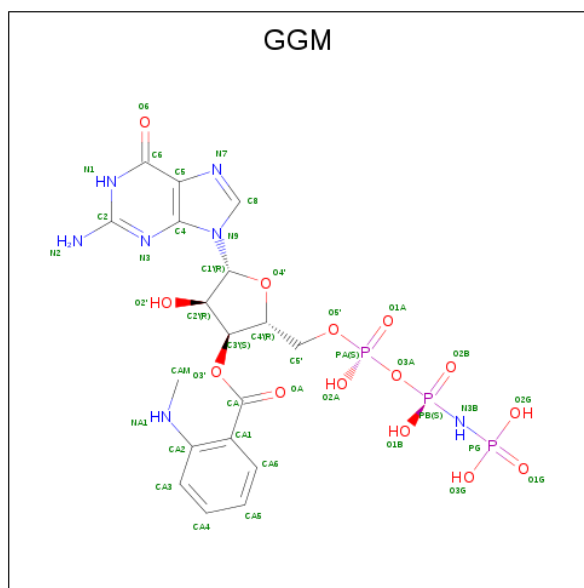
- Molecule 21 is a protein called Small ribosomal subunit biogenesis GTPase RsgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	323	Total	C	N	O	S	0	0
			2348	1463	397	479	9		

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	Z	1	Total	Zn	0
			1	1	

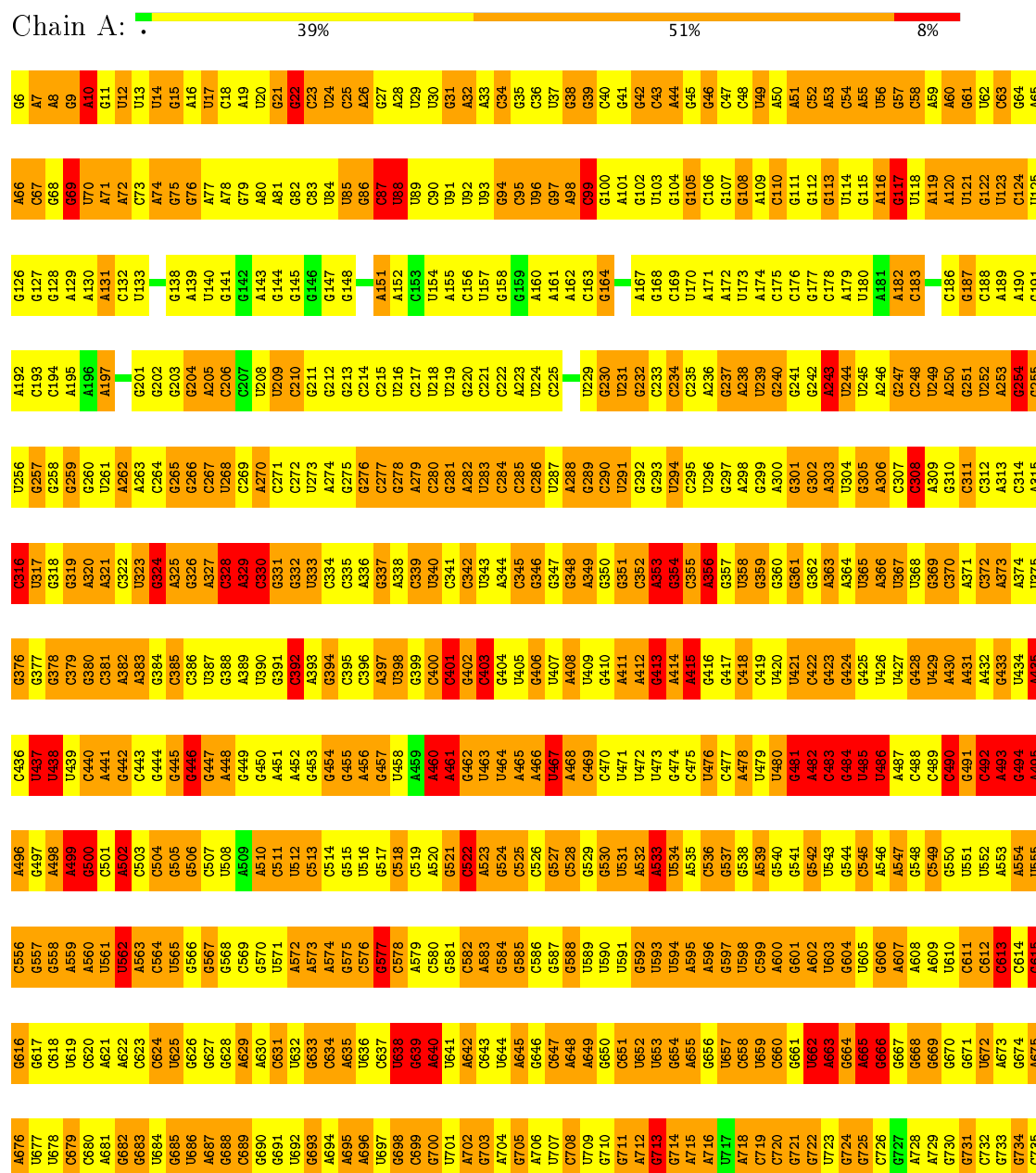
- Molecule 23 is 3'-O-(N-methylantraniloyl)-beta:gamma-imidoguanosine-5'-triphosphate (three-letter code: GGM) (formula: C₁₈H₂₄N₇O₁₄P₃).



3 Residue-property plots

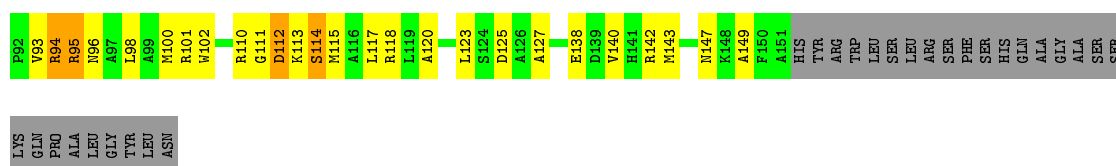
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 16S RIBOSOMAL RNA

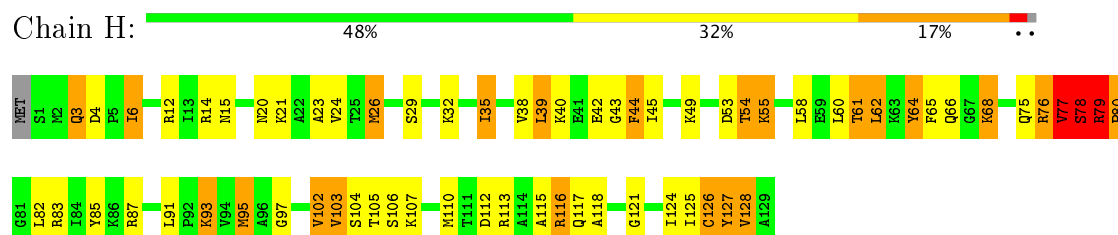


- Molecule 2: 30S ribosomal protein S3

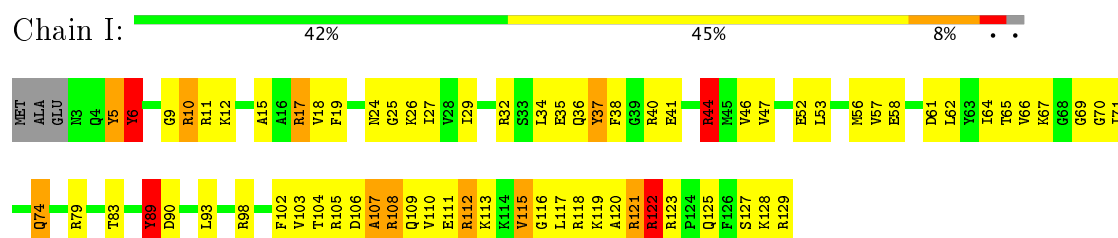
Met	G1	Q2	K3	V4	H5	P6	N7	G8	I9	R10	L11	G12	I13	V14	K15	P16	V17	I18	S19	T20	W21	F22	A23	G24	T25	K26	E27	F28	N31	L32	D33	S34	D35	F36			R39	Q40	Y41		V51		I54	V55	I56	E57	R58	P59	A60	K61	G62	I63	R64	V65	T66	I67	H68			I70
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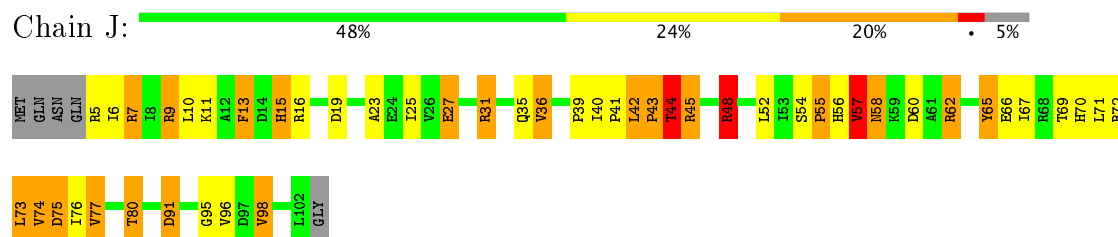
• Molecule 7: 30S ribosomal protein S8



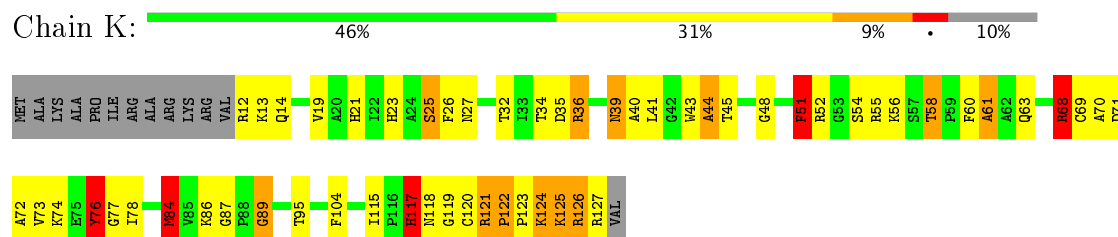
• Molecule 8: 30S ribosomal protein S9



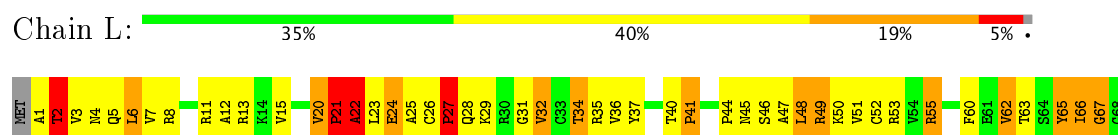
• Molecule 9: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S11



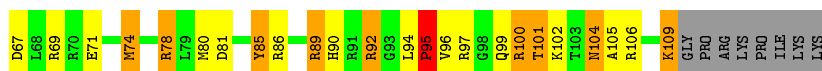
• Molecule 11: 30S ribosomal protein S12





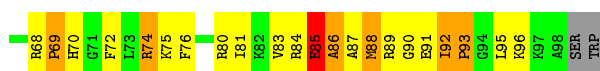
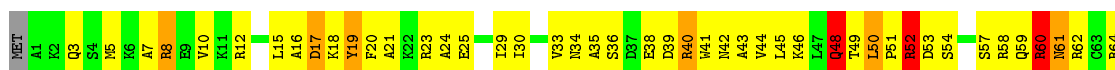
• Molecule 12: 30S ribosomal protein S13

Chain M: 32% 42% 18% 8%



• Molecule 13: 30S ribosomal protein S14

Chain N: 31% 50% 12%



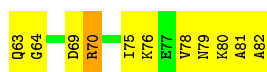
• Molecule 14: 30S ribosomal protein S15

Chain O: 42% 39% 10% 6%



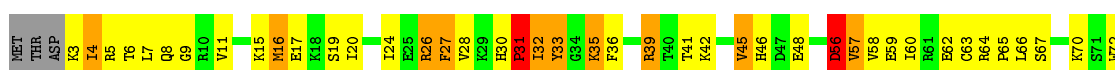
• Molecule 15: 30S ribosomal protein S16

Chain P: 32% 52% 15%

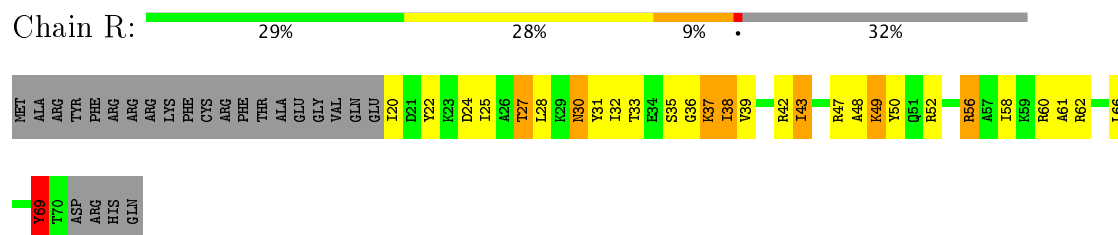


• Molecule 16: 30S ribosomal protein S17

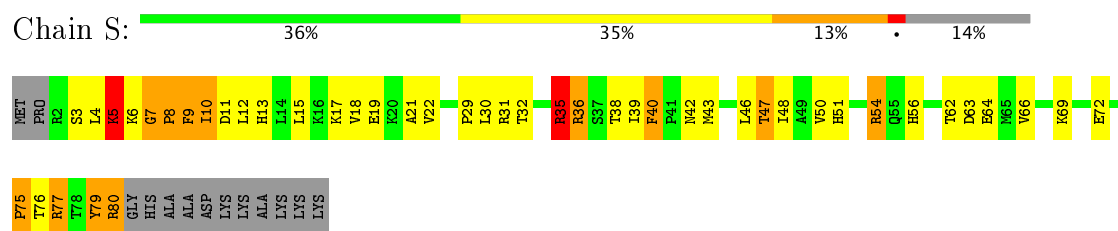
Chain Q: 37% 43% 13% 5%



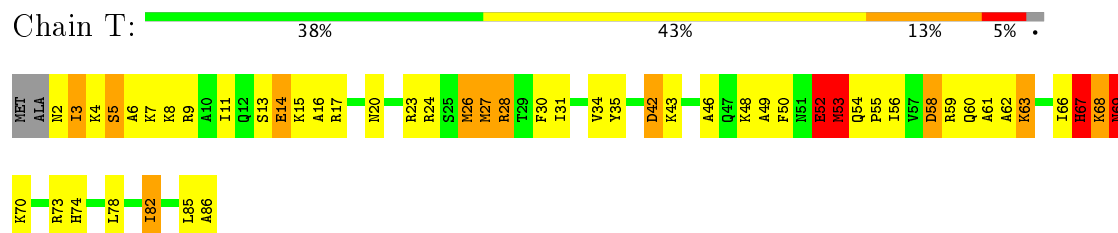
- Molecule 17: 30S ribosomal protein S18



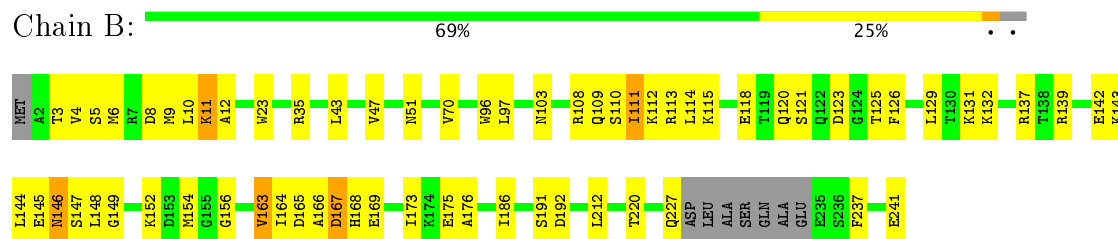
- Molecule 18: 30S ribosomal protein S19



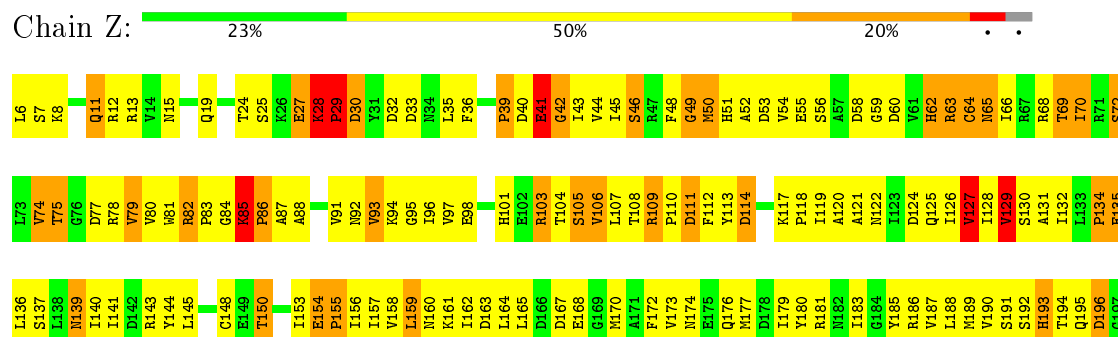
- Molecule 19: 30S ribosomal protein S20

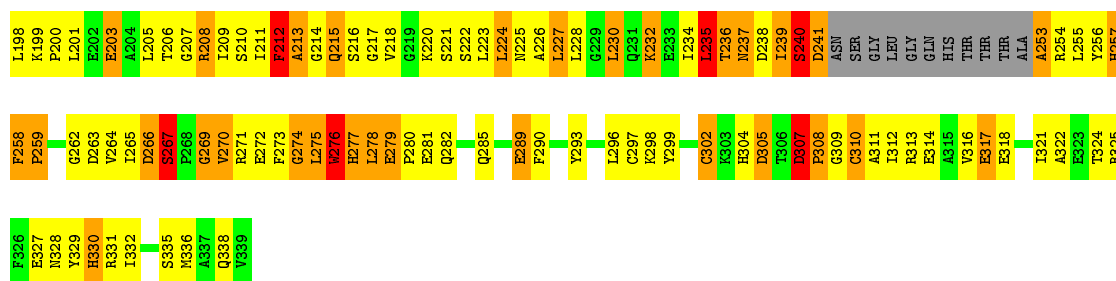


- Molecule 20: 30S ribosomal protein S2



- Molecule 21: Small ribosomal subunit biogenesis GTPase RsgA





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	130462	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	34482	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GGM, ZN

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	2.66	229/36645 (0.6%)	1.59	597/57061 (1.0%)
10	K	1.32	0/885	1.53	15/1195 (1.3%)
11	L	1.76	6/965 (0.6%)	1.79	23/1296 (1.8%)
12	M	1.31	0/851	1.44	9/1136 (0.8%)
13	N	1.67	2/769 (0.3%)	1.36	5/1026 (0.5%)
14	O	1.51	0/708	1.55	11/946 (1.2%)
15	P	1.68	0/659	1.72	12/884 (1.4%)
16	Q	1.57	0/657	1.70	10/881 (1.1%)
17	R	1.16	0/420	1.27	4/565 (0.7%)
18	S	1.15	0/633	1.35	6/853 (0.7%)
19	T	1.60	0/671	1.60	7/888 (0.8%)
2	C	1.47	1/1651 (0.1%)	1.59	23/2225 (1.0%)
20	B	0.54	2/1864 (0.1%)	0.92	6/2511 (0.2%)
21	Z	0.79	16/2388 (0.7%)	1.28	60/3259 (1.8%)
3	D	1.67	6/1661 (0.4%)	1.66	27/2223 (1.2%)
4	E	1.78	5/1118 (0.4%)	1.72	21/1504 (1.4%)
5	F	1.33	0/835	1.61	10/1128 (0.9%)
6	G	1.30	1/1173 (0.1%)	1.58	13/1573 (0.8%)
7	H	1.65	3/985 (0.3%)	1.71	15/1322 (1.1%)
8	I	1.44	0/1034	1.65	12/1375 (0.9%)
9	J	1.41	1/796 (0.1%)	1.66	19/1077 (1.8%)
All	All	2.28	272/57368 (0.5%)	1.57	905/84928 (1.1%)

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
1	A	1	7
10	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	L	0	7
12	M	0	2
13	N	0	3
14	O	0	6
15	P	0	5
16	Q	0	2
17	R	0	2
18	S	0	4
19	T	0	4
2	C	0	20
21	Z	0	11
3	D	0	17
4	E	0	9
5	F	0	6
6	G	0	6
7	H	0	5
8	I	0	10
9	J	0	7
All	All	1	135

The worst 5 of 272 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	801	U	O3'-P	-90.89	0.52	1.61
1	A	1012	A	O3'-P	-90.78	0.52	1.61
1	A	901	A	O3'-P	-87.79	0.55	1.61
1	A	1310	G	O3'-P	-83.62	0.60	1.61
1	A	354	G	O3'-P	-82.82	0.61	1.61

The worst 5 of 905 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	801	U	P-O3'-C3'	-77.19	27.07	119.70
1	A	639	G	OP2-P-O3'	-41.14	14.70	105.20
1	A	944	G	P-O3'-C3'	40.49	168.28	119.70
1	A	804	U	P-O3'-C3'	37.59	164.81	119.70
1	A	1508	A	P-O3'-C3'	35.20	161.94	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1243	C	C3'

5 of 135 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	437	U	Sidechain
1	A	438	U	Sidechain
1	A	496	A	Sidechain
1	A	521	G	Sidechain

5.2 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 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	32767	0	16531	9892	0
2	C	1624	0	1699	134	0
3	D	1639	0	1699	141	0
4	E	1105	0	1148	92	0
5	F	817	0	808	114	0
6	G	1160	0	1207	89	0
7	H	975	0	1023	77	0
8	I	1022	0	1070	103	0
9	J	786	0	828	62	0
10	K	869	0	877	116	0
11	L	951	0	1007	125	0
12	M	845	0	900	135	0
13	N	759	0	789	179	0
14	O	700	0	723	68	0
15	P	649	0	665	50	0
16	Q	648	0	690	79	0
17	R	414	0	439	85	0
18	S	619	0	628	155	0
19	T	665	0	710	54	0
20	B	1830	0	1839	147	0
21	Z	2348	0	2103	553	0
22	Z	1	0	0	0	0
23	Z	32	0	12	32	0
All	All	53225	0	37395	11485	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 128.

The worst 5 of 11485 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)
1:A:1088:G:C2	1:A:1098:C:N3	1.67	1.59
1:A:714:G:H2'	1:A:715:A:C8	1.08	1.58
1:A:510:A:O3'	1:A:511:C:P	1.16	1.54
1:A:317:U:C4	1:A:337:G:C2	1.98	1.51
1:A:253:A:N6	1:A:274:A:C6	1.79	1.51

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 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	
2	C	204/233 (88%)	149 (73%)	40 (20%)	15 (7%)	1	18
3	D	203/206 (98%)	162 (80%)	25 (12%)	16 (8%)	1	17
4	E	148/167 (89%)	119 (80%)	23 (16%)	6 (4%)	3	30
5	F	98/131 (75%)	76 (78%)	10 (10%)	12 (12%)	0	7
6	G	147/179 (82%)	115 (78%)	25 (17%)	7 (5%)	2	27
7	H	127/130 (98%)	104 (82%)	18 (14%)	5 (4%)	3	31
8	I	125/130 (96%)	93 (74%)	22 (18%)	10 (8%)	1	17
9	J	96/103 (93%)	70 (73%)	16 (17%)	10 (10%)	0	10
10	K	114/129 (88%)	86 (75%)	19 (17%)	9 (8%)	1	17
11	L	121/124 (98%)	81 (67%)	26 (22%)	14 (12%)	0	8
12	M	105/118 (89%)	78 (74%)	18 (17%)	9 (9%)	1	15
13	N	96/101 (95%)	61 (64%)	24 (25%)	11 (12%)	0	8
14	O	84/89 (94%)	68 (81%)	13 (16%)	3 (4%)	4	34
15	P	80/82 (98%)	64 (80%)	9 (11%)	7 (9%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	78/84 (93%)	50 (64%)	22 (28%)	6 (8%)	1	17
17	R	49/75 (65%)	35 (71%)	12 (24%)	2 (4%)	3	30
18	S	77/92 (84%)	55 (71%)	15 (20%)	7 (9%)	1	14
19	T	83/87 (95%)	72 (87%)	4 (5%)	7 (8%)	1	15
20	B	231/241 (96%)	218 (94%)	11 (5%)	2 (1%)	20	63
21	Z	319/334 (96%)	259 (81%)	41 (13%)	19 (6%)	2	22
All	All	2585/2835 (91%)	2015 (78%)	393 (15%)	177 (7%)	3	20

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	62	SER
2	C	158	GLY
2	C	174	LEU
2	C	178	ARG
2	C	195	ILE

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	
2	C	170/190 (90%)	156 (92%)	14 (8%)	13	44
3	D	171/173 (99%)	141 (82%)	30 (18%)	2	14
4	E	113/126 (90%)	100 (88%)	13 (12%)	6	28
5	F	87/112 (78%)	81 (93%)	6 (7%)	18	51
6	G	121/147 (82%)	109 (90%)	12 (10%)	9	34
7	H	103/105 (98%)	92 (89%)	11 (11%)	8	31
8	I	105/107 (98%)	94 (90%)	11 (10%)	8	32
9	J	86/90 (96%)	75 (87%)	11 (13%)	5	25
10	K	89/99 (90%)	77 (86%)	12 (14%)	4	24
11	L	102/104 (98%)	92 (90%)	10 (10%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	88/96 (92%)	77 (88%)	11 (12%)	5	26
13	N	74/84 (88%)	67 (90%)	7 (10%)	10	36
14	O	74/77 (96%)	68 (92%)	6 (8%)	14	44
15	P	65/65 (100%)	54 (83%)	11 (17%)	2	16
16	Q	74/78 (95%)	68 (92%)	6 (8%)	14	44
17	R	43/65 (66%)	37 (86%)	6 (14%)	4	23
18	S	66/79 (84%)	62 (94%)	4 (6%)	22	55
19	T	65/66 (98%)	55 (85%)	10 (15%)	3	19
20	B	194/199 (98%)	189 (97%)	5 (3%)	51	75
21	Z	234/286 (82%)	204 (87%)	30 (13%)	5	25
All	All	2124/2348 (90%)	1898 (89%)	226 (11%)	12	31

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	66	GLU
11	L	89	LEU
21	Z	195	GLN
9	J	80	THR
10	K	68	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
7	H	66	GLN
11	L	4	ASN
21	Z	62	HIS
10	K	39	ASN
10	K	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1486/1527 (97%)	735 (49%)	92 (6%)

5 of 735 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	8	A
1	A	9	G
1	A	10	A
1	A	14	U

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	615	G
1	A	804	U
1	A	1445	U
1	A	633	G
1	A	666	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	GGM	Z	402	21	29,34,45	2.20	9 (31%)	30,54,69	2.63	12 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GGM	Z	402	21	-	0/13/38/48	0/3/3/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	402	GGM	C2'-C1'	-4.06	1.47	1.53
23	Z	402	GGM	C3'-C2'	-3.08	1.45	1.53
23	Z	402	GGM	PG-N3B	2.13	1.69	1.63
23	Z	402	GGM	PG-O2G	2.29	1.63	1.56
23	Z	402	GGM	PB-O2B	2.55	1.49	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	402	GGM	N3-C2-N1	-6.09	118.57	127.46
23	Z	402	GGM	C1'-N9-C4	-4.68	118.54	126.64
23	Z	402	GGM	O1G-PG-N3B	-4.48	105.09	111.79
23	Z	402	GGM	C2'-C3'-C4'	-4.45	93.95	102.62
23	Z	402	GGM	C6-C5-C4	-3.06	117.80	120.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Z	402	GGM	32	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	195

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Mol	Chain	Number of breaks
21	Z	4
20	B	1
13	N	1
12	M	1

The worst 5 of 202 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1249:C	O3'	1250:A	P	3.76
1	A	646:G	O3'	647:C	P	3.66
1	A	886:G	O3'	887:G	P	3.56
1	A	1309:G	O3'	1310:G	P	3.30
1	A	317:U	O3'	318:G	P	3.28