wwPDB EM Validation Summary Report ⓘ

Nov 3, 2022 – 12:25 AM EDT

PDB ID	:	5UQ7
EMDB ID	:	EMD-8596
Title	:	70S ribosome complex with dnaX mRNA stemloop and E-site tRNA ("in" conformation)
Authors	:	Zhang, Y.; Hong, S.; Skiniotis, G.; Dunham, C.M.
Deposited on	:	2017-02-07
Resolution	:	3.50 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:

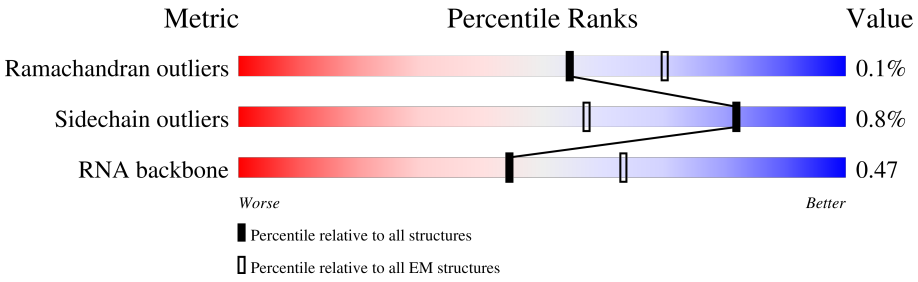
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2915	15% 75% 23%
2	B	120	17% 80% 20%
3	D	275	49% 100%
4	E	204	52% 100%
5	F	203	65% 98%
6	G	181	91% 98%
7	H	173	90% 99%
8	I	146	99% 100%

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Mol	Chain	Length	Quality of chain
9	N	140	65% 99%
10	O	122	60% 99%
11	P	149	67% 100%
12	Q	141	60% 99%
13	R	118	55% 100%
14	S	110	67% 99%
15	T	131	65% 99%
16	U	116	51% 100%
17	V	101	72% 99%
18	W	112	57% 99%
19	X	95	69% 100%
20	Y	107	80% 97%
21	Z	187	89% 99%
22	0	77	53% 99%
23	1	97	67% 99%
24	2	70	73% 100%
25	3	59	69% 100%
26	4	69	91% 97%
27	5	59	59% 98%
28	6	53	68% 98%
29	7	48	52% 100%
30	8	64	59% 100%
31	9	37	62% 100%
32	a	1521	21% 76% 22%
33	b	231	91% 99%

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Mol	Chain	Length	Quality of chain
34	c	206	82% 100%
35	d	208	80% 100%
36	e	148	73% 99%
37	f	100	90% 100%
38	g	155	88% 99%
39	h	137	66% 100%
40	i	126	90% 98%
41	j	96	92% 99%
42	k	114	82% 100%
43	l	122	74% 98%
44	m	114	89% 99%
45	n	60	80% 97%
46	o	88	70% 99%
47	p	82	66% 99%
48	q	99	70% 100%
49	r	68	85% 100%
50	s	83	94% 100%
51	t	98	83% 99%
52	u	23	96% 100%
53	y	77	84% 82% 18%
54	C	226	100% 99%
55	z	76	100% 55% 43%
56	x	55	96% 56% 42%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 148590 atoms, of which 4 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2867	61758	27491	11552	19850	2865	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2573	1146	476	832	119	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	275	2136	1349	423	361	3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	204	1559	985	298	270	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	203	1580	1007	297	274	2	0	1

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	181	1424	912	259	249	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	173	Total	C	N	O	S	0	0
			1324	842	247	234	1		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	146	Total	C	N	O	S	0	0
			1076	687	186	202	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	140	Total	C	N	O	S	0	0
			1117	719	207	187	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	122	Total	C	N	O	S	0	0
			933	588	171	170	4		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	149	Total	C	N	O	S	0	0
			1135	706	230	196	3		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0
			1122	715	212	188	7		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	118	Total	C	N	O	S	0	0
			968	604	203	160	1		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	S	110	Total 870	C 549	N 173	O 148	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	131	Total 1083	C 675	N 224	O 183	S 1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	116	Total 959	C 608	N 201	O 149	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	101	Total 771	C 495	N 140	O 135	S 1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	112	Total 886	C 557	N 174	O 153	S 2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	95	Total 750	C 488	N 135	O 126	S 1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	107	Total 810	C 519	N 153	O 132	S 6	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	187	Total	C	N	O	S	0	0
			1459	932	257	268	2		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	77	Total	C	N	O	S	0	0
			608	375	129	103	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	97	Total	C	N	O	S	0	0
			759	478	149	131	1		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	70	Total	C	N	O	S	0	0
			592	368	119	103	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	3	59	Total	C	N	O	0	0
			464	296	90	78		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	69	Total	C	N	O	S	0	0
			536	342	98	91	5		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	59	Total	C	N	O	S	0	0
			455	285	89	76	5		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	53	Total	C	N	O	S	0	0
			449	279	91	75	4		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	48	Total	C	N	O	S	0	0
			418	257	104	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	64	Total	C	N	O	S	0	0
			517	331	102	82	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1513	Total	C	N	O	P	0	0
			32532	14488	6021	10510	1513		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1542	G	-	insertion	GB 55771382
a	1543	C	-	insertion	GB 55771382
a	1544	U	-	insertion	GB 55771382

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	231	Total	C	N	O	S	0	0
			1825	1167	326	327	5		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1542	968	300	273	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	208	Total	C	N	O	S	0	0
			1668	1047	330	284	7		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	148	Total	C	N	O	S	0	0
			1133	716	214	199	4		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			816	516	146	151	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	155	Total	C	N	O	S	0	0
			1229	766	241	216	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	137	Total	C	N	O	S	0	0
			1088	689	206	191	2		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	i	126	Total	C	N	O	0	0
			966	613	186	167		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	j	96	Total	C	N	O	0	0
			710	442	137	131		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	114	Total	C	N	O	S	0	0
			833	519	156	155	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	122	Total	C	N	O	S	0	0
			932	586	185	159	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	114	Total	C	N	O	S	0	0
			895	550	186	157	2		

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	88	Total	C	N	O	S	0	0
			728	456	144	126	2		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	82	Total	C	N	O	S	0	0
			677	430	133	113	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
49	r	68	Total	C	N	O	0	0
			555	355	108	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	83	Total	C	N	O	S	0	0
			645	410	118	115	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	98	Total	C	N	O	S	0	0
			733	451	154	126	2		

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	u	23	Total	C	N	O	0	0
			199	122	48	29		

- Molecule 53 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	77	Total	C	N	O	P	0	0
			1640	732	298	534	76		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	17B	C	U	conflict	GB 1126835761

- Molecule 54 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	C	225	Total	C	N	O	S	0	0
			1718	1085	315	316	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	MET	deletion	UNP Q5SLP7

- Molecule 55 is a RNA chain called E-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

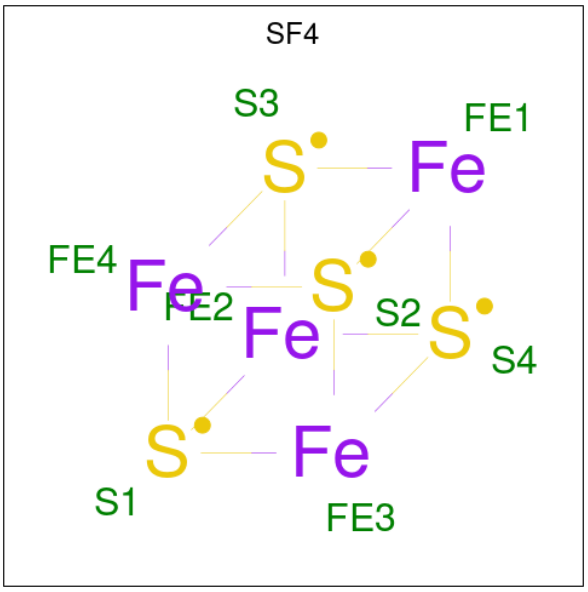
- Molecule 56 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	x	55	Total	C	H	N	O	P	0	0
			1180	527	4	219	376	54		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	Y	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	
57	5	1	Total	Zn	0
			1	1	
57	6	1	Total	Zn	0
			1	1	
57	9	1	Total	Zn	0
			1	1	
57	n	1	Total	Zn	0
			1	1	

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



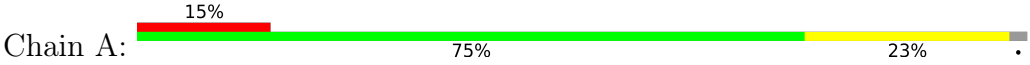
Mol	Chain	Residues	Atoms			AltConf
58	d	1	Total	Fe	S	0
			8	4	4	

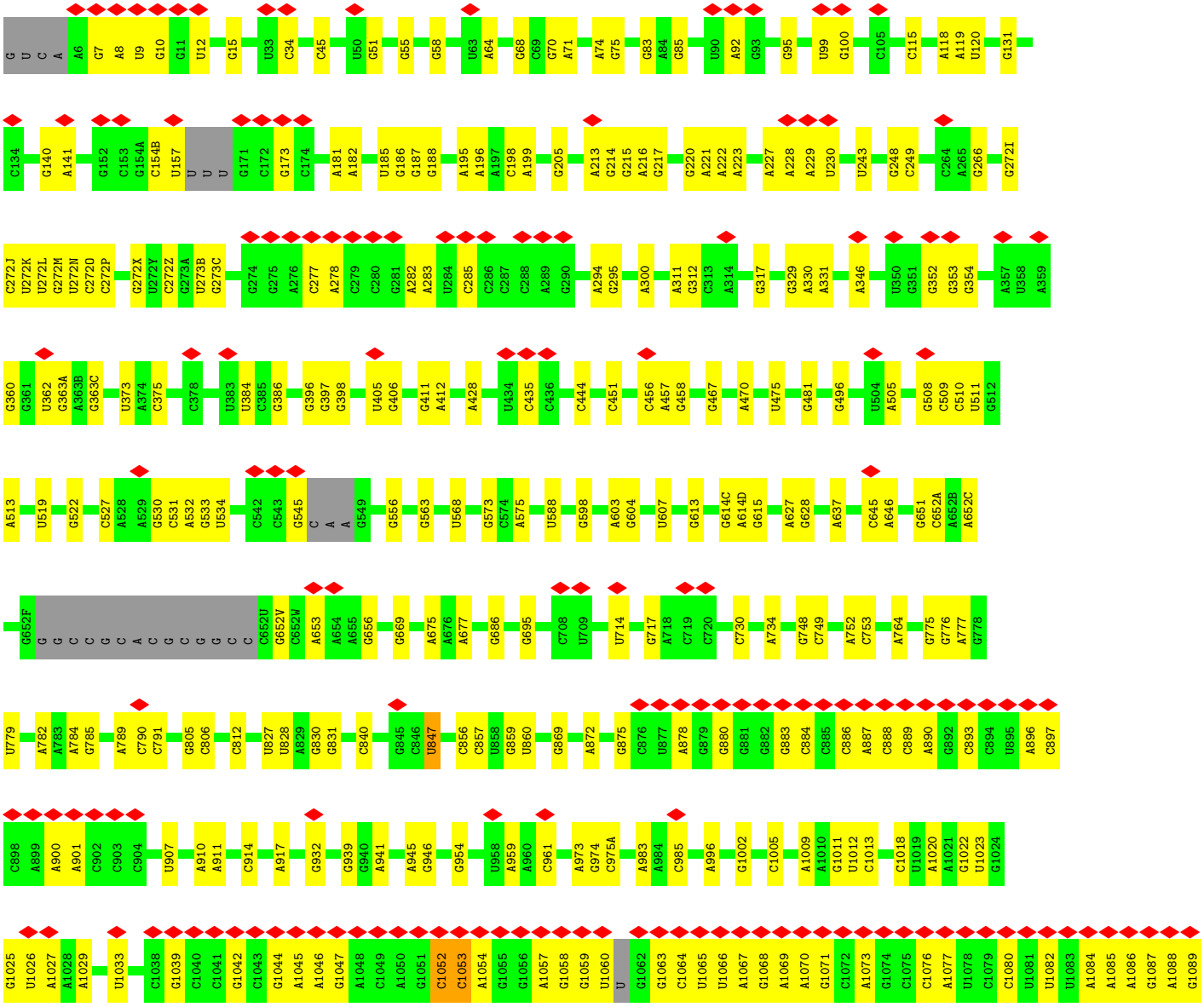
3 Residue-property plots (i)

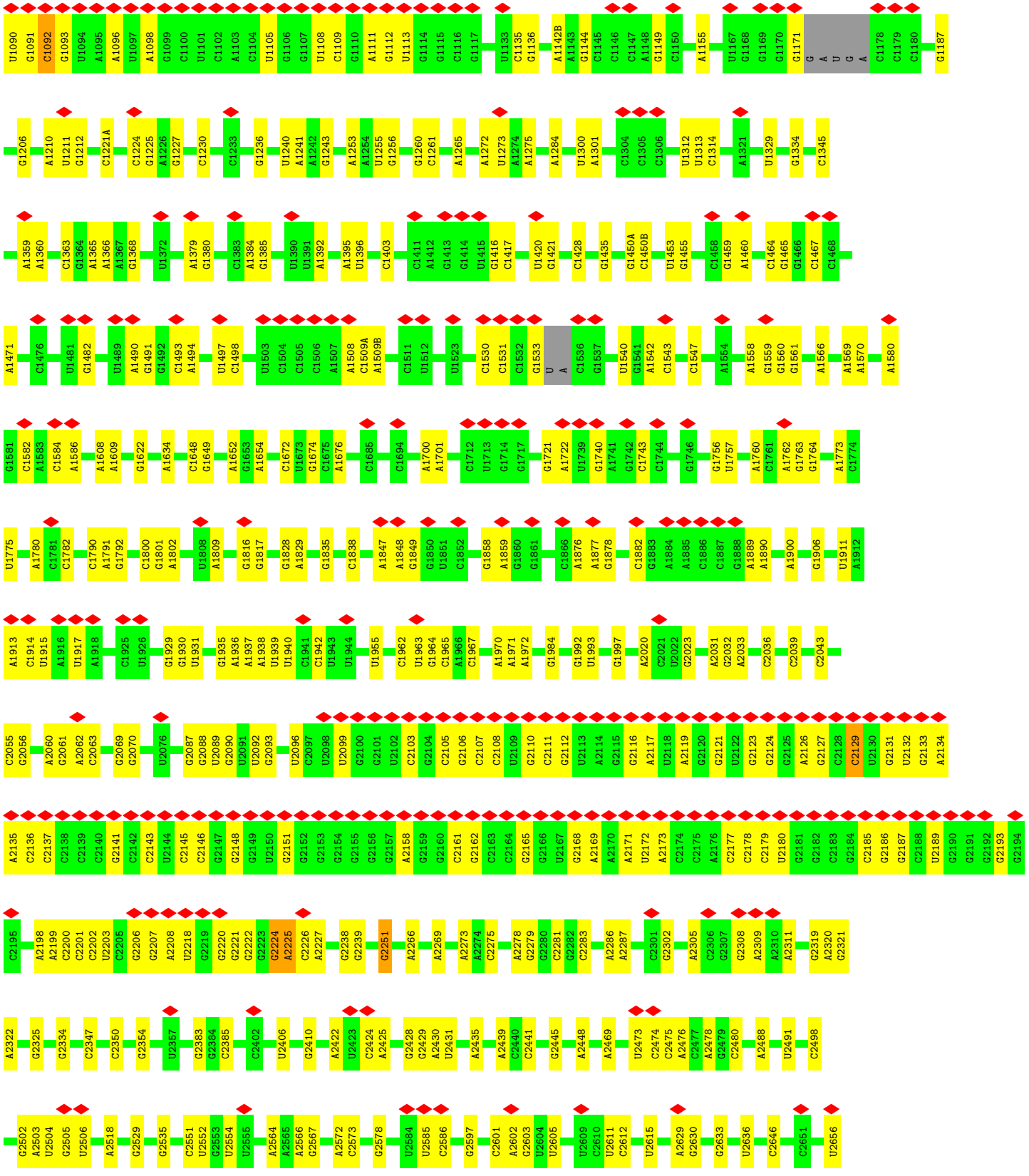
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

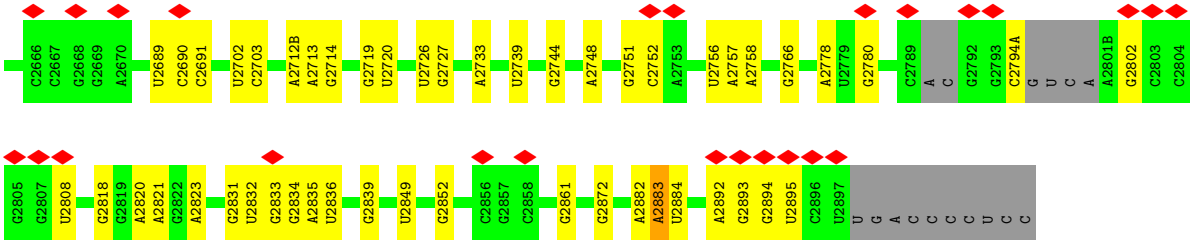
- Molecule 1: 23S rRNA

Chain A:



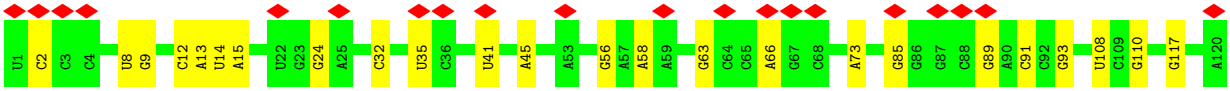



U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 C1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 U1133 C1135 G1136 A1142B A1143 G1144 C1145 C1146 C1147 A1148 G1149 C1150 A1155 U1167 G1168 G1169 G1170 G1171 G A U G A C1178 C1179 C1180 G1187
G1206 A1210 U1211 G1212 C1221A C1224 G1225 A1226 G1227 C1230 C1233 G1236 U1240 A1241 A1242 G1243 A1253 A1254 U1255 G1256 G1260 C1261 A1265 A1272 U1273 A1274 A1275 A1284 U1300 A1301 C1304 C1305 C1306 U1312 U1313 C1314 A1321 U1329 G1334 C1345
A1359 A1360 C1363 G1364 A1365 A1366 A1367 G1368 U1372 A1379 G1380 C1383 A1384 G1385 U1390 U1391 A1392 A1395 U1396 C1403 C1411 A1412 G1413 G1414 U1415 G1416 C1417 U1420 G1421 C1428 G1435 G1450A C1450B U1453 G1455 C1458 G1459 A1460 C1464 G1465 G1466 C1467 C1468
A1471 C1476 U1481 G1482 U1489 A1490 G1491 G1492 C1493 A1494 U1497 C1498 U1503 C1504 C1505 C1506 A1507 A1508 C1509A A1509B C1511 U1512 U1523 C1530 C1531 C1532 G1533 U A C1536 G1537 U1540 G1541 A1542 C1543 C1547 A1554 A1558 G1559 G1560 G1561 A1566 A1569 A1570 A1580
G1581 C1582 A1583 C1584 A1586 A1608 A1609 G1622 A1634 C1648 G1649 A1652 G1653 A1654 C1672 U1673 G1674 C1675 A1676 C1685 C1694 A1700 A1701 C1712 U1713 G1714 G1717 G1721 A1722 U1739 G1740 A1741 G1742 C1743 C1744 G1746 G1756 U1757 A1760 C1761 A1762 G1763 G1764 A1773 C1774
U1775 A1780 C1781 C1782 C1790 A1791 G1792 C1800 G1801 A1802 U1808 A1809 G1816 G1817 G1828 A1829 G1835 C1838 A1847 A1848 G1849 G1850 U1851 C1852 G1858 A1859 G1860 G1861 C1866 A1876 A1877 G1878 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 A1890 A1900 G1906 U1911 A1912
A1913 C1914 U1915 A1916 U1917 A1918 C1925 U1926 G1929 G1930 U1931 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 U1955 C1962 U1963 G1964 C1965 A1966 C1967 A1970 A1971 A1972 G1984 G1992 U1993 G1997 A2020 C2021 U2022 G2023 A2031 G2032 A2033 C2036 C2039 C2043
C2055 G2056 A2060 G2061 A2062 C2063 G2069 G2070 U2076 G2087 G2088 U2089 G2090 U2091 U2092 G2093 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134
A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 G2194
C2195 A2198 A2199 C2200 C2201 C2202 U2203 C2205 G2206 G2207 A2208 U2218 G2219 G2220 G2221 G2222 G2223 G2224 A2225 C2226 A2227 G2238 G2239 G2251 A2266 A2269 A2273 A2274 C2275 A2278 G2279 G2280 C2281 G2282 C2283 A2286 A2287 C2301 G2302 A2305 C2306 G2307 G2308 A2309 A2310 A2311 G2319 A2320 G2321
A2322 G2325 G2334 C2347 C2350 G2354 U2357 G2383 G2384 C2385 C2402 U2406 G2410 A2422 U2423 C2424 A2425 G2428 G2429 A2430 U2431 A2435 A2439 C2440 C2441 G2445 A2448 A2469 U2473 C2474 C2475 A2476 C2477 A2478 G2479 C2480 A2488 U2491 C2498
G2502 A2503 U2504 G2505 U2506 A2518 G2529 G2535 C2551 U2552 G2553 U2554 U2555 A2564 A2565 A2566 G2567 A2572 C2573 G2578 U2584 U2585 C2586 G2597 C2601 A2602 G2603 U2604 U2605 U2609 C2610 U2611 C2612 U2615 A2629 G2630 G2633 U2636 C2646 C2651 U2656



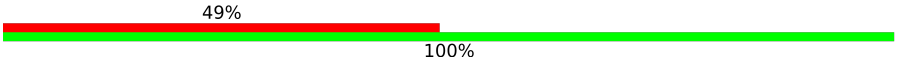
• Molecule 2: 5S rRNA

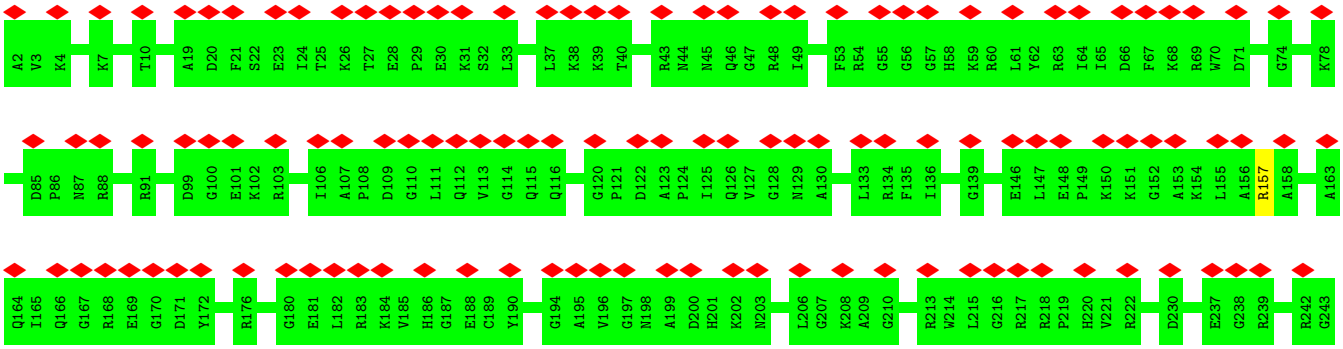
Chain B:



• Molecule 3: 50S ribosomal protein L2

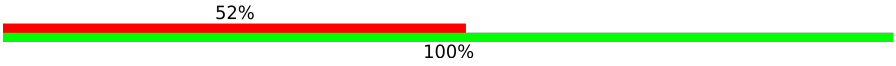
Chain D:

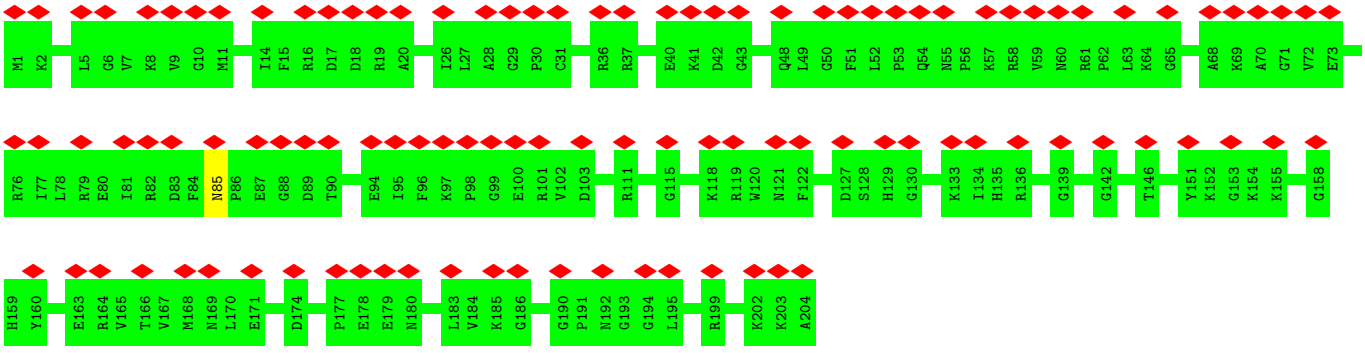




• Molecule 4: 50S ribosomal protein L3

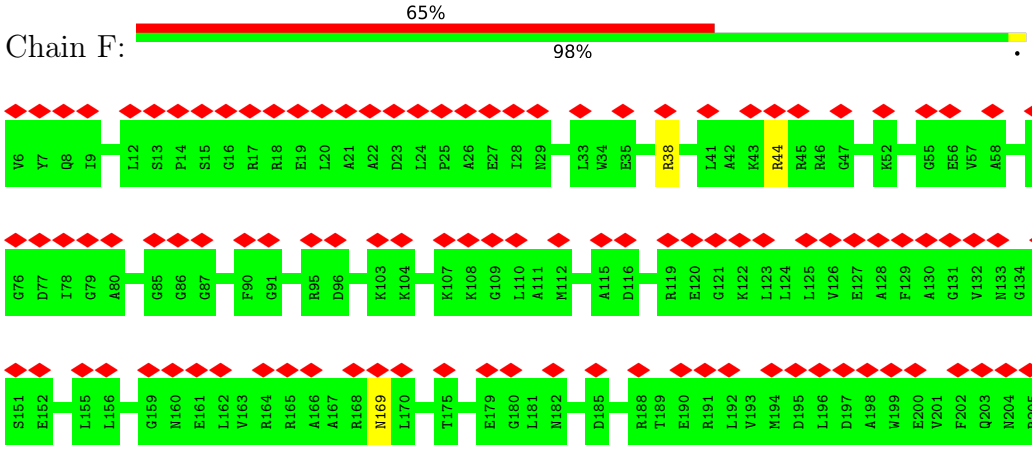
Chain E:





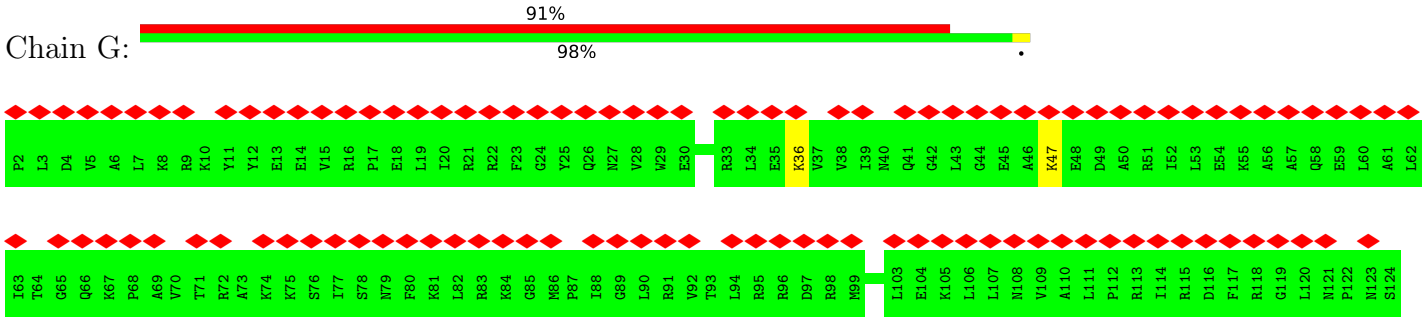
• Molecule 5: 50S ribosomal protein L4

Chain F:



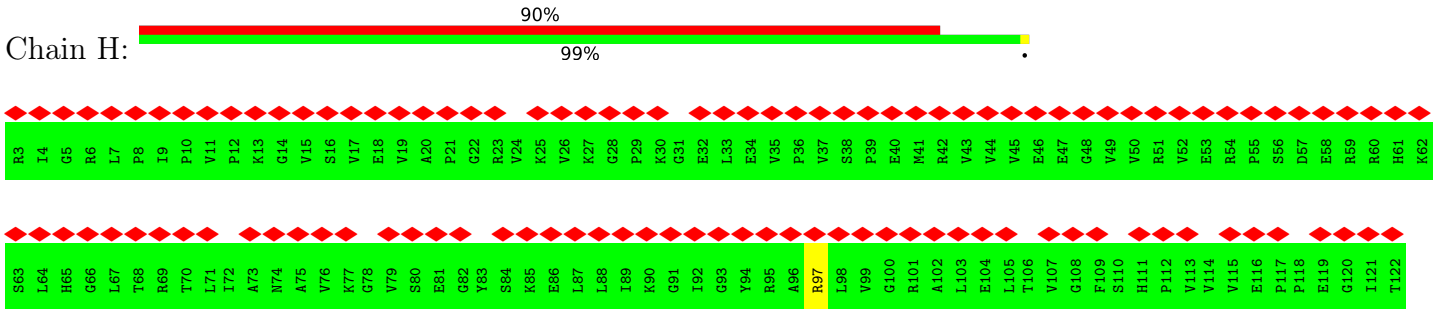
• Molecule 6: 50S ribosomal protein L5

Chain G:



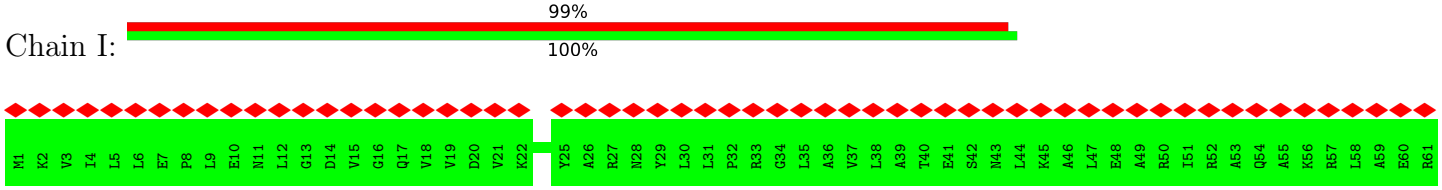
• Molecule 7: 50S ribosomal protein L6

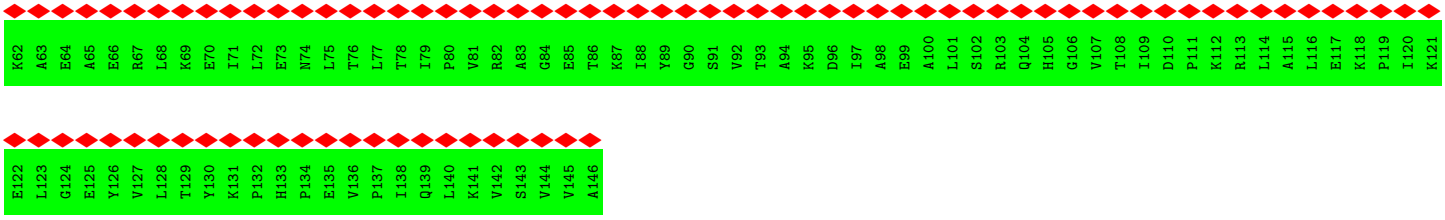
Chain H:



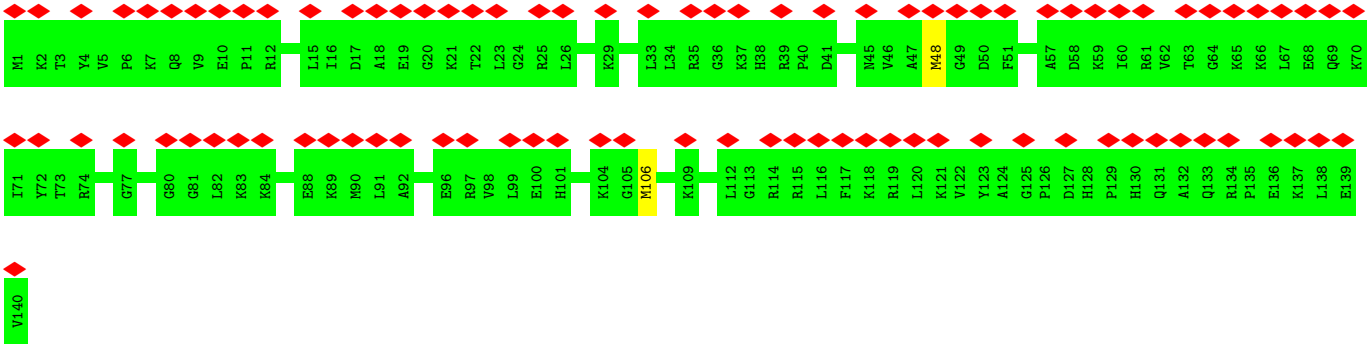
• Molecule 8: 50S ribosomal protein L9

Chain I:

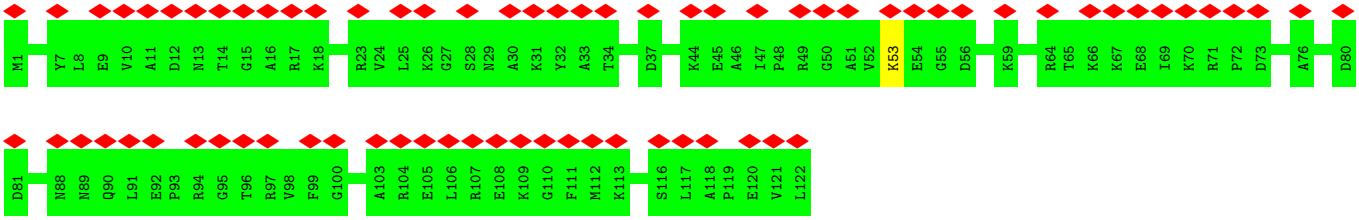




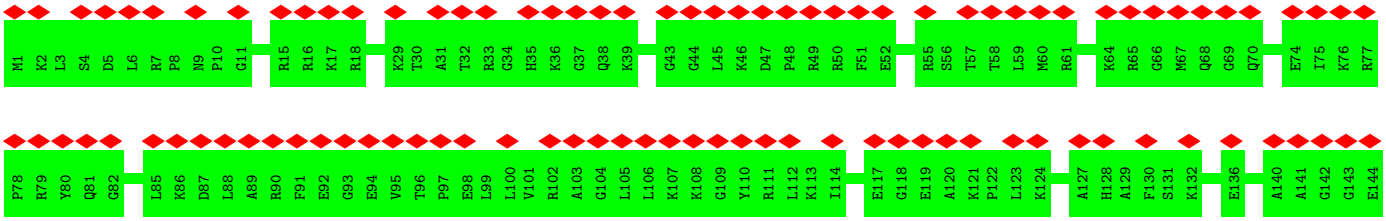
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14

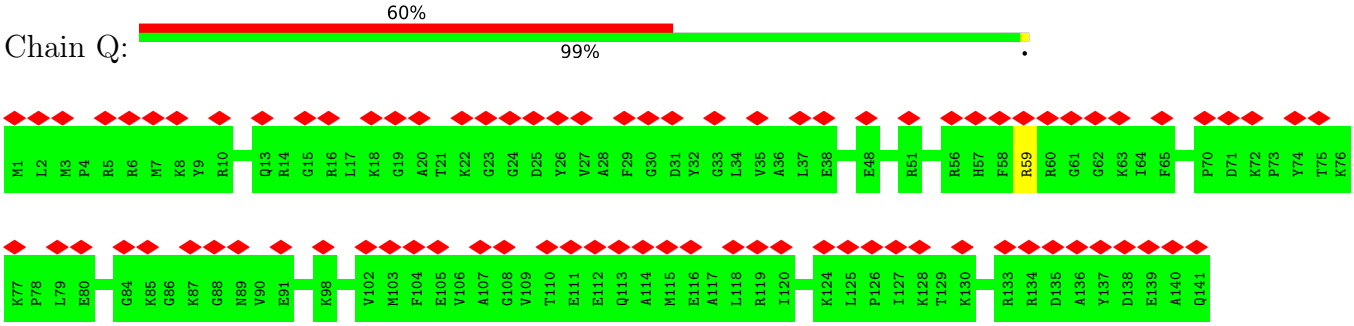


• Molecule 11: 50S ribosomal protein L15



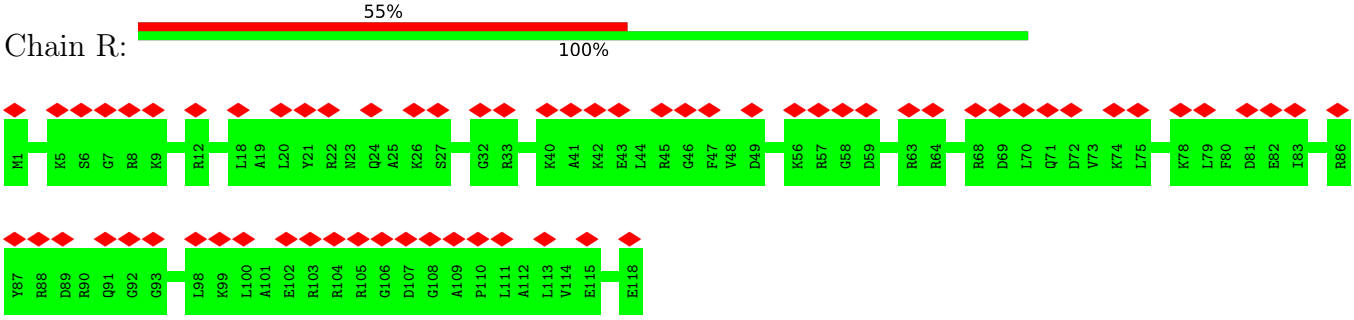
• Molecule 12: 50S ribosomal protein L16

Chain Q:



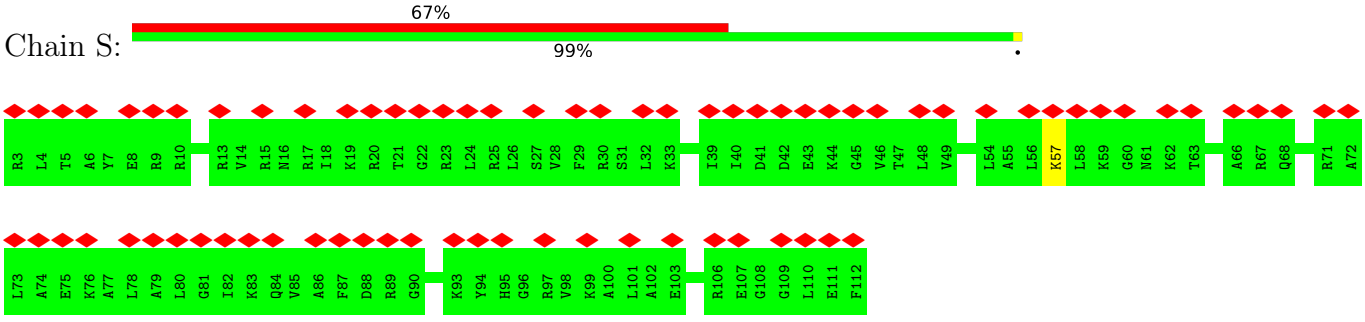
• Molecule 13: 50S ribosomal protein L17

Chain R:



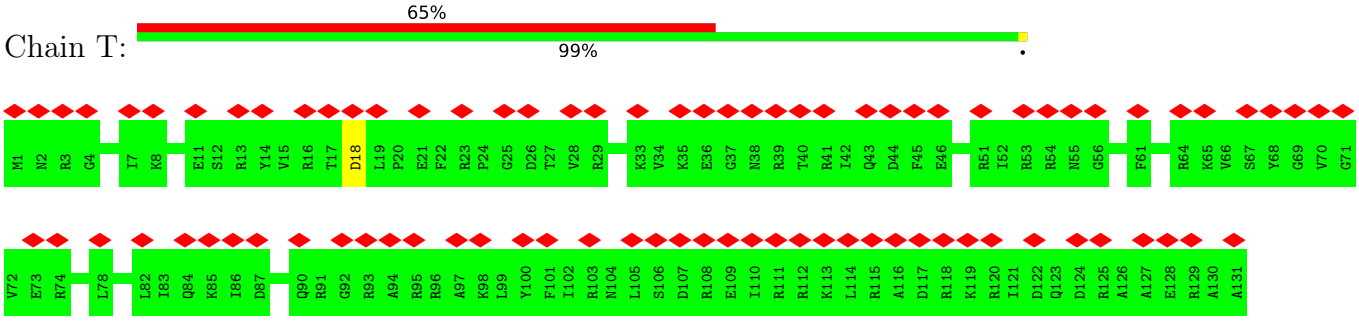
• Molecule 14: 50S ribosomal protein L18

Chain S:



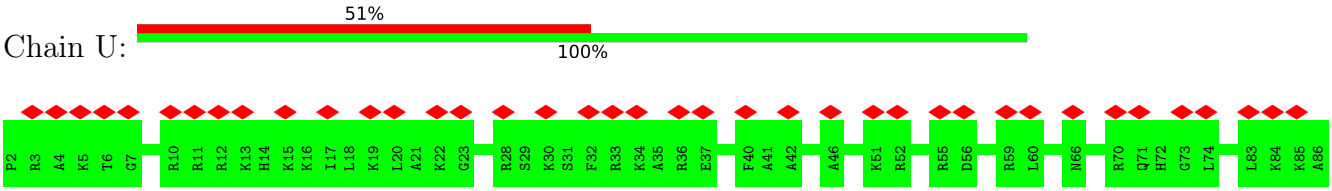
• Molecule 15: 50S ribosomal protein L19

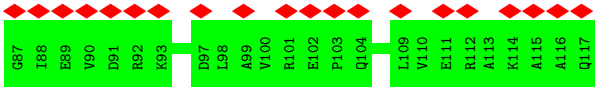
Chain T:



• Molecule 16: 50S ribosomal protein L20

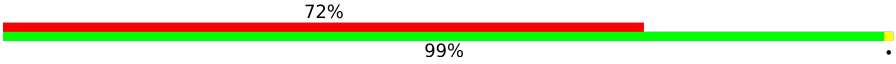
Chain U:

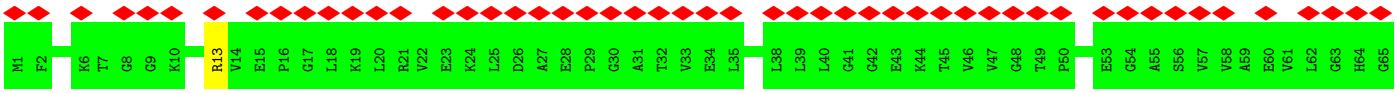


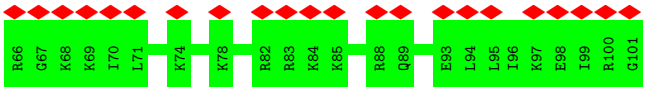


• Molecule 17: 50S ribosomal protein L21

Chain V:

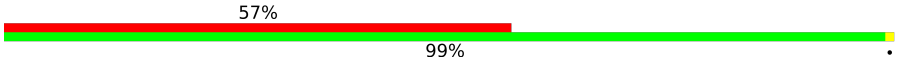


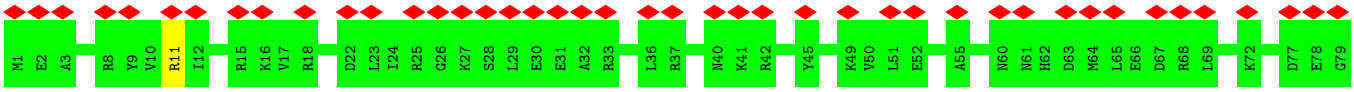


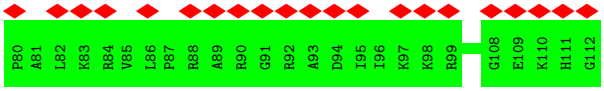


• Molecule 18: 50S ribosomal protein L22

Chain W:

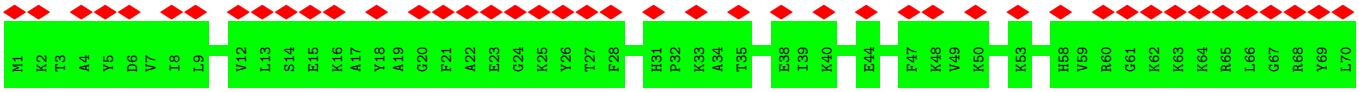


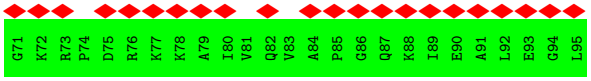




• Molecule 19: 50S ribosomal protein L23

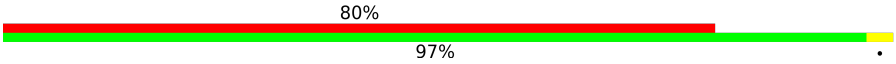
Chain X:

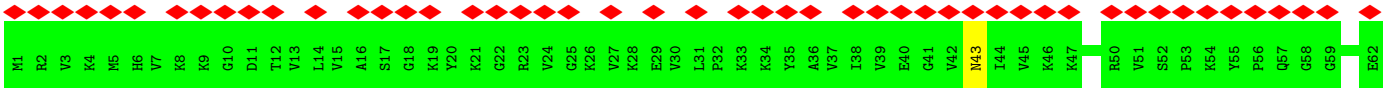


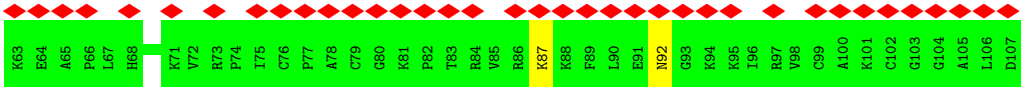


• Molecule 20: 50S ribosomal protein L24

Chain Y:

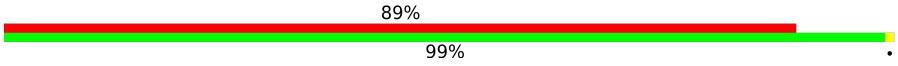


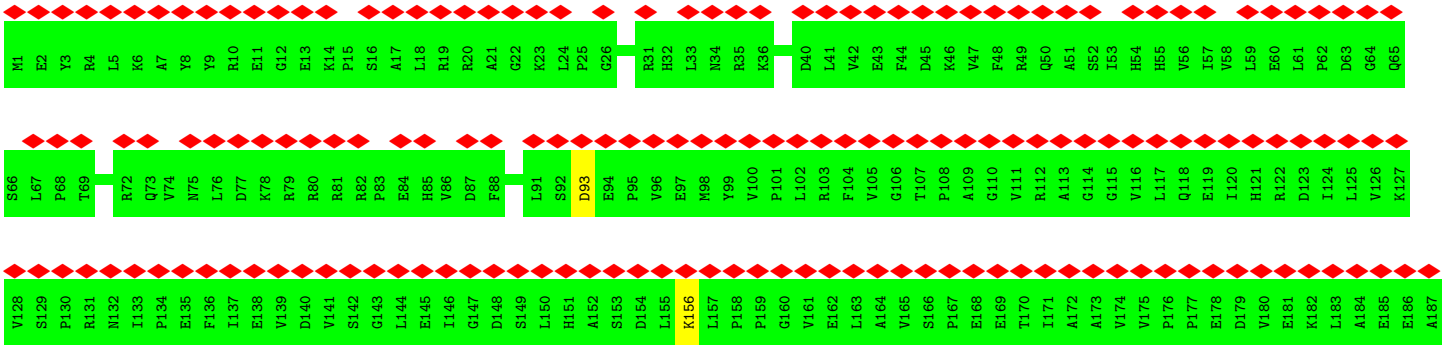




• Molecule 21: 50S ribosomal protein L25

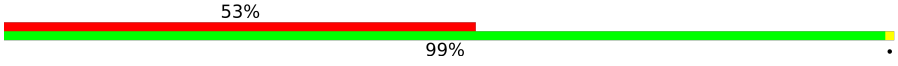
Chain Z:

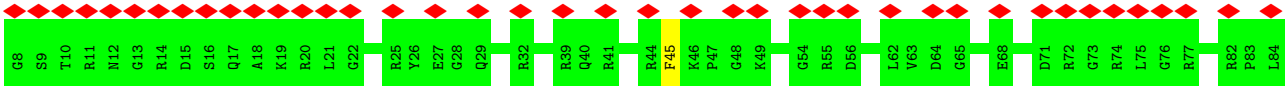




- Molecule 22: 50S ribosomal protein L27

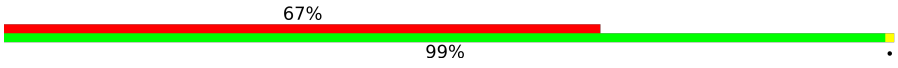
Chain 0:

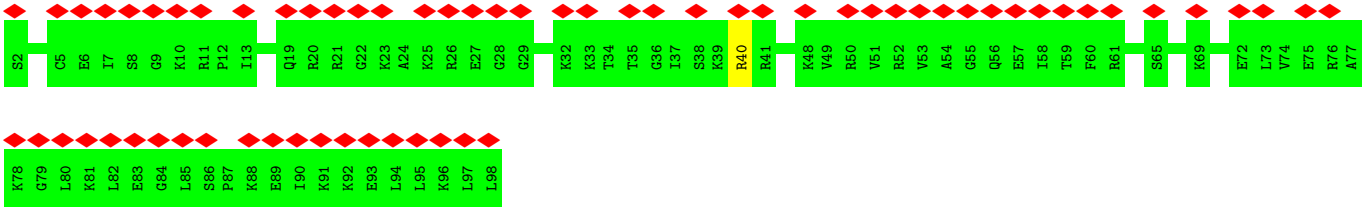




- Molecule 23: 50S ribosomal protein L28

Chain 1:



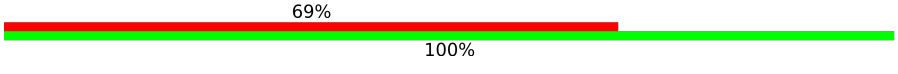


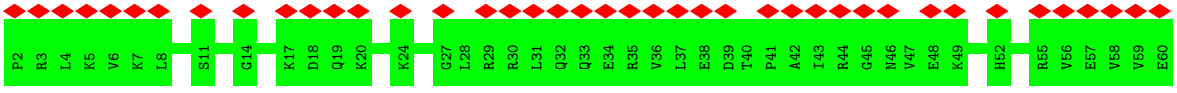
- Molecule 24: 50S ribosomal protein L29

Chain 2:

- Molecule 25: 50S ribosomal protein L30

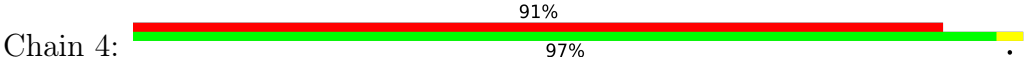
Chain 3:

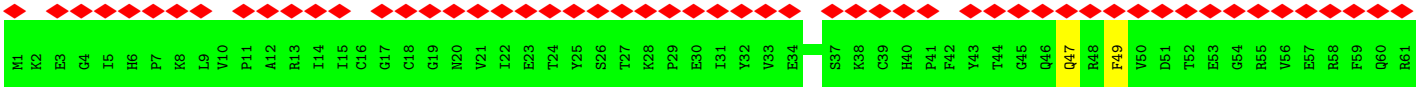


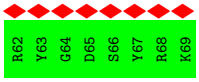


• Molecule 26: 50S ribosomal protein L31

Chain 4:

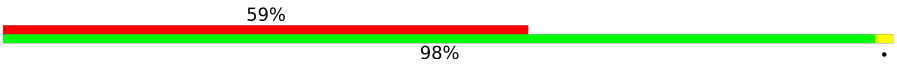


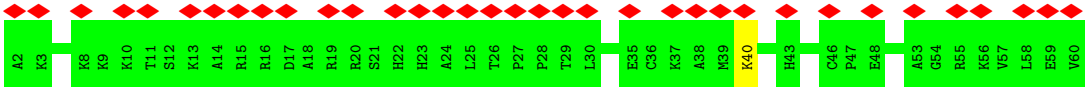




• Molecule 27: 50S ribosomal protein L32

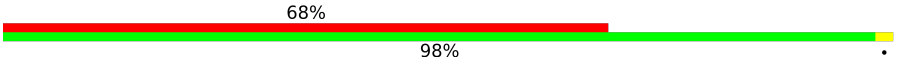
Chain 5:

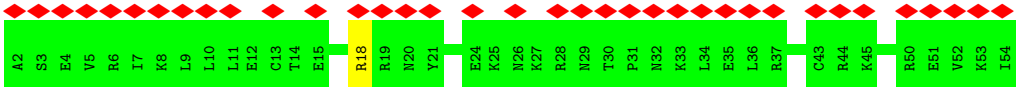




• Molecule 28: 50S ribosomal protein L33

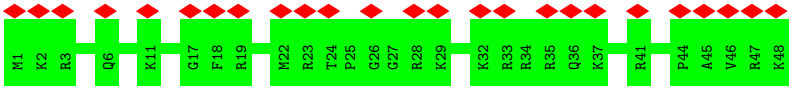
Chain 6:





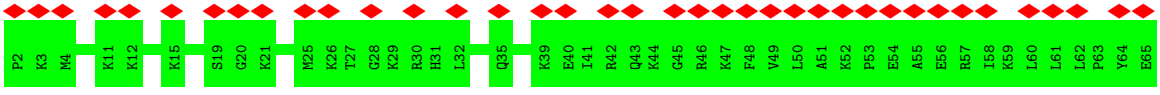
• Molecule 29: 50S ribosomal protein L34

Chain 7:



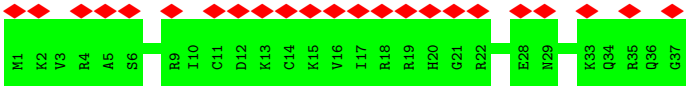
• Molecule 30: 50S ribosomal protein L35

Chain 8:



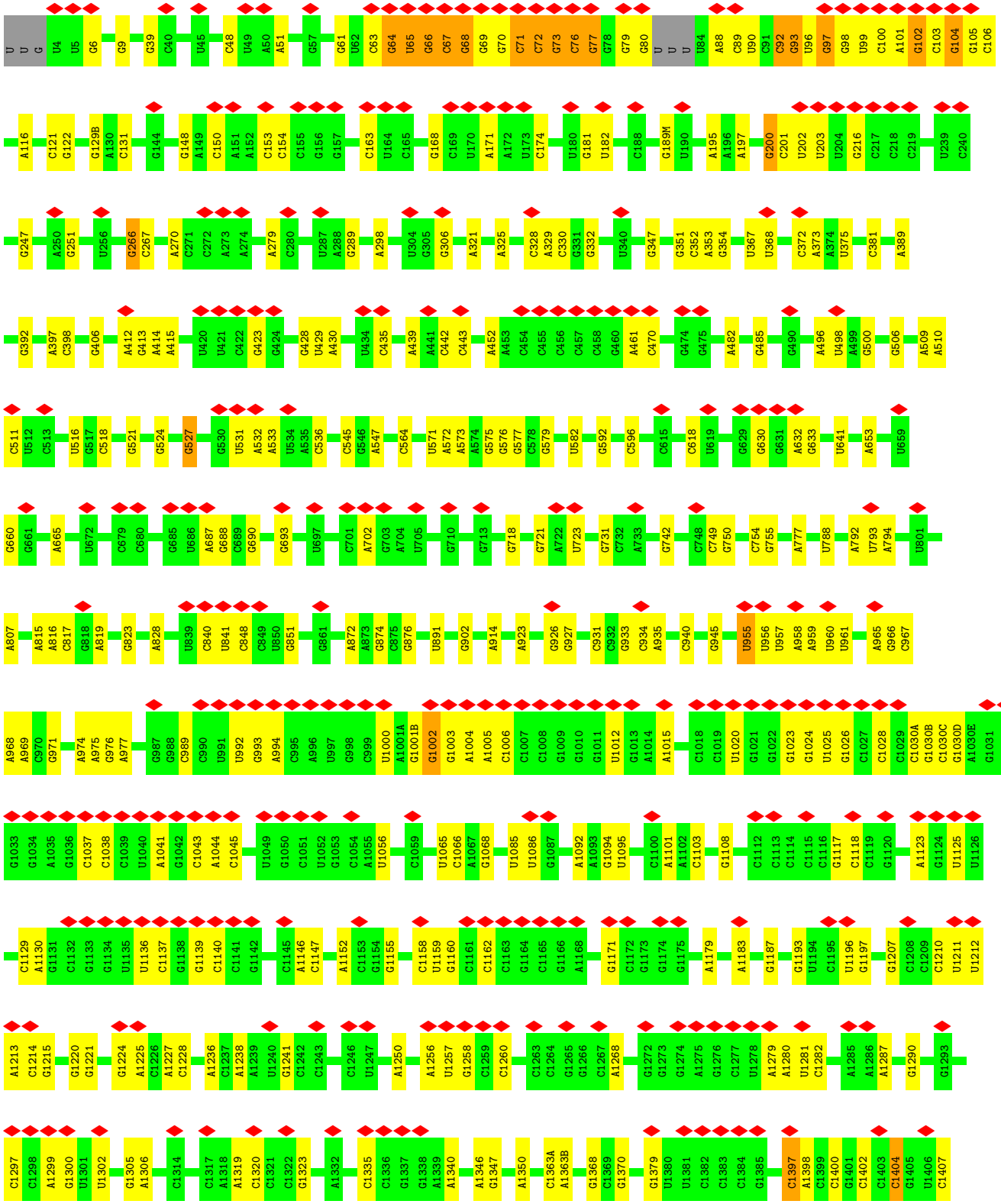
• Molecule 31: 50S ribosomal protein L36

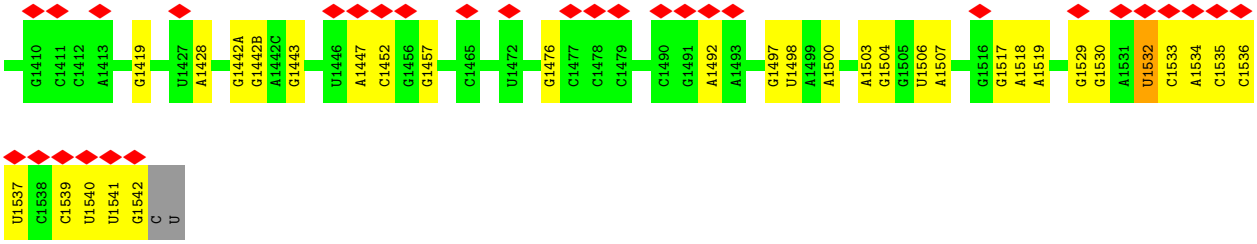
Chain 9:



• Molecule 32: 16S rRNA

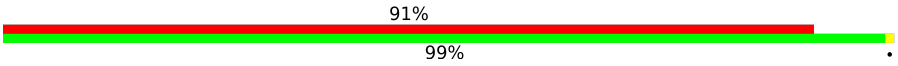
Chain a:





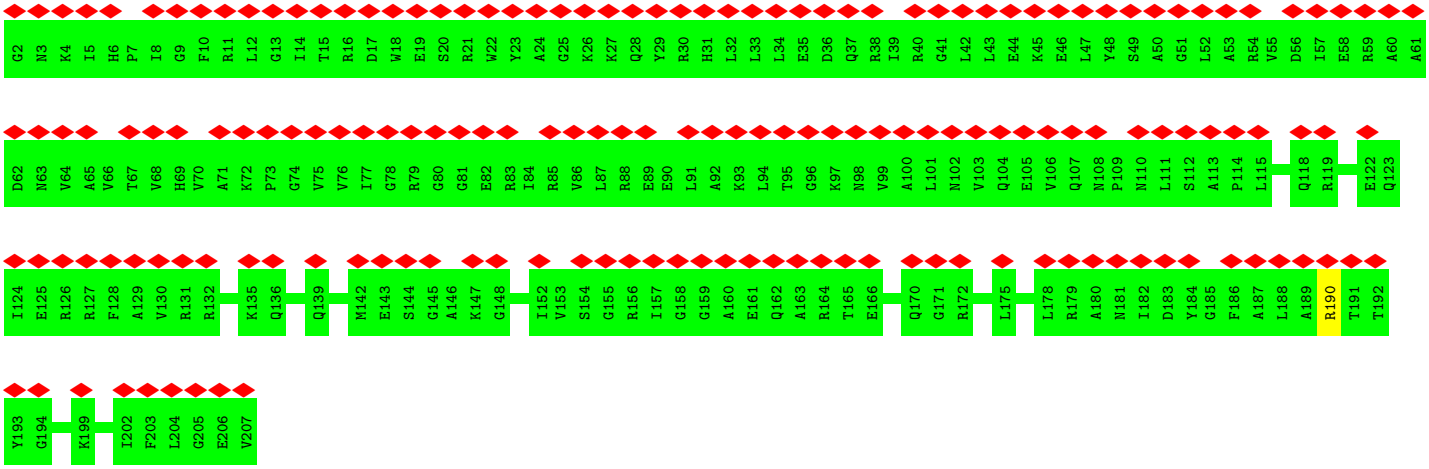
• Molecule 33: 30S ribosomal protein S2

Chain b:



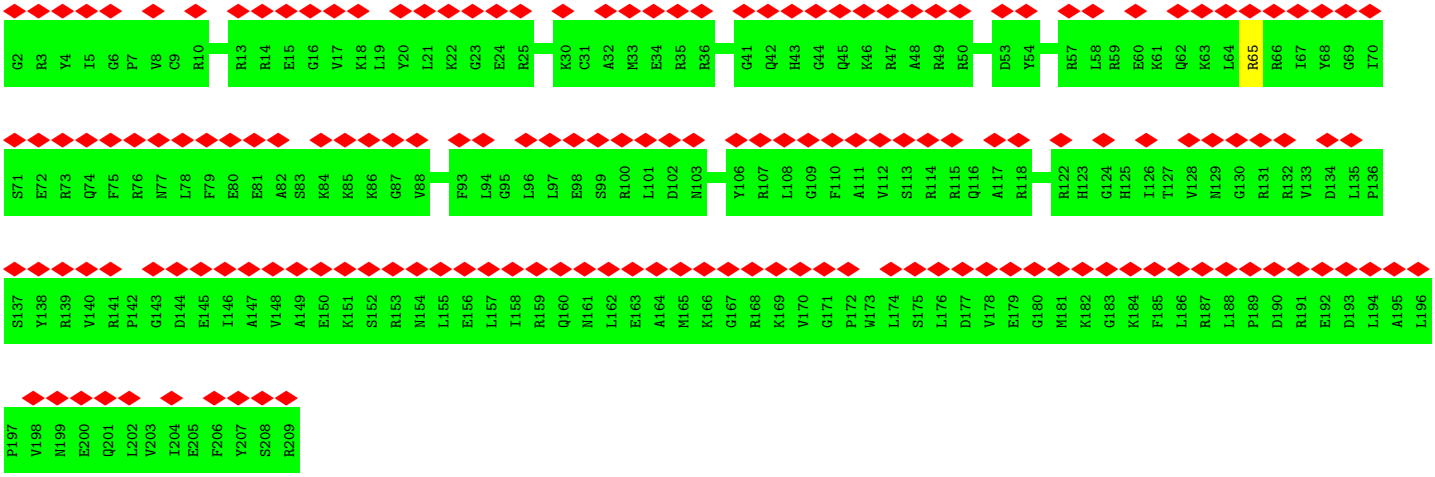
• Molecule 34: 30S ribosomal protein S3

Chain c:



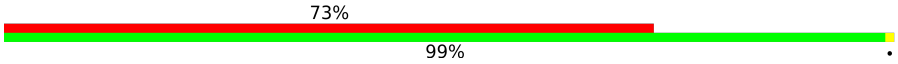
• Molecule 35: 30S ribosomal protein S4

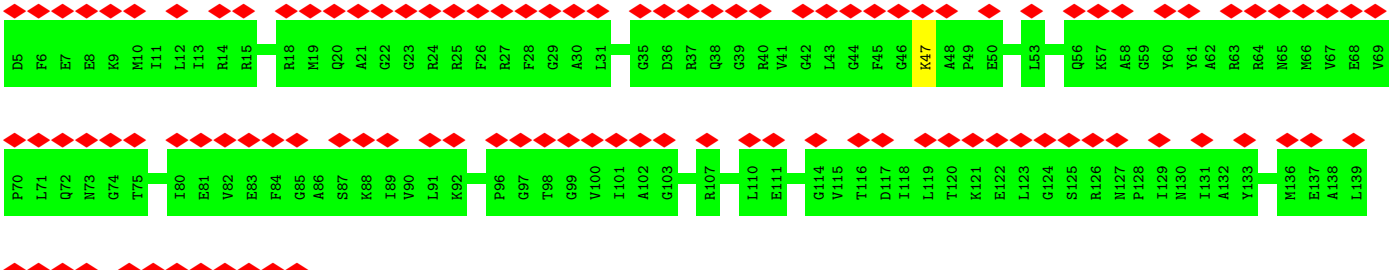
Chain d:



• Molecule 36: 30S ribosomal protein S5

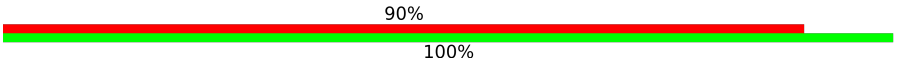
Chain e:

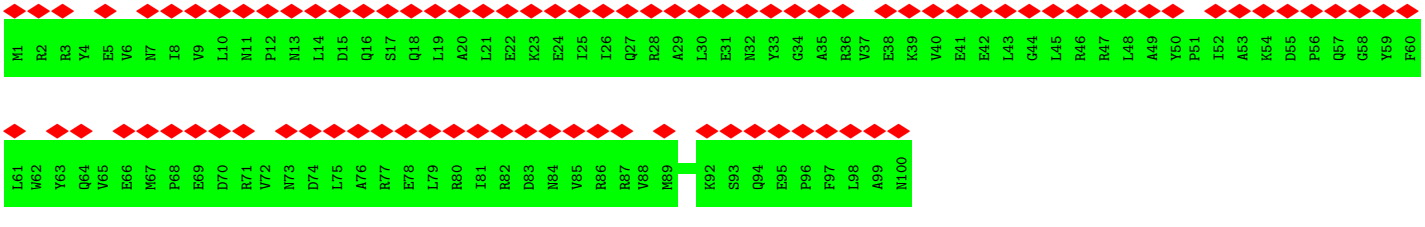




• Molecule 37: 30S ribosomal protein S6

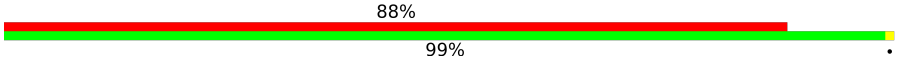
Chain f:

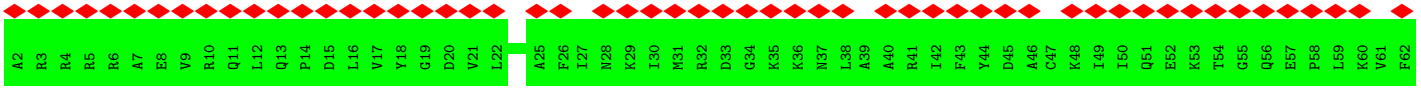


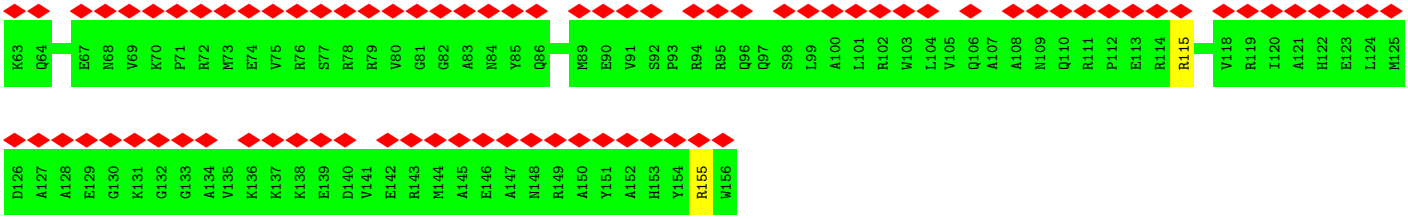


• Molecule 38: 30S ribosomal protein S7

Chain g:

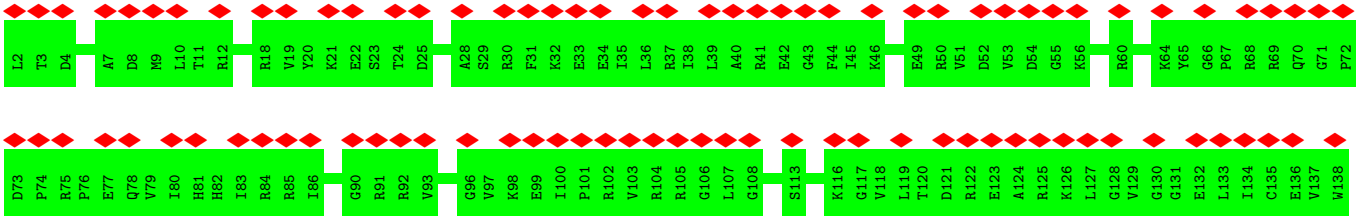






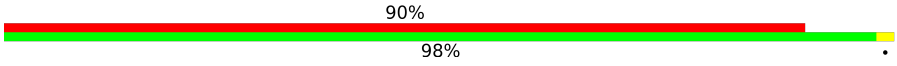
• Molecule 39: 30S ribosomal protein S8

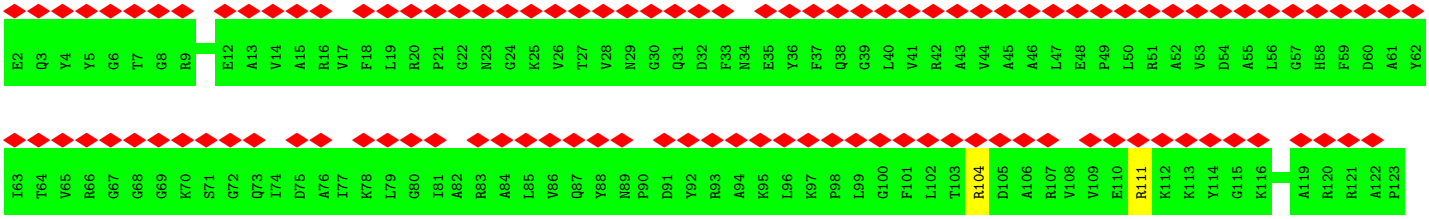
Chain h:



• Molecule 40: 30S ribosomal protein S9

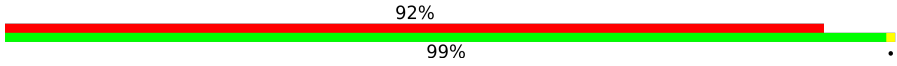
Chain i:

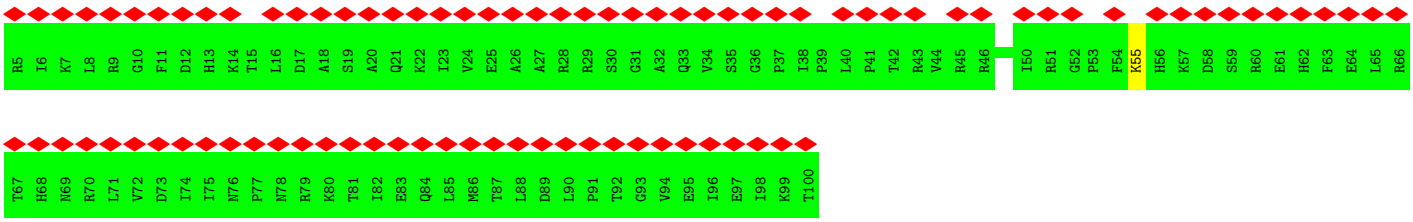




• Molecule 41: 30S ribosomal protein S10

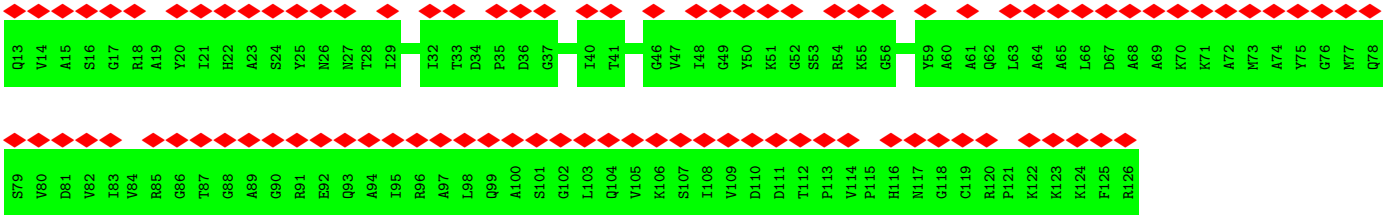
Chain j:





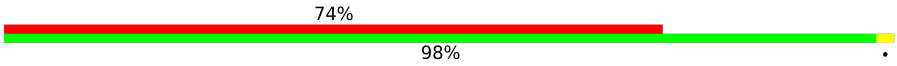
• Molecule 42: 30S ribosomal protein S11

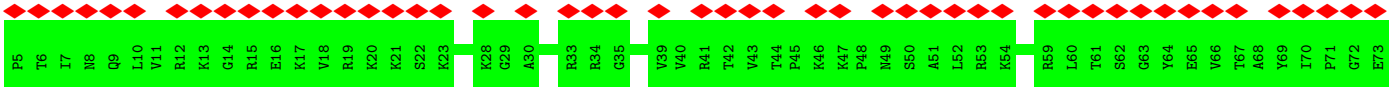
Chain k:



• Molecule 43: 30S ribosomal protein S12

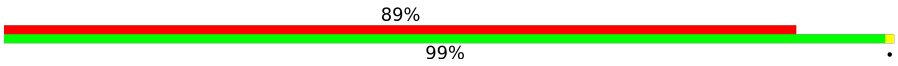
Chain l:





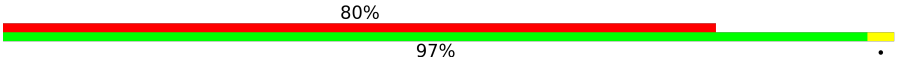
• Molecule 44: 30S ribosomal protein S13

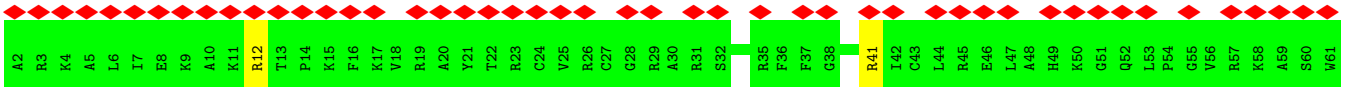
Chain m:



• Molecule 45: 30S ribosomal protein S14 type Z

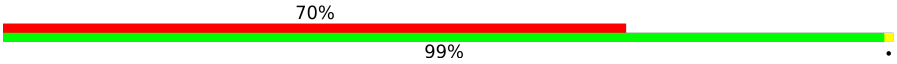
Chain n:

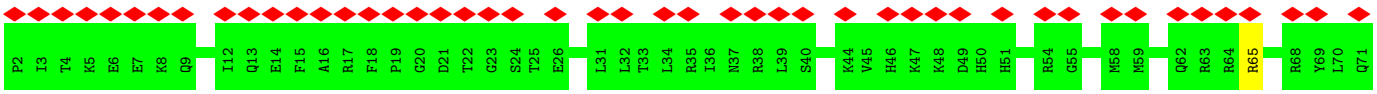




• Molecule 46: 30S ribosomal protein S15

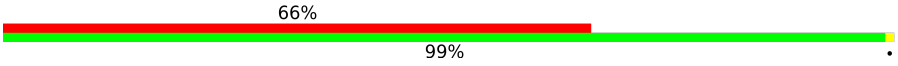
Chain o:

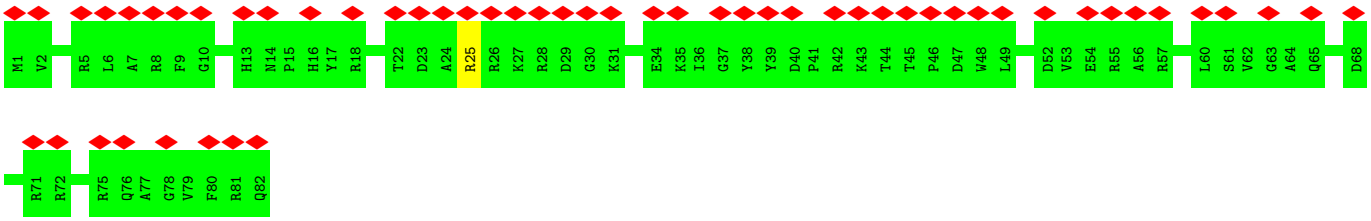




• Molecule 47: 30S ribosomal protein S16

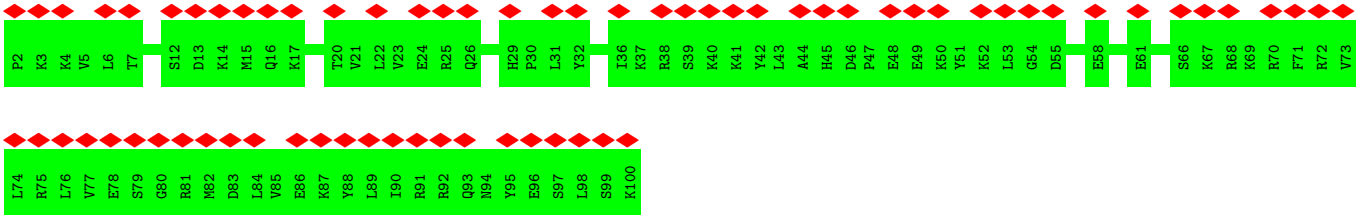
Chain p:





• Molecule 48: 30S ribosomal protein S17

Chain q:

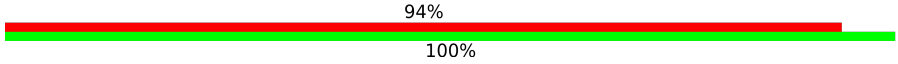


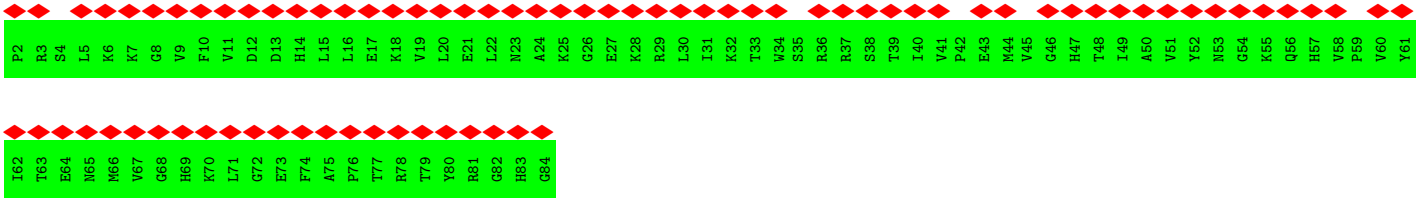
• Molecule 49: 30S ribosomal protein S18

Chain r:

• Molecule 50: 30S ribosomal protein S19

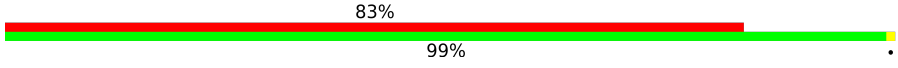
Chain s:

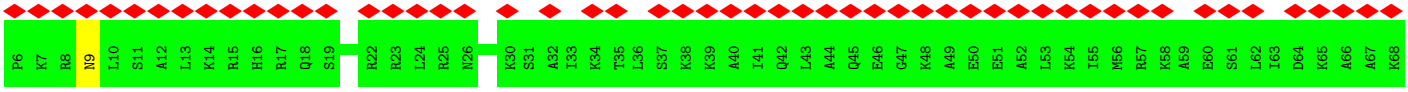


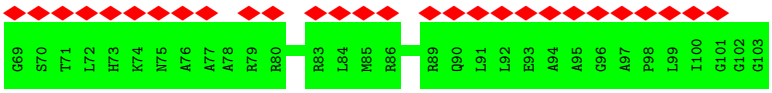


• Molecule 51: 30S ribosomal protein S20

Chain t:

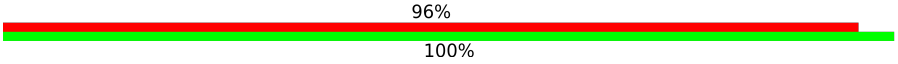


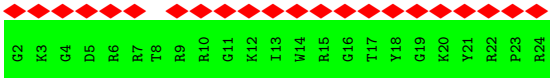




• Molecule 52: 30S ribosomal protein Thx

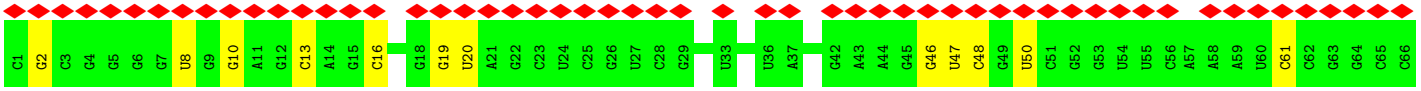
Chain u:

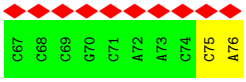




• Molecule 53: P-site tRNA fMet

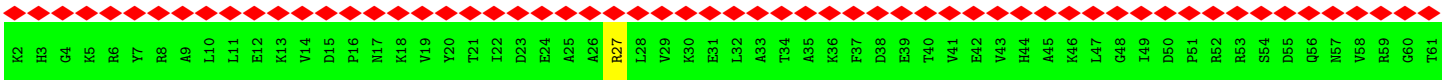
Chain y:

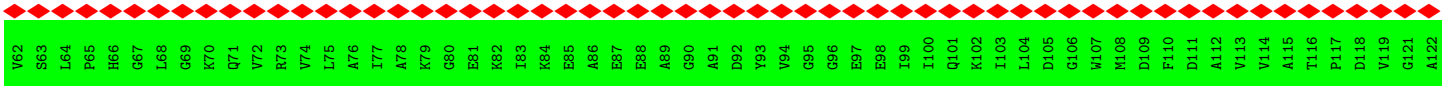


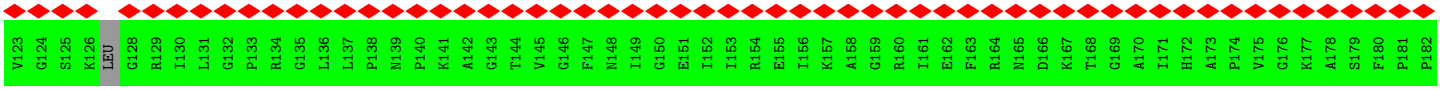


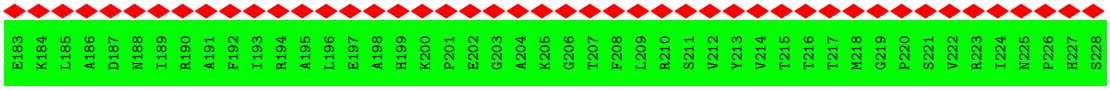
• Molecule 54: 50S ribosomal protein L1

Chain C:



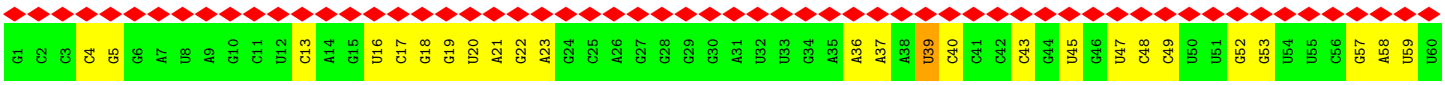


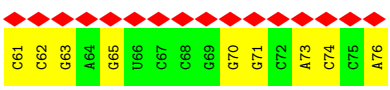




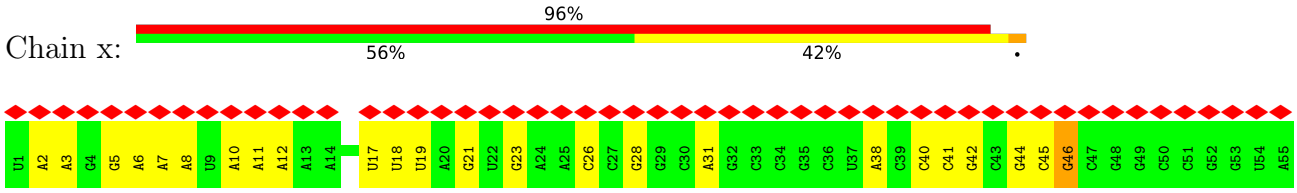
• Molecule 55: E-site tRNA Phe

Chain z:





• Molecule 56: messenger RNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, MA6, ZN, 2MA, 5MU, UR3, 2MU, PSU, 0TD, 2MG, 4OC, M2G, 7MG, 5MC, SF4

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	A	0.77	0/68899	0.93	22/107536 (0.0%)
2	B	0.67	0/2878	0.91	0/4490
3	D	0.41	0/2186	0.51	0/2944
4	E	0.39	0/1592	0.52	0/2149
5	F	0.38	0/1615	0.47	0/2188
6	G	0.35	0/1449	0.49	0/1957
7	H	0.34	0/1347	0.46	0/1817
8	I	0.29	0/1091	0.47	0/1490
9	N	0.39	0/1144	0.49	1/1543 (0.1%)
10	O	0.41	0/943	0.51	0/1269
11	P	0.37	0/1152	0.51	0/1533
12	Q	0.40	0/1143	0.49	0/1527
13	R	0.35	0/982	0.52	0/1312
14	S	0.34	0/880	0.46	0/1172
15	T	0.39	0/1097	0.54	1/1468 (0.1%)
16	U	0.38	0/977	0.44	0/1301
17	V	0.38	0/782	0.49	0/1049
18	W	0.38	0/897	0.48	0/1205
19	X	0.37	0/764	0.46	0/1025
20	Y	0.34	0/823	0.47	0/1100
21	Z	0.34	0/1491	0.47	0/2029
22	0	0.40	0/616	0.55	1/821 (0.1%)
23	1	0.37	0/766	0.49	0/1018
24	2	0.31	0/594	0.42	0/785
25	3	0.37	0/469	0.48	0/630
26	4	0.34	0/549	0.54	0/741
27	5	0.38	0/469	0.46	0/635
28	6	0.39	0/456	0.54	0/608
29	7	0.36	0/426	0.49	0/561
30	8	0.37	0/525	0.47	0/691
31	9	0.38	0/310	0.44	0/407
32	a	1.56	10/36110 (0.0%)	0.99	72/56345 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.32	0/1860	0.45	0/2518
34	c	0.35	0/1566	0.46	0/2119
35	d	0.36	0/1698	0.44	0/2277
36	e	0.38	0/1149	0.50	0/1548
37	f	0.35	0/829	0.48	0/1123
38	g	0.32	0/1248	0.42	0/1676
39	h	0.38	0/1108	0.49	0/1494
40	i	0.34	0/985	0.45	0/1329
41	j	0.31	0/723	0.50	0/984
42	k	0.35	0/848	0.47	0/1149
43	l	0.37	0/937	0.52	0/1260
44	m	0.32	0/905	0.45	0/1217
45	n	0.38	0/501	0.46	0/664
46	o	0.33	0/739	0.47	0/985
47	p	0.39	0/693	0.47	0/935
48	q	0.38	0/836	0.47	0/1117
49	r	0.32	0/560	0.47	0/746
50	s	0.33	0/660	0.49	0/893
51	t	0.32	0/736	0.47	0/976
52	u	0.38	0/203	0.47	0/266
53	y	0.56	0/1832	0.89	0/2855
54	C	0.28	0/1748	0.49	0/2354
55	z	0.45	0/1809	0.91	2/2819 (0.1%)
56	x	0.33	0/1315	1.02	6/2046 (0.3%)
All	All	0.93	10/160910 (0.0%)	0.85	105/240696 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	71	C	N1-C6	136.75	2.19	1.37
32	a	71	C	N3-C4	114.97	2.14	1.33
32	a	71	C	C2-N3	101.01	2.16	1.35
32	a	71	C	C5-C6	94.30	2.09	1.34
32	a	71	C	C4-C5	93.34	2.17	1.43

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	64	G	P-O3'-C3'	36.13	163.05	119.70
56	x	46	G	C5-N7-C8	17.91	113.25	104.30
32	a	71	C	C2-N3-C4	13.87	126.84	119.90
56	x	46	G	C4-C5-N7	13.18	116.07	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2224	G	OP1-P-O3'	-12.98	76.64	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
3	D	273/275 (99%)	252 (92%)	21 (8%)	0	100	100
4	E	202/204 (99%)	187 (93%)	15 (7%)	0	100	100
5	F	201/203 (99%)	192 (96%)	8 (4%)	1 (0%)	29	68
6	G	179/181 (99%)	164 (92%)	15 (8%)	0	100	100
7	H	166/173 (96%)	156 (94%)	10 (6%)	0	100	100
8	I	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
9	N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
10	O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	P	147/149 (99%)	134 (91%)	13 (9%)	0	100	100
12	Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
13	R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
15	T	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
16	U	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
17	V	99/101 (98%)	85 (86%)	14 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	W	110/112 (98%)	98 (89%)	12 (11%)	0	100	100
19	X	93/95 (98%)	84 (90%)	9 (10%)	0	100	100
20	Y	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
21	Z	185/187 (99%)	163 (88%)	21 (11%)	1 (0%)	29	68
22	0	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
23	1	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
24	2	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
25	3	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
26	4	67/69 (97%)	54 (81%)	11 (16%)	2 (3%)	4	30
27	5	57/59 (97%)	52 (91%)	5 (9%)	0	100	100
28	6	51/53 (96%)	44 (86%)	7 (14%)	0	100	100
29	7	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
30	8	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
31	9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	b	229/231 (99%)	205 (90%)	24 (10%)	0	100	100
34	c	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
35	d	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
36	e	146/148 (99%)	137 (94%)	9 (6%)	0	100	100
37	f	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
38	g	153/155 (99%)	142 (93%)	11 (7%)	0	100	100
39	h	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
40	i	124/126 (98%)	113 (91%)	11 (9%)	0	100	100
41	j	94/96 (98%)	82 (87%)	11 (12%)	1 (1%)	14	52
42	k	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
43	l	119/122 (98%)	108 (91%)	11 (9%)	0	100	100
44	m	112/114 (98%)	99 (88%)	13 (12%)	0	100	100
45	n	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
46	o	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
47	p	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
48	q	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
49	r	66/68 (97%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	s	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
51	t	96/98 (98%)	84 (88%)	12 (12%)	0	100	100
52	u	21/23 (91%)	20 (95%)	1 (5%)	0	100	100
54	C	221/226 (98%)	196 (89%)	25 (11%)	0	100	100
All	All	5919/6028 (98%)	5459 (92%)	455 (8%)	5 (0%)	54	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	4	49	PHE
26	4	47	GLN
41	j	55	LYS
21	Z	93	ASP
5	F	207	GLY

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	
3	D	215/217 (99%)	214 (100%)	1 (0%)	88	94
4	E	164/165 (99%)	163 (99%)	1 (1%)	86	94
5	F	159/161 (99%)	156 (98%)	3 (2%)	57	80
6	G	142/155 (92%)	139 (98%)	3 (2%)	53	79
7	H	143/144 (99%)	142 (99%)	1 (1%)	84	93
8	I	108/122 (88%)	108 (100%)	0	100	100
9	N	118/119 (99%)	117 (99%)	1 (1%)	81	91
10	O	100/100 (100%)	99 (99%)	1 (1%)	76	88
11	P	115/116 (99%)	115 (100%)	0	100	100
12	Q	111/111 (100%)	110 (99%)	1 (1%)	78	90
13	R	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	S	85/87 (98%)	84 (99%)	1 (1%)	71 87
15	T	113/115 (98%)	113 (100%)	0	100 100
16	U	93/93 (100%)	93 (100%)	0	100 100
17	V	80/82 (98%)	79 (99%)	1 (1%)	69 86
18	W	90/91 (99%)	89 (99%)	1 (1%)	73 88
19	X	77/77 (100%)	77 (100%)	0	100 100
20	Y	86/88 (98%)	83 (96%)	3 (4%)	36 67
21	Z	156/164 (95%)	155 (99%)	1 (1%)	86 94
22	0	61/62 (98%)	61 (100%)	0	100 100
23	1	81/82 (99%)	80 (99%)	1 (1%)	71 87
24	2	66/66 (100%)	66 (100%)	0	100 100
25	3	50/51 (98%)	50 (100%)	0	100 100
26	4	54/62 (87%)	54 (100%)	0	100 100
27	5	50/51 (98%)	49 (98%)	1 (2%)	55 79
28	6	50/51 (98%)	49 (98%)	1 (2%)	55 79
29	7	41/41 (100%)	41 (100%)	0	100 100
30	8	54/54 (100%)	54 (100%)	0	100 100
31	9	34/34 (100%)	34 (100%)	0	100 100
33	b	187/199 (94%)	185 (99%)	2 (1%)	73 88
34	c	140/160 (88%)	139 (99%)	1 (1%)	84 93
35	d	172/180 (96%)	171 (99%)	1 (1%)	86 94
36	e	114/114 (100%)	113 (99%)	1 (1%)	78 90
37	f	85/90 (94%)	85 (100%)	0	100 100
38	g	119/126 (94%)	117 (98%)	2 (2%)	60 82
39	h	114/118 (97%)	114 (100%)	0	100 100
40	i	88/97 (91%)	86 (98%)	2 (2%)	50 77
41	j	68/86 (79%)	68 (100%)	0	100 100
42	k	83/86 (96%)	83 (100%)	0	100 100
43	l	96/102 (94%)	95 (99%)	1 (1%)	76 88
44	m	87/93 (94%)	86 (99%)	1 (1%)	73 88
45	n	49/49 (100%)	47 (96%)	2 (4%)	30 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	o	78/79 (99%)	77 (99%)	1 (1%)	69 86
47	p	68/71 (96%)	67 (98%)	1 (2%)	65 84
48	q	94/94 (100%)	94 (100%)	0	100 100
49	r	59/59 (100%)	59 (100%)	0	100 100
50	s	67/72 (93%)	67 (100%)	0	100 100
51	t	70/76 (92%)	69 (99%)	1 (1%)	67 85
52	u	18/18 (100%)	18 (100%)	0	100 100
54	C	177/178 (99%)	176 (99%)	1 (1%)	86 94
All	All	4830/5009 (96%)	4791 (99%)	39 (1%)	82 91

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	g	155	ARG
46	o	65	ARG
40	i	104	ARG
44	m	102	ARG
51	t	9	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
33	b	40	HIS
47	p	65	GLN
35	d	123	HIS
46	o	62	GLN
50	s	47	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2853/2915 (97%)	658 (23%)	41 (1%)
2	B	119/120 (99%)	24 (20%)	0
32	a	1505/1521 (98%)	344 (22%)	0
53	y	76/77 (98%)	14 (18%)	0
55	z	75/76 (98%)	34 (45%)	0
56	x	54/55 (98%)	23 (42%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4682/4764 (98%)	1097 (23%)	41 (0%)

5 of 1097 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	A
1	A	10	G
1	A	12	U
1	A	15	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2126	A
1	A	2601	C
1	A	2171	A
1	A	2321	G
1	A	2689	U

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

24 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	$\#\|Z\| > 2$
1	5MC	A	1962	1	18,22,23	0.95	2 (11%)	26,32,35	1.25	3 (11%)
1	PSU	A	2605	1	18,21,22	1.40	3 (16%)	22,30,33	2.07	4 (18%)
43	0TD	l	92	43	7,9,10	1.42	1 (14%)	6,11,13	1.27	1 (16%)
32	5MC	a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.19	2 (7%)
32	5MC	a	1407	32	18,22,23	0.98	2 (11%)	26,32,35	1.28	3 (11%)
1	2MU	A	2552	1	19,22,24	1.33	4 (21%)	26,31,36	2.08	6 (23%)
1	4OC	A	1920	1	19,22,24	0.82	0	26,31,35	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	5MC	a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.23	3 (11%)
32	MA6	a	1518	32	19,26,27	0.89	1 (5%)	18,38,41	1.81	6 (33%)
1	2MA	A	2503	1	17,25,26	1.05	2 (11%)	17,37,40	0.95	2 (11%)
1	5MU	A	1915	1	19,22,23	1.46	5 (26%)	28,32,35	2.36	9 (32%)
32	M2G	a	966	32	20,27,28	1.39	3 (15%)	22,40,43	1.07	2 (9%)
1	OMG	A	2251	1,53	18,26,27	1.01	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A	1917	1	18,21,22	1.41	3 (16%)	22,30,33	2.01	5 (22%)
32	2MG	a	1207	32	18,26,27	0.99	1 (5%)	16,38,41	1.14	3 (18%)
32	7MG	a	527	32	22,26,27	1.42	4 (18%)	29,39,42	2.61	7 (24%)
32	5MC	a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.15	2 (7%)
1	5MU	A	1939	1	19,22,23	1.42	4 (21%)	28,32,35	2.13	6 (21%)
1	5MC	A	1942	1	18,22,23	0.92	2 (11%)	26,32,35	1.22	1 (3%)
32	4OC	a	1402	32	20,23,24	0.77	0	26,32,35	0.91	2 (7%)
32	MA6	a	1519	32	19,26,27	0.91	1 (5%)	18,38,41	1.99	6 (33%)
32	UR3	a	1498	32	19,22,23	0.94	0	26,32,35	1.47	2 (7%)
1	PSU	A	1911	1	18,21,22	1.38	3 (16%)	22,30,33	1.95	4 (18%)
32	PSU	a	516	32	18,21,22	1.37	4 (22%)	22,30,33	1.94	4 (18%)

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
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
43	0TD	l	92	43	-	4/7/12/14	-
32	5MC	a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	a	1407	32	-	0/7/25/26	0/2/2/2
1	2MU	A	2552	1	-	0/9/27/28	0/2/2/2
1	4OC	A	1920	1	-	0/9/27/30	0/2/2/2
32	5MC	a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	a	1518	32	-	1/7/29/30	0/3/3/3
1	2MA	A	2503	1	-	1/3/25/26	0/3/3/3
1	5MU	A	1915	1	-	2/7/25/26	0/2/2/2
32	M2G	a	966	32	-	0/7/29/30	0/3/3/3
1	OMG	A	2251	1,53	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
32	2MG	a	1207	32	-	0/5/27/28	0/3/3/3
32	7MG	a	527	32	-	3/7/37/38	0/3/3/3
32	5MC	a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	a	1519	32	-	5/7/29/30	0/3/3/3
32	UR3	a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	a	516	32	-	0/7/25/26	0/2/2/2

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	966	M2G	C2-N3	4.05	1.35	1.30
32	a	527	7MG	C4-N9	-3.78	1.33	1.37
1	A	2605	PSU	C4-N3	-3.23	1.32	1.38
1	A	1939	5MU	C4-N3	-3.16	1.33	1.38
1	A	1911	PSU	C4-N3	-3.15	1.33	1.38

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	527	7MG	N9-C4-N3	9.31	139.39	125.47
1	A	2605	PSU	N1-C2-N3	6.46	122.44	115.13
1	A	1917	PSU	N1-C2-N3	6.31	122.27	115.13
1	A	1911	PSU	N1-C2-N3	6.12	122.06	115.13
32	a	516	PSU	N1-C2-N3	6.01	121.93	115.13

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1915	5MU	O4'-C1'-N1-C2
1	A	1915	5MU	O4'-C1'-N1-C6
32	a	527	7MG	C3'-C4'-C5'-O5'
32	a	1519	MA6	O4'-C4'-C5'-O5'
32	a	1519	MA6	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	d	301	35	0,12,12	-	-	-		

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	SF4	d	301	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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	a	4
7	H	3
1	A	2

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1029:C	O3'	1030(A):C	P	5.11
1	a	1000:U	O3'	1001(A):A	P	4.99
1	A	2180:U	O3'	2181:G	P	4.52
1	a	1030(E):A	O3'	1031:G	P	3.85
1	H	3:ARG	C	4:ILE	N	3.28

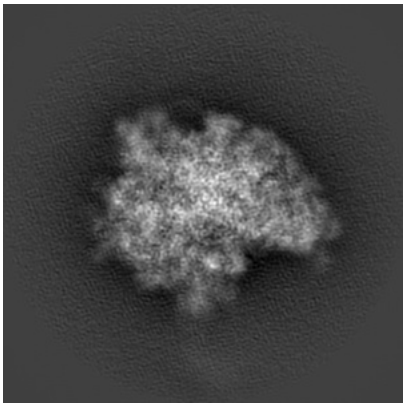
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8596. These allow visual inspection of the internal detail of the map and identification of artifacts.

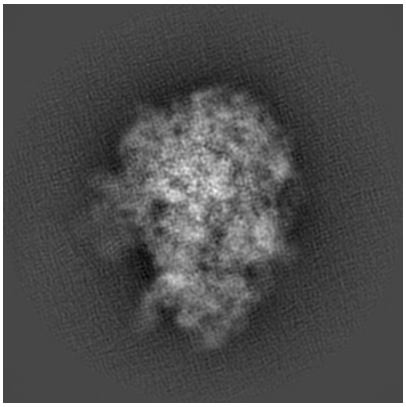
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

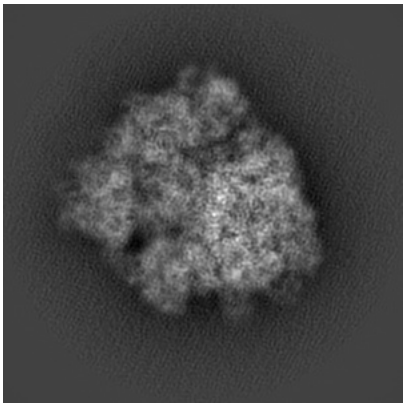
6.1.1 Primary map



X



Y

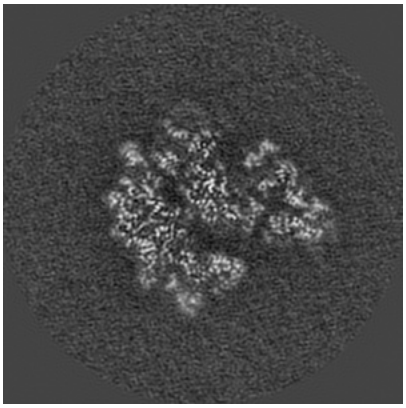


Z

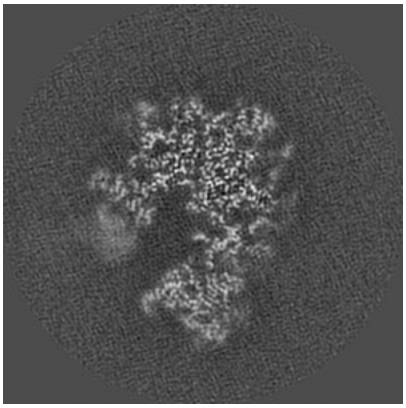
The images above show the map projected in three orthogonal directions.

6.2 Central slices

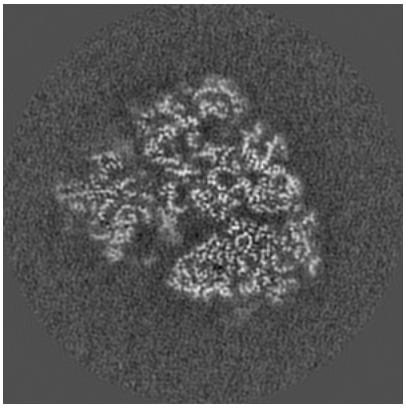
6.2.1 Primary map



X Index: 192



Y Index: 192

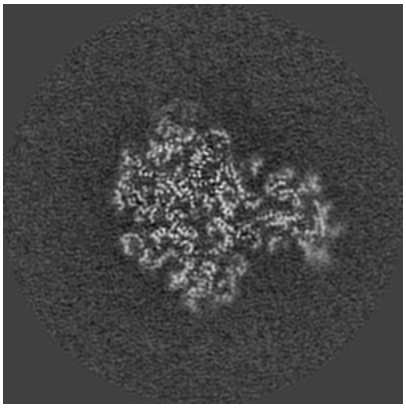


Z Index: 192

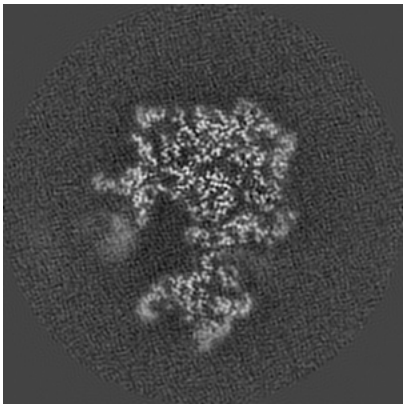
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

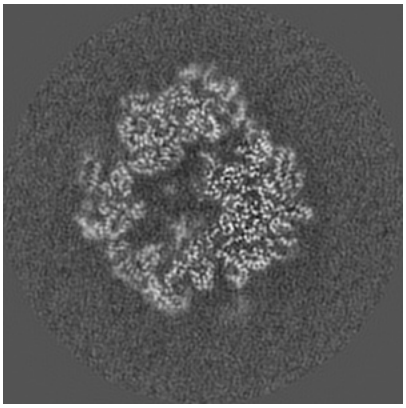
6.3.1 Primary map



X Index: 203



Y Index: 200



Z Index: 173

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

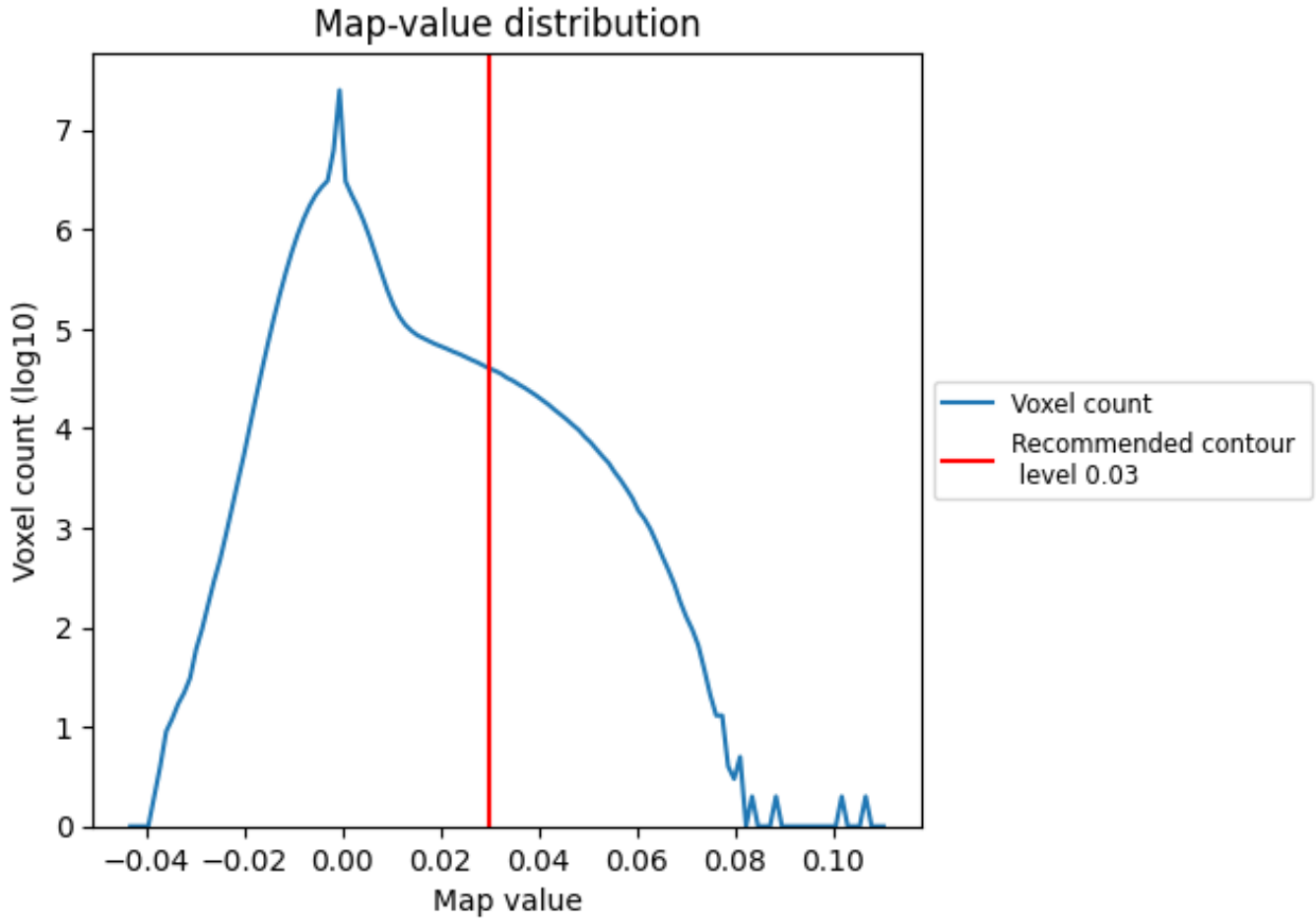
6.5 Mask visualisation (i)

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

7 Map analysis

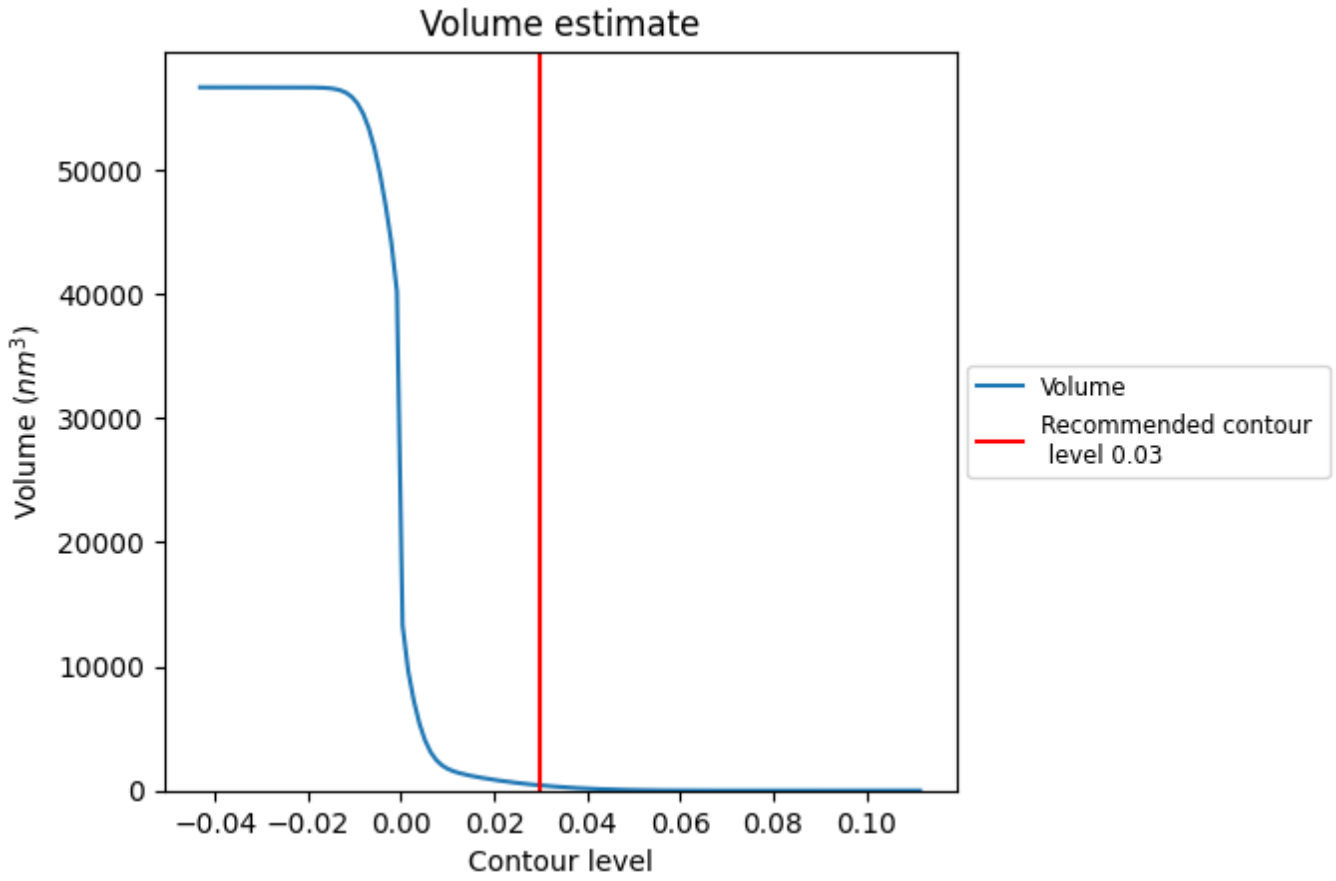
This section contains the results of statistical analysis of the map.

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.

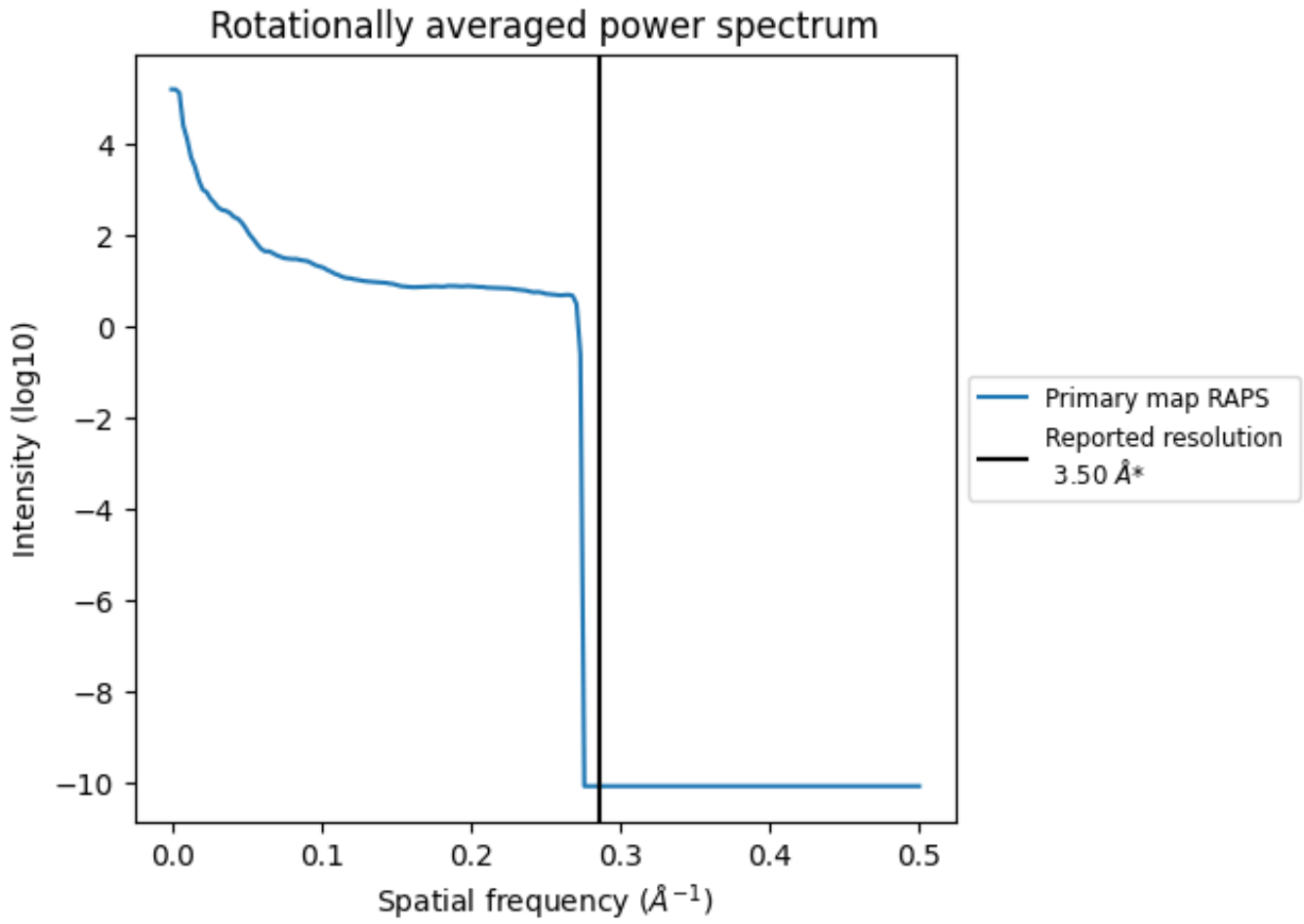
7.2 Volume estimate (i)



The volume at the recommended contour level is 418 nm^3; this corresponds to an approximate mass of 378 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 0.286 Å^{-1}

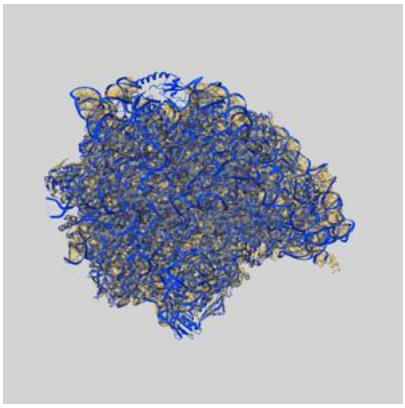
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

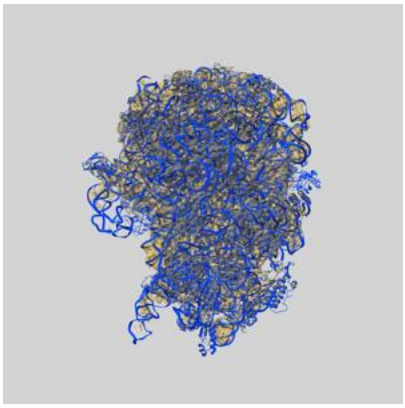
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8596 and PDB model 5UQ7. Per-residue inclusion information can be found in section 3 on page 15.

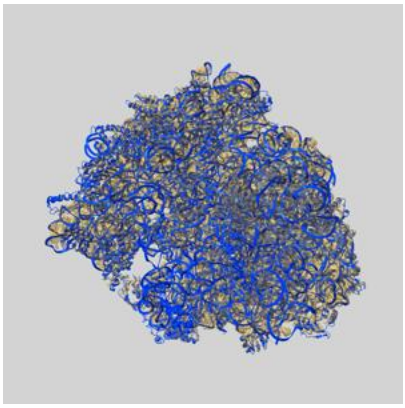
9.1 Map-model overlay



X



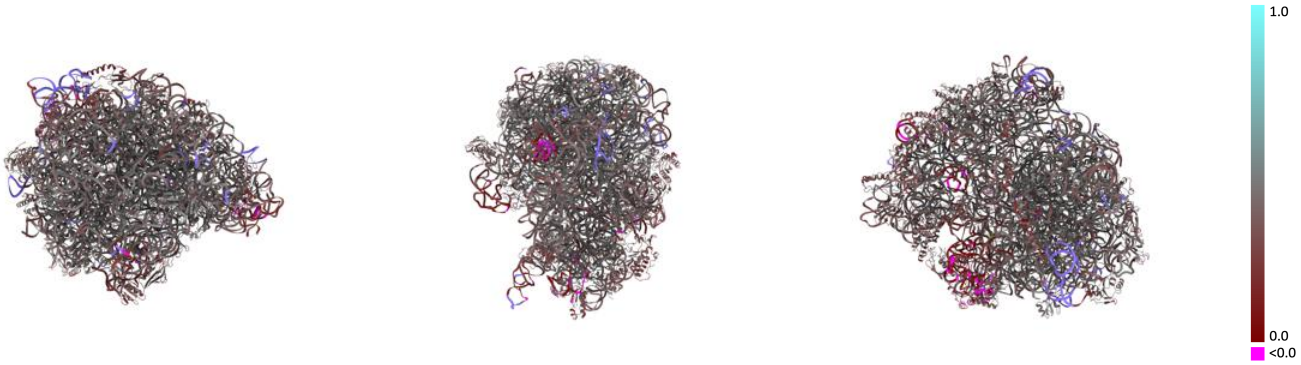
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

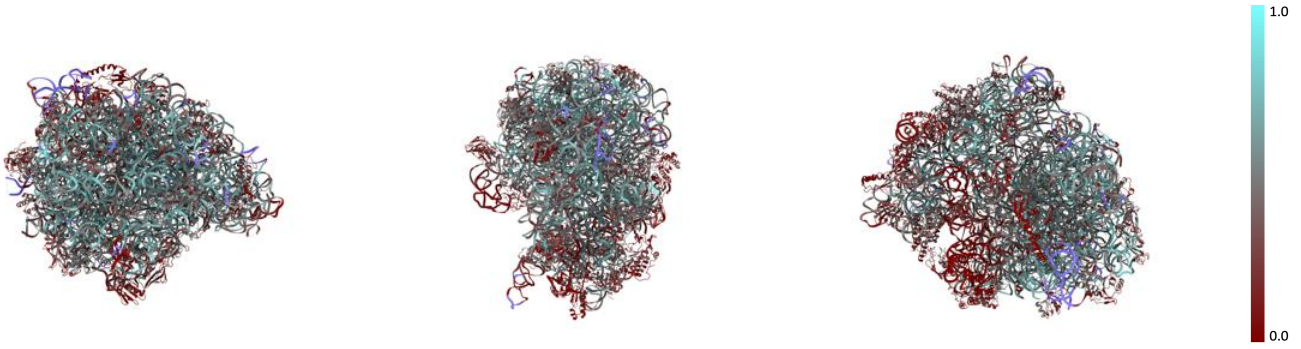
9.2 Q-score mapped to coordinate model



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.

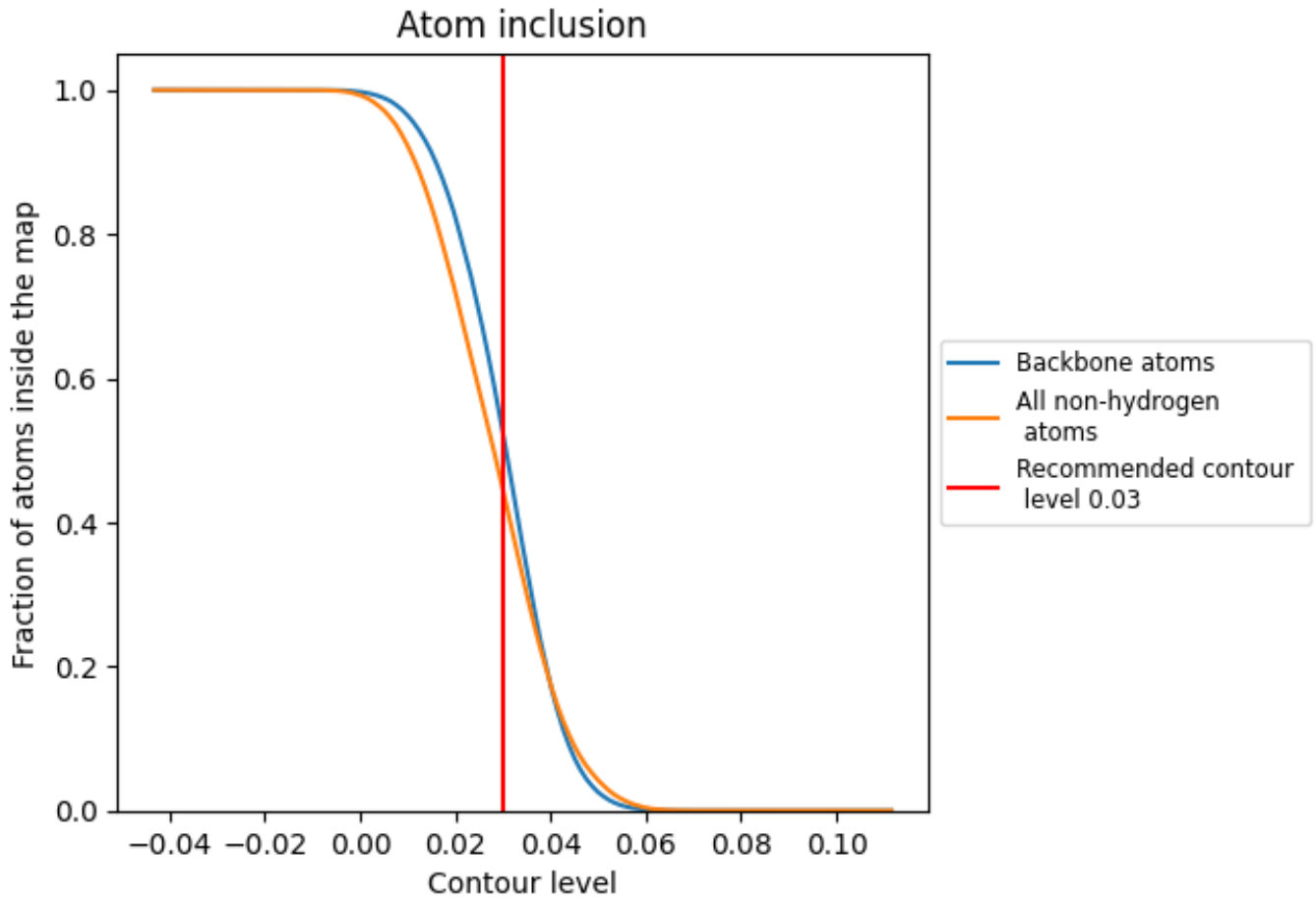
9.3 Atom inclusion mapped to coordinate model



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 45% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4457	0.3970
0	0.3672	0.4460
1	0.3080	0.4260
2	0.3129	0.3660
3	0.3348	0.4200
4	0.0942	0.2850
5	0.3829	0.4500
6	0.3233	0.3960
7	0.4021	0.4440
8	0.3723	0.4570
9	0.3932	0.4280
A	0.5580	0.4120
B	0.5468	0.4020
C	0.0000	0.1230
D	0.3943	0.4600
E	0.3825	0.4450
F	0.3375	0.4210
G	0.1926	0.3680
H	0.1709	0.3570
I	0.0237	0.2910
N	0.3511	0.4260
O	0.3337	0.4440
P	0.3203	0.4320
Q	0.3475	0.4350
R	0.4132	0.4390
S	0.3050	0.3890
T	0.3450	0.4270
U	0.4253	0.4270
V	0.2905	0.4280
W	0.3798	0.4360
X	0.3102	0.4220
Y	0.2469	0.4090
Z	0.1523	0.3560
a	0.5202	0.3980
b	0.1728	0.3540

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Chain	Atom inclusion	Q-score
c	0.2351	0.4020
d	0.2777	0.3860
e	0.3151	0.4250
f	0.1696	0.3470
g	0.2099	0.3680
h	0.3464	0.4180
i	0.2028	0.3810
j	0.1460	0.3620
k	0.2485	0.3960
l	0.2764	0.4370
m	0.1972	0.3540
n	0.2821	0.4080
o	0.3196	0.3800
p	0.3483	0.4210
q	0.3208	0.4260
r	0.2041	0.3680
s	0.1506	0.3660
t	0.2813	0.3750
u	0.2527	0.3660
x	0.0264	0.1470
y	0.1762	0.3590
z	0.0290	0.2070