wwPDB EM Validation Summary Report (i)

Apr 29, 2024 – 07:16 pm BST

PDB ID	:	5AKA
EMDB ID	:	EMD-2917
Title	:	EM structure of ribosome-SRP-FtsY complex in closed state
Authors	:	von Loeffelholz, O.; Jiang, Q.; Ariosa, A.; Karuppasamy, M.; Huard, K.; Berger, I.; Shan, S.; Schaffitzel, C.
Deposited on	:	2015-03-03
Resolution	:	5.70 Å(reported)

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

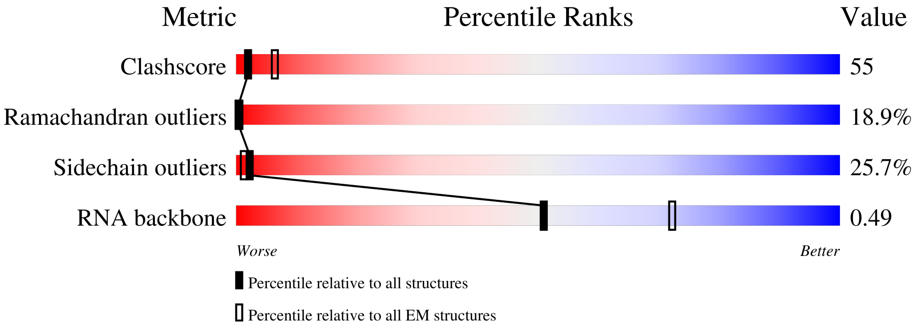
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

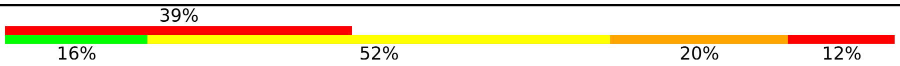
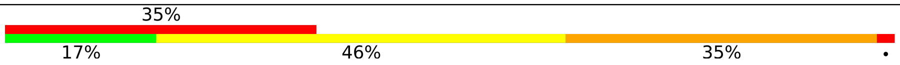
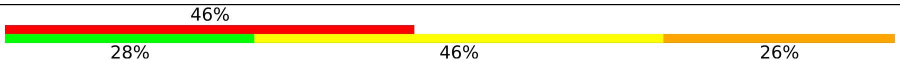
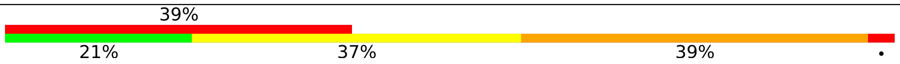
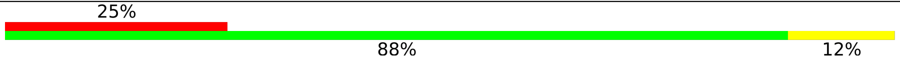
The reported resolution of this entry is 5.70 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	56	 39% 16% 52% 20% 12%
2	1	54	 35% 17% 46% 35% •
3	2	46	 46% 28% 46% 26%
4	3	64	 67% 23% 42% 33% •
5	4	38	 39% 21% 37% 39% •
6	5	109	 49% 44% 50% 6%
7	6	8	 25% 88% 12%

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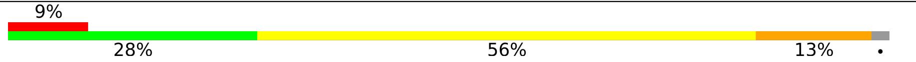
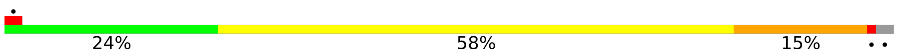
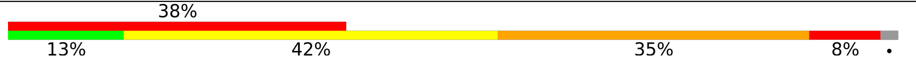
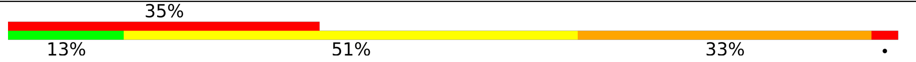
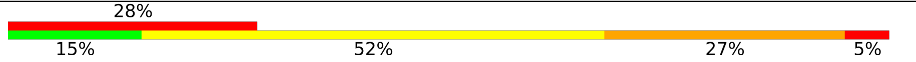
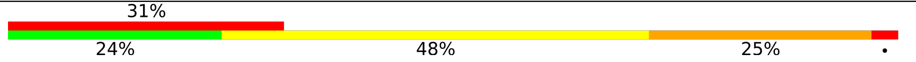
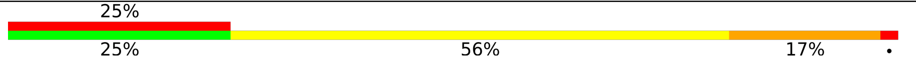
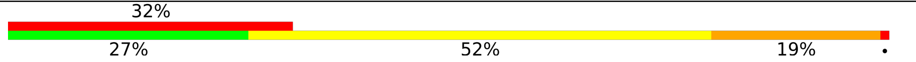
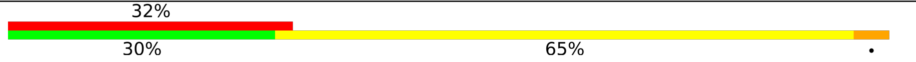
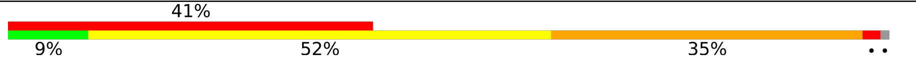
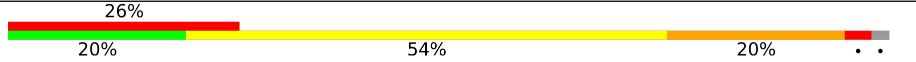
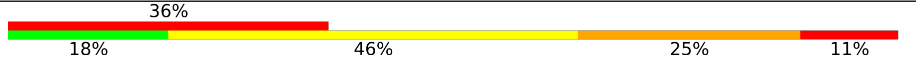
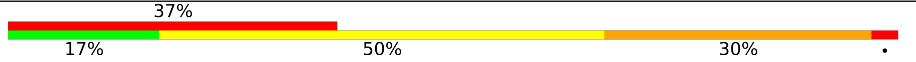
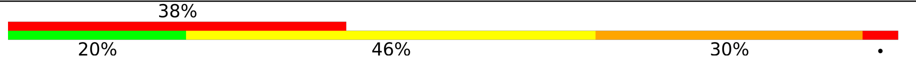
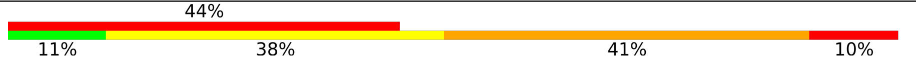
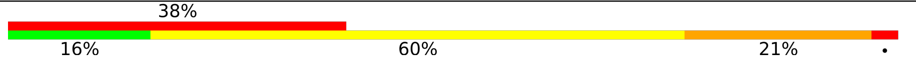
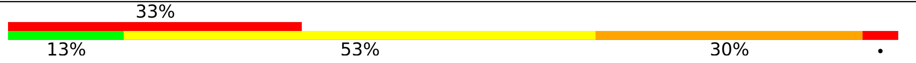
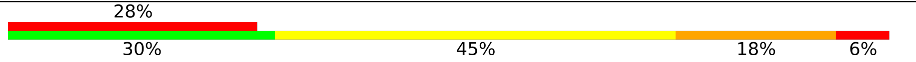
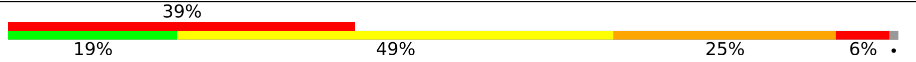
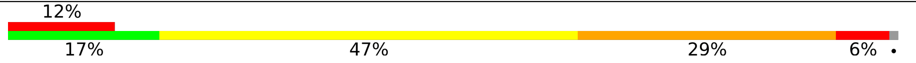
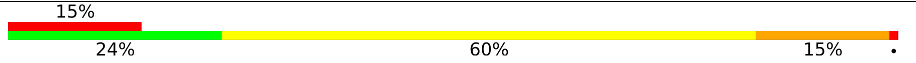
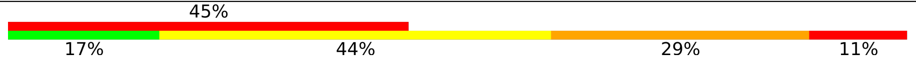
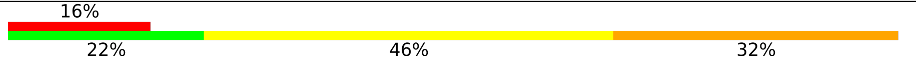
Mol	Chain	Length	Quality of chain
8	7	74	
9	A	120	
10	B	2904	
11	C	273	
12	D	209	
13	E	201	
14	F	178	
15	G	176	
16	H	149	
17	I	141	
18	J	142	
19	K	123	
20	L	144	
21	M	136	
22	N	127	
23	O	117	
24	P	114	
25	Q	117	
26	R	103	
27	S	110	
28	T	100	
29	U	103	
30	V	94	
31	W	84	
32	X	63	

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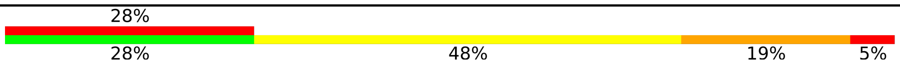
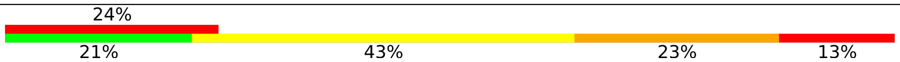
Mol	Chain	Length	Quality of chain
33	Y	58	
34	Z	70	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 92737 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 protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	56	444	269	94	80	1	0	0

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	54	441	284	81	76	0	0

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	109	850	523	159	153	15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	406	SER	CYS	conflict	UNP P0AGD7

- Molecule 7 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	6	8	41	24	8	9	0	0

- Molecule 8 is a RNA chain called 4.5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	7	74	1591	709	298	511	73	0	0

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A	117	2507	1116	459	815	117	0	0

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	B	2841	60995	27210	11229	19715	2841	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2798	U	UNK	conflict	GB 731469900
B	2800	A	UNK	conflict	GB 731469900

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	267	2053	1271	416	359	7	0	0

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	209	1565	979	288	294	4	0	0

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	201	1552	974	283	290	5	0	0

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	178	1420	905	251	258	6	0	0

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	176	1323	832	243	246	2	0	0

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	149	1111	699	197	214	1	0	0

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	141	1032	651	179	196	6	0	0

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	140	1112	704	210	194	4	0	0

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	121	Total 930	C 582	N 179	O 164	S 5	0	0

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	138	Total 1002	C 623	N 197	O 181	S 1	0	0

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	136	Total 1074	C 686	N 205	O 177	S 6	0	0

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	127	Total 1008	C 621	N 204	O 178	S 5	0	0

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	117	Total 900	C 557	N 179	O 163	S 1	0	0

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	114	Total 917	C 574	N 179	O 163	S 1	0	0

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Q	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	103	816	516	153	145	2	0	0

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S	110	857	532	166	156	3	0	0

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	99	777	491	145	139	2	0	0

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	U	102	779	492	146	141	0	0

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	94	753	479	137	134	3	0	0

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	84	634	391	129	113	1	0	0

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X	63	509	313	99	95	2	0	0

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y	58	449	281	87	79	2	0	0

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Z	70	549	339	104	100	6	0	0

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
35	B	110	110	110	0

- Molecule 36 is water.

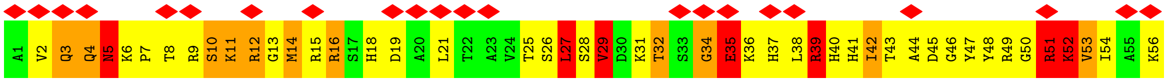
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	B	497	497	497	0
			Total	O	
36	C	1	1	1	0
			Total	O	
36	E	5	5	5	0
			Total	O	
36	L	2	2	2	0
			Total	O	
36	N	1	1	1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

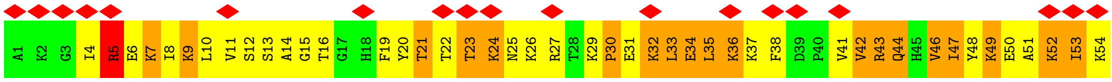
- Molecule 1: 50S RIBOSOMAL PROTEIN L32

Chain 0:



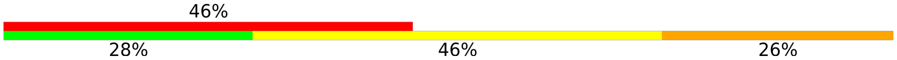
- Molecule 2: 50S RIBOSOMAL PROTEIN L33

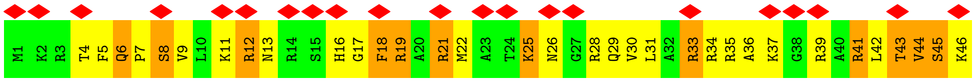
Chain 1:



- Molecule 3: 50S RIBOSOMAL PROTEIN L34

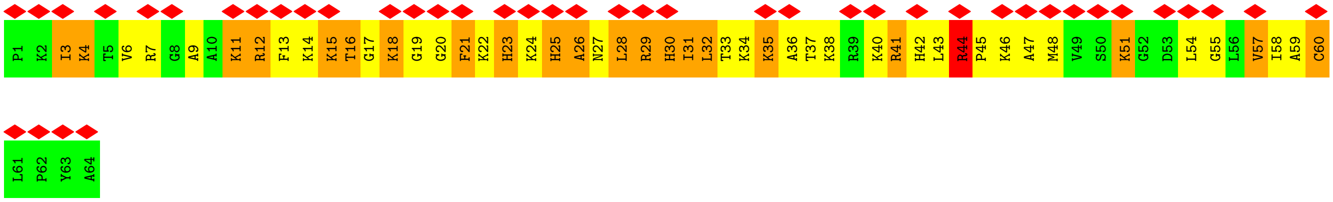
Chain 2:





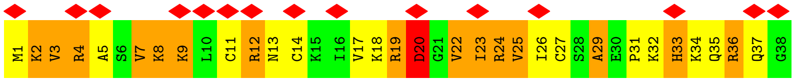
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:



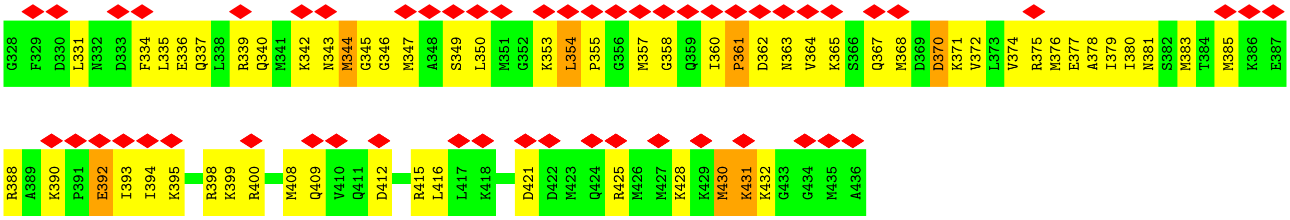
- Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain 4:



- Molecule 6: SIGNAL RECOGNITION PARTICLE PROTEIN

Chain 5:



- Molecule 7: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

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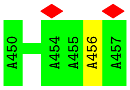

- Molecule 8: 4.5S ribosomal RNA

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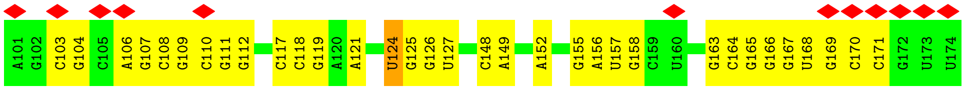

- Molecule 9: 5S ribosomal RNA

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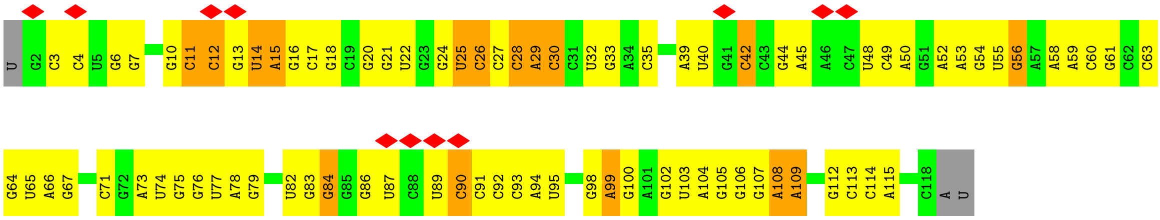

- Molecule 10: 23S ribosomal RNA

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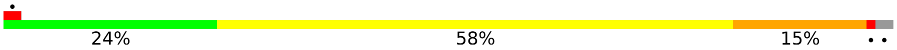

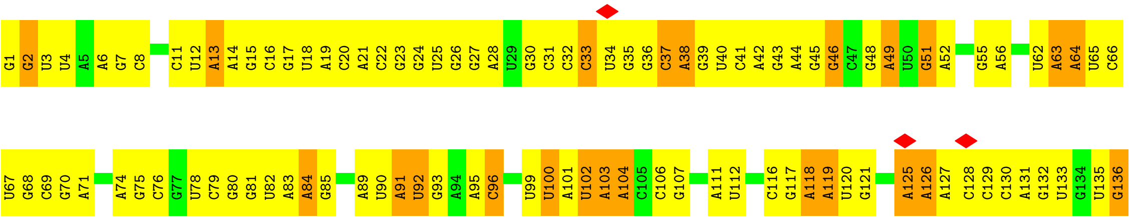

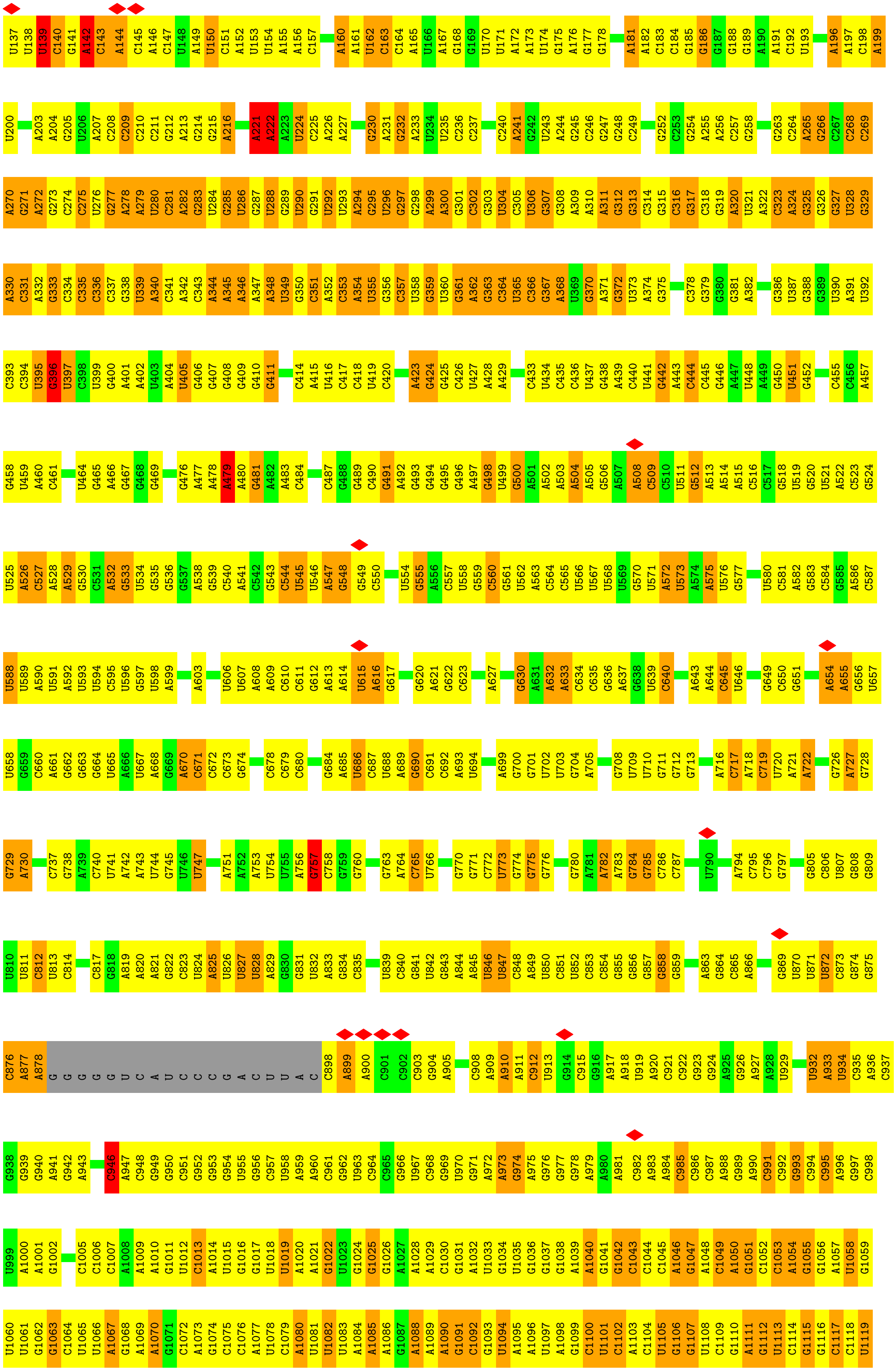
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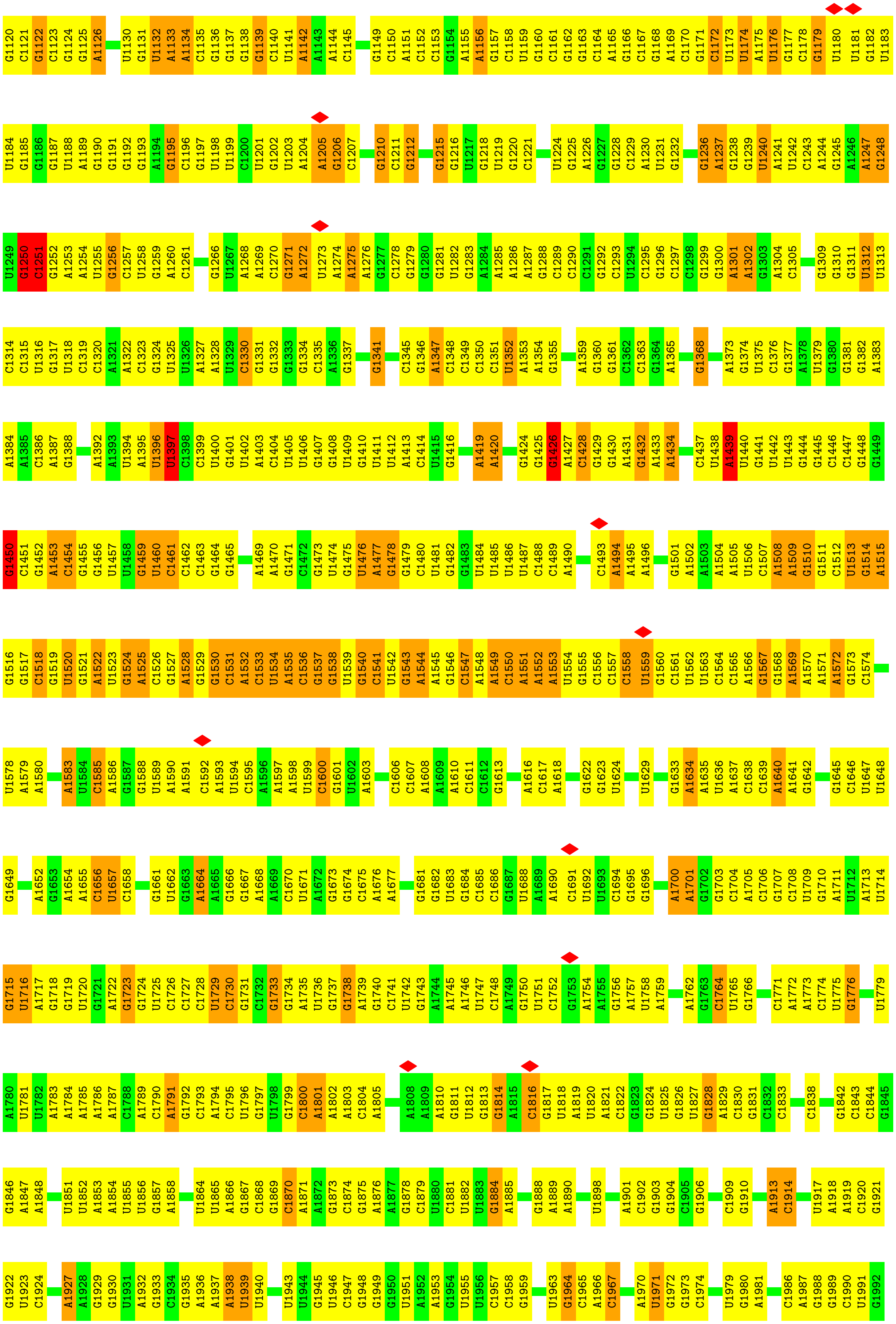
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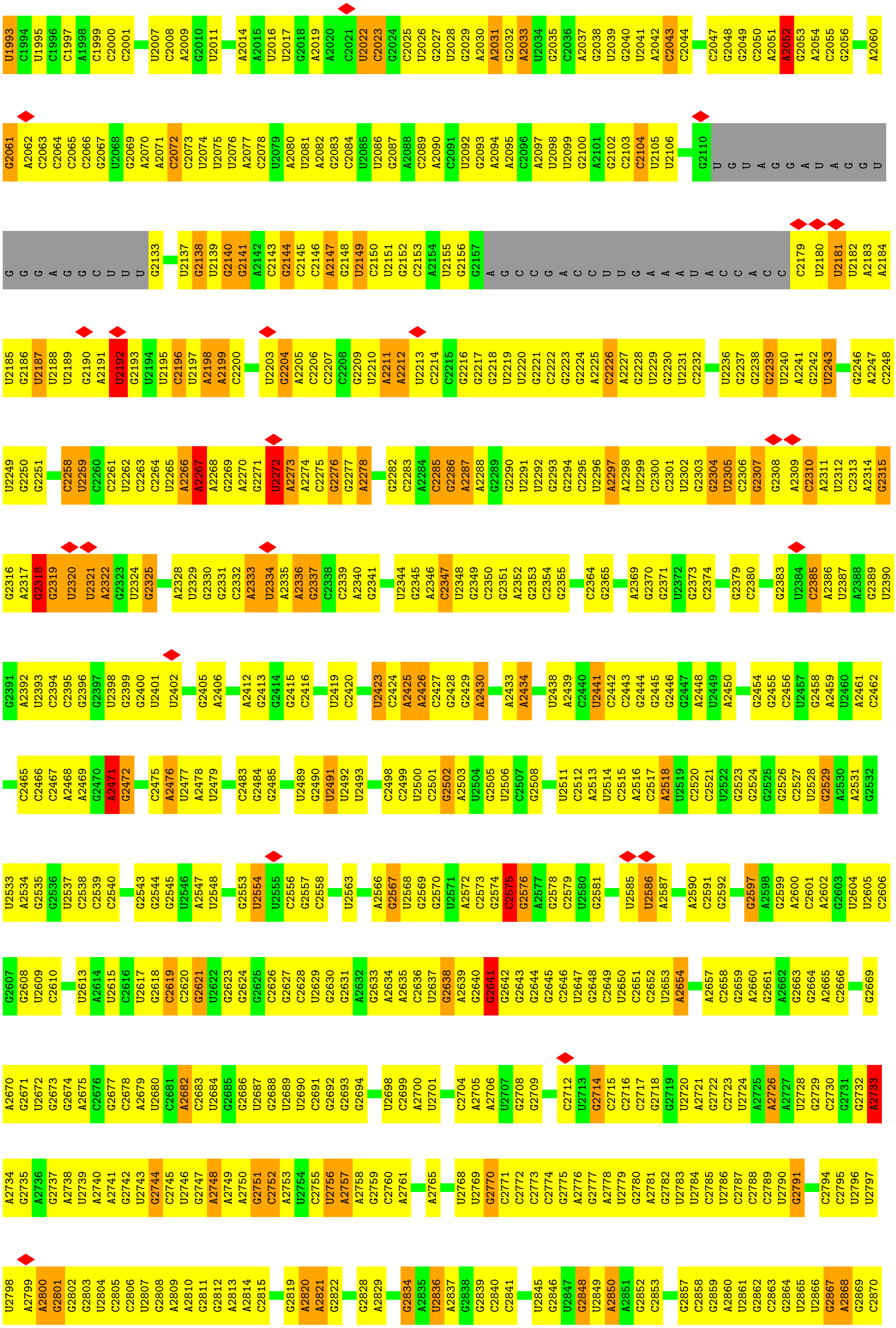
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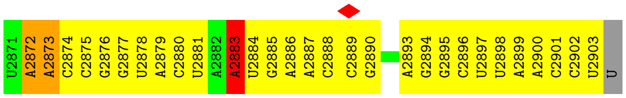
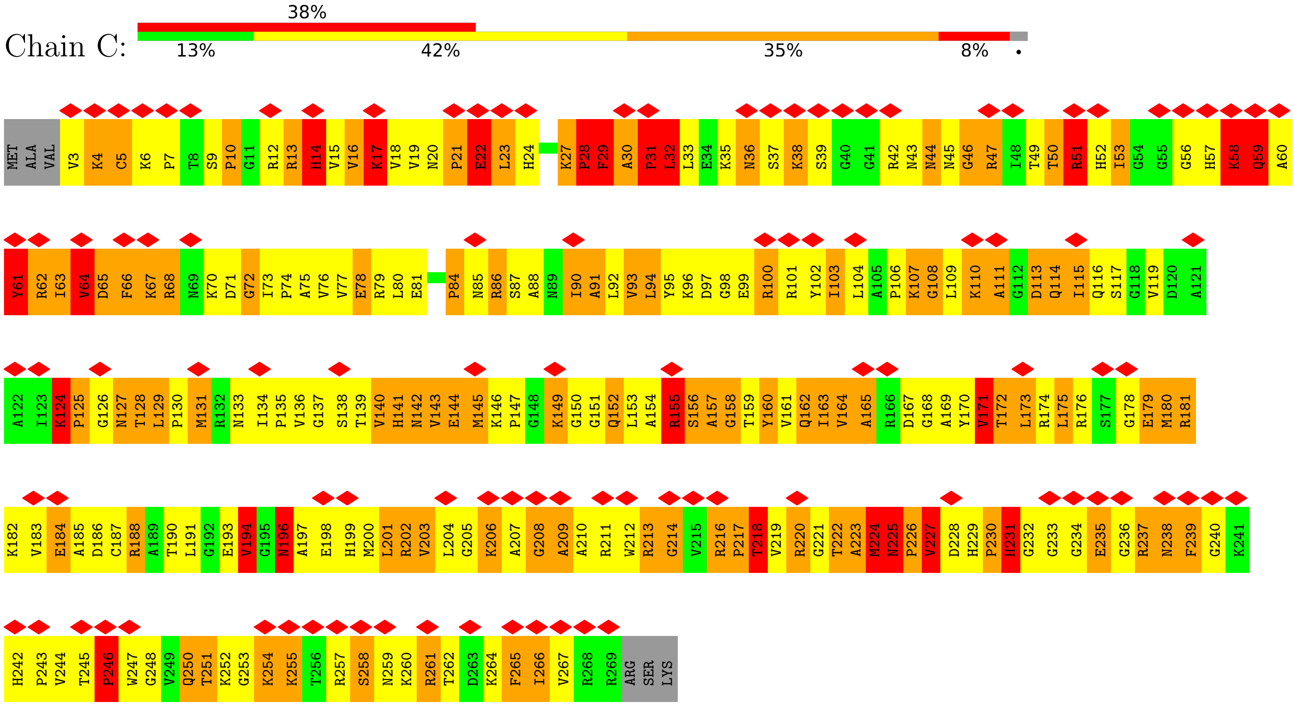
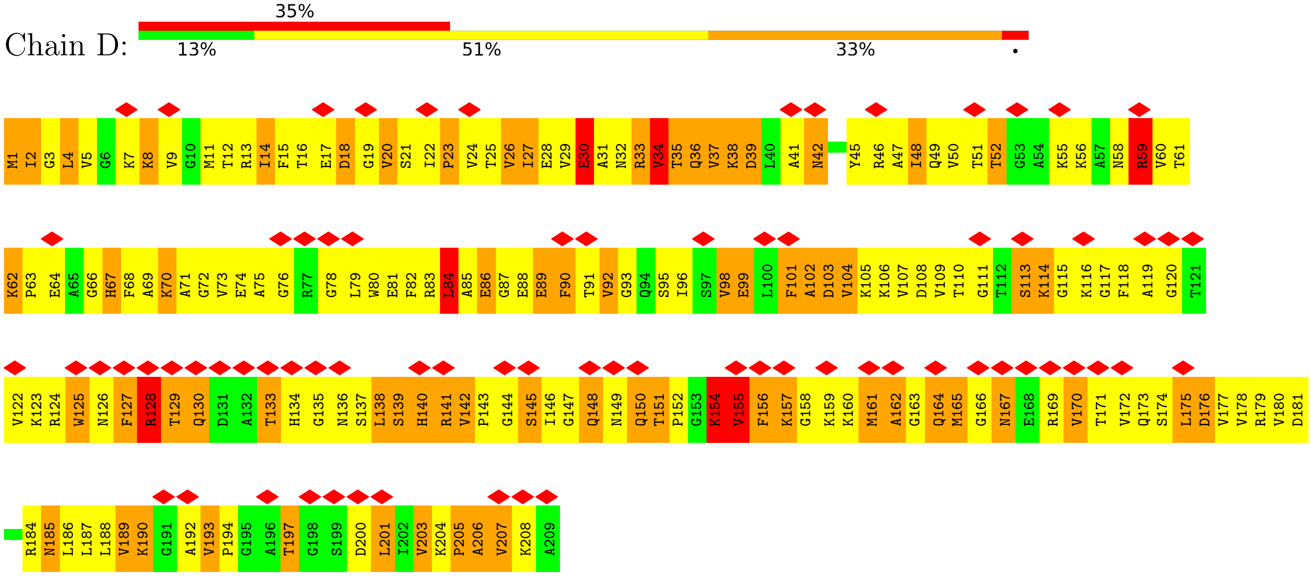


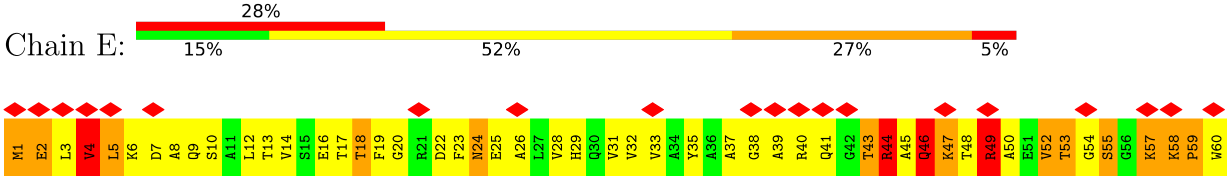
- Molecule 11: 50S RIBOSOMAL PROTEIN L2

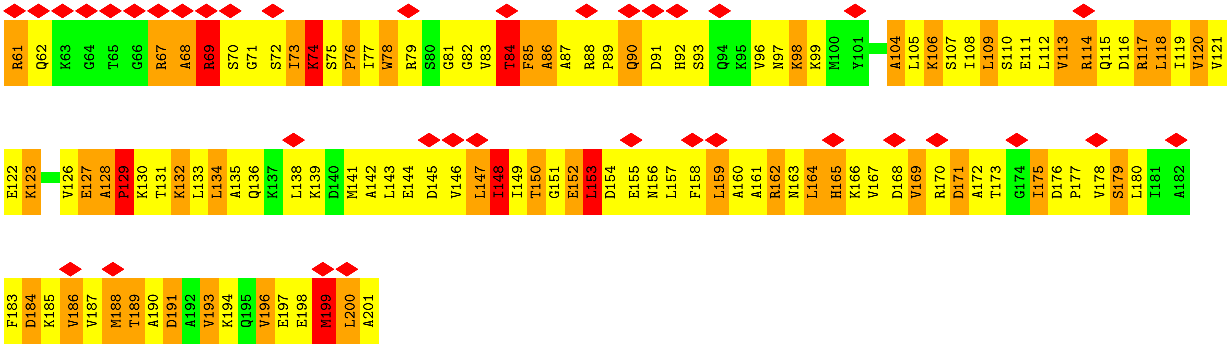


- Molecule 12: 50S RIBOSOMAL PROTEIN L3



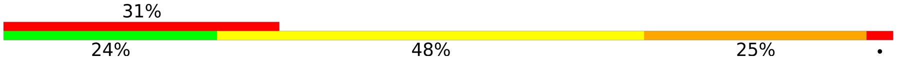
- Molecule 13: 50S RIBOSOMAL PROTEIN L4

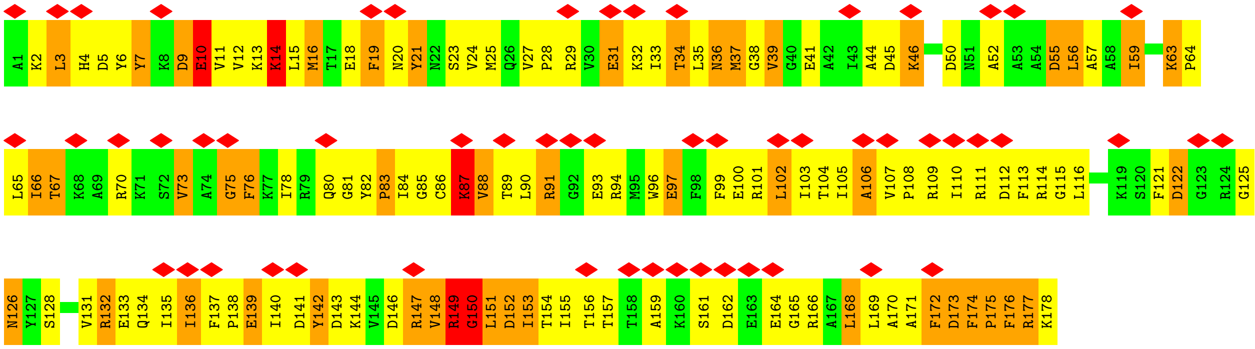




- Molecule 14: 50S RIBOSOMAL PROTEIN L5

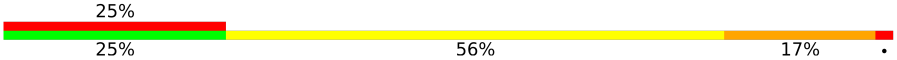
Chain F:

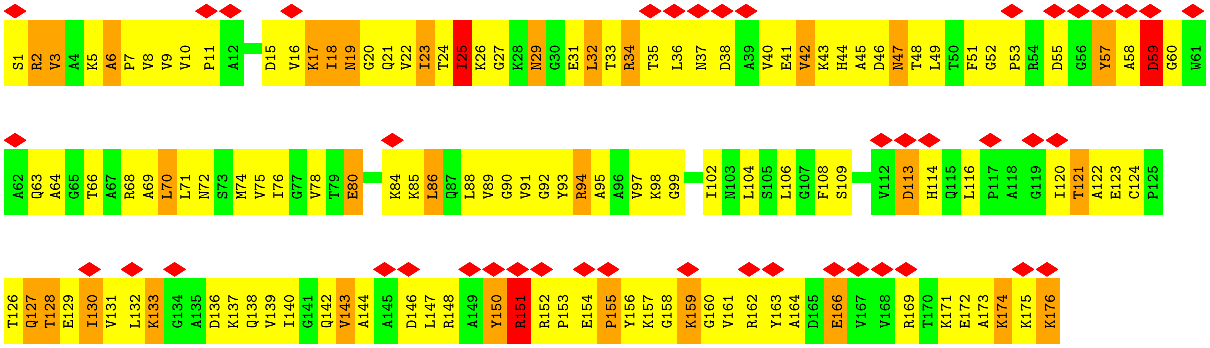




- Molecule 15: 50S RIBOSOMAL PROTEIN L6

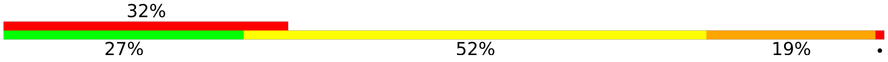
Chain G:

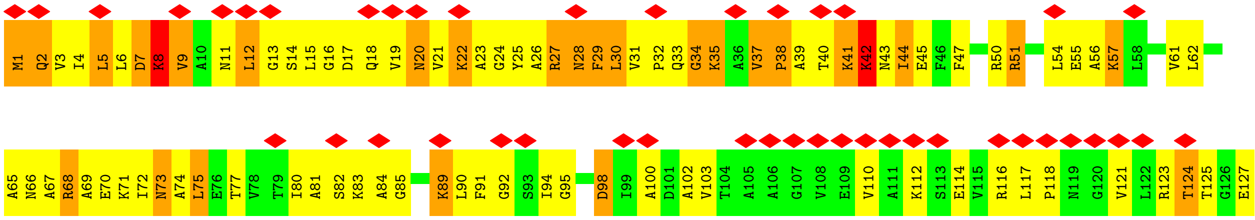




- Molecule 16: 50S RIBOSOMAL PROTEIN L9

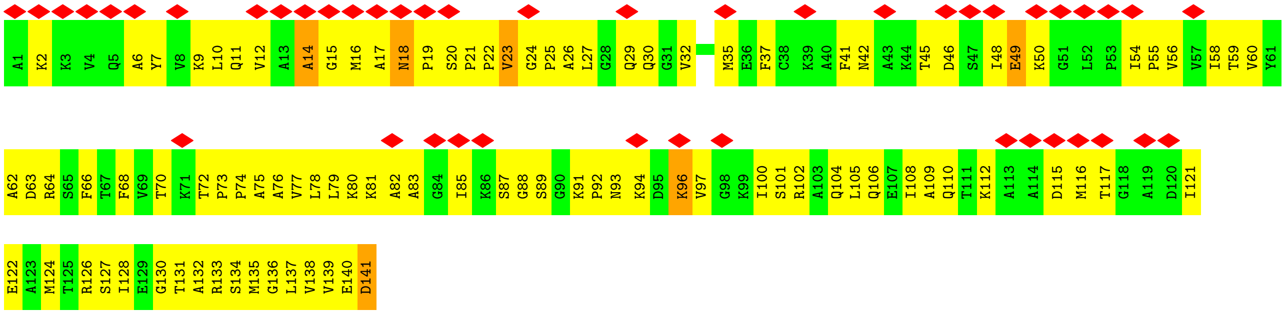
Chain H:





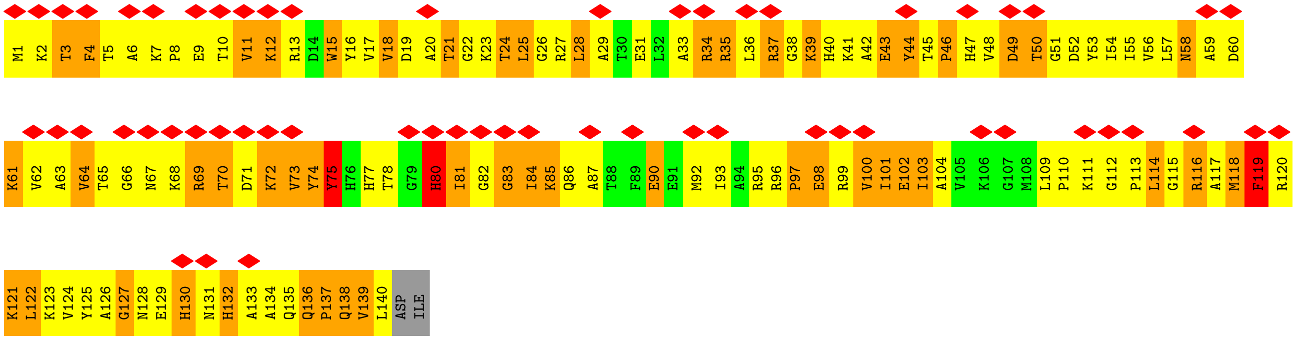
- Molecule 17: 50S RIBOSOMAL PROTEIN L11

Chain I:



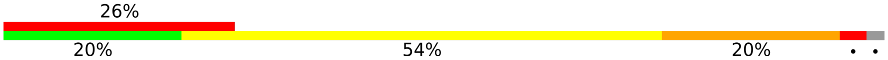
- Molecule 18: 50S RIBOSOMAL PROTEIN L13

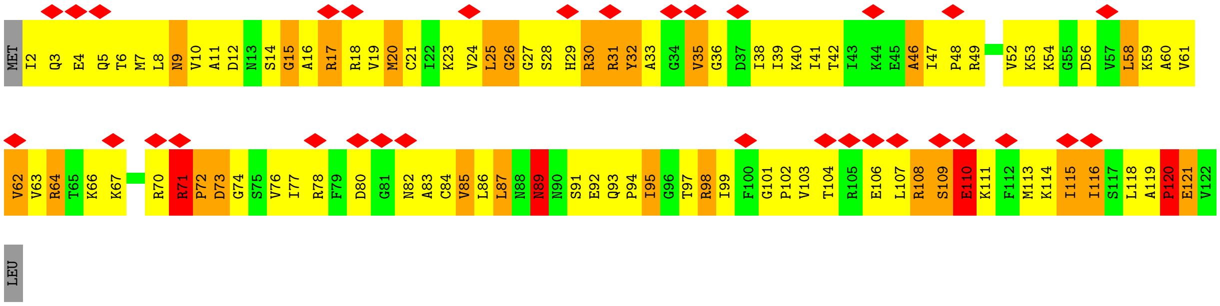
Chain J:



- Molecule 19: 50S RIBOSOMAL PROTEIN L14

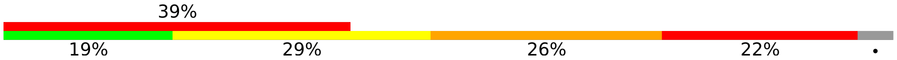
Chain K:

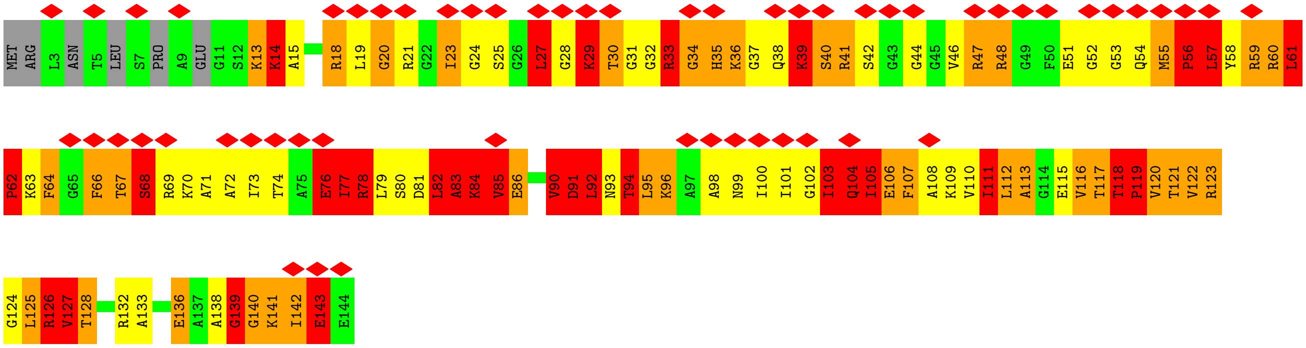




- Molecule 20: 50S RIBOSOMAL PROTEIN L15

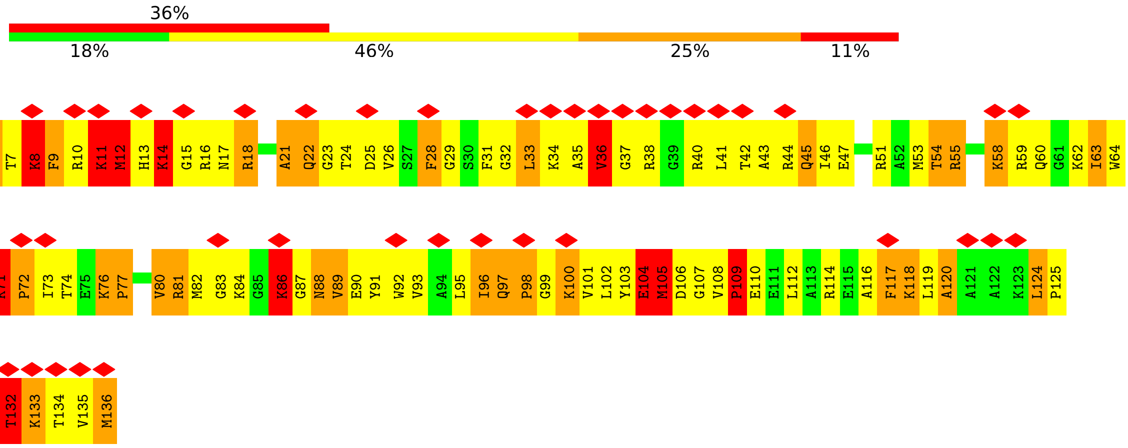
Chain L:





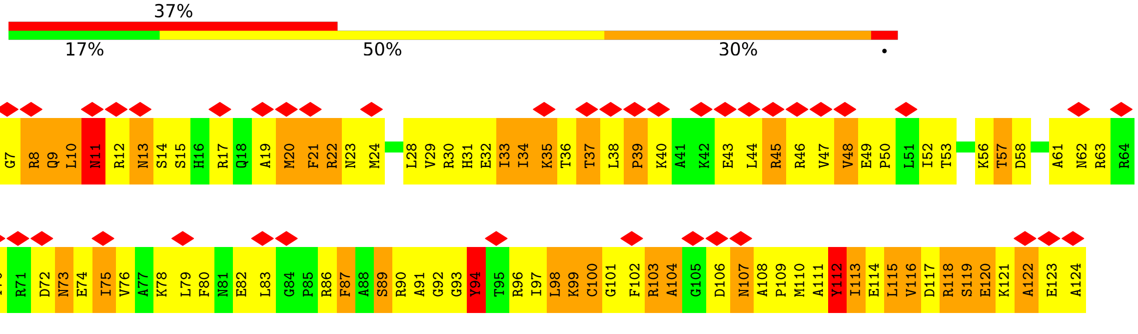
- Molecule 21: 50S RIBOSOMAL PROTEIN L16

Chain M:



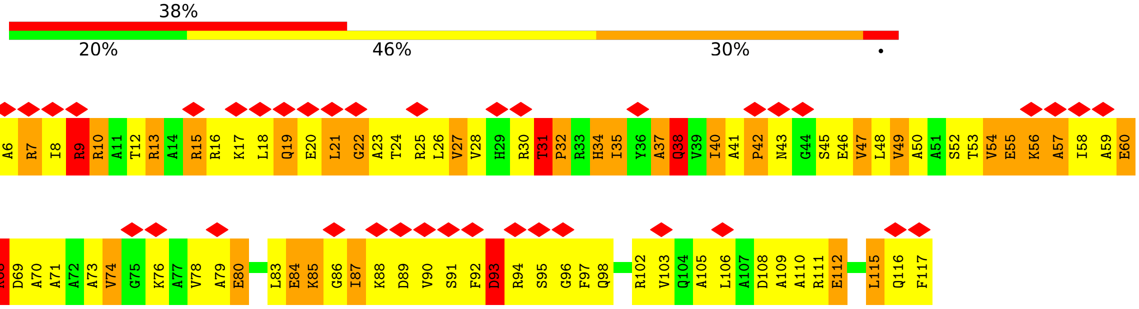
- Molecule 22: 50S RIBOSOMAL PROTEIN L17

Chain N:

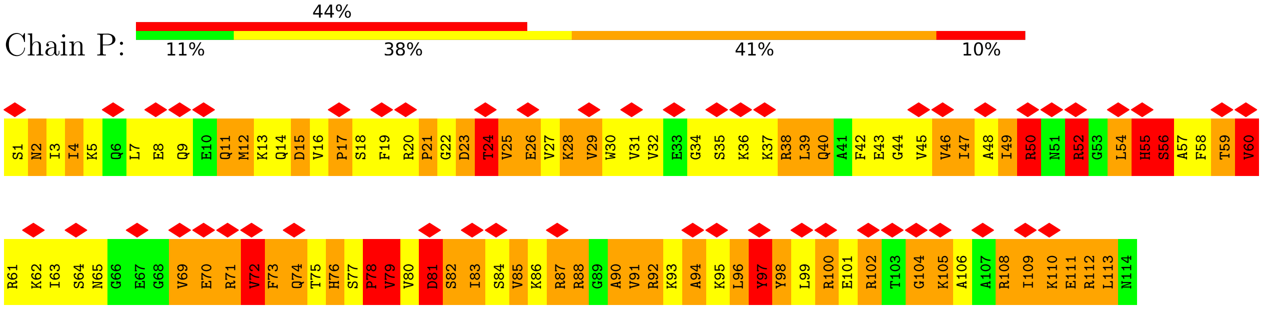


- Molecule 23: 50S RIBOSOMAL PROTEIN L18

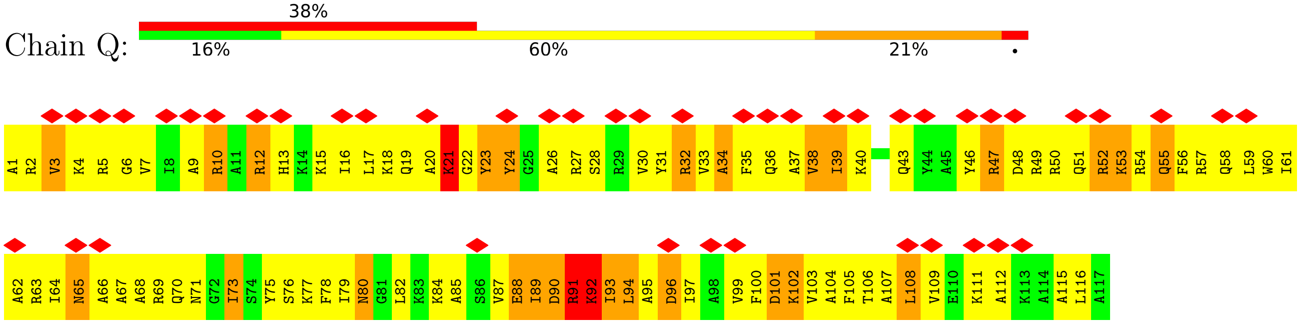
Chain O:



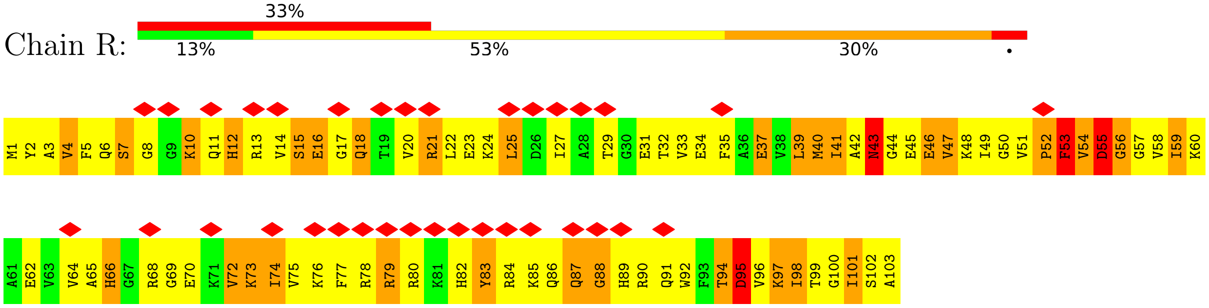
- Molecule 24: 50S RIBOSOMAL PROTEIN L19



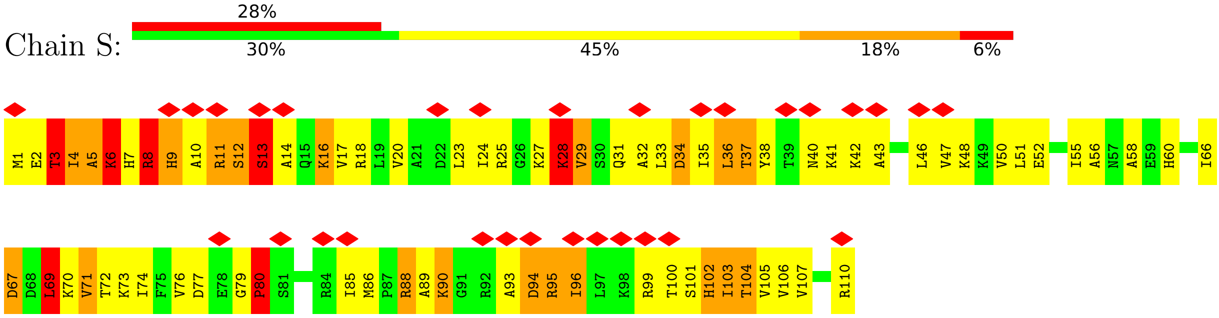
- Molecule 25: 50S RIBOSOMAL PROTEIN L20



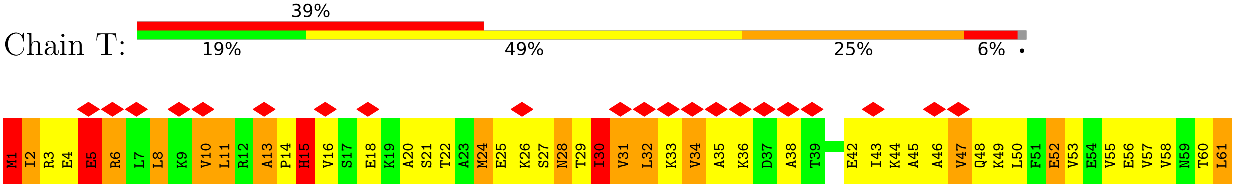
- Molecule 26: 50S RIBOSOMAL PROTEIN L21

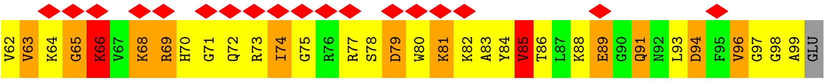


- Molecule 27: 50S RIBOSOMAL PROTEIN L22

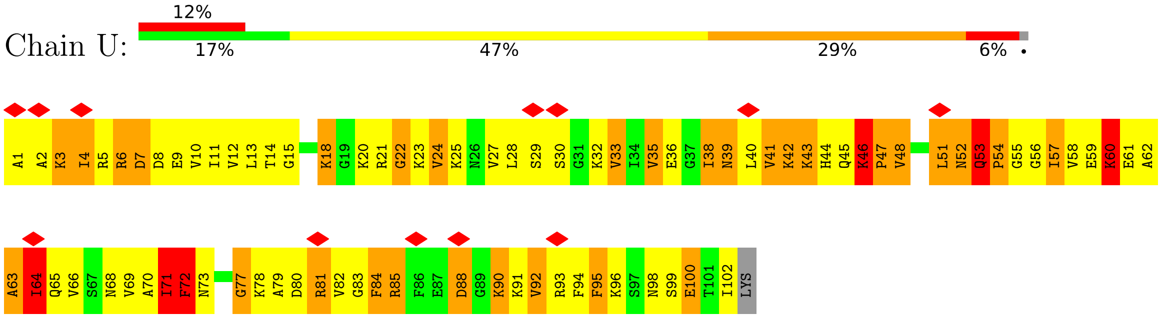


- Molecule 28: 50S RIBOSOMAL PROTEIN L23

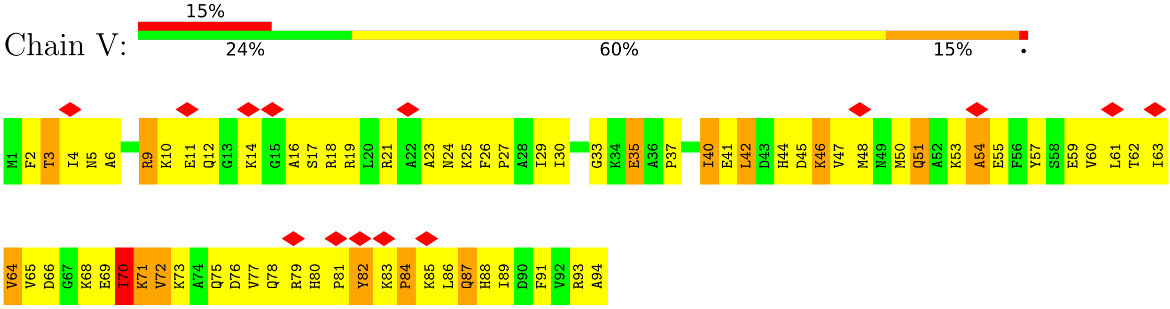




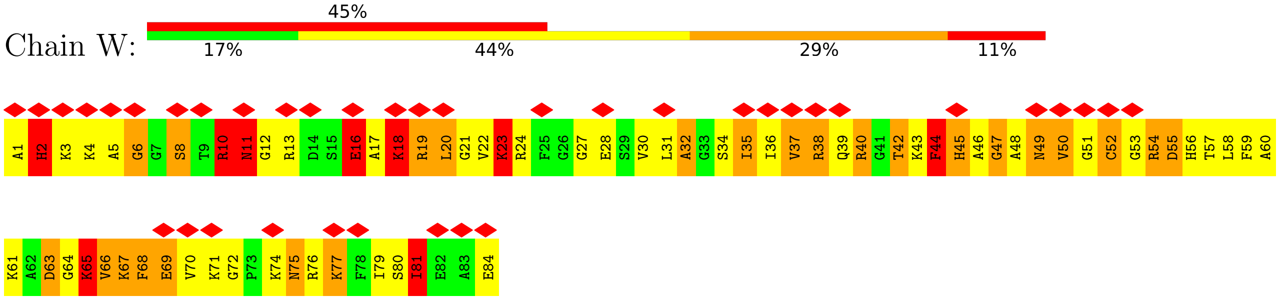
- Molecule 29: 50S RIBOSOMAL PROTEIN L24



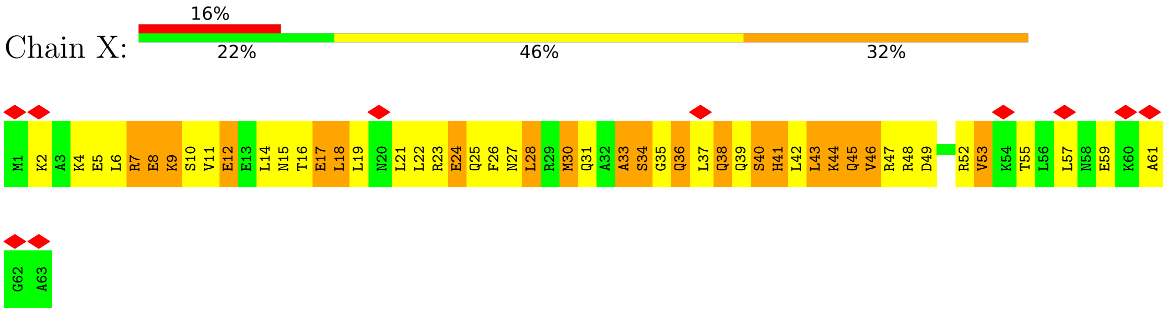
- Molecule 30: 50S RIBOSOMAL PROTEIN L25



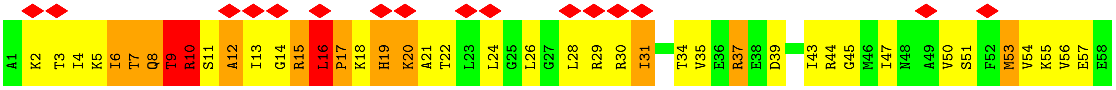
- Molecule 31: 50S RIBOSOMAL PROTEIN L27



- Molecule 32: 50S RIBOSOMAL PROTEIN L29

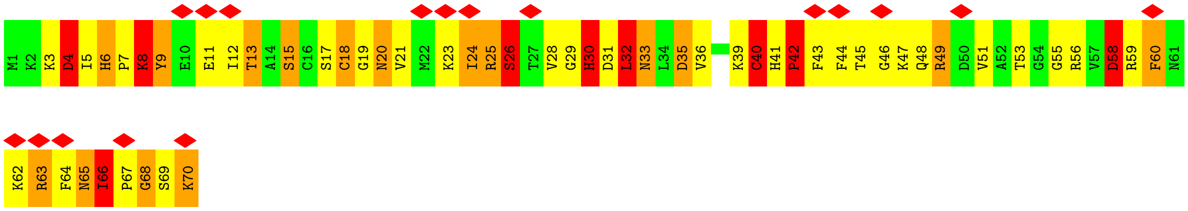


- Molecule 33: 50S RIBOSOMAL PROTEIN L30



- Molecule 34: 50S RIBOSOMAL PROTEIN L31

Chain Z:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32170	Depositor
Resolution determination method	Not provided	
CTF correction method	PER MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	24	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	77769	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.158	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	360.0, 360.0, 360.0	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.0, 2.0, 2.0	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.53	1/450 (0.2%)	1.15	7/599 (1.2%)
2	1	0.36	0/448	0.71	0/594
3	2	0.33	0/380	0.64	0/498
4	3	0.47	0/513	0.96	1/676 (0.1%)
5	4	0.40	0/303	0.73	0/397
6	5	0.24	0/855	0.38	0/1124
7	6	0.37	0/40	0.26	0/53
8	7	0.13	0/1781	0.63	0/2779
9	A	0.27	0/2803	0.74	0/4371
10	B	0.32	11/68314 (0.0%)	0.77	54/106569 (0.1%)
11	C	0.40	0/2092	0.88	7/2813 (0.2%)
12	D	0.40	0/1586	0.80	2/2134 (0.1%)
13	E	0.45	1/1571 (0.1%)	0.88	6/2113 (0.3%)
14	F	0.33	0/1444	0.87	5/1937 (0.3%)
15	G	0.31	0/1343	0.69	0/1816
16	H	0.27	0/1122	0.59	0/1515
17	I	0.26	0/1046	0.58	0/1410
18	J	0.41	1/1135 (0.1%)	0.72	3/1529 (0.2%)
19	K	0.35	0/939	0.99	2/1258 (0.2%)
20	L	0.71	0/1006	1.61	29/1331 (2.2%)
21	M	0.48	0/1093	1.03	8/1460 (0.5%)
22	N	0.34	0/1021	0.78	4/1364 (0.3%)
23	O	0.30	0/910	0.67	1/1219 (0.1%)
24	P	0.55	0/929	1.40	16/1242 (1.3%)
25	Q	0.41	0/960	0.86	2/1278 (0.2%)
26	R	1.06	6/829 (0.7%)	1.42	13/1107 (1.2%)
27	S	0.28	0/864	0.69	1/1156 (0.1%)
28	T	0.38	0/784	0.77	4/1048 (0.4%)
29	U	0.48	0/787	0.74	3/1051 (0.3%)
30	V	0.30	0/766	0.53	0/1025
31	W	0.36	0/642	0.96	5/848 (0.6%)
32	X	0.29	0/509	0.81	1/674 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Y	0.30	0/453	0.64	0/605
34	Z	0.48	0/559	1.04	5/745 (0.7%)
All	All	0.35	20/100277 (0.0%)	0.80	179/150338 (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
10	B	0	55
11	C	0	3
18	J	0	2
20	L	0	1
24	P	0	1
25	Q	0	1
26	R	0	1
All	All	0	64

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	53	PHE	CB-CG	17.81	1.81	1.51
26	R	54	VAL	N-CA	-11.64	1.23	1.46
26	R	54	VAL	CA-CB	11.12	1.78	1.54
10	B	2196	C	O3'-P	10.16	1.73	1.61
10	B	2052	A	C4'-C3'	-8.24	1.44	1.53

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	2791	G	O5'-P-OP1	-28.73	76.22	110.70
10	B	2791	G	O5'-P-OP2	18.24	132.59	110.70
26	R	53	PHE	CA-C-N	-17.34	79.05	117.20
26	R	54	VAL	CB-CA-C	15.12	140.12	111.40
10	B	2790	U	OP1-P-O3'	14.24	136.52	105.20

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	B	136	G	Sidechain
10	B	139	U	Sidechain
10	B	142	A	Sidechain
10	B	143	C	Sidechain
10	B	51	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	0	444	0	461	105	0
2	1	441	0	485	68	0
3	2	377	0	418	50	0
4	3	504	0	574	108	0
5	4	302	0	343	45	0
6	5	850	0	897	94	0
7	6	41	0	39	1	0
8	7	1591	0	806	24	0
9	A	2507	0	1270	86	0
10	B	60995	0	30659	4160	0
11	C	2053	0	2122	432	0
12	D	1565	0	1616	377	0
13	E	1552	0	1617	282	0
14	F	1420	0	1460	167	0
15	G	1323	0	1374	165	0
16	H	1111	0	1148	190	0
17	I	1032	0	1088	199	0
18	J	1112	0	1147	217	0
19	K	930	0	1000	119	0
20	L	1002	0	1070	287	0
21	M	1074	0	1157	244	0
22	N	1008	0	1036	232	0
23	O	900	0	935	129	0
24	P	917	0	965	205	0
25	Q	947	0	1022	173	0
26	R	816	0	838	166	0
27	S	857	0	922	120	0
28	T	777	0	840	129	0
29	U	779	0	831	255	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	V	753	0	780	104	0
31	W	634	0	656	157	0
32	X	509	0	541	68	0
33	Y	449	0	491	57	0
34	Z	549	0	552	114	0
35	B	110	0	0	0	0
36	B	497	0	0	17	0
36	C	1	0	0	0	0
36	E	5	0	0	0	0
36	L	2	0	0	0	0
36	N	1	0	0	0	0
All	All	92737	0	61160	8365	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 55.

The worst 5 of 8365 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)
10:B:1062:G:H21	17:I:134:SER:CB	1.09	1.62
10:B:1059:G:C5'	17:I:117:THR:HG23	1.22	1.60
26:R:54:VAL:CA	26:R:54:VAL:CB	1.78	1.59
26:R:53:PHE:CB	26:R:53:PHE:CG	1.81	1.58
10:B:80:G:C5'	10:B:346:A:C8	1.88	1.53

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	
1	0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	52/54 (96%)	19 (36%)	23 (44%)	10 (19%)	0	2
3	2	44/46 (96%)	23 (52%)	14 (32%)	7 (16%)	0	3
4	3	62/64 (97%)	30 (48%)	25 (40%)	7 (11%)	0	7
5	4	36/38 (95%)	18 (50%)	9 (25%)	9 (25%)	0	1
6	5	107/109 (98%)	83 (78%)	19 (18%)	5 (5%)	2	21
7	6	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
11	C	265/273 (97%)	103 (39%)	82 (31%)	80 (30%)	0	0
12	D	207/209 (99%)	90 (44%)	69 (33%)	48 (23%)	0	1
13	E	199/201 (99%)	98 (49%)	60 (30%)	41 (21%)	0	2
14	F	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	2
15	G	174/176 (99%)	118 (68%)	39 (22%)	17 (10%)	0	9
16	H	147/149 (99%)	85 (58%)	47 (32%)	15 (10%)	0	8
17	I	139/141 (99%)	124 (89%)	11 (8%)	4 (3%)	4	29
18	J	138/142 (97%)	67 (49%)	42 (30%)	29 (21%)	0	2
19	K	119/123 (97%)	71 (60%)	32 (27%)	16 (13%)	0	4
20	L	132/144 (92%)	55 (42%)	36 (27%)	41 (31%)	0	0
21	M	134/136 (98%)	69 (52%)	37 (28%)	28 (21%)	0	2
22	N	125/127 (98%)	71 (57%)	34 (27%)	20 (16%)	0	3
23	O	115/117 (98%)	64 (56%)	26 (23%)	25 (22%)	0	2
24	P	112/114 (98%)	39 (35%)	36 (32%)	37 (33%)	0	0
25	Q	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	0	8
26	R	101/103 (98%)	44 (44%)	31 (31%)	26 (26%)	0	1
27	S	108/110 (98%)	63 (58%)	27 (25%)	18 (17%)	0	3
28	T	97/100 (97%)	41 (42%)	39 (40%)	17 (18%)	0	3
29	U	100/103 (97%)	30 (30%)	47 (47%)	23 (23%)	0	1
30	V	92/94 (98%)	62 (67%)	22 (24%)	8 (9%)	1	11
31	W	82/84 (98%)	29 (35%)	26 (32%)	27 (33%)	0	0
32	X	60/63 (95%)	28 (47%)	20 (33%)	12 (20%)	0	2
33	Y	56/58 (97%)	29 (52%)	17 (30%)	10 (18%)	0	3
34	Z	68/70 (97%)	29 (43%)	26 (38%)	13 (19%)	0	2
All	All	3422/3507 (98%)	1793 (52%)	982 (29%)	647 (19%)	0	2

5 of 647 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	10	SER
1	0	29	VAL
1	0	35	GLU
2	1	46	VAL
3	2	4	THR

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	
1	0	47/47 (100%)	31 (66%)	16 (34%)	0	1
2	1	48/48 (100%)	33 (69%)	15 (31%)	0	2
3	2	38/38 (100%)	27 (71%)	11 (29%)	0	2
4	3	51/51 (100%)	33 (65%)	18 (35%)	0	1
5	4	34/34 (100%)	22 (65%)	12 (35%)	0	1
6	5	92/92 (100%)	89 (97%)	3 (3%)	38	61
11	C	213/218 (98%)	145 (68%)	68 (32%)	0	2
12	D	164/164 (100%)	112 (68%)	52 (32%)	0	2
13	E	165/165 (100%)	115 (70%)	50 (30%)	0	2
14	F	149/149 (100%)	119 (80%)	30 (20%)	1	7
15	G	137/137 (100%)	105 (77%)	32 (23%)	1	4
16	H	114/114 (100%)	87 (76%)	27 (24%)	1	4
17	I	109/109 (100%)	106 (97%)	3 (3%)	43	64
18	J	114/116 (98%)	84 (74%)	30 (26%)	0	3
19	K	102/104 (98%)	78 (76%)	24 (24%)	1	4
20	L	97/103 (94%)	57 (59%)	40 (41%)	0	0
21	M	109/109 (100%)	77 (71%)	32 (29%)	0	2
22	N	103/103 (100%)	78 (76%)	25 (24%)	0	4
23	O	87/87 (100%)	58 (67%)	29 (33%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	P	99/99 (100%)	77 (78%)	22 (22%)	1	6
25	Q	89/89 (100%)	66 (74%)	23 (26%)	0	3
26	R	84/84 (100%)	68 (81%)	16 (19%)	1	8
27	S	93/93 (100%)	72 (77%)	21 (23%)	1	5
28	T	83/84 (99%)	60 (72%)	23 (28%)	0	3
29	U	83/84 (99%)	58 (70%)	25 (30%)	0	2
30	V	78/78 (100%)	66 (85%)	12 (15%)	2	14
31	W	62/62 (100%)	46 (74%)	16 (26%)	0	3
32	X	55/55 (100%)	40 (73%)	15 (27%)	0	3
33	Y	48/48 (100%)	36 (75%)	12 (25%)	0	3
34	Z	62/62 (100%)	43 (69%)	19 (31%)	0	2
All	All	2809/2826 (99%)	2088 (74%)	721 (26%)	2	3

5 of 721 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	N	1	MET
26	R	66	HIS
22	N	57	THR
21	M	136	MET
24	P	24	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
19	K	82	ASN
24	P	2	ASN
34	Z	30	HIS
20	L	38	GLN
22	N	73	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	2837/2904 (97%)	552 (19%)	19 (0%)
8	7	73/74 (98%)	3 (4%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	A	116/120 (96%)	23 (19%)	0
All	All	3026/3098 (97%)	578 (19%)	19 (0%)

5 of 578 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	121	A
8	7	124	U
8	7	168	U
9	A	11	C
9	A	12	C

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	B	2258	C
10	B	2425	A
10	B	2756	U
10	B	2336	A
10	B	1236	G

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 110 ligands modelled in this entry, 110 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
32	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	1:MET	C	2:LYS	N	3.26

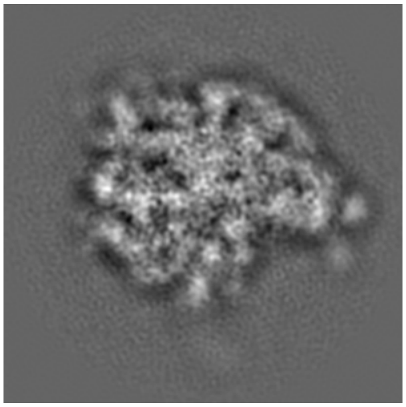
6 Map visualisation ⓘ

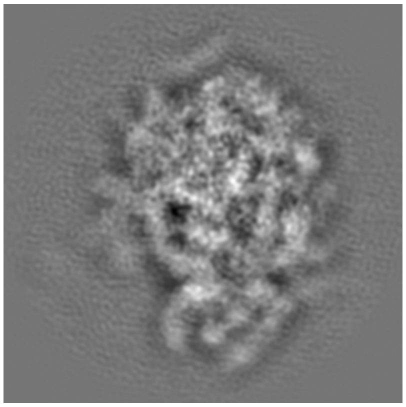
This section contains visualisations of the EMDB entry EMD-2917. These allow visual inspection of the internal detail of the map and identification of artifacts.

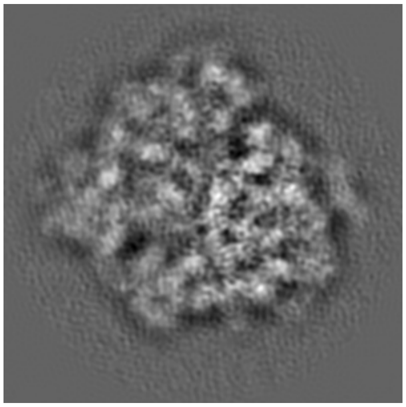
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map


X

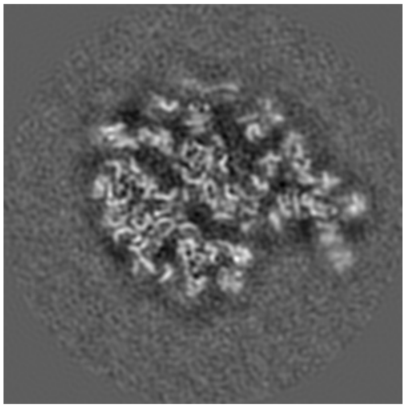

Y

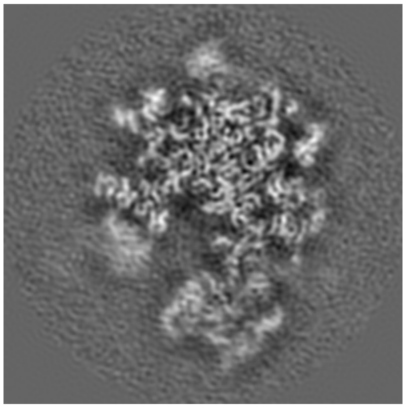

Z

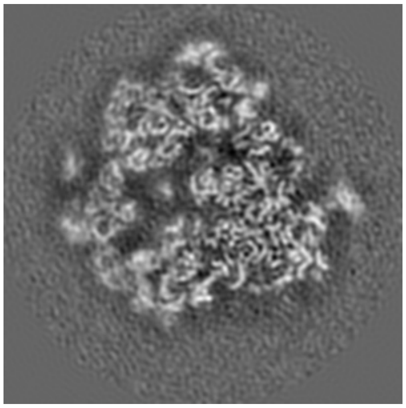
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map


X Index: 90

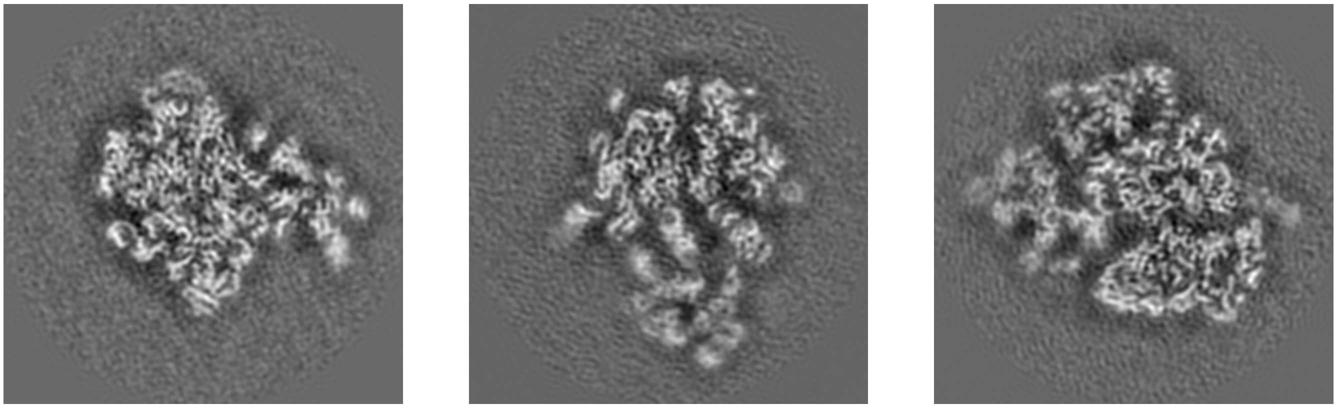

Y Index: 90


Z Index: 90

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

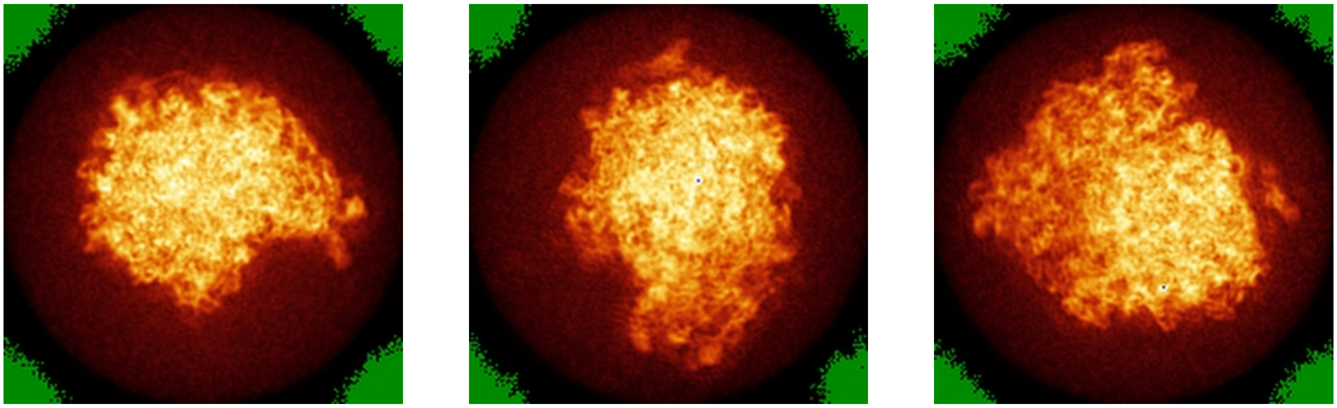
6.3.1 Primary map


X Index: 95 Y Index: 79 Z Index: 98

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map


X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

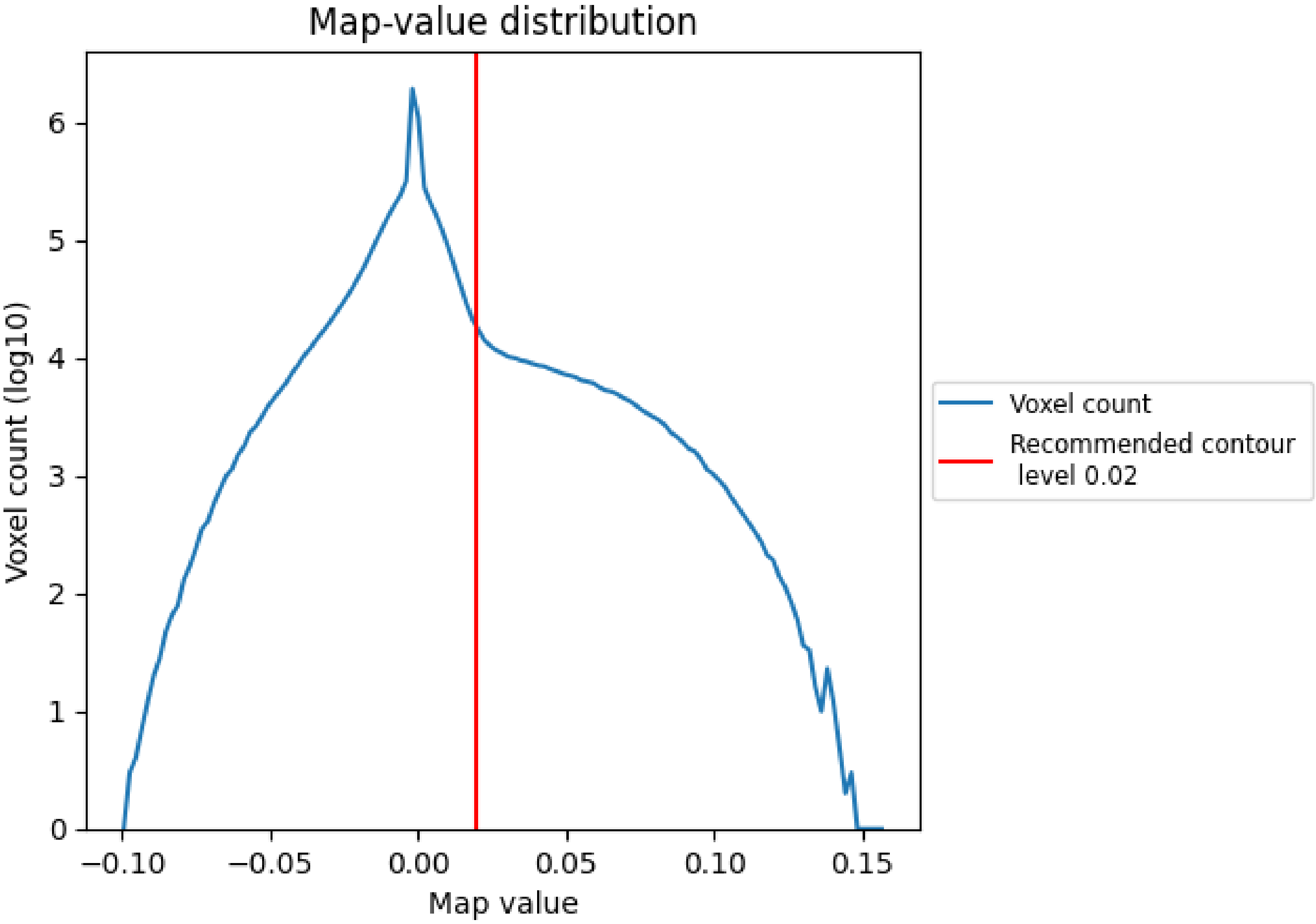
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

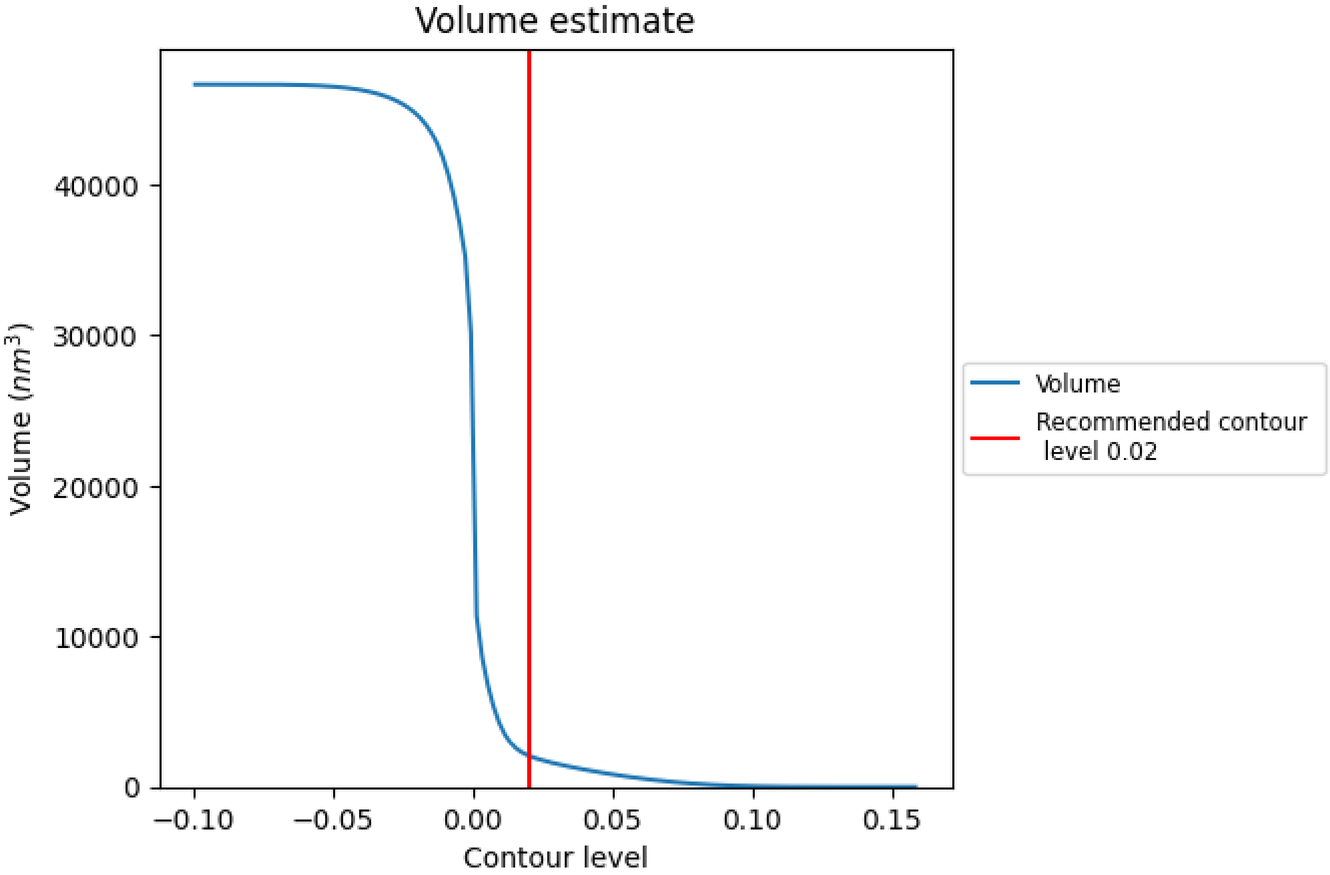
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

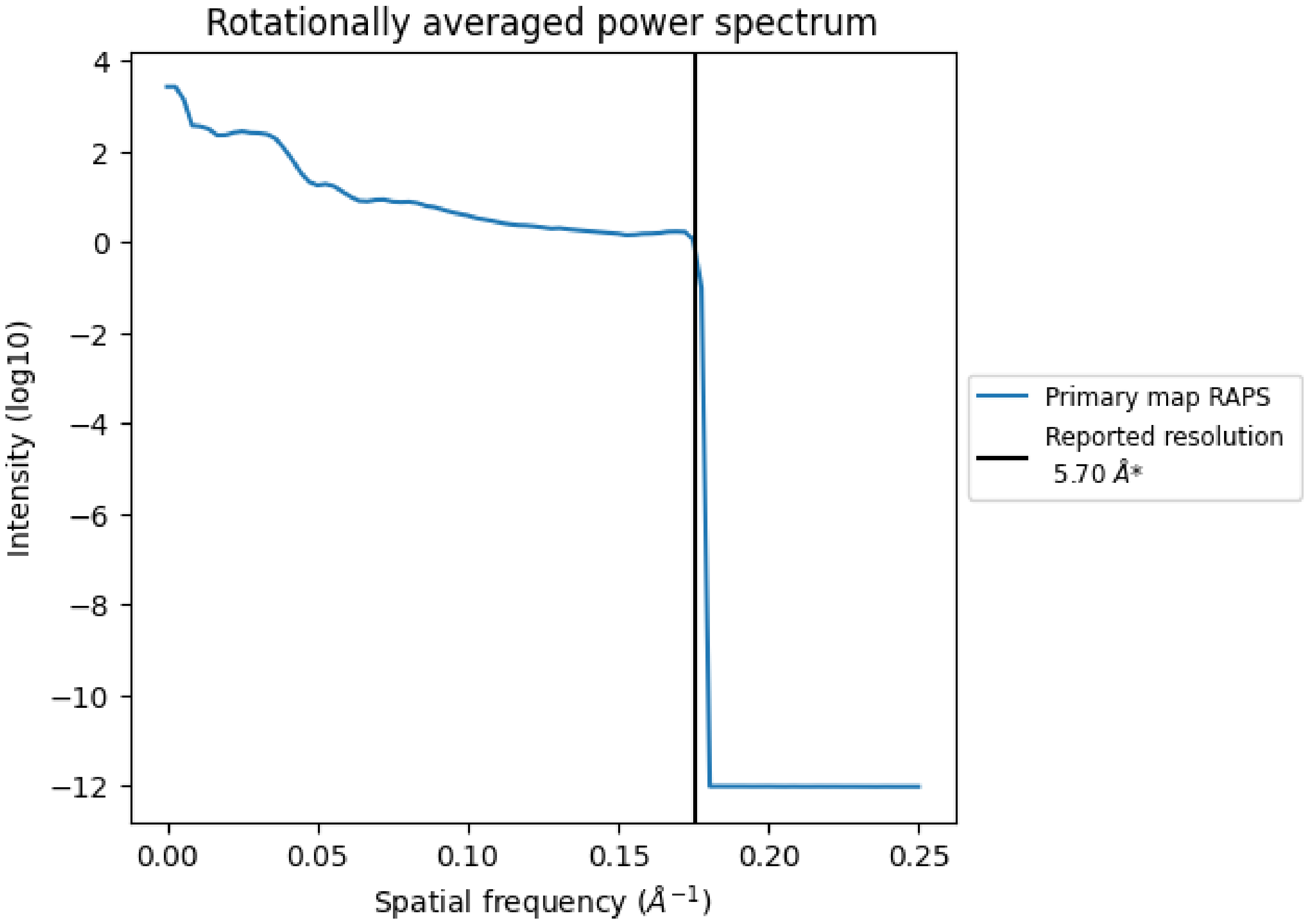
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2076 nm^3; this corresponds to an approximate mass of 1875 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

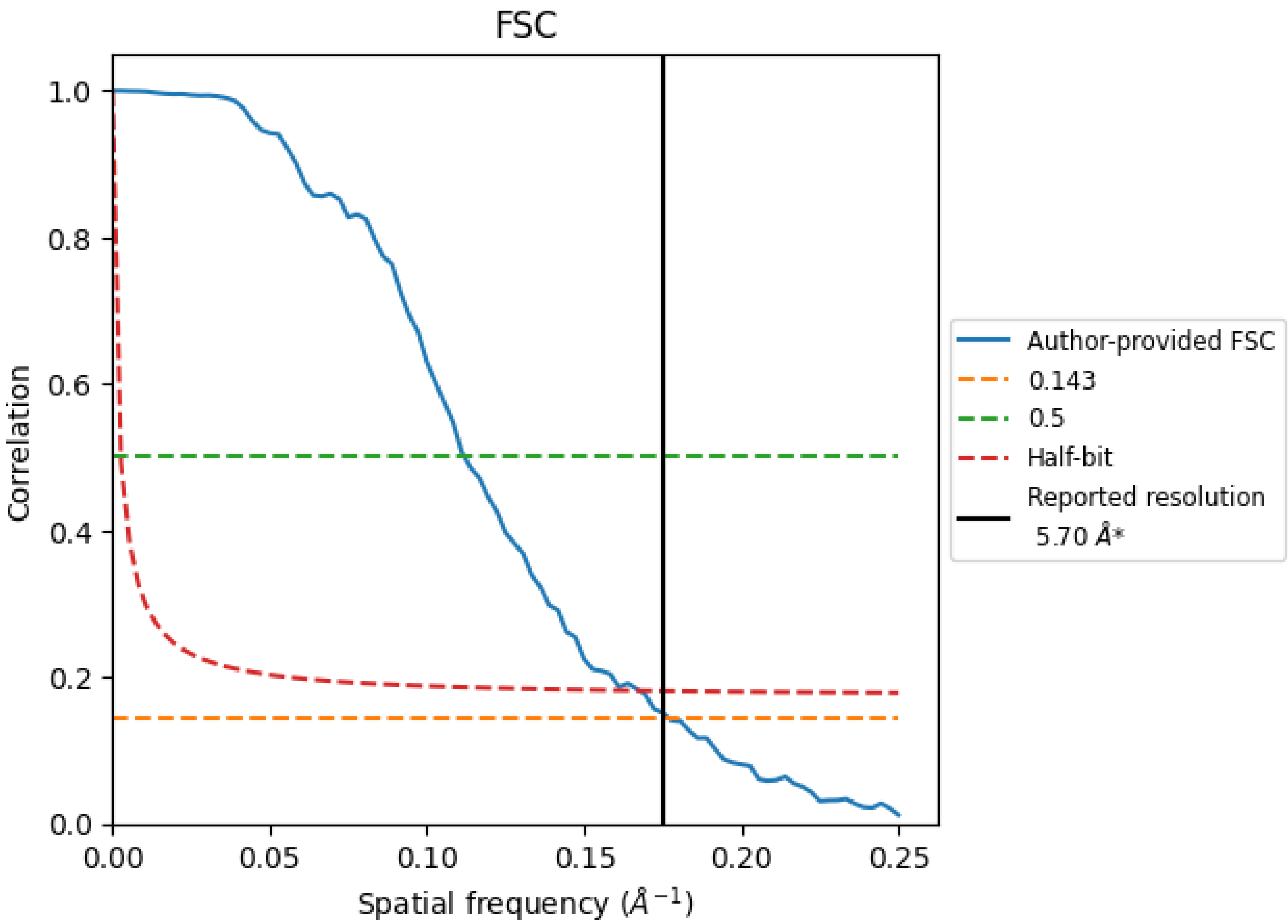


*Reported resolution corresponds to spatial frequency of 0.175 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.175 Å^{-1}

8.2 Resolution estimates ⓘ

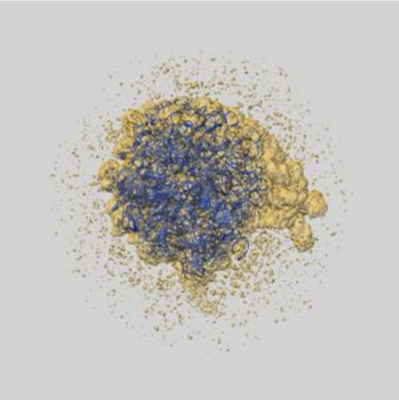
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	5.64	8.93	5.97
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

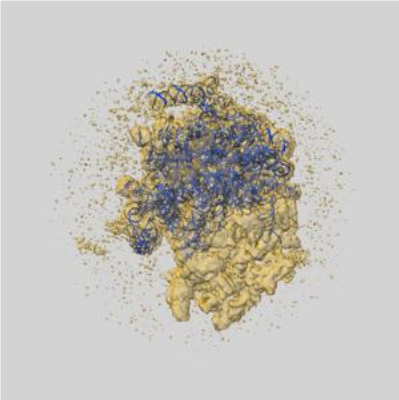
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2917 and PDB model 5AKA. Per-residue inclusion information can be found in section 3 on page 11.

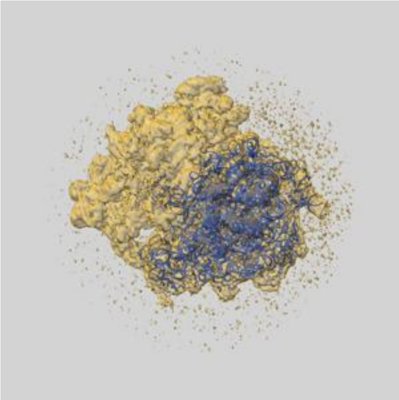
9.1 Map-model overlay



X



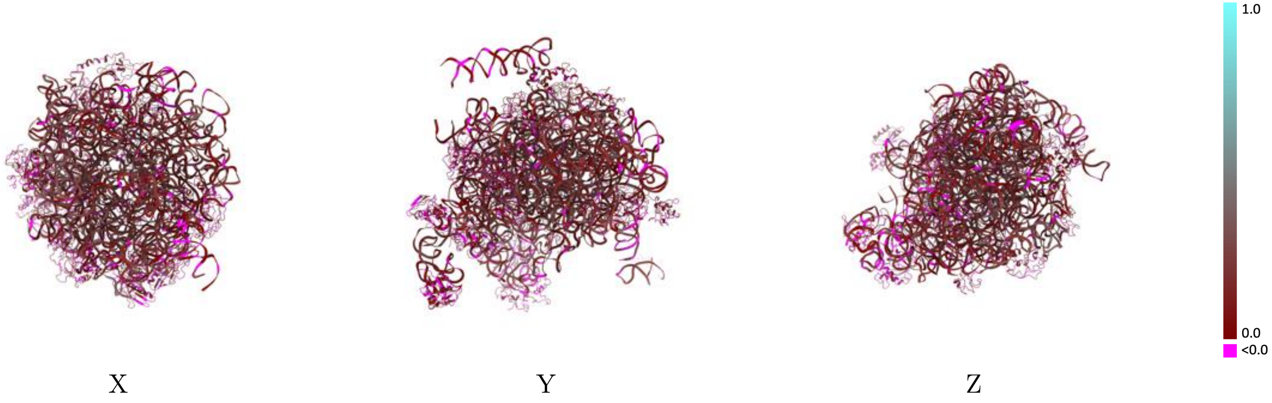
Y



Z

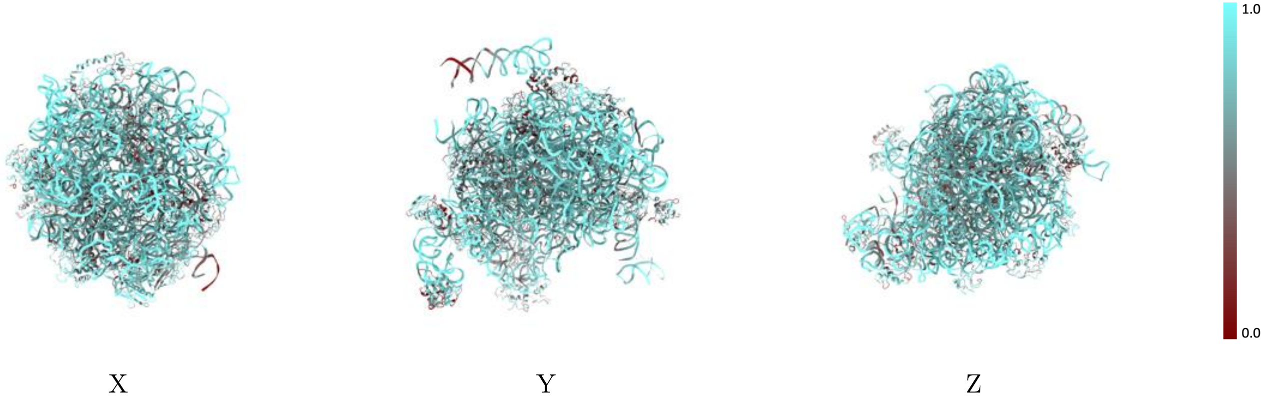
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



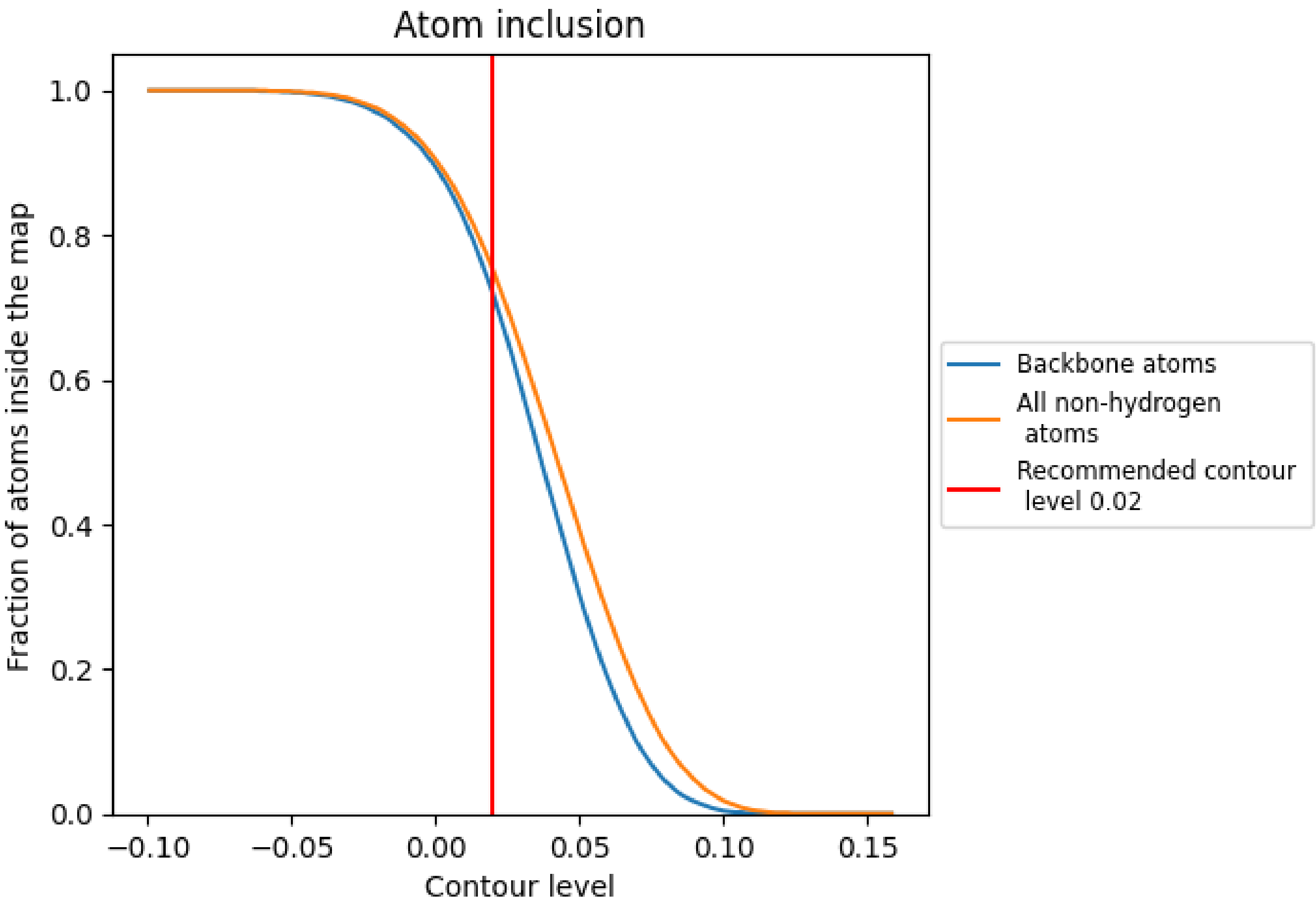
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.1560
0	0.5400	0.1450
1	0.5500	0.0750
2	0.4200	0.1470
3	0.3120	0.1210
4	0.4380	0.0500
5	0.4330	0.1280
6	0.6580	0.3100
7	0.7370	0.0860
A	0.7890	0.1070
B	0.8420	0.1890
C	0.5050	0.0930
D	0.5270	0.0790
E	0.5940	0.1120
F	0.6180	0.0300
G	0.6460	0.0390
H	0.5770	0.1080
I	0.5860	0.0720
J	0.5010	0.0970
K	0.5710	0.1020
L	0.4920	0.0690
M	0.5100	0.0930
N	0.5260	0.1220
O	0.5300	0.0150
P	0.4710	0.0770
Q	0.5370	0.0980
R	0.5850	0.0930
S	0.5290	0.1330
T	0.4910	0.1170
U	0.7500	0.1510
V	0.6980	0.0690
W	0.4470	0.0640
X	0.6740	0.1360
Y	0.6130	0.1120
Z	0.5450	0.0960