



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 03:10 AM UTC

PDB ID : 9NLB / pdb_00009nlb
EMDB ID : EMD-40929
Title : E. coli initiation complex with EQ2-EttA in Hydrolytic 2 conformation
Authors : Singh, S.; Hunt, J.F.
Deposited on : 2025-03-03
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

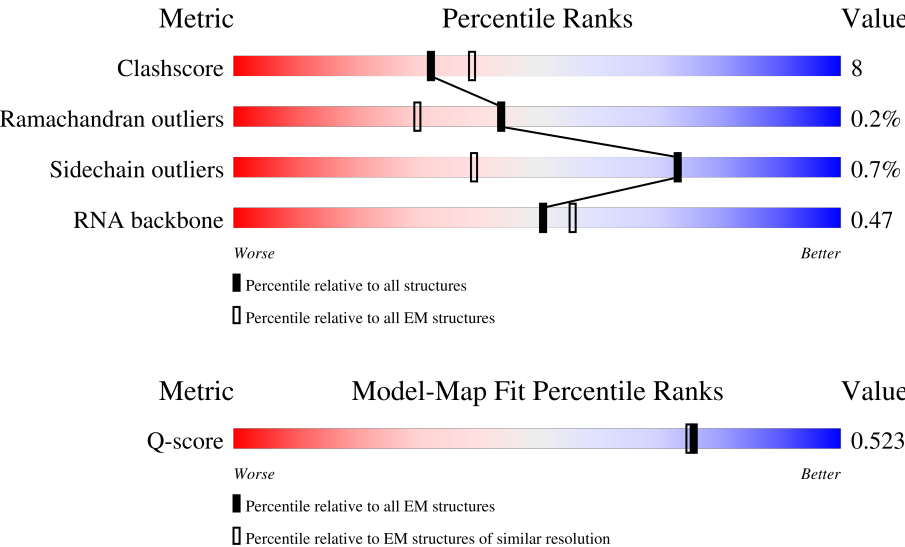
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

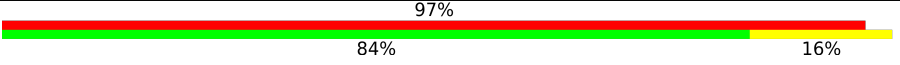
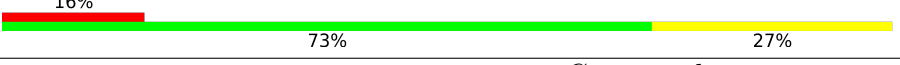
The reported resolution of this entry is 3.20 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 $\leq 5\%$. 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	1	220	
2	13	142	
3	14	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	15	143	8% 83% 17%
5	16	136	15% 79% 21%
6	17	120	5% 84% 16%
7	18	116	22% 80% 20%
8	19	114	14% 80% 19%
9	2	271	9% 82% 18%
10	20	117	• 90% 10%
11	21	103	17% 67% 33%
12	22	110	11% 82% 17%
13	23	93	17% 74% 26%
14	24	102	27% 74% 26%
15	25	94	26% 74% 26%
16	27	76	5% 87% 12%
17	28	77	19% 83% 17%
18	29	63	22% 83% 17%
19	3	209	9% 80% 20%
20	30	58	14% 81% 19%
21	31	66	94% 73% 27%
22	32	56	12% 62% 38%
23	33	50	28% 78% 22%
24	34	46	• 85% 15%
25	35	64	5% 78% 17% 5%
26	36	38	13% 66% 32%
27	4	201	18% 82% 18%
28	5	177	60% 71% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	6	176	
30	9	149	
31	E	552	
32	M	9	
33	R1	2903	
34	R2	119	
35	R3	1531	
36	T	77	
37	sb	218	
38	sc	206	
39	sd	205	
40	se	157	
41	sf	100	
42	sg	151	
43	sh	129	
44	si	127	
45	sj	98	
46	sk	116	
47	sl	123	
48	sm	114	
49	sn	100	
50	so	88	
51	sp	82	
52	sq	80	
53	sr	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	ss	79	
55	st	85	
56	su	70	

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
36	H2U	T	20	X	-	-	-
36	4OC	T	32	X	-	-	-
36	MUM	T	54	X	-	-	-
36	PSU	T	55	X	-	-	-
36	4SU	T	8	X	-	-	-

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 150087 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 Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	220	Total	C	N	O	S	0	0
			1353	804	270	277	2		

- Molecule 2 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	13	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 3 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	14	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 4 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	15	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 5 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	16	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	17	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	18	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 8 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	19	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 10 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	20	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 11 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	21	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 12 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	22	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	23	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	24	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	25	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	27	76	Total	C	N	O	S		
			582	360	117	104	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	28	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	29	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	209	Total	C	N	O	S		
			1565	979	288	294	4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	30	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	33	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called Energy-dependent translational throttle protein EttA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	552	Total	C	N	O	S	0	0
			4360	2745	774	829	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	188	GLN	GLU	conflict	UNP P0A9W3
E	341	SER	ASP	conflict	UNP P0A9W3
E	470	GLN	GLU	conflict	UNP P0A9W3

- Molecule 32 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	9	Total	C	N	O	P	0	0
			195	88	40	58	9		

- Molecule 33 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R1	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R1	1847	G	A	conflict	GB 2019144442

- Molecule 34 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R2	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	R3	1531	Total	C	N	O	P	0	0
			32850	14652	6028	10640	1530		

- Molecule 36 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	T	77	Total	C	N	O	P	S	0	0
			1639	734	294	534	76	1		

- Molecule 37 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 38 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	se	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 41 is a protein called 30S ribosomal protein S6, non-modified isoform.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	sg	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

- Molecule 44 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 47 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	sn	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 50 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	so	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 51 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 52 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	sr	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 54 is a protein called 30S ribosomal protein S19.

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

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

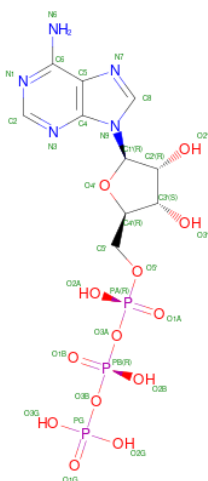
- Molecule 56 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	su	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	15	1	Total	Mg	0
			1	1	
57	2	1	Total	Mg	0
			1	1	
57	32	1	Total	Mg	0
			1	1	
57	R1	199	Total	Mg	0
			199	199	
57	R3	77	Total	Mg	0
			77	77	

- Molecule 58 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

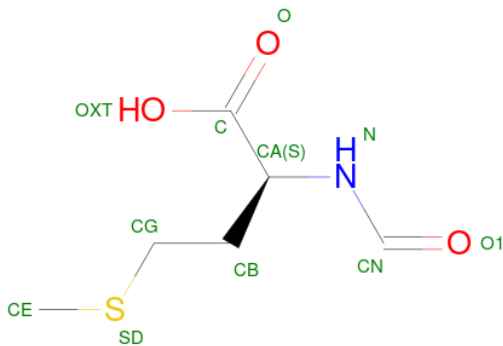


Mol	Chain	Residues	Atoms					AltConf
58	E	1	Total 31	C 10	N 5	O 13	P 3	0
58	E	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 59 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
59	E	2	Total 2	Na 2	0

- Molecule 60 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $\text{C}_6\text{H}_{11}\text{NO}_3\text{S}$).

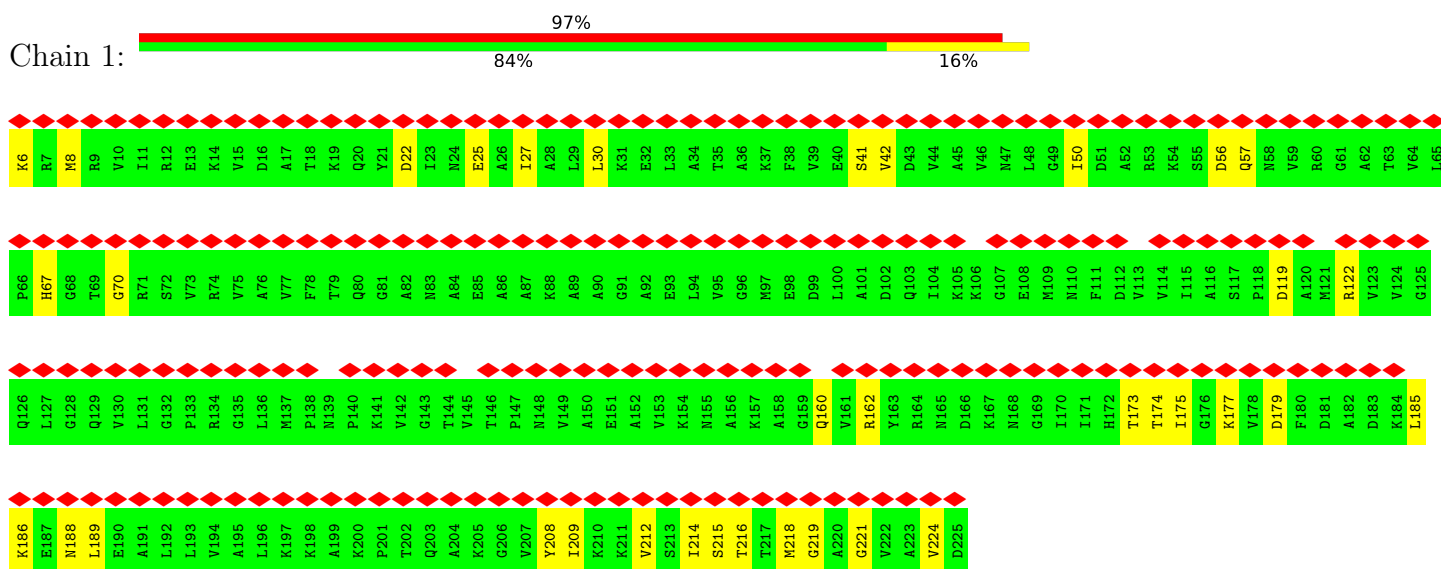


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	T	1	10	6	1	2	1	0

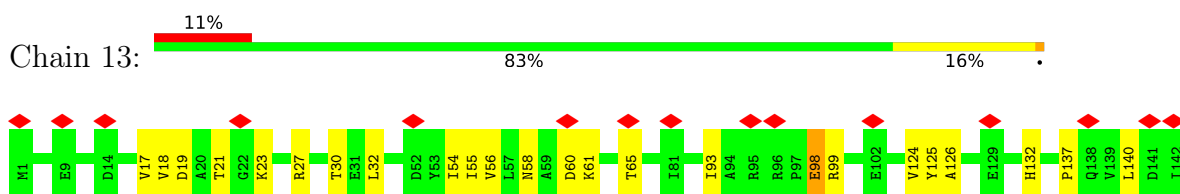
3 Residue-property plots

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.

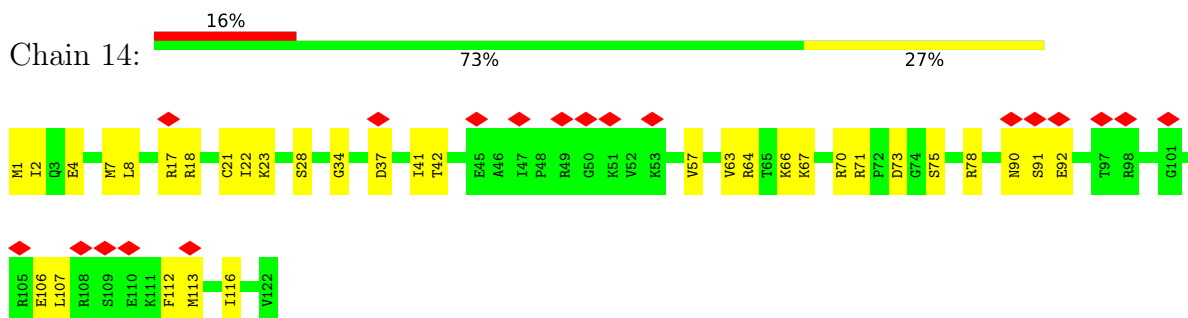
• Molecule 1: Large ribosomal subunit protein uL1



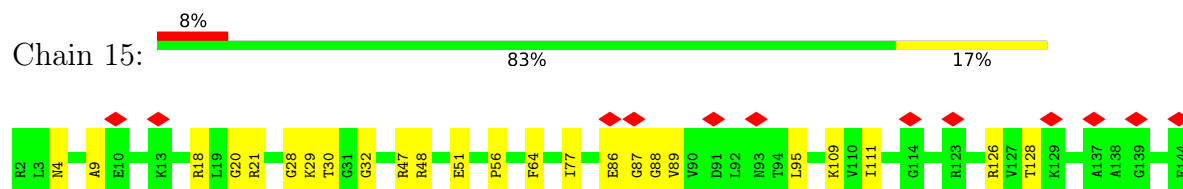
• Molecule 2: Large ribosomal subunit protein uL13



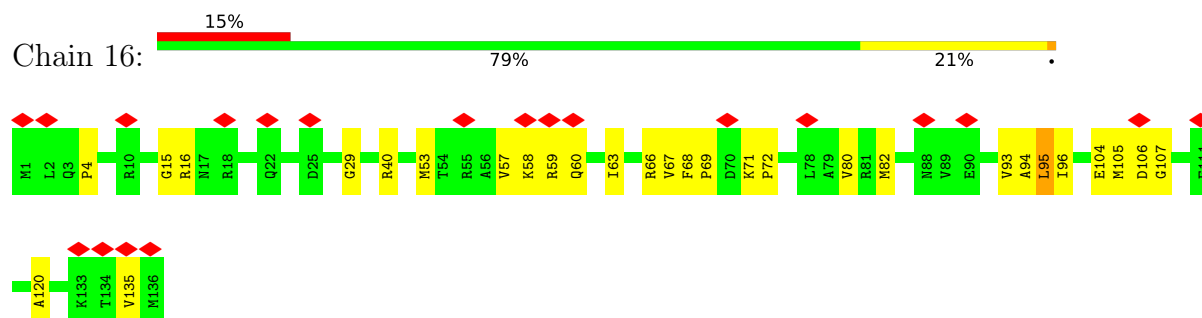
• Molecule 3: 50S ribosomal protein L14



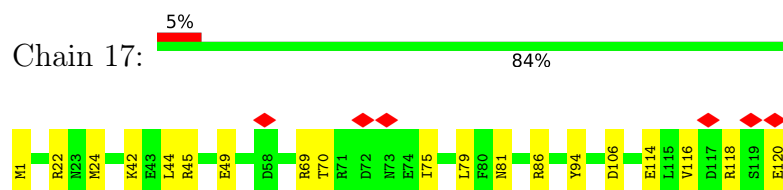
- Molecule 4: 50S ribosomal protein L15



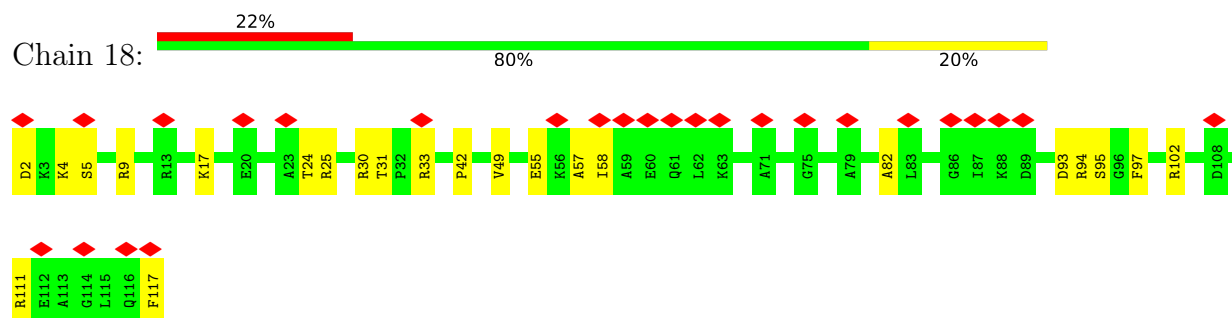
- Molecule 5: 50S ribosomal protein L16



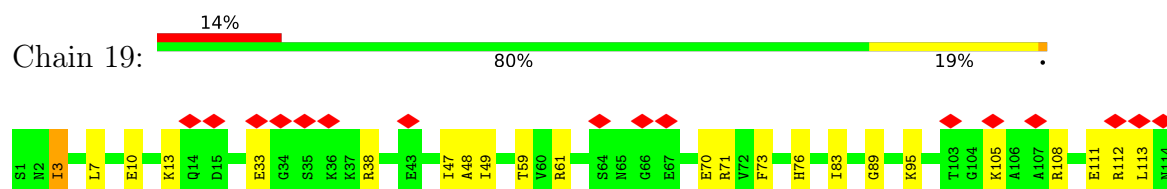
- Molecule 6: Large ribosomal subunit protein bL17



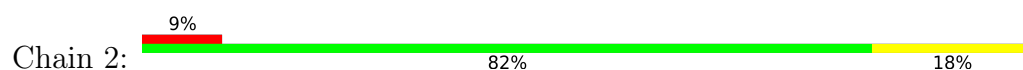
- Molecule 7: Large ribosomal subunit protein uL18

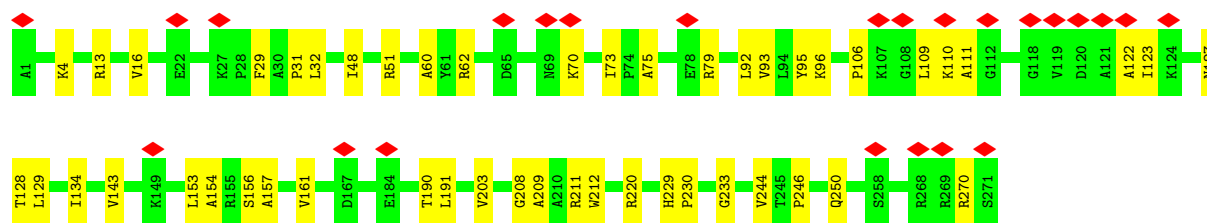


- Molecule 8: 50S ribosomal protein L19

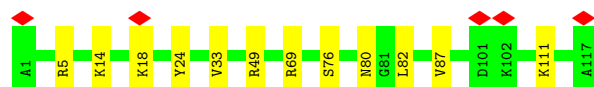


- Molecule 9: 50S ribosomal protein L2

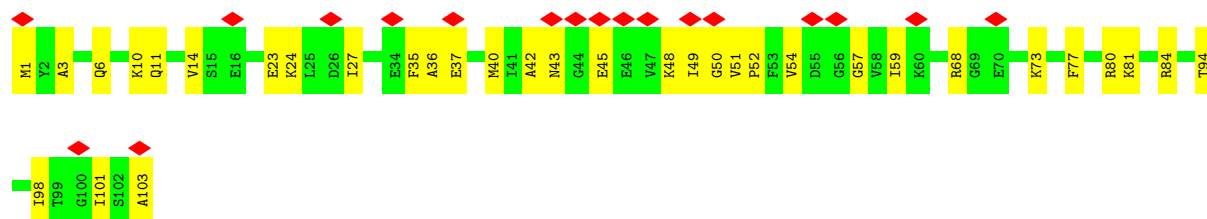




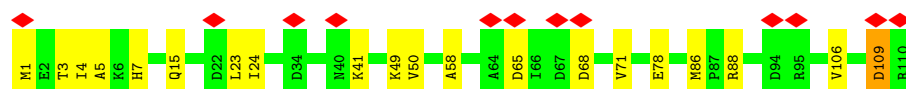
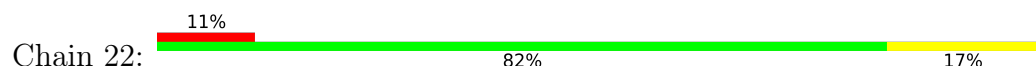
- Molecule 10: Large ribosomal subunit protein bL20



- Molecule 11: Large ribosomal subunit protein bL21



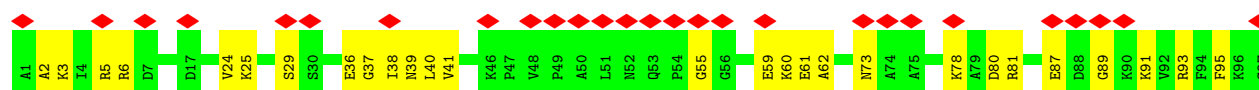
- Molecule 12: Large ribosomal subunit protein uL22



- Molecule 13: Large ribosomal subunit protein uL23

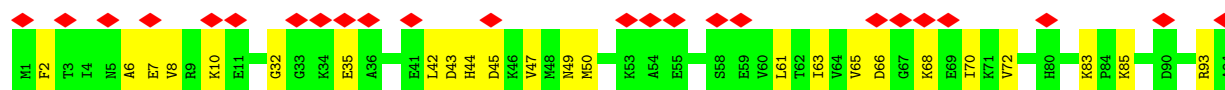
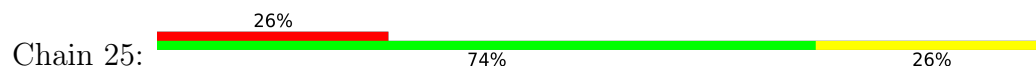


- Molecule 14: Large ribosomal subunit protein uL24





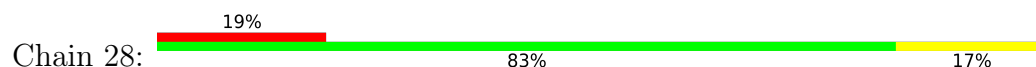
- Molecule 15: Large ribosomal subunit protein bL25



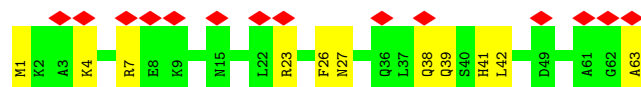
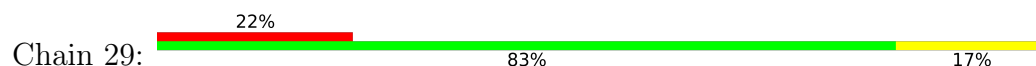
- Molecule 16: Large ribosomal subunit protein bL27



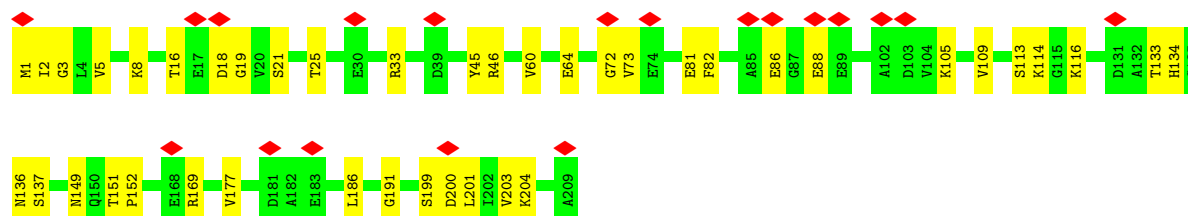
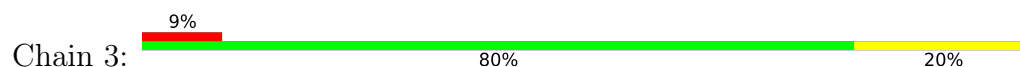
- Molecule 17: 50S ribosomal protein L28



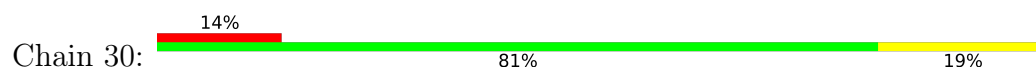
- Molecule 18: Large ribosomal subunit protein uL29

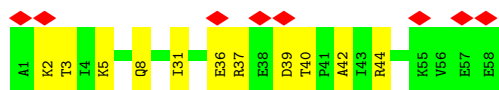


- Molecule 19: 50S ribosomal protein L3

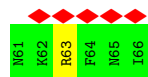
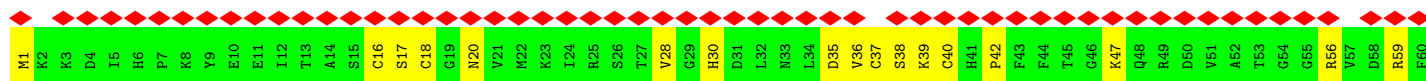
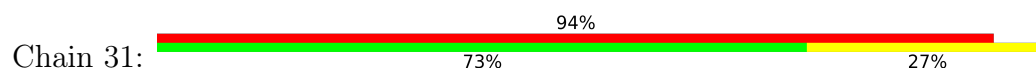


- Molecule 20: 50S ribosomal protein L30

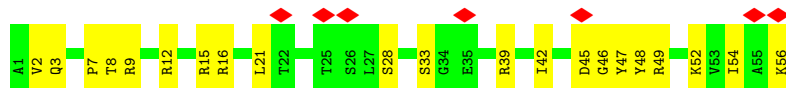




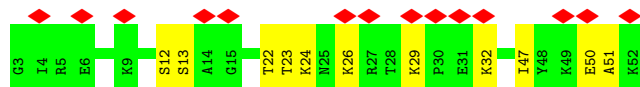
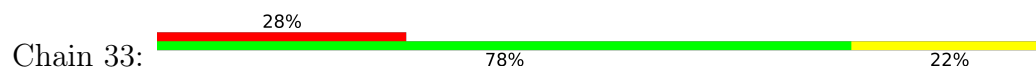
- Molecule 21: Large ribosomal subunit protein bL31



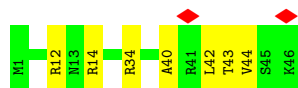
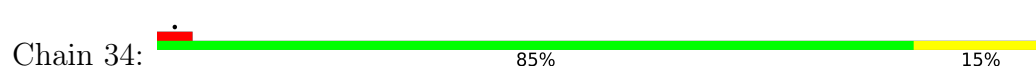
- Molecule 22: 50S ribosomal protein L32



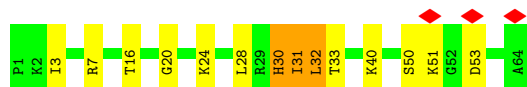
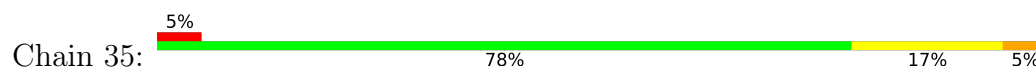
- Molecule 23: Large ribosomal subunit protein bL33



- Molecule 24: 50S ribosomal protein L34



- Molecule 25: Large ribosomal subunit protein bL35

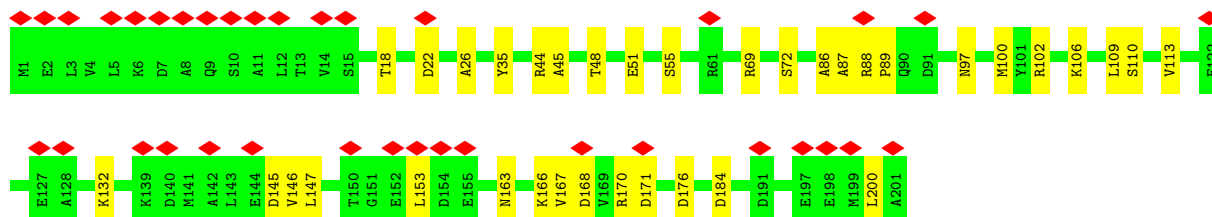
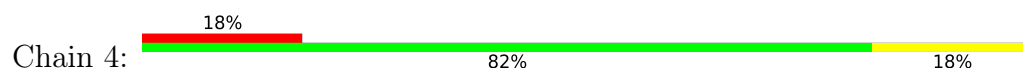


- Molecule 26: 50S ribosomal protein L36

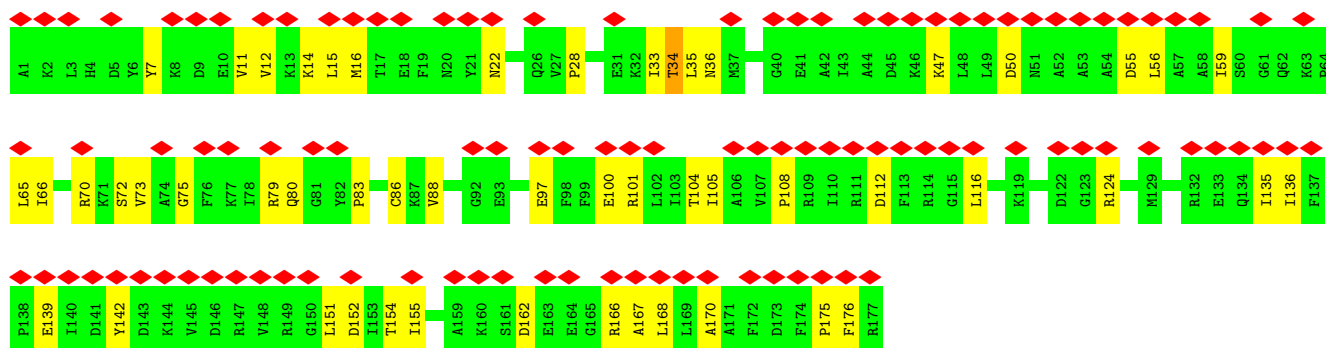




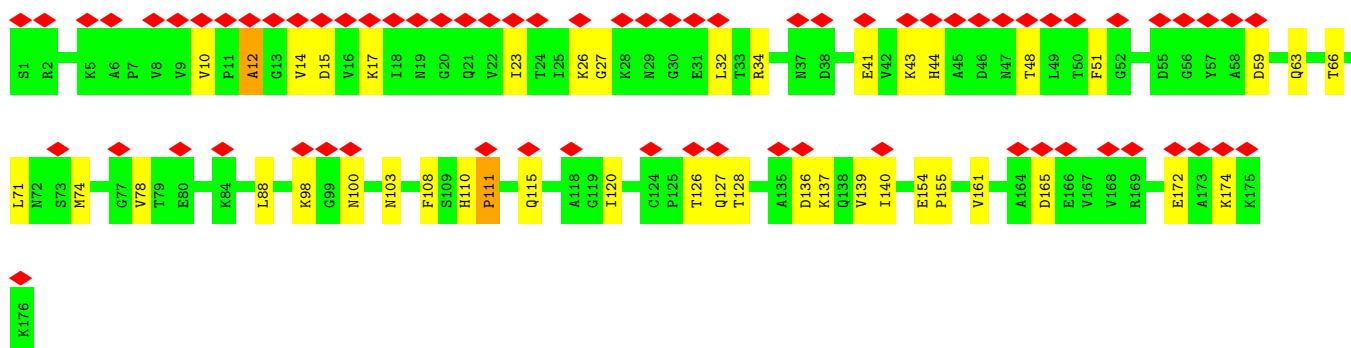
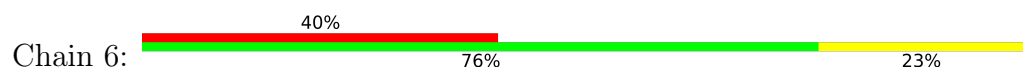
- Molecule 27: Large ribosomal subunit protein uL4



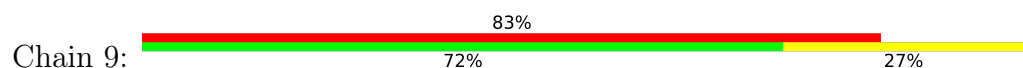
- Molecule 28: 50S ribosomal protein L5

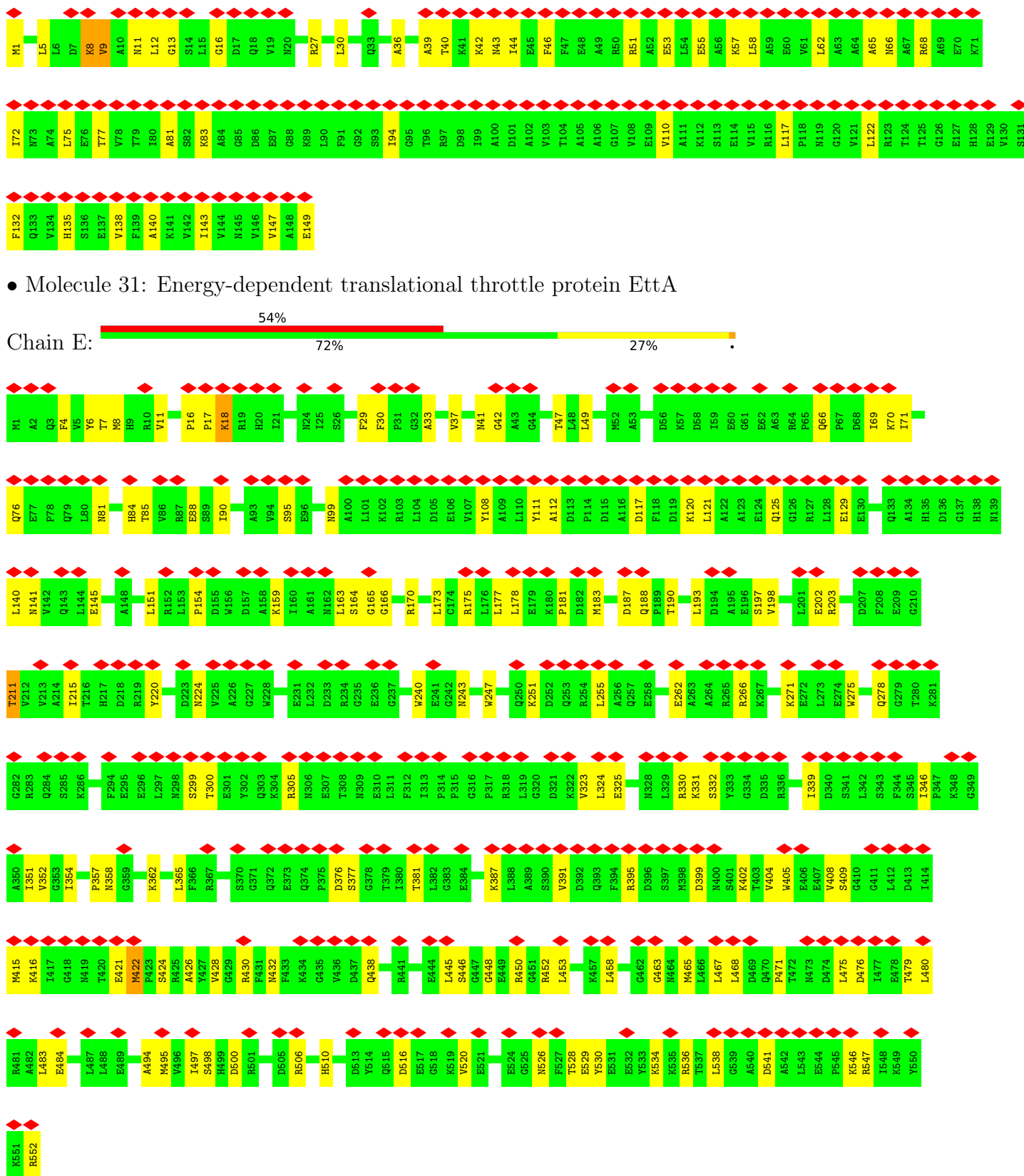


- Molecule 29: Large ribosomal subunit protein uL6

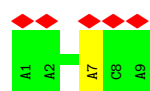
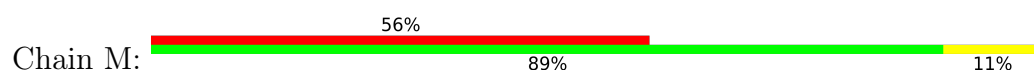


- Molecule 30: Large ribosomal subunit protein bL9

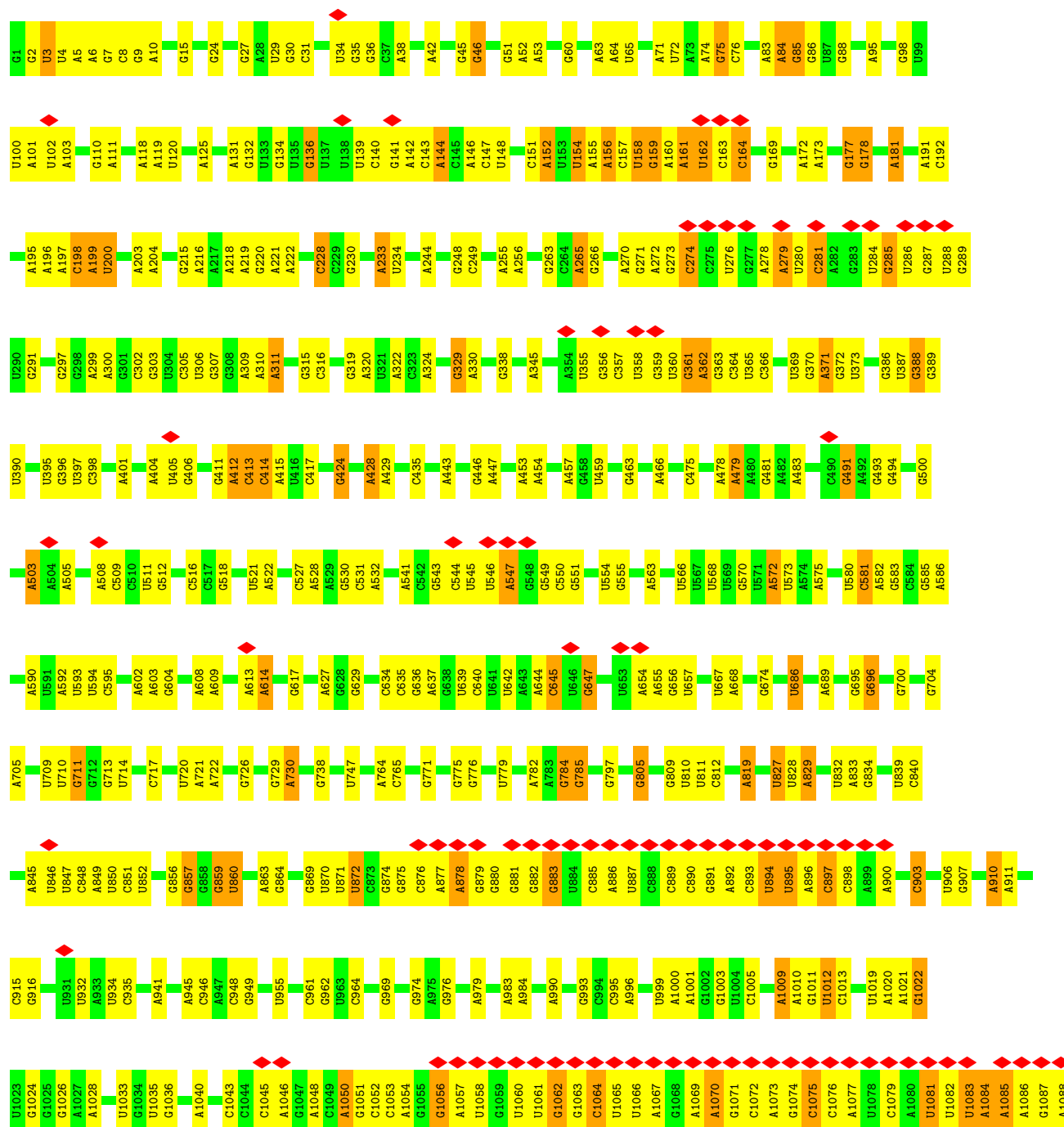




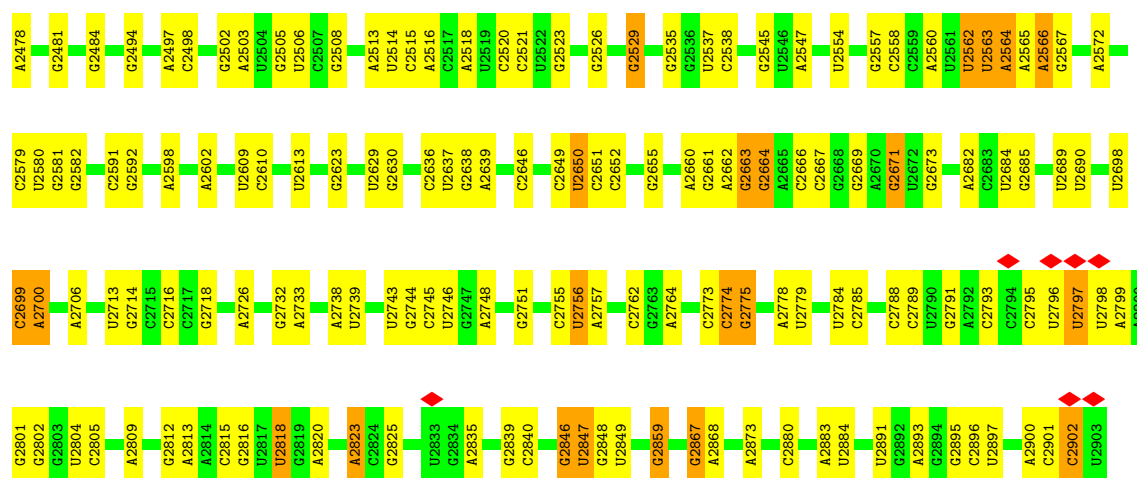
• Molecule 32: mRNA



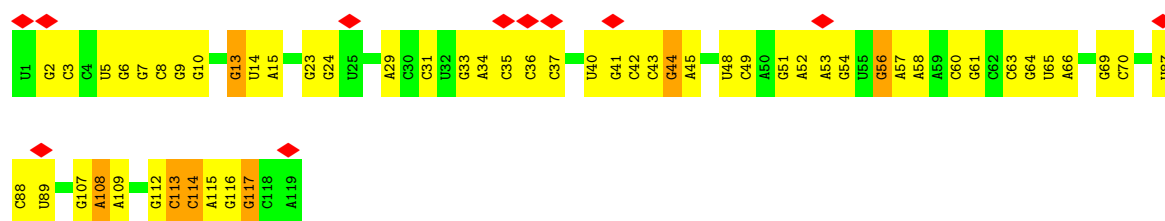
• Molecule 33: 23S ribosomal RNA



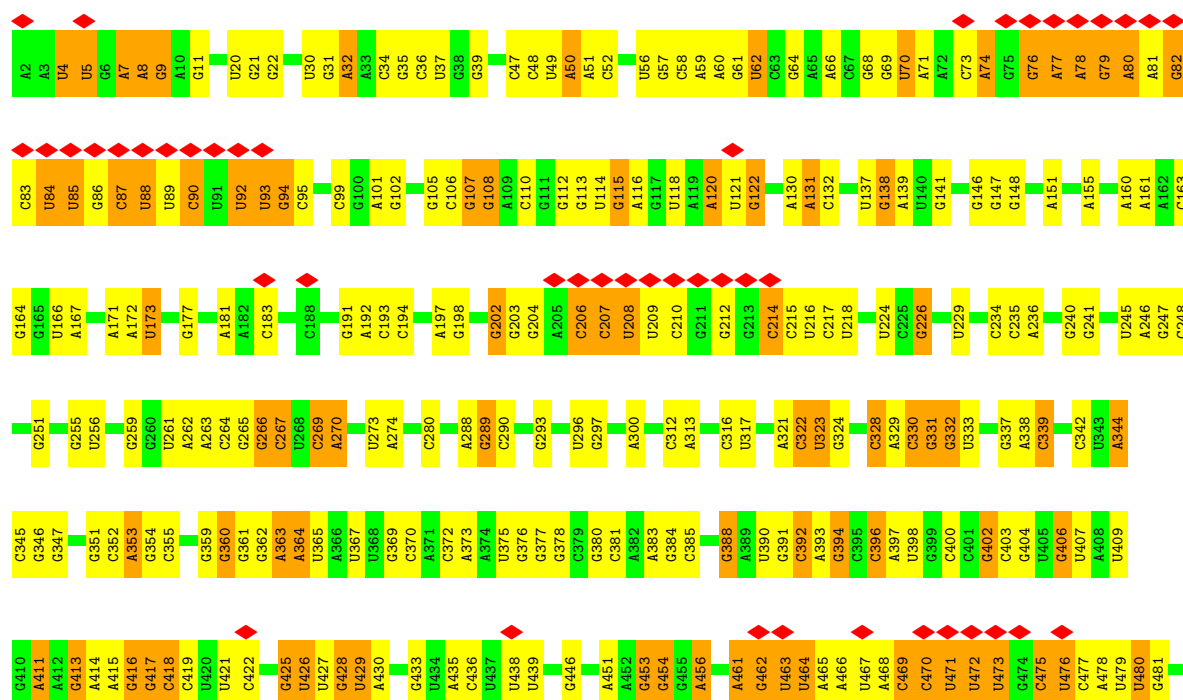
C2248	C2249	C2250	A2266	A2267	A2273	C2283	G2286	A2287	A2288	A2297	A2298	G2304	U2305	C2306	G2307	C2308	A2309	C2310	A2311	U2312	C2313	A2314	G2315	A2316	A2317	G2318	C2319	U2320	U2321	A2322	G2323	U2324	G2325	C2326	A2327	A2328	U2329	G2330	C2331	A2332	A2333	A2336	U2343	U2344	C2345	A2346	C2347	C2350	C2359										
A2169	A2170	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2185	G2186	U2187	U2188	U2189	A2190	A2191	U2192	G2193	A2198	A2199	C2200	U2203	G2204	C2208	A2211	A2212	U2213	C2214	G2217	G2221	A2225	C2226	U2229	U2233	G2234	U2238	G2239	U2243	U2244	U2245	G2246	A2247											
U2109	G2110	U2111	G2112	U2113	C2114	C2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	A2142	C2143	G2144	C2145	G2146	A2147	G2148	U2149	C2150	U2151	G2152	C2153	U2154	U2155	G2156	G2157	A2158	C2159	C2160	C2161	G2162	A2163	C2164	C2165	U2166	U2167	C2168
A1889	A1890	G1891	A1776	U1779	A1784	A1789	G1792	A1794	C1795	U1796	U1797	U1798	G1799	C1800	A1801	A1802	A1803	G1807	A1808	A1809	A1810	G1811	C1816	A1829	G1838	G1839	G1847	A1848	U1856	G1857	A1858	U1859	A1866	G1867	C1868	G1869	A1870	A1871	A1872	G1873	C1874	G1875	C1879	G1884															
U1648	G1649	A1654	A1655	C1656	U1657	G1667	G1674	C1675	G1682	U1683	A1689	A1690	U1693	C1694	G1707	U1714	G1715	U1716	U1720	G1721	G1724	U1725	G1726	C1727	C1728	U1729	C1730	G1731	G1732	U1736	G1737	G1738	A1739	G1740	C1741	A1744	A1745	A1746	U1747	G1756	A1757	U1758	C1764	C1771															
U1438	G1441	U1442	U1443	G1444	G1452	A1453	G1459	U1460	C1461	U1468	A1469	A1470	A1477	G1478	U1481	G1482	G1483	U1484	U1485	U1486	U1487	C1488	C1489	A1490	G1491	C1492	C1493	A1494	A1495	A1496	U1497	C1498	C1499	U1506	A1507	A1508	A1509	G1510	G1511	C1512	U1513	G1514	A1515	G1516	A1522	U1523	G1524	G1527	A1528	G1529									
G1530	C1531	A1532	C1533	U1534	A1535	C1536	U1537	G1538	U1539	G1540	C1541	U1542	G1543	A1544	A1548	A1549	U1559	G1560	U1563	C1564	C1565	A1566	A1569	U1578	A1583	U1584	C1585	A1590	A1591	C1592	A1593	U1594	C1595	A1596	A1597	A1598	C1607	A1608	A1609	A1610	G1622	A1626	G1631	A1632	A1633	A1634	U1647												
U1089	A1090	G1091	C1092	G1093	U1094	A1095	U1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	G1115	G1116	G1120	G1125	U1130	G1131	U1132	A1133	A1134	C1135	U1141	A1142	A1143	G1149	C1150	A1151	G1152	C1153	G1154	A1155	U1159	G1160	G1166	G1167	A1168	G1170	G1171									

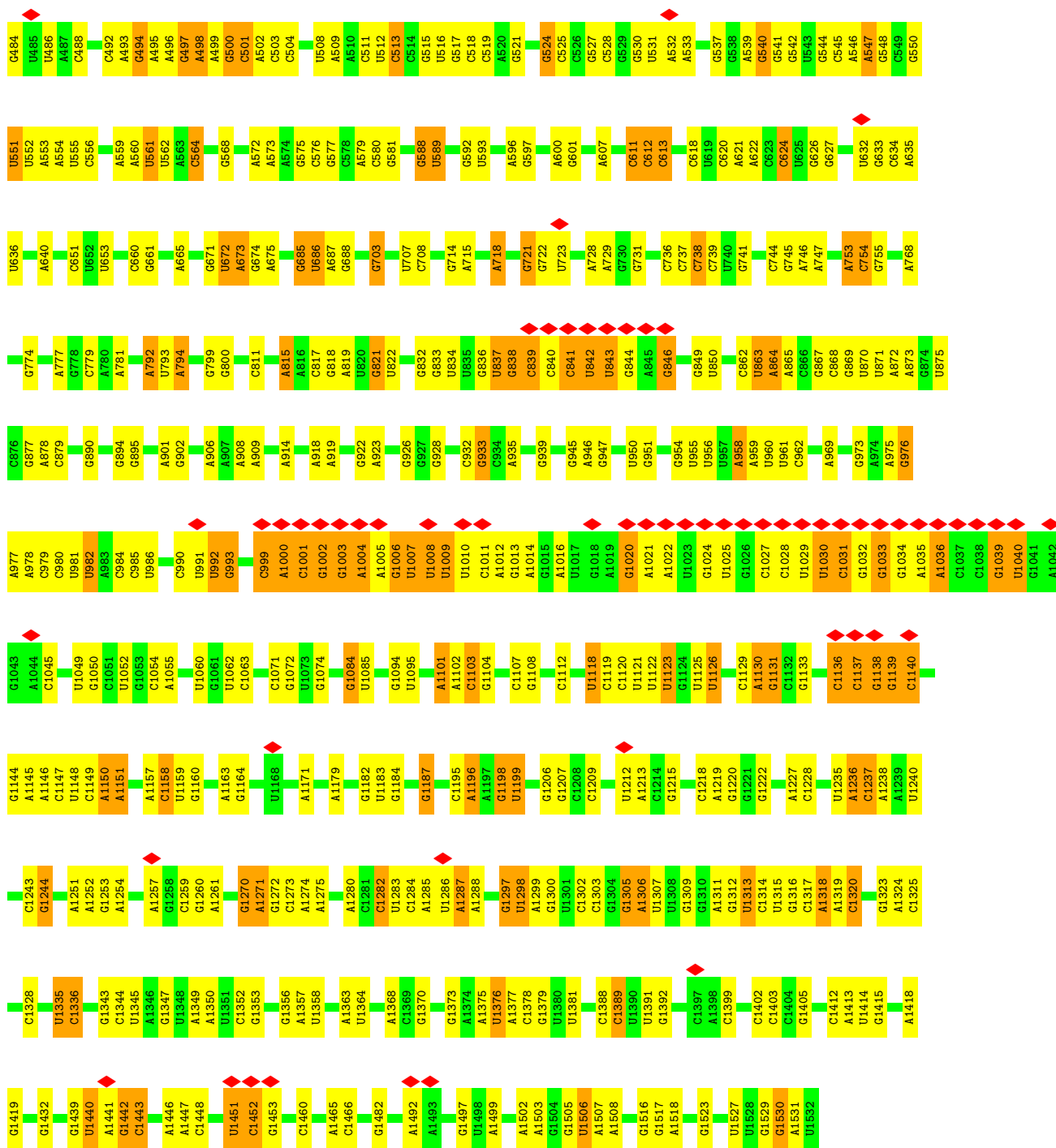


• Molecule 34: 5S ribosomal RNA

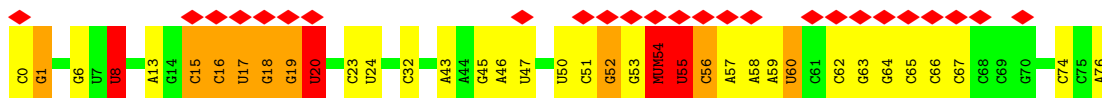


• Molecule 35: 16S ribosomal RNA

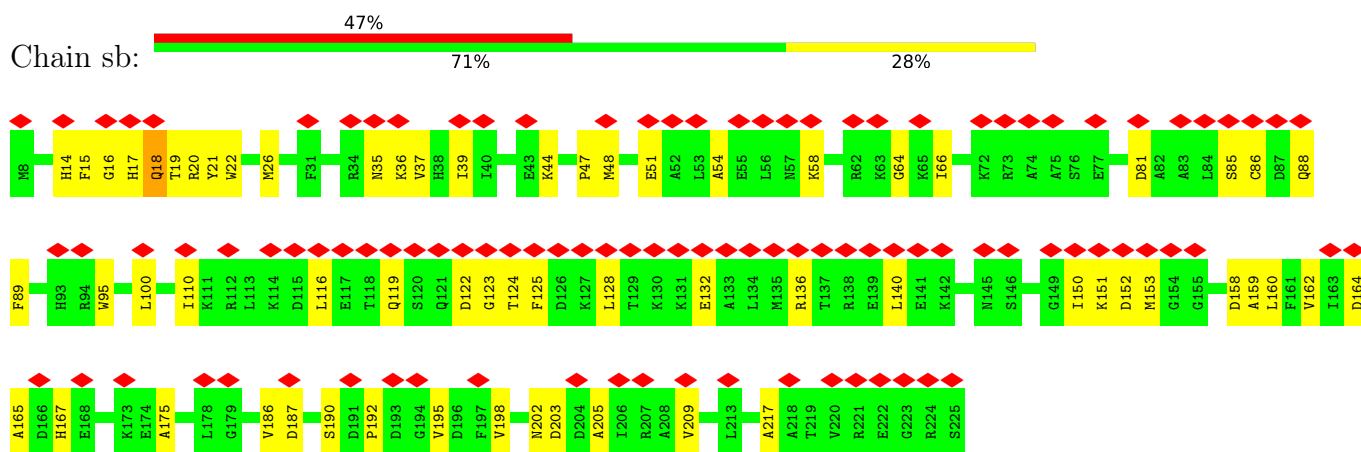




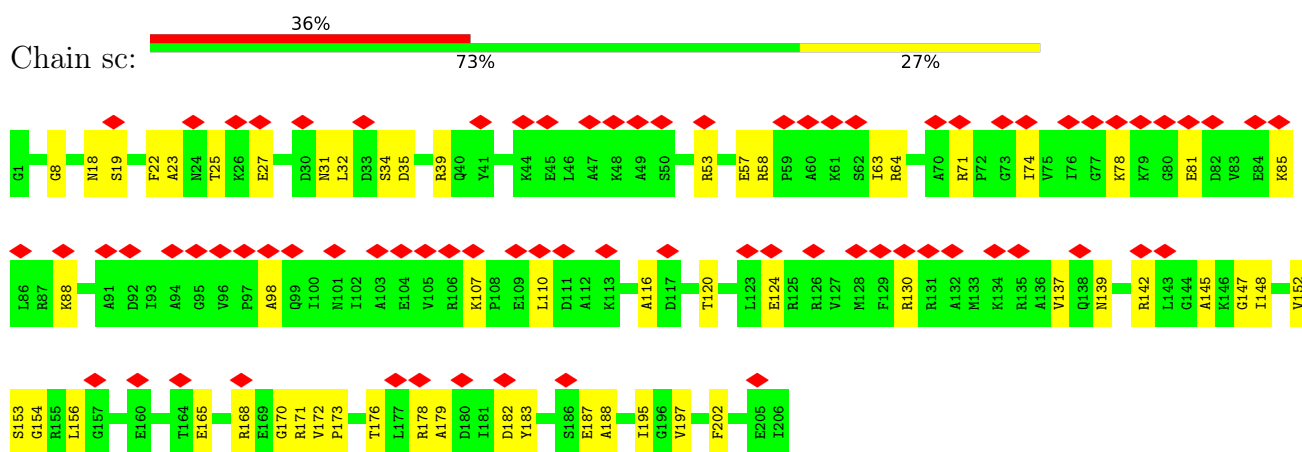
- Molecule 36: tRNA



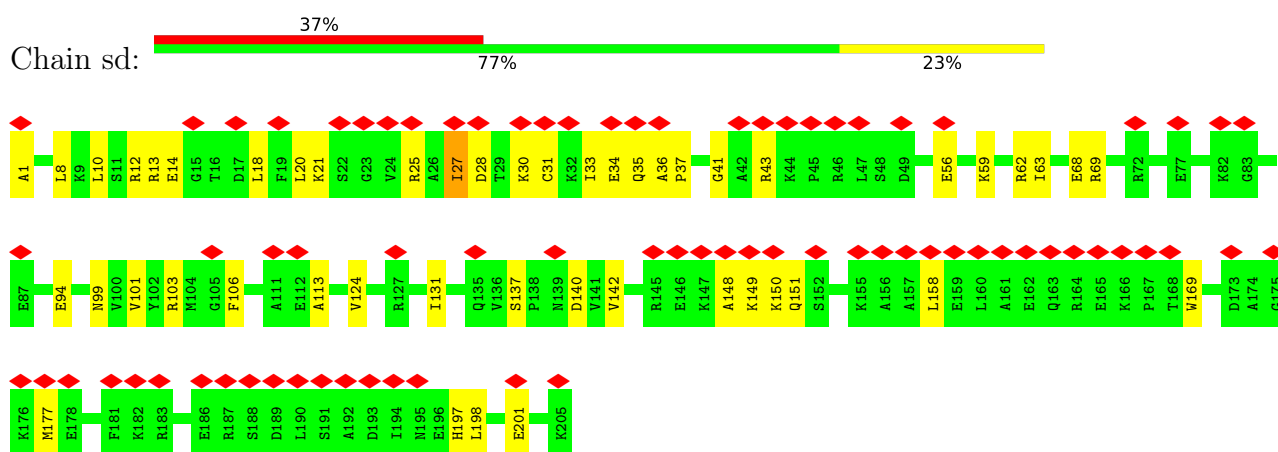
- Molecule 37: Small ribosomal subunit protein uS2



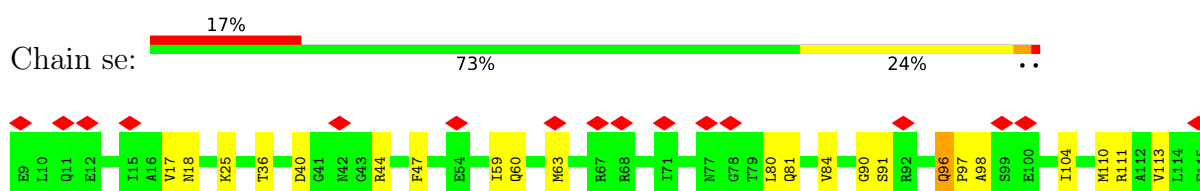
• Molecule 38: Small ribosomal subunit protein uS3

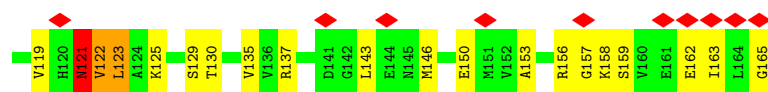


• Molecule 39: 30S ribosomal protein S4

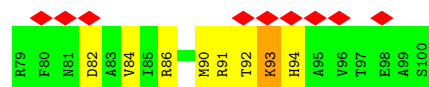


• Molecule 40: Small ribosomal subunit protein uS5

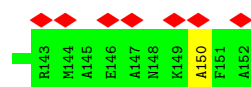
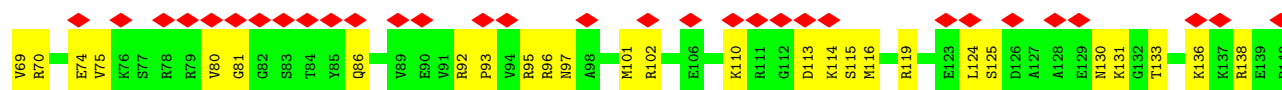
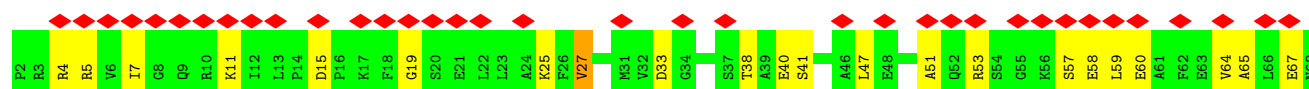




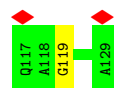
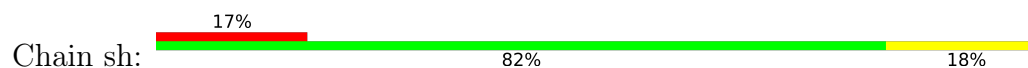
- Molecule 41: 30S ribosomal protein S6, non-modified isoform



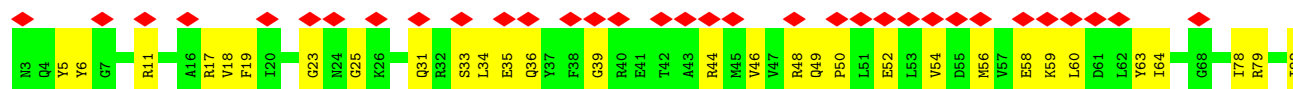
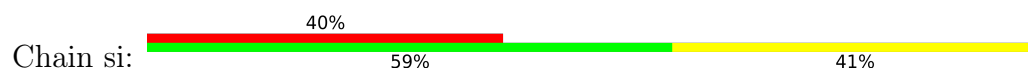
- Molecule 42: 30S ribosomal protein S7

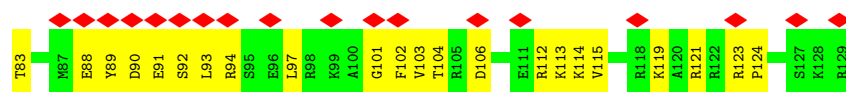


- Molecule 43: 30S ribosomal protein S8

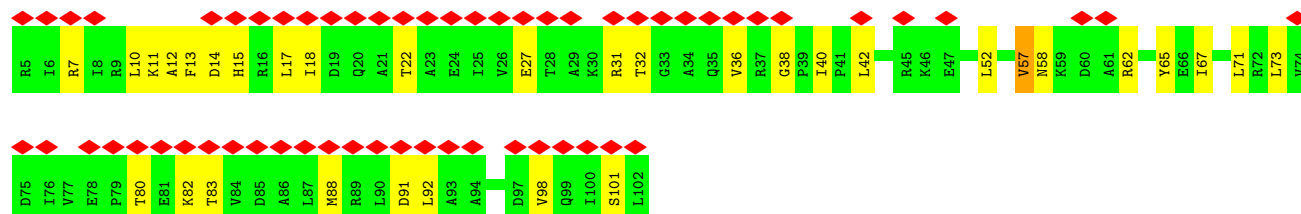


- Molecule 44: Small ribosomal subunit protein uS9

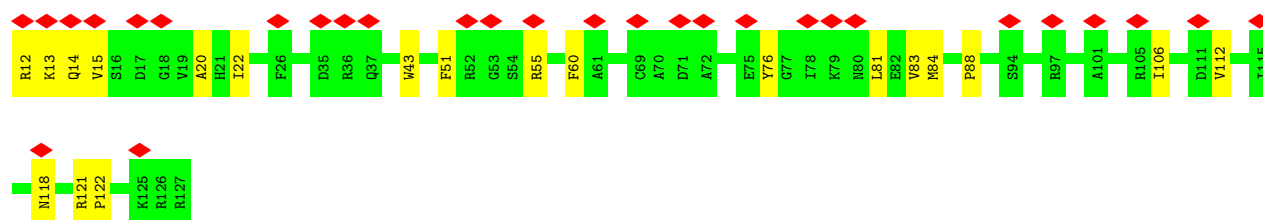
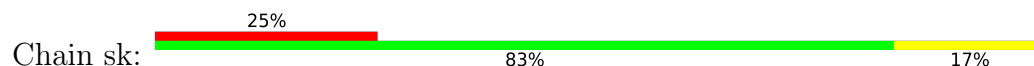




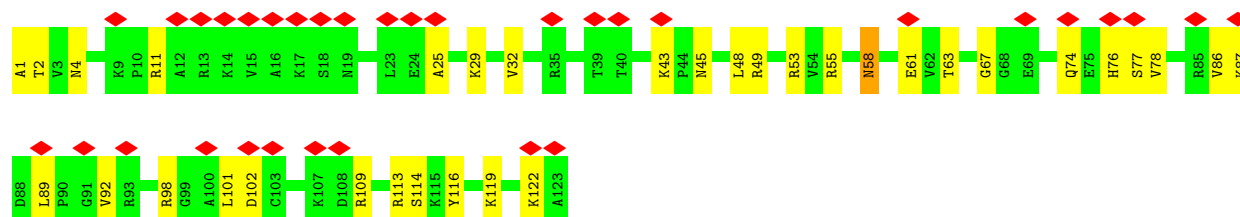
- Molecule 45: 30S ribosomal protein S10



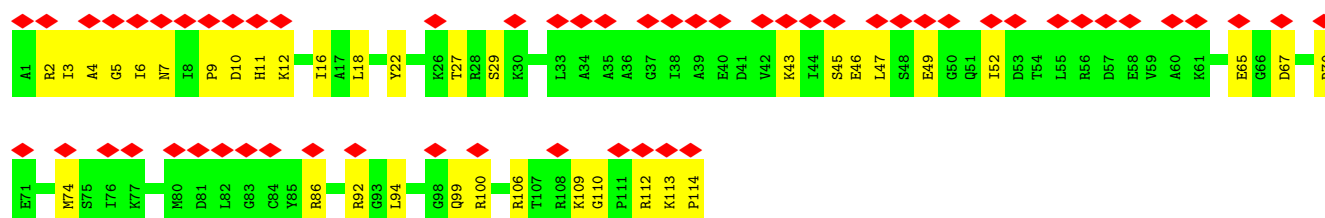
- Molecule 46: Small ribosomal subunit protein uS11



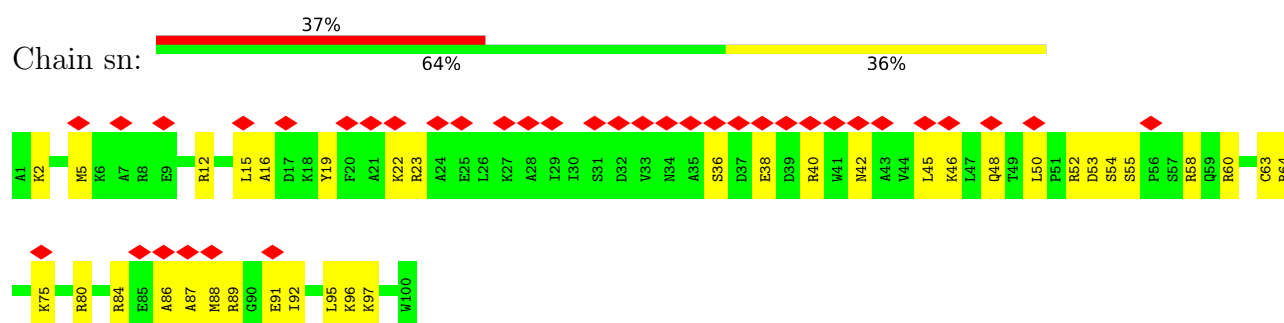
- Molecule 47: Small ribosomal subunit protein uS12



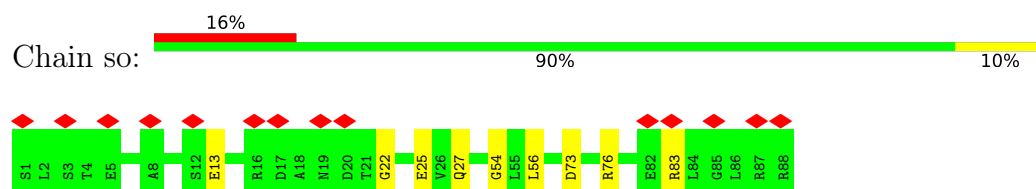
- Molecule 48: 30S ribosomal protein S13



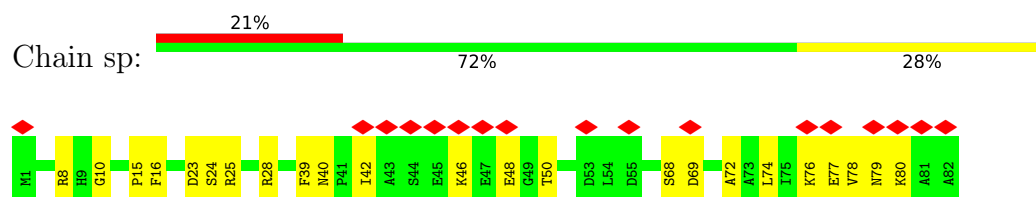
- Molecule 49: Small ribosomal subunit protein uS14



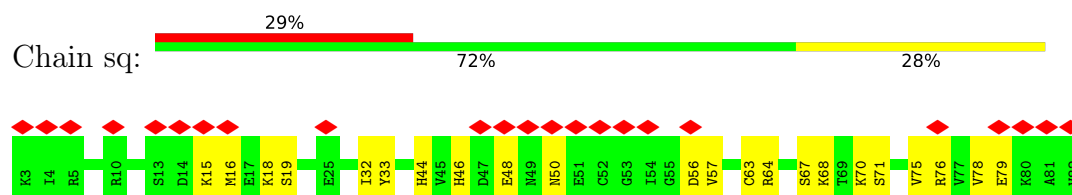
- Molecule 50: Small ribosomal subunit protein uS15



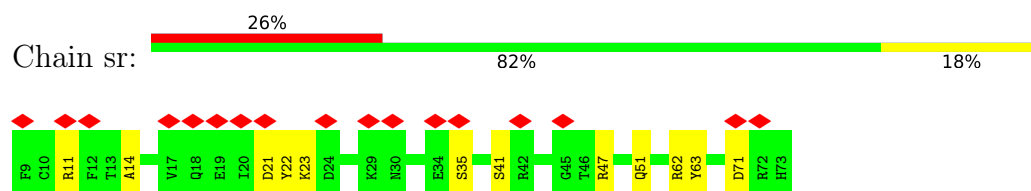
- Molecule 51: Small ribosomal subunit protein bS16



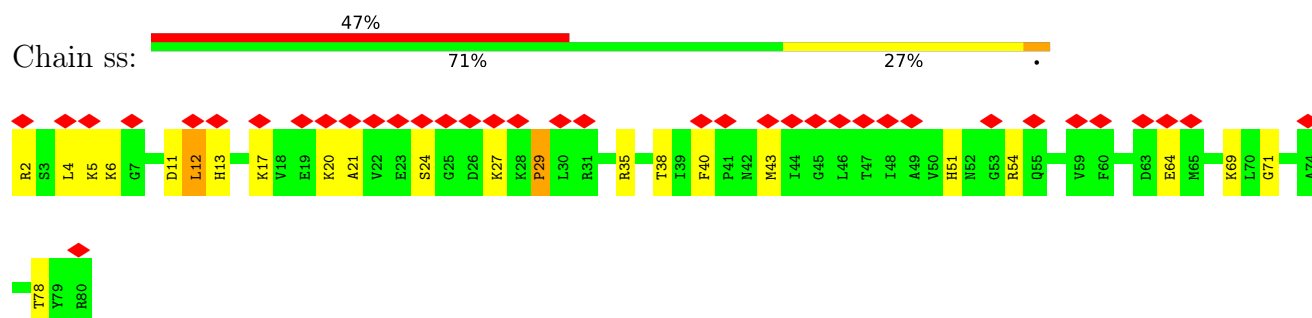
- Molecule 52: Small ribosomal subunit protein uS17



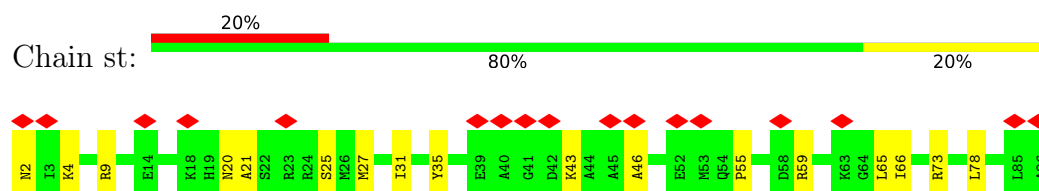
- Molecule 53: 30S ribosomal protein S18



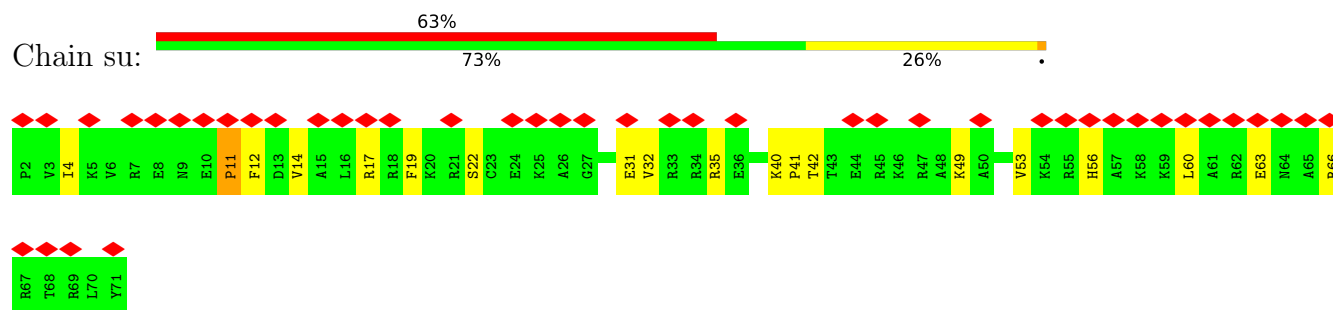
- Molecule 54: 30S ribosomal protein S19



● Molecule 55: 30S ribosomal protein S20



● Molecule 56: Small ribosomal subunit protein bS21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.378	Depositor
Minimum map value	-1.183	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, PSU, MUM, FME, NA, 4OC, ATP, MG, 4SU

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	1	0.11	0/1361	0.35	0/1796
2	13	0.23	0/1152	0.36	0/1551
3	14	0.23	0/947	0.40	0/1268
4	15	0.24	0/1054	0.40	0/1403
5	16	0.21	0/1093	0.39	0/1460
6	17	0.23	0/973	0.36	0/1301
7	18	0.16	0/902	0.28	0/1209
8	19	0.22	0/929	0.30	0/1242
9	2	0.25	0/2121	0.35	0/2852
10	20	0.25	0/960	0.30	0/1278
11	21	0.22	0/829	0.42	0/1107
12	22	0.22	0/864	0.33	0/1156
13	23	0.20	0/744	0.36	0/994
14	24	0.18	0/787	0.37	0/1051
15	25	0.18	0/766	0.35	0/1025
16	27	0.23	0/589	0.29	0/779
17	28	0.22	0/635	0.27	0/848
18	29	0.16	0/510	0.28	0/677
19	3	0.24	0/1586	0.38	0/2134
20	30	0.21	0/453	0.30	0/605
21	31	0.18	0/531	0.41	0/709
22	32	0.23	0/450	0.35	0/599
23	33	0.19	0/416	0.32	0/554
24	34	0.25	0/380	0.37	0/498
25	35	0.26	0/513	0.59	1/676 (0.1%)
26	36	0.23	0/303	0.30	0/397
27	4	0.21	0/1571	0.34	0/2113
28	5	0.16	0/1434	0.34	0/1926
29	6	0.74	3/1343 (0.2%)	1.00	5/1816 (0.3%)
30	9	0.15	0/1122	0.41	0/1515
31	E	0.18	0/4441	0.38	0/5993
32	M	0.16	0/219	0.25	0/339

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	R1	0.25	0/69797	0.31	0/108890
34	R2	0.20	0/2847	0.30	0/4440
35	R3	0.22	0/36782	0.33	0/57377
36	T	0.22	0/1716	0.31	0/2672
37	sb	0.18	0/1735	0.41	0/2338
38	sc	0.19	0/1651	0.30	0/2225
39	sd	0.17	0/1665	0.37	0/2227
40	se	0.20	0/1169	0.47	0/1573
41	sf	0.18	0/835	0.50	0/1128
42	sg	0.16	0/1195	0.33	0/1602
43	sh	0.20	0/989	0.35	0/1326
44	si	0.19	0/1034	0.46	0/1375
45	sj	0.19	0/796	0.45	0/1077
46	sk	0.19	0/885	0.32	0/1195
47	sl	0.21	0/969	0.45	0/1300
48	sm	0.18	0/892	0.38	0/1193
49	sn	0.18	0/817	0.44	0/1088
50	so	0.19	0/722	0.32	0/964
51	sp	0.21	0/659	0.36	0/884
52	sq	0.20	0/657	0.38	0/881
53	sr	0.19	0/544	0.35	0/731
54	ss	0.49	2/652 (0.3%)	1.09	4/877 (0.5%)
55	st	0.18	0/671	0.29	0/888
56	su	0.19	0/598	0.38	1/792 (0.1%)
All	All	0.24	5/162255 (0.0%)	0.35	11/241914 (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
25	35	0	1
29	6	0	1
30	9	0	1
36	T	8	0
39	sd	0	1
40	se	0	1
41	sf	0	1
49	sn	0	1
All	All	8	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	111	PRO	CG-CD	-20.34	0.81	1.50
29	6	111	PRO	CB-CG	15.36	2.26	1.49
54	ss	29	PRO	CG-CD	-8.65	1.21	1.50
54	ss	29	PRO	CB-CG	-7.25	1.13	1.49
29	6	111	PRO	N-CD	5.35	1.55	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	111	PRO	N-CD-CG	-20.10	73.05	103.20
54	ss	29	PRO	N-CD-CG	-18.37	75.64	103.20
29	6	111	PRO	N-CA-CB	-18.22	84.11	103.25
29	6	111	PRO	CA-CB-CG	-17.83	70.61	104.50
29	6	111	PRO	CB-CG-CD	-17.77	49.22	106.10

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	T	8	4SU	C2',C1'
36	T	20	H2U	C2'
36	T	32	4OC	C2'
36	T	54	MUM	C4',C3',C5
36	T	55	PSU	C4'

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	35	30	HIS	Peptide
29	6	12	ALA	Peptide
30	9	8	LYS	Peptide
39	sd	27	ILE	Peptide
40	se	121	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1353	0	1159	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	13	1129	0	1162	16	0
3	14	938	0	1012	24	0
4	15	1045	0	1117	24	0
5	16	1074	0	1157	17	0
6	17	960	0	1000	13	0
7	18	892	0	923	15	0
8	19	917	0	965	17	0
9	2	2082	0	2157	35	0
10	20	947	0	1022	12	0
11	21	816	0	839	26	0
12	22	857	0	922	15	0
13	23	738	0	807	16	0
14	24	779	0	834	23	0
15	25	753	0	780	13	0
16	27	582	0	599	7	0
17	28	625	0	655	10	0
18	29	509	0	543	9	0
19	3	1565	0	1616	30	0
20	30	449	0	491	7	0
21	31	522	0	524	14	0
22	32	444	0	461	18	0
23	33	409	0	440	9	0
24	34	377	0	418	5	0
25	35	504	0	574	15	0
26	36	302	0	343	10	0
27	4	1552	0	1619	27	0
28	5	1410	0	1447	40	0
29	6	1323	0	1374	30	0
30	9	1111	0	1148	29	0
31	E	4360	0	4336	105	0
32	M	195	0	99	0	0
33	R1	62318	0	31344	640	0
34	R2	2546	0	1292	37	0
35	R3	32850	0	16534	456	0
36	T	1639	0	831	29	0
37	sb	1704	0	1732	45	0
38	sc	1624	0	1699	41	0
39	sd	1643	0	1710	41	0
40	se	1156	0	1199	32	0
41	sf	817	0	808	24	0
42	sg	1181	0	1238	42	0
43	sh	979	0	1034	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	si	1022	0	1070	38	0
45	sj	786	0	828	24	0
46	sk	869	0	878	16	0
47	sl	955	0	1019	30	0
48	sm	883	0	944	29	0
49	sn	805	0	847	30	0
50	so	714	0	737	7	0
51	sp	649	0	666	20	0
52	sq	648	0	691	16	0
53	sr	535	0	552	8	0
54	ss	637	0	665	23	0
55	st	665	0	714	18	0
56	su	590	0	629	13	0
57	15	1	0	0	0	0
57	2	1	0	0	0	0
57	32	1	0	0	0	0
57	R1	199	0	0	0	0
57	R3	77	0	0	0	0
58	E	62	0	24	4	0
59	E	2	0	0	0	0
60	T	10	0	10	2	0
All	All	150087	0	102238	2088	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 8.

The worst 5 of 2088 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)
33:R1:136:G:N1	33:R1:142:A:C2	2.28	1.02
33:R1:134:G:H1	33:R1:144:A:N6	1.62	0.98
33:R1:136:G:N1	33:R1:142:A:H2	1.59	0.96
35:R3:359:G:HO2'	35:R3:360:G:H8	0.96	0.91
38:sc:8:GLY:HA3	49:sn:88:MET:HB3	1.54	0.89

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	1	218/220 (99%)	189 (87%)	29 (13%)	0	100	100
2	13	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
3	14	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
4	15	141/143 (99%)	123 (87%)	18 (13%)	0	100	100
5	16	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
6	17	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
7	18	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
8	19	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
9	2	269/271 (99%)	244 (91%)	25 (9%)	0	100	100
10	20	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
11	21	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
12	22	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
13	23	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
14	24	100/102 (98%)	90 (90%)	10 (10%)	0	100	100
15	25	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
16	27	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
17	28	75/77 (97%)	75 (100%)	0	0	100	100
18	29	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
19	3	207/209 (99%)	186 (90%)	21 (10%)	0	100	100
20	30	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
21	31	64/66 (97%)	54 (84%)	10 (16%)	0	100	100
22	32	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
23	33	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
24	34	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
25	35	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	7	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	36	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
27	4	199/201 (99%)	184 (92%)	15 (8%)	0	100	100
28	5	175/177 (99%)	160 (91%)	15 (9%)	0	100	100
29	6	174/176 (99%)	157 (90%)	17 (10%)	0	100	100
30	9	147/149 (99%)	126 (86%)	19 (13%)	2 (1%)	9	39
31	E	550/552 (100%)	496 (90%)	51 (9%)	3 (0%)	24	59
37	sb	216/218 (99%)	190 (88%)	25 (12%)	1 (0%)	24	59
38	sc	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
39	sd	203/205 (99%)	180 (89%)	23 (11%)	0	100	100
40	se	155/157 (99%)	135 (87%)	18 (12%)	2 (1%)	9	40
41	sf	98/100 (98%)	80 (82%)	18 (18%)	0	100	100
42	sg	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
43	sh	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
44	si	125/127 (98%)	106 (85%)	19 (15%)	0	100	100
45	sj	96/98 (98%)	85 (88%)	10 (10%)	1 (1%)	12	45
46	sk	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
47	sl	121/123 (98%)	91 (75%)	30 (25%)	0	100	100
48	sm	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
49	sn	98/100 (98%)	75 (76%)	23 (24%)	0	100	100
50	so	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
51	sp	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
52	sq	78/80 (98%)	66 (85%)	12 (15%)	0	100	100
53	sr	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
54	ss	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
55	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
56	su	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
All	All	6352/6454 (98%)	5731 (90%)	611 (10%)	10 (0%)	44	73

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	35	31	ILE
31	E	18	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	sb	18	GLN
40	se	122	VAL
31	E	211	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	1	106/171 (62%)	106 (100%)	0	100	100
2	13	116/116 (100%)	115 (99%)	1 (1%)	70	81
3	14	103/103 (100%)	103 (100%)	0	100	100
4	15	102/102 (100%)	102 (100%)	0	100	100
5	16	109/109 (100%)	106 (97%)	3 (3%)	38	68
6	17	100/100 (100%)	100 (100%)	0	100	100
7	18	86/86 (100%)	85 (99%)	1 (1%)	63	79
8	19	99/99 (100%)	97 (98%)	2 (2%)	48	72
9	2	216/216 (100%)	216 (100%)	0	100	100
10	20	89/89 (100%)	87 (98%)	2 (2%)	45	71
11	21	84/84 (100%)	84 (100%)	0	100	100
12	22	93/93 (100%)	91 (98%)	2 (2%)	45	71
13	23	80/80 (100%)	80 (100%)	0	100	100
14	24	83/83 (100%)	83 (100%)	0	100	100
15	25	78/78 (100%)	76 (97%)	2 (3%)	40	69
16	27	58/58 (100%)	57 (98%)	1 (2%)	53	75
17	28	67/67 (100%)	66 (98%)	1 (2%)	57	76
18	29	55/55 (100%)	55 (100%)	0	100	100
19	3	164/164 (100%)	164 (100%)	0	100	100
20	30	48/48 (100%)	48 (100%)	0	100	100
21	31	59/59 (100%)	59 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	32	47/47 (100%)	47 (100%)	0	100	100
23	33	45/45 (100%)	45 (100%)	0	100	100
24	34	38/38 (100%)	38 (100%)	0	100	100
25	35	51/51 (100%)	50 (98%)	1 (2%)	48	72
26	36	34/34 (100%)	32 (94%)	2 (6%)	18	50
27	4	165/165 (100%)	163 (99%)	2 (1%)	63	79
28	5	148/148 (100%)	144 (97%)	4 (3%)	39	68
29	6	137/137 (100%)	137 (100%)	0	100	100
30	9	114/114 (100%)	113 (99%)	1 (1%)	70	81
31	E	461/464 (99%)	460 (100%)	1 (0%)	87	89
37	sb	180/180 (100%)	179 (99%)	1 (1%)	78	84
38	sc	170/170 (100%)	169 (99%)	1 (1%)	78	84
39	sd	172/172 (100%)	172 (100%)	0	100	100
40	se	119/119 (100%)	115 (97%)	4 (3%)	32	64
41	sf	87/87 (100%)	86 (99%)	1 (1%)	65	79
42	sg	124/124 (100%)	123 (99%)	1 (1%)	73	82
43	sh	104/104 (100%)	104 (100%)	0	100	100
44	si	105/105 (100%)	105 (100%)	0	100	100
45	sj	86/86 (100%)	86 (100%)	0	100	100
46	sk	89/89 (100%)	89 (100%)	0	100	100
47	sl	103/103 (100%)	102 (99%)	1 (1%)	68	80
48	sm	92/92 (100%)	92 (100%)	0	100	100
49	sn	83/83 (100%)	83 (100%)	0	100	100
50	so	76/76 (100%)	76 (100%)	0	100	100
51	sp	65/65 (100%)	65 (100%)	0	100	100
52	sq	74/74 (100%)	74 (100%)	0	100	100
53	sr	56/56 (100%)	56 (100%)	0	100	100
54	ss	70/70 (100%)	68 (97%)	2 (3%)	37	67
55	st	65/65 (100%)	65 (100%)	0	100	100
56	su	60/60 (100%)	60 (100%)	0	100	100
All	All	5215/5283 (99%)	5178 (99%)	37 (1%)	73	83

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	se	17	VAL
54	ss	12	LEU
40	se	25	LYS
41	sf	73	GLU
15	25	49	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
31	E	139	ASN
39	sd	135	GLN
31	E	224	ASN
38	sc	101	ASN
41	sf	14	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	M	8/9 (88%)	1 (12%)	0
33	R1	2902/2903 (99%)	571 (19%)	21 (0%)
34	R2	118/119 (99%)	17 (14%)	0
35	R3	1529/1531 (99%)	390 (25%)	23 (1%)
36	T	76/77 (98%)	20 (26%)	3 (3%)
All	All	4633/4639 (99%)	999 (21%)	47 (1%)

5 of 999 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	M	7	A
33	R1	2	G
33	R1	3	U
33	R1	10	A
33	R1	15	G

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	R3	472	U
35	R3	685	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	R3	497	G
35	R3	588	G
35	R3	837	U

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
36	4SU	T	8	36	18,21,22	3.64	8 (44%)	25,30,33	2.27	5 (20%)
36	4OC	T	32	36	20,23,24	2.70	5 (25%)	25,32,35	1.09	2 (8%)
36	H2U	T	20	36	18,21,22	4.56	5 (27%)	19,30,33	3.83	6 (31%)
36	PSU	T	55	36	18,21,22	2.23	7 (38%)	21,30,33	2.16	5 (23%)
36	MUM	T	54	36	18,22,22	3.39	6 (33%)	19,32,32	2.17	5 (26%)

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
36	4SU	T	8	36	2/2/5/5	0/7/25/26	0/2/2/2
36	4OC	T	32	36	1/1/5/6	1/9/29/30	0/2/2/2
36	H2U	T	20	36	1/1/8/9	5/7/38/39	0/2/2/2
36	PSU	T	55	36	1/1/5/5	5/7/25/26	0/2/2/2
36	MUM	T	54	36	3/3/9/10	3/7/41/41	0/2/2/2

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	T	54	MUM	C6-N1	-12.32	1.31	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	T	20	H2U	O4-C4	11.19	1.45	1.23
36	T	8	4SU	O2-C2	10.65	1.41	1.23
36	T	20	H2U	C2-N1	9.58	1.48	1.35
36	T	32	4OC	O2-C2	9.31	1.41	1.23

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	T	20	H2U	O2-C2-N1	-10.22	110.81	123.10
36	T	20	H2U	O4-C4-N3	-7.61	108.56	120.30
36	T	8	4SU	C4-N3-C2	-6.81	120.78	127.31
36	T	55	PSU	N1-C2-N3	6.59	122.12	115.17
36	T	20	H2U	O4-C4-C5	-6.48	108.93	122.20

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	T	20	H2U	C2'
36	T	32	4OC	C2'
36	T	54	MUM	C4'
36	T	54	MUM	C3'
36	T	54	MUM	C5

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	T	20	H2U	O4'-C1'-N1-C2
36	T	20	H2U	O4'-C1'-N1-C6
36	T	54	MUM	O4'-C4'-C5'-O5'
36	T	54	MUM	C3'-C4'-C5'-O5'
36	T	54	MUM	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	T	20	H2U	2	0
36	T	55	PSU	1	0
36	T	54	MUM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 284 ligands modelled in this entry, 281 are monoatomic - leaving 3 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	$\# Z > 2$
58	ATP	E	601	59	32,33,33	0.59	1 (3%)	48,52,52	0.31	0
58	ATP	E	602	59	32,33,33	0.43	0	48,52,52	0.32	0
60	FME	T	101	36	8,9,10	0.96	0	8,9,11	1.00	0

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
58	ATP	E	601	59	-	5/22/38/38	0/3/3/3
58	ATP	E	602	59	-	4/22/38/38	0/3/3/3
60	FME	T	101	36	-	5/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	E	601	ATP	PA-O3A	-2.21	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	E	601	ATP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	E	601	ATP	C5'-O5'-PA-O2A
58	E	601	ATP	C5'-O5'-PA-O3A
58	E	602	ATP	PB-O3B-PG-O2G
60	T	101	FME	N-CA-CB-CG

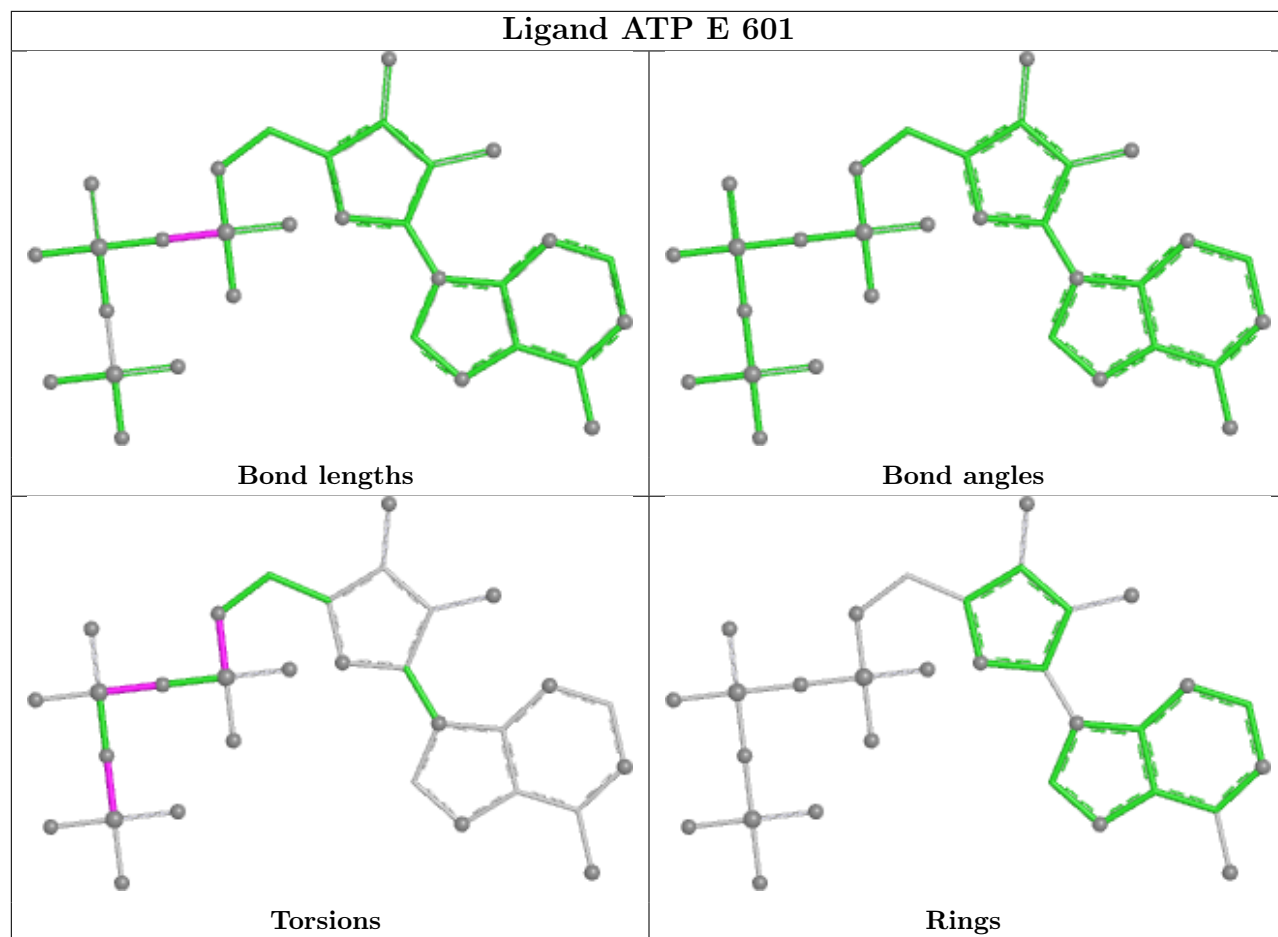
There are no ring outliers.

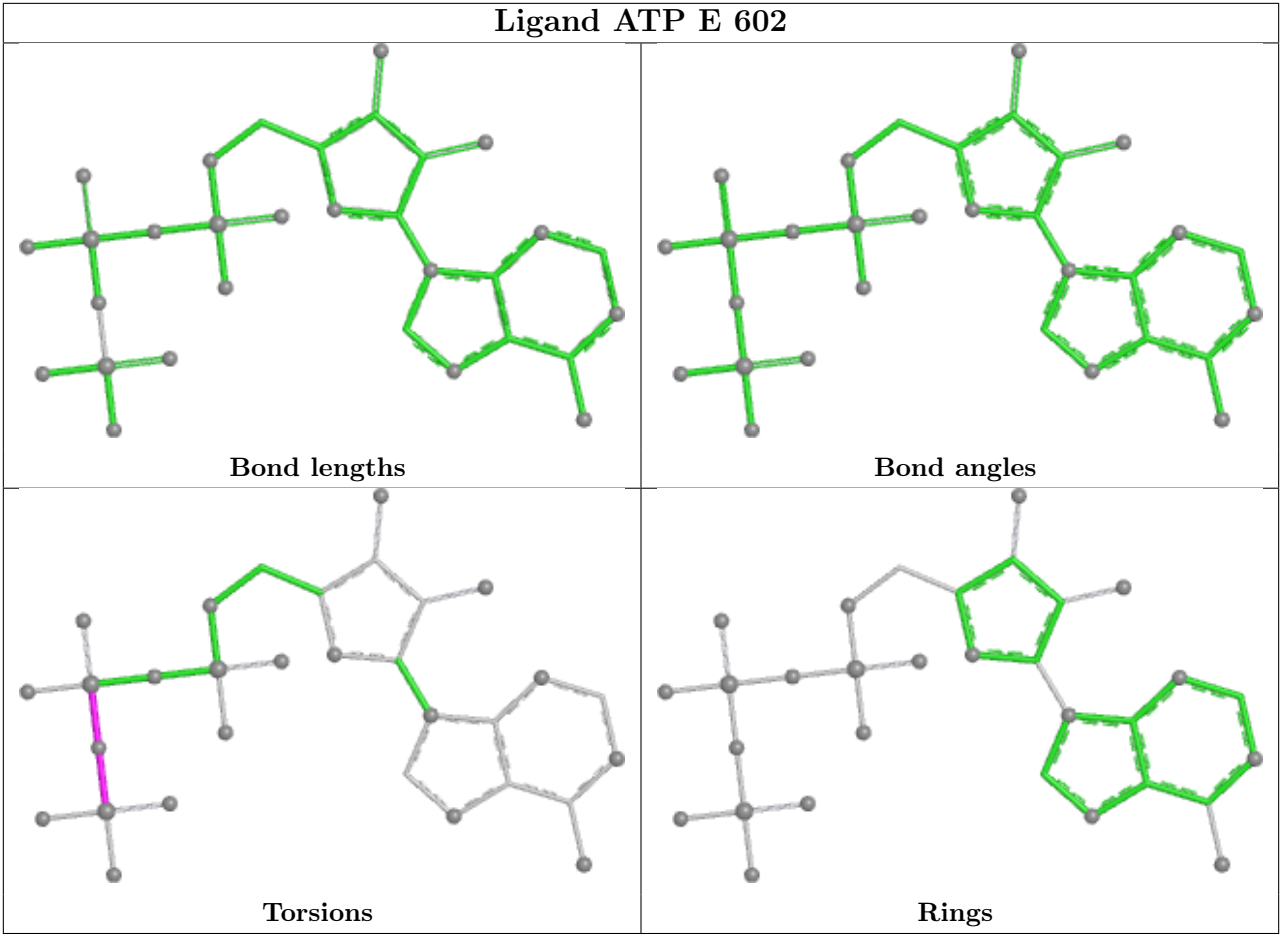
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	E	601	ATP	3	0
58	E	602	ATP	1	0
60	T	101	FME	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP E 601





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
35	R3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	460:A	O3'	461:A	P	5.06
1	R3	210:C	O3'	211:G	P	3.72

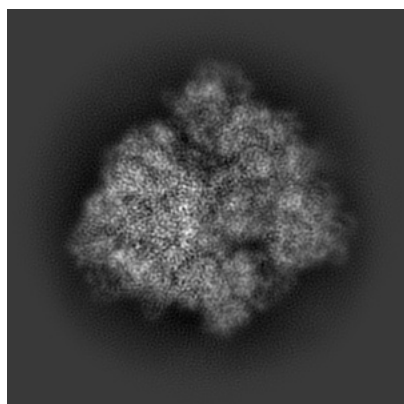
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40929. These allow visual inspection of the internal detail of the map and identification of artifacts.

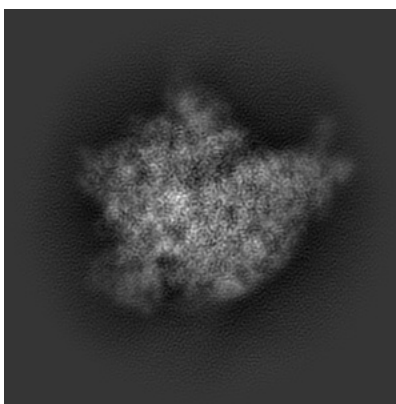
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

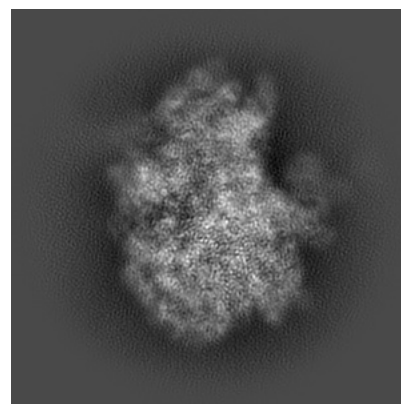
6.1.1 Primary map



X

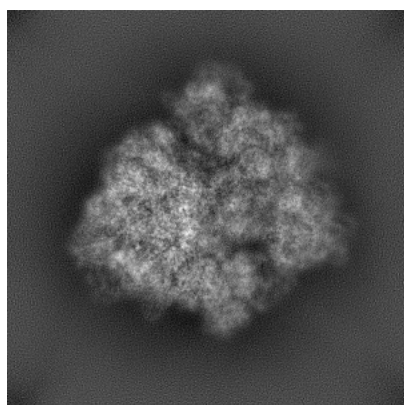


Y

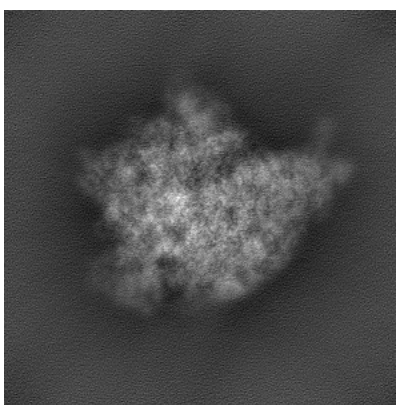


Z

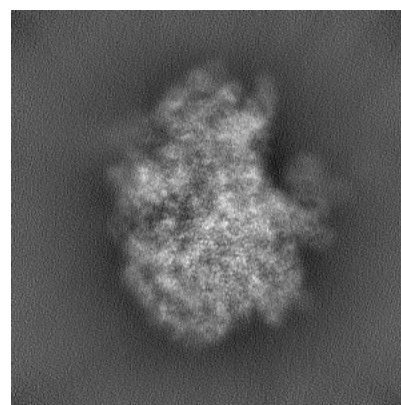
6.1.2 Raw map



X



Y

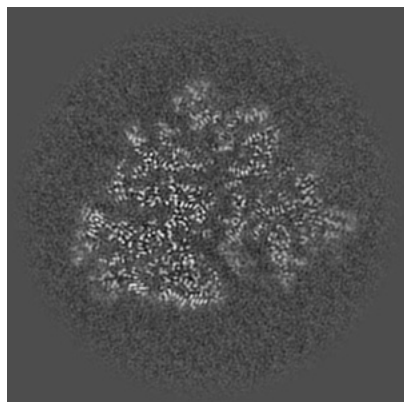


Z

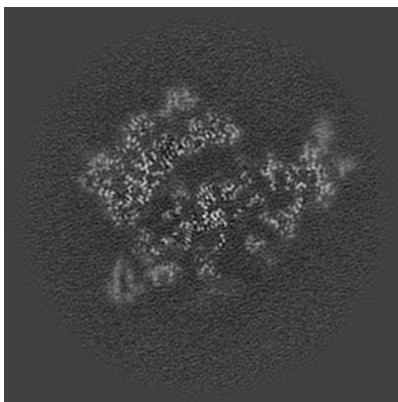
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

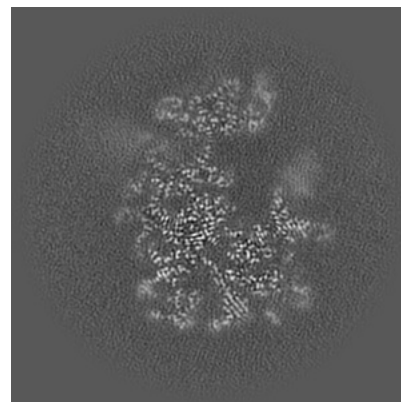
6.2.1 Primary map



X Index: 200

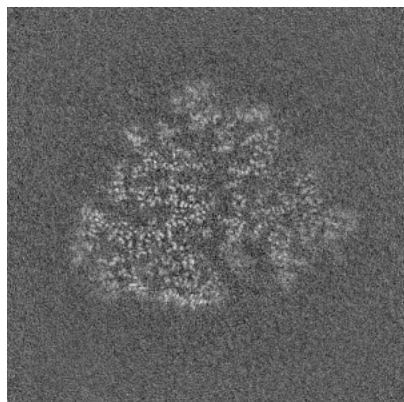


Y Index: 200

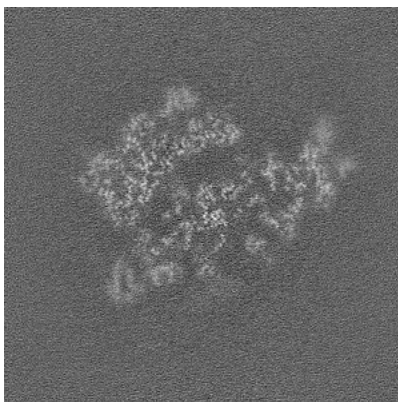


Z Index: 200

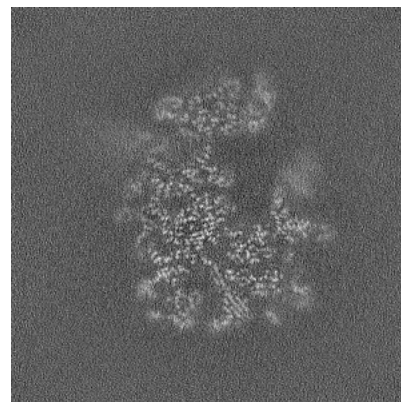
6.2.2 Raw map



X Index: 200



Y Index: 200

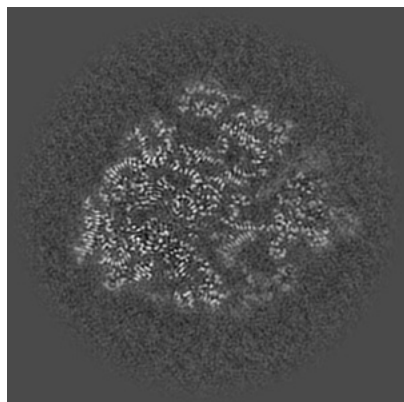


Z Index: 200

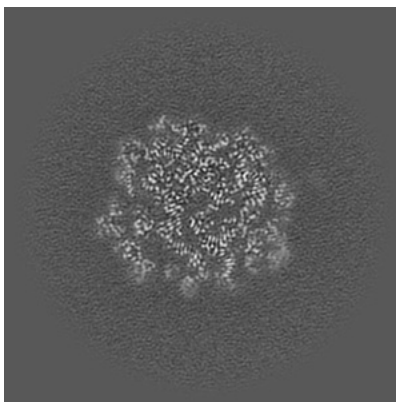
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

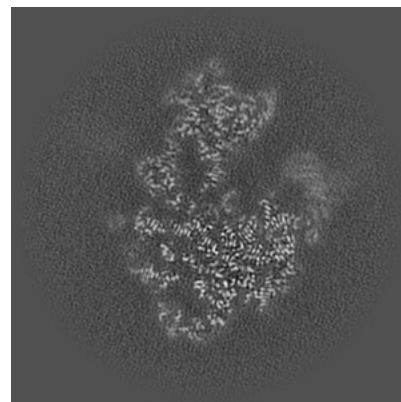
6.3.1 Primary map



X Index: 207

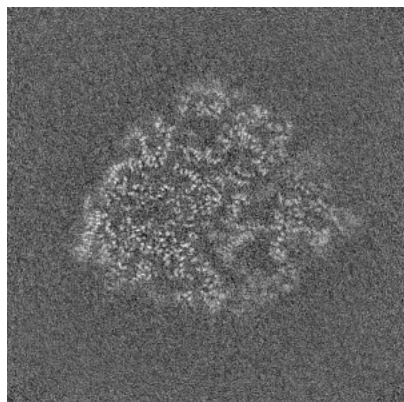


Y Index: 152

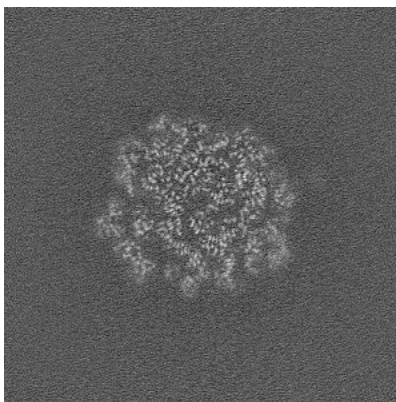


Z Index: 177

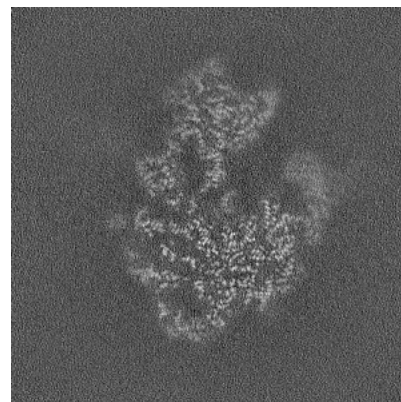
6.3.2 Raw map



X Index: 208



Y Index: 152

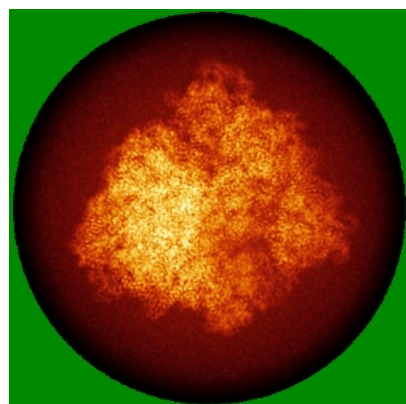


Z Index: 178

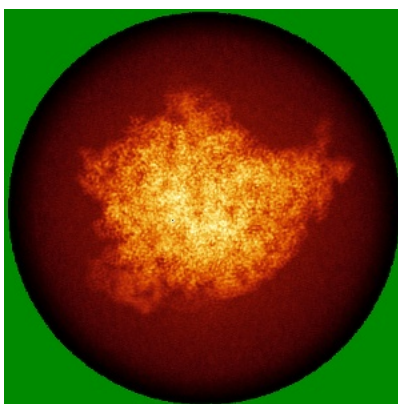
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

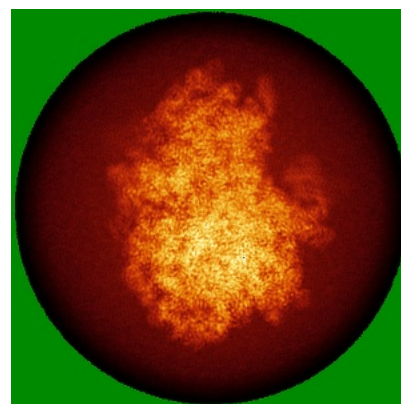
6.4.1 Primary map



X

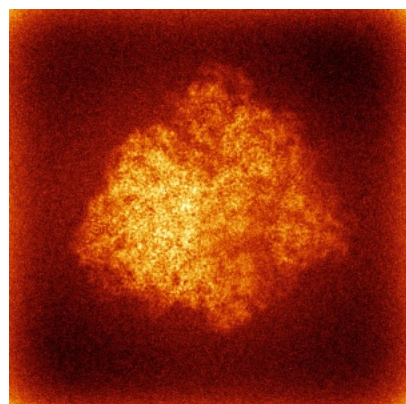


Y

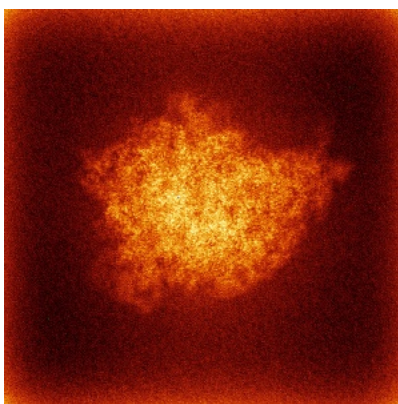


Z

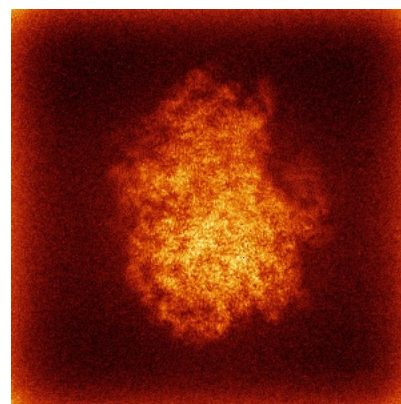
6.4.2 Raw map



X



Y

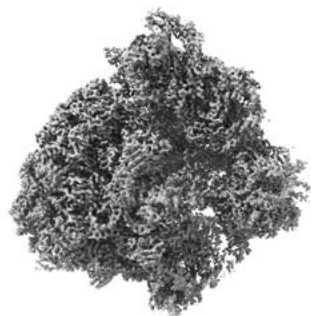


Z

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 [i](#)

6.5.1 Primary map



X



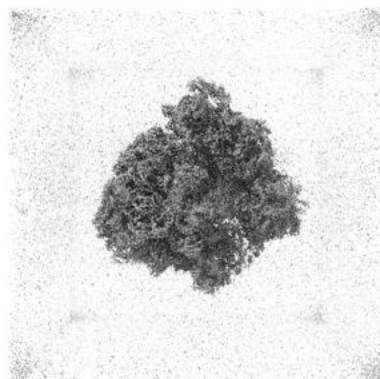
Y



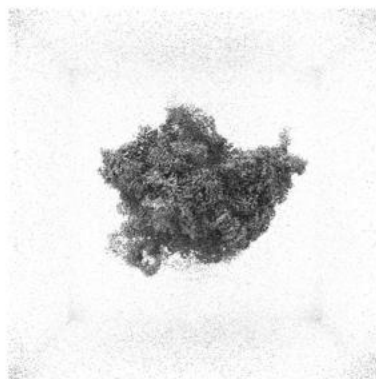
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

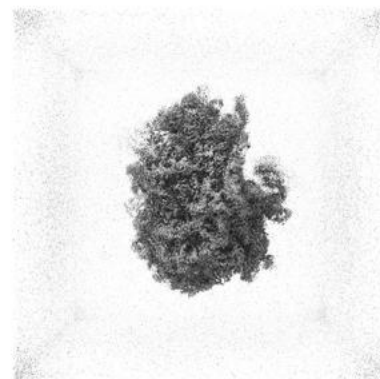
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

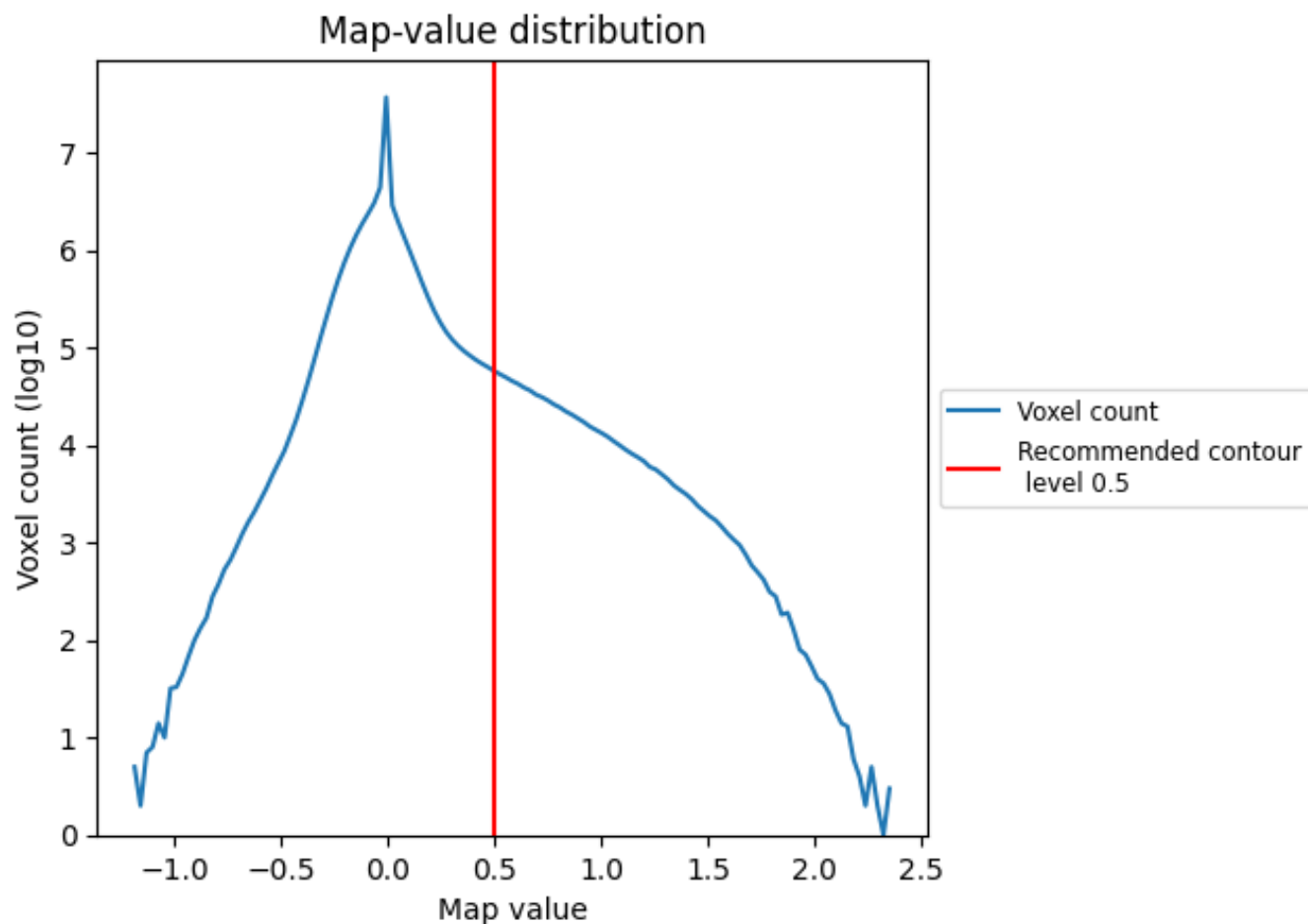
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

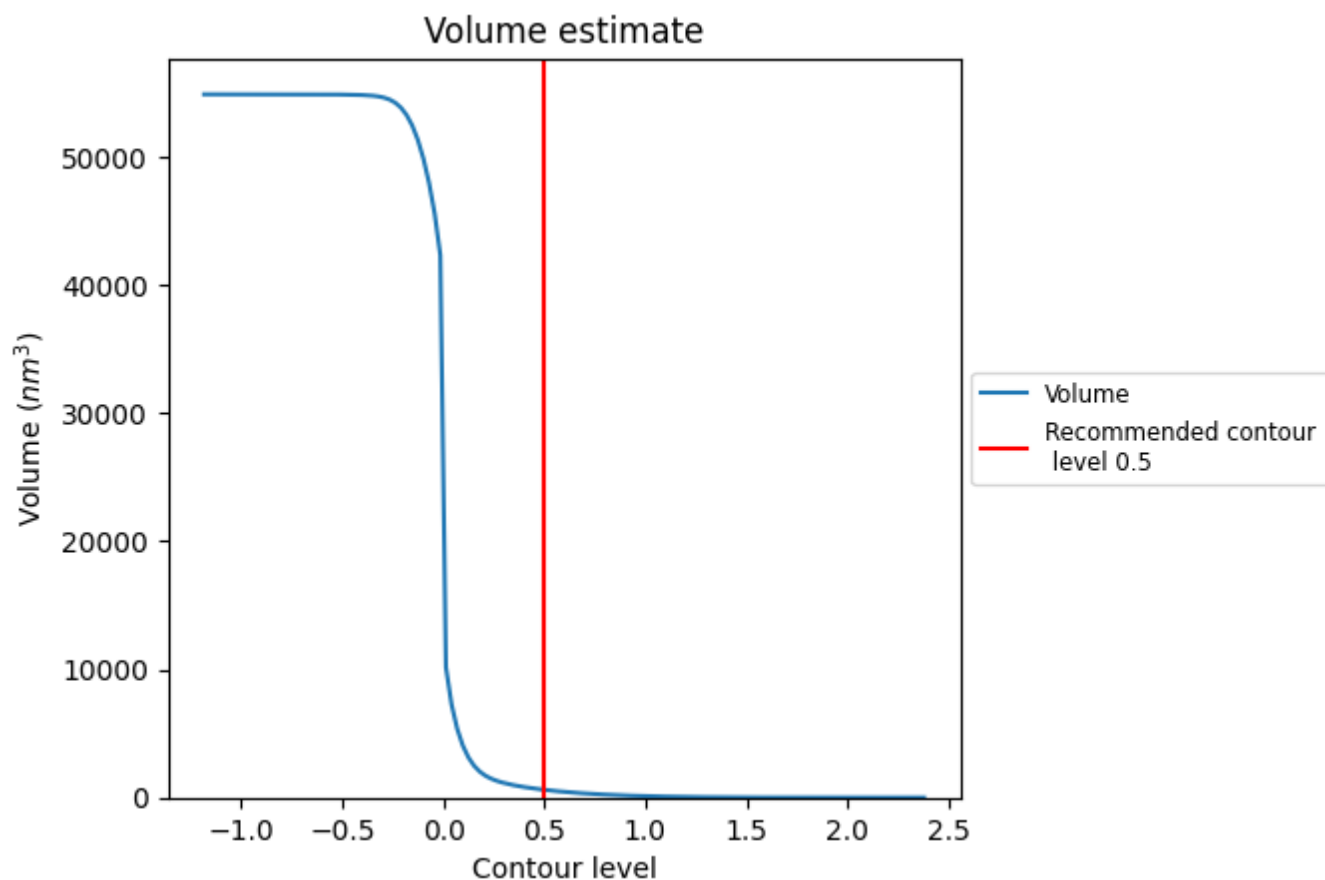
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

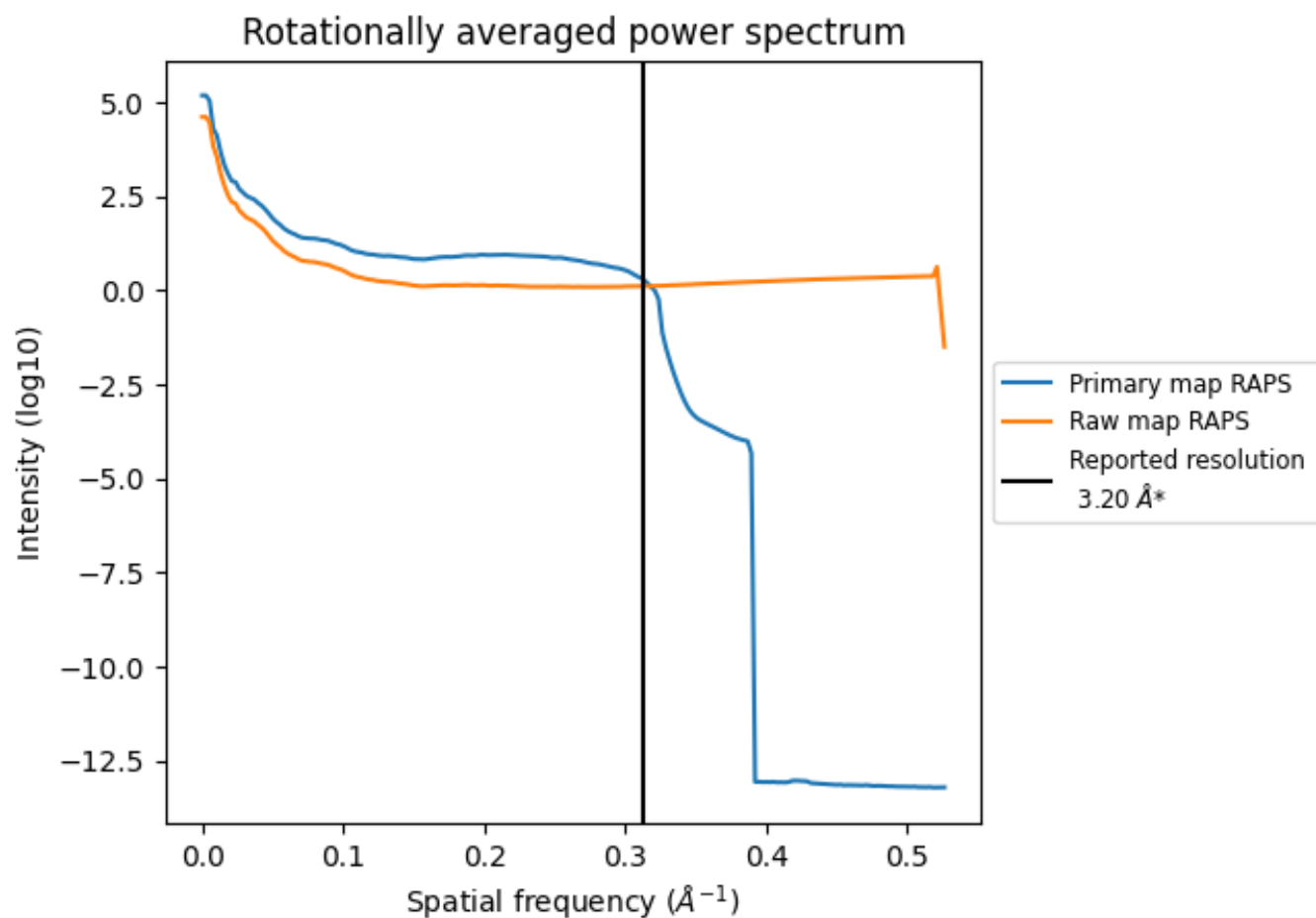
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 605 nm³; this corresponds to an approximate mass of 546 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 ⓘ

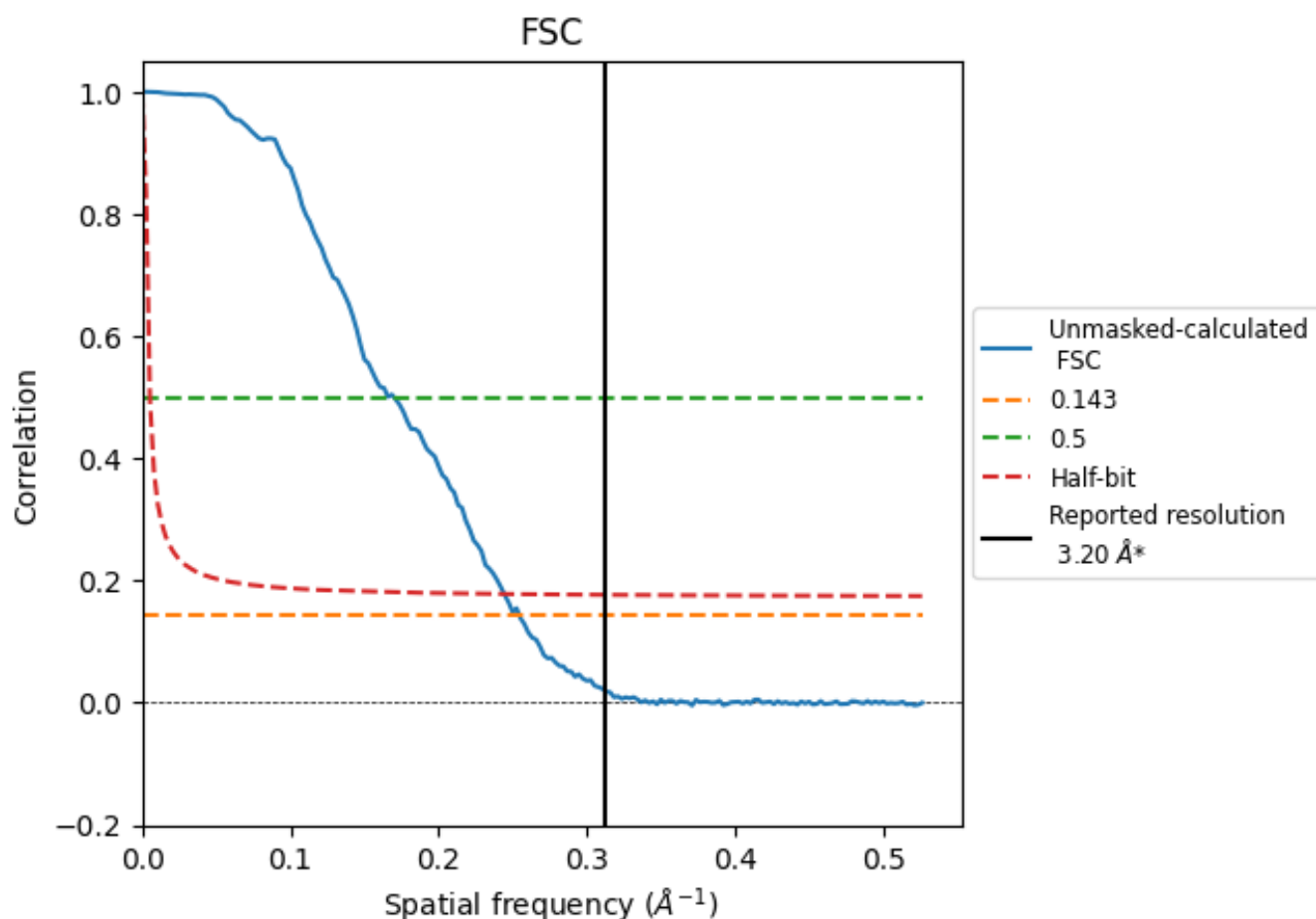


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

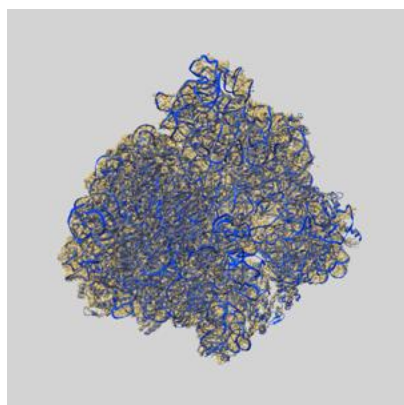
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.93	5.89	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.2 by more than 10 %

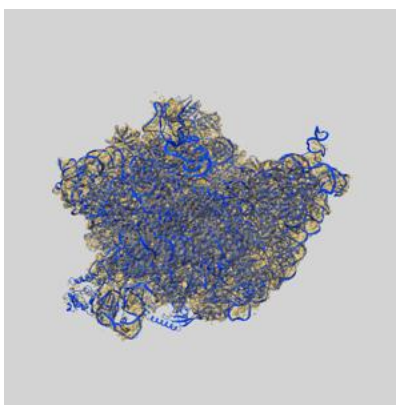
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40929 and PDB model 9NLB. Per-residue inclusion information can be found in section 3 on page 17.

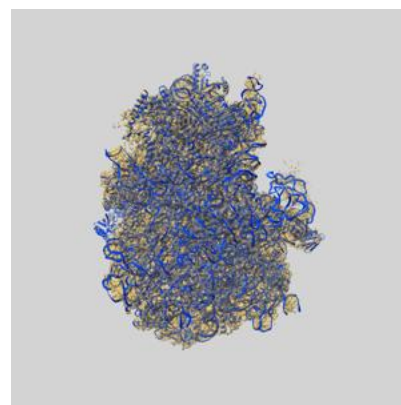
9.1 Map-model overlay [i](#)



X



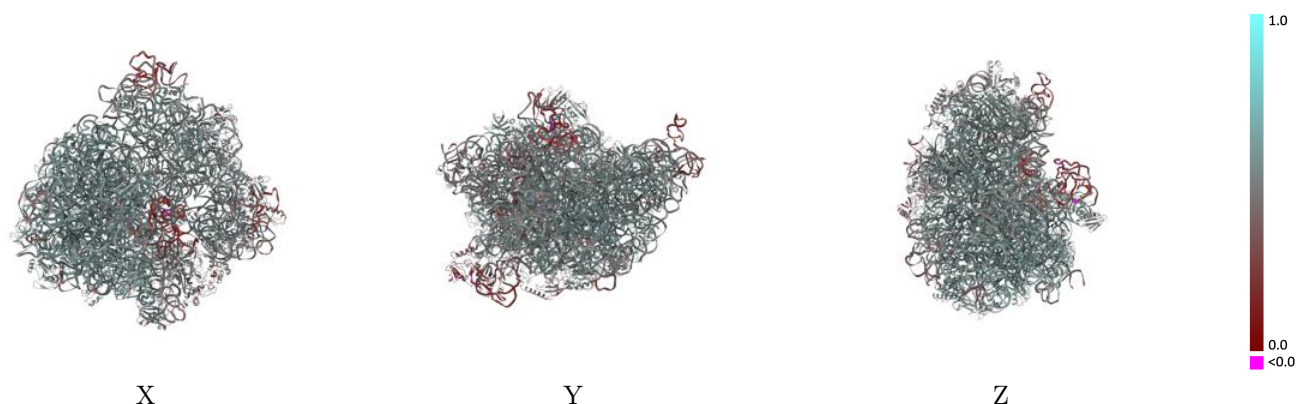
Y



Z

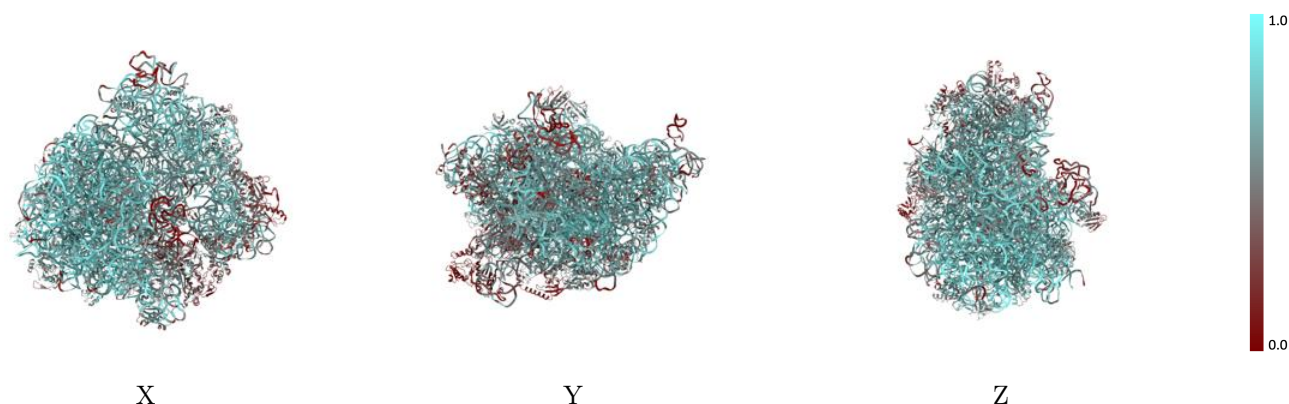
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



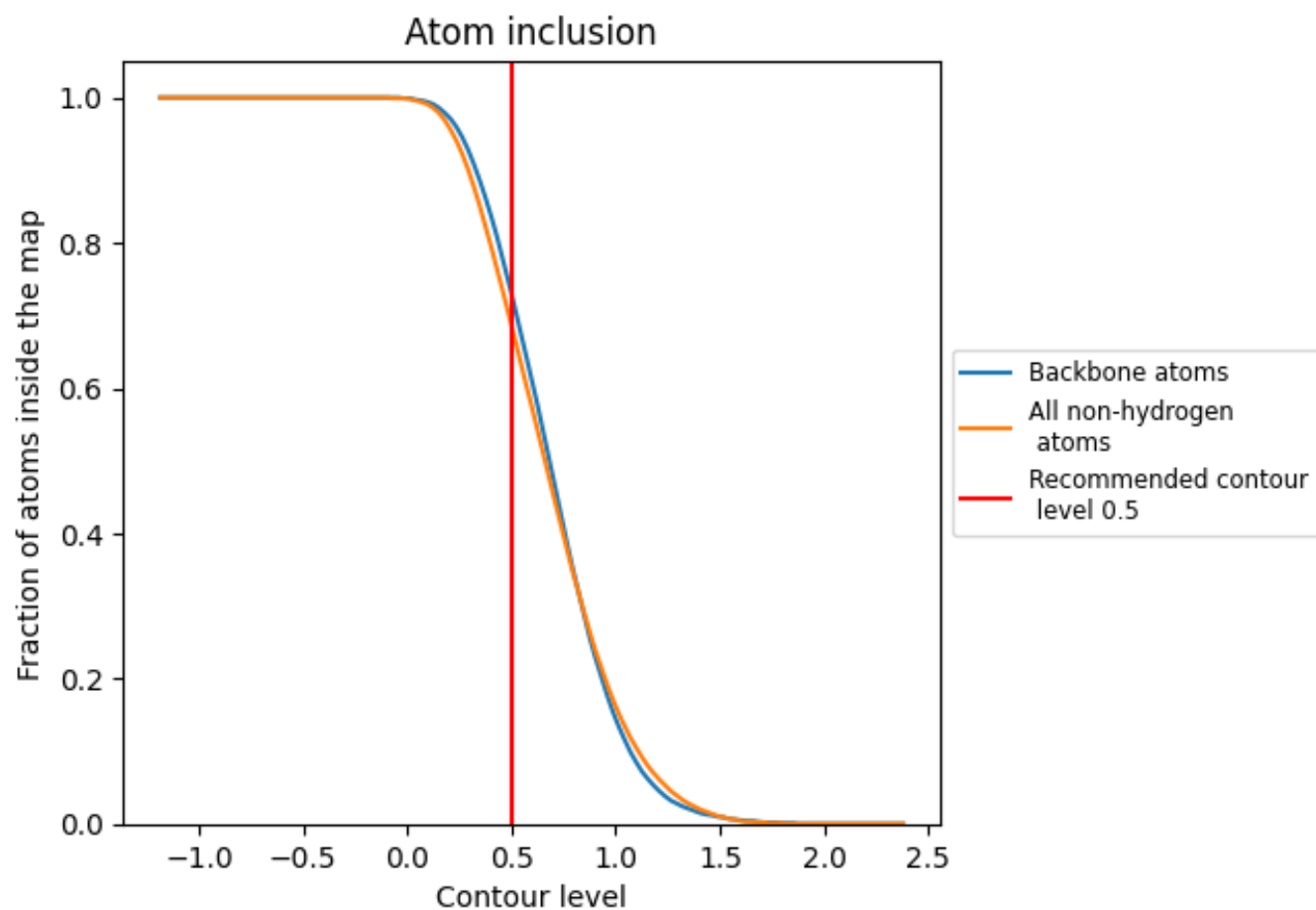
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 69% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.5230
1	 0.0970	 0.3300
13	 0.6700	 0.5680
14	 0.5980	 0.5620
15	 0.6640	 0.5600
16	 0.6180	 0.5660
17	 0.7220	 0.5740
18	 0.5430	 0.5200
19	 0.6310	 0.5640
2	 0.6780	 0.5790
20	 0.7190	 0.5810
21	 0.6410	 0.5450
22	 0.6600	 0.5620
23	 0.5910	 0.5410
24	 0.5370	 0.5150
25	 0.5850	 0.5430
27	 0.6910	 0.5770
28	 0.6440	 0.5760
29	 0.5760	 0.5160
3	 0.6640	 0.5640
30	 0.6340	 0.5480
31	 0.0920	 0.3690
32	 0.6690	 0.5620
33	 0.5590	 0.5530
34	 0.7210	 0.5910
35	 0.7190	 0.5870
36	 0.6470	 0.5680
4	 0.6110	 0.5490
5	 0.3430	 0.4720
6	 0.4430	 0.4950
9	 0.1590	 0.3960
E	 0.3970	 0.4980
M	 0.3690	 0.4910
R1	 0.7940	 0.5360
R2	 0.7270	 0.4920



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
R3	 0.7420	 0.5110
T	 0.5170	 0.4310
sb	 0.4240	 0.4720
sc	 0.4660	 0.5220
sd	 0.4960	 0.5130
se	 0.5950	 0.5350
sf	 0.5150	 0.5010
sg	 0.4180	 0.5020
sh	 0.5850	 0.5490
si	 0.4640	 0.4950
sj	 0.3720	 0.4720
sk	 0.5480	 0.5390
sl	 0.5340	 0.5350
sm	 0.4170	 0.4940
sn	 0.4920	 0.4970
so	 0.5910	 0.5490
sp	 0.5740	 0.5280
sq	 0.5320	 0.5330
sr	 0.5520	 0.5290
ss	 0.4330	 0.4930
st	 0.5510	 0.5260
su	 0.3660	 0.5190