wwPDB EM Validation Summary Report

Mar 24, 2025 – 11:01 AM EDT

PDB ID	:	9NLJ
EMDB ID	:	EMD-29399
Title	:	E.coli Initiation complex with Uup-EQ2
Authors	:	Singh, S.; Hunt, J.F.
Deposited on	:	2025-03-03
Resolution	:	3.10 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:

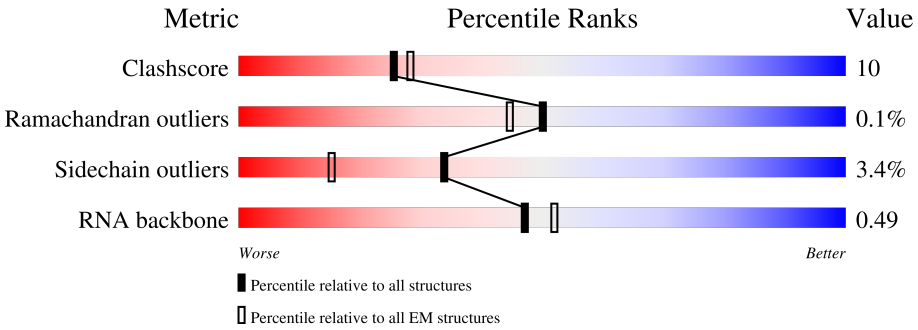
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	13	142	6% 85% 15%
2	14	122	9% 85% 15%
3	15	144	9% 77% 23%
4	16	136	7% 74% 24%
5	17	120	68% 32%
6	18	116	20% 73% 27%
7	19	114	11% 72% 26%

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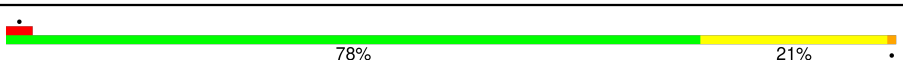
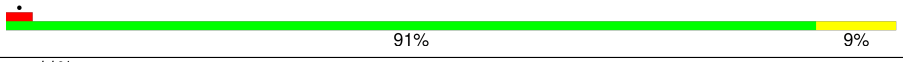
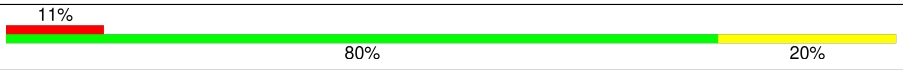
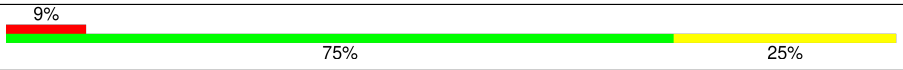
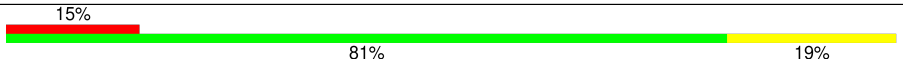
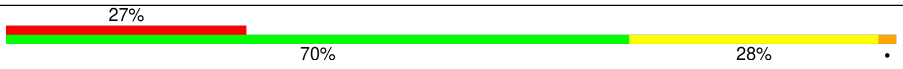
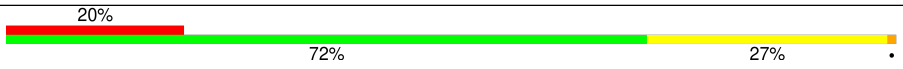
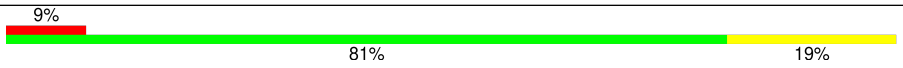
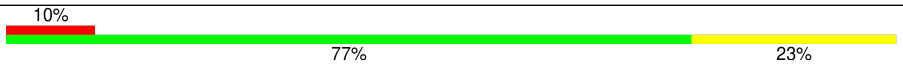
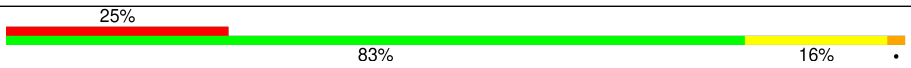
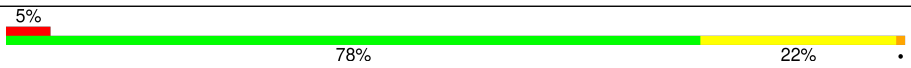
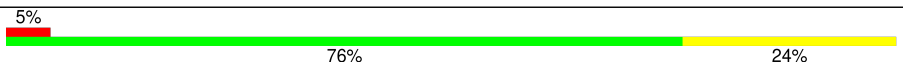
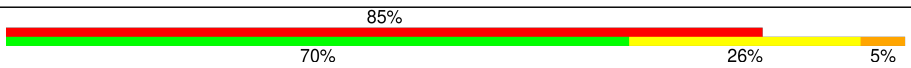
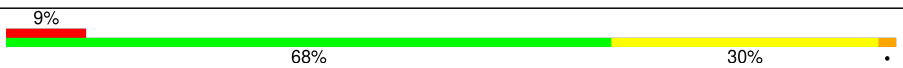
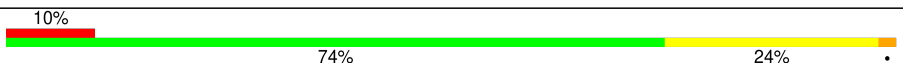
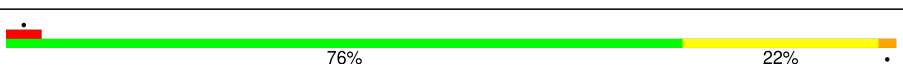
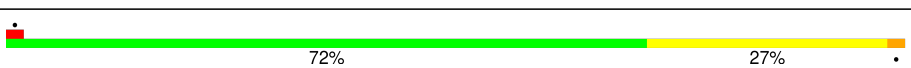
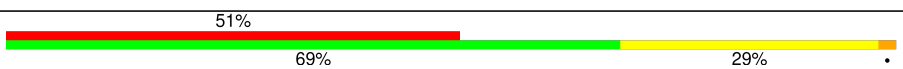
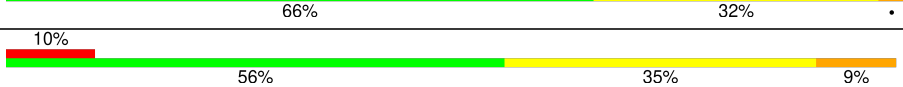
Mol	Chain	Length	Quality of chain
8	2	271	
9	20	117	
10	21	103	
11	22	110	
12	23	93	
13	24	102	
14	25	94	
15	27	85	
16	28	77	
17	29	63	
18	3	209	
19	30	58	
20	31	66	
21	32	56	
22	33	50	
23	34	46	
24	35	64	
25	36	38	
26	4	201	
27	5	177	
28	6	176	
29	9	149	
30	R1	2903	
31	R2	119	
32	R3	1531	

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Mol	Chain	Length	Quality of chain
33	sb	218	72% 95% 5%
34	sc	206	47% 97%
35	sd	205	60% 97%
36	se	157	20% 99%
37	sf	100	41% 97%
38	sg	151	36% 99%
39	sh	129	15% 93% 7%
40	si	127	43% 95% 5%
41	sj	98	70% 99%
42	sk	116	24% 98%
43	sl	123	50% 98%
44	sm	114	58% 97%
45	sn	100	57% 93% 7%
46	so	88	22% 97%
47	sp	82	40% 96%
48	sq	80	44% 94% 6%
49	sr	65	35% 95% 5%
50	ss	79	73% 94% 6%
51	st	85	54% 98%
52	su	65	58% 94% 6%
53	T	78	9% 54% 33% 8% 5%
54	U	537	37% 61% 36%
55	1	220	91% 71% 28%
56	M	9	22% 78% 22%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	H2U	T	20	X	-	-	-
53	4OC	T	32	X	-	-	-
53	5MU	T	54	X	-	-	-
53	PSU	T	55	X	-	-	-
53	4SU	T	8	X	-	-	-

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 150042 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 uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	13	142	1129	714	212	199	4	0	0

- Molecule 2 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	14	122	938	587	180	165	6	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	15	144	1053	654	207	190	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	16	136	1074	686	205	177	6	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	18	116	892	552	178	162	0	0

- Molecule 7 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	19	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 9 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	20	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 10 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	21	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 11 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	22	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	23	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 13 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	24	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 14 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	25	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 15 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	27	85	Total	C	N	O	S	0	0
			642	396	130	114	2		

- Molecule 16 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	28	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 17 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	29	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 18 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 19 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	30	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 20 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	33	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 24 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 25 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 33 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 34 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6, non-modified isoform.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 43 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 46 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 47 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

- Molecule 52 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	su	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	T	78	Total	C	N	O	P	S	0	0
			1649	740	295	536	76	2		

- Molecule 54 is a protein called Uup.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	U	537	Total	C	N	O	S	0	0
			4295	2690	778	810	17		

- Molecule 55 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1	220	Total	C	N	O	S	0	0
			1353	804	270	277	2		

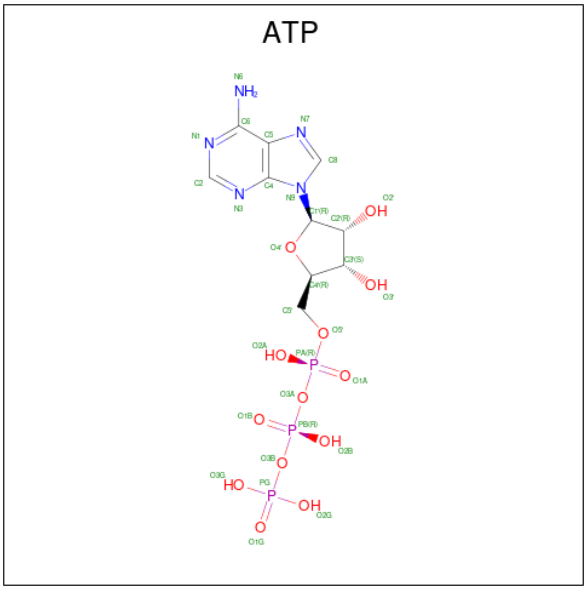
- Molecule 56 is a RNA chain called mRNA.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: 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	20	1	Total	Mg	0
			1	1	
57	32	1	Total	Mg	0
			1	1	
57	R1	192	Total	Mg	0
			192	192	
57	R3	81	Total	Mg	0
			81	81	

- Molecule 58 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 59 is SODIUM ION (three-letter code: NA) (formula: Na).

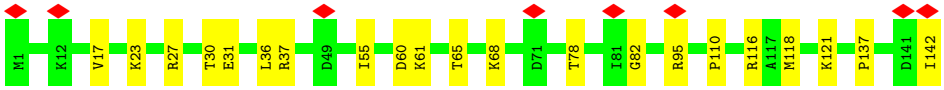
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
59	U	2	2	2	0

3 Residue-property plots (i)

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.

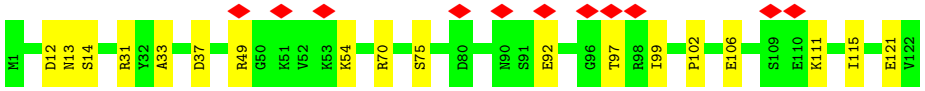
• Molecule 1: Large ribosomal subunit protein uL13

Chain 13:



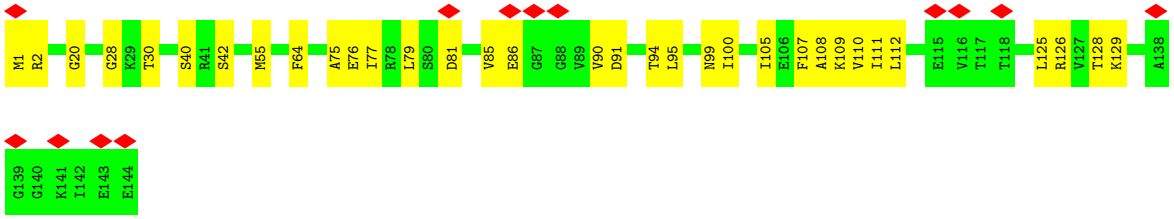
• Molecule 2: 50S ribosomal protein L14

Chain 14:



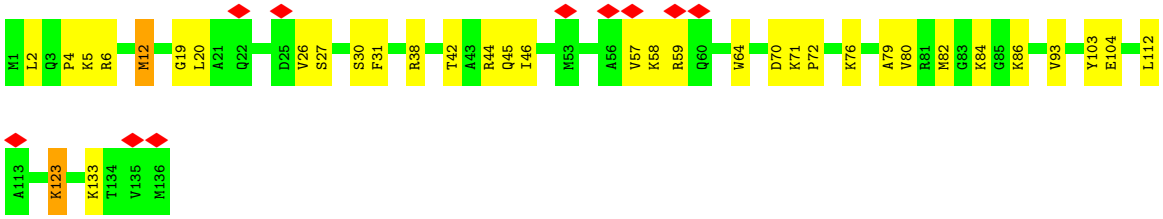
• Molecule 3: Large ribosomal subunit protein uL15

Chain 15:



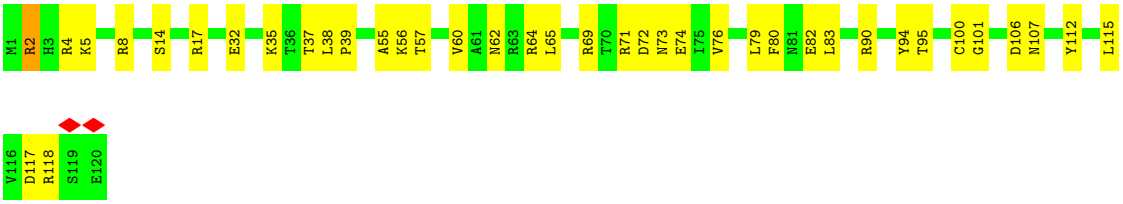
• Molecule 4: 50S ribosomal protein L16

Chain 16:



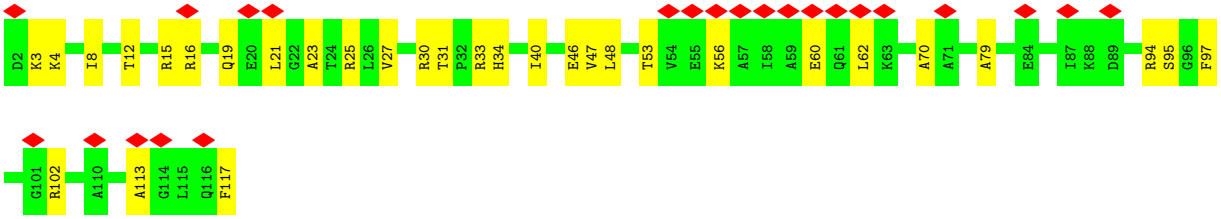
• Molecule 5: Large ribosomal subunit protein bL17

Chain 17:



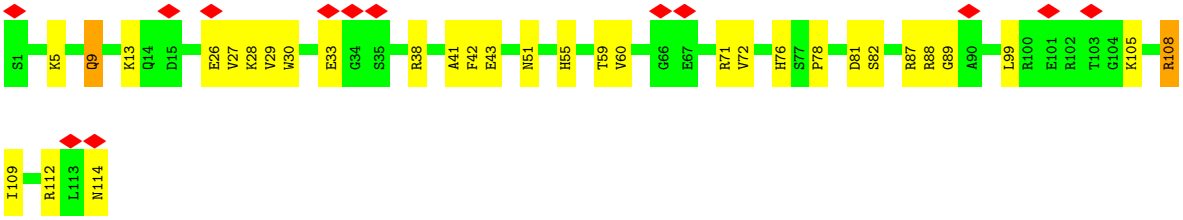
• Molecule 6: Large ribosomal subunit protein uL18

Chain 18:



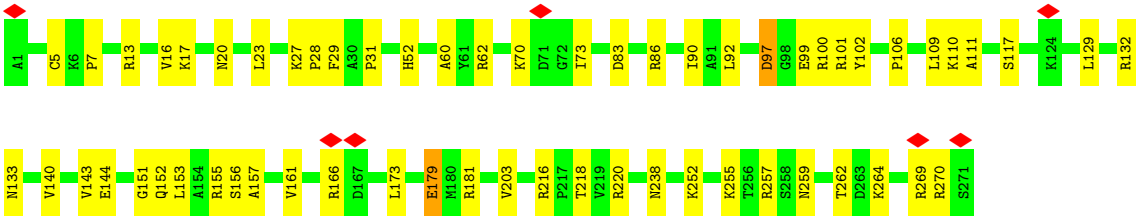
• Molecule 7: 50S ribosomal protein L19

Chain 19:



• Molecule 8: 50S ribosomal protein L2

Chain 2:

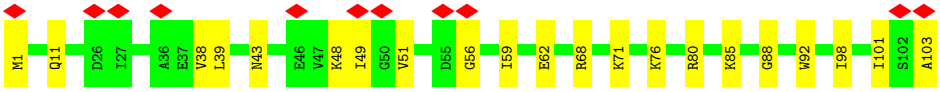


• Molecule 9: Large ribosomal subunit protein bL20

Chain 20:

• Molecule 10: Large ribosomal subunit protein bL21

Chain 21:

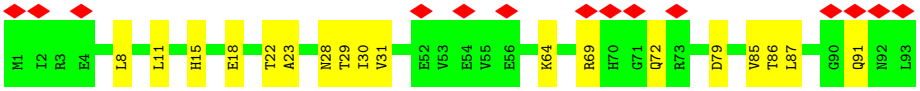


• Molecule 11: Large ribosomal subunit protein uL22

Chain 22:

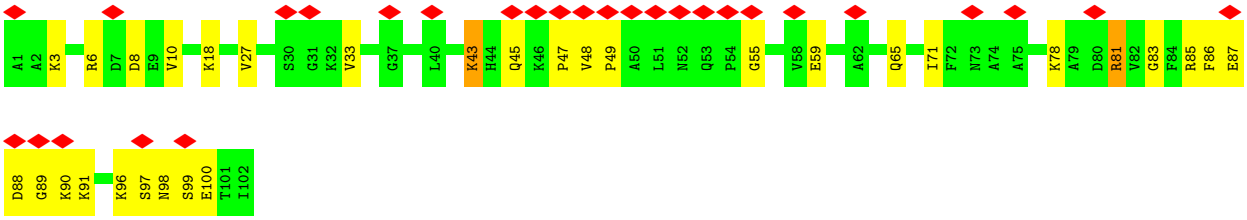
• Molecule 12: Large ribosomal subunit protein uL23

Chain 23:



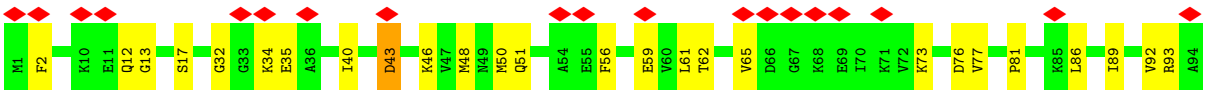
• Molecule 13: Large ribosomal subunit protein uL24

Chain 24:



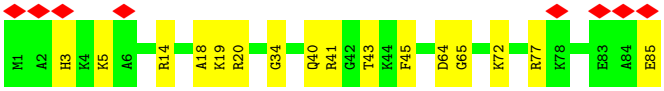
• Molecule 14: Large ribosomal subunit protein bL25

Chain 25:

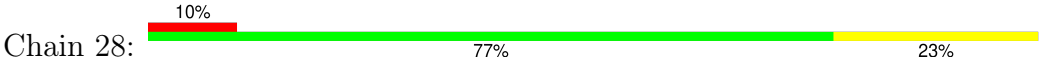


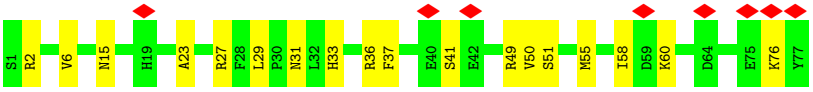
• Molecule 15: Large ribosomal subunit protein bL27

Chain 27:

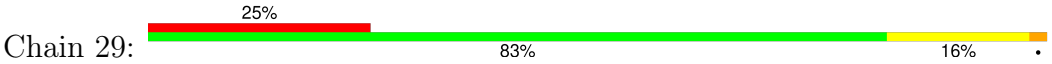


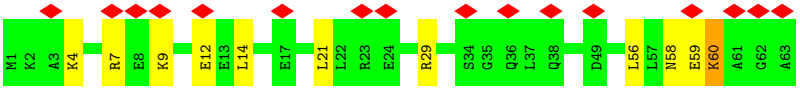
• Molecule 16: 50S ribosomal protein L28



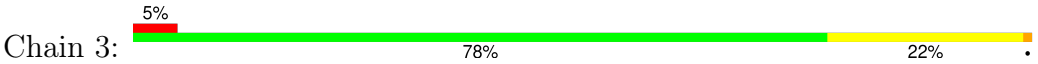


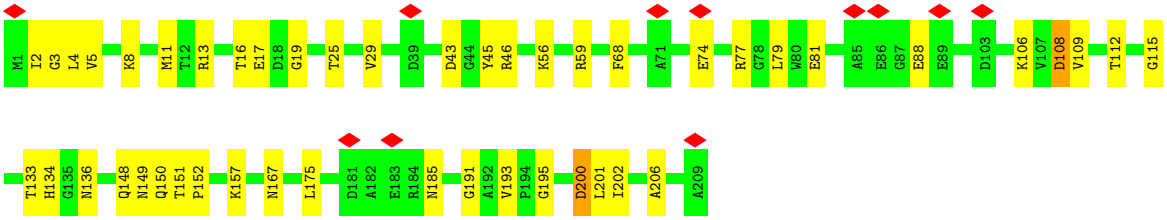
• Molecule 17: Large ribosomal subunit protein uL29



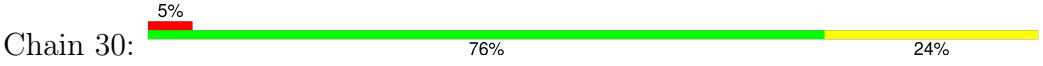


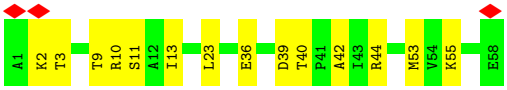
• Molecule 18: 50S ribosomal protein L3



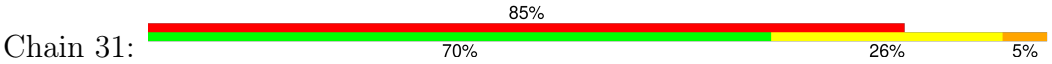


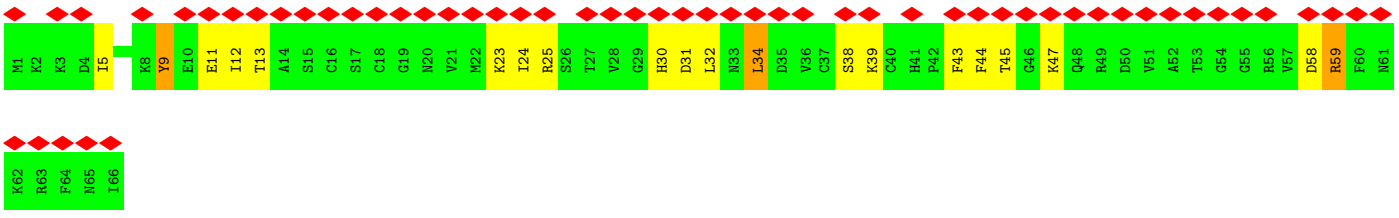
• Molecule 19: 50S ribosomal protein L30





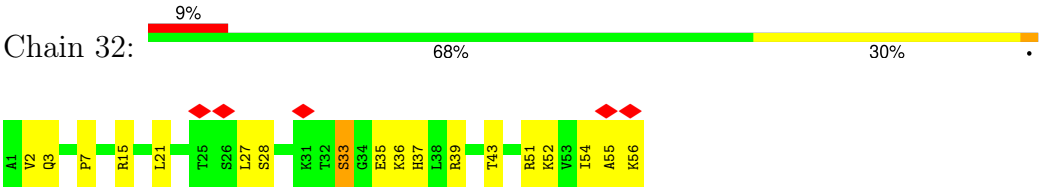
• Molecule 20: Large ribosomal subunit protein bL31





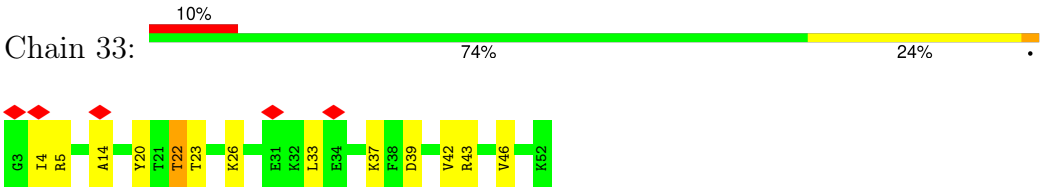
• Molecule 21: 50S ribosomal protein L32

Chain 32:



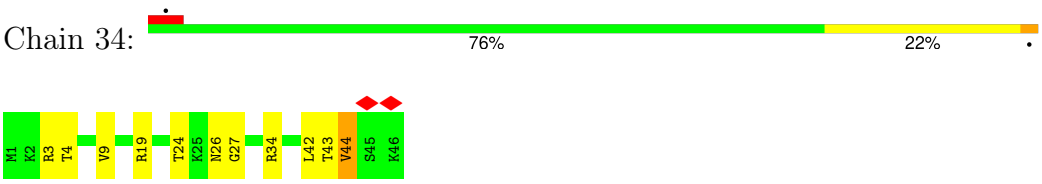
• Molecule 22: Large ribosomal subunit protein bL33

Chain 33:



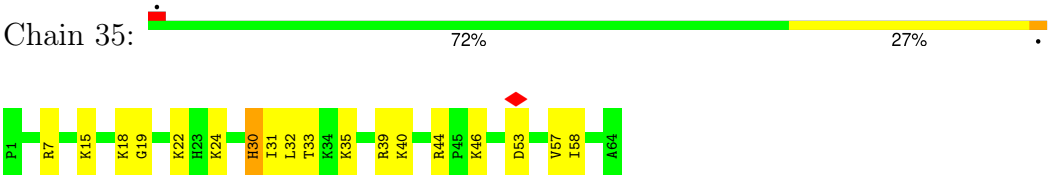
• Molecule 23: 50S ribosomal protein L34

Chain 34:



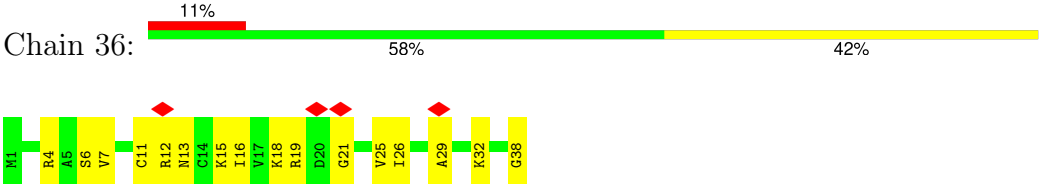
• Molecule 24: Large ribosomal subunit protein bL35

Chain 35:



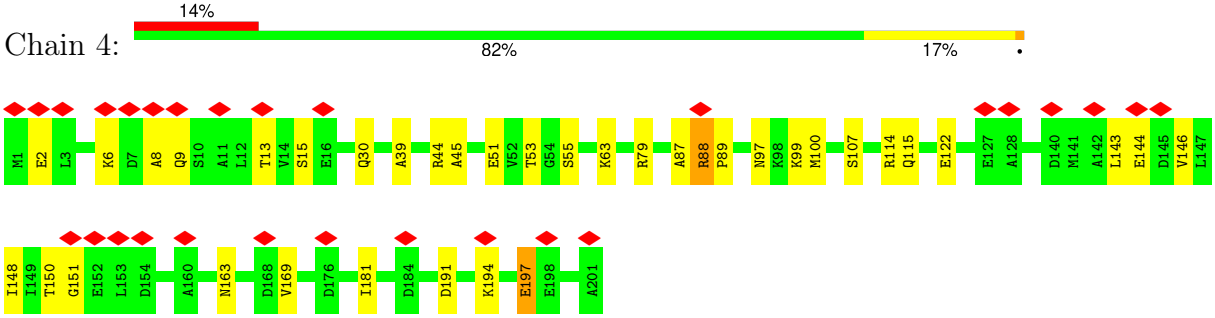
• Molecule 25: 50S ribosomal protein L36

Chain 36:



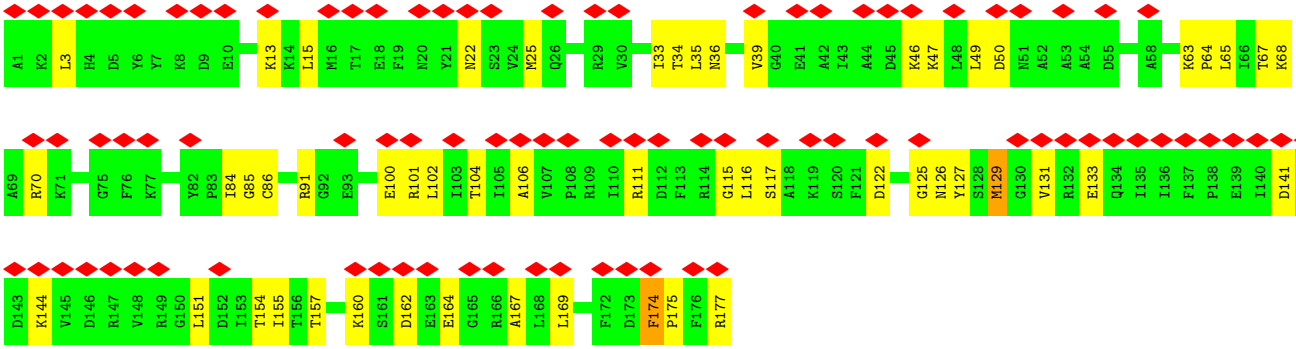
• Molecule 26: Large ribosomal subunit protein uL4

Chain 4:



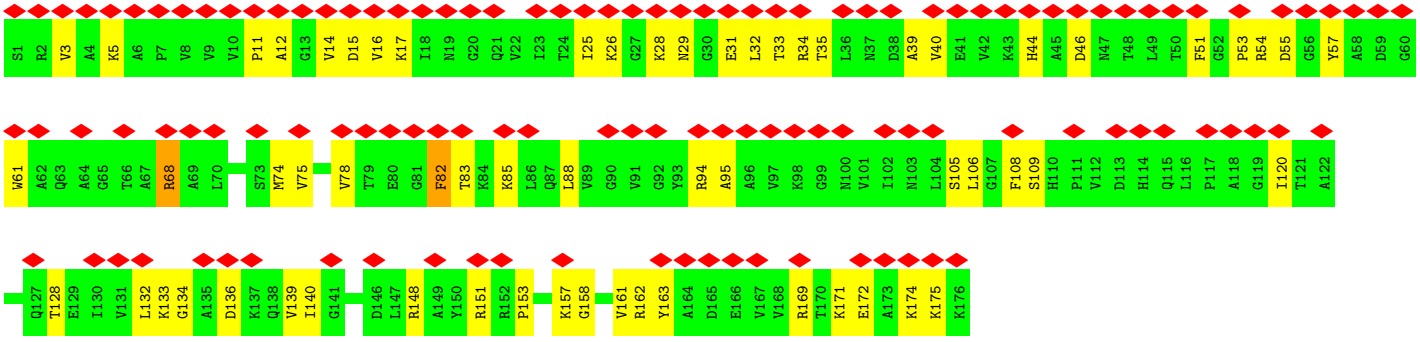
• Molecule 27: 50S ribosomal protein L5

Chain 5:



• Molecule 28: Large ribosomal subunit protein uL6

Chain 6:

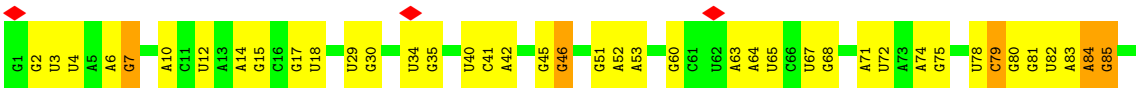


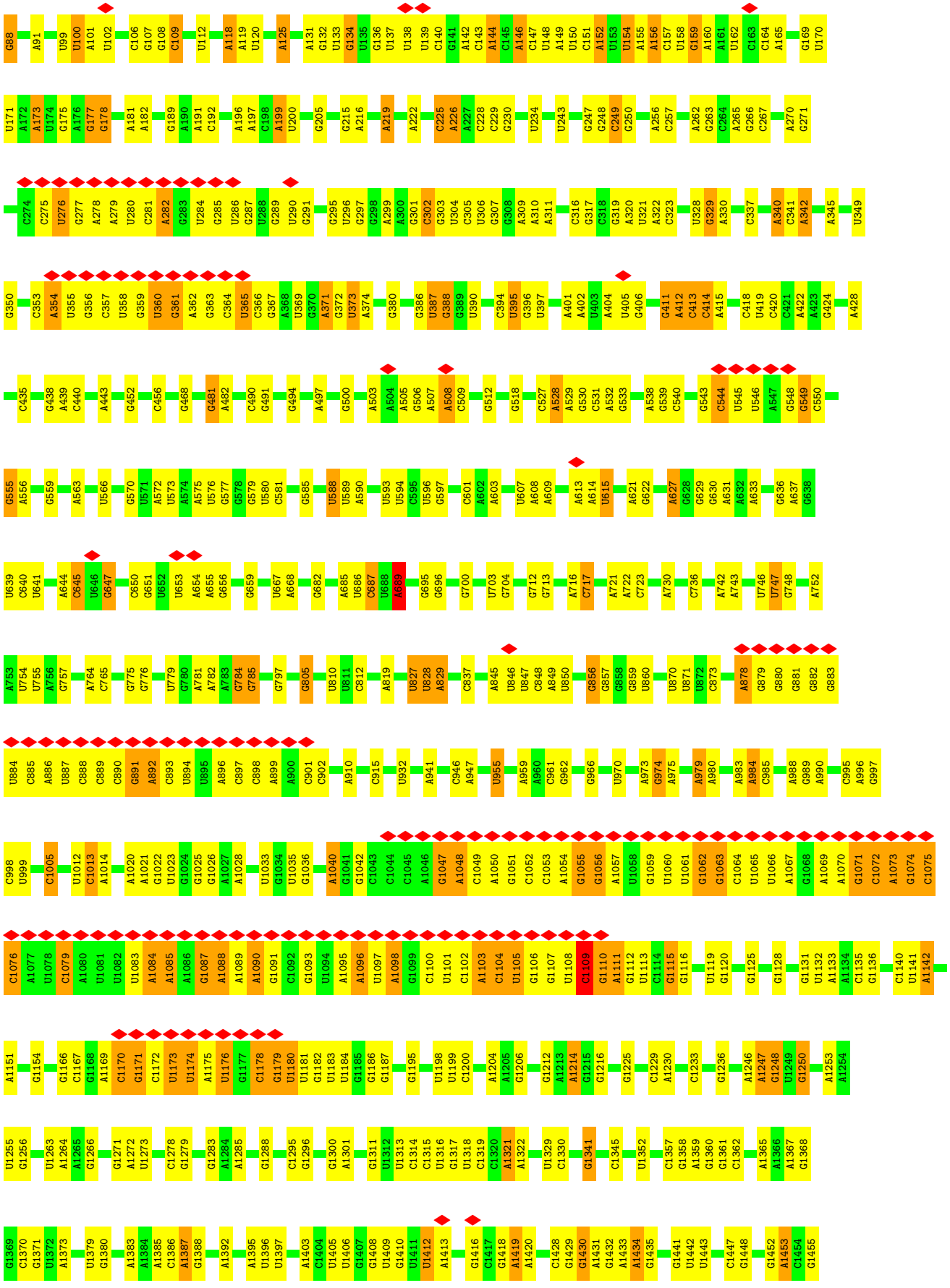
• Molecule 29: Large ribosomal subunit protein bL9

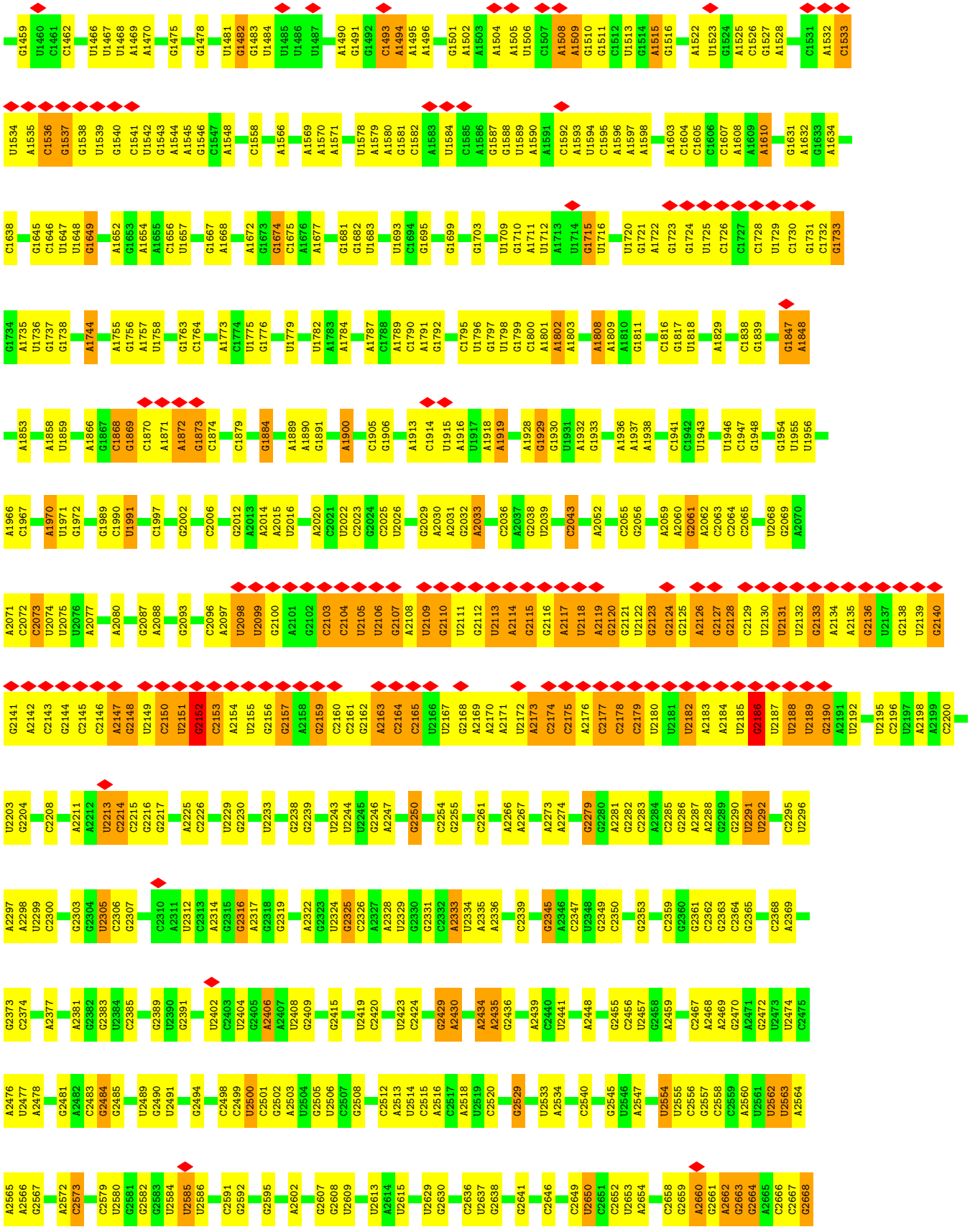
Chain 9:

• Molecule 30: 23S ribosomal RNA

Chain R1:



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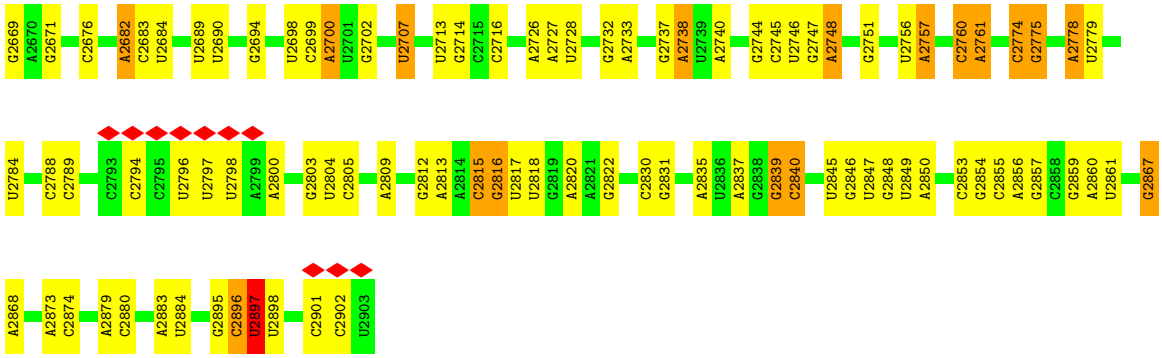
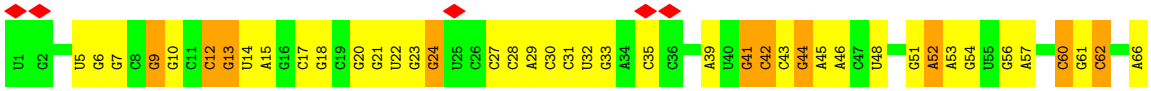
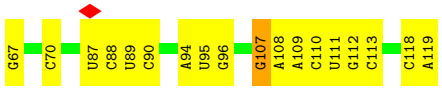
U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1544 A1545 G1546 G1547 A1548 C1558 A1566 A1569 A1570 A1571 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 C1595 A1596 A1597 A1598 A1603 C1604 C1605 C1606 C1607 A1608 A1609 A1610 G1631 A1632 G1633 A1634
C1638 G1645 C1646 U1647 U1648 G1649 A1652 G1653 A1654 A1655 C1656 U1657 G1667 A1668 A1672 G1673 G1674 C1675 A1676 A1677 G1681 G1682 U1683 U1693 C1694 G1695 G1699 G1703 U1709 G1710 A1711 U1712 A1713 U1714 G1715 U1716 U1720 G1721 A1722 G1723 G1724 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732 G1733
G1734 A1735 U1736 G1737 G1738 A1744 A1755 G1756 A1757 U1758 G1763 C1764 A1773 C1774 U1775 G1776 U1779 U1782 A1783 A1784 A1787 C1788 A1789 C1790 A1791 G1792 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 A1808 A1809 A1810 G1811 C1816 G1817 U1818 A1829 C1838 G1839 G1847 A1848
A1853 A1858 U1859 A1866 G1867 C1868 G1869 C1870 A1871 A1872 G1873 C1874 C1879 G1884 A1889 A1890 G1891 A1900 C1905 G1906 A1913 C1914 U1915 A1916 U1917 A1918 A1919 A1928 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 C1941 C1942 U1943 U1946 C1947 G1948 G1954 U1955 U1956
A1966 C1967 A1970 U1971 G1972 G1989 C1990 U1991 C1997 G2002 C2006 C2012 A2013 A2014 A2015 U2016 A2020 C2021 U2022 C2023 G2024 C2025 U2026 G2029 A2030 A2031 G2032 A2033 C2036 A2037 G2038 U2039 C2043 A2052 C2055 C2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 U2068 G2069 A2070
A2071 C2072 C2073 U2074 U2075 U2076 A2077 A2080 G2087 A2088 G2093 C2096 A2097 U2098 U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 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 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 A2182 A2183 A2184 U2185 G2186 U2187 U2188 U2189 G2190 A2191 U2192 U2195 C2196 U2197 A2198 A2199 C2200
U2203 G2204 C2208 A2211 A2212 U2213 C2214 C2215 G2216 G2217 A2225 C2226 U2229 G2230 U2233 G2238 G2239 U2243 U2244 U2245 G2246 A2247 G2250 C2254 G2255 C2261 A2266 A2267 A2273 A2274 G2279 G2280 A2281 G2282 C2283 A2284 C2285 G2286 A2287 A2288 G2289 G2290 U2291 U2292 C2295 U2296
A2297 A2298 U2299 C2300 G2303 G2304 U2305 C2306 G2307 C2310 A2311 U2312 C2313 A2314 G2315 G2316 A2317 G2318 G2319 A2322 G2323 U2324 G2325 C2326 A2327 A2328 U2329 G2330 G2331 C2332 A2333 U2334 A2335 A2336 C2339 G2345 A2346 C2347 U2348 G2349 C2350 G2353 C2359 G2360 G2361 C2362 G2363 C2364 G2365 C2368 A2369
G2373 C2374 A2377 A2381 G2382 G2383 U2384 C2385 G2389 U2390 G2391 U2402 C2403 U2404 G2405 A2406 A2407 U2408 G2409 G2415 U2419 C2420 U2423 C2424 G2429 A2430 A2434 A2435 G2436 A2439 C2440 U2441 A2448 G2455 C2456 U2457 G2458 A2459 C2467 A2468 A2469 G2470 A2471 G2472 U2473 U2474 C2475
A2476 U2477 A2478 G2481 A2482 C2483 G2484 G2485 U2489 G2490 U2491 G2494 C2498 C2499 U2500 C2501 G2502 A2503 U2504 G2505 U2506 C2507 G2508 C2512 A2513 U2514 C2515 A2516 C2517 A2518 U2519 C2520 G2529 U2533 A2534 C2540 G2545 U2546 A2547 U2554 U2555 C2556 G2557 C2558 C2559 A2560 U2561 U2562 U2563 A2564
A2565 A2566 G2567 A2572 C2573 C2579 U2580 G2581 G2582 G2583 U2584 U2585 U2586 C2591 G2592 G2595 A2602 G2607 G2608 U2609 U2613 A2614 U2615 U2629 G2630 C2636 U2637 G2638 G2641 C2646 C2649 U2650 C2651 C2652 U2653 A2654 C2658 G2659 A2660 G2661 A2662 G2663 G2664 A2665 C2666 C2667 G2668



• Molecule 31: 5S ribosomal RNA

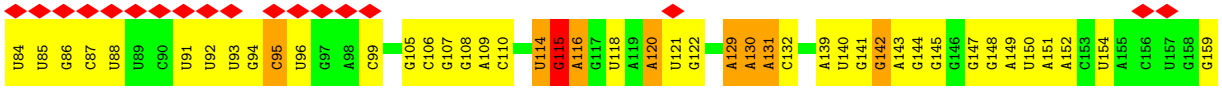
Chain R2:

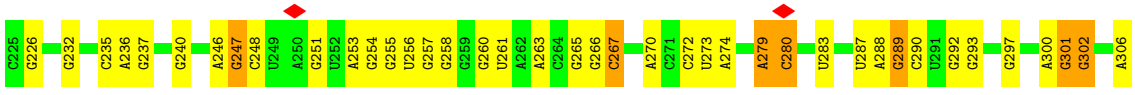


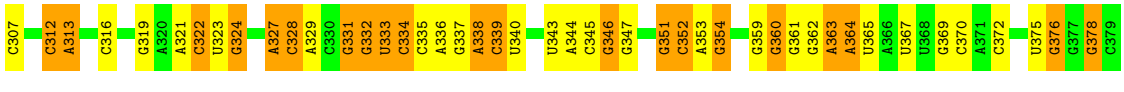


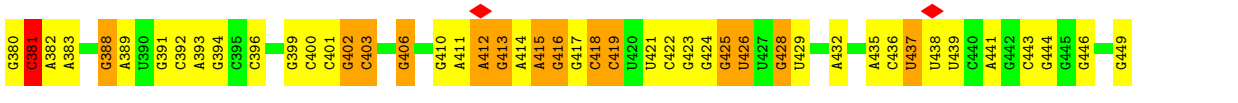
• Molecule 32: 16S ribosomal RNA

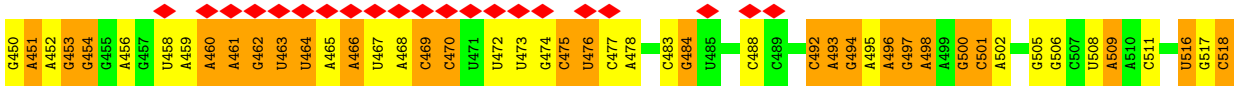
Chain R3:

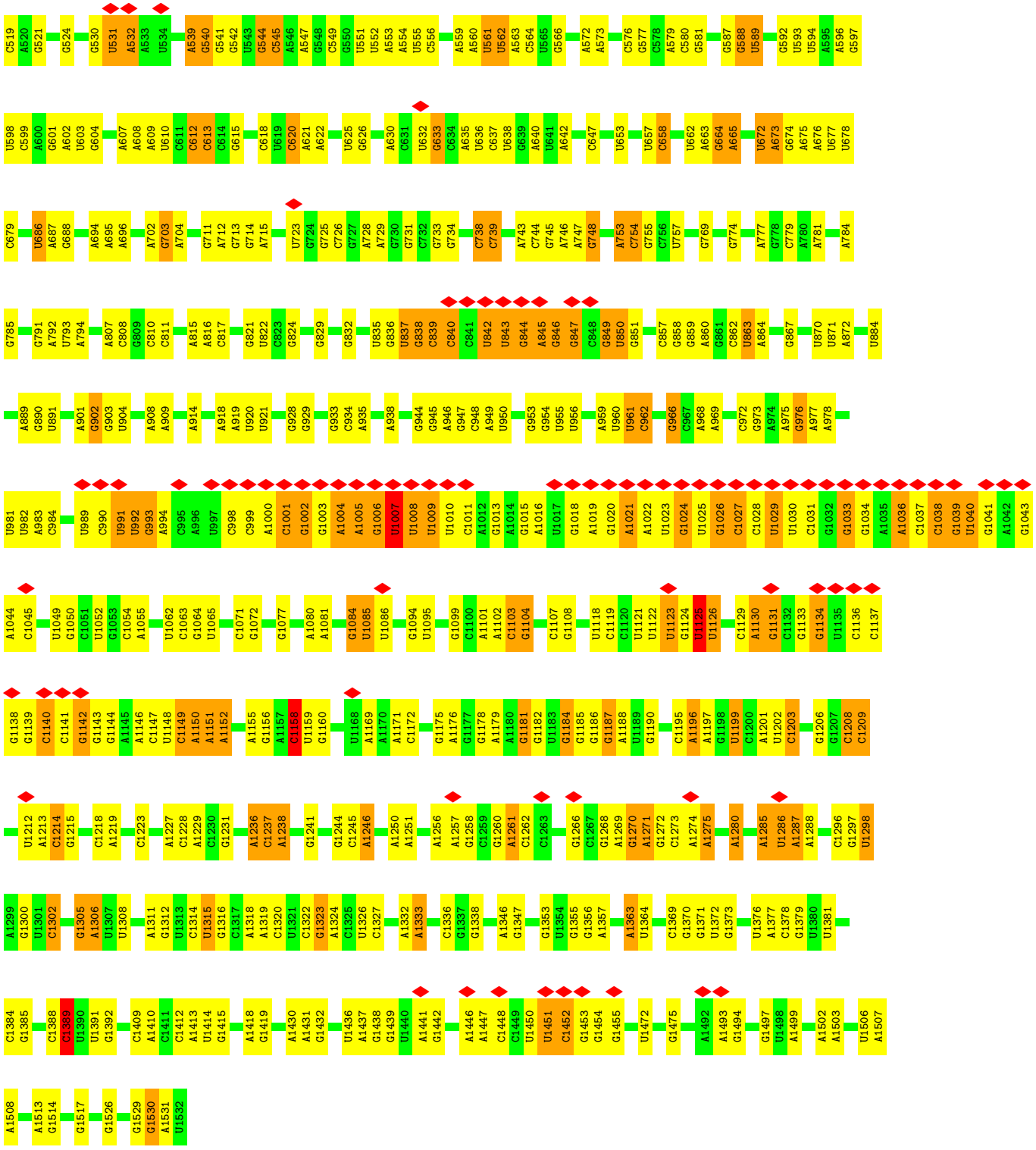






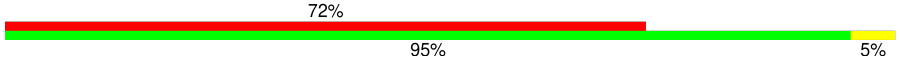






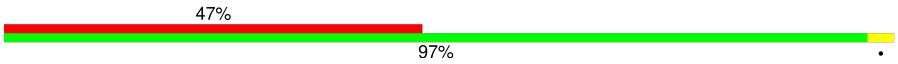
• Molecule 33: Small ribosomal subunit protein uS2

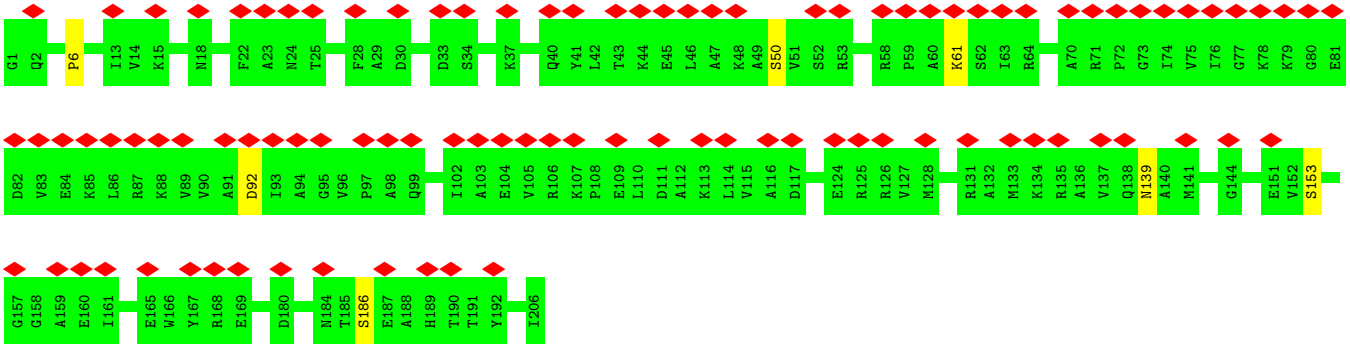
Chain sb:



• Molecule 34: Small ribosomal subunit protein uS3

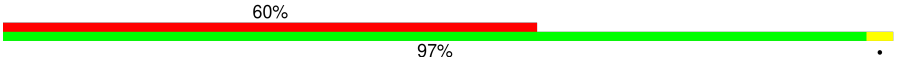
Chain sc:

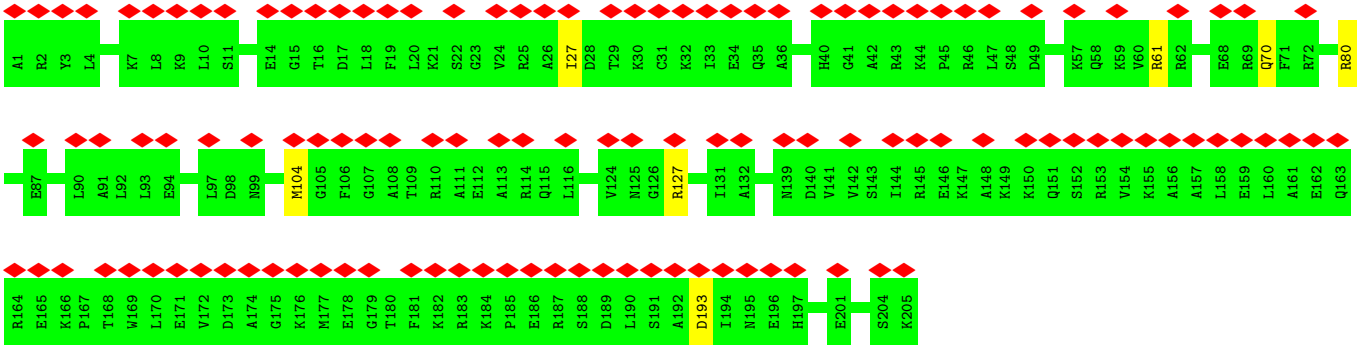




• Molecule 35: 30S ribosomal protein S4

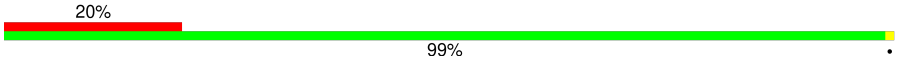
Chain sd:

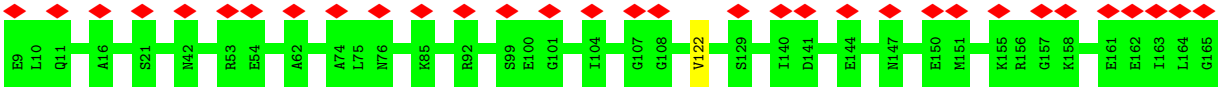




• Molecule 36: Small ribosomal subunit protein uS5

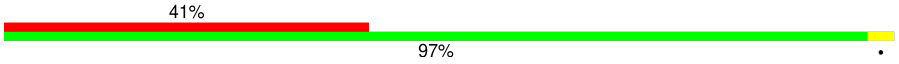
Chain se:

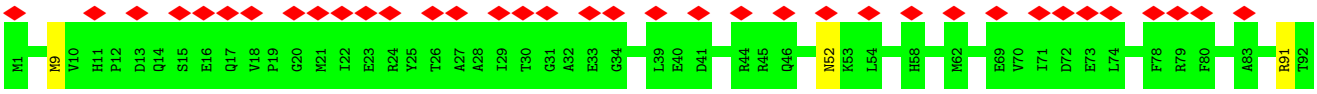


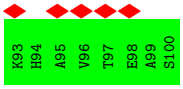


• Molecule 37: 30S ribosomal protein S6, non-modified isoform

Chain sf:

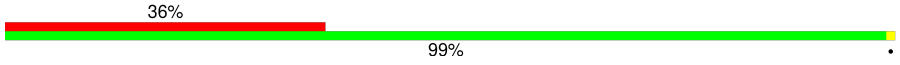


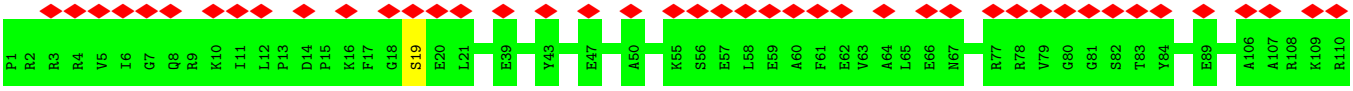


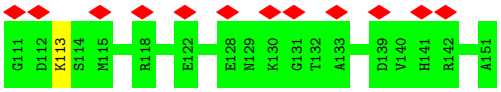


• Molecule 38: 30S ribosomal protein S7

Chain sg:

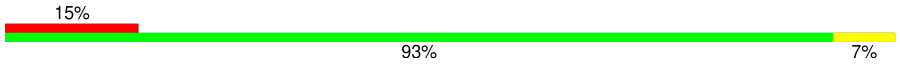


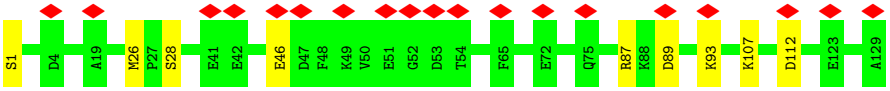




• Molecule 39: 30S ribosomal protein S8

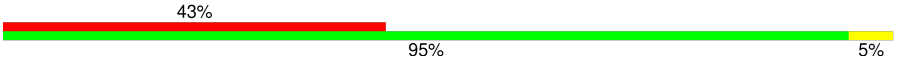
Chain sh:

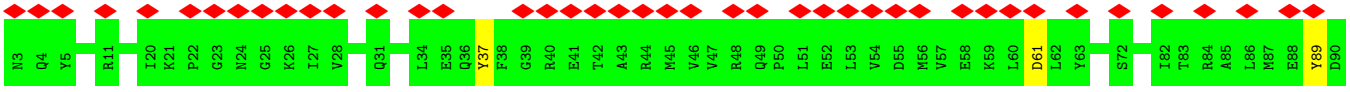


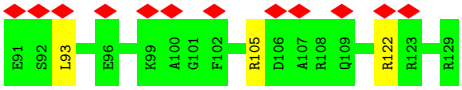


• Molecule 40: Small ribosomal subunit protein uS9

Chain si:

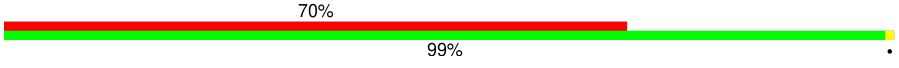






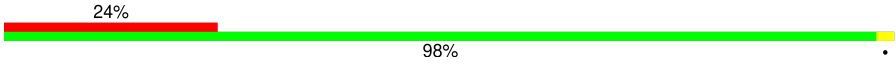
• Molecule 41: 30S ribosomal protein S10

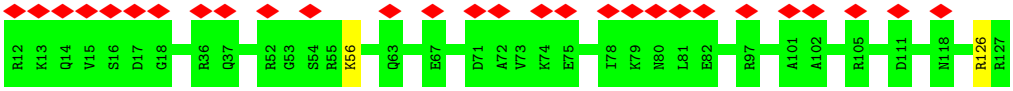
Chain sj:



• Molecule 42: Small ribosomal subunit protein uS11

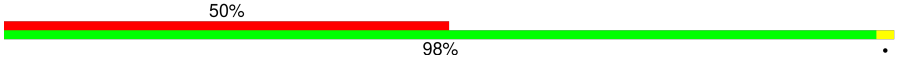
Chain sk:

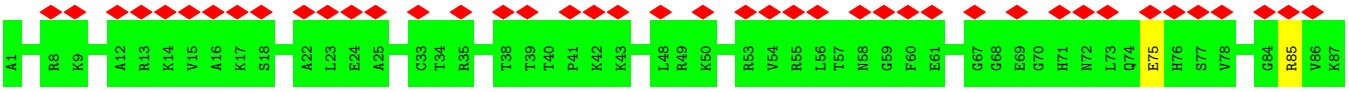


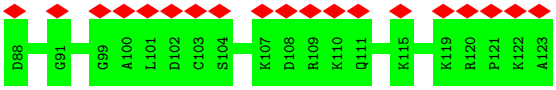


• Molecule 43: Small ribosomal subunit protein uS12

Chain sl:

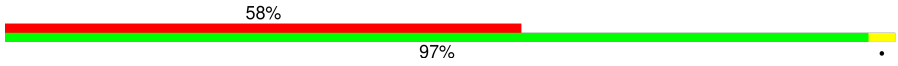


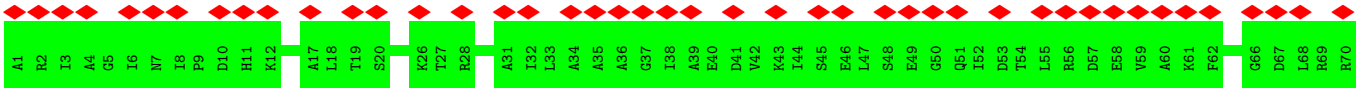


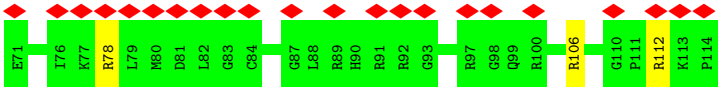


• Molecule 44: 30S ribosomal protein S13

Chain sm:

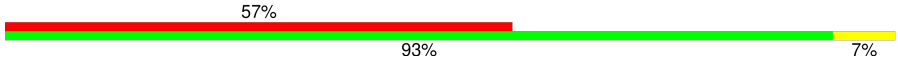


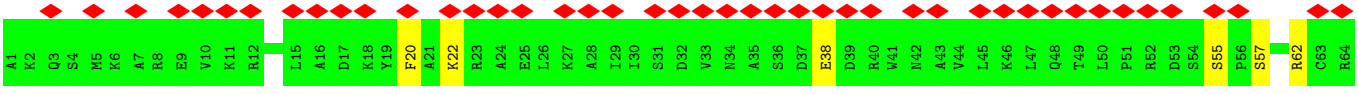


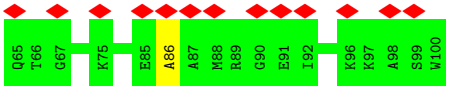


• Molecule 45: Small ribosomal subunit protein uS14

Chain sn:

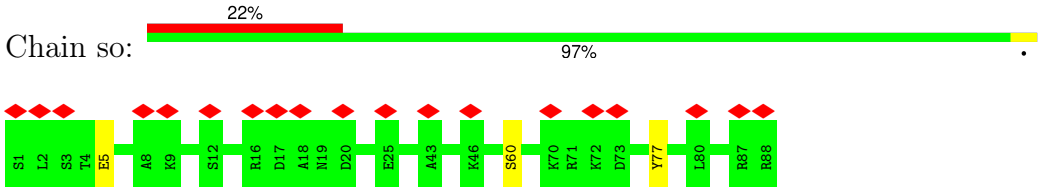






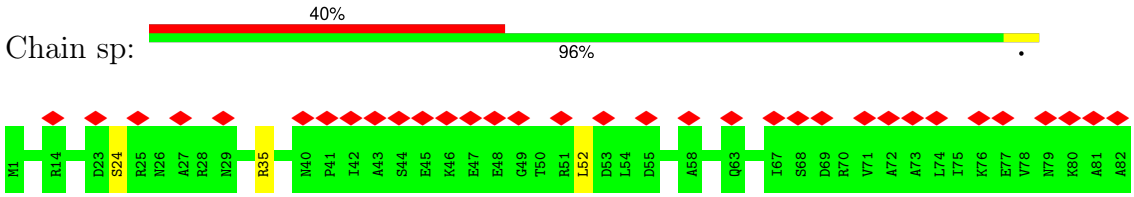
• Molecule 46: Small ribosomal subunit protein uS15

Chain so:



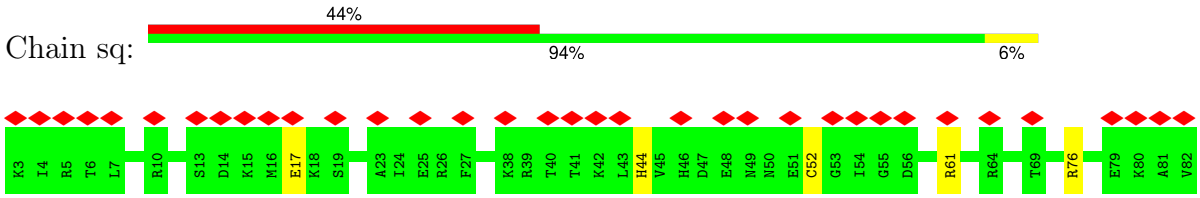
• Molecule 47: Small ribosomal subunit protein bS16

Chain sp:



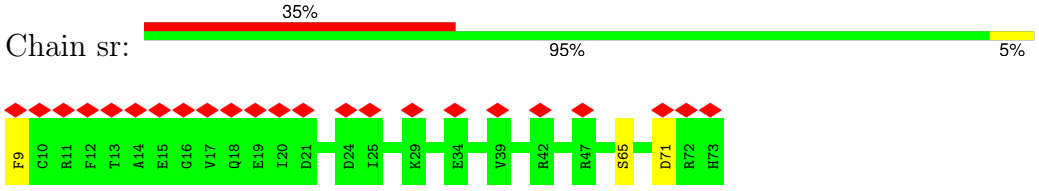
• Molecule 48: Small ribosomal subunit protein uS17

Chain sq:



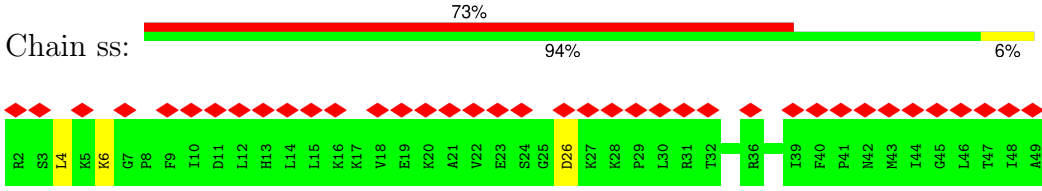
• Molecule 49: 30S ribosomal protein S18

Chain sr:



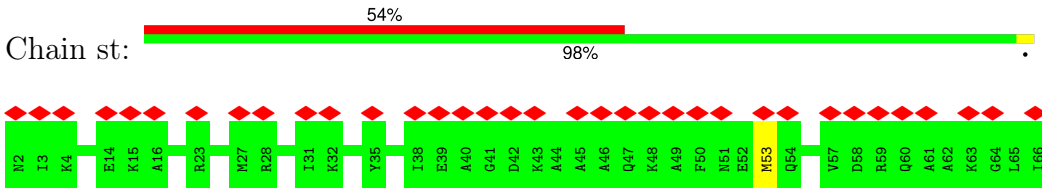
• Molecule 50: 30S ribosomal protein S19

Chain ss:



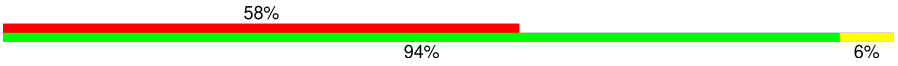
• Molecule 51: 30S ribosomal protein S20

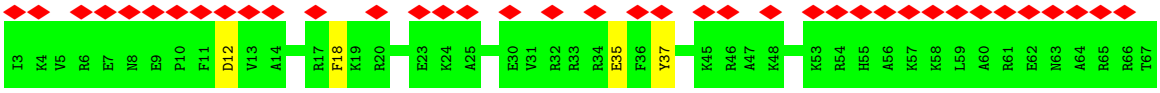
Chain st:



• Molecule 52: Small ribosomal subunit protein bS21

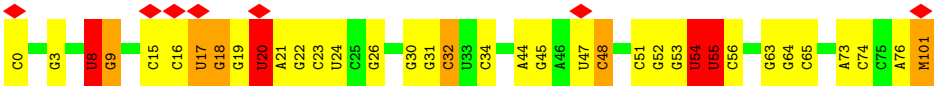
Chain su:





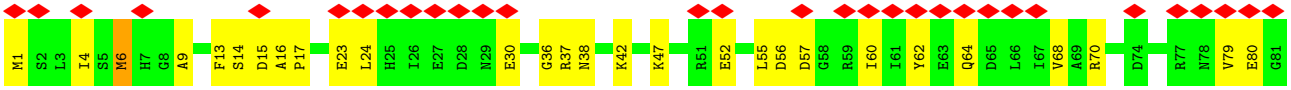
• Molecule 53: tRNA

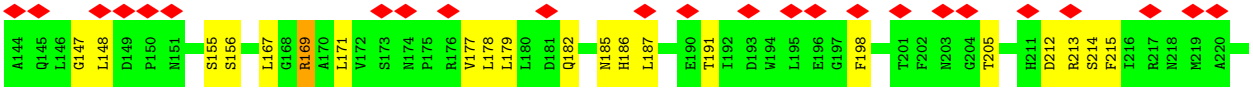
Chain T:

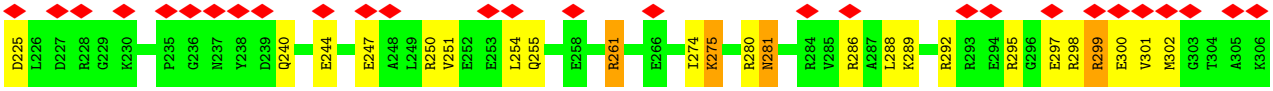


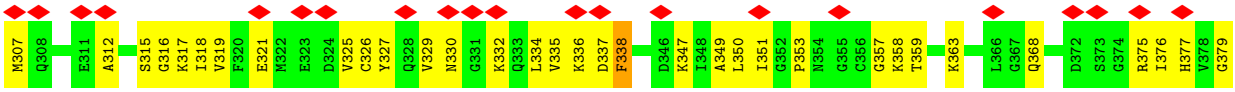
• Molecule 54: Uup

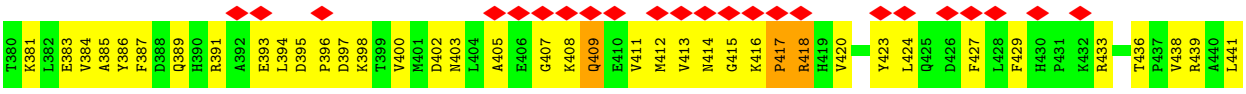
Chain U:

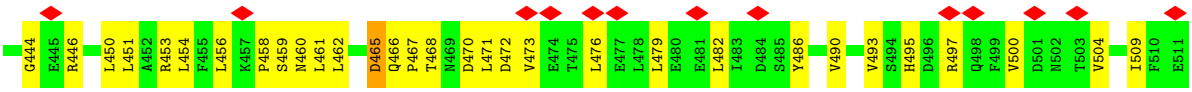


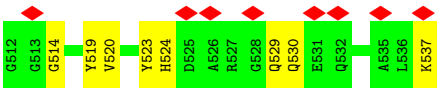






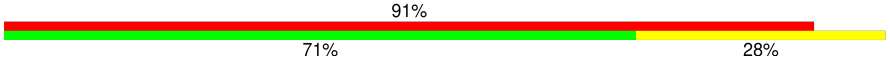


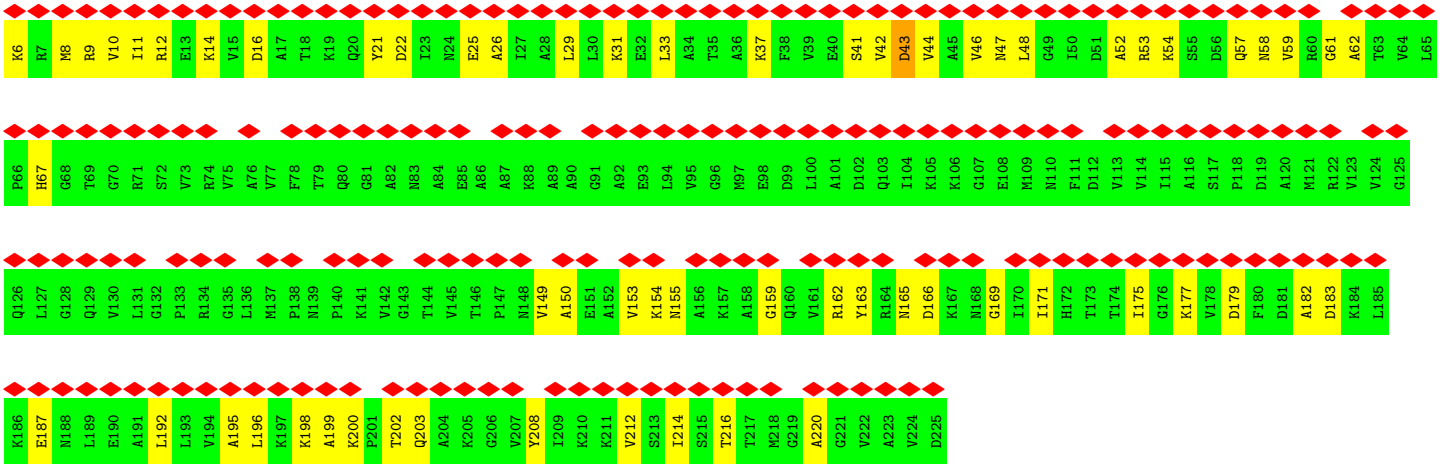




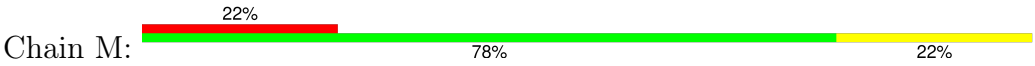
• Molecule 55: Large ribosomal subunit protein uL1

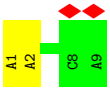
Chain 1:





• Molecule 56: mRNA





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61688	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 ($e^-/Å^2$)	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	3.670	Depositor
Minimum map value	-2.176	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.55	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: 4SU, ATP, H2U, 4OC, MG, PSU, 5MU, FME, NA

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	13	0.31	0/1152	0.51	0/1551
2	14	0.32	0/947	0.61	0/1268
3	15	0.31	0/1062	0.61	0/1413
4	16	0.31	0/1093	0.60	0/1460
5	17	0.30	0/973	0.60	0/1301
6	18	0.27	0/902	0.58	0/1209
7	19	0.32	0/929	0.56	0/1242
8	2	0.33	0/2121	0.59	0/2852
9	20	0.36	0/960	0.55	0/1278
10	21	0.32	0/829	0.57	0/1107
11	22	0.31	0/864	0.55	0/1156
12	23	0.29	0/744	0.54	0/994
13	24	0.29	0/787	0.55	0/1051
14	25	0.28	0/766	0.55	0/1025
15	27	0.32	0/650	0.56	0/858
16	28	0.30	0/635	0.57	0/848
17	29	0.24	0/510	0.54	0/677
18	3	0.33	0/1586	0.56	0/2134
19	30	0.28	0/453	0.61	0/605
20	31	0.26	0/531	0.57	0/709
21	32	0.31	0/450	0.58	0/599
22	33	0.31	0/416	0.53	0/554
23	34	0.29	0/380	0.65	0/498
24	35	0.30	0/513	0.54	0/676
25	36	0.29	0/303	0.62	0/397
26	4	0.30	0/1571	0.52	0/2113
27	5	0.28	0/1434	0.54	0/1926
28	6	0.27	0/1343	0.53	0/1816
29	9	0.27	0/1122	0.56	0/1515
30	R1	0.55	0/69797	0.85	28/108890 (0.0%)
31	R2	0.39	0/2847	0.86	4/4440 (0.1%)
32	R3	0.41	0/36782	0.86	34/57377 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	sb	0.26	0/1735	0.51	0/2338
34	sc	0.27	0/1651	0.56	1/2225 (0.0%)
35	sd	0.27	0/1665	0.56	0/2227
36	se	0.29	0/1169	0.57	0/1573
37	sf	0.29	0/835	0.56	0/1128
38	sg	0.26	0/1195	0.55	0/1602
39	sh	0.27	0/989	0.56	0/1326
40	si	0.30	0/1034	0.64	0/1375
41	sj	0.27	0/796	0.61	0/1077
42	sk	0.28	0/885	0.56	0/1195
43	sl	0.28	0/969	0.60	0/1300
44	sm	0.26	0/892	0.60	0/1193
45	sn	0.29	0/817	0.64	1/1088 (0.1%)
46	so	0.25	0/722	0.54	0/964
47	sp	0.26	0/659	0.59	0/884
48	sq	0.30	0/657	0.59	0/881
49	sr	0.28	0/544	0.56	0/731
50	ss	0.27	0/652	0.57	0/877
51	st	0.25	0/671	0.52	0/888
52	su	0.28	0/550	0.72	0/728
53	T	0.43	0/1716	0.80	0/2672
54	U	0.28	0/4363	0.57	2/5884 (0.0%)
55	1	0.26	0/1361	0.54	0/1796
56	M	0.38	0/219	0.77	0/339
All	All	0.44	0/162198	0.78	70/241830 (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
29	9	0	1
35	sd	0	1
45	sn	0	1
53	T	7	0
All	All	7	3

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	R1	2668	G	O4'-C1'-N9	7.95	114.56	108.20
32	R3	1208	C	C2-N1-C1'	7.58	127.14	118.80
54	U	417	PRO	N-CD-CG	-7.02	92.67	103.20
32	R3	470	C	C2-N1-C1'	6.87	126.35	118.80
30	R1	544	C	C2-N1-C1'	6.71	126.18	118.80

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	T	8	4SU	C3',C2'
53	T	20	H2U	C1',C2'
53	T	32	4OC	C2'
53	T	54	5MU	C4'
53	T	55	PSU	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	9	8	LYS	Peptide
35	sd	27	ILE	Peptide
45	sn	86	ALA	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	13	1129	0	1162	14	0
2	14	938	0	1012	12	0
3	15	1053	0	1129	28	0
4	16	1074	0	1157	27	0
5	17	960	0	1000	28	0
6	18	892	0	923	24	0
7	19	917	0	965	23	0
8	2	2082	0	2157	44	0
9	20	947	0	1022	14	0
10	21	816	0	839	17	0
11	22	857	0	922	20	0
12	23	738	0	807	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	24	779	0	834	22	0
14	25	753	0	780	15	0
15	27	642	0	665	15	0
16	28	625	0	655	12	0
17	29	509	0	543	9	0
18	3	1565	0	1616	33	0
19	30	449	0	491	11	0
20	31	522	0	524	16	0
21	32	444	0	461	16	0
22	33	409	0	440	10	0
23	34	377	0	418	9	0
24	35	504	0	574	13	0
25	36	302	0	343	10	0
26	4	1552	0	1619	31	0
27	5	1410	0	1447	37	0
28	6	1323	0	1374	45	0
29	9	1111	0	1148	38	0
30	R1	62318	0	31345	772	0
31	R2	2546	0	1292	42	0
32	R3	32850	0	16534	451	0
33	sb	1704	0	1732	0	0
34	sc	1624	0	1699	0	0
35	sd	1643	0	1710	0	0
36	se	1156	0	1199	0	0
37	sf	817	0	808	0	0
38	sg	1181	0	1240	0	0
39	sh	979	0	1034	0	0
40	si	1022	0	1070	0	0
41	sj	786	0	828	0	0
42	sk	869	0	878	0	0
43	sl	955	0	1019	0	0
44	sm	883	0	944	0	0
45	sn	805	0	847	0	0
46	so	714	0	737	0	0
47	sp	649	0	666	0	0
48	sq	648	0	691	0	0
49	sr	535	0	552	0	0
50	ss	637	0	665	0	0
51	st	665	0	714	0	0
52	su	544	0	579	0	0
53	T	1649	0	853	23	0
54	U	4295	0	4302	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1	1353	0	1159	43	0
56	M	195	0	99	1	0
57	15	1	0	0	0	0
57	2	1	0	0	0	0
57	20	1	0	0	0	0
57	32	1	0	0	0	0
57	R1	192	0	0	0	0
57	R3	81	0	0	0	0
58	U	62	0	24	4	0
59	U	2	0	0	0	0
All	All	150042	0	102247	1879	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 10.

The worst 5 of 1879 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)
30:R1:156:A:H2	30:R1:169:G:N1	1.28	1.26
30:R1:156:A:C2	30:R1:169:G:N1	2.03	1.24
32:R3:359:G:HO2'	32:R3:360:G:H8	1.03	0.97
30:R1:947:A:HO2'	30:R1:984:A:H2	1.09	0.92
30:R1:2073:C:H5	30:R1:2436:G:H1	1.20	0.89

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
2	14	120/122 (98%)	111 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	15	142/144 (99%)	126 (89%)	16 (11%)	0	100	100
4	16	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
5	17	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
6	18	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
7	19	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
8	2	269/271 (99%)	247 (92%)	22 (8%)	0	100	100
9	20	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
10	21	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
11	22	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
12	23	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
13	24	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	13	42
14	25	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
15	27	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
16	28	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
17	29	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
18	3	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
19	30	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
20	31	64/66 (97%)	52 (81%)	12 (19%)	0	100	100
21	32	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
22	33	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
23	34	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	23
24	35	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	36	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
26	4	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
27	5	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
28	6	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
29	9	147/149 (99%)	128 (87%)	19 (13%)	0	100	100
33	sb	216/218 (99%)	193 (89%)	22 (10%)	1 (0%)	25	58
34	sc	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
35	sd	203/205 (99%)	177 (87%)	26 (13%)	0	100	100
36	se	155/157 (99%)	129 (83%)	25 (16%)	1 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	sf	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
38	sg	149/151 (99%)	133 (89%)	16 (11%)	0	100	100
39	sh	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
40	si	125/127 (98%)	106 (85%)	19 (15%)	0	100	100
41	sj	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
42	sk	114/116 (98%)	102 (90%)	12 (10%)	0	100	100
43	sl	121/123 (98%)	92 (76%)	29 (24%)	0	100	100
44	sm	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
45	sn	98/100 (98%)	76 (78%)	22 (22%)	0	100	100
46	so	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
47	sp	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
48	sq	78/80 (98%)	66 (85%)	12 (15%)	0	100	100
49	sr	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
50	ss	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
51	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
52	su	63/65 (97%)	45 (71%)	17 (27%)	1 (2%)	8	31
54	U	535/537 (100%)	484 (90%)	50 (9%)	1 (0%)	44	74
55	1	218/220 (99%)	189 (87%)	29 (13%)	0	100	100
All	All	6342/6444 (98%)	5707 (90%)	629 (10%)	6 (0%)	50	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	24	88	ASP
52	su	35	GLU
54	U	275	LYS
36	se	122	VAL
33	sb	18	GLN

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	13	116/116 (100%)	115 (99%)	1 (1%)	75 88
2	14	103/103 (100%)	101 (98%)	2 (2%)	52 75
3	15	103/103 (100%)	101 (98%)	2 (2%)	52 75
4	16	109/109 (100%)	106 (97%)	3 (3%)	38 66
5	17	100/100 (100%)	98 (98%)	2 (2%)	50 74
6	18	86/86 (100%)	85 (99%)	1 (1%)	67 83
7	19	99/99 (100%)	97 (98%)	2 (2%)	50 74
8	2	216/216 (100%)	212 (98%)	4 (2%)	52 75
9	20	89/89 (100%)	89 (100%)	0	100 100
10	21	84/84 (100%)	83 (99%)	1 (1%)	67 83
11	22	93/93 (100%)	89 (96%)	4 (4%)	25 55
12	23	80/80 (100%)	80 (100%)	0	100 100
13	24	83/83 (100%)	78 (94%)	5 (6%)	16 44
14	25	78/78 (100%)	75 (96%)	3 (4%)	28 59
15	27	63/63 (100%)	62 (98%)	1 (2%)	58 79
16	28	67/67 (100%)	63 (94%)	4 (6%)	16 44
17	29	55/55 (100%)	54 (98%)	1 (2%)	54 76
18	3	164/164 (100%)	161 (98%)	3 (2%)	54 76
19	30	48/48 (100%)	47 (98%)	1 (2%)	48 72
20	31	59/59 (100%)	55 (93%)	4 (7%)	13 40
21	32	47/47 (100%)	45 (96%)	2 (4%)	25 55
22	33	45/45 (100%)	44 (98%)	1 (2%)	47 71
23	34	38/38 (100%)	38 (100%)	0	100 100
24	35	51/51 (100%)	50 (98%)	1 (2%)	50 74
25	36	34/34 (100%)	33 (97%)	1 (3%)	37 65
26	4	165/165 (100%)	158 (96%)	7 (4%)	25 56
27	5	148/148 (100%)	141 (95%)	7 (5%)	22 52
28	6	137/137 (100%)	133 (97%)	4 (3%)	37 65
29	9	114/114 (100%)	109 (96%)	5 (4%)	24 54
33	sb	180/180 (100%)	170 (94%)	10 (6%)	17 46
34	sc	170/170 (100%)	164 (96%)	6 (4%)	31 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	sd	172/172 (100%)	166 (96%)	6 (4%)	31 61
36	se	119/119 (100%)	119 (100%)	0	100 100
37	sf	87/87 (100%)	84 (97%)	3 (3%)	32 62
38	sg	124/124 (100%)	122 (98%)	2 (2%)	58 79
39	sh	104/104 (100%)	95 (91%)	9 (9%)	8 31
40	si	105/105 (100%)	99 (94%)	6 (6%)	17 46
41	sj	86/86 (100%)	85 (99%)	1 (1%)	67 83
42	sk	89/89 (100%)	87 (98%)	2 (2%)	47 71
43	sl	103/103 (100%)	101 (98%)	2 (2%)	52 75
44	sm	92/92 (100%)	89 (97%)	3 (3%)	33 62
45	sn	83/83 (100%)	78 (94%)	5 (6%)	16 44
46	so	76/76 (100%)	73 (96%)	3 (4%)	27 58
47	sp	65/65 (100%)	62 (95%)	3 (5%)	23 52
48	sq	74/74 (100%)	69 (93%)	5 (7%)	13 40
49	sr	56/56 (100%)	53 (95%)	3 (5%)	18 47
50	ss	70/70 (100%)	65 (93%)	5 (7%)	12 39
51	st	65/65 (100%)	63 (97%)	2 (3%)	35 63
52	su	55/55 (100%)	52 (94%)	3 (6%)	18 47
54	U	462/462 (100%)	438 (95%)	24 (5%)	19 48
55	1	106/171 (62%)	103 (97%)	3 (3%)	38 66
All	All	5217/5282 (99%)	5039 (97%)	178 (3%)	34 62

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	sk	56	LYS
50	ss	26	ASP
44	sm	78	ARG
47	sp	24	SER
52	su	37	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
35	sd	115	GLN
54	U	495	HIS
36	se	121	ASN
55	1	188	ASN
50	ss	55	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	R1	2902/2903 (99%)	621 (21%)	13 (0%)
31	R2	118/119 (99%)	22 (18%)	1 (0%)
32	R3	1529/1531 (99%)	433 (28%)	24 (1%)
53	T	75/78 (96%)	18 (24%)	3 (4%)
56	M	8/9 (88%)	0	0
All	All	4632/4640 (99%)	1094 (23%)	41 (0%)

5 of 1094 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	R1	3	U
30	R1	4	U
30	R1	10	A
30	R1	12	U
30	R1	14	A

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	R3	753	A
32	R3	1270	G
32	R3	837	U
32	R3	1124	G
32	R3	1305	G

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

6 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	$\#\|Z\| > 2$
53	5MU	T	54	53	19,22,23	2.72	8 (42%)	27,32,35	2.26	8 (29%)
53	PSU	T	55	53	18,21,22	2.20	9 (50%)	21,30,33	1.87	4 (19%)
53	H2U	T	20	53	18,21,22	4.33	5 (27%)	19,30,33	4.14	6 (31%)
53	4SU	T	8	53	18,21,22	3.99	7 (38%)	25,30,33	2.34	6 (24%)
53	FME	T	101	53	8,9,10	0.95	0	8,9,11	1.20	1 (12%)
53	4OC	T	32	53	20,23,24	2.38	4 (20%)	25,32,35	2.02	5 (20%)

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
53	5MU	T	54	53	1/1/5/5	3/7/25/26	0/2/2/2
53	PSU	T	55	53	1/1/5/5	1/7/25/26	0/2/2/2
53	H2U	T	20	53	2/2/8/9	5/7/38/39	0/2/2/2
53	4SU	T	8	53	2/2/5/5	3/7/25/26	0/2/2/2
53	FME	T	101	53	-	2/7/9/11	-
53	4OC	T	32	53	1/1/5/6	4/9/29/30	0/2/2/2

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	T	8	4SU	O2-C2	11.92	1.44	1.23
53	T	20	H2U	O4-C4	10.47	1.44	1.23
53	T	8	4SU	C4-S4	9.53	1.85	1.68
53	T	54	5MU	O4-C4	-9.24	1.06	1.23
53	T	20	H2U	C2-N1	9.14	1.48	1.35

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	T	20	H2U	O2-C2-N1	-11.63	109.12	123.10
53	T	20	H2U	O4-C4-N3	-7.68	108.45	120.30
53	T	8	4SU	C4-N3-C2	-6.65	120.94	127.31
53	T	20	H2U	O4-C4-C5	-6.62	108.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	T	20	H2U	O2-C2-N3	-6.23	110.00	121.49

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	T	8	4SU	C3'
53	T	8	4SU	C2'
53	T	20	H2U	C1'
53	T	20	H2U	C2'
53	T	32	4OC	C2'

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	T	20	H2U	O4'-C4'-C5'-O5'
53	T	20	H2U	O4'-C1'-N1-C6
53	T	20	H2U	C2'-C1'-N1-C2
53	T	54	5MU	C4'-C5'-O5'-P
53	T	101	FME	CB-CA-N-CN

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	T	54	5MU	4	0
53	T	55	PSU	2	0
53	T	20	H2U	1	0
53	T	8	4SU	1	0
53	T	101	FME	1	0
53	T	32	4OC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 281 ligands modelled in this entry, 279 are monoatomic - leaving 2 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	U	602	59	28,33,33	0.71	0	34,52,52	0.60	1 (2%)
58	ATP	U	601	59	28,33,33	0.71	0	34,52,52	0.60	1 (2%)

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	U	602	59	-	6/18/38/38	0/3/3/3
58	ATP	U	601	59	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	U	601	ATP	C5-C6-N6	2.31	123.83	120.31
58	U	602	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	U	602	ATP	C5'-O5'-PA-O2A
58	U	602	ATP	O4'-C4'-C5'-O5'
58	U	602	ATP	C3'-C4'-C5'-O5'
58	U	602	ATP	C5'-O5'-PA-O1A
58	U	602	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	U	602	ATP	2	0

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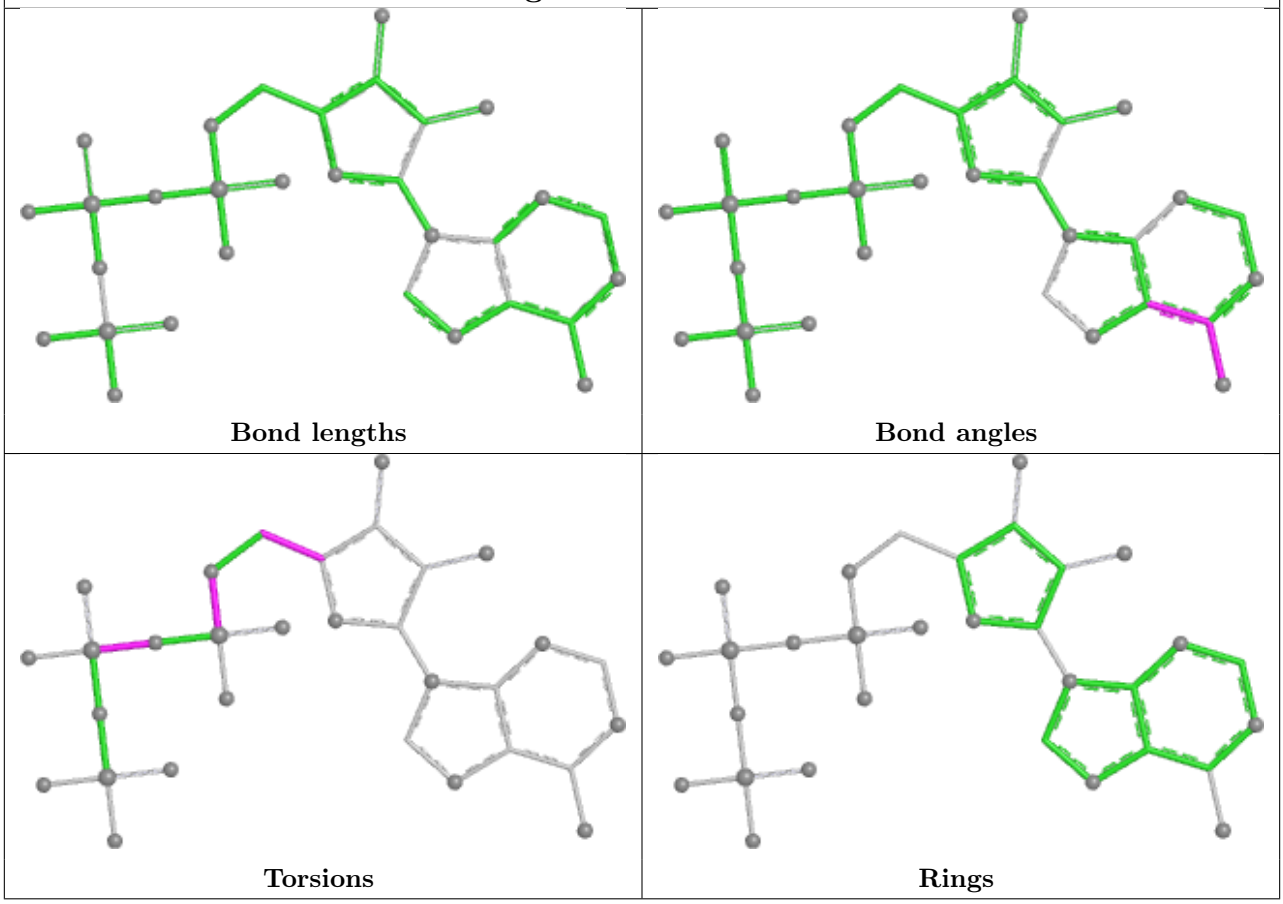
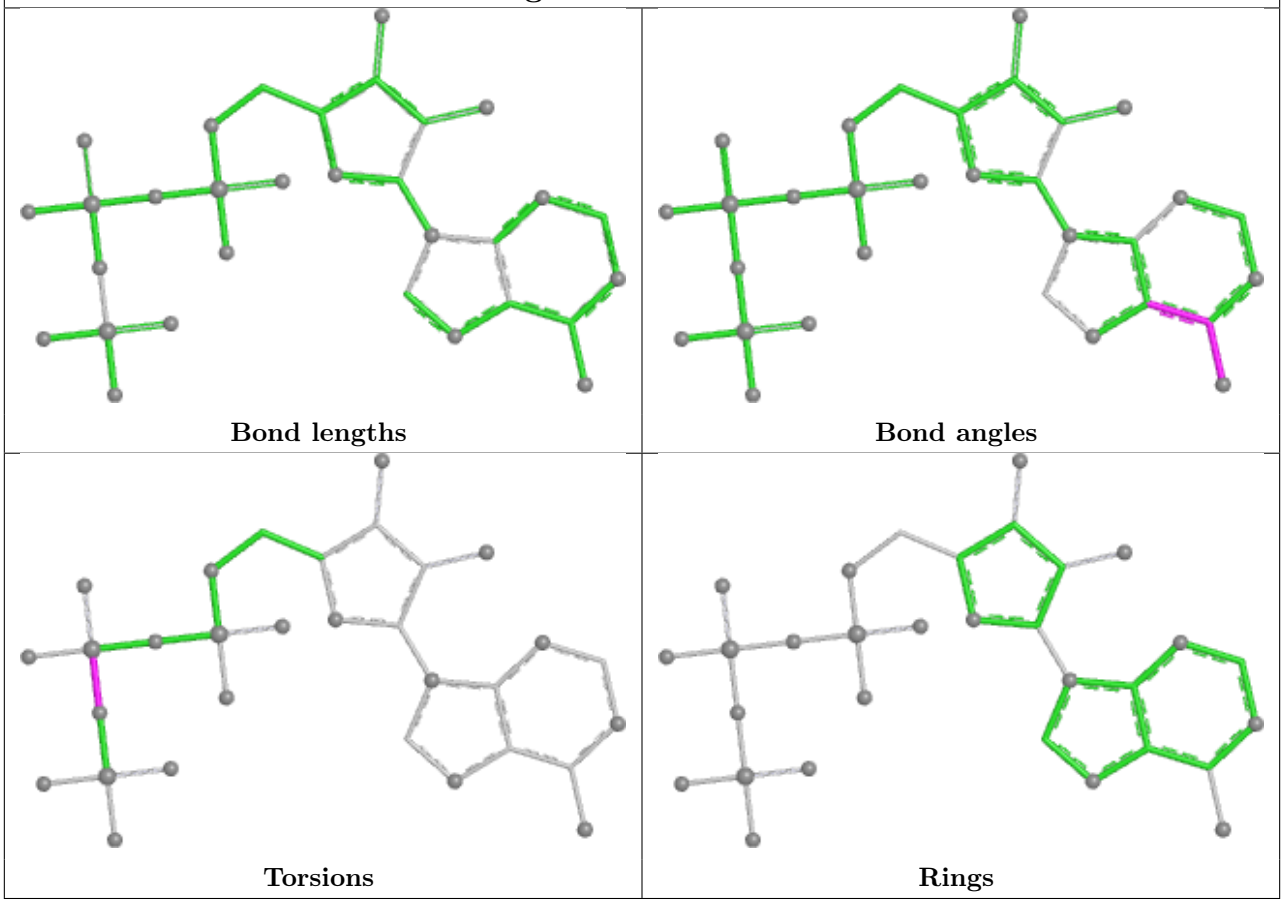
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	U	601	ATP	2	0

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 then 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 U 602



Ligand ATP U 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	R3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	210:C	O3'	211:G	P	7.40
1	R3	460:A	O3'	461:A	P	4.00

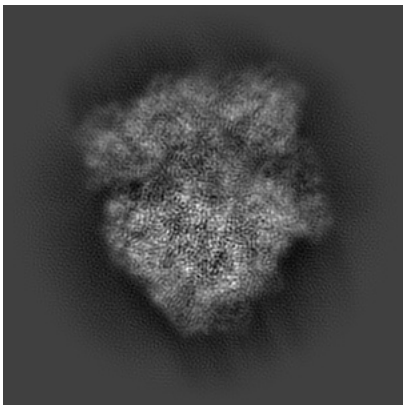
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29399. These allow visual inspection of the internal detail of the map and identification of artifacts.

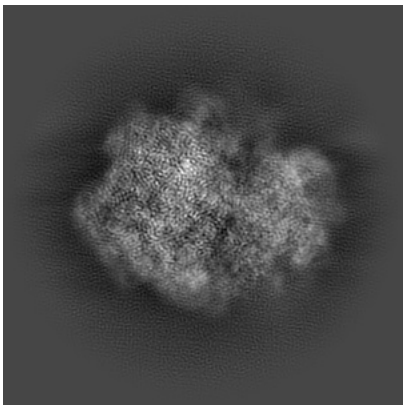
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

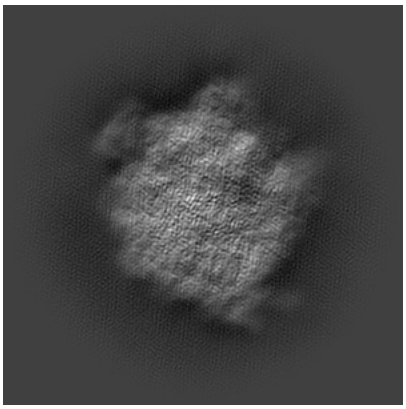
6.1.1 Primary map



X

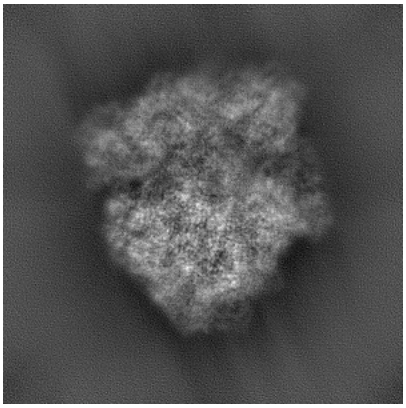


Y

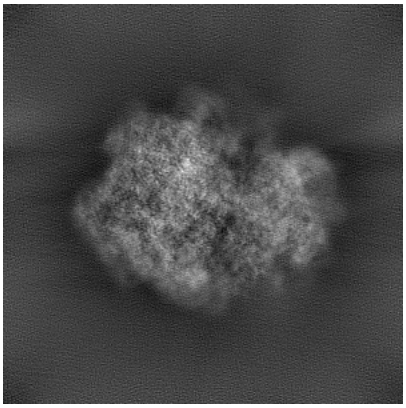


Z

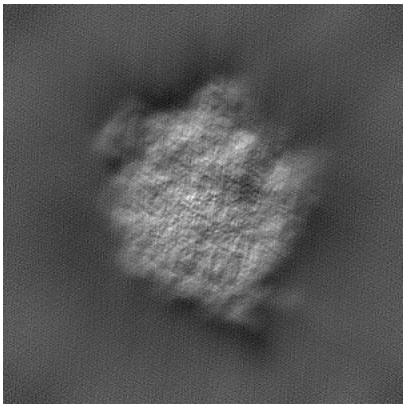
6.1.2 Raw map



X



Y

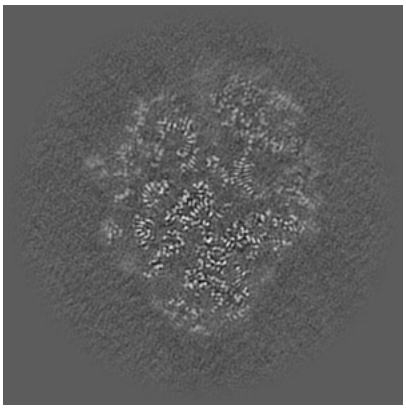


Z

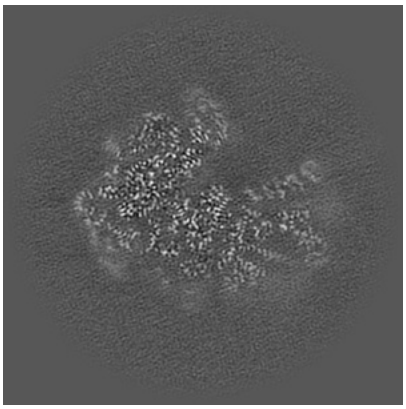
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

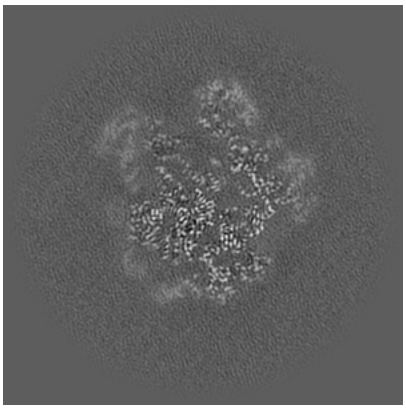
6.2.1 Primary map



X Index: 200

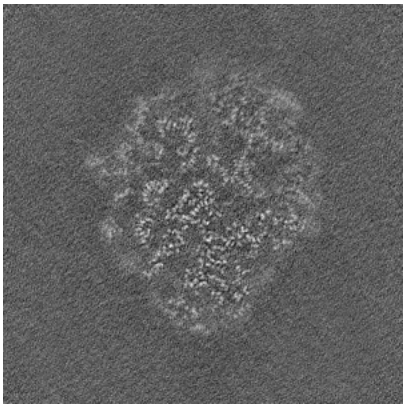


Y Index: 200

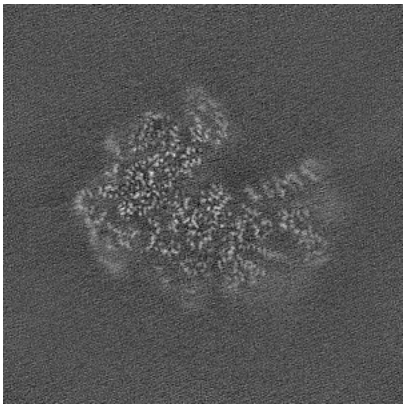


Z Index: 200

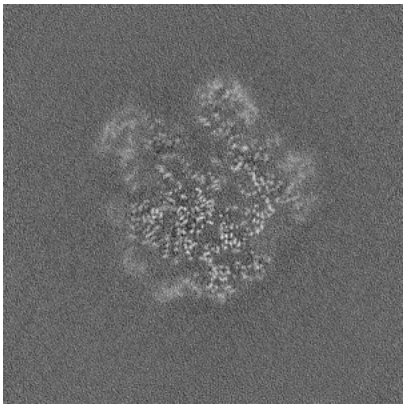
6.2.2 Raw map



X Index: 200



Y Index: 200

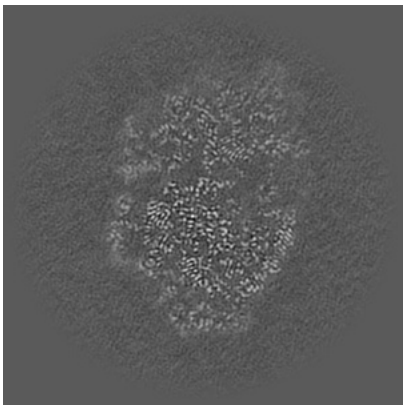


Z Index: 200

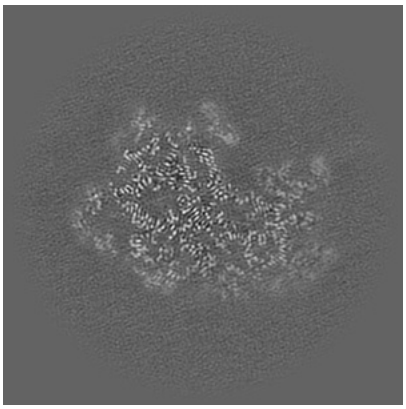
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

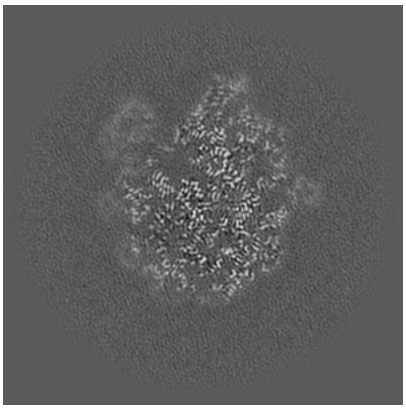
6.3.1 Primary map



X Index: 188

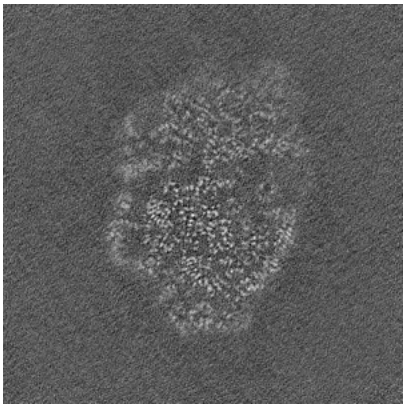


Y Index: 184

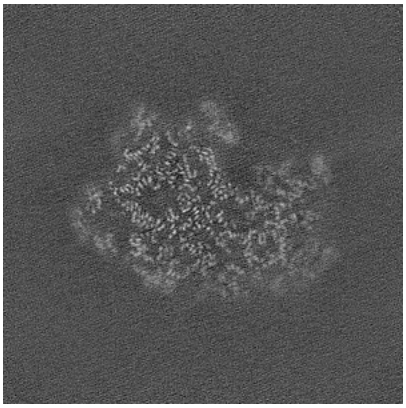


Z Index: 184

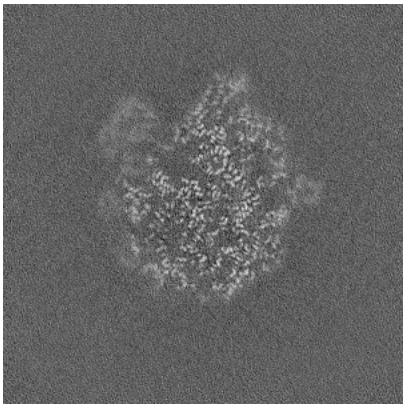
6.3.2 Raw map



X Index: 188



Y Index: 184

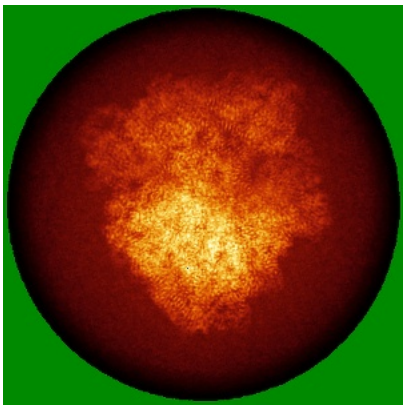


Z Index: 184

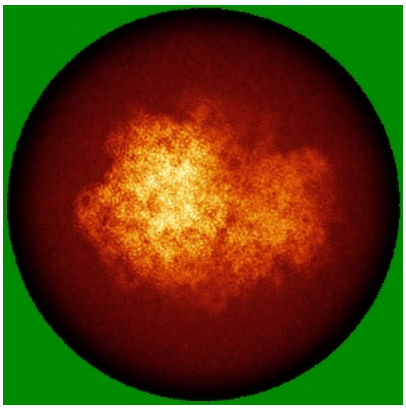
The images above show the largest variance slices of the map in three orthogonal directions.

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

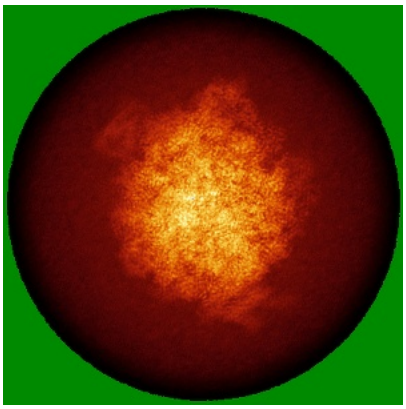
6.4.1 Primary map



X

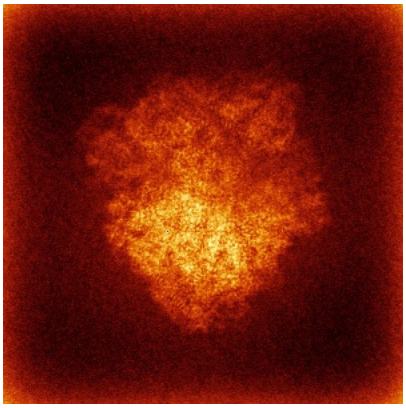


Y

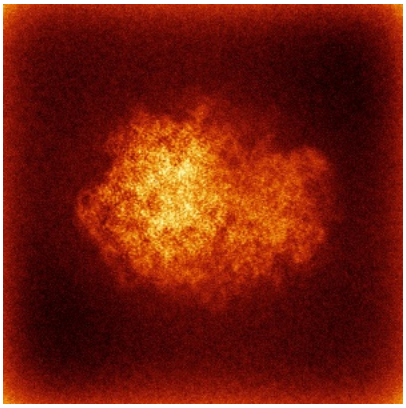


Z

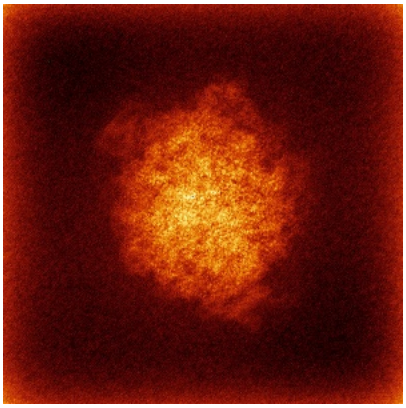
6.4.2 Raw map



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

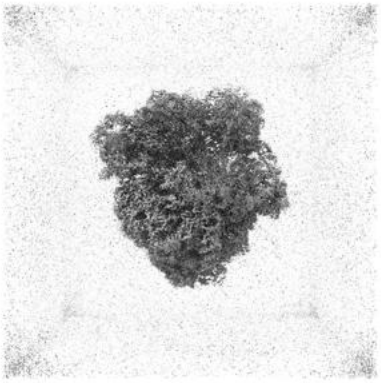
X

Y

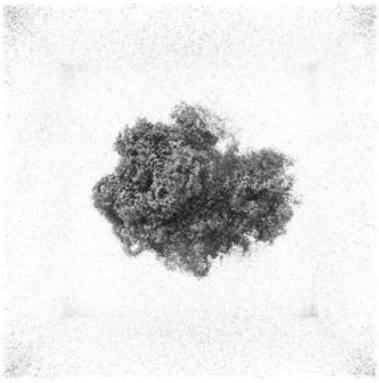
Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

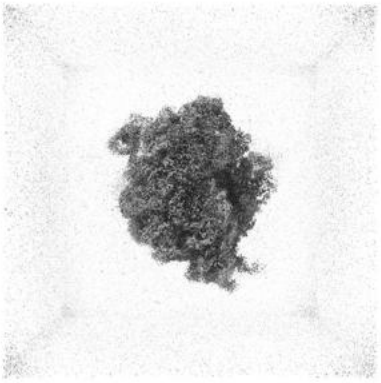
6.5.2 Raw map



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.

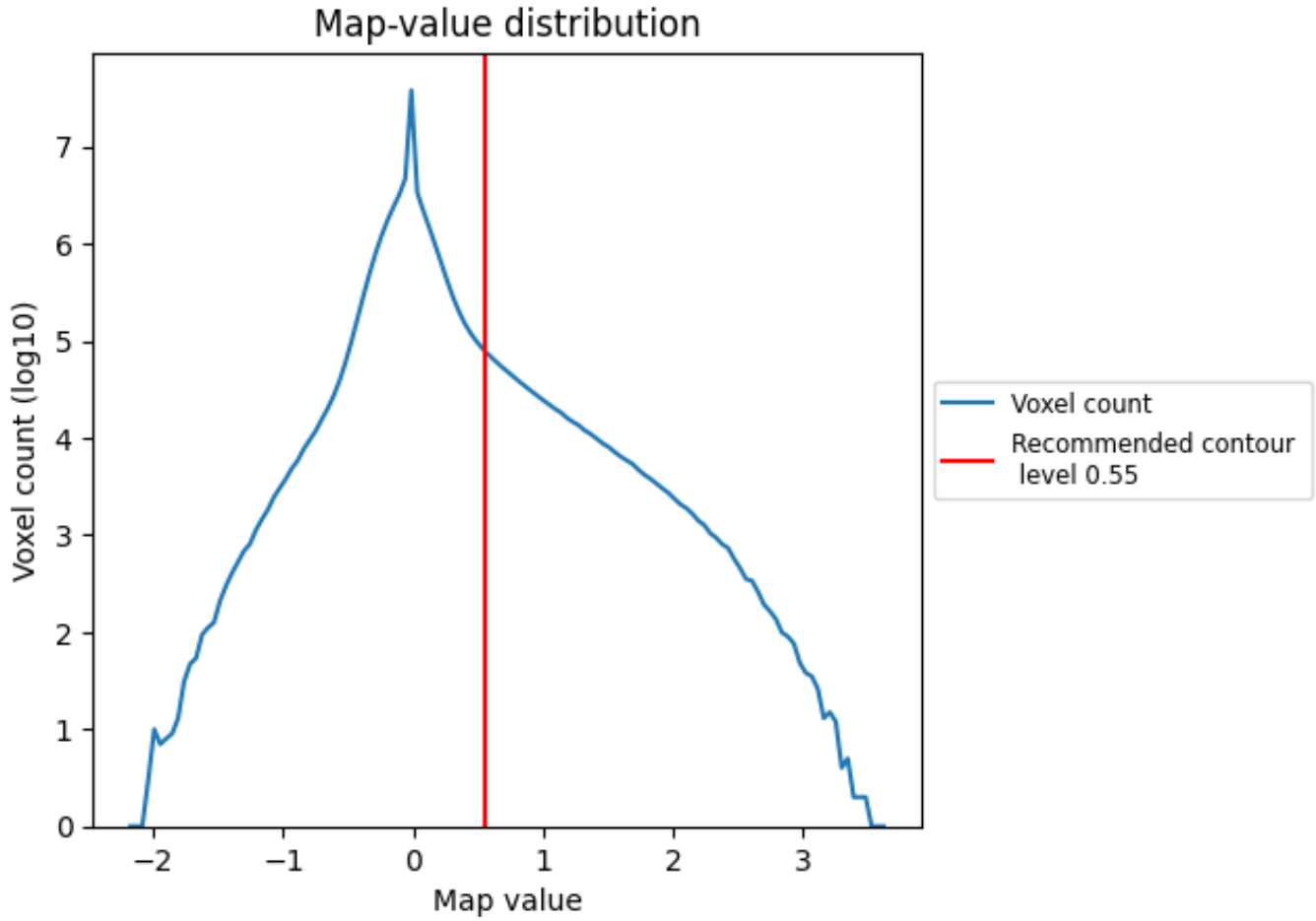
6.6 Mask visualisation (i)

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

7 Map analysis

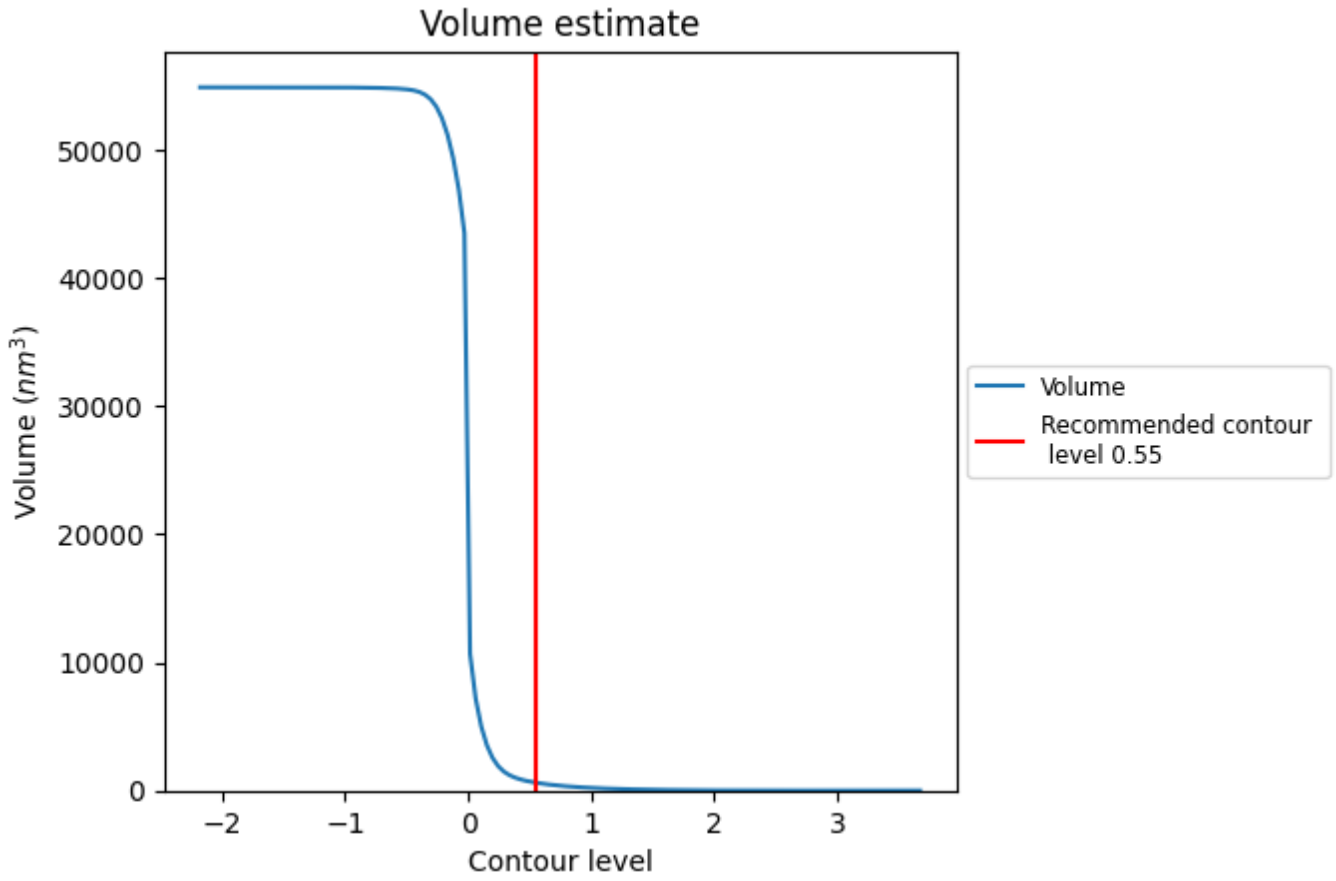
This section contains the results of statistical analysis of the map.

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.

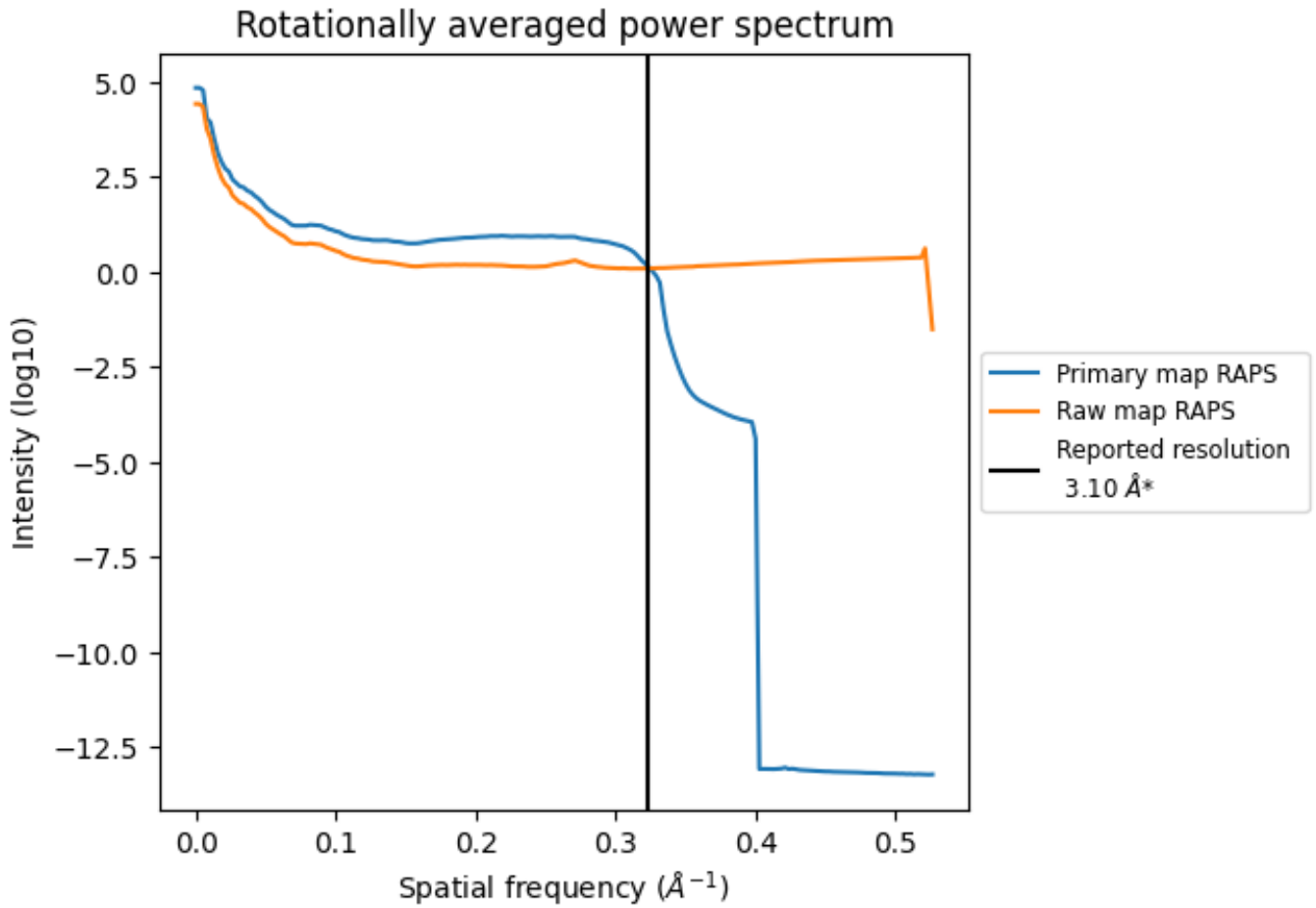
7.2 Volume estimate (i)



The volume at the recommended contour level is 616 nm^3; this corresponds to an approximate mass of 556 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 (i)

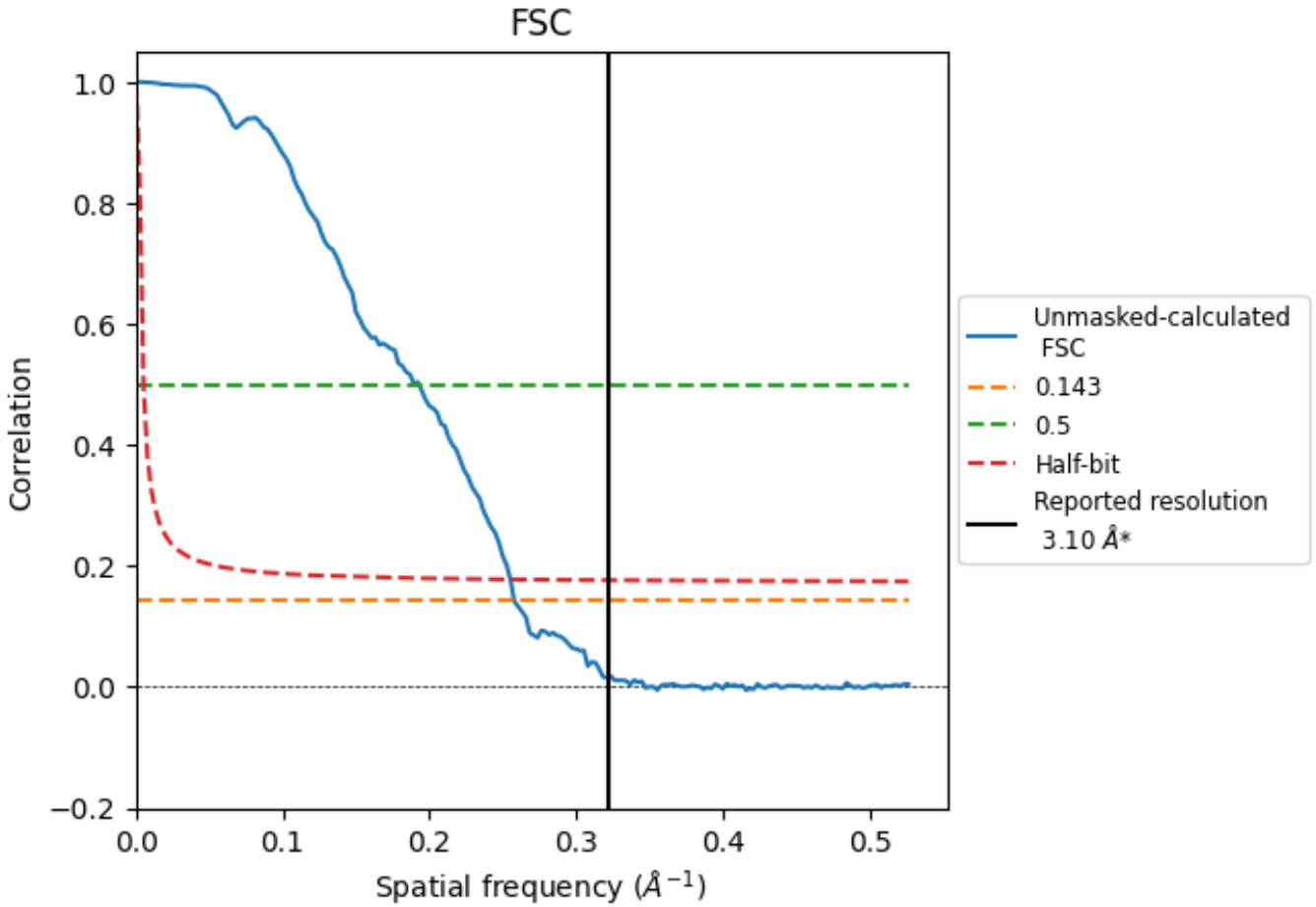


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

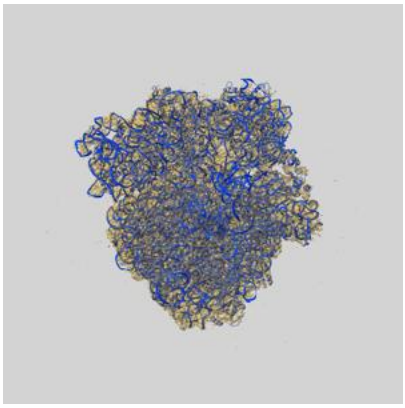
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	5.19	3.92

*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 3.88 differs from the reported value 3.1 by more than 10 %

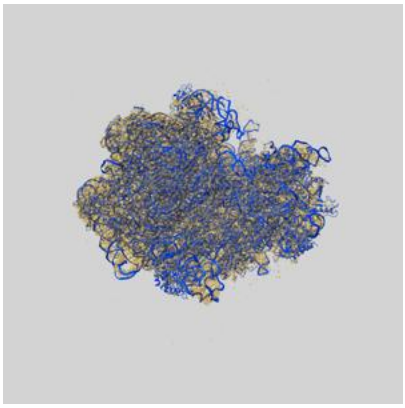
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29399 and PDB model 9NLJ. Per-residue inclusion information can be found in section 3 on page 16.

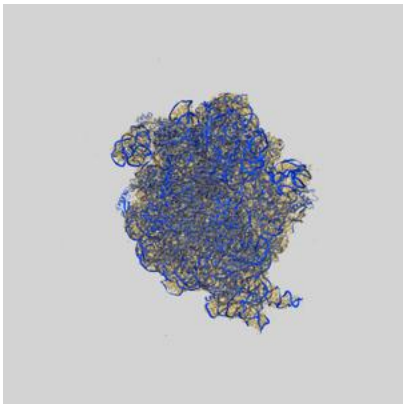
9.1 Map-model overlay



X



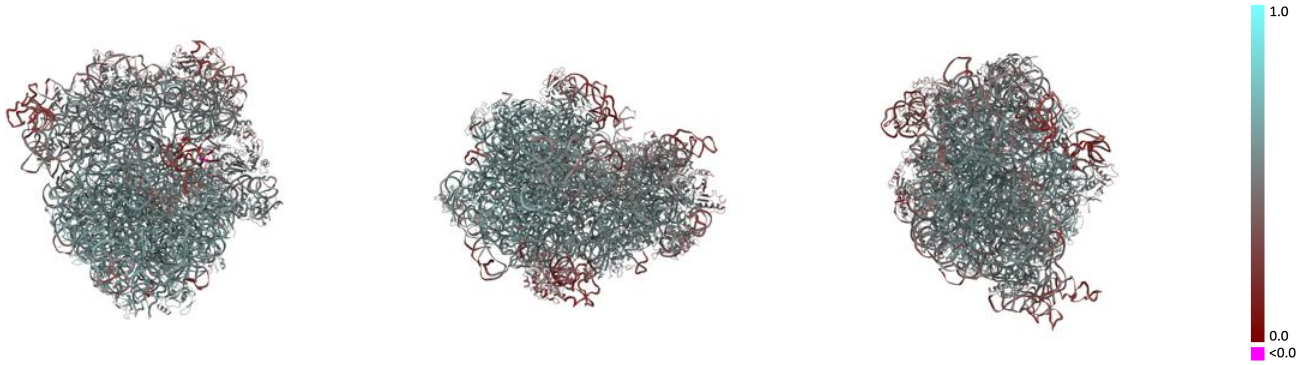
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

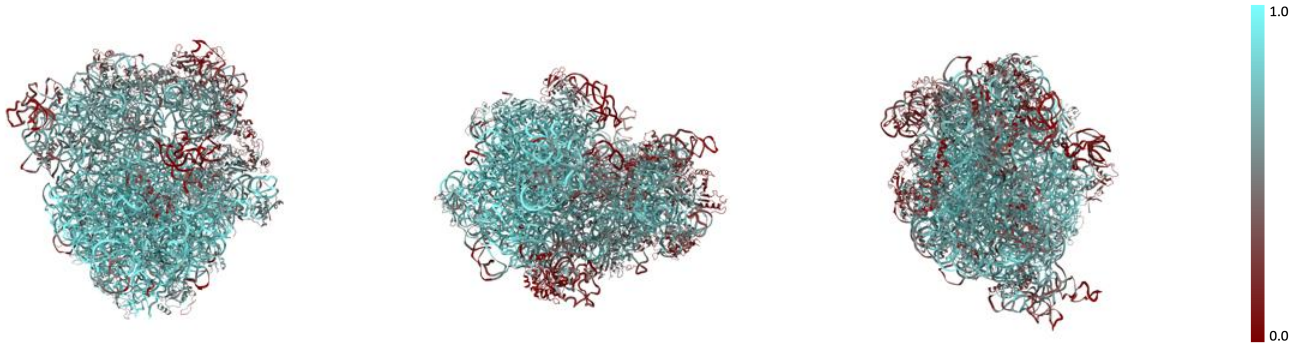
9.2 Q-score mapped to coordinate model



X Y Z

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.

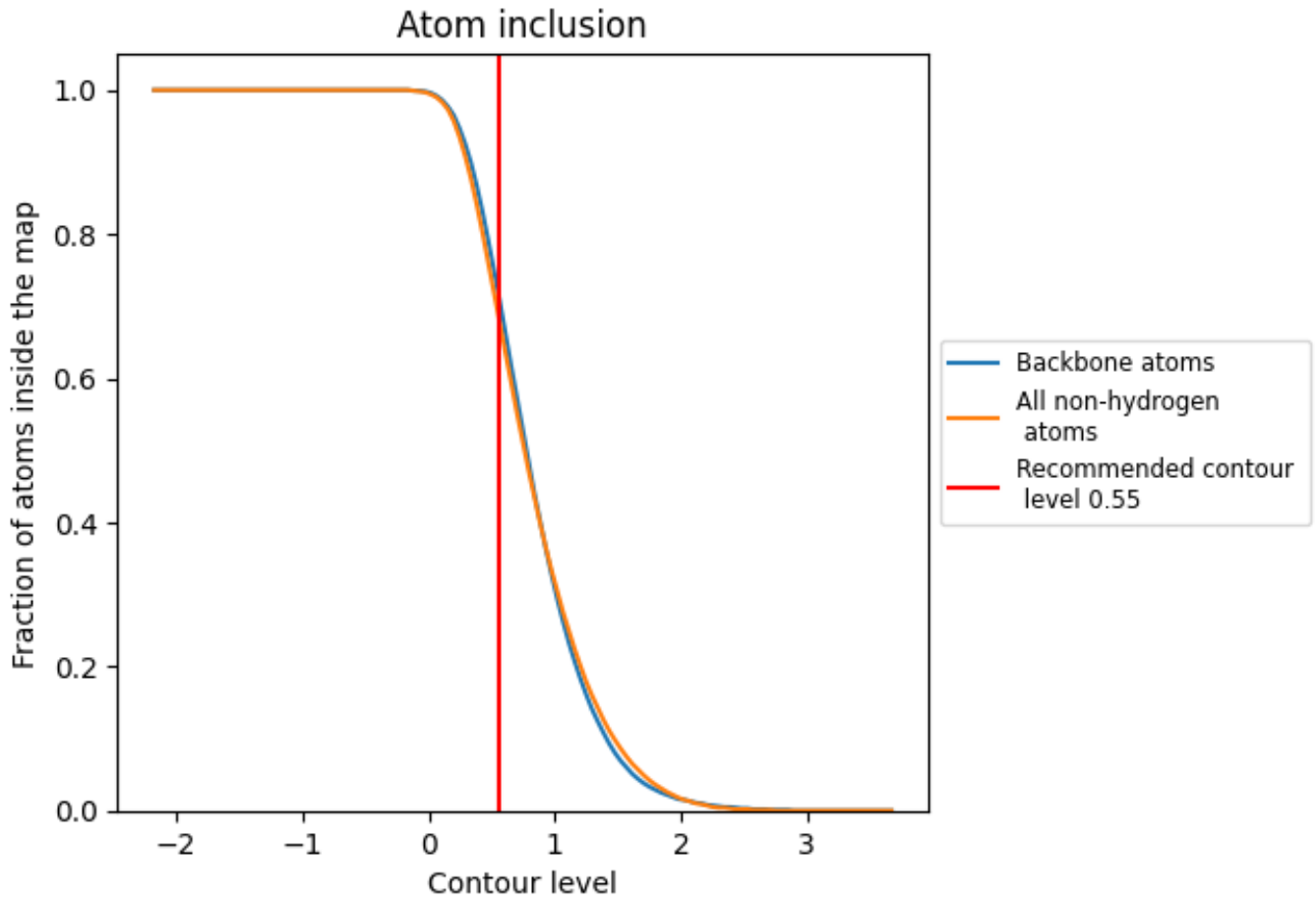
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 72% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6900	0.5200
1	0.1170	0.3350
13	0.7500	0.5890
14	0.7150	0.5820
15	0.7360	0.5620
16	0.7170	0.5740
17	0.8160	0.5810
18	0.5540	0.5190
19	0.6900	0.5700
2	0.7360	0.5870
20	0.7940	0.5910
21	0.6670	0.5520
22	0.7200	0.5710
23	0.6190	0.5480
24	0.5410	0.5200
25	0.5980	0.5270
27	0.7430	0.5800
28	0.6960	0.5740
29	0.5760	0.5130
3	0.7740	0.5800
30	0.7390	0.5700
31	0.1740	0.3730
32	0.7370	0.5750
33	0.7080	0.5760
34	0.8030	0.5970
35	0.8310	0.6080
36	0.6540	0.5610
4	0.6520	0.5520
5	0.4030	0.4830
6	0.2940	0.4200
9	0.1110	0.3510
M	0.6560	0.5380
R1	0.8100	0.5400
R2	0.7600	0.4990
R3	0.6950	0.4920

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Chain	Atom inclusion	Q-score
T	0.7420	0.5500
U	0.4790	0.5230
sb	0.2780	0.4310
sc	0.4320	0.5000
sd	0.3490	0.4730
se	0.5690	0.5190
sf	0.4850	0.4790
sg	0.4850	0.5090
sh	0.5820	0.5330
si	0.4310	0.4760
sj	0.2820	0.4450
sk	0.5850	0.5470
sl	0.4160	0.5130
sm	0.3840	0.4790
sn	0.3760	0.4700
so	0.5640	0.5170
sp	0.4510	0.4960
sq	0.4640	0.4960
sr	0.5040	0.5020
ss	0.2880	0.4460
st	0.4080	0.4750
su	0.3480	0.4410