wwPDB EM Validation Summary Report (i)

Jul 14, 2024 – 09:15 pm BST

PDB ID	:	8C8X
EMDB ID	:	EMD-16494
Title	:	Cryo-EM captures early ribosome assembly in action
Authors	:	Lauer, S.; Nikolay, R.; Qin, B.
Deposited on	:	2023-01-21
Resolution	:	3.93 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 (i) 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 (i)) were used in the production of this report:

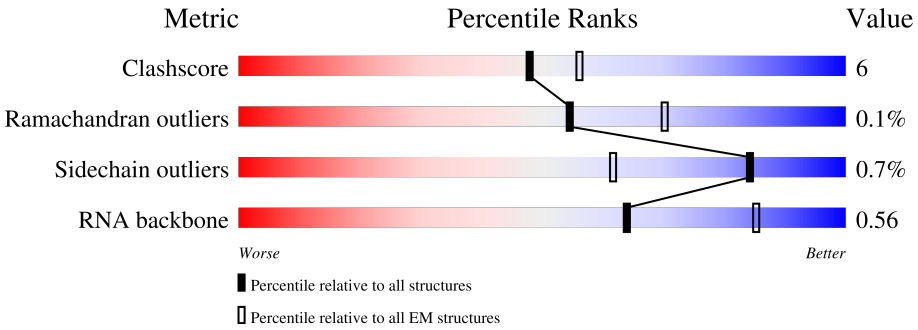
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.93 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	C	273	5% 70% 18% 12%
2	D	209	13% 75% 14% 11%
3	E	201	15% 84% 10% 5%
4	F	179	77% 84% 15%
5	H	149	13% 21% 11% 66%
6	J	142	13% 82% 18%
7	K	123	37% 81% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	L	144	33% 83% 17%
9	N	127	9% 78% 17% 6%
10	O	117	26% 86% 13%
11	P	115	23% 79% 19%
12	Q	118	8% 87% 12%
13	R	103	15% 85% 15%
14	S	110	14% 79% 21%
15	T	100	13% 73% 18% 7%
16	U	104	12% 91% 7%
17	V	94	37% 89% 11%
18	W	85	22% 72% 18% 11%
19	X	78	23% 72% 27%
20	Y	63	11% 71% 25%
21	Z	59	17% 73% 25%
22	0	57	19% 72% 26%
23	1	55	36% 73% 18% 9%
24	2	46	15% 85% 15%
25	3	65	74% 80% 18%
26	M	136	82% 78% 13% 9%
27	A	2904	13% 61% 27% 5% 7%
28	B	119	5% 77% 20%

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 82776 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	241	1858	1149	379	324	6	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	186	1393	880	250	259	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	190	1462	918	262	277	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	50	384	247	68	68	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

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

- Molecule 9 is a protein called 50S ribosomal protein L17.

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

- Molecule 10 is a protein called 50S ribosomal protein L18.

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

- Molecule 11 is a protein called 50S ribosomal protein L19.

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

- Molecule 12 is a protein called 50S ribosomal protein L20.

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

- Molecule 13 is a protein called 50S ribosomal protein L21.

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

- Molecule 14 is a protein called 50S ribosomal protein L22.

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

- Molecule 15 is a protein called 50S ribosomal protein L23.

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

- Molecule 16 is a protein called 50S ribosomal protein L24.

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

- Molecule 17 is a protein called 50S ribosomal protein L25.

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

- Molecule 18 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	76	Total 575	C 356	N 117	O 101	S 1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L28.

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

- Molecule 20 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	61	Total 499	C 308	N 97	O 92	S 2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	50	Total	C	N	O	0	0
			409	263	75	71		

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

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

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	124	Total	C	N	O	S	0	0
			984	629	187	163	5		

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A	2705	Total	C	N	O	P	0	0
			58086	25911	10706	18764	2705		

- Molecule 28 is a RNA chain called 5S rRNA.

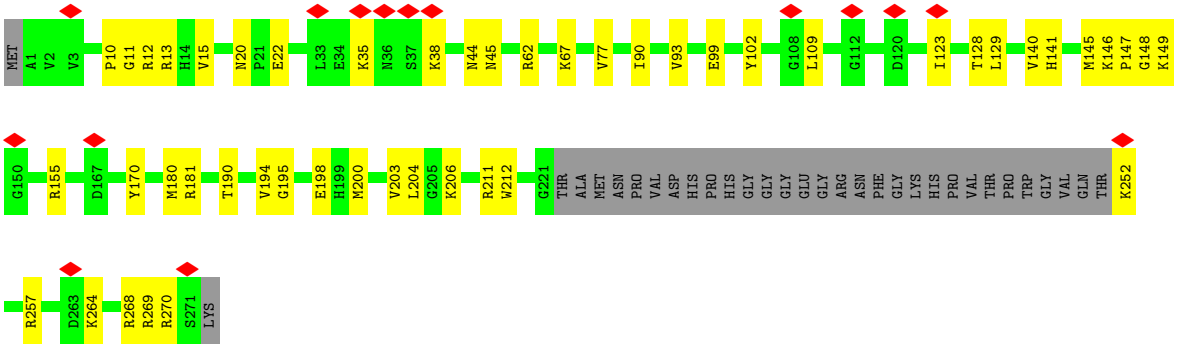
Mol	Chain	Residues	Atoms					AltConf	Trace
28	B	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

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.

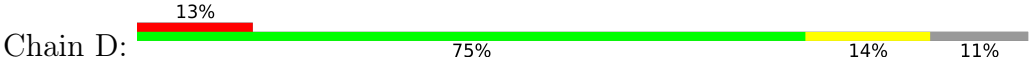
• Molecule 1: 50S ribosomal protein L2

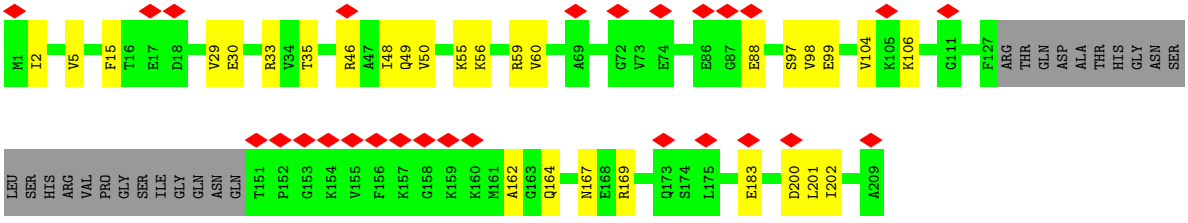
Chain C:



• Molecule 2: 50S ribosomal protein L3

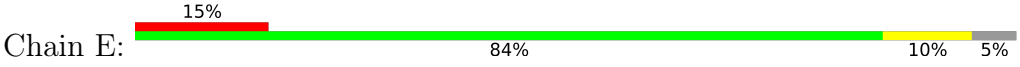
Chain D:

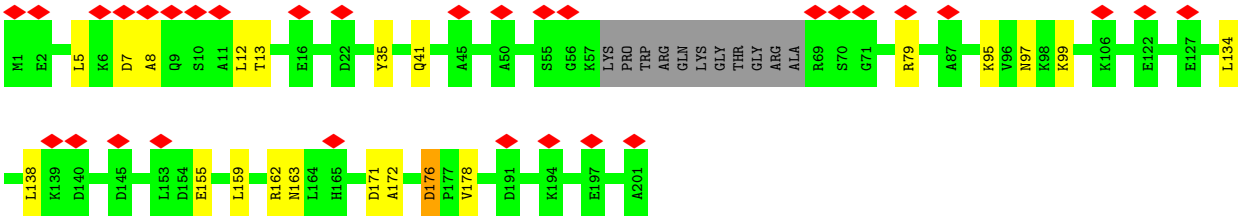




• Molecule 3: 50S ribosomal protein L4

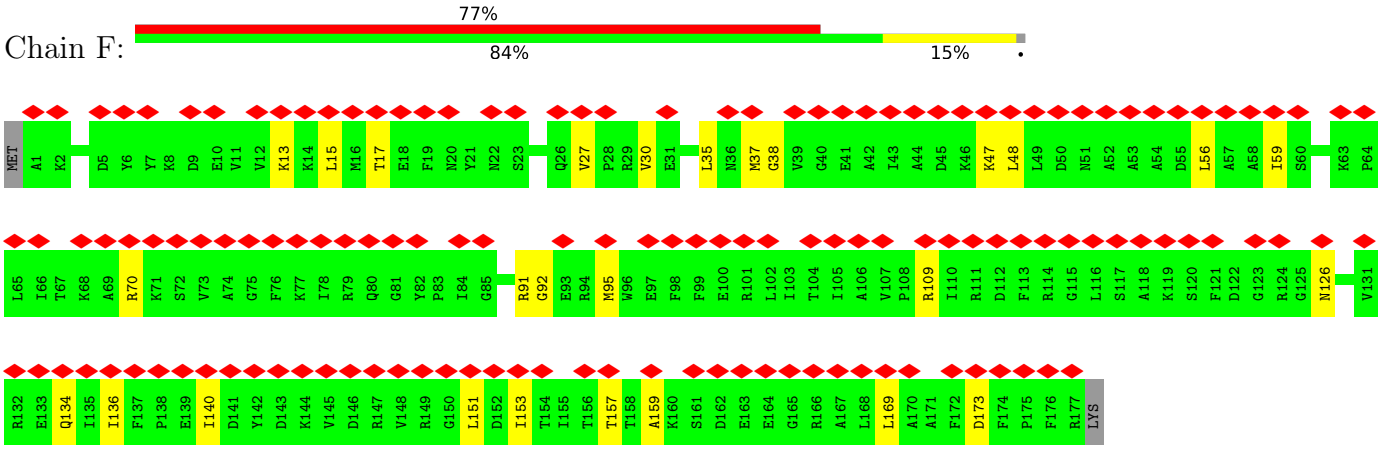
Chain E:





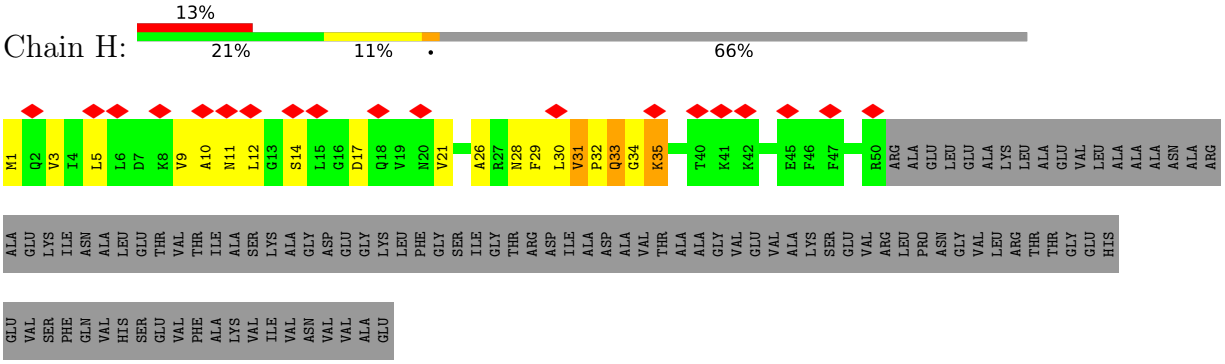
• Molecule 4: 50S ribosomal protein L5

Chain F:



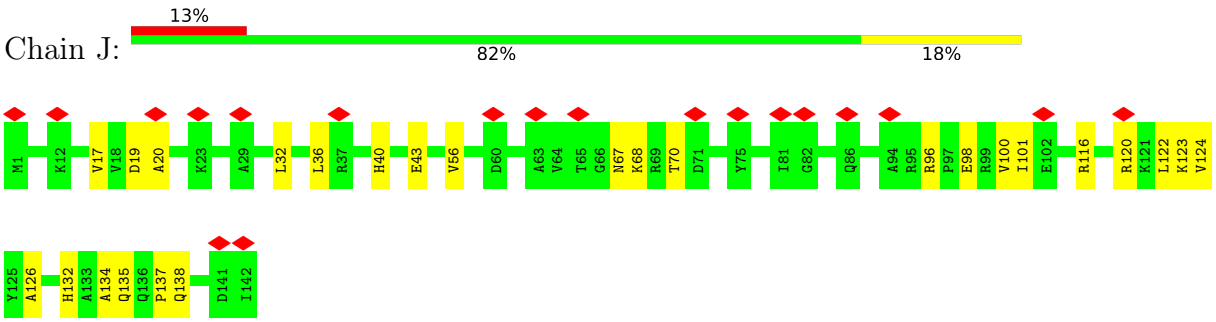
• Molecule 5: 50S ribosomal protein L9

Chain H:



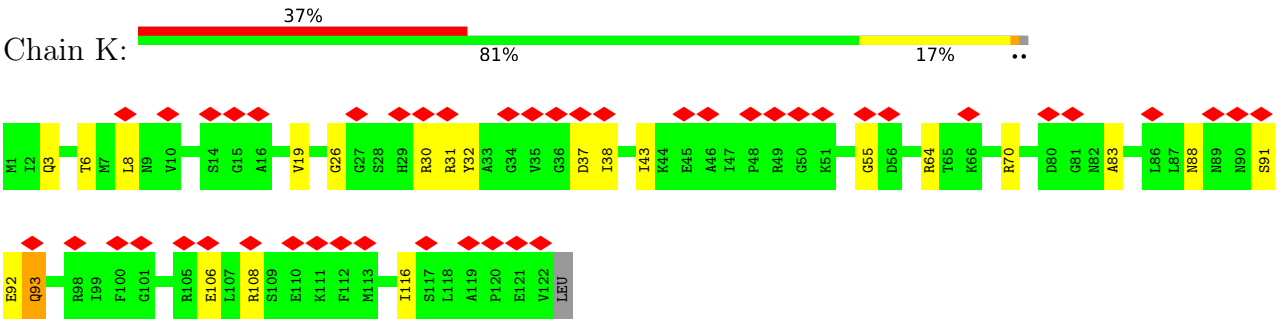
• Molecule 6: 50S ribosomal protein L13

Chain J:



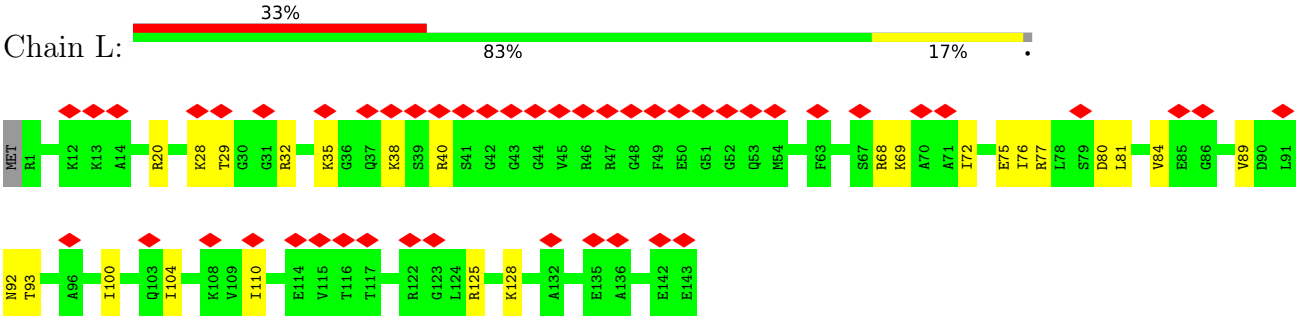
• Molecule 7: 50S ribosomal protein L14

Chain K:



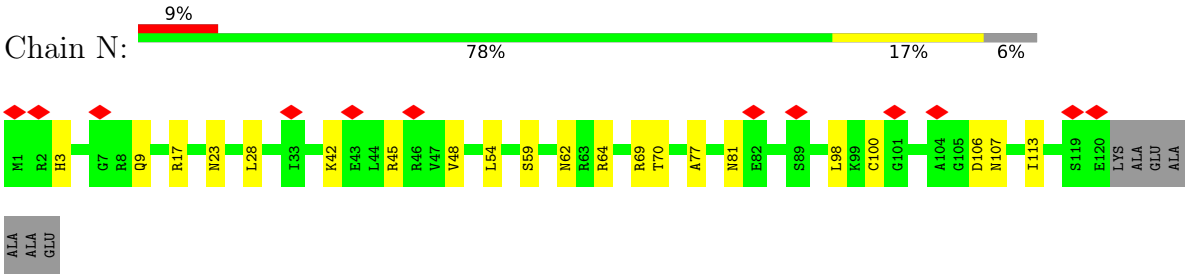
• Molecule 8: 50S ribosomal protein L15

Chain L:



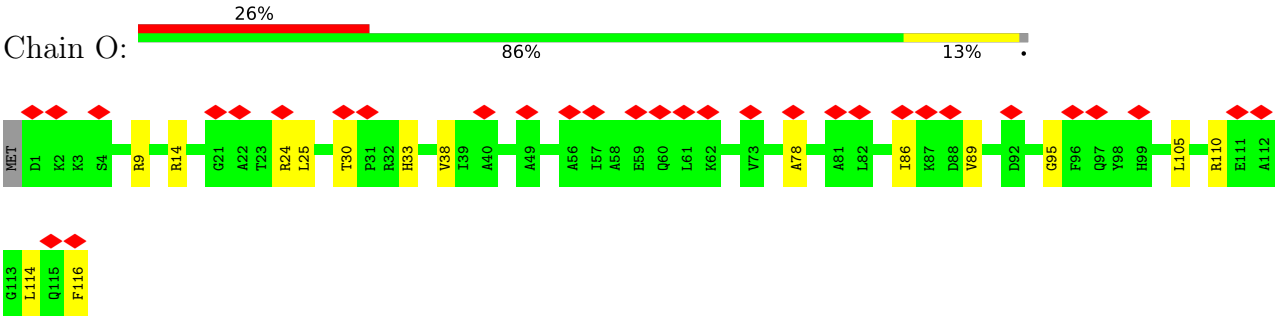
• Molecule 9: 50S ribosomal protein L17

Chain N:



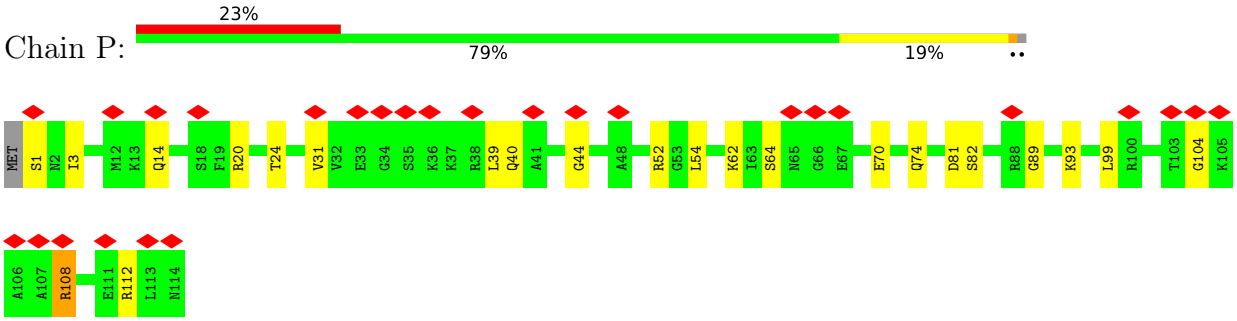
• Molecule 10: 50S ribosomal protein L18

Chain O:



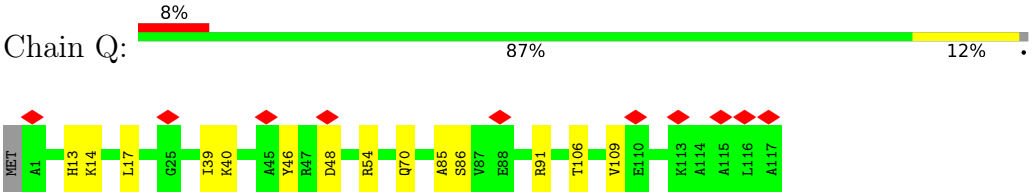
• Molecule 11: 50S ribosomal protein L19

Chain P:



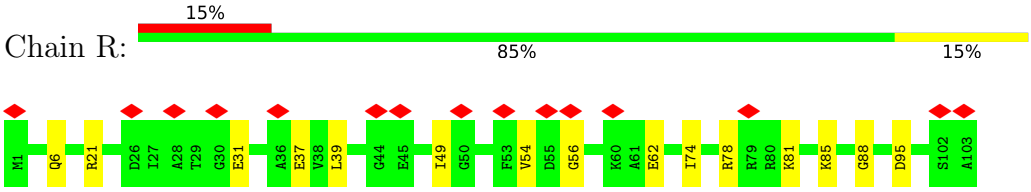
• Molecule 12: 50S ribosomal protein L20

Chain Q:



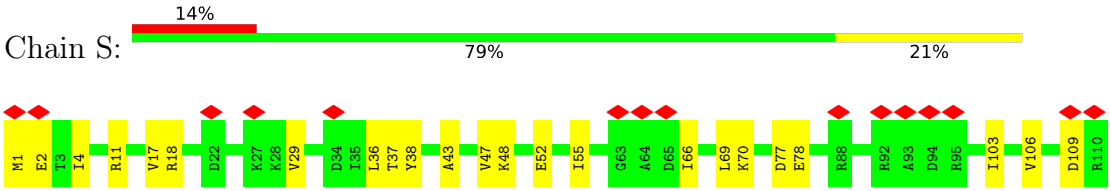
• Molecule 13: 50S ribosomal protein L21

Chain R:



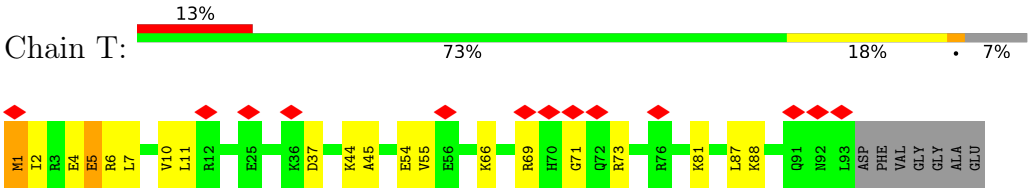
• Molecule 14: 50S ribosomal protein L22

Chain S:



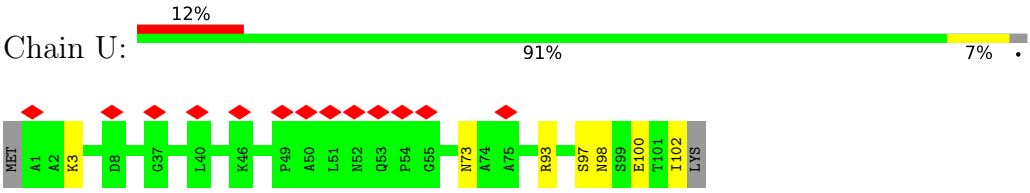
• Molecule 15: 50S ribosomal protein L23

Chain T:



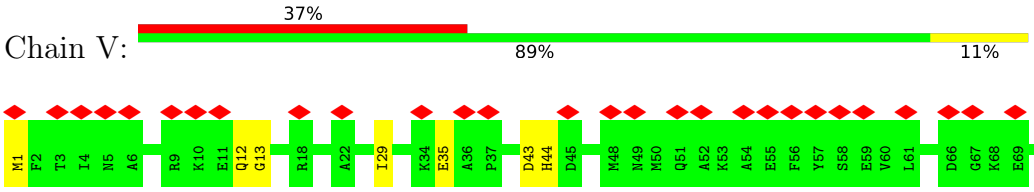
• Molecule 16: 50S ribosomal protein L24

Chain U:



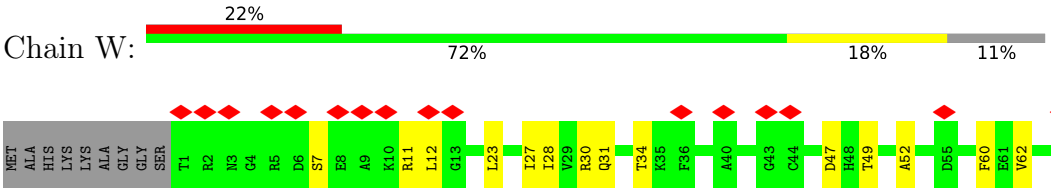
• Molecule 17: 50S ribosomal protein L25

Chain V:



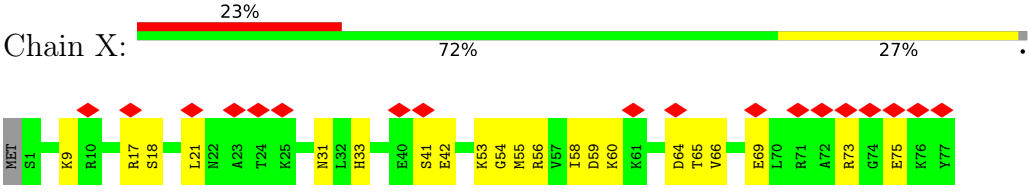
• Molecule 18: 50S ribosomal protein L27

Chain W:



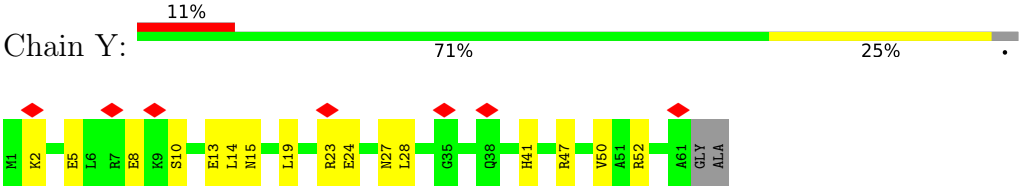
• Molecule 19: 50S ribosomal protein L28

Chain X:



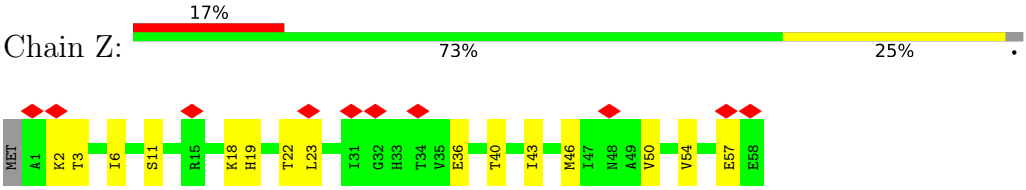
• Molecule 20: 50S ribosomal protein L29

Chain Y:



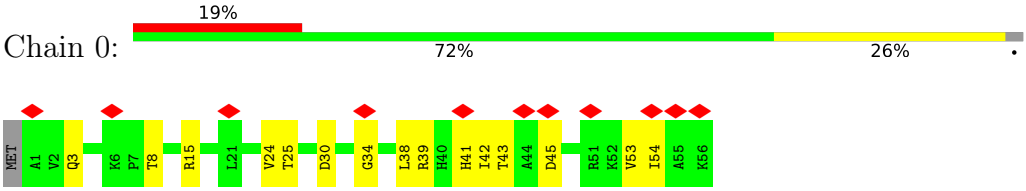
• Molecule 21: 50S ribosomal protein L30

Chain Z:



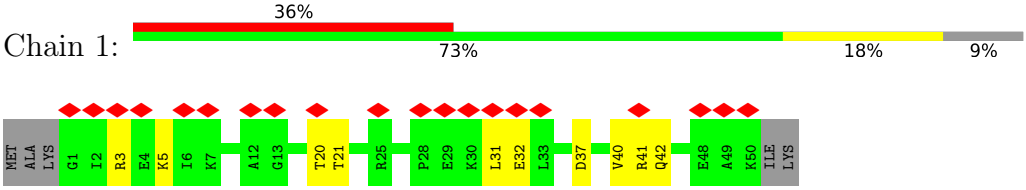
• Molecule 22: 50S ribosomal protein L32

Chain 0:



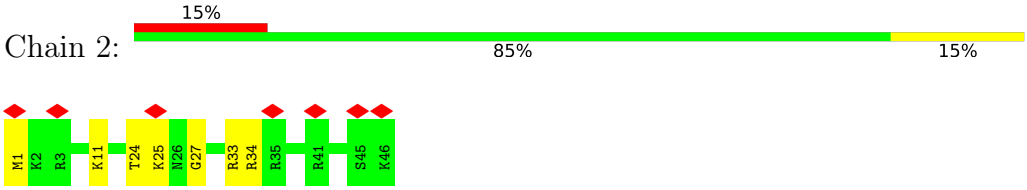
• Molecule 23: 50S ribosomal protein L33

Chain 1:



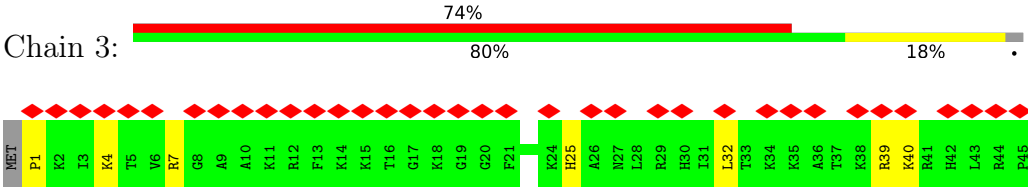
• Molecule 24: 50S ribosomal protein L34

Chain 2:



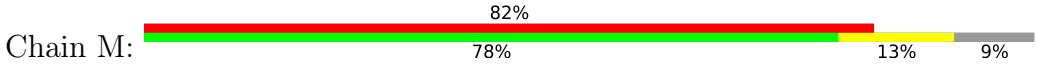
• Molecule 25: 50S ribosomal protein L35

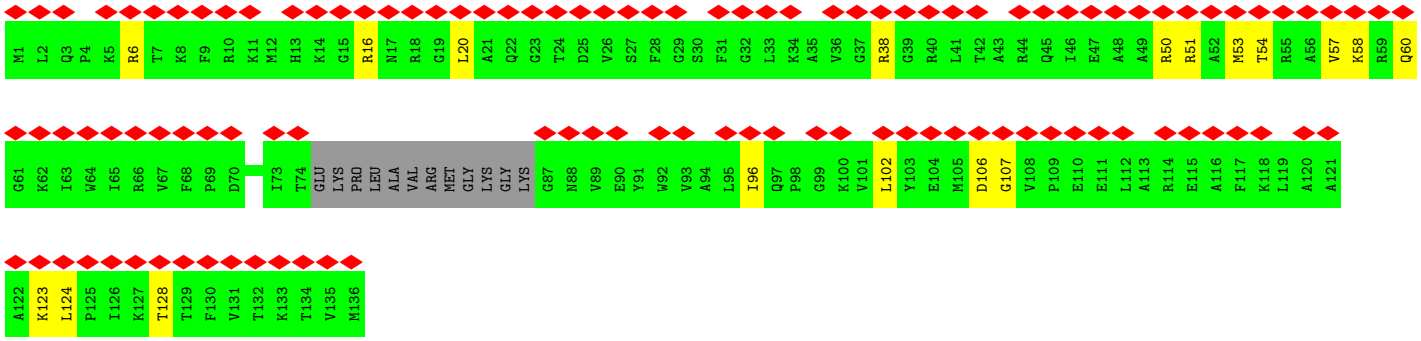
Chain 3:



• Molecule 26: 50S ribosomal protein L16

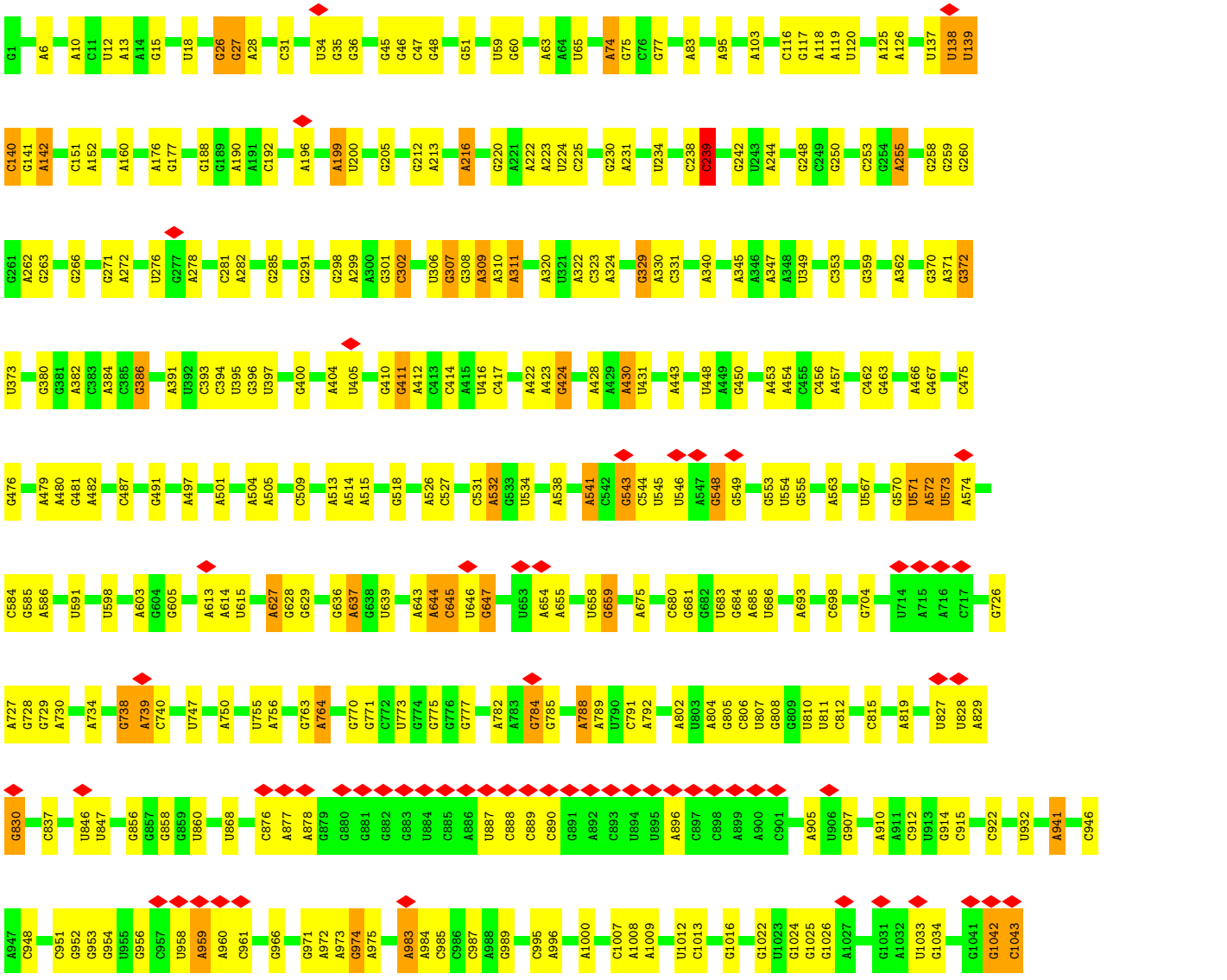
Chain M:

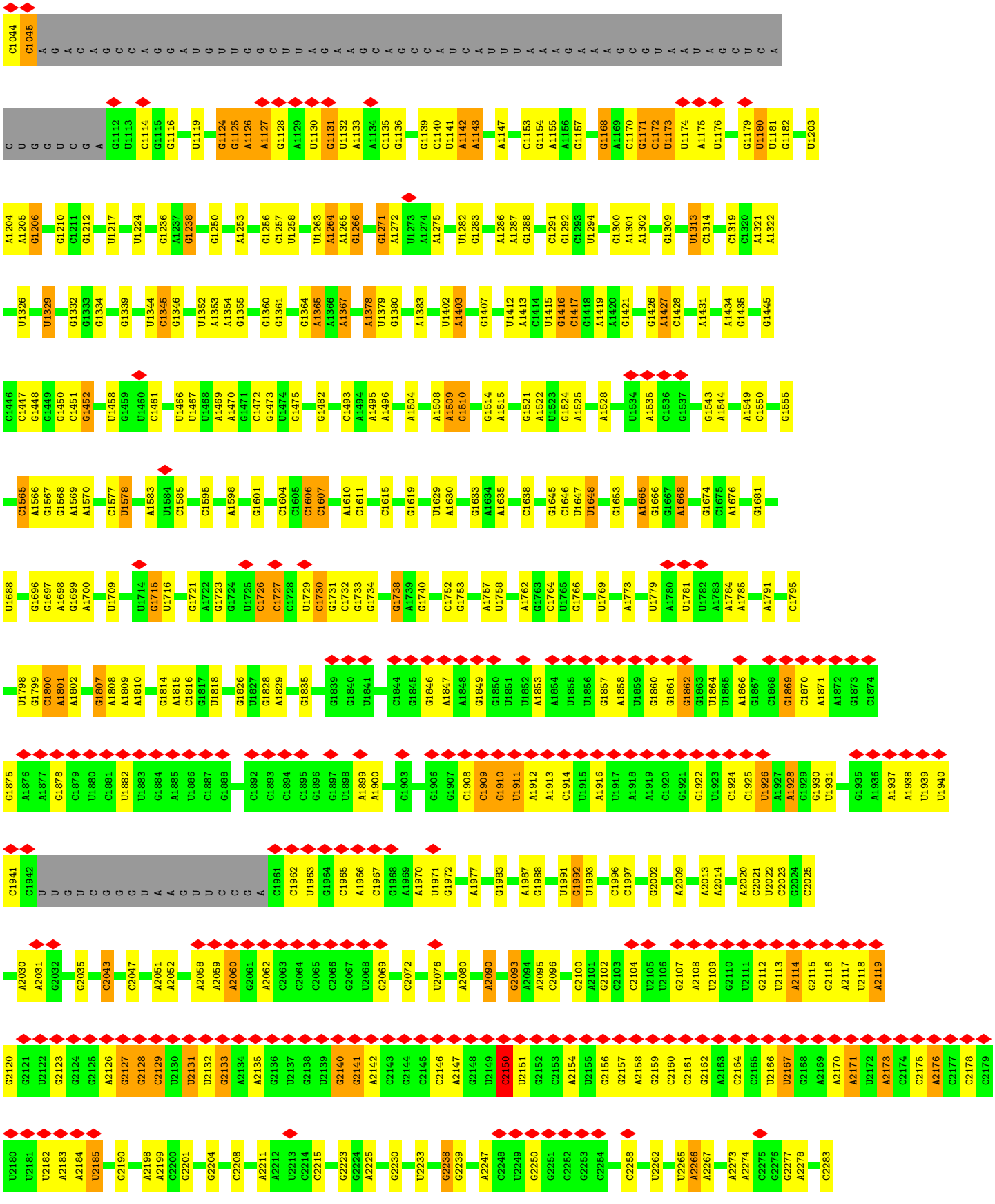


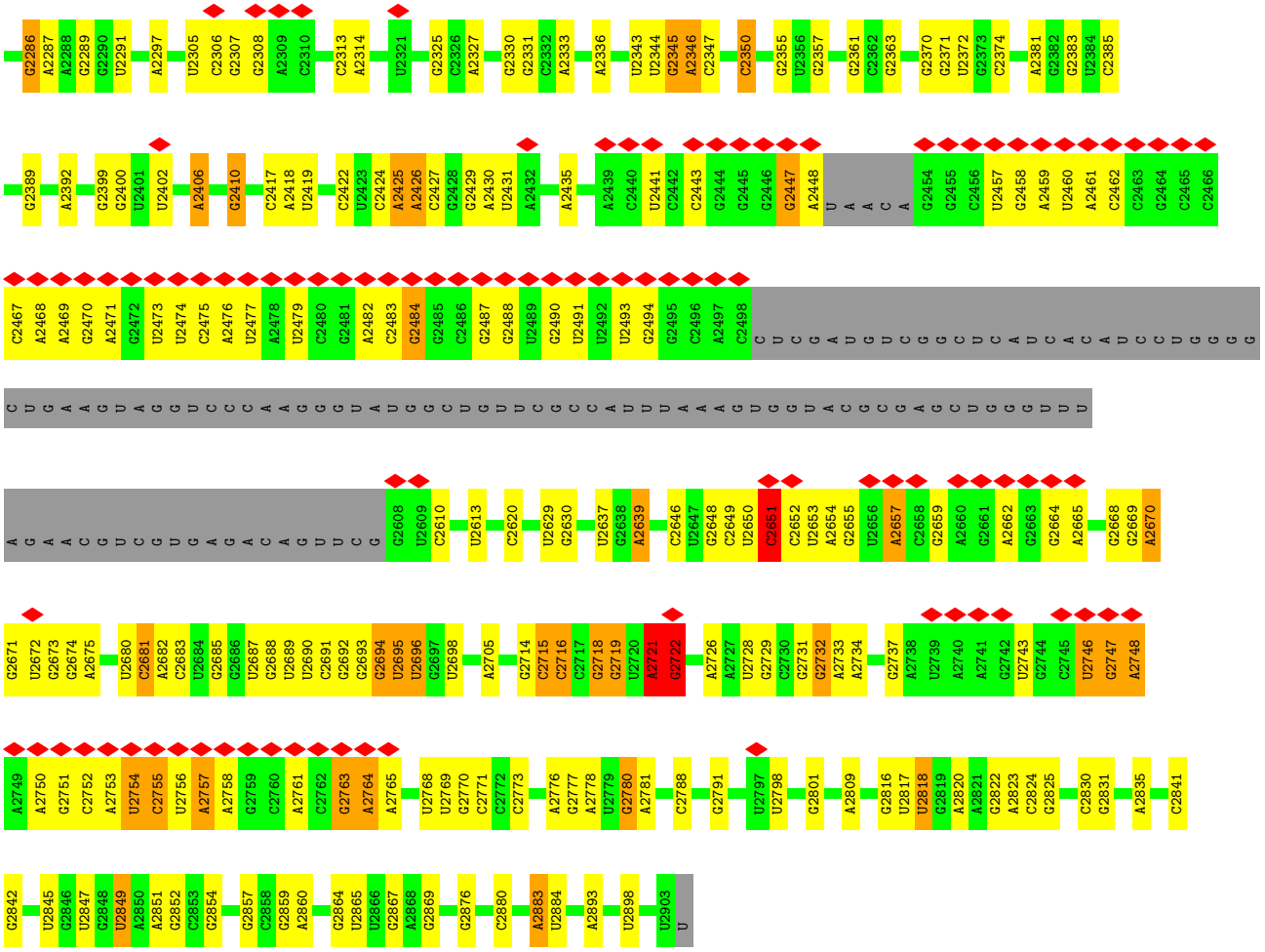


• Molecule 27: 23S rRNA

Chain A:

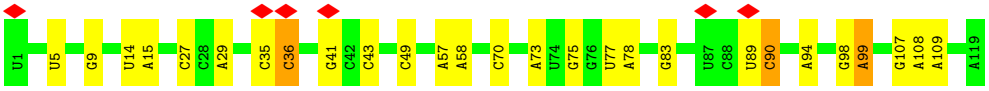



C1044 C1045 A G A C A G C C C A G G A U G U U G G C U U A G A A G C C C A A U C A U U U A A A G A A A G C A A G C C C A A U C U C A
C U U G G U C G A G1112 U1113 C1114 G1115 G1116 U1119 G1124 G1125 A1126 A1127 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 C1140 U1141 A1142 A1143 A1147 C1153 G1154 A1155 A1156 G1157 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1179 U1180 U1181 G1182 U1203
A1204 A1205 G1206 G1210 C1211 G1212 U1217 U1224 G1236 A1237 G1238 G1250 A1253 G1256 C1257 U1258 U1263 A1264 A1265 G1266 G1271 A1272 U1273 A1274 A1275 U1282 G1283 A1286 A1287 G1288 C1291 G1292 C1293 U1294 G1300 A1301 A1302 G1309 U1313 C1314 C1319 C1320 A1321 A1322
U1326 U1329 G1332 G1333 G1334 G1339 U1344 C1345 G1346 U1352 A1353 A1354 G1355 G1360 G1361 G1364 A1365 A1366 A1367 A1378 U1379 G1380 A1383 U1402 A1403 G1407 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1426 A1427 C1428 A1431 A1434 G1435 G1445
C1446 C1447 G1448 G1449 G1450 C1451 G1452 U1458 G1459 U1460 C1461 U1466 U1467 U1468 A1469 A1470 G1471 C1472 G1473 U1474 G1475 G1482 C1493 A1494 A1495 A1496 A1504 A1508 A1509 G1510 G1514 A1515 G1521 A1522 U1523 G1524 A1525 A1528 U1534 A1535 C1536 G1537 G1543 A1544 A1549 C1550 G1555
C1565 A1566 G1567 G1568 A1569 A1570 C1577 U1578 A1583 U1584 C1585 C1595 A1598 G1601 C1604 C1605 C1606 C1607 A1610 C1611 C1615 G1619 U1629 A1630 G1633 A1634 A1635 C1638 G1645 C1646 U1647 U1648 G1653 A1665 G1666 G1667 A1668 G1674 C1675 A1676 G1681
U1688 G1696 G1697 A1698 G1699 A1700 U1709 U1714 G1715 U1716 G1721 A1722 G1723 G1724 U1725 C1726 C1727 C1728 U1729 C1730 C1731 C1732 G1733 G1734 G1738 A1739 G1740 C1752 G1753 A1757 U1758 A1762 G1763 C1764 U1765 G1766 U1769 A1773 U1779 A1780 U1781 U1782 A1783 A1784 A1785 A1791 C1796
U1798 G1799 C1800 A1801 A1802 G1807 A1808 A1809 A1810 G1814 A1815 C1816 G1817 U1818 G1826 U1827 G1828 A1829 G1835 G1839 G1840 U1841 C1844 G1845 G1846 A1847 A1848 G1849 G1850 U1851 U1852 A1853 A1854 U1855 U1856 G1857 A1858 U1859 G1860 G1861 G1862 G1863 U1864 U1865 A1866 G1867 C1868 G1869 C1870 A1871 A1872 G1873 C1874
G1875 A1876 A1877 G1878 C1879 U1880 C1881 U1882 U1883 G1884 A1885 U1886 C1887 G1888 C1892 C1893 C1894 C1895 G1896 G1897 U1898 A1899 A1900 G1903 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 G1935 A1936 A1937 A1938 U1939 U1940
C1941 C1942 U U G U C G G G U A A G U U C C C G A C1961 C1962 C1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 A1977 G1983 A1987 G1988 U1991 G1992 U1993 C1996 C1997 G2002 A2009 A2013 A2014 A2020 C2021 U2022 C2023 G2024 C2025
A2030 A2031 G2032 G2035 C2043 C2047 A2051 A2052 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 C2072 U2076 A2080 A2090 G2093 A2094 A2095 C2096 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 C2125 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 C2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179
U2180 U2181 U2182 A2183 A2184 U2185 G2190 A2198 A2199 C2200 G2201 G2204 C2208 A2211 A2212 U2213 C2214 C2215 G2223 G2224 A2225 G2230 U2233 G2238 G2239 A2247 C2248 U2249 G2250 G2251 G2252 G2253 C2254 C2258 U2262 U2265 A2266 A2267 A2273 A2274 C2275 G2276 G2277 A2278 C2283



• Molecule 28: 5S rRNA

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5772	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 ($e^-/Å^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.778	Depositor
Minimum map value	-0.642	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	375.0, 375.0, 375.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	0.24	0/1886	0.56	0/2528
2	D	0.24	0/1410	0.51	0/1894
3	E	0.24	0/1477	0.48	0/1986
4	F	0.24	0/1434	0.50	0/1926
5	H	0.33	0/389	0.53	0/523
6	J	0.24	0/1152	0.49	0/1551
7	K	0.24	0/947	0.55	0/1268
8	L	0.25	0/1054	0.58	0/1403
9	N	0.24	0/973	0.58	0/1301
10	O	0.24	0/902	0.53	0/1209
11	P	0.24	0/929	0.54	0/1242
12	Q	0.24	0/960	0.52	0/1278
13	R	0.25	0/829	0.53	0/1107
14	S	0.24	0/864	0.51	0/1156
15	T	0.26	0/744	0.51	0/994
16	U	0.26	0/787	0.51	0/1051
17	V	0.24	0/766	0.47	0/1025
18	W	0.25	0/582	0.55	0/769
19	X	0.23	0/635	0.57	0/848
20	Y	0.25	0/500	0.53	0/665
21	Z	0.24	0/453	0.55	0/605
22	0	0.23	0/450	0.55	0/599
23	1	0.27	0/416	0.49	0/554
24	2	0.25	0/380	0.64	0/498
25	3	0.24	0/513	0.52	0/676
26	M	0.24	0/1001	0.53	0/1338
27	A	0.54	12/65058 (0.0%)	0.79	38/101492 (0.0%)
28	B	0.13	0/2847	0.69	0/4440
All	All	0.47	12/90338 (0.0%)	0.74	38/135926 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2721	A	C6-N1	66.09	1.81	1.35
27	A	2721	A	N3-C4	61.58	1.71	1.34
27	A	2721	A	N1-C2	43.25	1.73	1.34
27	A	2721	A	C2-N3	39.85	1.69	1.33
27	A	2722	G	C1'-N9	37.11	2.04	1.48

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	2722	G	C8-N9-C4	-74.01	76.80	106.40
27	A	2722	G	N7-C8-N9	39.14	132.67	113.10
27	A	2722	G	N9-C4-C5	37.02	120.21	105.40
27	A	2721	A	N1-C2-N3	-30.08	114.26	129.30
27	A	2722	G	N3-C4-C5	-26.49	115.36	128.60

There are no chirality outliers.

There are no planarity outliers.

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	C	1858	0	1952	37	0
2	D	1393	0	1454	21	0
3	E	1462	0	1523	15	0
4	F	1410	0	1447	21	0
5	H	384	0	405	30	0
6	J	1129	0	1162	19	0
7	K	938	0	1012	17	0
8	L	1045	0	1120	19	0
9	N	960	0	1000	18	0
10	O	892	0	926	10	0
11	P	917	0	965	18	0
12	Q	947	0	1022	10	0
13	R	816	0	839	14	0
14	S	857	0	922	15	0
15	T	738	0	807	21	0
16	U	779	0	834	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	V	753	0	780	7	0
18	W	575	0	592	18	0
19	X	625	0	655	16	0
20	Y	499	0	535	10	0
21	Z	449	0	491	10	0
22	0	444	0	461	17	0
23	1	409	0	443	11	0
24	2	377	0	418	6	0
25	3	504	0	574	11	0
26	M	984	0	1051	12	0
27	A	58086	0	29218	502	0
28	B	2546	0	1292	16	0
All	All	82776	0	53900	805	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 6.

The worst 5 of 805 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)
27:A:2721:A:C2	27:A:2722:G:H1'	1.28	1.68
27:A:2721:A:N3	27:A:2721:A:C4	1.71	1.58
27:A:2721:A:C2	27:A:2721:A:N3	1.69	1.55
27:A:2721:A:C2	27:A:2721:A:N1	1.73	1.55
27:A:2721:A:N1	27:A:2721:A:C6	1.81	1.48

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	C	237/273 (87%)	223 (94%)	14 (6%)	0	100	100
2	D	182/209 (87%)	177 (97%)	5 (3%)	0	100	100
3	E	186/201 (92%)	183 (98%)	3 (2%)	0	100	100
4	F	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
5	H	48/149 (32%)	38 (79%)	9 (19%)	1 (2%)	7	38
6	J	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
7	K	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
8	L	141/144 (98%)	126 (89%)	15 (11%)	0	100	100
9	N	118/127 (93%)	112 (95%)	6 (5%)	0	100	100
10	O	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
11	P	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
12	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
13	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
14	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
15	T	91/100 (91%)	82 (90%)	8 (9%)	1 (1%)	14	50
16	U	100/104 (96%)	86 (86%)	14 (14%)	0	100	100
17	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
18	W	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
19	X	75/78 (96%)	75 (100%)	0	0	100	100
20	Y	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
21	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
22	0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
23	1	48/55 (87%)	48 (100%)	0	0	100	100
24	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	3	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
26	M	120/136 (88%)	113 (94%)	7 (6%)	0	100	100
All	All	2772/3052 (91%)	2636 (95%)	134 (5%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	35	LYS
15	T	5	GLU

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	C	193/218 (88%)	192 (100%)	1 (0%)	88 93
2	D	145/164 (88%)	145 (100%)	0	100 100
3	E	157/165 (95%)	156 (99%)	1 (1%)	86 91
4	F	148/150 (99%)	148 (100%)	0	100 100
5	H	40/114 (35%)	38 (95%)	2 (5%)	24 52
6	J	116/116 (100%)	116 (100%)	0	100 100
7	K	103/104 (99%)	102 (99%)	1 (1%)	76 85
8	L	102/103 (99%)	101 (99%)	1 (1%)	76 85
9	N	100/103 (97%)	100 (100%)	0	100 100
10	O	86/87 (99%)	85 (99%)	1 (1%)	71 83
11	P	99/100 (99%)	98 (99%)	1 (1%)	76 85
12	Q	89/90 (99%)	89 (100%)	0	100 100
13	R	84/84 (100%)	84 (100%)	0	100 100
14	S	93/93 (100%)	93 (100%)	0	100 100
15	T	80/84 (95%)	79 (99%)	1 (1%)	69 81
16	U	83/85 (98%)	83 (100%)	0	100 100
17	V	78/78 (100%)	78 (100%)	0	100 100
18	W	56/63 (89%)	56 (100%)	0	100 100
19	X	67/68 (98%)	67 (100%)	0	100 100
20	Y	55/55 (100%)	52 (94%)	3 (6%)	21 50
21	Z	48/49 (98%)	48 (100%)	0	100 100
22	0	47/48 (98%)	47 (100%)	0	100 100
23	1	45/49 (92%)	45 (100%)	0	100 100
24	2	38/38 (100%)	37 (97%)	1 (3%)	46 67
25	3	51/52 (98%)	50 (98%)	1 (2%)	55 73
26	M	100/109 (92%)	98 (98%)	2 (2%)	55 73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2303/2469 (93%)	2287 (99%)	16 (1%)	84 90

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	M	6	ARG
25	3	40	LYS
15	T	1	MET
24	2	25	LYS
11	P	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
20	Y	27	ASN
20	Y	38	GLN
5	H	18	GLN
5	H	33	GLN
9	N	81	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	A	2701/2904 (93%)	468 (17%)	22 (0%)
28	B	118/119 (99%)	10 (8%)	0
All	All	2819/3023 (93%)	478 (16%)	22 (0%)

5 of 478 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	A	10	A
27	A	12	U
27	A	26	G
27	A	27	G
27	A	34	U

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	A	2140	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	2470	G
27	A	2457	U
27	A	2694	G
27	A	1126	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

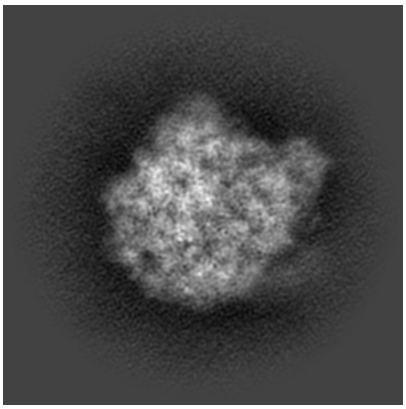
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16494. These allow visual inspection of the internal detail of the map and identification of artifacts.

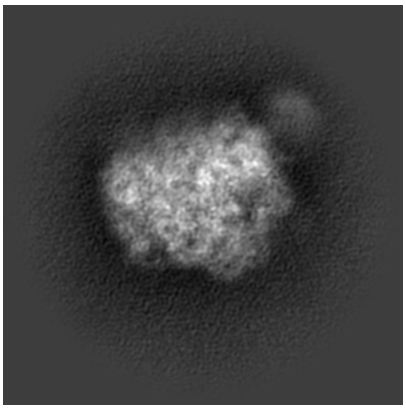
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

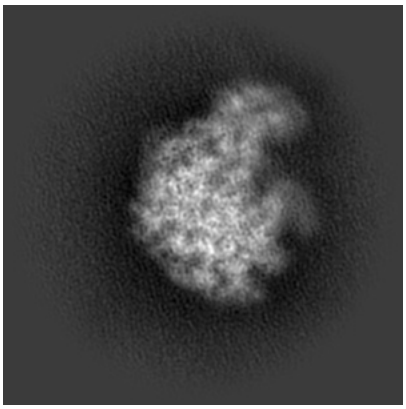
6.1.1 Primary map



X

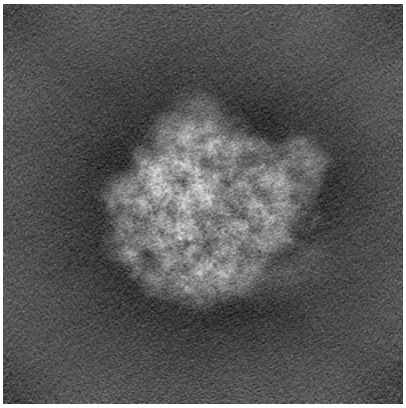


Y

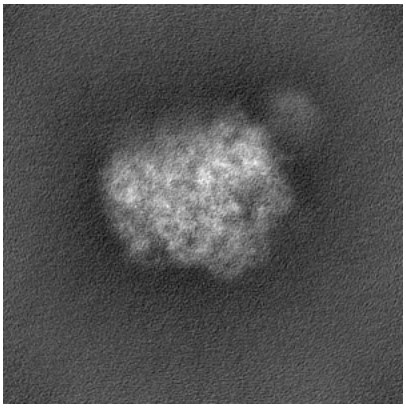


Z

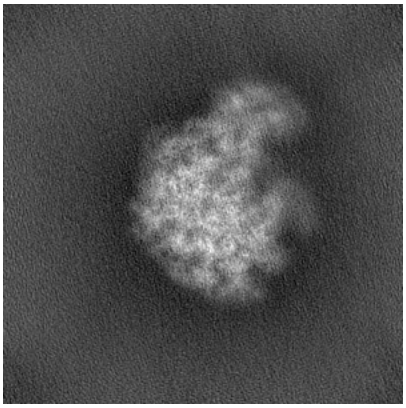
6.1.2 Raw map



X



Y

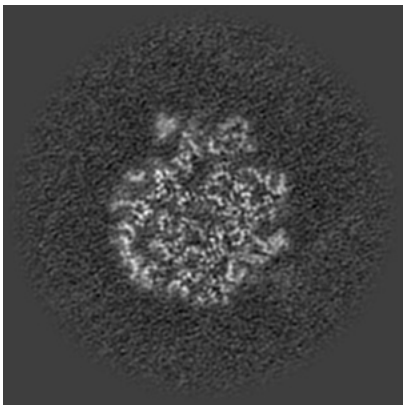


Z

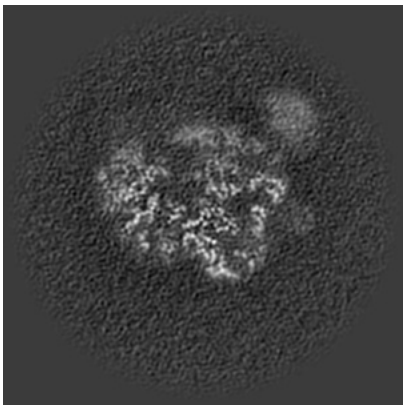
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

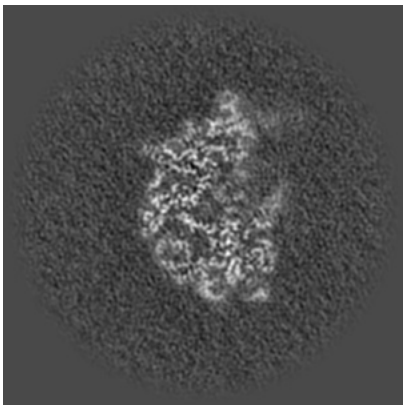
6.2.1 Primary map



X Index: 150

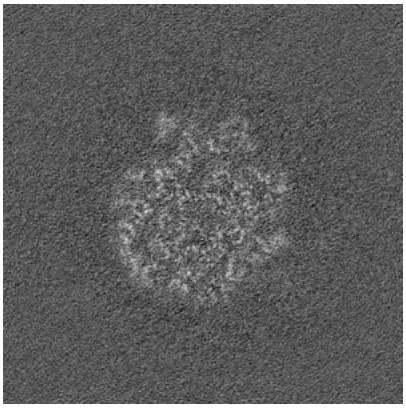


Y Index: 150

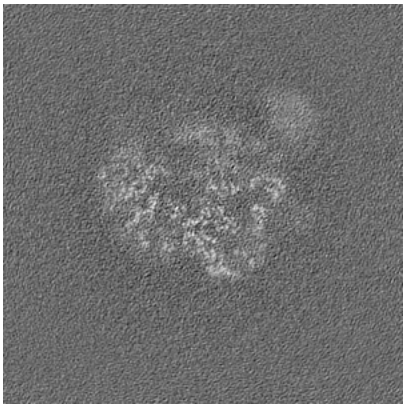


Z Index: 150

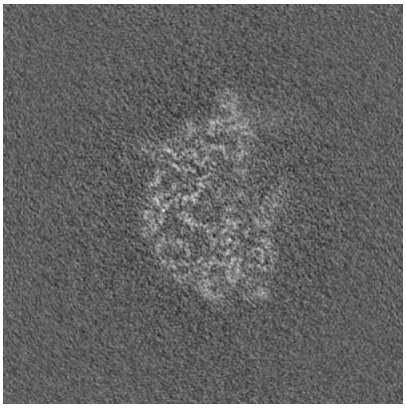
6.2.2 Raw map



X Index: 150



Y Index: 150

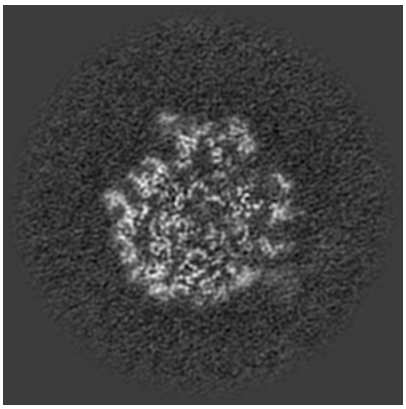


Z Index: 150

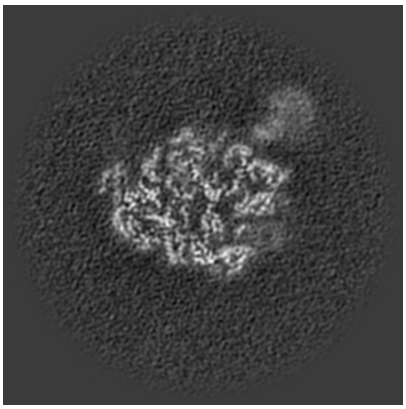
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

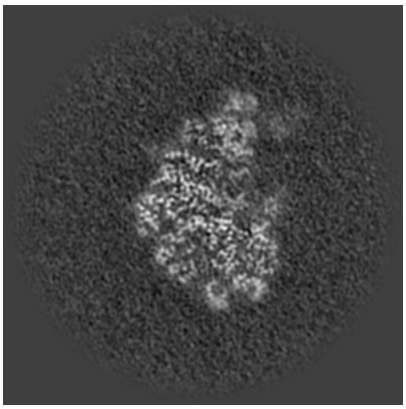
6.3.1 Primary map



X Index: 154

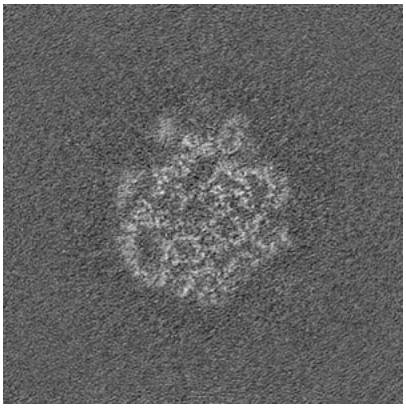


Y Index: 139

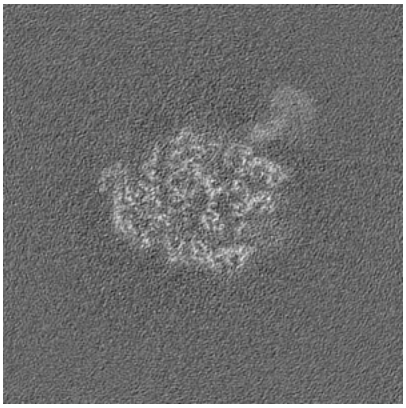


Z Index: 154

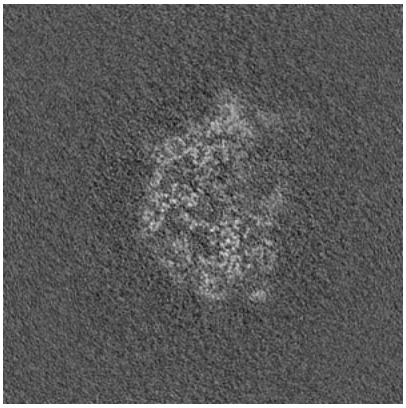
6.3.2 Raw map



X Index: 147



Y Index: 138

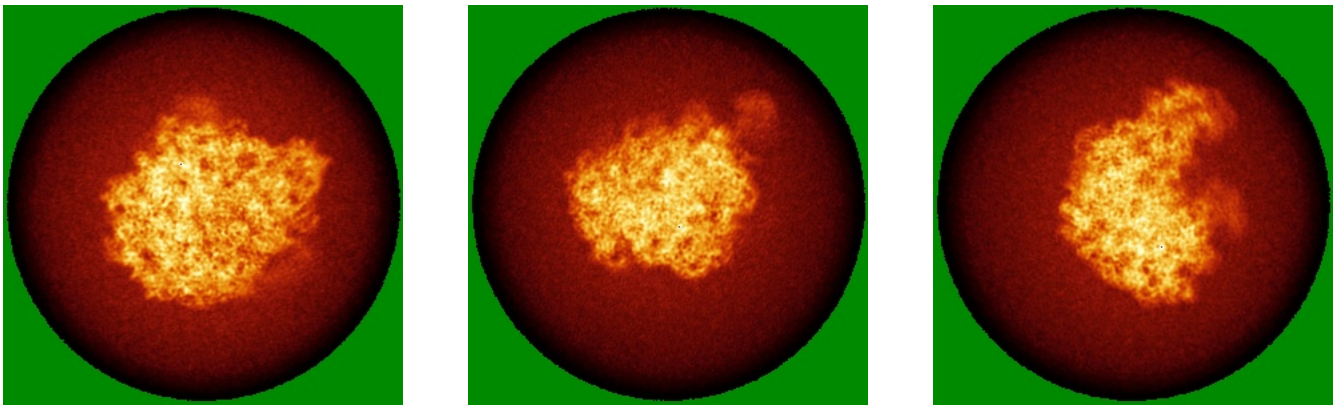


Z Index: 149

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

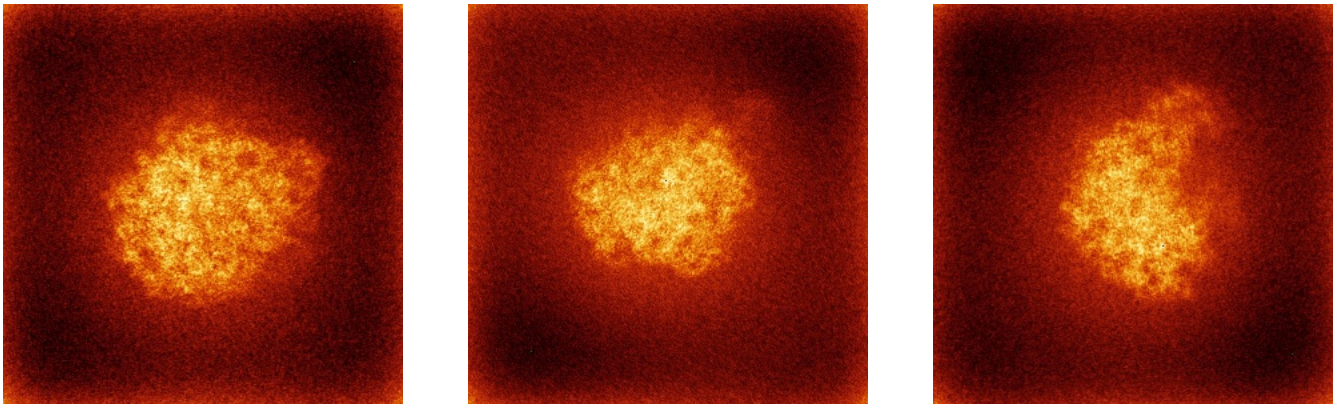
6.4 Orthogonal standard-deviation projections (False-color) (i)

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.

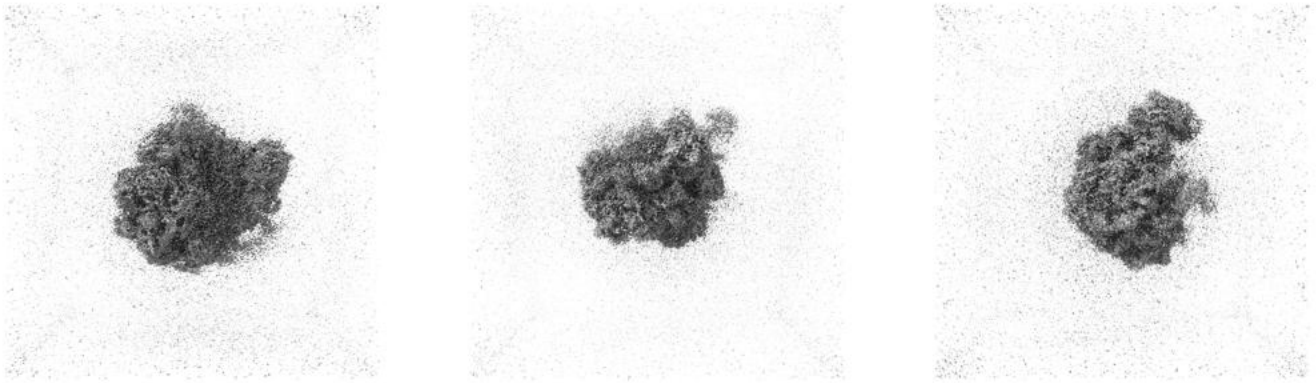
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

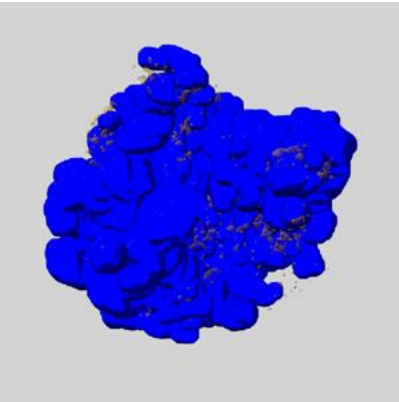
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

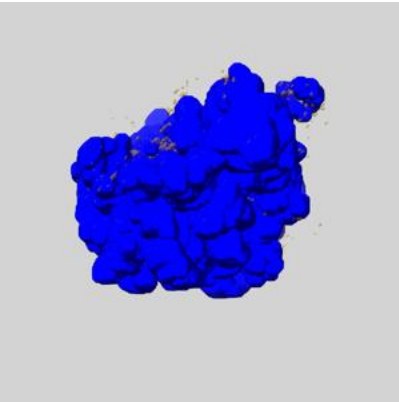
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

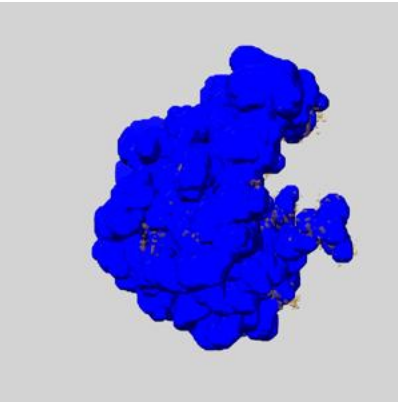
6.6.1 emd_16494_msk_1.map (i)



X



Y

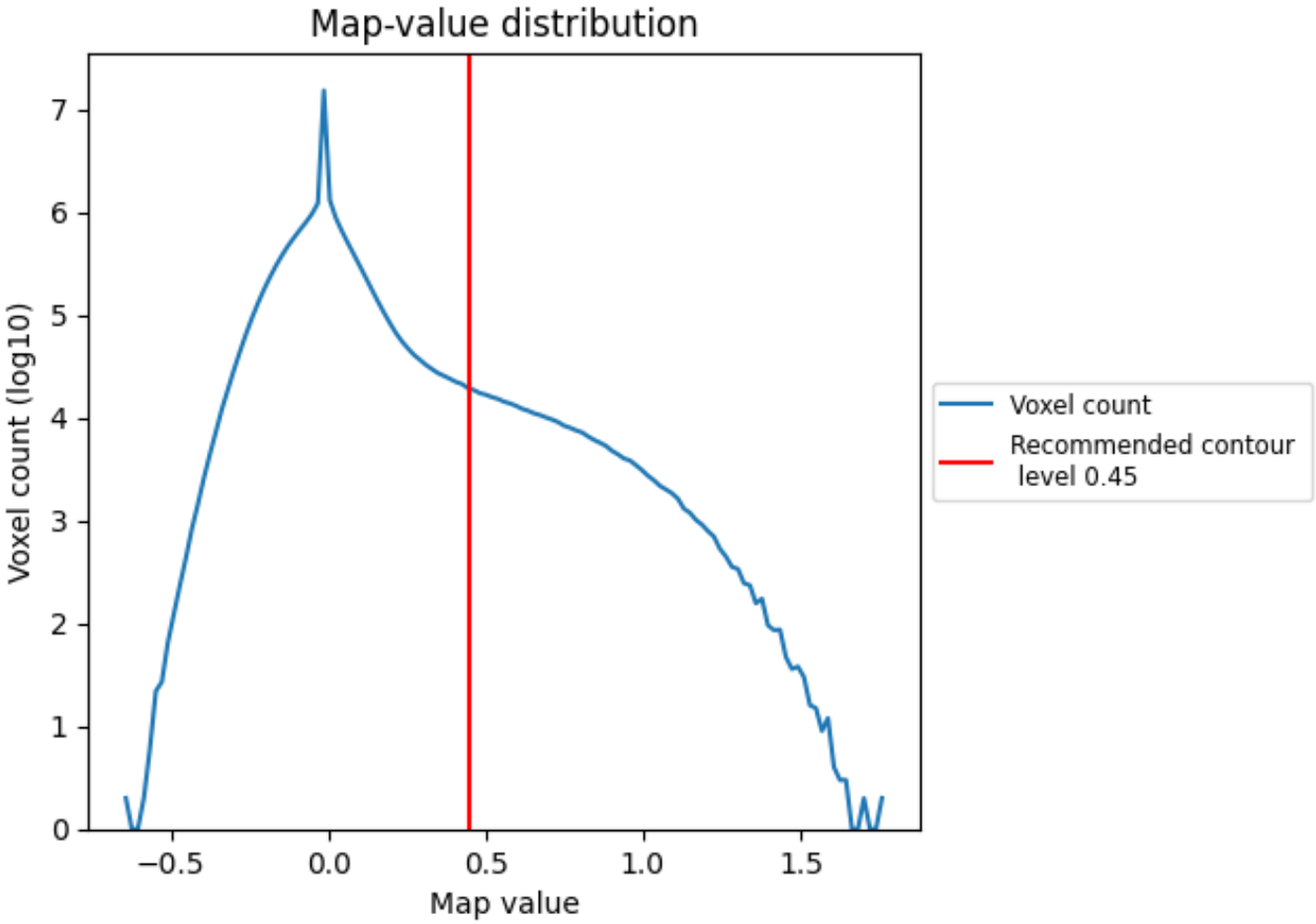


Z

7 Map analysis

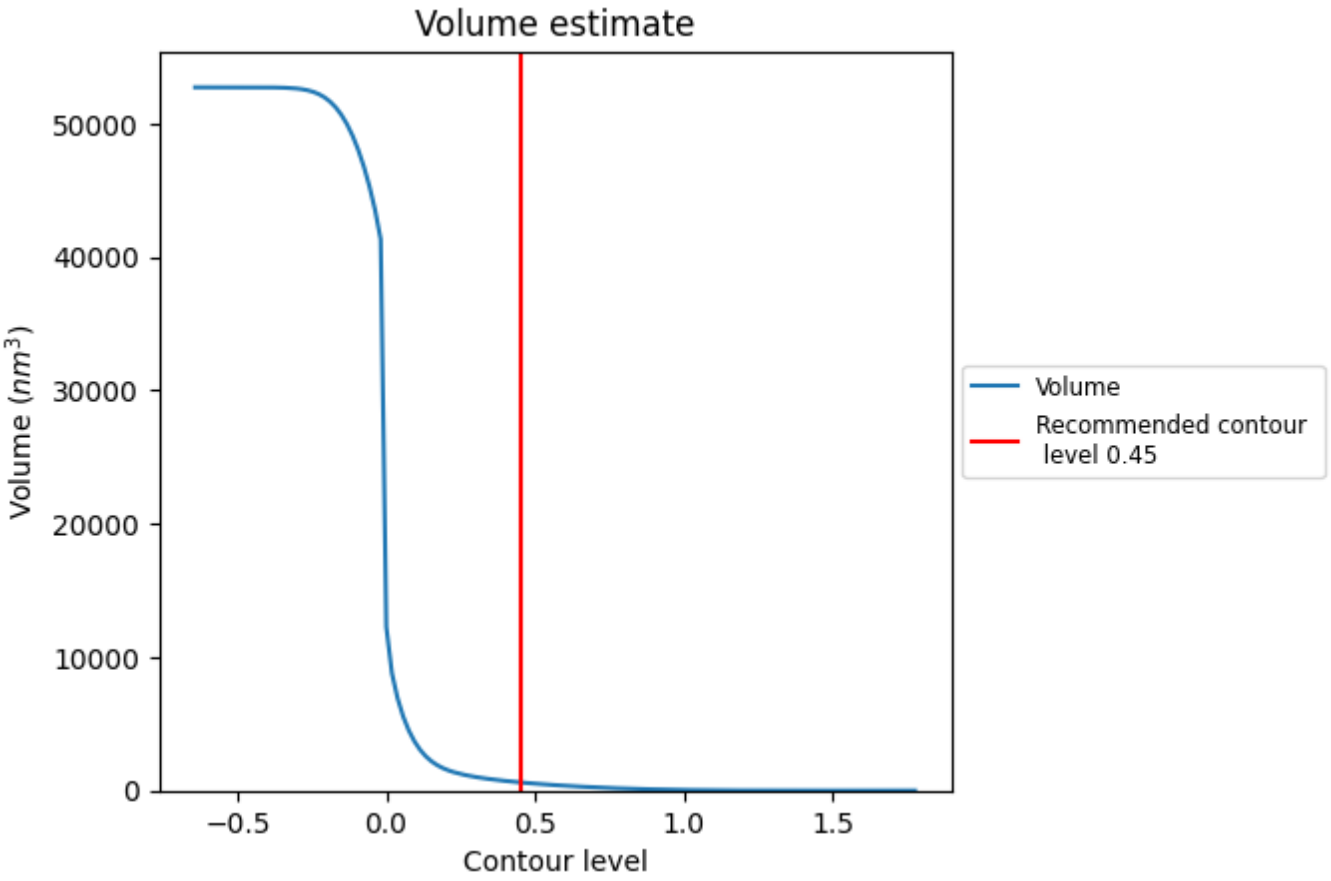
This section contains the results of statistical analysis of the map.

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.

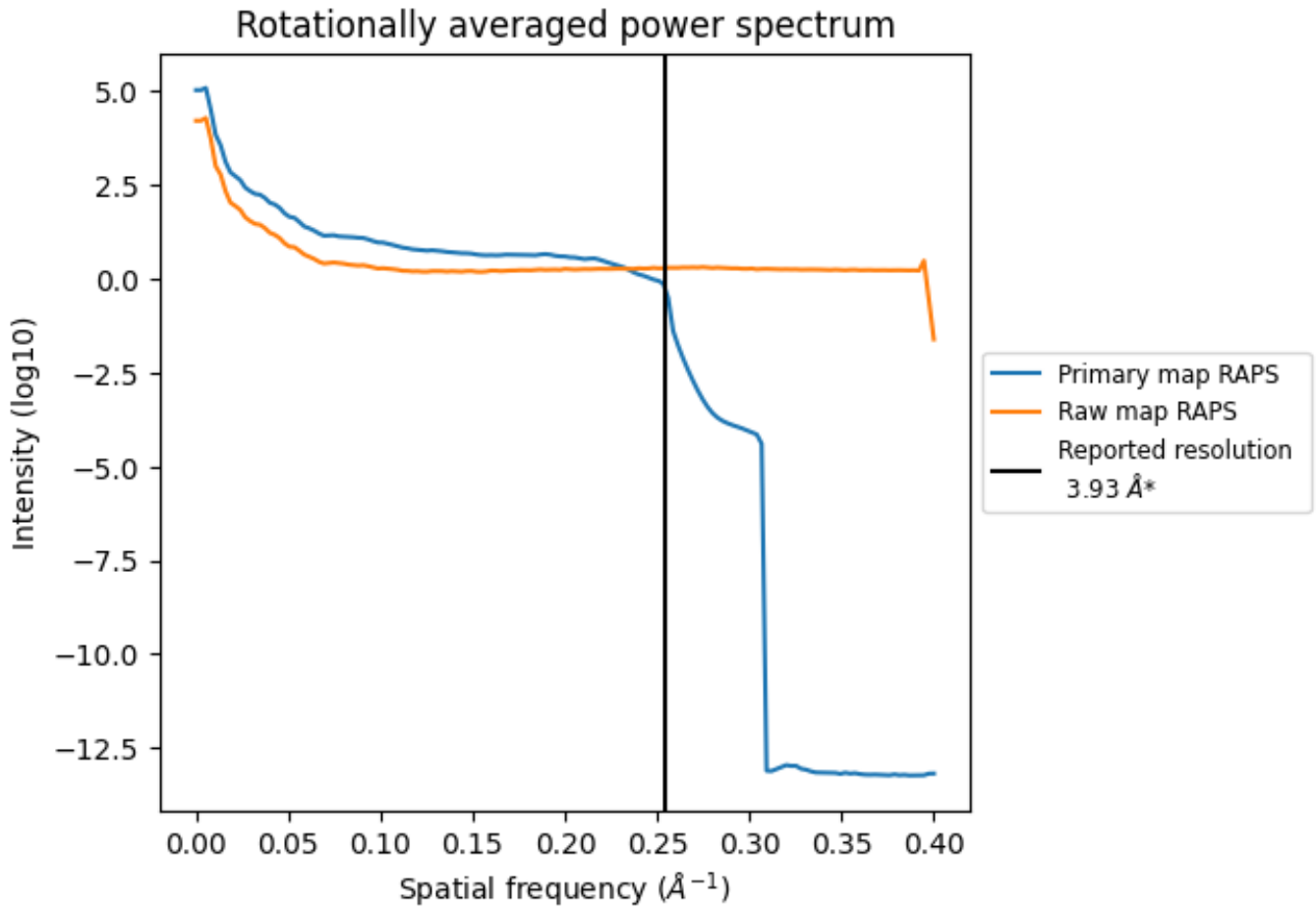
7.2 Volume estimate (i)



The volume at the recommended contour level is 612 nm^3; this corresponds to an approximate mass of 553 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)

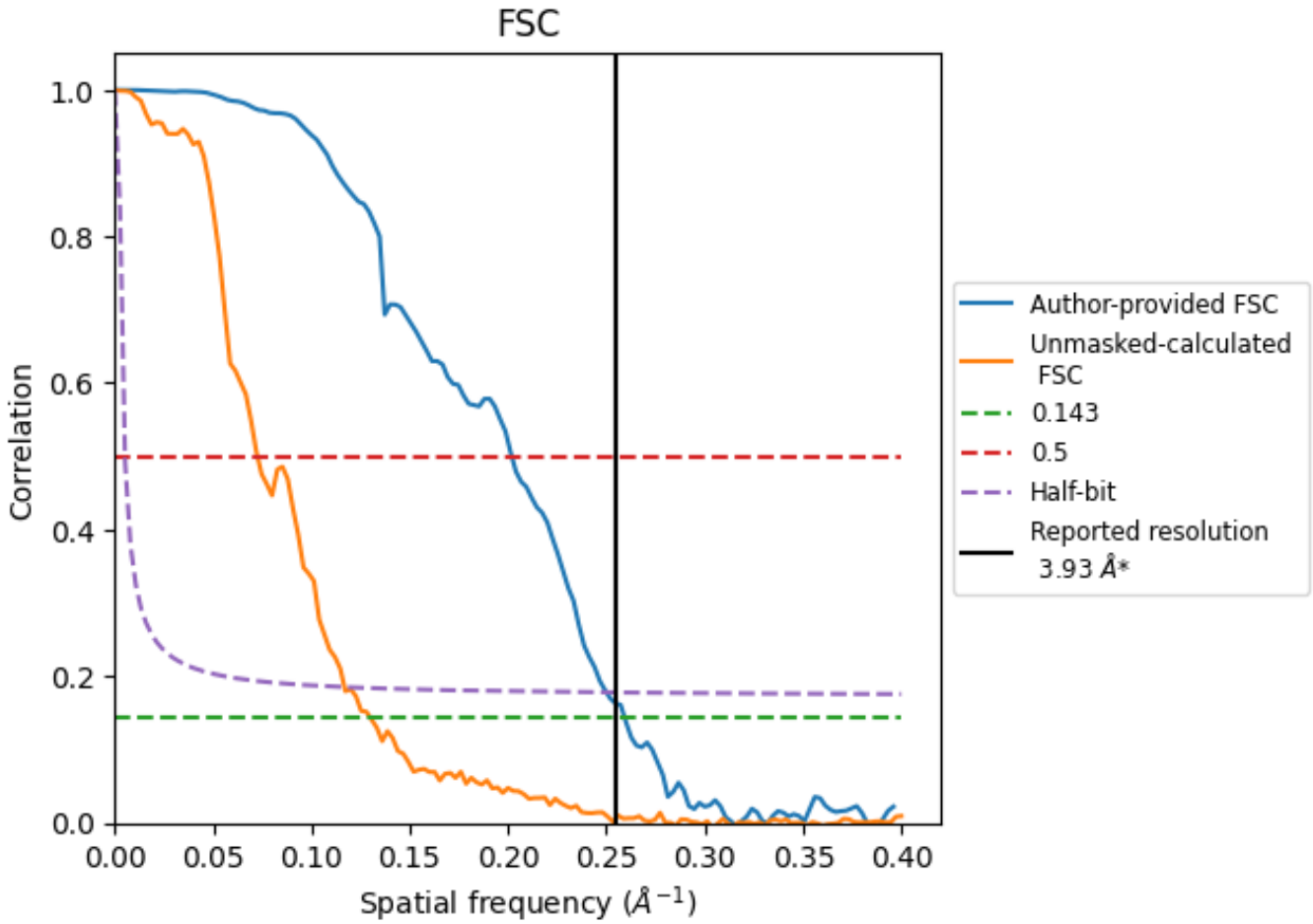


*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

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 0.254 Å^{-1}

8.2 Resolution estimates (i)

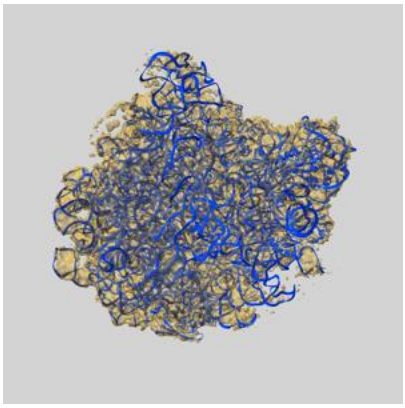
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.86	4.95	4.00
Unmasked-calculated*	7.70	13.77	8.56

*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 7.70 differs from the reported value 3.93 by more than 10 %

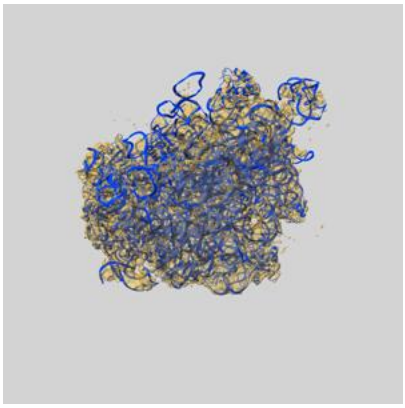
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16494 and PDB model 8C8X. Per-residue inclusion information can be found in section 3 on page 9.

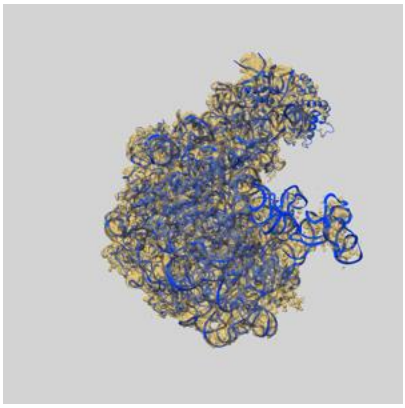
9.1 Map-model overlay



X



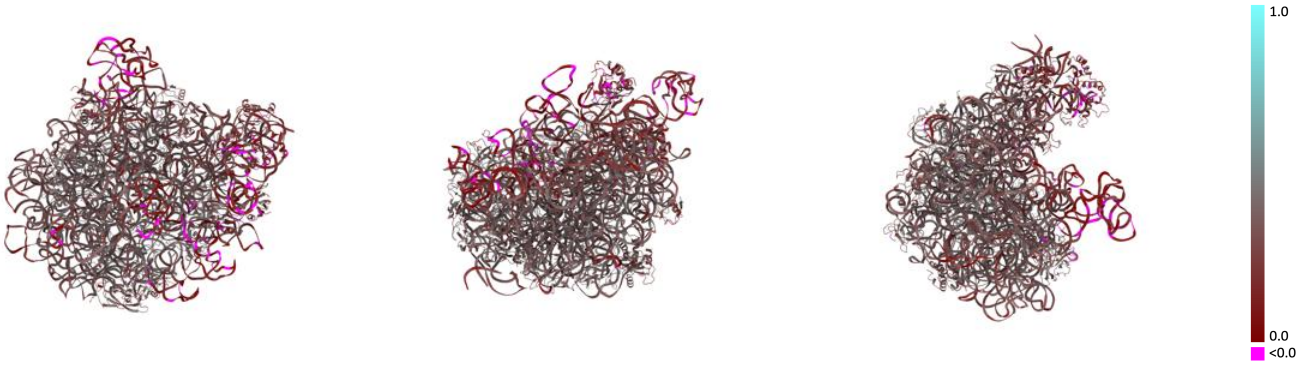
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

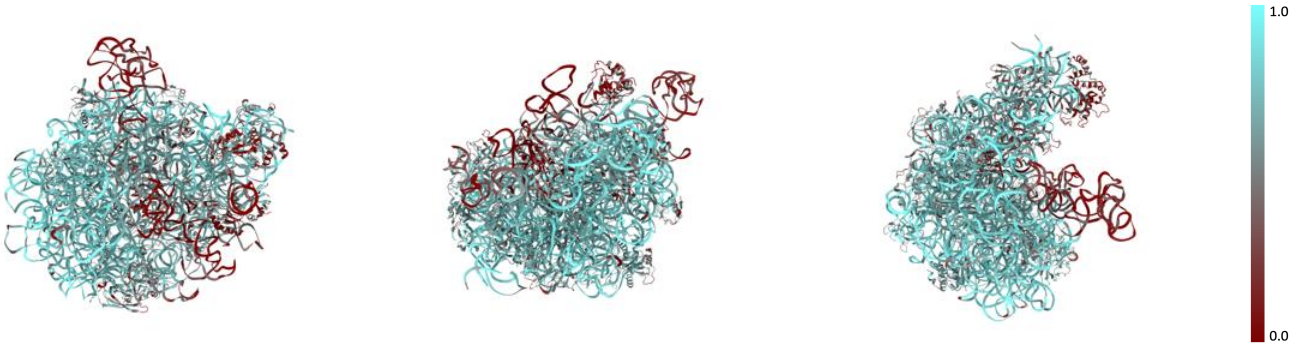
9.2 Q-score mapped to coordinate model (i)



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.

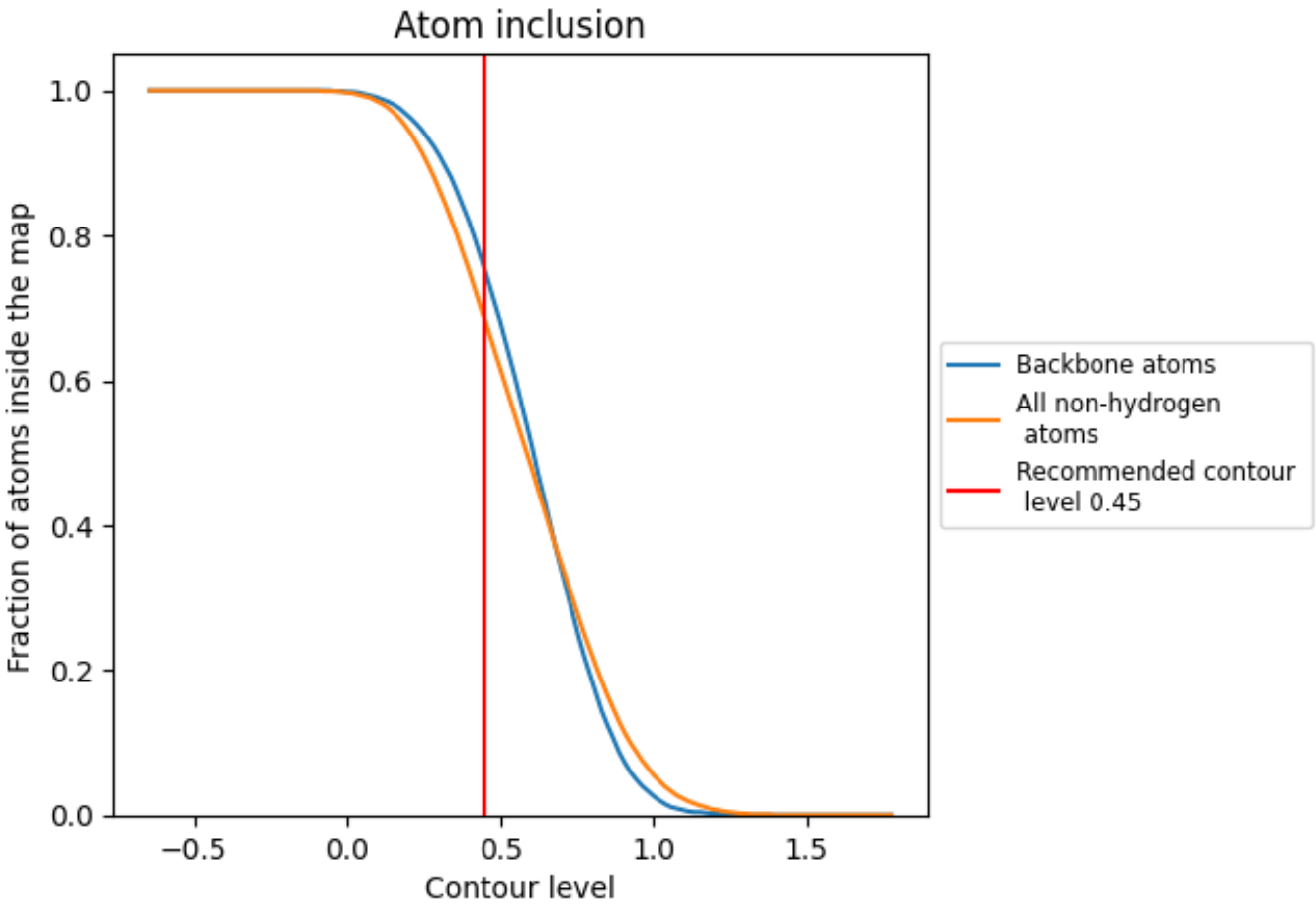
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6840	0.3180
0	0.6010	0.3750
1	0.4440	0.3000
2	0.6170	0.4100
3	0.2810	0.3510
A	0.7340	0.3120
B	0.7880	0.2660
C	0.6840	0.3840
D	0.6120	0.3930
E	0.6010	0.3600
F	0.2100	0.1850
H	0.5040	0.2750
J	0.6050	0.3760
K	0.4480	0.3360
L	0.5170	0.3380
M	0.1380	0.2710
N	0.6590	0.3720
O	0.5660	0.2520
P	0.5630	0.3620
Q	0.6790	0.3820
R	0.5830	0.3690
S	0.5990	0.3980
T	0.6140	0.3620
U	0.6310	0.3460
V	0.5160	0.2910
W	0.5210	0.3400
X	0.5820	0.3750
Y	0.6100	0.3110
Z	0.5930	0.3800