wwPDB EM Validation Summary Report ⓘ

Mar 4, 2024 – 11:22 AM EST

PDB ID	:	5V7Q
EMDB ID	:	EMD-8641
Title	:	Cryo-EM structure of the large ribosomal subunit from Mycobacterium tuberculosis bound with a potent linezolid analog
Authors	:	Yang, K.; Chang, J.-Y.; Cui, Z.; Zhang, J.
Deposited on	:	2017-03-20
Resolution	:	3.70 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:

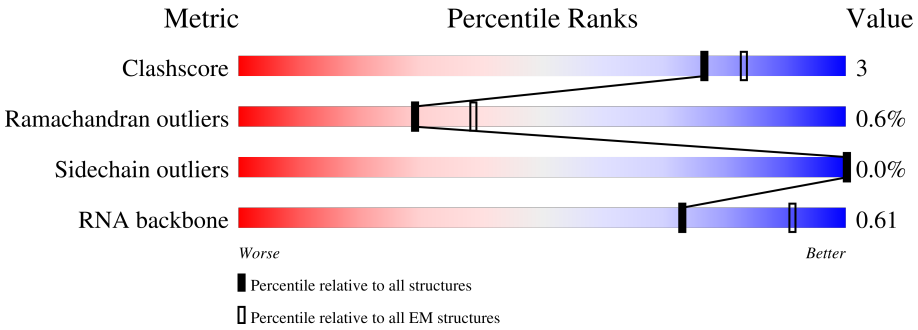
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.70 Å.

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



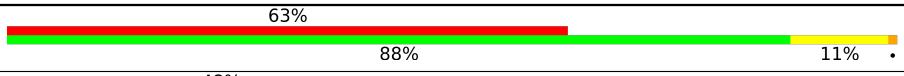
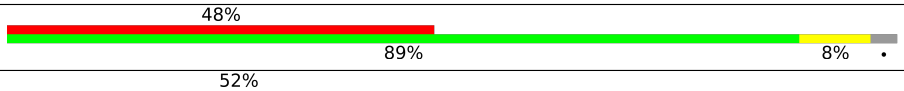
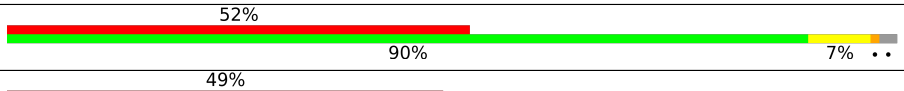
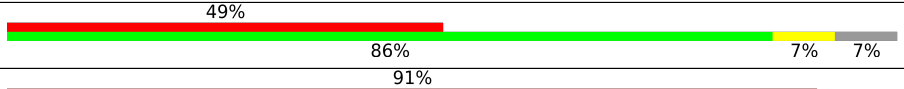
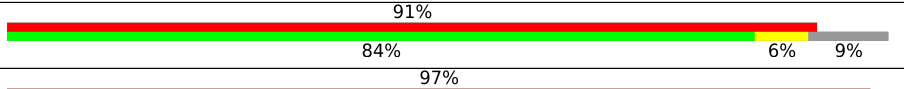
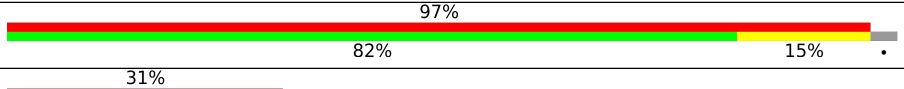
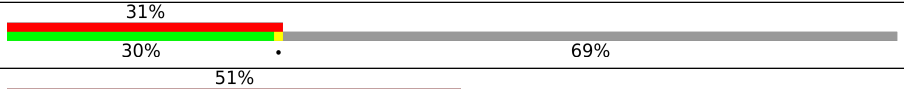
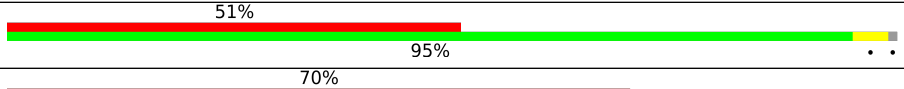
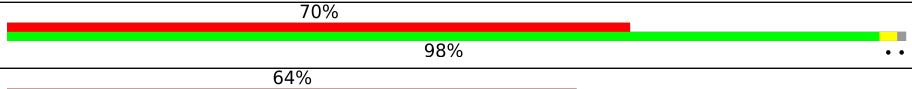
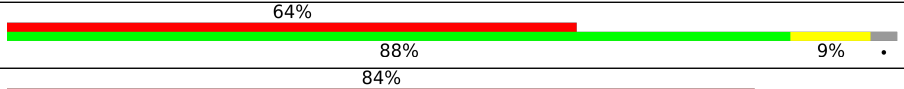
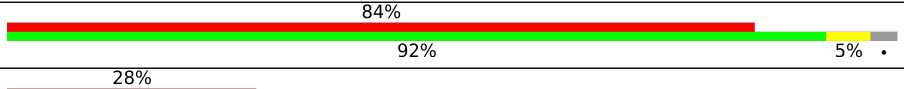
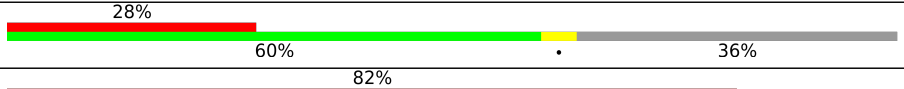
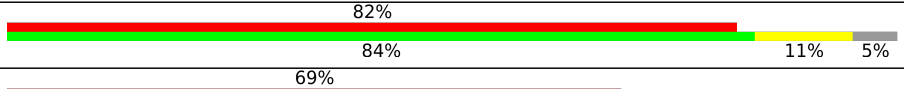
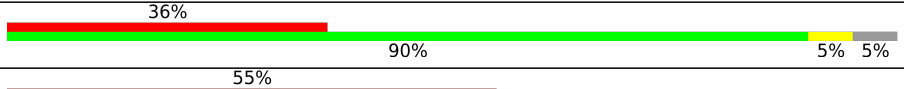
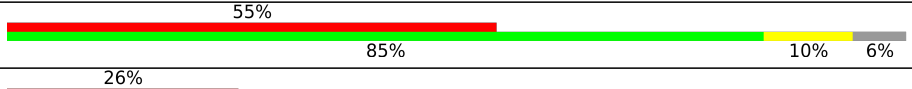
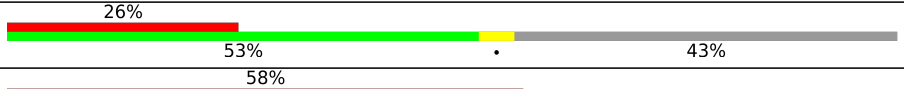
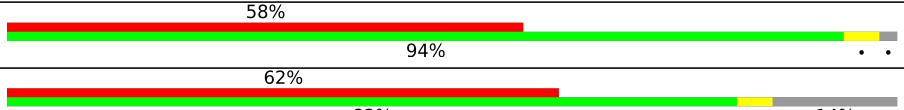
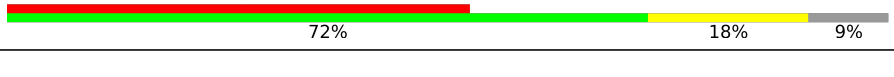
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	57	60%, 86%, 7%, 7%
2	1	55	56%, 82%, 5%, 13%
3	2	47	32%, 79%, 11%, 11%
4	3	64	59%, 86%, 11%, ·
5	4	37	86%, 81%, 19%
6	6	80	56%, 51%, 5%, 44%
7	A	3138	33%, 76%, 20%, · ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	B	115	
9	C	280	
10	D	217	
11	E	223	
12	F	187	
13	G	179	
14	H	152	
15	J	147	
16	K	122	
17	L	146	
18	M	138	
19	N	180	
20	O	122	
21	P	113	
22	Q	129	
23	R	104	
24	S	197	
25	T	100	
26	U	105	
27	V	215	
28	W	86	
29	X	64	
30	Y	77	
31	Z	65	

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 94306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	53	421	262	93	66	0	0

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	48	400	245	84	67	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	42	358	212	94	51	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	3	62	494	298	112	84	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	37	299	182	66	47	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	MET	conflict	UNP A0A1L6JSF4

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	45	Total	C	N	O	S	0	0
			345	214	60	66	5		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	3118	Total	C	N	O	P	0	0
			66956	29845	12340	21653	3118		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	115	Total	C	N	O	P	0	0
			2458	1097	456	790	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2088	1277	437	369	5		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	213	Total	C	N	O	S	0	0
			1590	985	307	292	6		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	207	Total	C	N	O	S	0	0
			1552	958	303	289	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	170	Total	C	N	O	S	0	0
			1335	834	254	242	5		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	174	Total	C	N	O	S	0	0
			1330	836	249	244	1		

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			350	220	64	65	1		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	146	Total	C	N	O	S	0	0
			1143	724	217	199	3		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	121	Total	C	N	O	S	0	0
			934	585	179	168	2		

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	142	Total	C	N	O	S	0	0
			1060	656	215	187	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	VAL	MET	conflict	UNP A0A0T7M0A0

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1072	679	215	177	1		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	116	Total 908	C 574	N 175	O 158	S 1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	O	116	Total 886	C 541	N 188	O 157	0	0

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	112	Total 907	C 573	N 174	O 159	S 1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Q	122	Total 980	C 608	N 205	O 167	0	0

- Molecule 23 is a protein called LSU ribosomal protein L21p.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	98	Total 742	C 472	N 136	O 134	0	0

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	S	113	Total 860	C 533	N 178	O 149	0	0

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	T	98	Total 759	C 480	N 141	O 138	0	0

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	90	Total	C	N	O	S	0	0
			699	430	138	129	2		

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	V	177	Total	C	N	O	0	0
			1319	822	243	254		

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	W	74	Total	C	N	O	0	0
			546	336	111	99		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	S	0	0
			476	289	101	81	5		

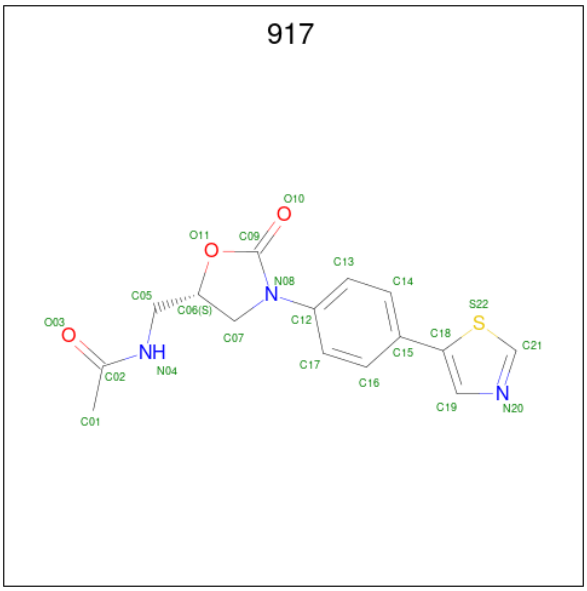
- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	65	Total	C	N	O	S	0	0
			541	331	106	103	1		

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	59	Total	C	N	O	0	0
			476	293	101	82		

- Molecule 32 is N-({(5S)-2-oxo-3-[4-(1,3-thiazol-5-yl)phenyl]-1,3-oxazolidin-5-yl}methyl)acetamide (three-letter code: 917) (formula: $C_{15}H_{15}N_3O_3S$).



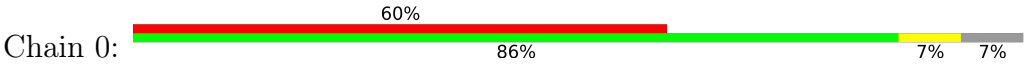
Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	N	O	S	0
			22	15	3	3	1	

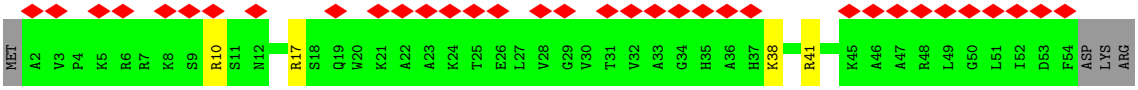
3 Residue-property plots (i)

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 L32

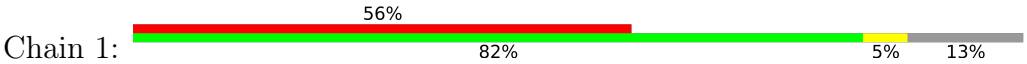
Chain 0:

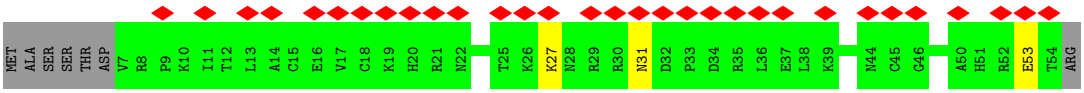




• Molecule 2: 50S ribosomal protein L33

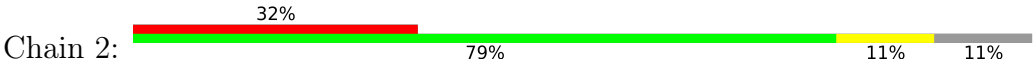
Chain 1:

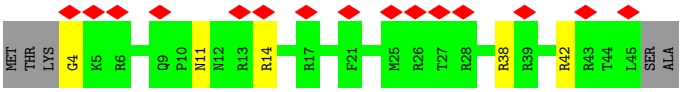




• Molecule 3: 50S ribosomal protein L34

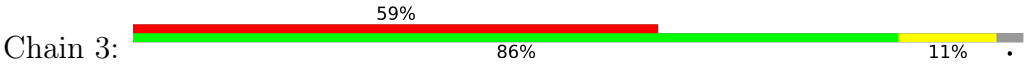
Chain 2:

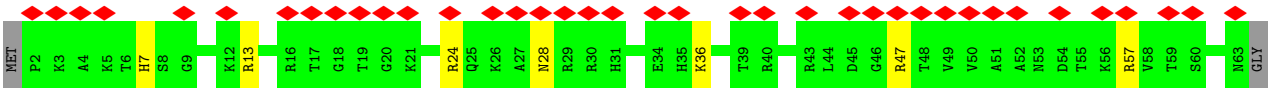




• Molecule 4: 50S ribosomal protein L35

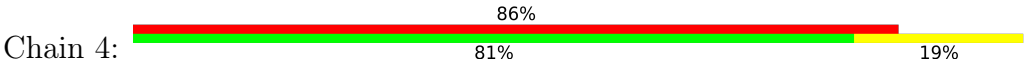
Chain 3:

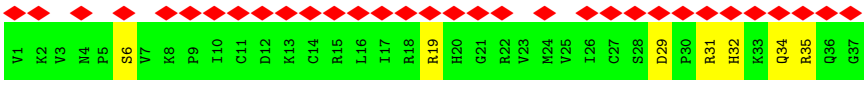




• Molecule 5: 50S ribosomal protein L36

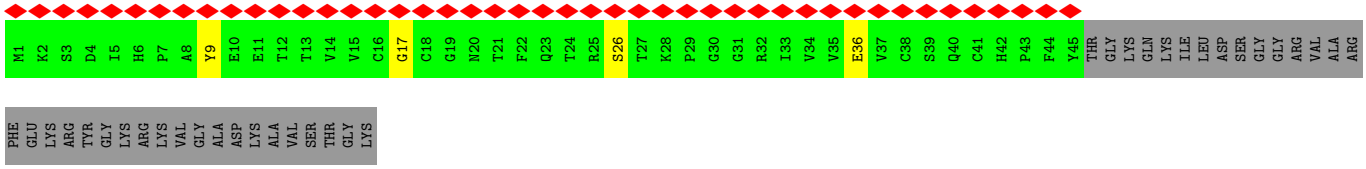
Chain 4:





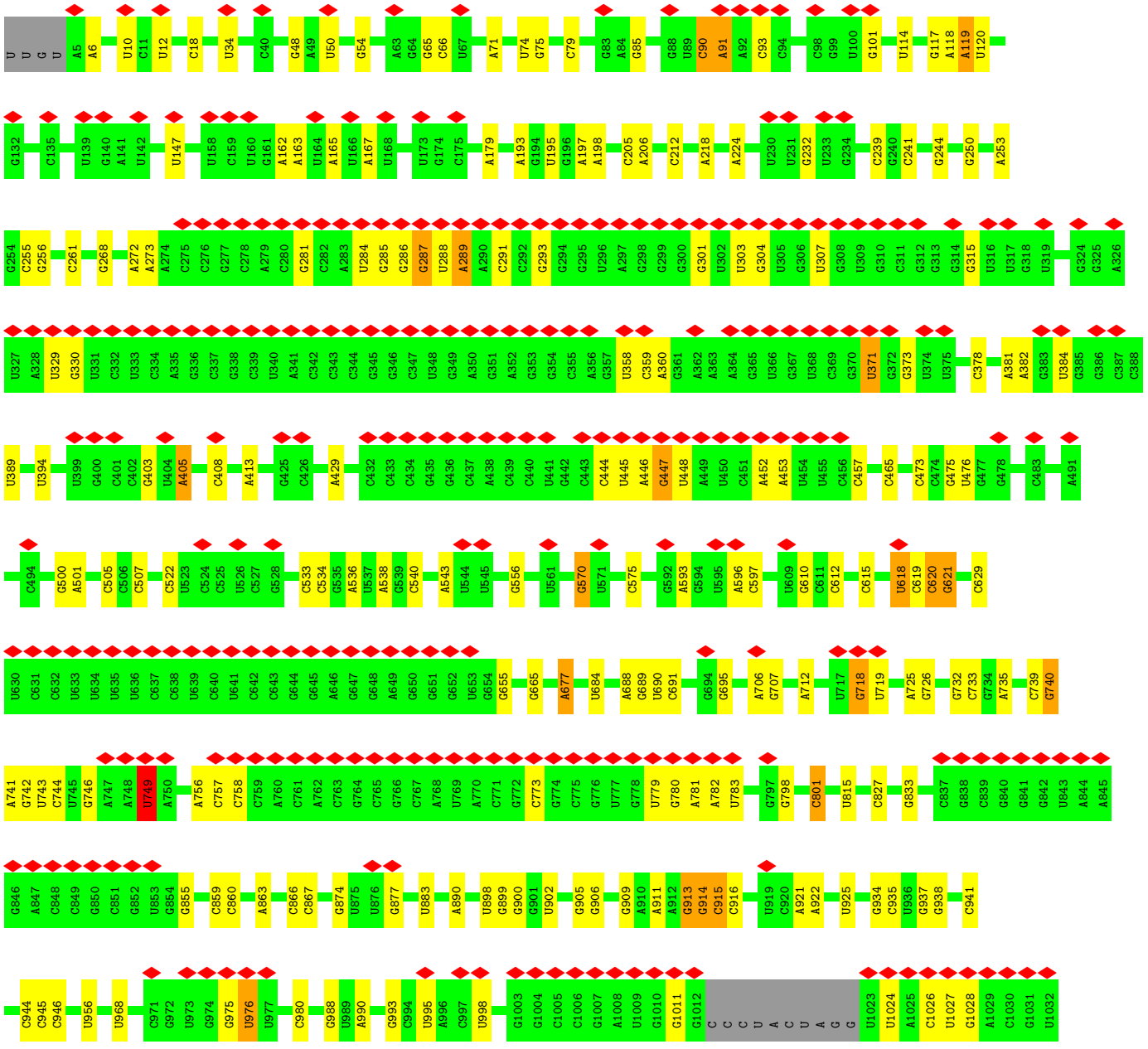
• Molecule 6: 50S ribosomal protein L31

Chain 6:

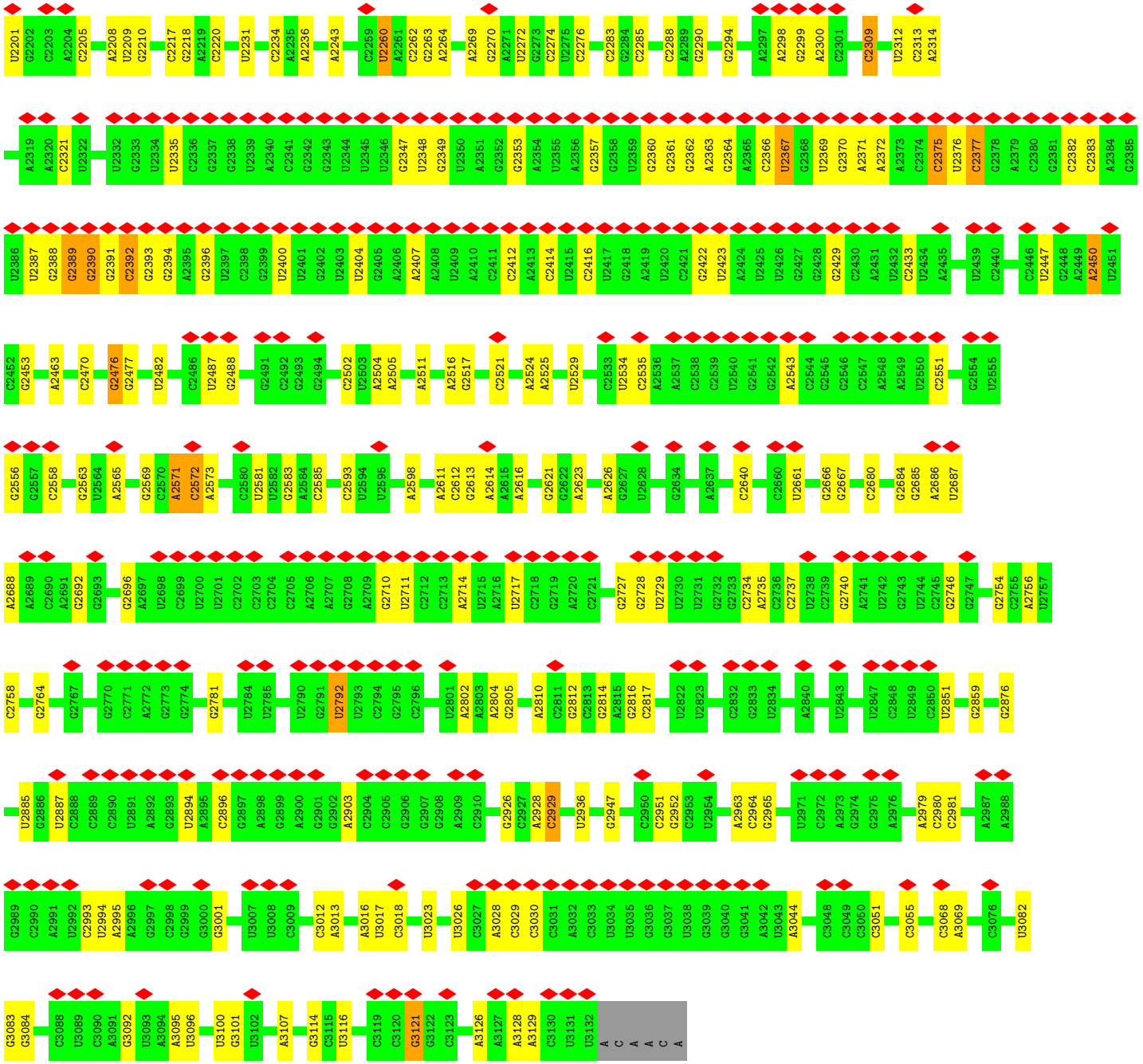


• Molecule 7: 23S rRNA

Chain A:

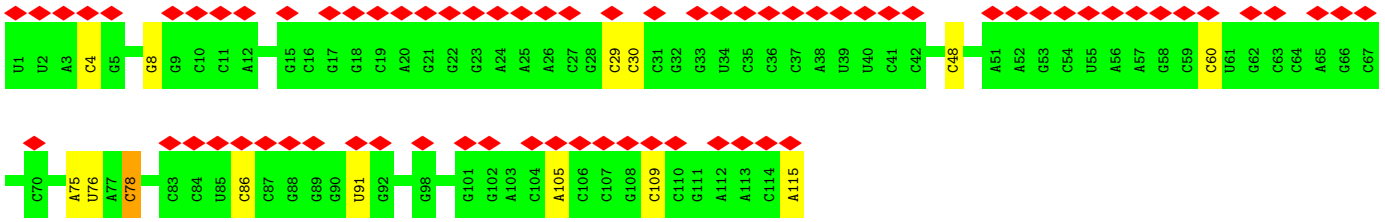



C1033 A1034 G1035 A1039 C1043 C1044 G1045 A1046 G1049 G1057 U1058 A1059 A1060 A1061 G1062 C1063 G1064 C1068 G1074 A1075 C1076 G1080 G1081 U1086 A1087 A1088 G1089 G1094 U1095 A1096 C1097 C1100 G1101 A1102 A1103 C1114 A1119 G1122 C1136 C1141 G1142 U1145 G1146 C1147
U1148 A1149 A1150 G1151 U1152 G1153 G1154 G1155 A1161 U1162 G1163 U1164 G1165 C1166 A1167 G1168 U1169 C1170 G1171 C1172 A1173 A1174 A1175 G1176 A1177 C1178 A1179 A1180 C1181 C1182 A1183 G1184 G1185 A1186 G1187 G1188 U1189 U1190 G1191 G1192 C1193 U1194 U1195 A1196 G1197 A1198 A1199 G1200 C1201 A1202 G1203 C1204 C1205 A1206 C1207 C1208 C1209 U1210 U1211
G1212 A1213 A1214 A1215 G1216 A1217 G1218 U1219 G1220 C1221 G1222 U1223 A1224 A1225 U1226 A1227 G1228 C1229 U1230 C1231 A1232 C1233 U1234 G1235 G1236 U1237 C1238 A1239 A1240 G1241 U1242 G1243 A1244 U1245 U1246 G1247 U1248 G1249 U1256 A1257 A1258 A1262 G1263 C1264 C1269 U1270 C1271 A1272 A1273 C1277 A1278 C1283 G1287
U1298 C1299 C1300 A1301 C1302 C1303 U1304 U1305 G1306 U1307 G1308 G1309 U1310 G1311 G1312 G1313 U1314 G1323 C1333 U1334 U1338 C1342 G1343 G1354 A1357 G1367 G1381 U1386 G1387 A1393 U1394 G1397 A1403 C1404 U1422 G1423 C1426 G1427 A1432 C1437 U1444 C1445
C1452 A1453 U1460 C1461 C1462 G1463 U1471 A1480 C1481 G1486 G1487 C1488 G1492 G1495 A1496 C1497 A1498 G1499 G1500 A1509 U1510 C1514 A1515 A1516 C1517 G1518 U1522 A1526 U1527 U1528 C1529 C1530 C1531 C1537 G1538 U1539 G1540 U1541 G1542 U1543 G1544 G1545 G1546 C1547 G1548 C1549 C1550 C1551 G1552
U1553 G1554 A1555 C1556 G1557 A1558 A1559 U1560 C1561 A1562 G1563 C1564 G1565 G1566 U1567 A1568 C1569 U1570 A1571 A1572 C1573 C1574 A1575 C1576 C1577 C1578 A1579 A1580 A1581 A1582 C1583 C1584 G1585 G1586 A1587 U1588 C1589 G1590 A1591 U1592 C1593 A1594 C1595 U1596 C1597 C1598 C1599 C1600 U1601 U1602 C1603 G1604 G1605 G1606 G1607 G1608 U1609 G1610 U1611 G1612
G1613 A1614 G1615 U1616 U1617 C1618 U1619 G1620 G1621 G1622 G1623 C1624 U1625 G1626 C1627 G1628 U1629 G1630 G1631 G1632 A1633 A1634 C1635 U1636 U1637 C1638 G1639 C1640 U1641 G1642 G1643 U1644 A1645 G1646 U1647 A1648 G1649 U1650 C1651 A1652 A1653 G1654 C1655 G1656 A1657 A1658 G1659 U1663 C1666 G1670 G1671 A1672 A1673 G1678 U1682
A1683 C1689 A1690 G1691 U1692 U1695 A1696 A1697 C1698 A1699 G1705 C1706 A1707 C1711 G1712 G1713 U1714 A1715 G1716 G1717 C1718 A1719 G1720 A1721 G1722 C1723 G1724 A1725 U1726 A1727 C1730 A1731 A1732 A1733 U1734 C1739 G1740 C1741 U1742 C1743 A1744 C1745 U1746 A1747 A1748 U1749 C1750 C1751 U1752 G1753 G1758 U1759 G1760
A1761 C1762 G1763 U1766 A1767 G1768 C1769 C1770 G1771 G1772 U1773 U1774 G1775 A1776 G1777 G1778 C1779 U1784 U1791 C1795 U1796 G1797 A1803 A1807 C1812 U1815 A1816 G1817 C1818 G1819 A1820 G1821 C1822 A1823 C1824 A1825 C1826 A1827 C1828 A1829 C1830 G1831 G1832 C1842 A1843 A1844 A1845 A1851 C1852 A1853
U1856 U1859 C1860 A1861 C1873 U1881 A1882 C1883 U1888 A1889 A1890 A1903 A1904 C1905 G1908 G1909 G1916 C1917 C1918 C1919 C1920 C1921 A1924 U1927 U1928 C1929 G1930 G1934 G1937 G1938 G1939 A1947 A1948 U1949 A1950 U1951 C1952 G1953 U1954 C1958 A1959 C1960 C1961 C1962 U1963 U1964
G1965 C1966 G1967 G1968 U1969 G1970 G1971 G1972 A1973 G1974 C1975 G1976 G1977 G1978 A1979 U1980 C1981 C1982 U1985 A1991 A1992 G1997 U1998 A2007 C2008 U2009 G2010 U2011 U2012 U2013 A2014 C2015 U2016 A2017 A2018 A2019 A2020 A2021 C2022 A2023 C2024 A2025 C2030 G2031 U2032 G2033 C2034 G2035 C2040 G2041 C2042 A2043 U2050
G2061 G2062 C2067 G2074 U2075 G2076 C2077 U2078 G2079 G2080 A2081 A2082 G2083 G2084 U2085 U2086 A2090 G2091 G2092 A2093 C2094 C2095 C2096 U2099 A2100 A2101 C2102 C2103 C2104 G2105 C2106 A2107 A2108 G2109 G2110 G2111 U2112 G2113 A2114 A2115 G2116 A2120 G2121 A2122 A2123 U2124 U2125 U2126 C2130 C2131 C2132 C2133 A2134
G2135 U2136 A2139 G2144 G2145 U2146 G2147 G2148 U2149 A2150 A2151 C2152 U2153 A2154 U2155 A2156 A2157 C2158 C2159 A2160 U2161 C2162 C2163 U2164 G2167 C2168 U2169 A2170 C2171 C2172 G2173 A2174 A2175 A2176 U2177 U2178 C2179 C2180 U2181 U2182 G2183 U2184 C2185 G2186 G2187 G2188 U2189 A2190 A2191 C2192 U2193 U2194 G2197 A2198 C2199 C2200



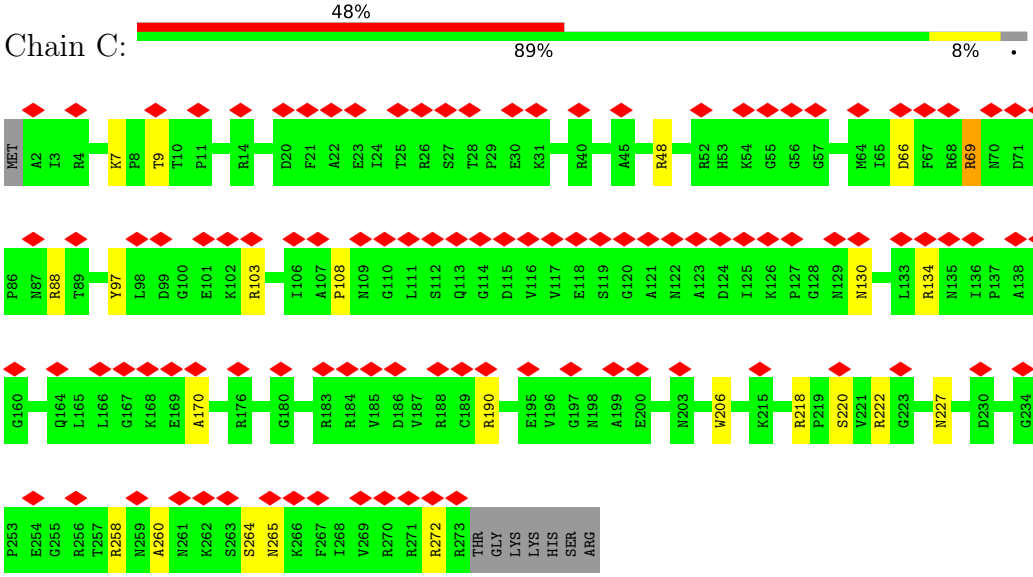
• Molecule 8: 5S ribosomal RNA

Chain B:



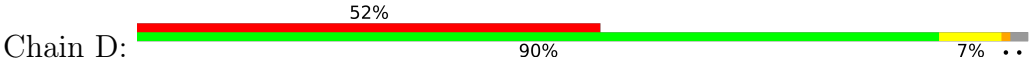
• Molecule 9: 50S ribosomal protein L2

Chain C:



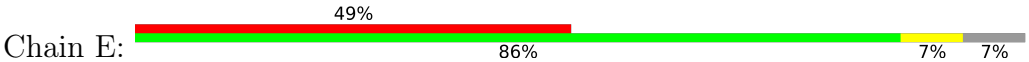
• Molecule 10: 50S ribosomal protein L3

Chain D:



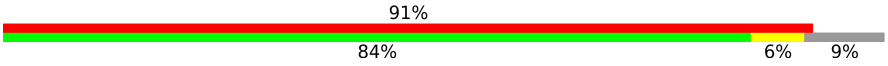
• Molecule 11: 50S ribosomal protein L4

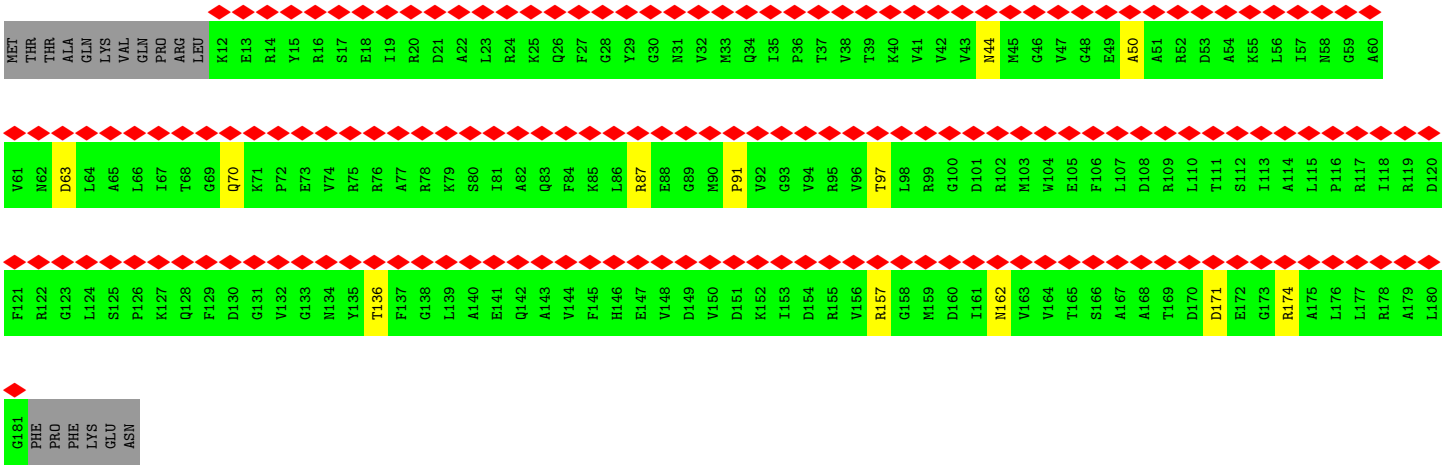
Chain E:



• Molecule 12: 50S ribosomal protein L5

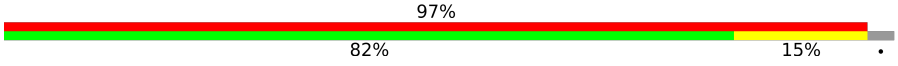
Chain F:

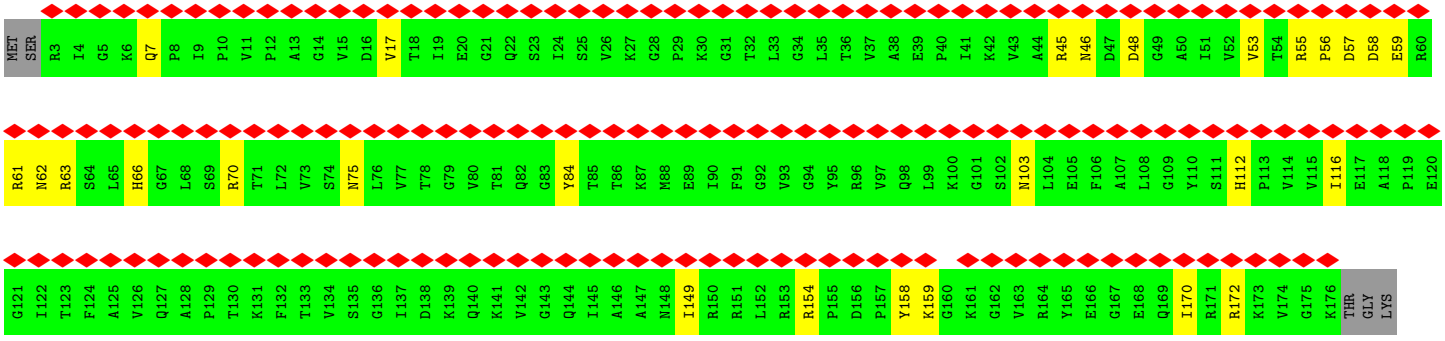




• Molecule 13: 50S ribosomal protein L6

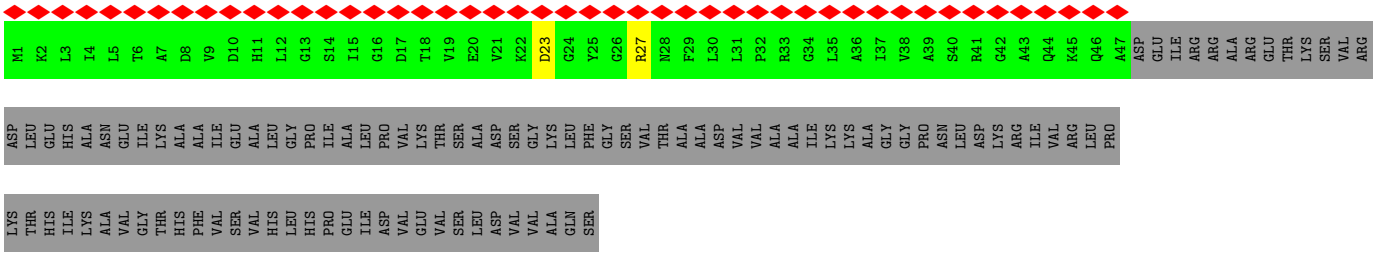
Chain G:





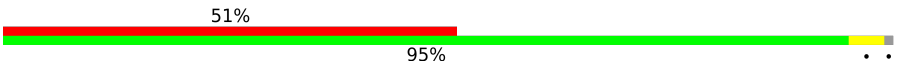
• Molecule 14: 50S ribosomal protein L9

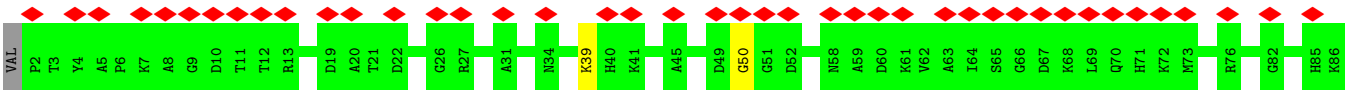
Chain H:

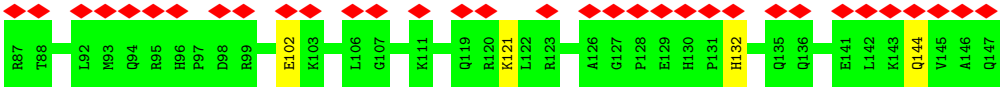


• Molecule 15: 50S ribosomal protein L13

Chain J:

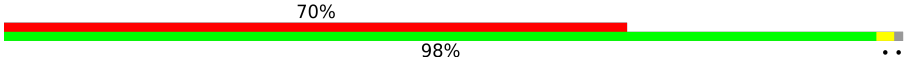


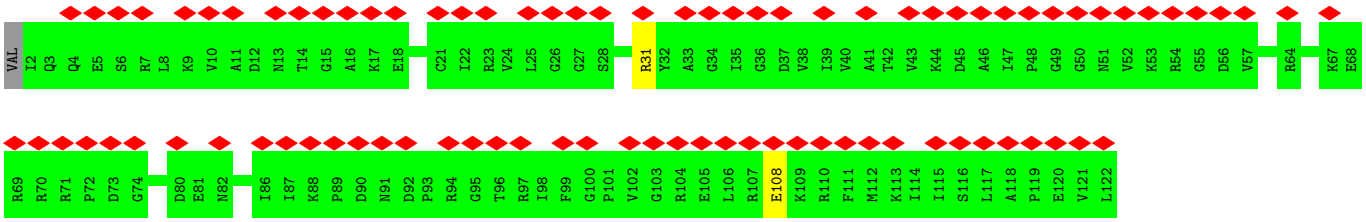




• Molecule 16: 50S ribosomal protein L14

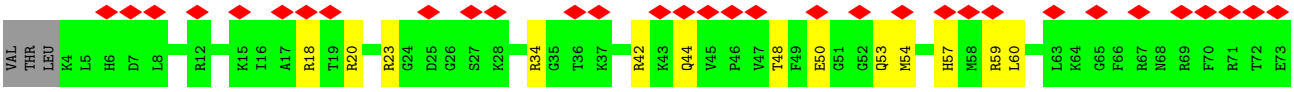
Chain K:

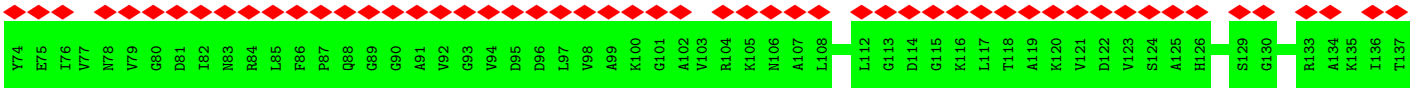


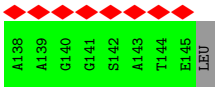


• Molecule 17: 50S ribosomal protein L15

Chain L:

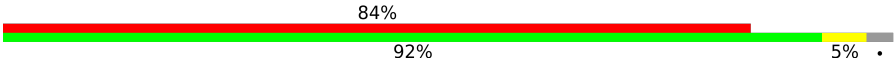


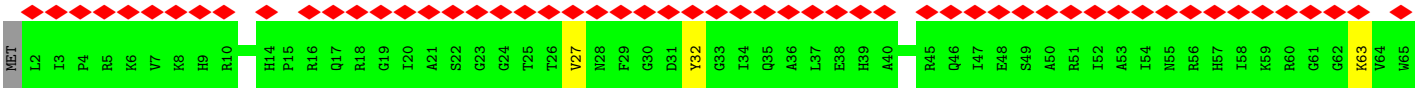


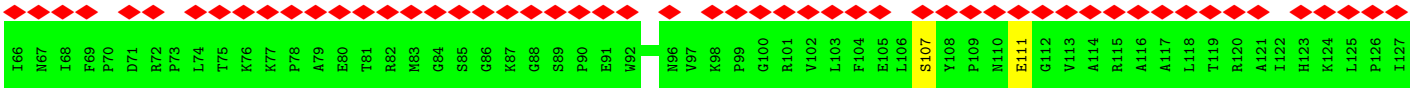


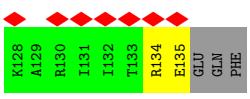
• Molecule 18: 50S ribosomal protein L16

Chain M:



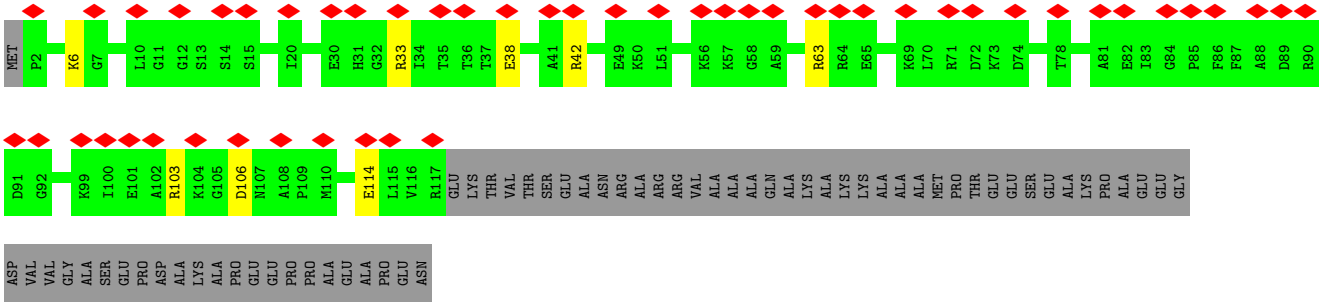






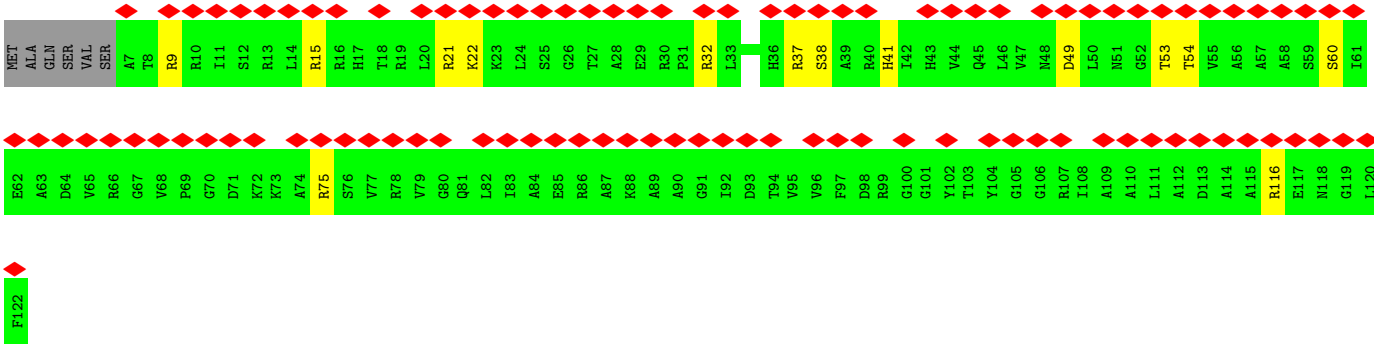
• Molecule 19: 50S ribosomal protein L17

Chain N:



• Molecule 20: 50S ribosomal protein L18

Chain O:

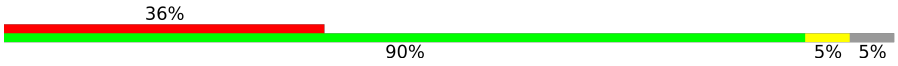


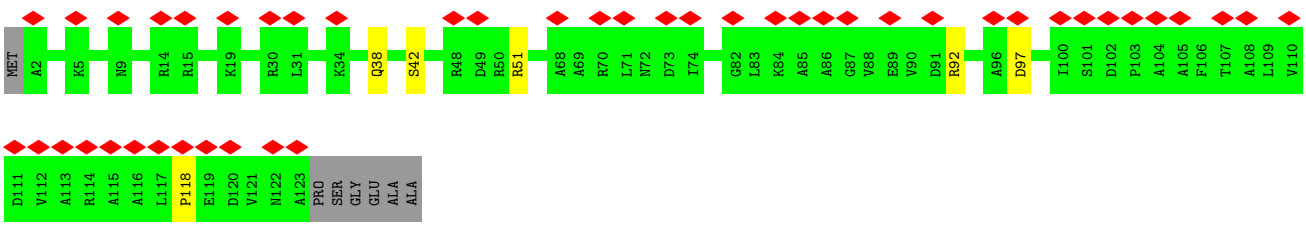
• Molecule 21: 50S ribosomal protein L19

Chain P:

• Molecule 22: 50S ribosomal protein L20

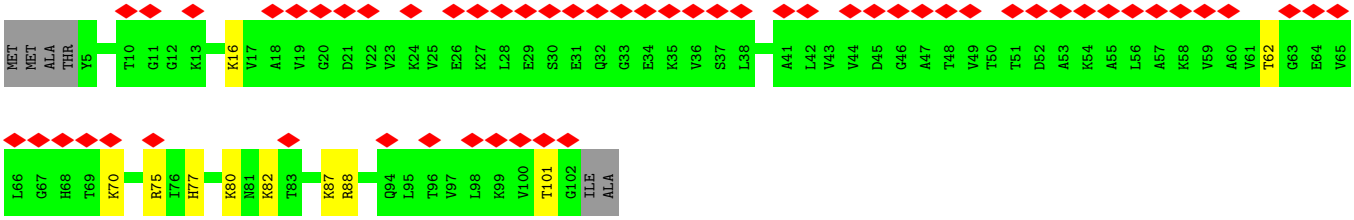
Chain Q:





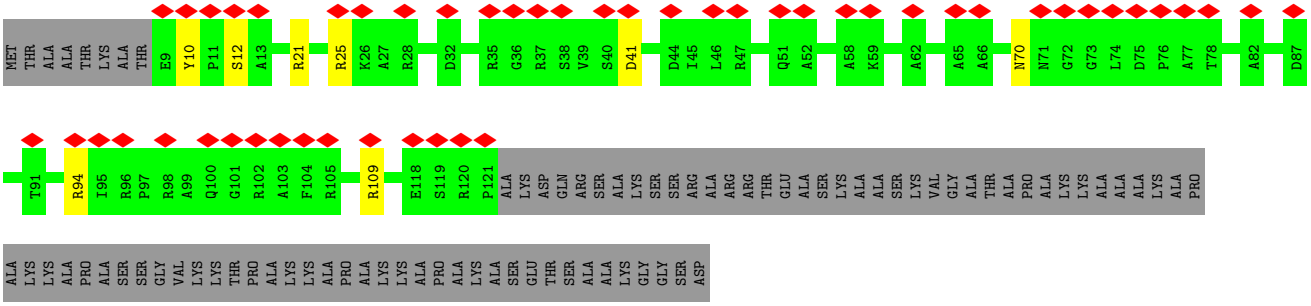
• Molecule 23: LSU ribosomal protein L21p

Chain R:



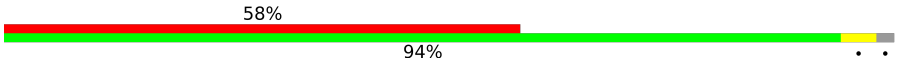
• Molecule 24: 50S ribosomal protein L22

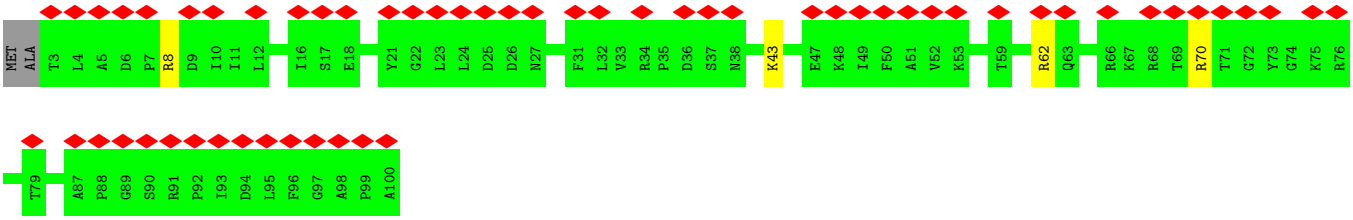
Chain S:



• Molecule 25: 50S ribosomal protein L23

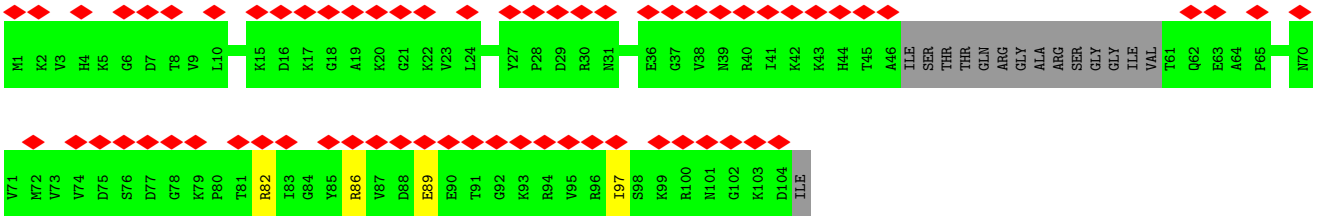
Chain T:





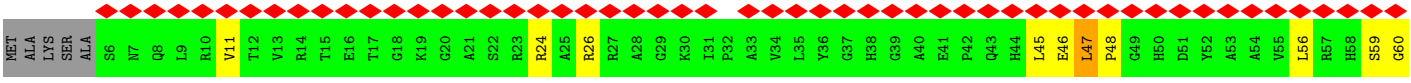
• Molecule 26: 50S ribosomal protein L24

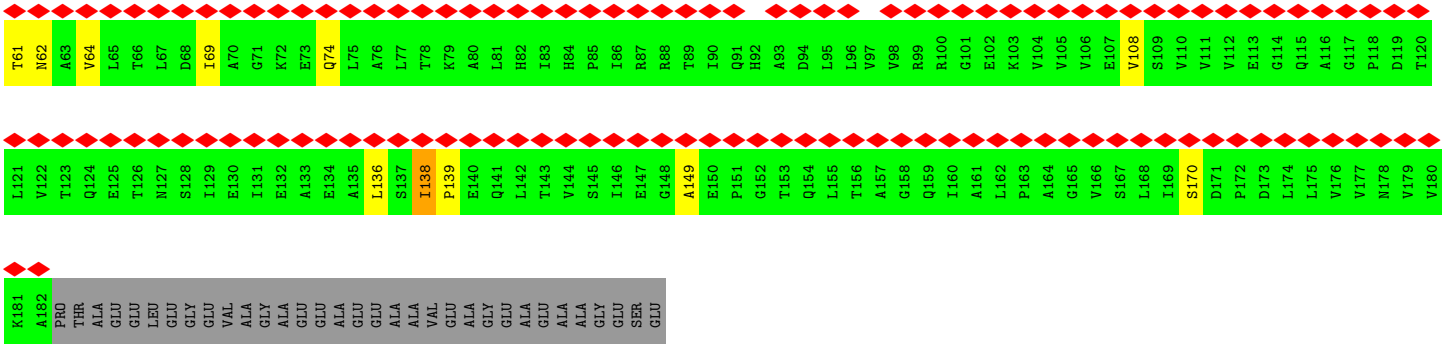
Chain U:



• Molecule 27: 50S ribosomal protein L25

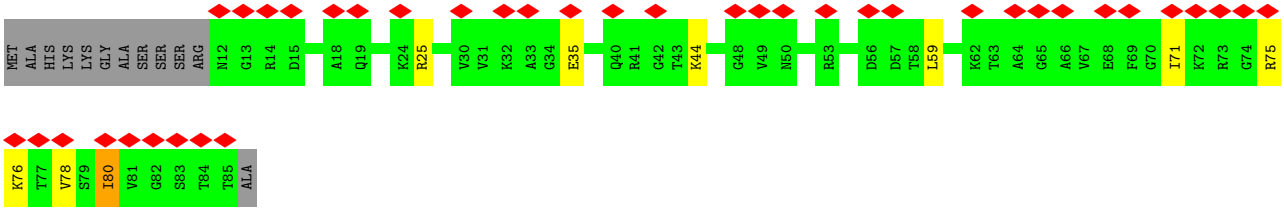
Chain V:





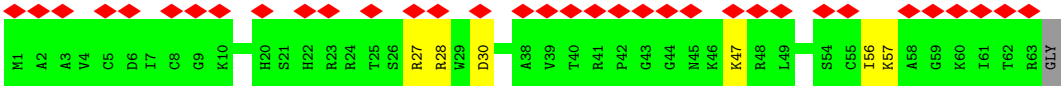
• Molecule 28: 50S ribosomal protein L27

Chain W:



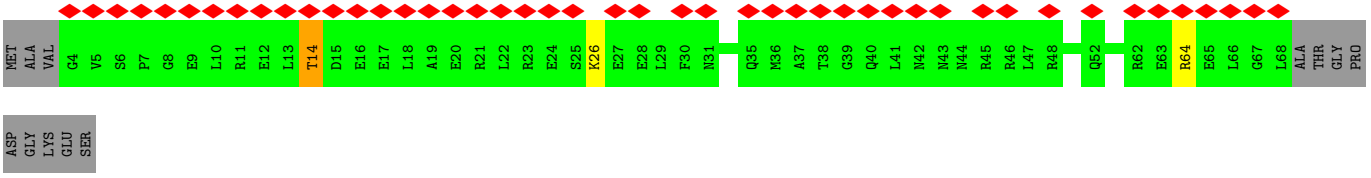
• Molecule 29: 50S ribosomal protein L28

Chain X:



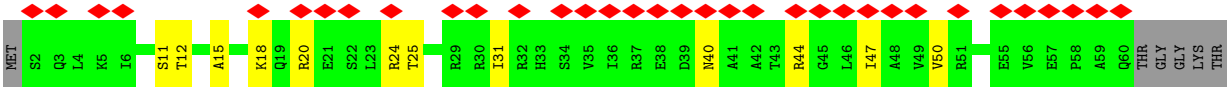
• Molecule 30: 50S ribosomal protein L29

Chain Y:



• Molecule 31: 50S ribosomal protein L30

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.37	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	0.307	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	298.47998, 298.47998, 298.47998	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.435, 1.435, 1.435	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 917

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.40	0/427	0.66	0/570
2	1	0.41	0/407	0.64	0/543
3	2	0.54	0/361	0.78	0/473
4	3	0.43	0/499	0.68	0/664
5	4	0.37	0/303	0.74	0/402
6	6	0.31	0/353	0.56	0/478
7	A	0.72	2/74973 (0.0%)	1.10	219/116979 (0.2%)
8	B	0.54	0/2749	1.02	7/4284 (0.2%)
9	C	0.42	0/2129	0.69	1/2861 (0.0%)
10	D	0.43	1/1613 (0.1%)	0.68	0/2174
11	E	0.41	0/1575	0.63	0/2129
12	F	0.31	0/1352	0.67	0/1817
13	G	0.31	0/1351	0.58	0/1824
14	H	0.32	0/353	0.58	0/474
15	J	0.43	0/1170	0.67	0/1584
16	K	0.40	0/944	0.67	0/1268
17	L	0.40	0/1073	0.67	0/1432
18	M	0.36	0/1098	0.62	0/1481
19	N	0.42	0/925	0.64	0/1242
20	O	0.35	0/895	0.69	0/1202
21	P	0.37	0/922	0.59	0/1236
22	Q	0.47	0/992	0.68	0/1329
23	R	0.42	0/751	0.61	0/1009
24	S	0.42	0/874	0.68	0/1186
25	T	0.37	0/770	0.67	0/1038
26	U	0.33	0/705	0.53	0/941
27	V	0.27	0/1336	0.57	0/1820
28	W	0.40	0/551	0.69	0/735
29	X	0.52	0/484	0.73	0/648
30	Y	0.37	0/544	0.65	0/727
31	Z	0.39	0/480	0.71	0/645
All	All	0.65	3/102959 (0.0%)	1.01	227/155195 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	146	ARG	C-N	5.43	1.46	1.34
7	A	1658	A	N9-C4	5.22	1.41	1.37
7	A	1816	A	N7-C5	-5.04	1.36	1.39

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	507	C	N3-C4-N4	9.97	124.98	118.00
7	A	507	C	C5-C4-N4	-9.80	113.34	120.20
7	A	866	C	N3-C4-N4	9.44	124.61	118.00
7	A	946	C	N3-C2-O2	-9.28	115.41	121.90
7	A	3012	C	N3-C4-N4	9.28	124.49	118.00

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	0	421	0	461	4	0
2	1	400	0	413	3	0
3	2	358	0	390	5	0
4	3	494	0	533	7	0
5	4	299	0	326	5	0
6	6	345	0	332	2	0
7	A	66956	0	33720	280	0
8	B	2458	0	1253	10	0
9	C	2088	0	2123	21	0
10	D	1590	0	1633	12	0
11	E	1552	0	1593	12	0
12	F	1335	0	1372	7	0
13	G	1330	0	1390	16	0
14	H	350	0	367	2	0
15	J	1143	0	1173	5	0
16	K	934	0	993	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1060	0	1119	12	0
18	M	1072	0	1115	4	0
19	N	908	0	956	5	0
20	O	886	0	924	11	0
21	P	907	0	947	7	0
22	Q	980	0	1028	5	0
23	R	742	0	799	8	0
24	S	860	0	903	7	0
25	T	759	0	809	4	0
26	U	699	0	738	2	0
27	V	1319	0	1365	13	0
28	W	546	0	567	5	0
29	X	476	0	496	4	0
30	Y	541	0	551	2	0
31	Z	476	0	509	8	0
32	A	22	0	0	0	0
All	All	94306	0	60898	391	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 3.

The worst 5 of 391 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)
7:A:1557:G:N3	7:A:1648:A:N6	2.10	0.97
13:G:103:ASN:ND2	13:G:116:ILE:O	2.10	0.84
7:A:1731:A:C2	7:A:1816:A:O2'	2.31	0.83
7:A:1627:C:N3	9:C:134:ARG:NH2	2.30	0.78
7:A:2746:G:O2'	7:A:2792:U:O2'	2.02	0.78

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	0	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
2	1	46/55 (84%)	41 (89%)	5 (11%)	0	100	100
3	2	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
4	3	60/64 (94%)	53 (88%)	7 (12%)	0	100	100
5	4	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
6	6	43/80 (54%)	36 (84%)	7 (16%)	0	100	100
9	C	270/280 (96%)	240 (89%)	29 (11%)	1 (0%)	34	69
10	D	211/217 (97%)	186 (88%)	22 (10%)	3 (1%)	11	45
11	E	205/223 (92%)	176 (86%)	29 (14%)	0	100	100
12	F	168/187 (90%)	152 (90%)	16 (10%)	0	100	100
13	G	172/179 (96%)	147 (86%)	24 (14%)	1 (1%)	25	62
14	H	45/152 (30%)	39 (87%)	6 (13%)	0	100	100
15	J	144/147 (98%)	135 (94%)	9 (6%)	0	100	100
16	K	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
17	L	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
18	M	132/138 (96%)	116 (88%)	16 (12%)	0	100	100
19	N	114/180 (63%)	108 (95%)	6 (5%)	0	100	100
20	O	114/122 (93%)	102 (90%)	12 (10%)	0	100	100
21	P	110/113 (97%)	96 (87%)	14 (13%)	0	100	100
22	Q	120/129 (93%)	112 (93%)	7 (6%)	1 (1%)	19	56
23	R	96/104 (92%)	87 (91%)	8 (8%)	1 (1%)	15	51
24	S	111/197 (56%)	104 (94%)	7 (6%)	0	100	100
25	T	96/100 (96%)	88 (92%)	8 (8%)	0	100	100
26	U	86/105 (82%)	71 (83%)	14 (16%)	1 (1%)	13	48
27	V	175/215 (81%)	143 (82%)	26 (15%)	6 (3%)	3	30
28	W	72/86 (84%)	65 (90%)	5 (7%)	2 (3%)	5	33
29	X	61/64 (95%)	50 (82%)	10 (16%)	1 (2%)	9	43
30	Y	63/77 (82%)	60 (95%)	2 (3%)	1 (2%)	9	43
31	Z	57/65 (88%)	51 (90%)	5 (9%)	1 (2%)	8	41
All	All	3156/3688 (86%)	2815 (89%)	322 (10%)	19 (1%)	29	62

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	108	PRO
10	D	91	ALA
10	D	92	ALA
22	Q	118	PRO
27	V	61	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	43/47 (92%)	43 (100%)	0	100	100
2	1	45/51 (88%)	45 (100%)	0	100	100
3	2	36/40 (90%)	36 (100%)	0	100	100
4	3	53/54 (98%)	53 (100%)	0	100	100
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	40/66 (61%)	40 (100%)	0	100	100
9	C	212/219 (97%)	212 (100%)	0	100	100
10	D	163/166 (98%)	162 (99%)	1 (1%)	86	93
11	E	159/172 (92%)	159 (100%)	0	100	100
12	F	139/155 (90%)	139 (100%)	0	100	100
13	G	143/147 (97%)	143 (100%)	0	100	100
14	H	36/121 (30%)	36 (100%)	0	100	100
15	J	120/121 (99%)	120 (100%)	0	100	100
16	K	100/101 (99%)	100 (100%)	0	100	100
17	L	106/110 (96%)	106 (100%)	0	100	100
18	M	110/114 (96%)	110 (100%)	0	100	100
19	N	94/139 (68%)	94 (100%)	0	100	100
20	O	88/93 (95%)	88 (100%)	0	100	100
21	P	98/99 (99%)	98 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	Q	95/99 (96%)	95 (100%)	0	100	100
23	R	79/83 (95%)	79 (100%)	0	100	100
24	S	87/140 (62%)	87 (100%)	0	100	100
25	T	82/83 (99%)	82 (100%)	0	100	100
26	U	77/88 (88%)	77 (100%)	0	100	100
27	V	142/164 (87%)	142 (100%)	0	100	100
28	W	54/62 (87%)	54 (100%)	0	100	100
29	X	52/52 (100%)	52 (100%)	0	100	100
30	Y	58/66 (88%)	58 (100%)	0	100	100
31	Z	51/55 (93%)	51 (100%)	0	100	100
All	All	2597/2942 (88%)	2596 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	D	76	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
18	M	123	HIS
24	S	70	ASN
27	V	62	ASN
9	C	227	ASN
10	D	76	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	3116/3138 (99%)	297 (9%)	1 (0%)
8	B	114/115 (99%)	2 (1%)	0
All	All	3230/3253 (99%)	299 (9%)	1 (0%)

5 of 299 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	10	U
7	A	50	U
7	A	71	A
7	A	74	U
7	A	75	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1567	U

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)

1 ligand is 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	$\#\|Z\| > 2$
32	917	A	5001	-	21,24,24	3.02	7 (33%)	28,33,33	3.16	12 (42%)

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
32	917	A	5001	-	-	4/13/25/25	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	5001	917	C09-N08	9.37	1.45	1.36
32	A	5001	917	O11-C09	6.78	1.44	1.35
32	A	5001	917	C02-N04	3.93	1.45	1.34
32	A	5001	917	C07-N08	-3.30	1.41	1.47
32	A	5001	917	C07-C06	-3.07	1.47	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	5001	917	C07-N08-C09	-8.15	106.56	111.28
32	A	5001	917	C19-N20-C21	6.66	116.17	105.78
32	A	5001	917	C06-C07-N08	5.41	107.26	101.81
32	A	5001	917	C07-C06-C05	-4.85	107.71	113.08
32	A	5001	917	C18-C19-N20	4.26	117.43	108.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	5001	917	N04-C05-C06-C07
32	A	5001	917	C13-C12-N08-C09
32	A	5001	917	C17-C12-N08-C09
32	A	5001	917	C06-C05-N04-C02

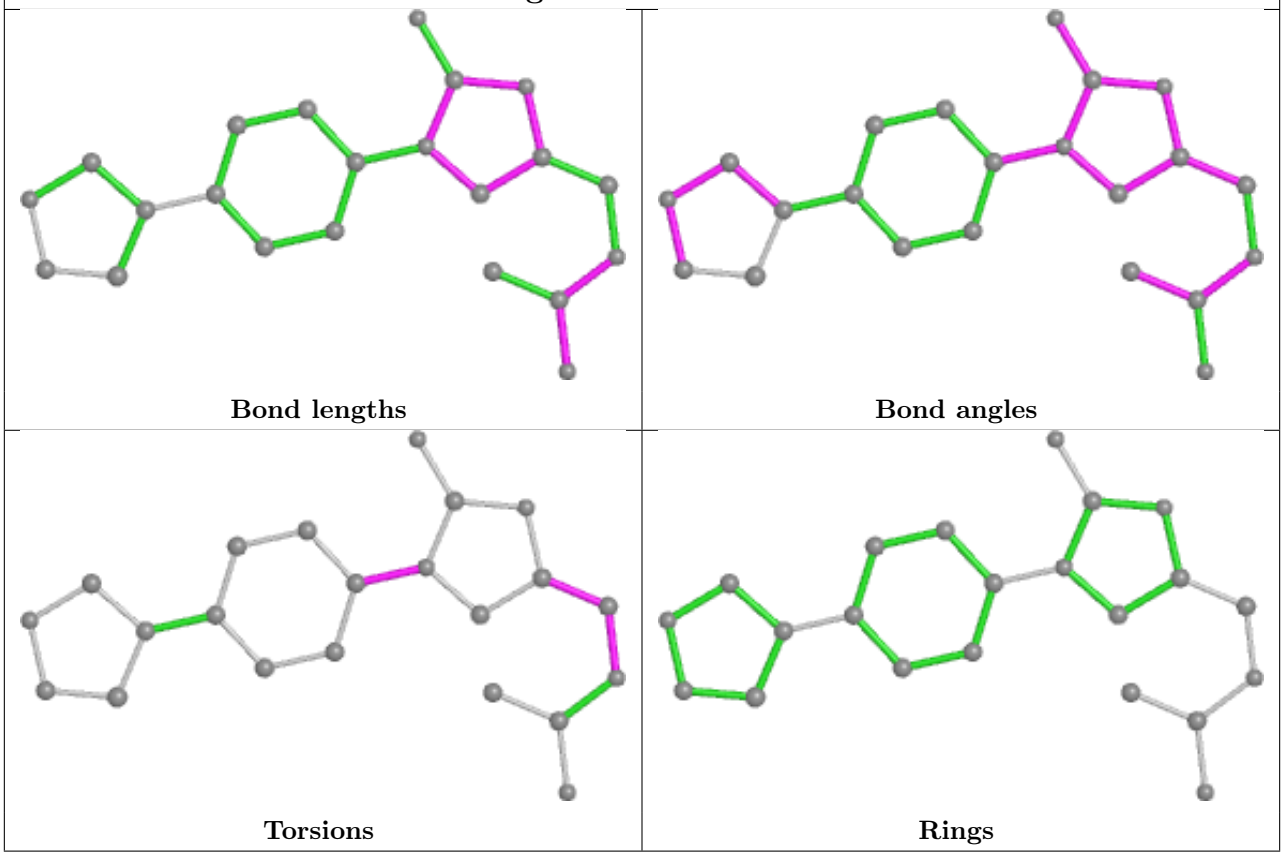
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 917 A 5001



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.

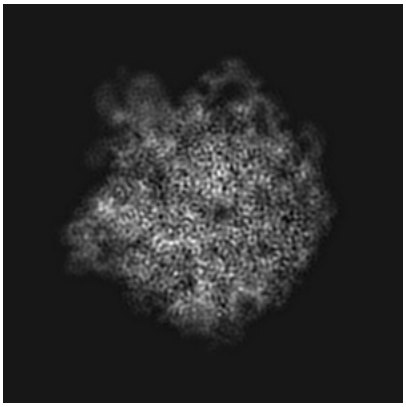
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8641. These allow visual inspection of the internal detail of the map and identification of artifacts.

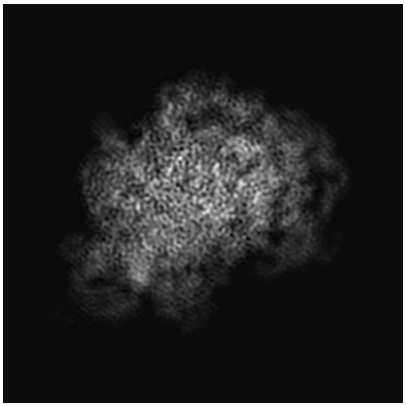
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

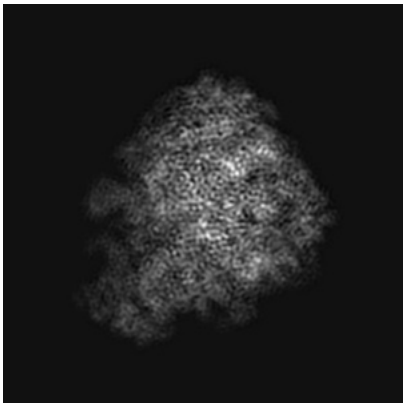
6.1.1 Primary map



X



Y

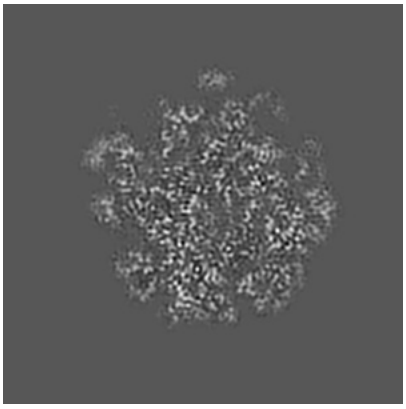


Z

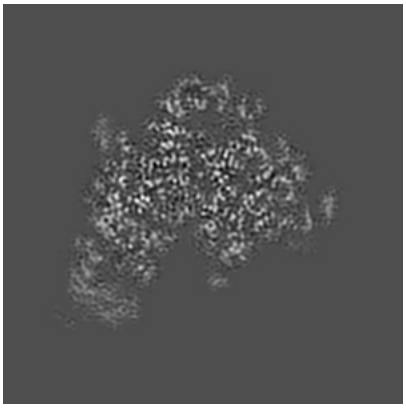
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 104



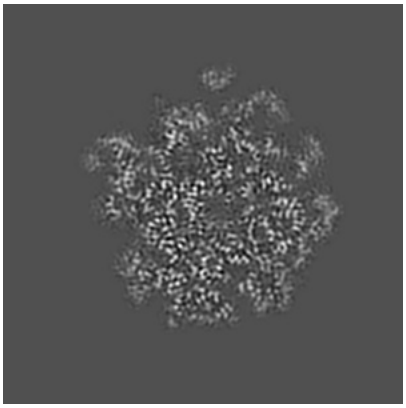
Y Index: 104

Z Index: 104

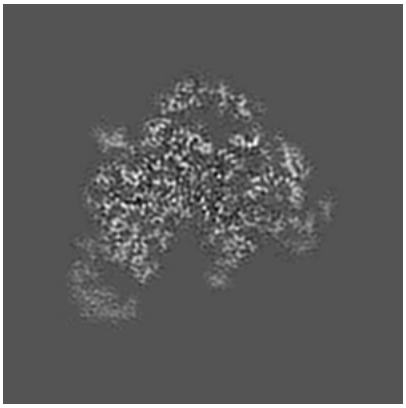
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

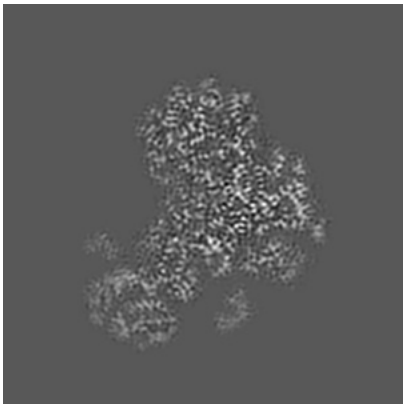
6.3.1 Primary map



X Index: 106



Y Index: 102

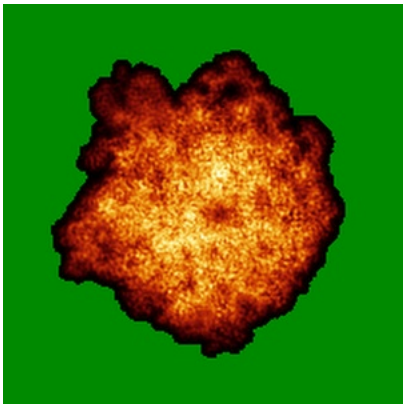


Z Index: 87

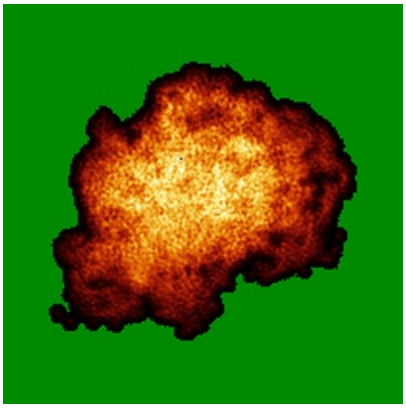
The images above show the largest variance slices of the map in three orthogonal directions.

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

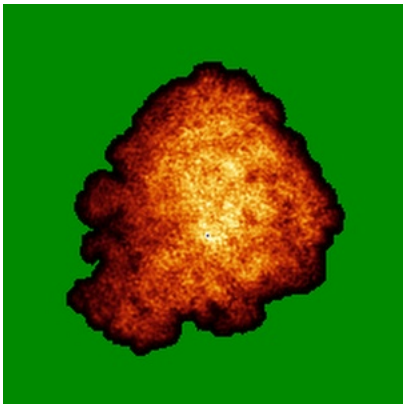
6.4.1 Primary map



X



Y



Z

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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

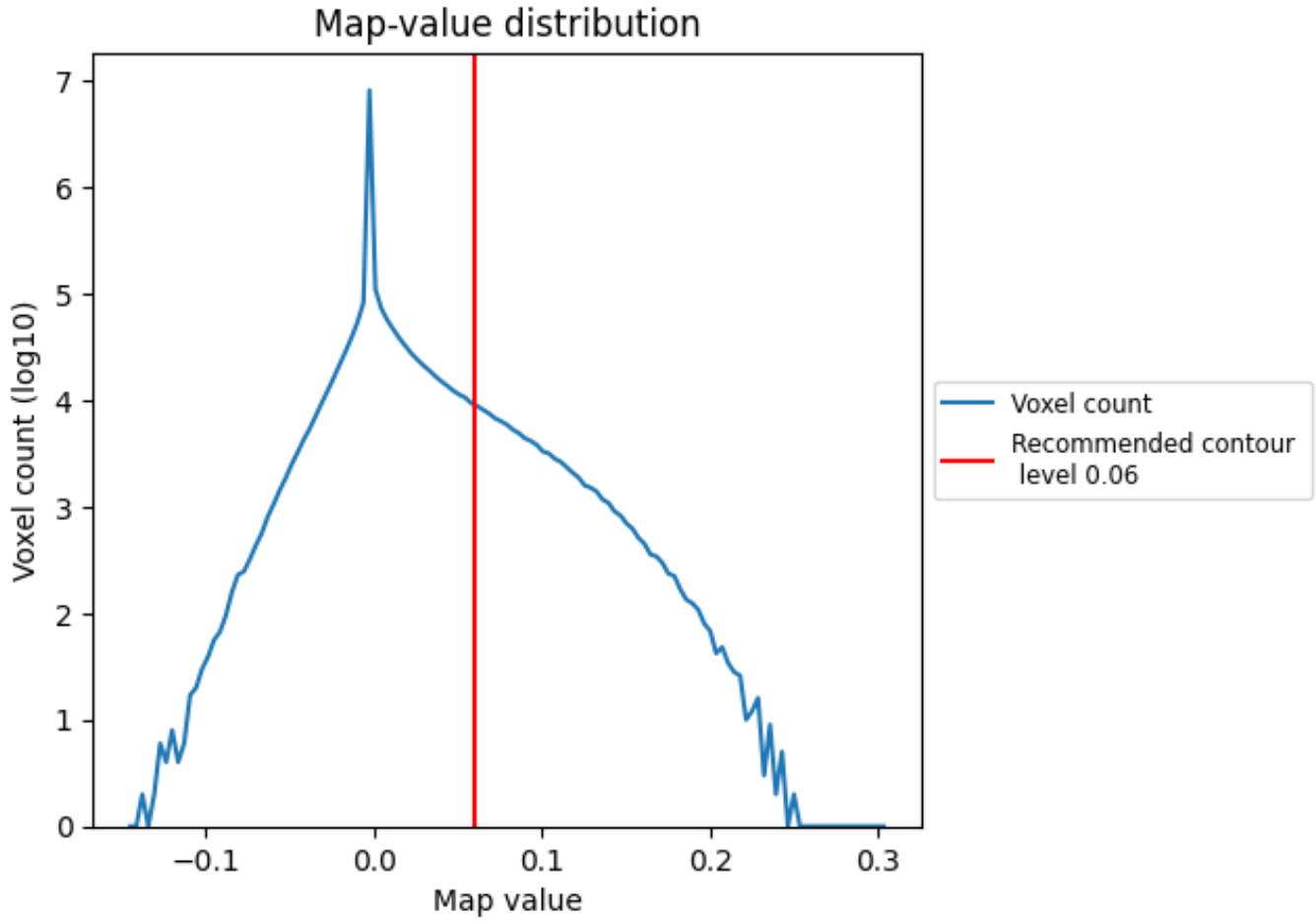
6.6 Mask visualisation (i)

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

7 Map analysis

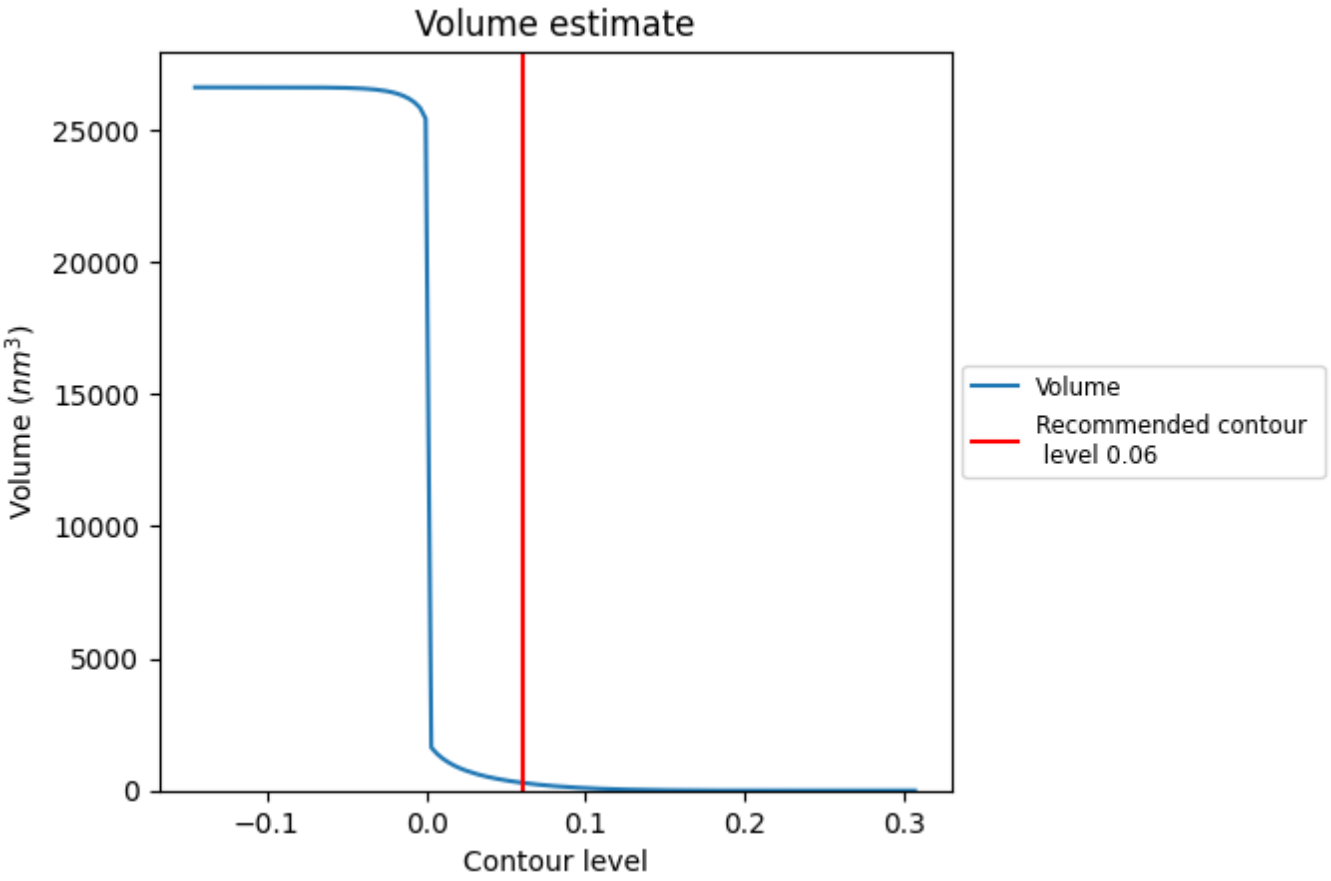
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

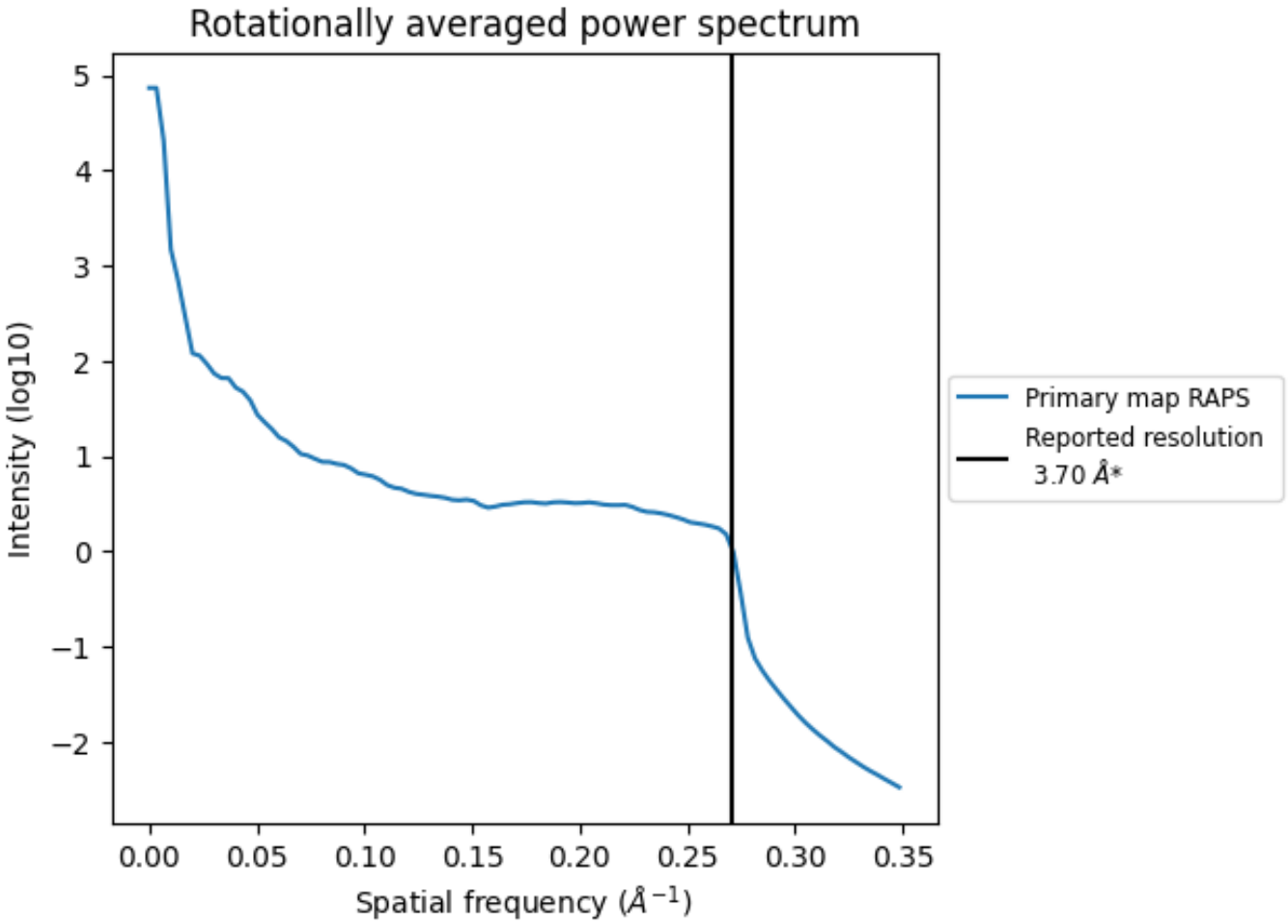
7.2 Volume estimate (i)



The volume at the recommended contour level is 296 nm^3; this corresponds to an approximate mass of 268 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)

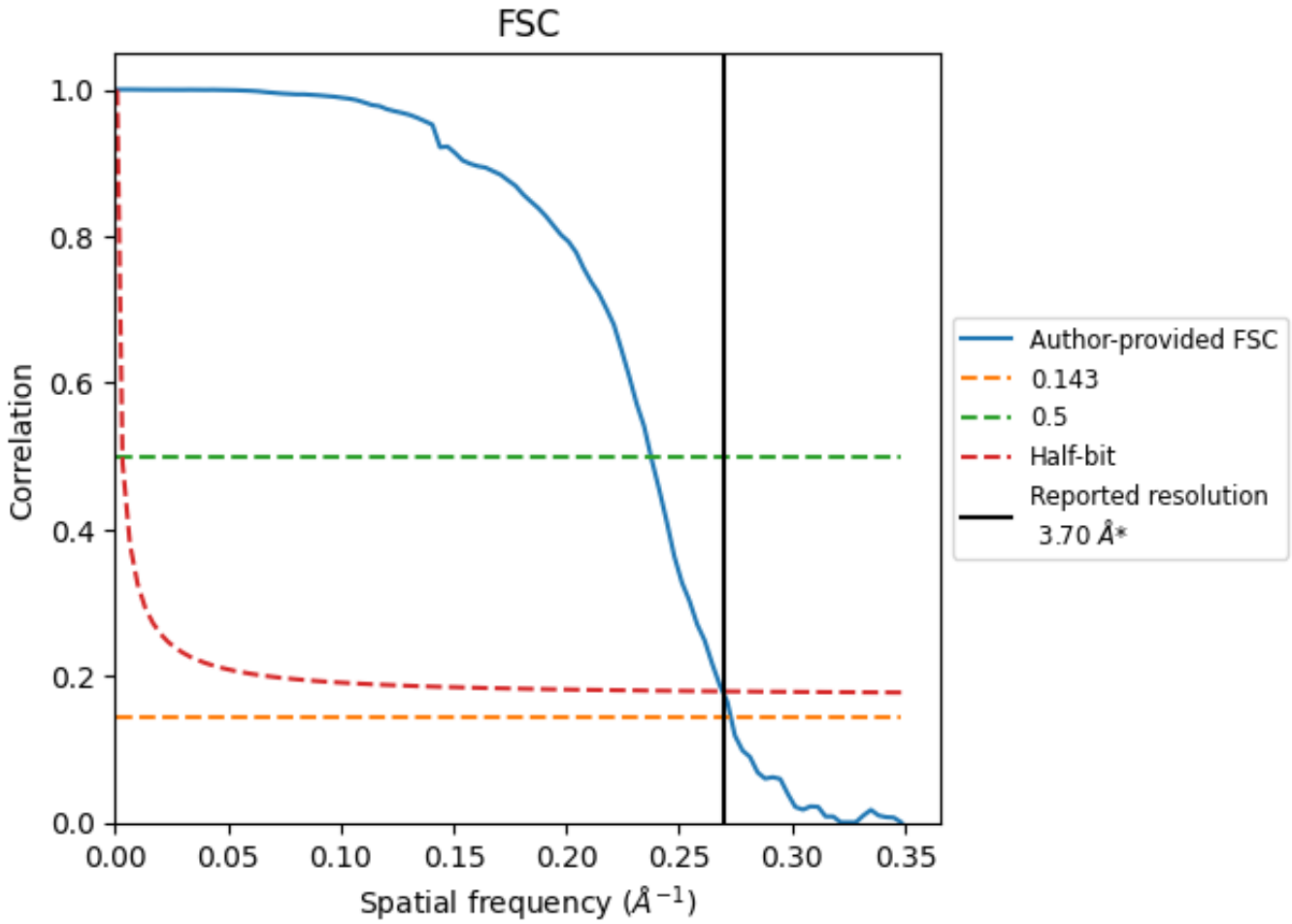


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

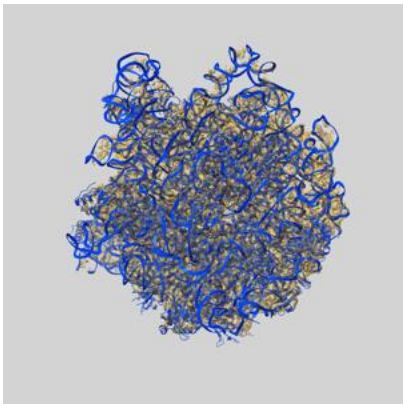
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.66	4.21	3.71
Unmasked-calculated*	-	-	-

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

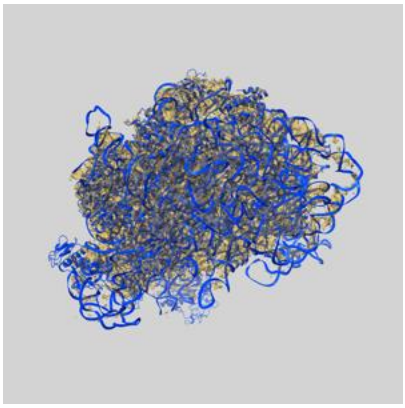
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8641 and PDB model 5V7Q. Per-residue inclusion information can be found in section 3 on page 10.

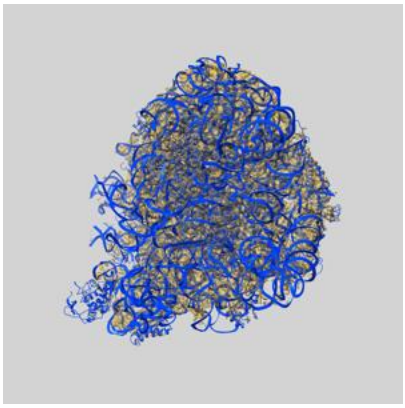
9.1 Map-model overlay



X



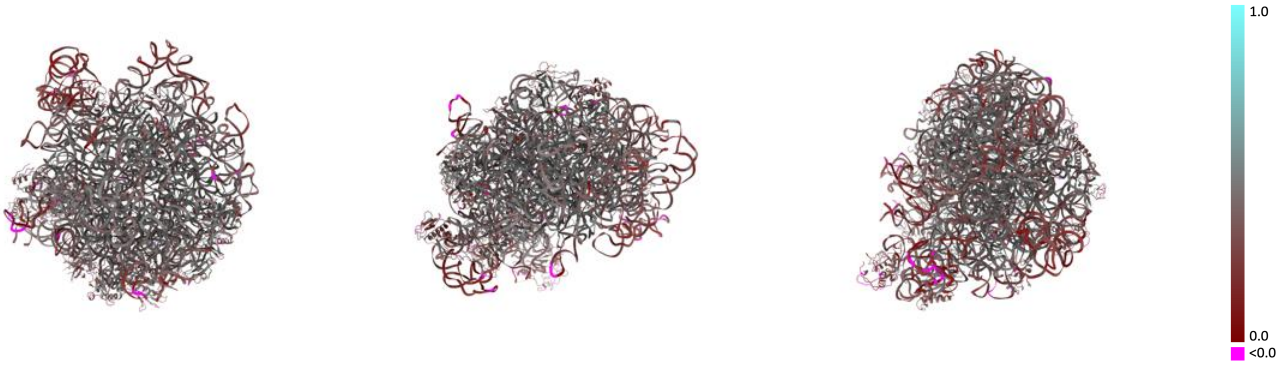
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

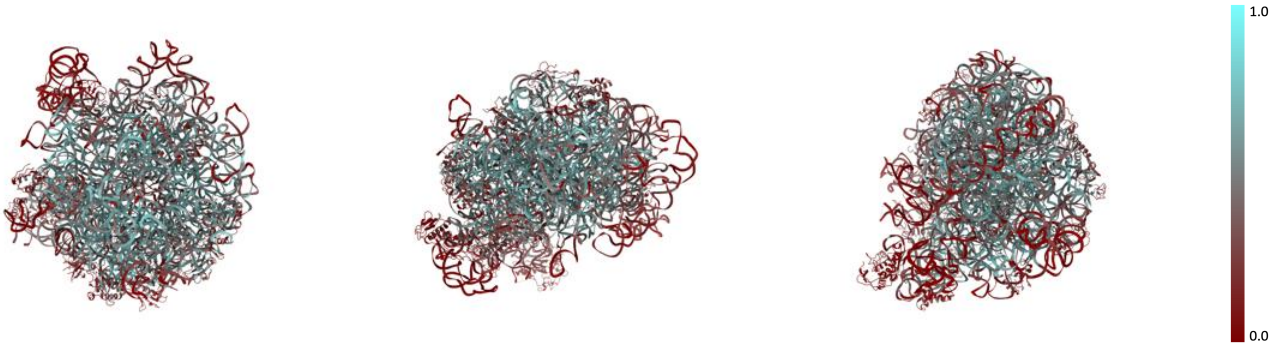
9.2 Q-score mapped to coordinate model (i)



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.

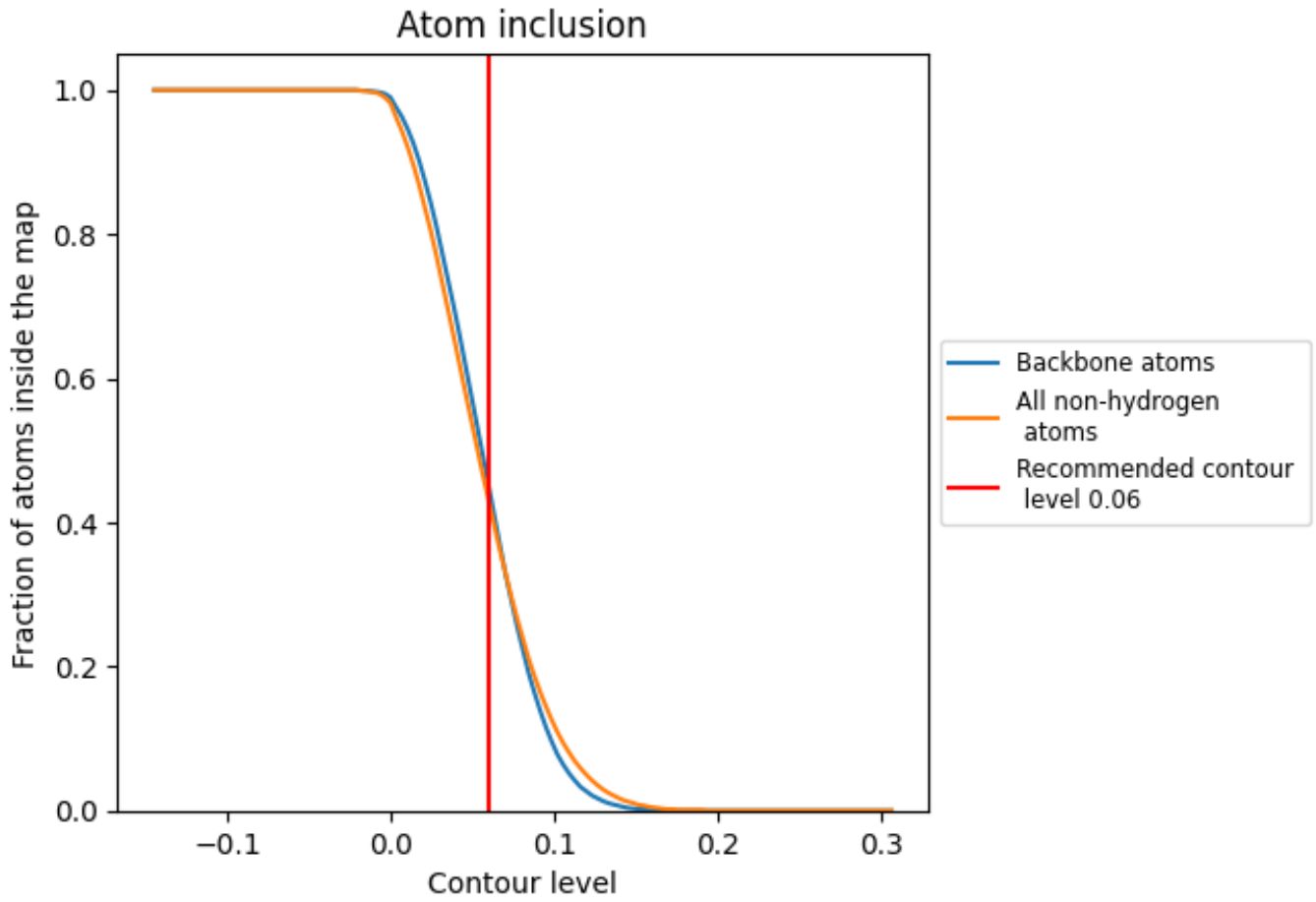
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 45% of all backbone atoms, 43% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4280	0.3840
0	0.3230	0.3740
1	0.3310	0.4080
2	0.5210	0.4160
3	0.3770	0.4140
4	0.2160	0.3840
6	0.0060	0.1110
A	0.4810	0.3920
B	0.3550	0.3550
C	0.4090	0.4180
D	0.3780	0.4180
E	0.3710	0.3890
F	0.0280	0.2370
G	0.0610	0.2710
H	0.0200	0.2620
J	0.3840	0.3960
K	0.2790	0.3770
L	0.3340	0.4010
M	0.1850	0.3590
N	0.4430	0.4180
O	0.2090	0.3260
P	0.2560	0.3540
Q	0.4880	0.4220
R	0.3080	0.3730
S	0.4140	0.4100
T	0.3100	0.3710
U	0.2570	0.3490
V	0.0430	0.2480
W	0.3890	0.4110
X	0.4010	0.4050
Y	0.3280	0.3690
Z	0.3540	0.4160