



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:07 PM BST

PDB ID : 4ADV
EMDB ID: : EMD-2017
Title : Structure of the E. coli methyltransferase KsgA bound to the E. coli 30S ribosomal subunit
Authors : Boehringer, D.; O'Farrell, H.C.; Rife, J.P.; Ban, N.
Deposited on : 2012-01-03
Resolution : 13.50 Å(reported)
Based on PDB ID : 2AVY, 1QYR

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

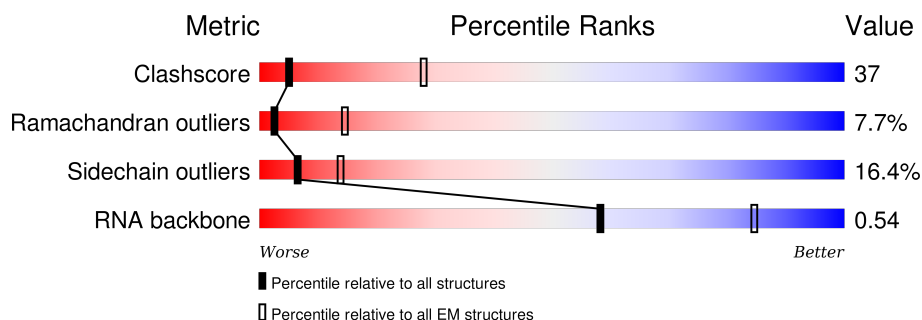
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	1542	<div> <div>23%</div> <div>55%</div> <div>13%</div> <div>9%</div> </div>
2	B	240	<div> <div>19%</div> <div>52%</div> <div>19%</div> <div>• 9%</div> </div>
3	C	232	<div> <div>27%</div> <div>48%</div> <div>13%</div> <div>• 11%</div> </div>
4	D	205	<div> <div>27%</div> <div>53%</div> <div>19%</div> <div>•</div> </div>
5	E	166	<div> <div>28%</div> <div>50%</div> <div>11%</div> <div>• 10%</div> </div>
6	F	135	<div> <div>24%</div> <div>37%</div> <div>11%</div> <div>• 26%</div> </div>
7	G	178	<div> <div>26%</div> <div>46%</div> <div>11%</div> <div>• 16%</div> </div>
8	H	129	<div> <div>40%</div> <div>50%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	129	
10	J	103	
11	K	128	
12	L	123	
13	M	117	
14	N	100	
15	O	89	
16	P	82	
17	Q	83	
18	R	74	
19	S	91	
20	T	86	
21	U	71	
22	V	252	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 50888 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	1410	Total	C	N	O	P	0	0
			30262	13496	5559	9797	1410		

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a protein called RIBOSOMAL RNA SMALL SUBUNIT METHYLTRANSFERASE A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	252	Total	C	N	O	S	0	0
			1949	1241	336	359	13		

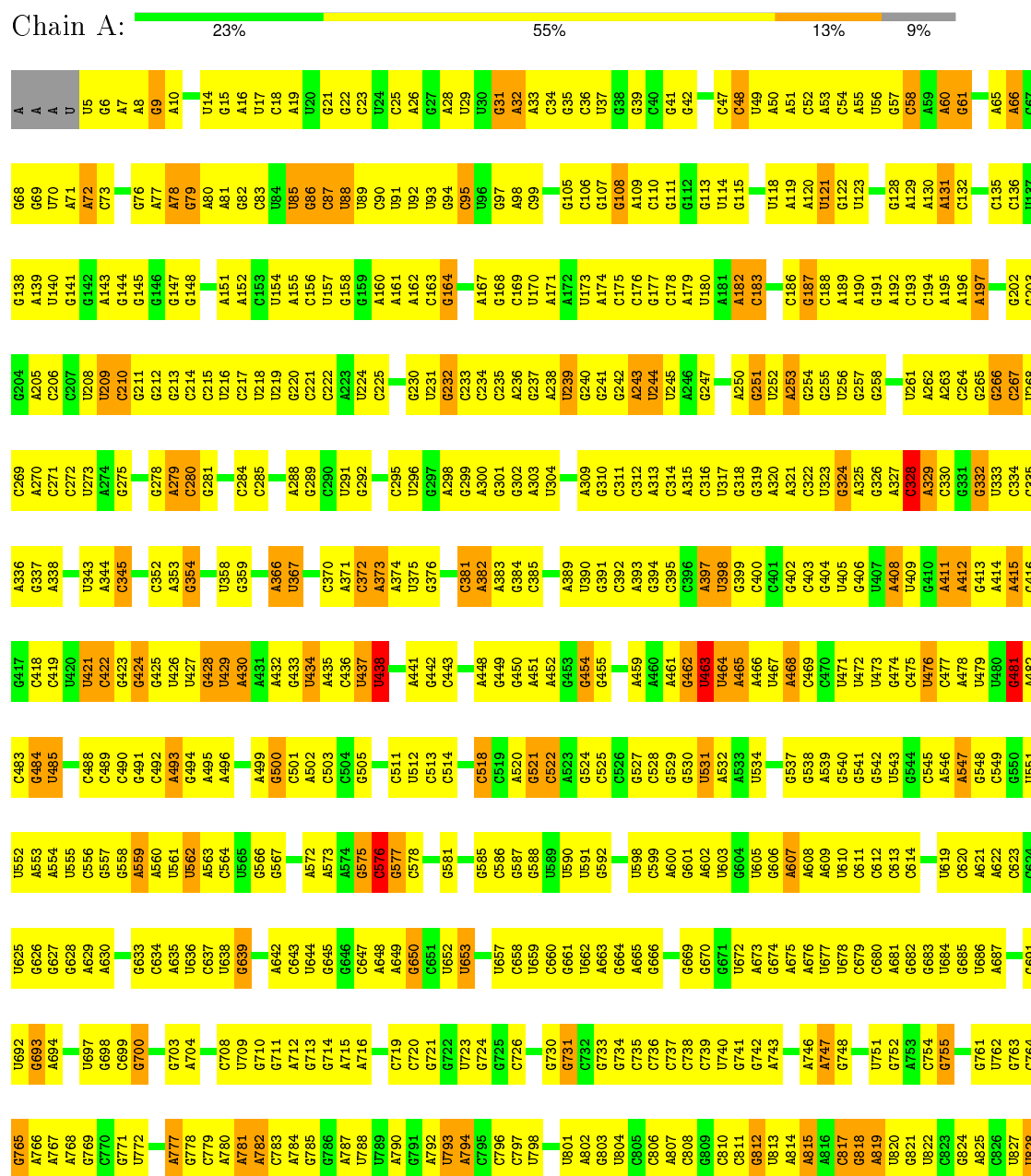
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	V	139	Total	O	0
			139	139	

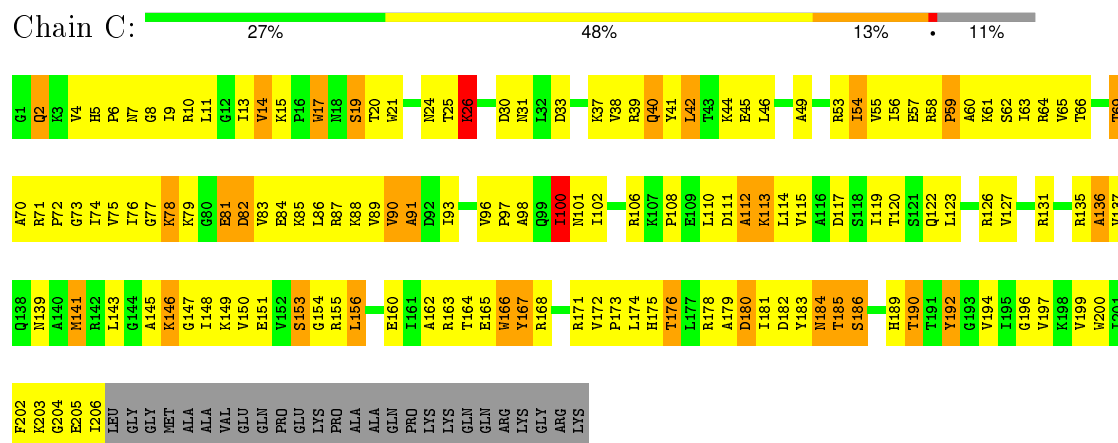
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

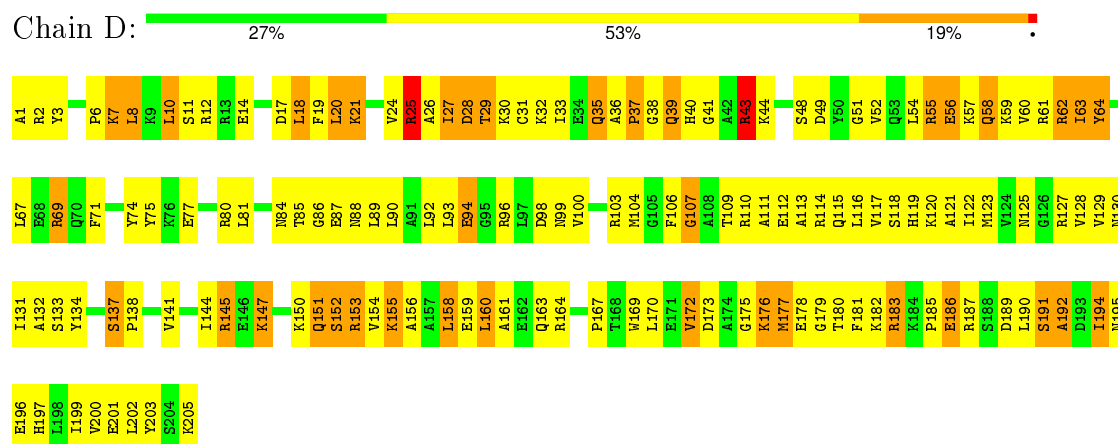
• Molecule 1: 16S RIBOSOMAL RNA



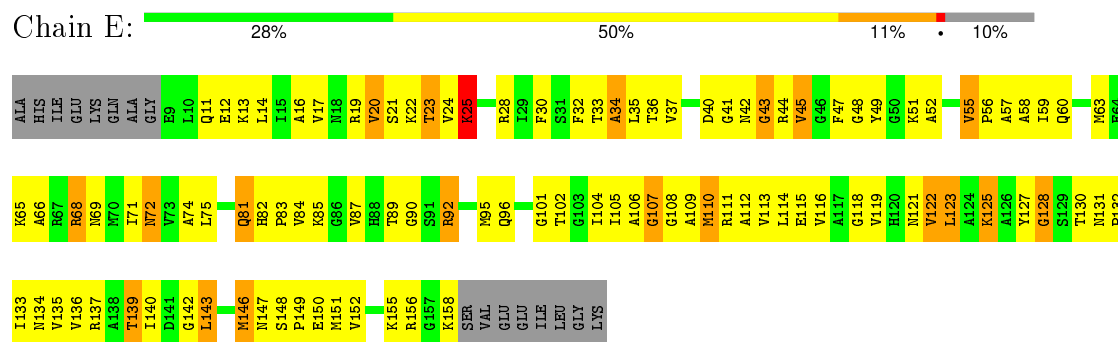
6829	6830	6831	6832	6833	6834	6835	6836	6837	6838	6839	6840	6841	6842	6843	6844	6845	6846	6847	6848	6849
6850	6851	6852	6853	6854	6855	6856	6857	6858	6859	6860	6861	6862	6863	6864	6865	6866	6867	6868	6869	6870
6871	6872	6873	6874	6875	6876	6877	6878	6879	6880	6881	6882	6883	6884	6885	6886	6887	6888	6889	6890	6891
6892	6893	6894	6895	6896	6897	6898	6899	6900	6901	6902	6903	6904	6905	6906	6907	6908	6909	6910	6911	6912
6913	6914	6915	6916	6917	6918	6919	6920	6921	6922	6923	6924	6925	6926	6927	6928	6929	6930	6931	6932	6933
6934	6935	6936	6937	6938	6939	6940	6941	6942	6943	6944	6945	6946	6947	6948	6949	6950	6951	6952	6953	6954
6955	6956	6957	6958	6959	6960	6961	6962	6963	6964	6965	6966	6967	6968	6969	6970	6971	6972	6973	6974	6975
6976	6977	6978	6979	6980	6981	6982	6983	6984	6985	6986	6987	6988	6989	6990	6991	6992	6993	6994	6995	6996
6997	6998	6999	7000	7001	7002	7003	7004	7005	7006	7007	7008	7009	7010	7011	7012	7013	7014	7015	7016	7017
7018	7019	7020	7021	7022	7023	7024	7025	7026	7027	7028	7029	7030	7031	7032	7033	7034	7035	7036	7037	7038
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7228	7229	7230	7231	7232	7233	7234	7235	7236	7237	7238	7239	7240	7241	7242	7243	7244	7245	7246	7247	7248
7249	7250	7251	7252	7253	7254	7255	7256	7257	7258	7259	7260	7261	7262	7263	7264	7265	7266	7267	7268	7269
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7312	7313	7314	7315	7316	7317	7318	7319	7320	7321	7322	7323	7324	7325	7326	7327	7328	7329	7330	7331	7332
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7396	7397	7398	7399	7400	7401	7402	7403	7404	7405	7406	7407	7408	7409	7410	7411	7412	7413	7414	7415	7416
7417	7418	7419	7420	7421	7422	7423	7424	7425	7426	7427	7428	7429	7430	7431	7432	7433	7434	7435	7436	7437
7438	7439	7440	7441	7442	7443	7444	7445	7446	7447	7448	7449	7450	7451	7452	7453	7454	7455	7456	7457	7458
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7606	7607	7608	7609	7610	7611	7612	7613	7614	7615	7616	7617	7618	7619	7620	7621	7622	7623	7624	7625	7626
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7942	7943	7944	7945	7946	7947	7948	7949	7950	7951	7952	7953	7954	7955	7956	7957	7958	7959	7960	7961	7962
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7984	7985	7986	7987	7988	7989	7990	7991	7992	7993	7994	7995	7996	7997	7998	7999	8000	8001	8002	8003	8004
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8047	8048	8049	8050	8051	8052	8053	8054	8055	8056	8057	8058	8059	8060	8061	8062	8063	8064	8065	8066	8067
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8152	8153	8154																		



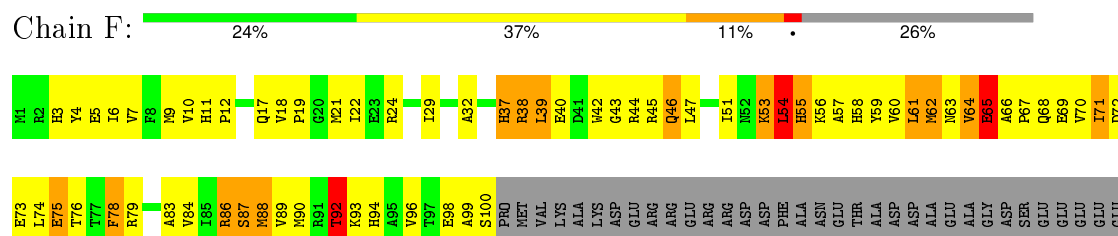
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 5: 30S RIBOSOMAL PROTEIN S5



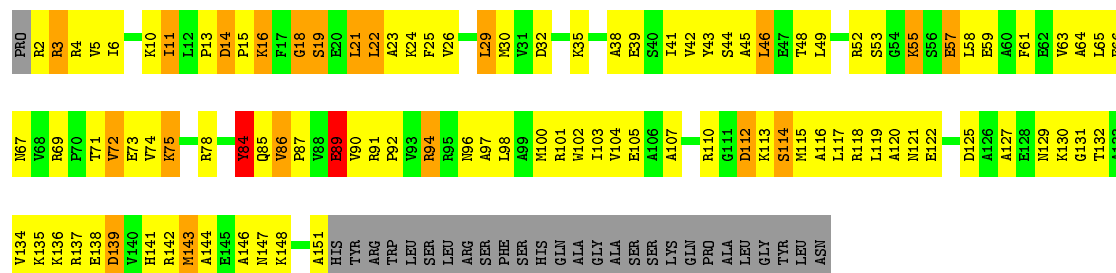
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



GLU

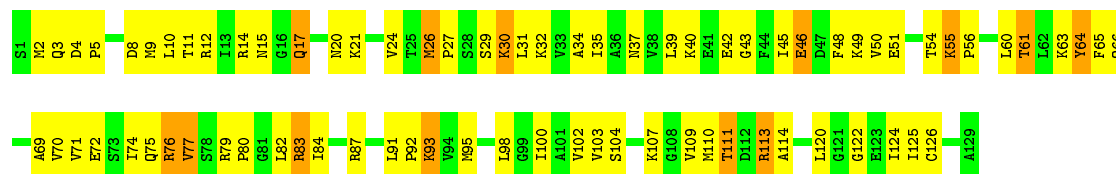
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



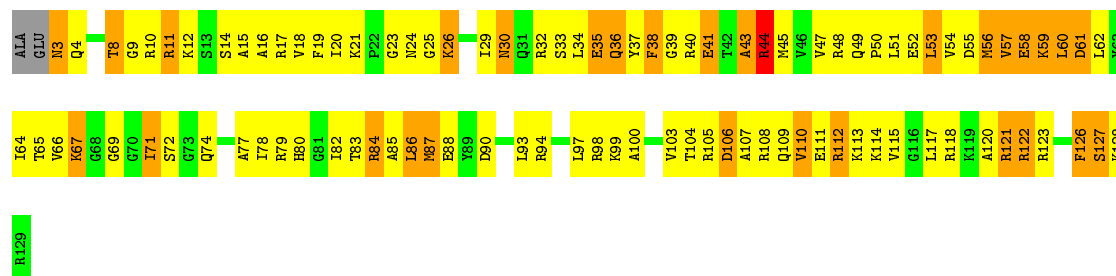
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H: 40% 50% 10%



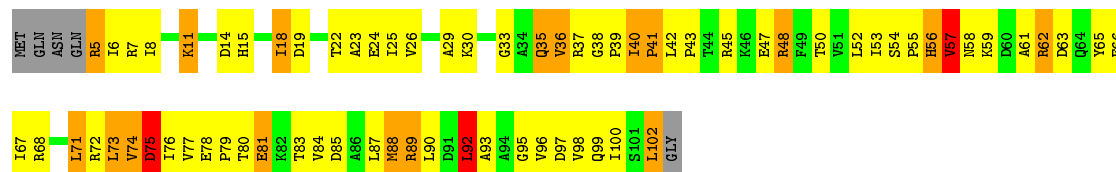
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I: 22% 53% 22% 3%



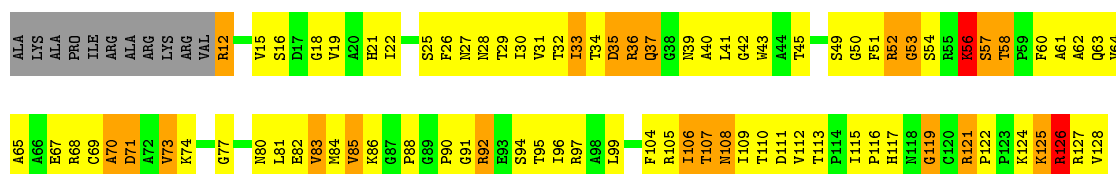
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J: 25% 50% 17% • 5%



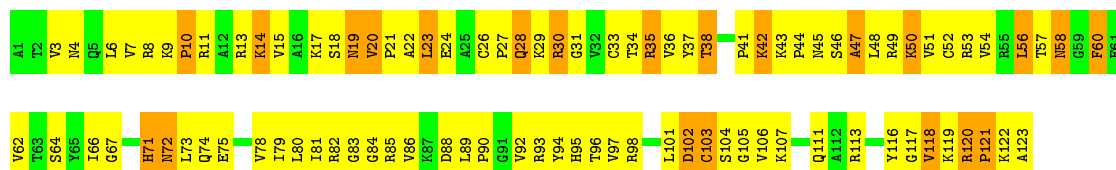
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K: 24% 49% 16% 9%



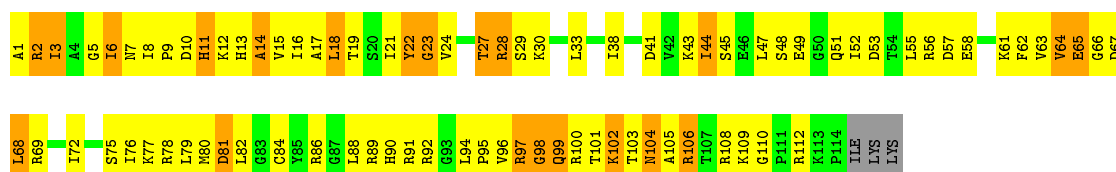
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 24% 59% 18%



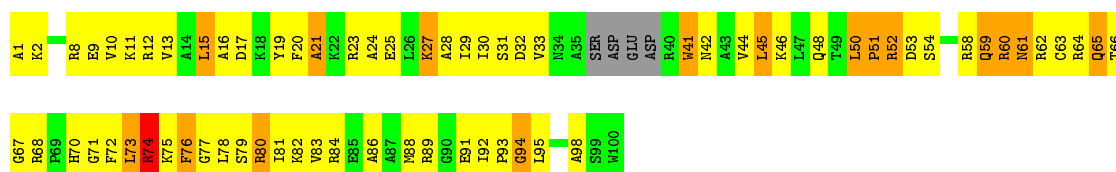
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 26% 54% 18%



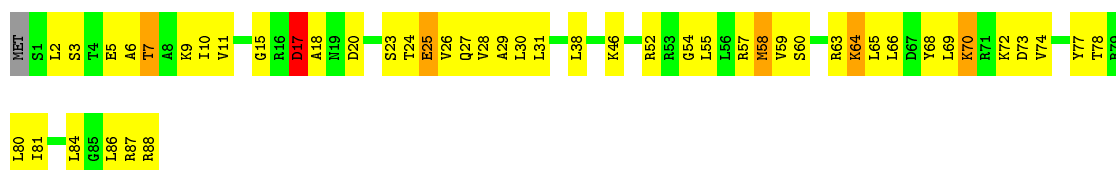
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N: 26% 53% 16%



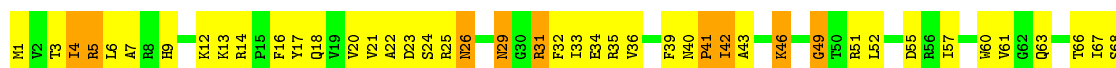
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O: 45% 47% 6%



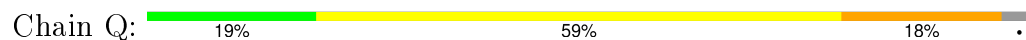
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 35% 54% 11%





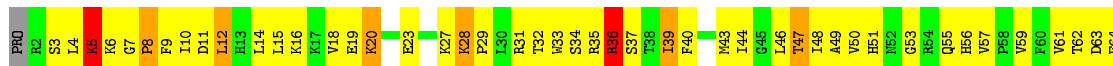
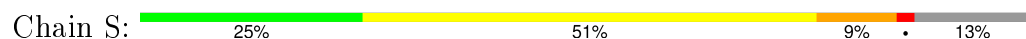
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



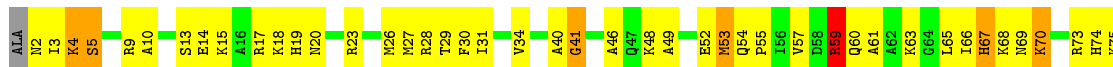
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



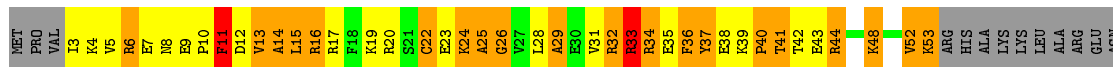
• Molecule 19: 30S RIBOSOMAL PROTEIN S19




• Molecule 20: 30S RIBOSOMAL PROTEIN S20

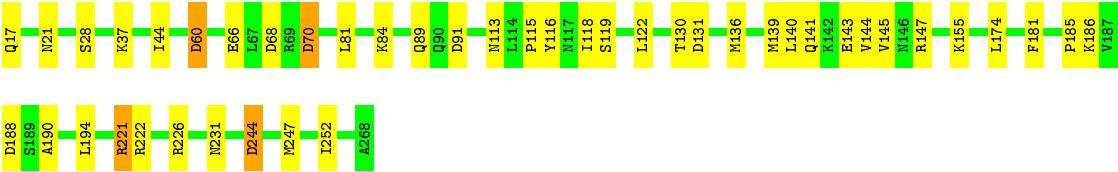


• Molecule 21: 30S RIBOSOMAL PROTEIN S21



● Molecule 22: RIBOSOMAL RNA SMALL SUBUNIT METHYLTRANSFERASE A

Chain V:  83% 16% ●



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER IMAGE, CTFFIND3	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	62000	Depositor
Image detector	GATAN US4000	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.27	2/33885 (0.0%)	0.75	7/52858 (0.0%)
10	J	0.23	0/796	0.49	0/1077
11	K	0.24	0/893	0.46	0/1205
12	L	0.22	0/969	0.47	0/1300
13	M	0.21	0/892	0.48	0/1193
14	N	0.25	0/785	0.46	0/1043
15	O	0.23	0/724	0.45	0/966
16	P	0.26	0/659	0.44	0/884
17	Q	0.24	0/657	0.46	0/881
18	R	0.23	0/462	0.46	0/621
19	S	0.25	0/652	0.46	0/877
2	B	0.25	0/1735	0.47	0/2338
20	T	0.24	0/671	0.41	0/888
21	U	1.01	4/430 (0.9%)	0.74	2/570 (0.4%)
22	V	0.62	0/1991	0.80	7/2710 (0.3%)
3	C	0.23	0/1651	0.45	0/2225
4	D	0.23	0/1665	0.46	0/2227
5	E	0.23	0/1118	0.45	0/1504
6	F	0.25	0/835	0.48	0/1128
7	G	0.23	0/1187	0.44	0/1591
8	H	0.23	0/989	0.45	0/1326
9	I	0.24	0/1034	0.45	0/1375
All	All	0.29	6/54680 (0.0%)	0.68	16/80787 (0.0%)

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	0	15
21	U	0	1
All	All	0	16

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	15	LEU	C-N	-15.01	0.99	1.34
21	U	25	ALA	C-N	-9.28	1.16	1.33
1	A	463	U	O3'-P	-6.70	1.53	1.61
21	U	29	ALA	C-N	6.63	1.49	1.34
21	U	11	PHE	C-N	-5.36	1.21	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	G	N9-C1'-C2'	-8.16	103.02	112.00
22	V	221	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	438	U	N1-C1'-C2'	-6.29	105.08	112.00
22	V	221	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	232	G	C5'-C4'-C3'	-6.21	106.07	116.00

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	281	G	Sidechain
1	A	437	U	Sidechain
1	A	438	U	Sidechain
1	A	58	C	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	30262	0	15198	1460	0
2	B	1704	0	1720	428	0
3	C	1624	0	1699	158	0
4	D	1643	0	1710	176	0
5	E	1105	0	1145	170	0
6	F	817	0	808	76	0
7	G	1174	0	1230	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	979	0	1032	81	0
9	I	1022	0	1070	141	0
10	J	786	0	828	96	0
11	K	877	0	887	107	0
12	L	955	0	1019	103	0
13	M	883	0	944	84	0
14	N	774	0	827	92	0
15	O	716	0	742	50	0
16	P	649	0	666	78	0
17	Q	648	0	691	81	0
18	R	455	0	478	39	0
19	S	637	0	665	78	0
20	T	665	0	714	53	0
21	U	425	0	447	102	0
22	V	1949	0	1949	46	0
23	V	139	0	0	11	0
All	All	50888	0	36469	3247	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 37.

The worst 5 of 3247 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:870:U:C6	2:B:27:LYS:HD3	1.28	1.64
1:A:829:G:C3'	2:B:30:ILE:HG12	1.18	1.62
1:A:830:G:C4	2:B:22:TRP:HB3	1.40	1.53
1:A:17:U:C5'	1:A:1079:G:H5'	1.39	1.49
1:A:830:G:C5	2:B:22:TRP:HB3	1.47	1.49

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	B	216/240 (90%)	145 (67%)	53 (24%)	18 (8%)	1	18
3	C	204/232 (88%)	135 (66%)	49 (24%)	20 (10%)	1	14
4	D	203/205 (99%)	130 (64%)	55 (27%)	18 (9%)	1	17
5	E	148/166 (89%)	108 (73%)	33 (22%)	7 (5%)	3	32
6	F	98/135 (73%)	69 (70%)	23 (24%)	6 (6%)	2	26
7	G	148/178 (83%)	103 (70%)	37 (25%)	8 (5%)	2	29
8	H	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	7	47
9	I	125/129 (97%)	86 (69%)	28 (22%)	11 (9%)	1	17
10	J	96/103 (93%)	63 (66%)	21 (22%)	12 (12%)	0	8
11	K	115/128 (90%)	75 (65%)	27 (24%)	13 (11%)	0	10
12	L	121/123 (98%)	74 (61%)	30 (25%)	17 (14%)	0	6
13	M	112/117 (96%)	87 (78%)	14 (12%)	11 (10%)	1	14
14	N	92/100 (92%)	59 (64%)	24 (26%)	9 (10%)	1	14
15	O	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	8	48
16	P	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	3	31
17	Q	78/83 (94%)	48 (62%)	26 (33%)	4 (5%)	2	30
18	R	53/74 (72%)	27 (51%)	19 (36%)	7 (13%)	0	7
19	S	77/91 (85%)	57 (74%)	14 (18%)	6 (8%)	1	20
20	T	83/86 (96%)	69 (83%)	8 (10%)	6 (7%)	1	22
21	U	49/71 (69%)	22 (45%)	12 (24%)	15 (31%)	0	0
22	V	250/252 (99%)	247 (99%)	2 (1%)	1 (0%)	39	80
All	All	2561/2813 (91%)	1834 (72%)	529 (21%)	198 (8%)	2	20

5 of 198 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	19	THR
2	B	22	TRP
2	B	163	ILE
2	B	186	VAL
3	C	2	GLN

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	B	180/198 (91%)	142 (79%)	38 (21%)	1	9
3	C	170/189 (90%)	142 (84%)	28 (16%)	3	19
4	D	172/172 (100%)	140 (81%)	32 (19%)	2	14
5	E	113/125 (90%)	92 (81%)	21 (19%)	2	14
6	F	87/116 (75%)	68 (78%)	19 (22%)	1	9
7	G	123/146 (84%)	102 (83%)	21 (17%)	2	17
8	H	104/104 (100%)	87 (84%)	17 (16%)	3	20
9	I	105/106 (99%)	83 (79%)	22 (21%)	1	9
10	J	86/90 (96%)	66 (77%)	20 (23%)	1	7
11	K	90/98 (92%)	70 (78%)	20 (22%)	1	9
12	L	103/103 (100%)	88 (85%)	15 (15%)	4	24
13	M	92/95 (97%)	70 (76%)	22 (24%)	1	7
14	N	79/83 (95%)	67 (85%)	12 (15%)	3	22
15	O	76/77 (99%)	69 (91%)	7 (9%)	11	43
16	P	65/65 (100%)	56 (86%)	9 (14%)	4	27
17	Q	74/77 (96%)	60 (81%)	14 (19%)	2	13
18	R	48/64 (75%)	45 (94%)	3 (6%)	22	59
19	S	70/78 (90%)	60 (86%)	10 (14%)	4	25
20	T	65/65 (100%)	56 (86%)	9 (14%)	4	27
21	U	44/61 (72%)	36 (82%)	8 (18%)	2	15
22	V	213/216 (99%)	206 (97%)	7 (3%)	45	76
All	All	2159/2328 (93%)	1805 (84%)	354 (16%)	6	19

5 of 354 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	17	GLN
10	J	5	ARG

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Mol	Chain	Res	Type
19	S	47	THR
8	H	48	PHE
9	I	30	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	121	ASN
9	I	30	ASN
19	S	51	HIS
7	G	147	ASN
8	H	20	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1407/1542 (91%)	261 (18%)	24 (1%)

5 of 261 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	9	G
1	A	14	U
1	A	31	G
1	A	32	A

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	576	C
1	A	975	A
1	A	1302	C
1	A	913	A
1	A	960	U

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.