wwPDB EM Validation Summary Report

Dec 18, 2022 – 07:49 pm GMT

PDB ID	:	7BL4
EMDB ID	:	EMD-12217
Title	:	in vitro reconstituted 50S-ObgE-GMPPNP-RsfS particle
Authors	:	Hilal, T.; Nikolay, R.; Spahn, C.M.T.
Deposited on	:	2021-01-18
Resolution	:	2.40 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:

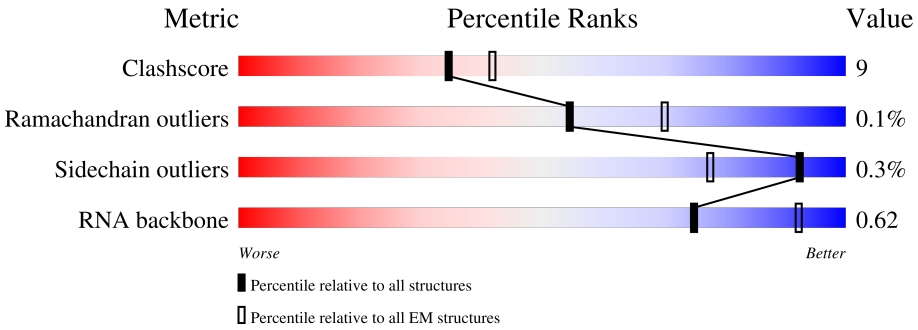
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.40 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	g	38	8% 100%
2	C	273	74% 25%
3	D	209	6% 78% 22%
4	E	201	7% 78% 18%
5	F	179	54% 65% 34%
6	G	177	19% 80% 18%
7	J	142	81% 19%

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Mol	Chain	Length	Quality of chain
8	L	144	5% 78% 22%
9	N	127	78% 17% 6%
10	O	117	15% 77% 22%
11	Q	118	86% 13%
12	R	103	7% 77% 23%
13	S	110	6% 73% 27%
14	T	100	5% 80% 13% 7%
15	U	104	12% 71% 27%
16	V	94	5% 79% 21%
17	W	85	78% 12% 11%
18	X	78	77% 22%
19	Y	63	11% 76% 24%
20	Z	59	75% 24%
21	0	57	7% 63% 35%
22	1	55	7% 64% 27% 9%
23	2	46	83% 17%
24	K	123	69% 30%
25	P	115	10% 77% 21%
26	M	136	82% 18%
27	H	149	76% 76% 24%
28	d	70	60% 67% 33%
29	A	2904	5% 56% 40%
30	B	119	58% 40%
31	6	105	9% 72% 25%
32	9	390	12% 66% 21% 13%

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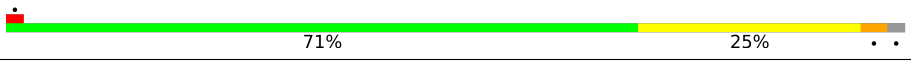
Mol	Chain	Length	Quality of chain
33	3	65	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 93560 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 L36.

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

- Molecule 2 is a protein called 50S ribosomal protein L2.

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

- Molecule 3 is a protein called 50S ribosomal protein L3.

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

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	193	Total	C	N	O	S	0	0
			1483	932	266	280	5		

- Molecule 5 is a protein called 50S ribosomal protein L5.

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

- Molecule 6 is a protein called 50S ribosomal protein L6.

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

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

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

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

- 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 L20.

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

- Molecule 12 is a protein called 50S ribosomal protein L21.

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

- Molecule 13 is a protein called 50S ribosomal protein L22.

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

- Molecule 14 is a protein called 50S ribosomal protein L23.

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

- Molecule 15 is a protein called 50S ribosomal protein L24.

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

- Molecule 16 is a protein called 50S ribosomal protein L25.

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

- Molecule 17 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	76	Total	C	N	O	S	0	0
			577	357	117	102	1		

- Molecule 18 is a protein called 50S ribosomal protein L28.

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

- Molecule 19 is a protein called 50S ribosomal protein L29.

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

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

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

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

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

- Molecule 22 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	1	50	Total	C	N	O	0	0
			409	263	75	71		

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

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

- Molecule 24 is a protein called 50S ribosomal protein L14.

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

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	113	Total	C	N	O	S	0	0
			911	571	178	161	1		

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

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

- Molecule 27 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 31 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	102	Total	C	N	O	S	0	0
			780	485	133	157	5		

- Molecule 32 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	338	Total	C	N	O	S	0	0
			2582	1626	453	490	13		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

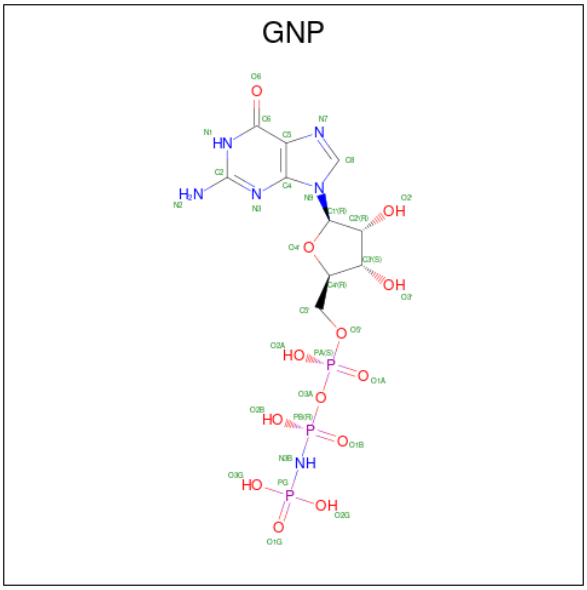
- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	g	1	Total	Zn	0
			1	1	
34	d	1	Total	Zn	0
			1	1	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
35	A	3	Total Mg 3 3	0
35	6	2	Total Mg 2 2	0
35	9	1	Total Mg 1 1	0

- Molecule 36 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
36	9	1	Total C N O P 32 10 6 13 3	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	AltConf
37	C	2	Total O 2 2	0
37	F	1	Total O 1 1	0
37	L	1	Total O 1 1	0
37	N	3	Total O 3 3	0
37	S	1	Total O 1 1	0

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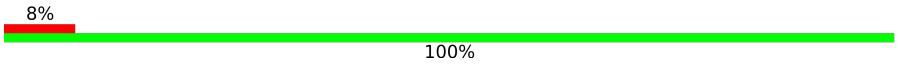
Mol	Chain	Residues	Atoms	AltConf
37	A	18	Total O 18 18	0
37	B	1	Total O 1 1	0
37	6	3	Total O 3 3	0
37	9	5	Total O 5 5	0

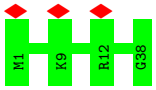
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 50S ribosomal protein L36

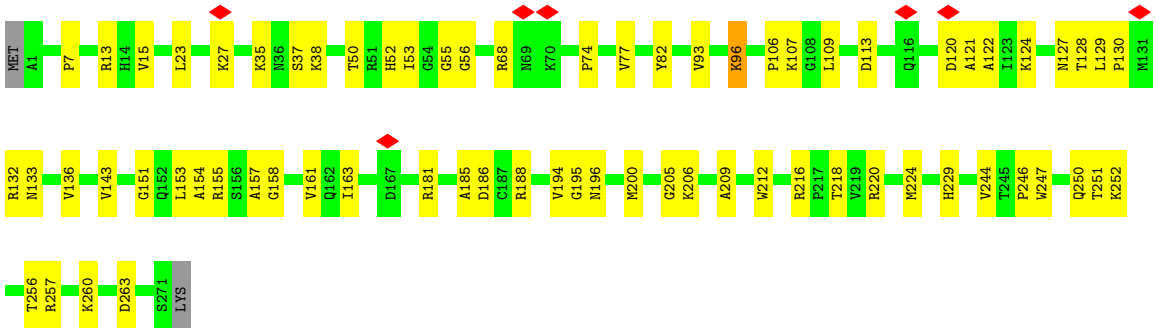
Chain g:





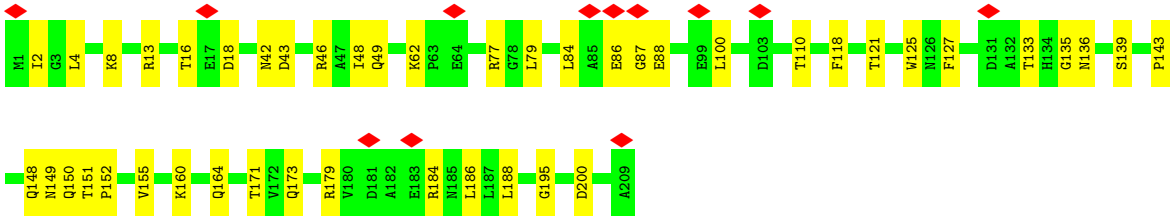
• Molecule 2: 50S ribosomal protein L2

Chain C:



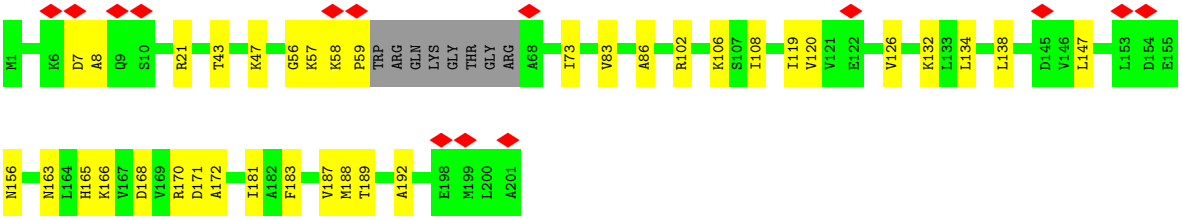
• Molecule 3: 50S ribosomal protein L3

Chain D:

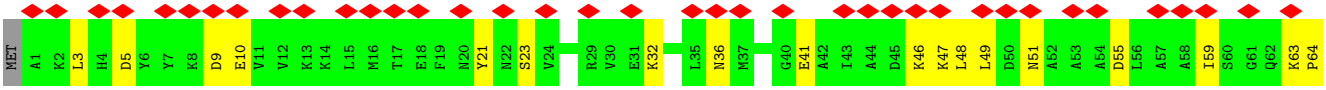


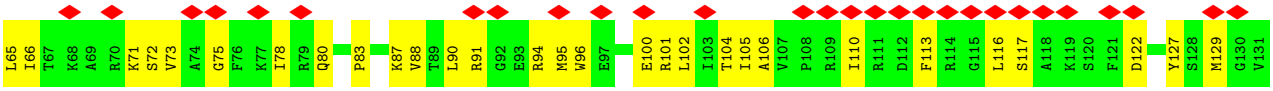
• Molecule 4: 50S ribosomal protein L4

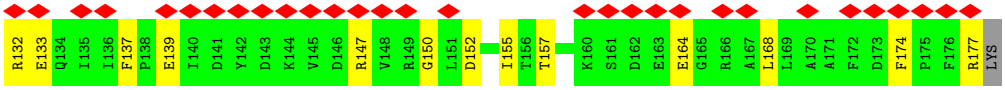
Chain E:



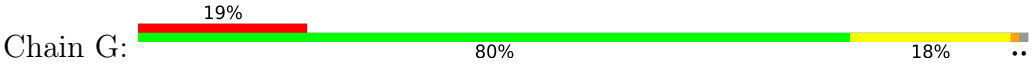
• Molecule 5: 50S ribosomal protein L5

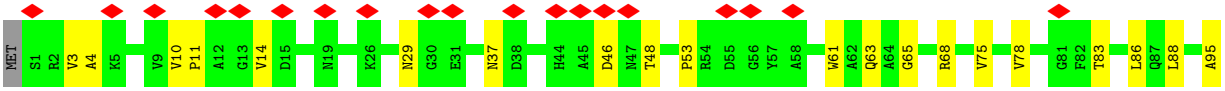


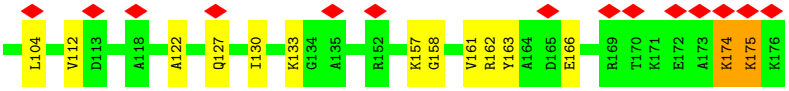




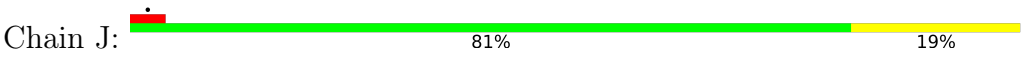
• Molecule 6: 50S ribosomal protein L6

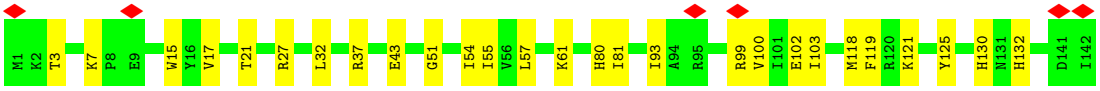




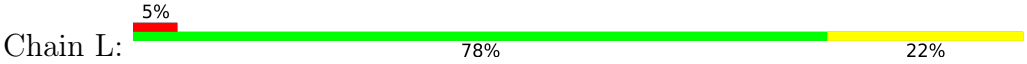


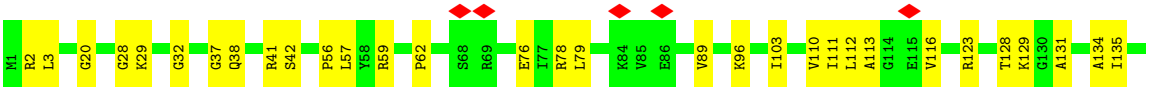
• Molecule 7: 50S ribosomal protein L13





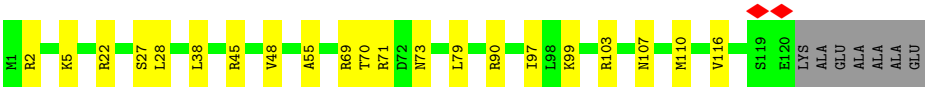
• Molecule 8: 50S ribosomal protein L15





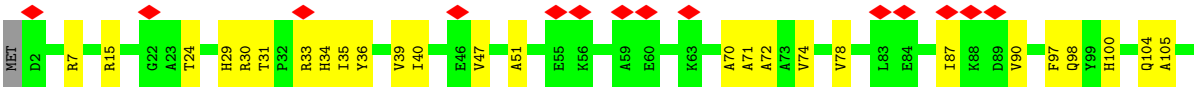
• Molecule 9: 50S ribosomal protein L17

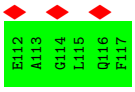
Chain N:



• Molecule 10: 50S ribosomal protein L18

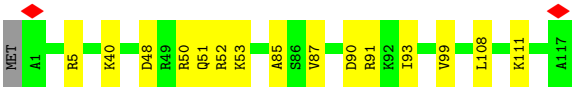
Chain O:





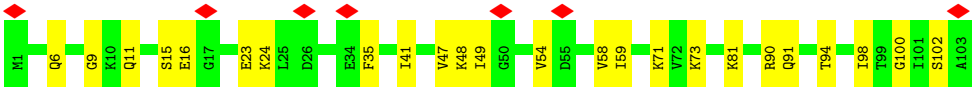
• Molecule 11: 50S ribosomal protein L20

Chain Q:



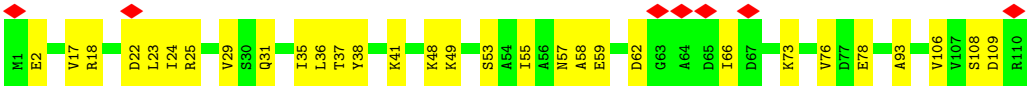
• Molecule 12: 50S ribosomal protein L21

Chain R:



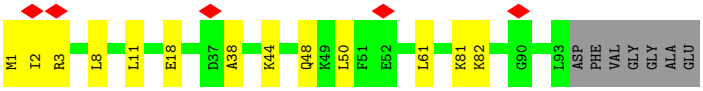
• Molecule 13: 50S ribosomal protein L22

Chain S:



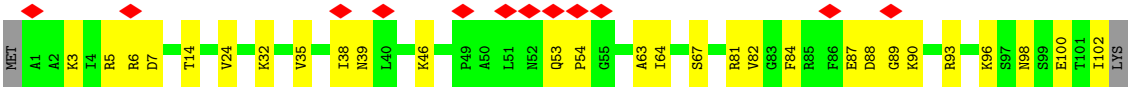
• Molecule 14: 50S ribosomal protein L23

Chain T:



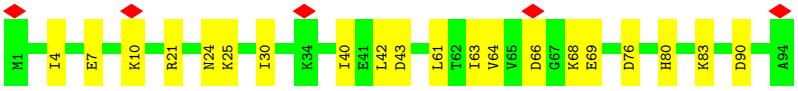
• Molecule 15: 50S ribosomal protein L24

Chain U:



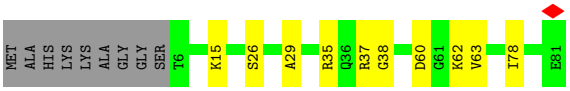
• Molecule 16: 50S ribosomal protein L25

Chain V:



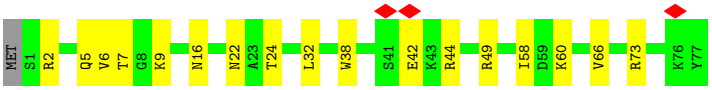
• Molecule 17: 50S ribosomal protein L27

Chain W:



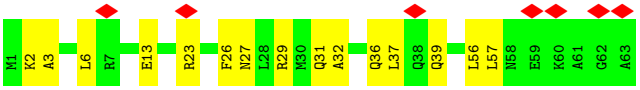
• Molecule 18: 50S ribosomal protein L28

Chain X:



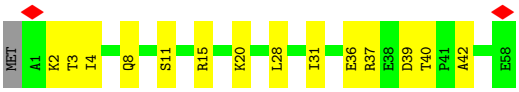
• Molecule 19: 50S ribosomal protein L29

Chain Y:



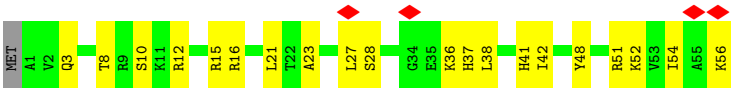
• Molecule 20: 50S ribosomal protein L30

Chain Z:



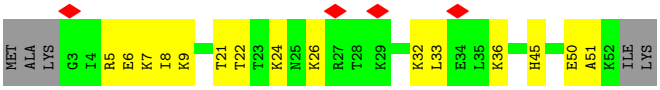
• Molecule 21: 50S ribosomal protein L32

Chain 0:



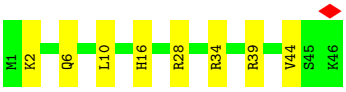
• Molecule 22: 50S ribosomal protein L33

Chain 1:



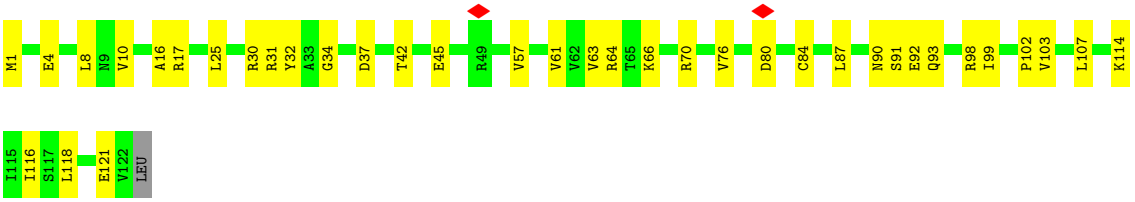
• Molecule 23: 50S ribosomal protein L34

Chain 2:



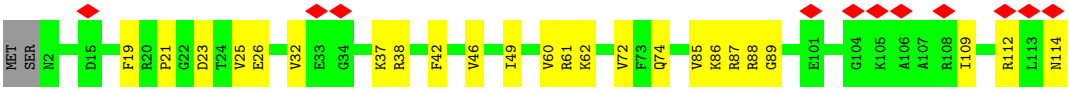
• Molecule 24: 50S ribosomal protein L14

Chain K:



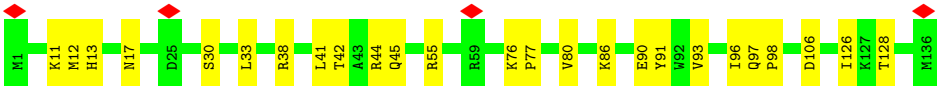
• Molecule 25: 50S ribosomal protein L19

Chain P:



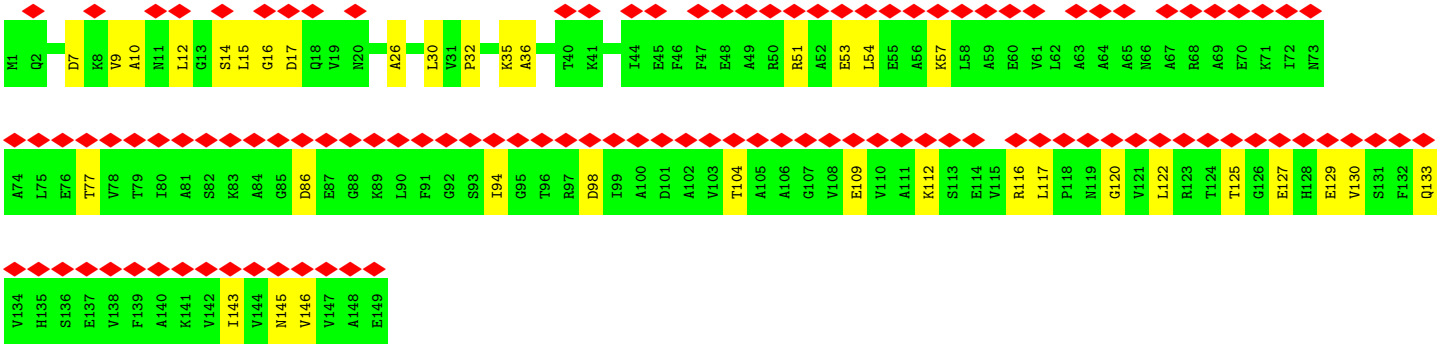
• Molecule 26: 50S ribosomal protein L16

Chain M:

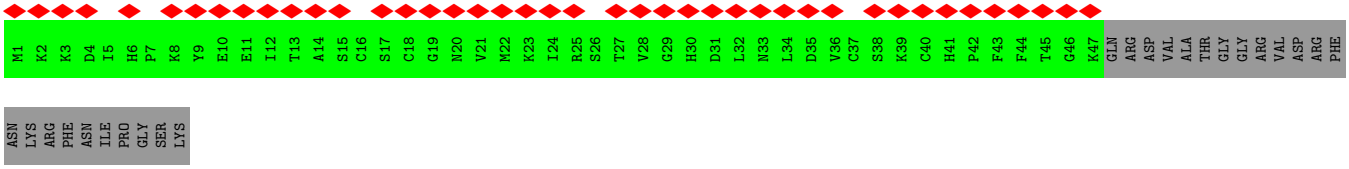


• Molecule 27: 50S ribosomal protein L9

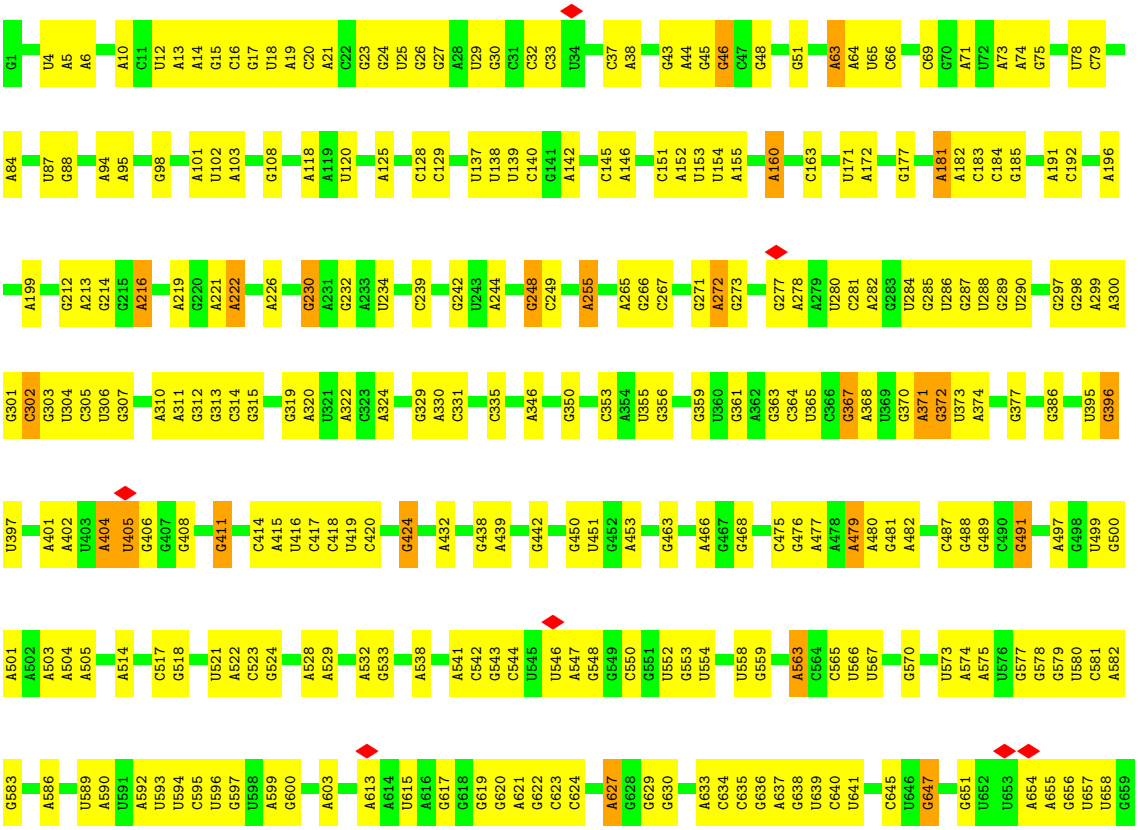
Chain H:

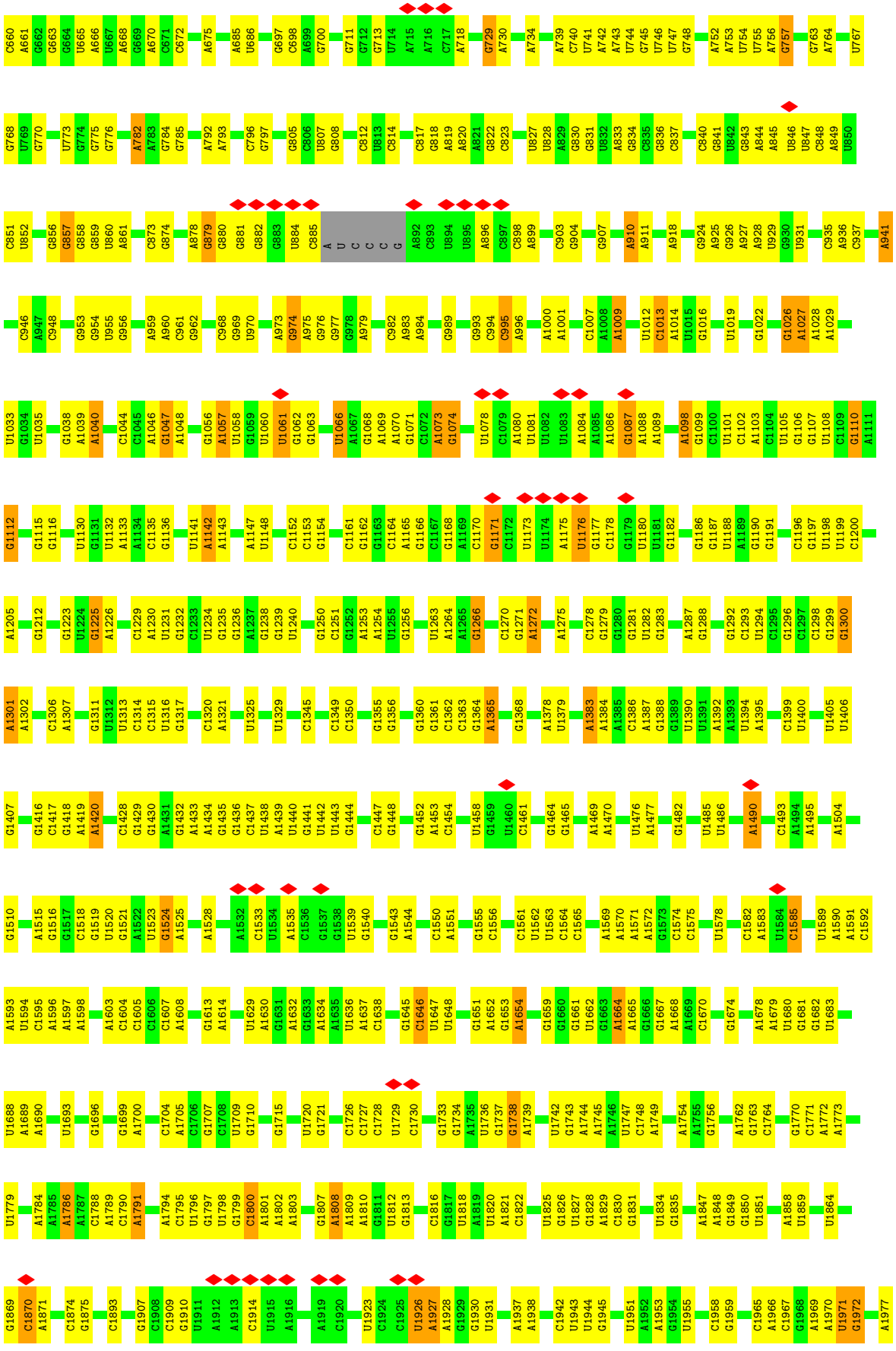


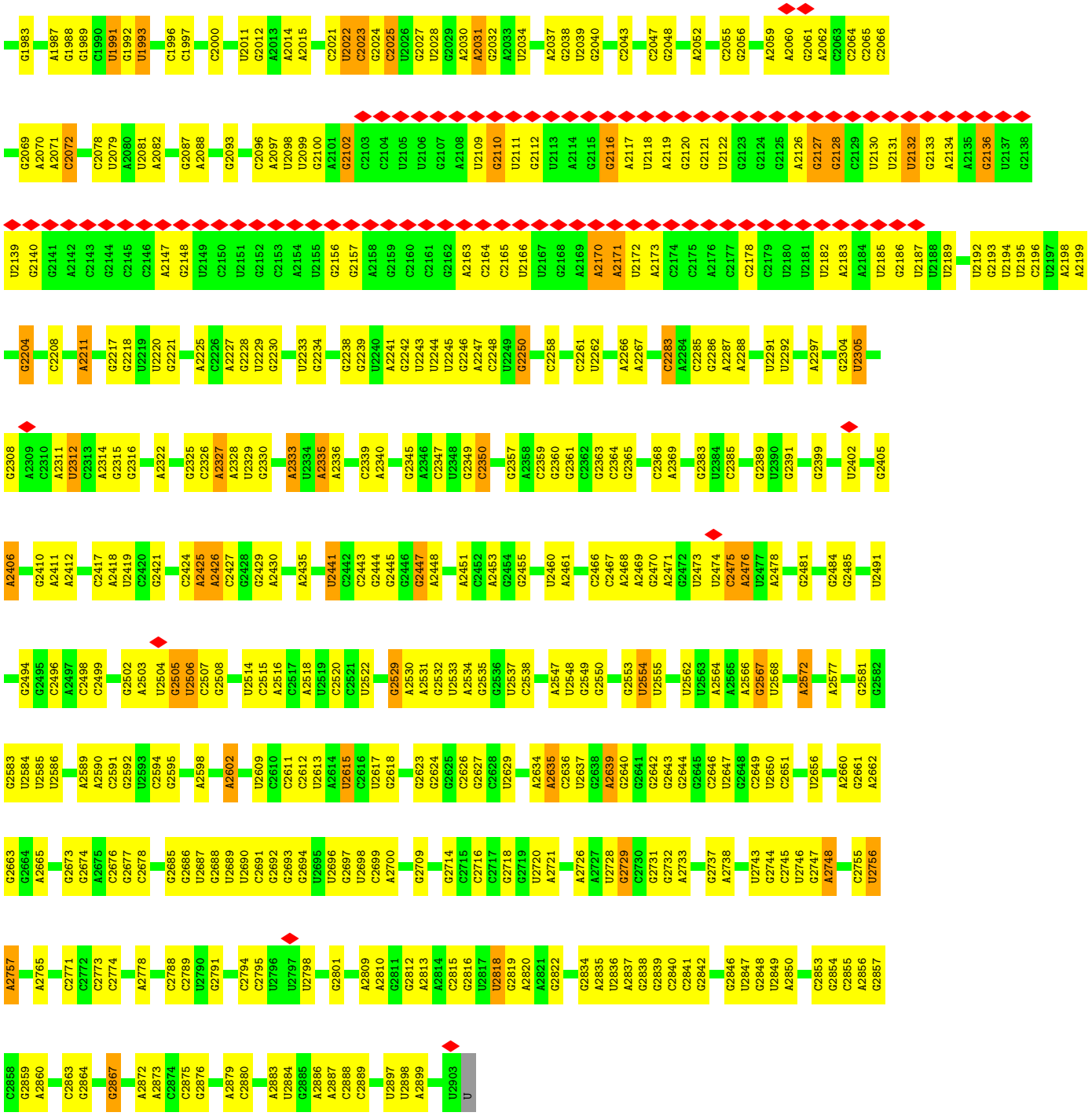
• Molecule 28: 50S ribosomal protein L31



• Molecule 29: 23S ribosomal RNA

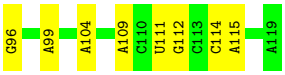



C660 A661 G662 G663 G664 U665 A666 U667 A668 G669 A670 C671 C672 A675 A685 U686 G697 C698 A699 G700 G711 G712 G713 U714 A715 A716 C717 A718 G729 A730 A734 A739 C740 U741 A742 A743 U744 G745 U746 U747 G748 A752 A753 U754 U755 A756 G757 G763 A764 U767
G768 U769 G770 U773 G774 G775 G776 A782 A783 G784 G785 A792 A793 C796 G797 G805 C806 U807 G808 C812 U813 C814 C817 G818 A819 A820 A821 G822 C823 U827 U828 A829 G830 G831 U832 A833 G834 C835 G836 C837 C840 G841 U842 G843 A844 A845 U846 U847 C848 A849 U850
C851 U852 G856 G857 G858 G859 U860 A861 C873 G874 A878 G879 G880 G881 G882 G883 U884 C885 A U C C C G A892 G893 U894 U895 A896 C897 C898 A899 C903 G904 G907 A910 A911 A918 G924 A925 G926 A927 A928 U929 G930 U931 C935 A936 C937 A941
C946 A947 C948 G953 G954 U955 G956 A959 A960 C961 G962 C968 G969 U970 A973 G974 A975 G976 G977 G978 A979 C982 A983 A984 G989 G993 C994 C995 A996 A1000 A1001 C1007 A1008 A1009 U1012 C1013 A1014 U1015 G1016 U1019 G1022 G1026 A1027 A1028 A1029
U1033 G1034 U1035 G1038 A1039 A1040 C1044 C1045 A1046 G1047 A1048 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111
G1112 G1115 G1116 U1130 G1131 U1132 A1133 A1134 C1135 G1136 U1141 A1142 A1143 A1147 U1148 C1152 C1153 G1154 C1161 G1162 G1163 C1164 A1165 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 G1186 G1187 U1188 A1189 G1190 G1191 C1196 G1197 U1198 U1199 C1200
A1205 G1212 G1223 U1224 G1225 A1226 C1229 A1230 U1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 G1250 C1251 G1252 A1253 A1254 U1255 G1256 U1263 A1264 A1265 G1266 C1270 G1271 A1272 A1275 C1278 G1279 G1280 G1281 U1282 G1283 A1287 G1288 G1292 C1293 U1294 C1295 G1296 C1297 C1298 G1299 G1300
A1301 A1302 C1306 A1307 G1311 U1312 U1313 C1314 C1315 U1316 G1317 C1320 A1321 U1325 U1329 C1345 C1349 C1350 G1355 G1356 G1360 G1361 C1362 C1363 G1364 A1365 G1368 A1378 U1379 A1383 A1384 A1385 C1386 A1387 G1388 G1389 U1390 U1391 A1392 A1393 U1394 A1395 C1399 U1400 U1405 U1406
G1407 G1416 C1417 G1418 A1419 A1420 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 G1436 C1437 U1438 A1439 U1440 G1441 U1442 U1443 G1444 C1447 G1448 G1452 A1453 C1454 U1458 G1459 U1460 C1461 G1464 G1465 A1469 A1470 U1476 A1477 G1482 U1485 U1486 A1490 C1493 A1494 A1495 A1504
G1510 A1515 G1516 G1517 C1518 G1519 U1520 G1521 A1522 U1523 G1524 A1525 A1528 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 G1543 A1544 C1550 A1551 G1555 C1556 C1561 U1562 U1563 C1564 C1565 A1569 A1570 A1571 A1572 G1573 C1574 C1575 U1578 C1582 A1583 U1584 C1585 U1589 A1590 A1591 C1592
A1593 U1594 C1595 A1596 A1597 A1598 A1603 C1604 C1605 C1606 C1607 A1608 G1613 A1614 U1629 A1630 G1631 A1632 G1633 A1634 A1635 U1636 A1637 C1638 G1645 C1646 U1647 U1648 G1651 A1652 G1653 A1654 G1659 G1660 G1661 U1662 G1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670 G1674 A1678 A1679 U1680 G1681 G1682 U1683
U1688 A1689 A1690 U1693 G1696 G1699 A1700 C1704 A1705 C1706 G1707 C1708 U1709 G1710 G1715 U1720 G1721 C1726 C1727 C1728 U1729 C1730 G1733 G1734 A1735 U1736 G1737 G1738 A1739 U1742 G1743 A1744 A1745 A1746 U1747 C1748 A1749 A1754 A1755 G1756 A1762 G1763 C1764 G1770 C1771 A1772 A1773
U1779 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 G1807 A1808 A1809 A1810 C1811 U1812 G1813 C1816 G1817 U1818 A1819 U1820 A1821 C1822 U1825 G1826 U1827 G1828 A1829 C1830 G1831 U1834 G1835 A1847 A1848 G1849 G1850 U1851 A1858 U1859 U1864
G1869 C1870 A1871 C1874 G1875 C1893 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 A1919 C1920 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1937 A1938 C1942 U1943 U1944 G1945 U1951 A1952 A1953 G1954 U1955 C1958 G1959 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 A1977



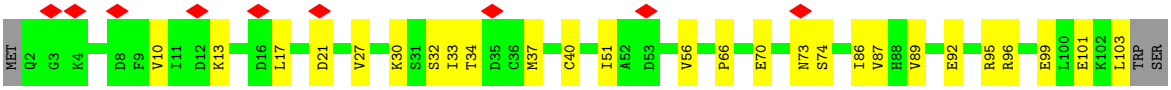
• Molecule 30: 5S ribosomal RNA

Chain B:



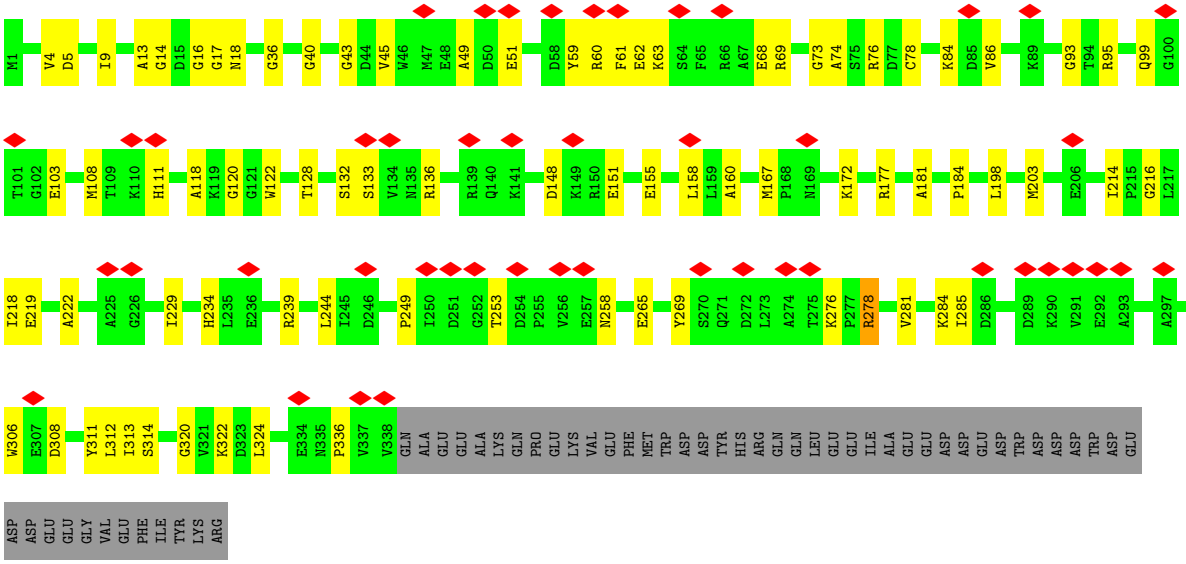
• Molecule 31: Ribosomal silencing factor RsfS

Chain 6:



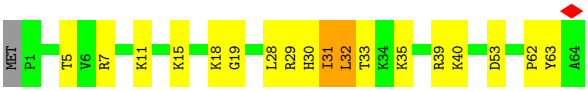
• Molecule 32: GTPase ObgE/CgtA

Chain 9:



• Molecule 33: 50S ribosomal protein L35

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	190393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	Not provided	
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	22.582	Depositor
Minimum map value	-9.349	Depositor
Average map value	-0.044	Depositor
Map value standard deviation	0.814	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	363.6, 363.6, 363.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GNP

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	g	0.23	0/303	0.44	0/397
2	C	0.24	0/2121	0.45	0/2852
3	D	0.25	0/1586	0.48	0/2134
4	E	0.24	0/1499	0.44	0/2016
5	F	0.25	0/1434	0.50	1/1926 (0.1%)
6	G	0.25	0/1343	0.45	0/1816
7	J	0.25	0/1152	0.43	0/1551
8	L	0.25	0/1062	0.50	0/1413
9	N	0.23	0/973	0.43	0/1301
10	O	0.24	0/902	0.43	0/1209
11	Q	0.25	0/960	0.40	0/1278
12	R	0.26	0/829	0.47	0/1107
13	S	0.24	0/864	0.41	0/1156
14	T	0.24	0/744	0.45	0/994
15	U	0.26	0/787	0.50	0/1051
16	V	0.24	0/766	0.44	0/1025
17	W	0.25	0/584	0.44	0/772
18	X	0.23	0/635	0.43	0/848
19	Y	0.23	0/510	0.49	0/677
20	Z	0.24	0/453	0.44	0/605
21	0	0.22	0/450	0.47	0/599
22	1	0.24	0/416	0.48	0/554
23	2	0.23	0/380	0.39	0/498
24	K	0.25	0/947	0.49	0/1268
25	P	0.24	0/923	0.43	0/1234
26	M	0.24	0/1093	0.43	0/1460
27	H	0.24	0/1121	0.44	0/1515
28	d	0.23	0/371	0.44	0/496
29	A	0.20	0/69659	0.73	4/108672 (0.0%)
30	B	0.16	0/2847	0.71	0/4440
31	6	0.24	0/787	0.46	0/1062
32	9	0.25	0/2626	0.46	0/3542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	3	0.24	0/513	0.51	0/676
All	All	0.21	0/101640	0.67	5/152144 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	1313	U	C2-N1-C1'	7.25	126.39	117.70
5	F	95	MET	CA-CB-CG	6.68	124.65	113.30
29	A	1893	C	N3-C2-O2	-6.13	117.61	121.90
29	A	1313	U	N1-C2-O2	5.65	126.75	122.80
29	A	1313	U	N3-C2-O2	-5.23	118.54	122.20

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	g	302	0	340	0	0
2	C	2082	0	2157	53	0
3	D	1565	0	1616	34	0
4	E	1483	0	1548	25	0
5	F	1410	0	1447	44	0
6	G	1323	0	1374	20	0
7	J	1129	0	1162	24	0
8	L	1053	0	1129	27	0
9	N	960	0	1000	17	0
10	O	892	0	923	16	0
11	Q	947	0	1022	17	0
12	R	816	0	839	17	0
13	S	857	0	922	22	0
14	T	738	0	807	9	0
15	U	779	0	834	27	0
16	V	753	0	780	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	W	577	0	594	8	0
18	X	625	0	655	12	0
19	Y	509	0	543	11	0
20	Z	449	0	491	10	0
21	0	444	0	461	16	0
22	1	409	0	440	10	0
23	2	377	0	418	5	0
24	K	938	0	1012	29	0
25	P	911	0	957	18	0
26	M	1074	0	1157	18	0
27	H	1110	0	1148	22	0
28	d	364	0	364	0	0
29	A	62195	0	31280	834	0
30	B	2548	0	1292	35	0
31	6	780	0	783	18	0
32	9	2582	0	2606	61	0
33	3	504	0	574	17	0
34	d	1	0	0	0	0
34	g	1	0	0	0	0
35	6	2	0	0	0	0
35	9	1	0	0	0	0
35	A	3	0	0	0	0
36	9	32	0	13	1	0
37	6	3	0	0	0	0
37	9	5	0	0	0	0
37	A	18	0	0	2	0
37	B	1	0	0	0	0
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	L	1	0	0	0	0
37	N	3	0	0	0	0
37	S	1	0	0	0	0
All	All	93560	0	62688	1321	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 9.

The worst 5 of 1321 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)
29:A:1040:A:N6	29:A:1115:G:H1	1.68	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:285:G:H1	29:A:355:U:H3	1.19	0.89
29:A:1040:A:H61	29:A:1115:G:H1	0.93	0.88
29:A:1171:G:N1	29:A:1178:C:N3	2.27	0.81
4:E:56:GLY:HA2	4:E:73:ILE:HG12	1.65	0.77

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	g	36/38 (95%)	36 (100%)	0	0	100	100
2	C	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
3	D	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
4	E	189/201 (94%)	185 (98%)	4 (2%)	0	100	100
5	F	175/179 (98%)	159 (91%)	16 (9%)	0	100	100
6	G	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
8	L	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
9	N	118/127 (93%)	108 (92%)	10 (8%)	0	100	100
10	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
11	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
12	R	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
13	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
14	T	91/100 (91%)	83 (91%)	8 (9%)	0	100	100
15	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
16	V	92/94 (98%)	92 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	W	74/85 (87%)	72 (97%)	2 (3%)	0	100 100
18	X	75/78 (96%)	75 (100%)	0	0	100 100
19	Y	61/63 (97%)	51 (84%)	10 (16%)	0	100 100
20	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
21	0	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
22	1	48/55 (87%)	48 (100%)	0	0	100 100
23	2	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
24	K	120/123 (98%)	111 (92%)	9 (8%)	0	100 100
25	P	111/115 (96%)	107 (96%)	4 (4%)	0	100 100
26	M	134/136 (98%)	131 (98%)	3 (2%)	0	100 100
27	H	147/149 (99%)	133 (90%)	14 (10%)	0	100 100
28	d	45/70 (64%)	44 (98%)	1 (2%)	0	100 100
31	6	100/105 (95%)	94 (94%)	6 (6%)	0	100 100
32	9	336/390 (86%)	319 (95%)	17 (5%)	0	100 100
33	3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4 3
All	All	3638/3832 (95%)	3452 (95%)	184 (5%)	2 (0%)	54 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	3	31	ILE
33	3	32	LEU

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	g	34/34 (100%)	34 (100%)	0	100 100
2	C	216/218 (99%)	215 (100%)	1 (0%)	88 95
3	D	164/164 (100%)	164 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	159/165 (96%)	159 (100%)	0	100 100
5	F	148/150 (99%)	148 (100%)	0	100 100
6	G	137/138 (99%)	134 (98%)	3 (2%)	52 71
7	J	116/116 (100%)	116 (100%)	0	100 100
8	L	103/103 (100%)	103 (100%)	0	100 100
9	N	100/103 (97%)	100 (100%)	0	100 100
10	O	86/87 (99%)	86 (100%)	0	100 100
11	Q	89/90 (99%)	89 (100%)	0	100 100
12	R	84/84 (100%)	84 (100%)	0	100 100
13	S	93/93 (100%)	93 (100%)	0	100 100
14	T	80/84 (95%)	80 (100%)	0	100 100
15	U	83/85 (98%)	83 (100%)	0	100 100
16	V	78/78 (100%)	77 (99%)	1 (1%)	69 84
17	W	57/63 (90%)	57 (100%)	0	100 100
18	X	67/68 (98%)	67 (100%)	0	100 100
19	Y	55/55 (100%)	55 (100%)	0	100 100
20	Z	48/49 (98%)	48 (100%)	0	100 100
21	0	47/48 (98%)	47 (100%)	0	100 100
22	1	45/49 (92%)	45 (100%)	0	100 100
23	2	38/38 (100%)	37 (97%)	1 (3%)	46 66
24	K	103/104 (99%)	103 (100%)	0	100 100
25	P	98/100 (98%)	98 (100%)	0	100 100
26	M	109/109 (100%)	109 (100%)	0	100 100
27	H	114/114 (100%)	113 (99%)	1 (1%)	78 90
28	d	43/62 (69%)	43 (100%)	0	100 100
31	6	88/91 (97%)	88 (100%)	0	100 100
32	9	273/321 (85%)	271 (99%)	2 (1%)	84 92
33	3	51/52 (98%)	51 (100%)	0	100 100
All	All	3006/3115 (96%)	2997 (100%)	9 (0%)	92 97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	9	203	MET
32	9	278	ARG
6	G	175	LYS
16	V	24	ASN
23	2	28	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
25	P	74	GLN
16	V	87	GLN
12	R	11	GLN
12	R	6	GLN
16	V	80	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	A	2895/2904 (99%)	377 (13%)	9 (0%)
30	B	118/119 (99%)	11 (9%)	0
All	All	3013/3023 (99%)	388 (12%)	9 (0%)

5 of 388 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	A	10	A
29	A	12	U
29	A	14	A
29	A	27	G
29	A	46	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	A	2505	G
29	A	2756	U
29	A	1057	A
29	A	1378	A
29	A	2127	G

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)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	GNP	9	402	35	29,34,34	1.60	7 (24%)	33,54,54	2.12	6 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GNP	9	402	35	-	3/14/38/38	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)
36	9	402	GNP	PB-O3A	4.34	1.64	1.59
36	9	402	GNP	C6-N1	3.08	1.38	1.33
36	9	402	GNP	PB-O1B	3.00	1.50	1.46
36	9	402	GNP	PG-N3B	2.90	1.70	1.63
36	9	402	GNP	PG-O1G	2.62	1.50	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	9	402	GNP	C5-C6-N1	-8.41	111.92	123.43
36	9	402	GNP	C2-N1-C6	5.82	125.17	115.93
36	9	402	GNP	N3-C2-N1	-2.73	123.59	127.22
36	9	402	GNP	PB-O3A-PA	-2.65	123.28	132.62
36	9	402	GNP	C4-C5-C6	-2.62	118.30	120.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	9	402	GNP	O4'-C4'-C5'-O5'
36	9	402	GNP	C4'-C5'-O5'-PA
36	9	402	GNP	C5'-O5'-PA-O3A

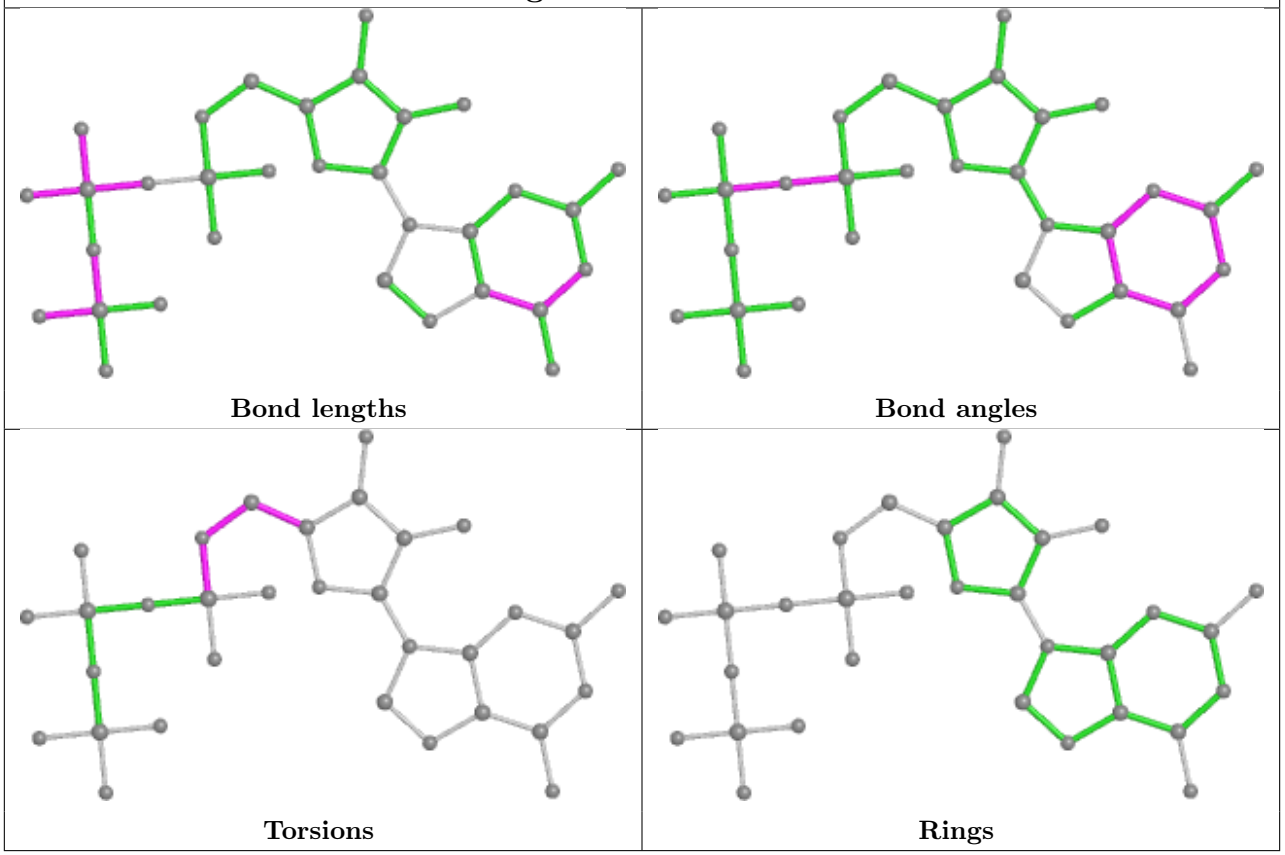
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	9	402	GNP	1	0

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

Ligand GNP 9 402



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.

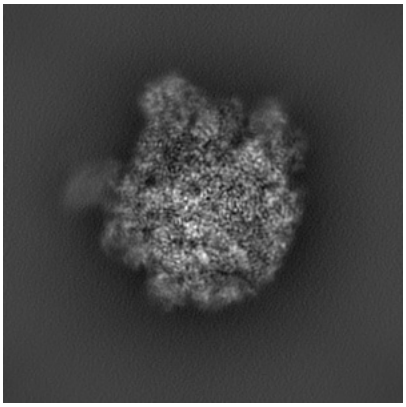
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12217. These allow visual inspection of the internal detail of the map and identification of artifacts.

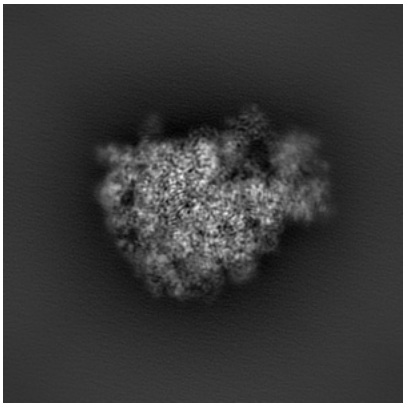
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

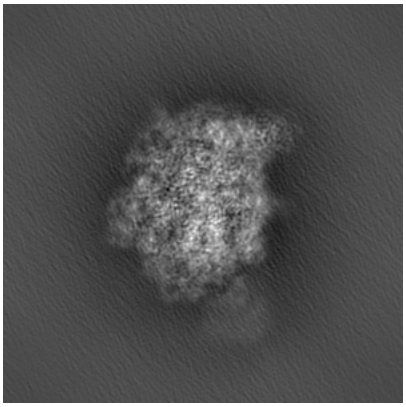
6.1.1 Primary map



X



Y

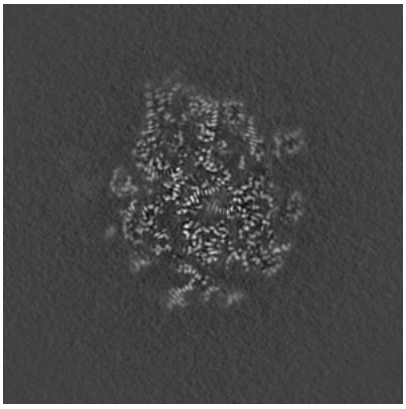


Z

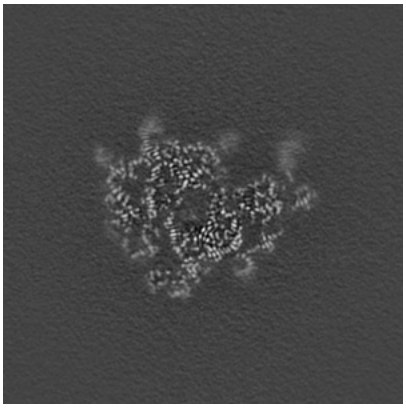
The images above show the map projected in three orthogonal directions.

6.2 Central slices

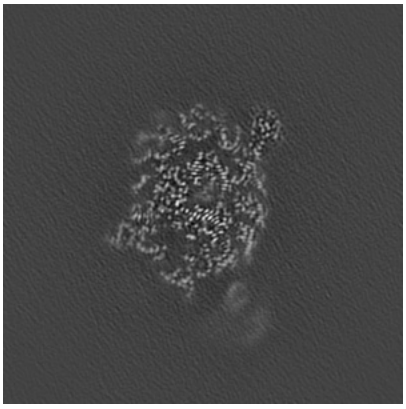
6.2.1 Primary map



X Index: 180



Y Index: 180

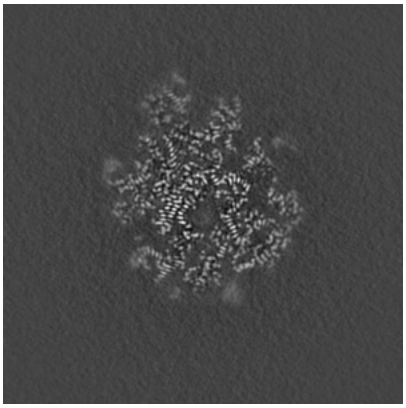


Z Index: 180

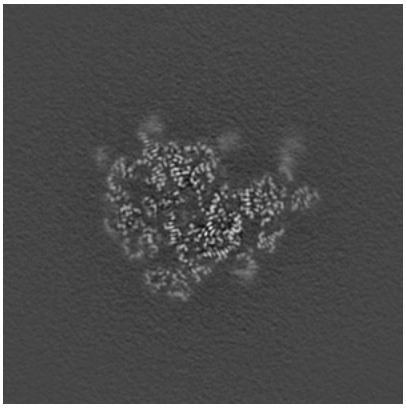
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

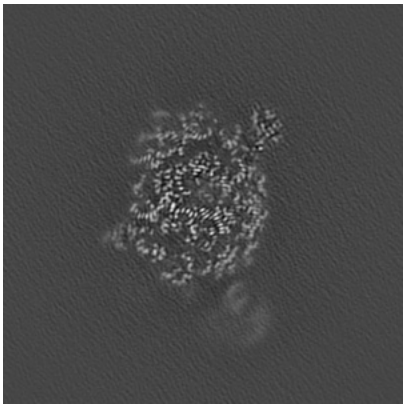
6.3.1 Primary map



X Index: 170



Y Index: 178

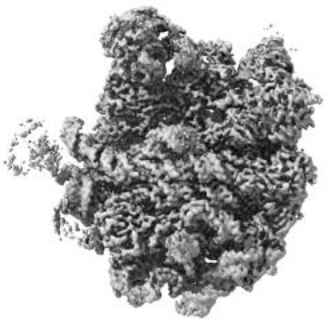


Z Index: 182

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

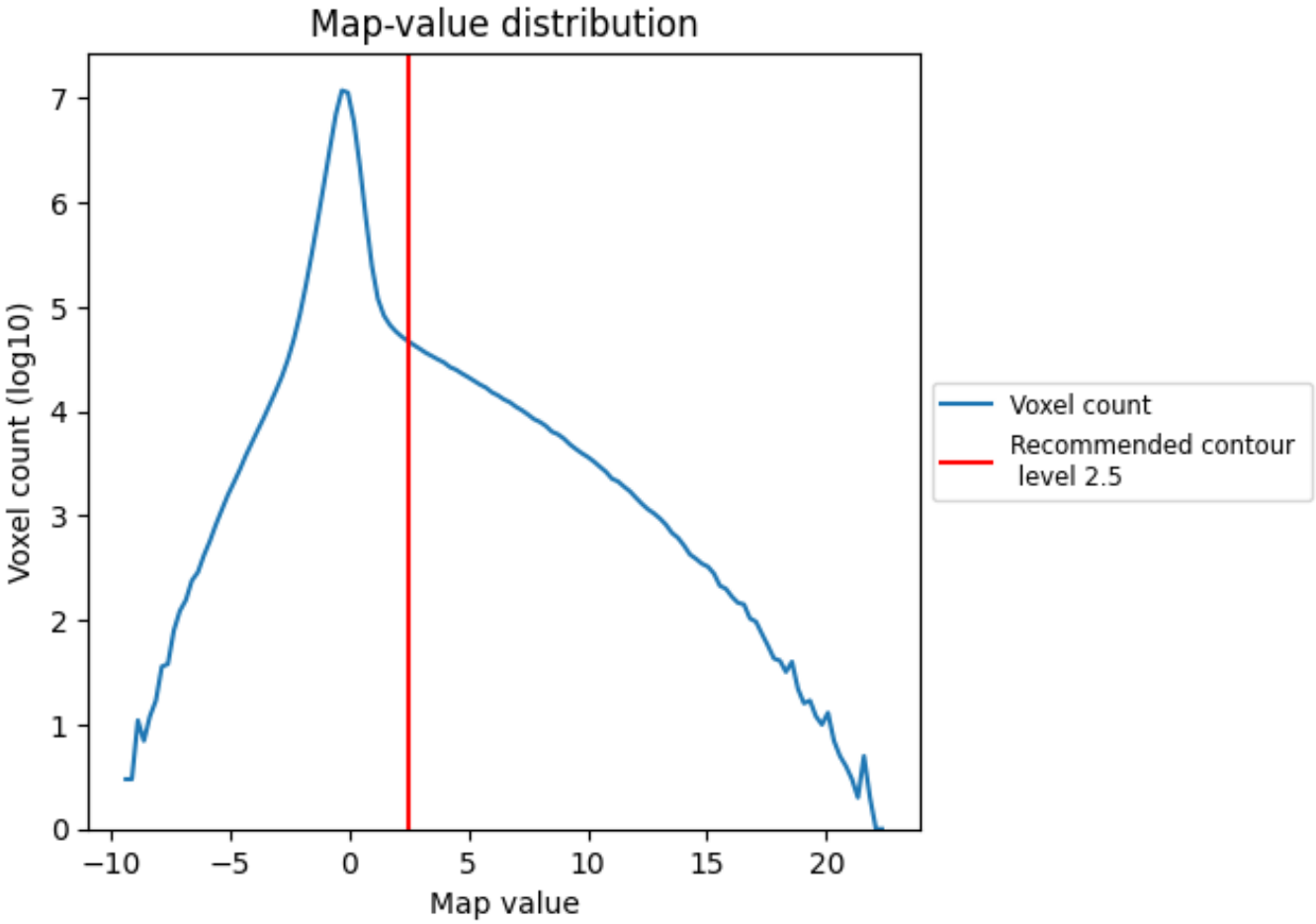
6.5 Mask visualisation (i)

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

7 Map analysis

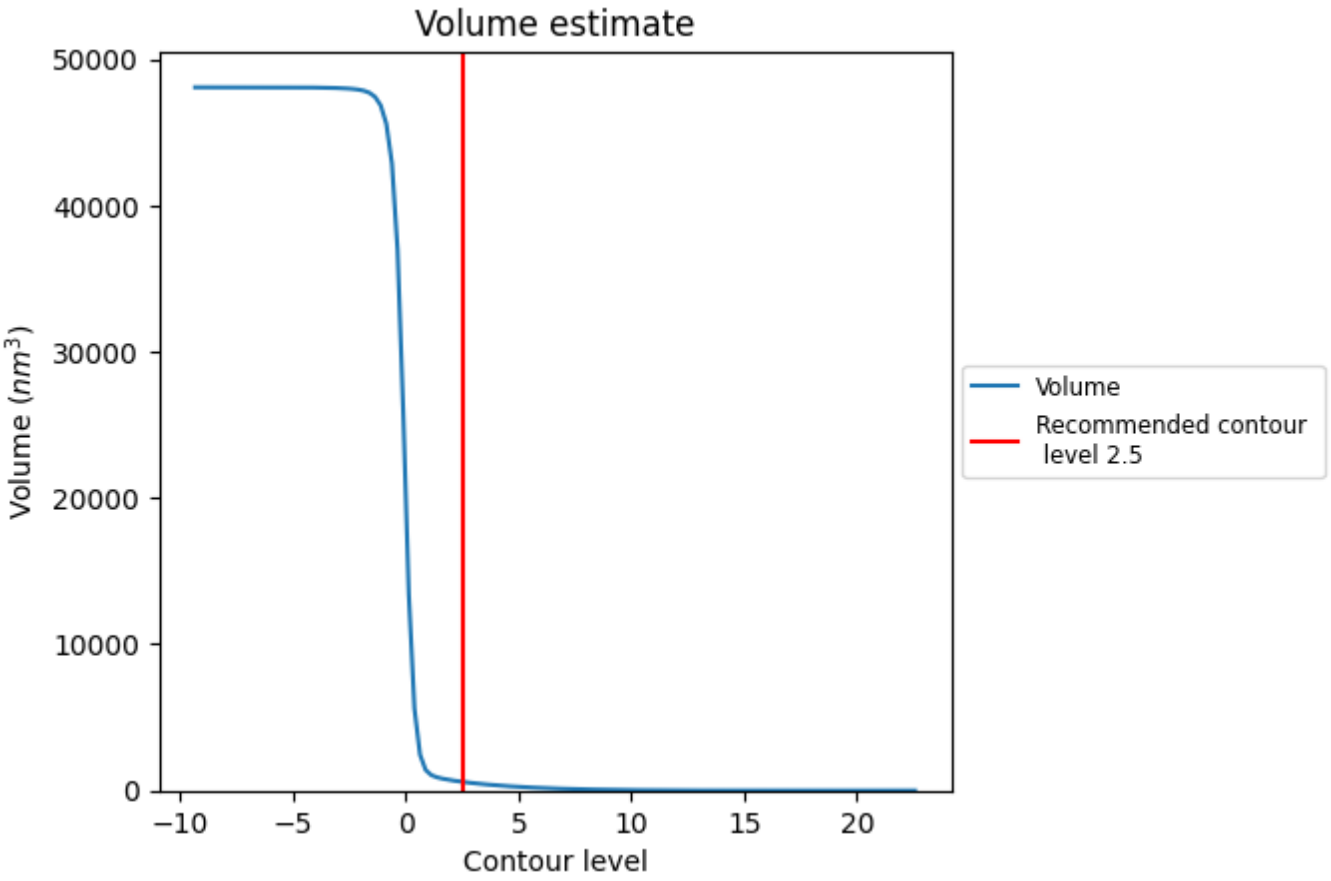
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

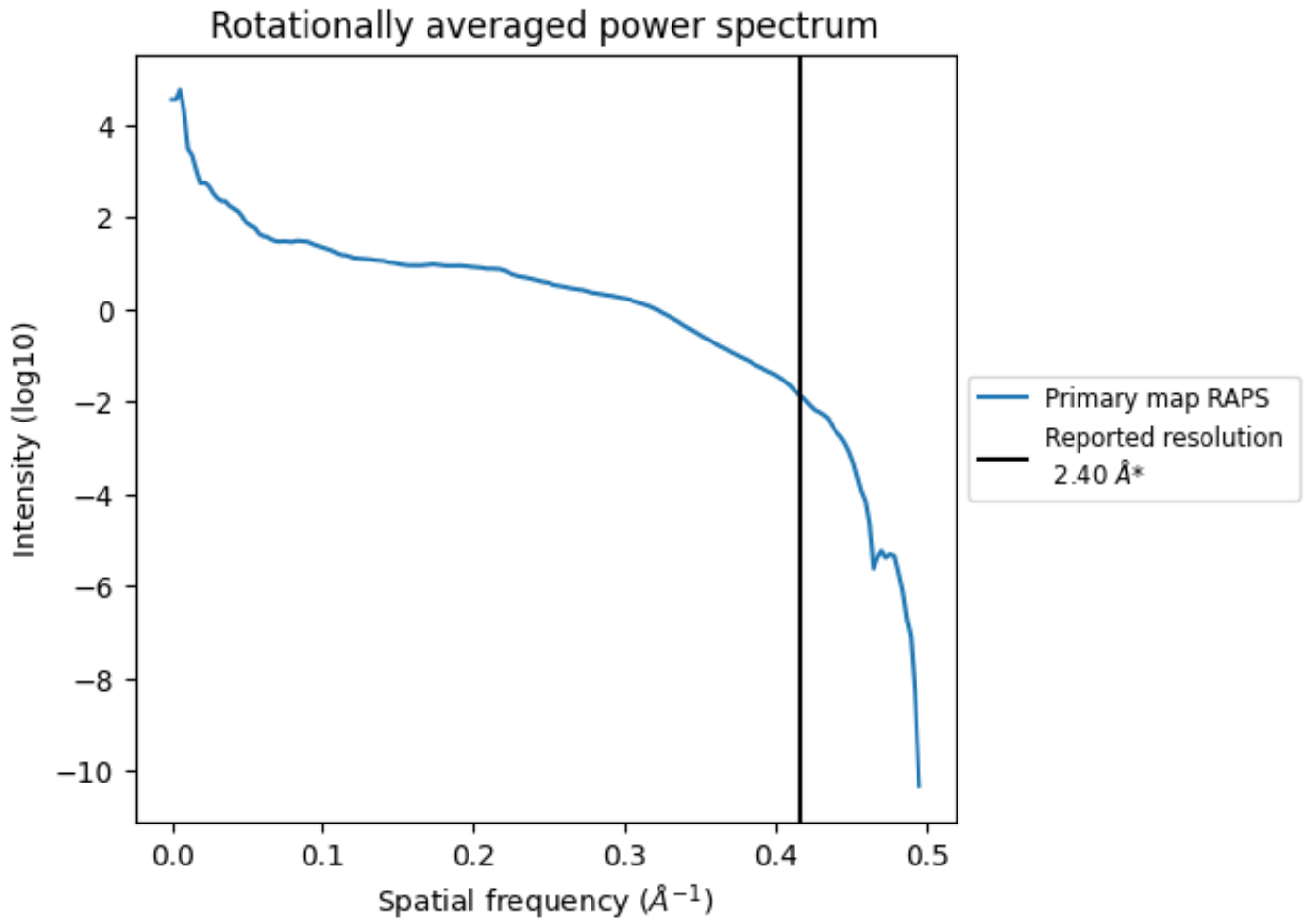
7.2 Volume estimate (i)



The volume at the recommended contour level is 597 nm^3; this corresponds to an approximate mass of 540 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)

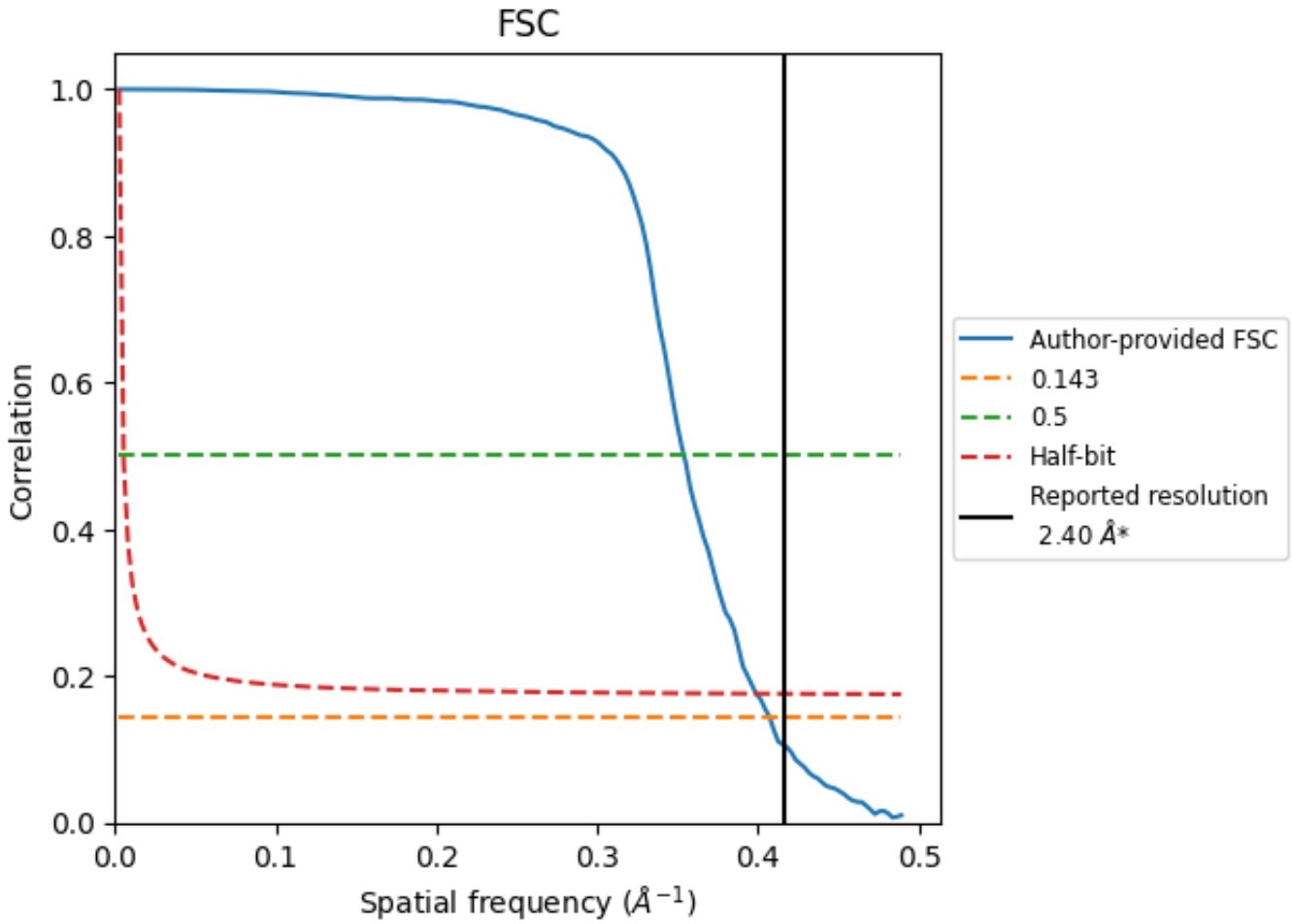


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

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 0.417 Å^{-1}

8.2 Resolution estimates (i)

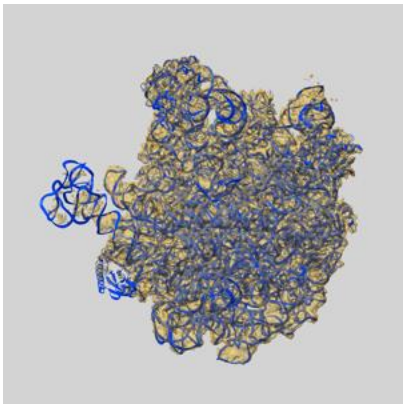
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.46	2.83	2.51
Unmasked-calculated*	-	-	-

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

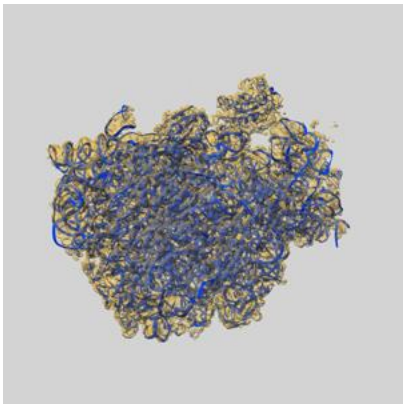
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12217 and PDB model 7BL4. Per-residue inclusion information can be found in section 3 on page 12.

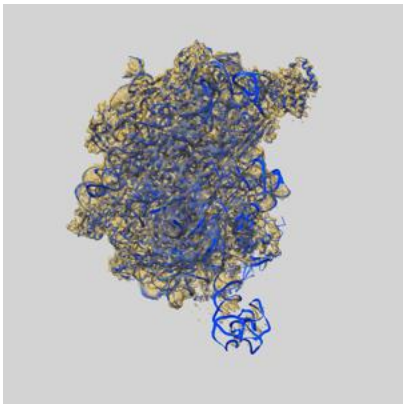
9.1 Map-model overlay



X



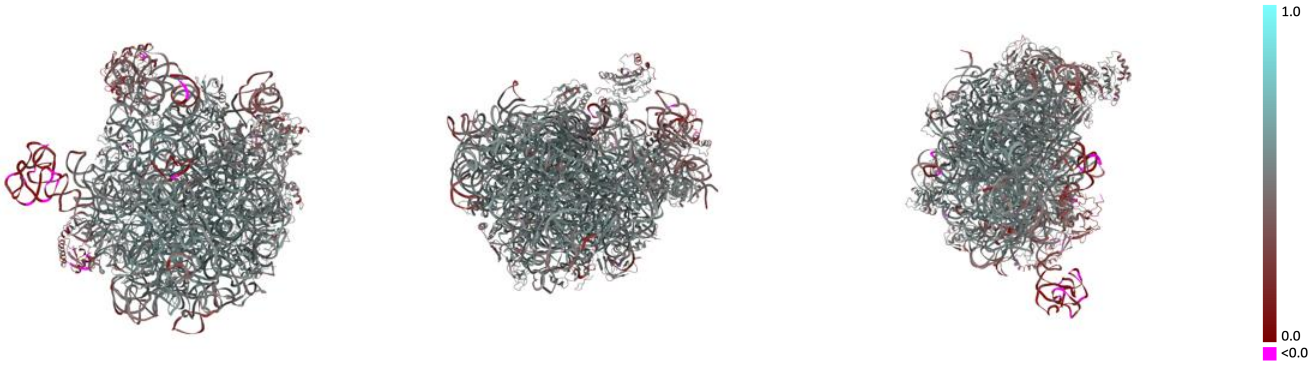
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

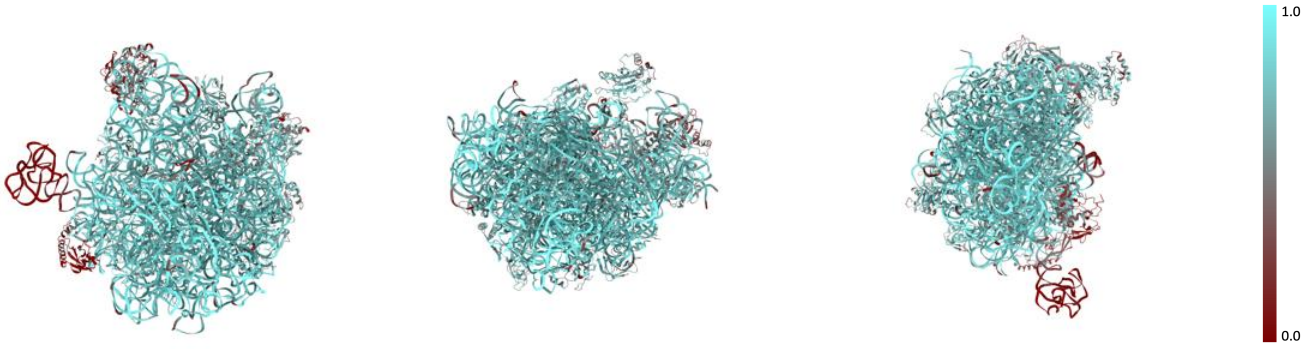
9.2 Q-score mapped to coordinate model (i)



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.

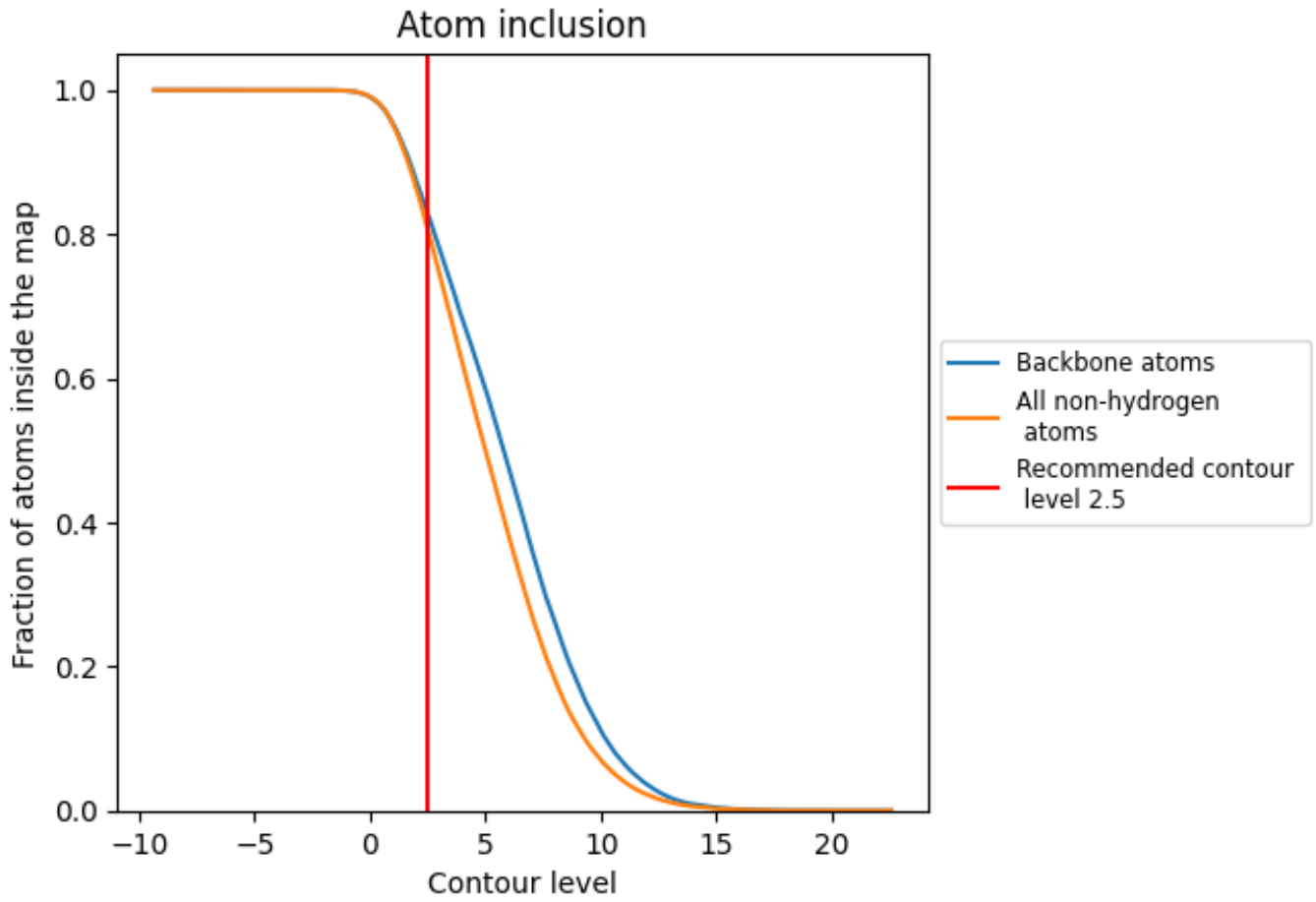
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 81% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8071	0.4920
0	0.7336	0.4890
1	0.7057	0.5000
2	0.8338	0.5840
3	0.8106	0.5410
6	0.7073	0.4610
9	0.6451	0.4460
A	0.8682	0.5010
B	0.8528	0.4730
C	0.7887	0.5260
D	0.7159	0.5110
E	0.6985	0.4970
F	0.3933	0.3250
G	0.5705	0.4280
H	0.2091	0.2510
J	0.7418	0.5190
K	0.7766	0.5130
L	0.7471	0.5010
M	0.7591	0.5180
N	0.7646	0.5210
O	0.6489	0.4340
P	0.7063	0.4870
Q	0.8062	0.5420
R	0.7365	0.4910
S	0.7608	0.5280
T	0.7161	0.5000
U	0.6323	0.4350
V	0.7141	0.4850
W	0.7861	0.5350
X	0.7737	0.5210
Y	0.6781	0.4250
Z	0.7391	0.4940
d	0.1961	0.2170
g	0.6451	0.5040