wwPDB EM Validation Summary Report

Oct 13, 2024 – 02:26 am BST

PDB ID	:	7PAS
EMDB ID	:	EMD-13282
Title	:	70S ribosome with P/E-site tRNA in Mycoplasma pneumoniae cells
Authors	:	Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.
Deposited on	:	2021-07-30
Resolution	:	16.00 Å(reported)
Based on initial models	:	4V7C, 7OOD, 7OOC

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:

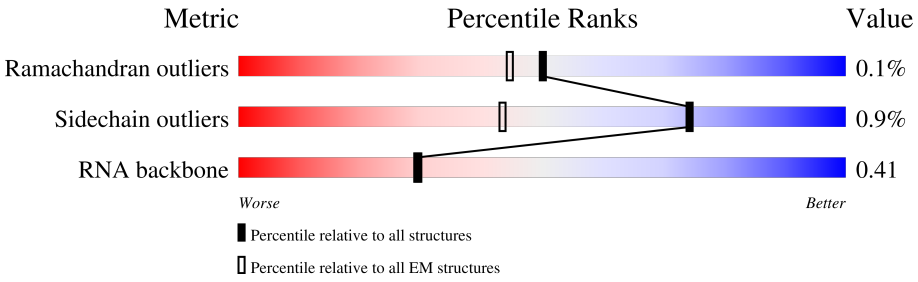
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 16.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	48	98% ·
2	1	59	100%
3	2	37	· 97% ·
4	A	294	25% 81% 18%
5	B	273	25% 79% 21%
6	C	205	12% 98% ··
7	D	219	8% 70% 30%
8	E	215	19% 77% · 22%

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Mol	Chain	Length	Quality of chain
9	F	155	23% 97%
10	G	142	16% 99%
11	H	132	20% 97%
12	I	108	25% 94% 6%
13	J	121	13% 94% 6%
14	K	139	93% 5%
15	L	124	34% 94% 5%
16	M	61	97%
17	N	86	8% 95%
18	O	94	84% 15%
19	P	85	13% 95%
20	Q	104	62% 38%
21	R	87	7% 95%
22	S	87	87% 11%
23	T	60	13% 88% 12%
24	a	287	99%
25	b	287	6% 80% 20%
26	c	212	11% 99%
27	d	180	28% 96%
28	e	184	22% 96%
29	f	149	54% 97%
30	g	161	38% 71% 7% 22%
31	h	137	53% 93% 7%
32	i	146	8% 98%
33	j	122	7% 100%

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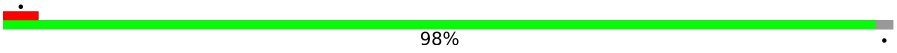
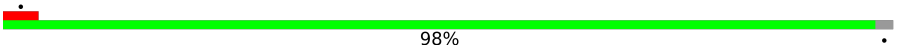
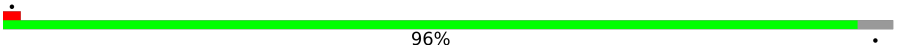
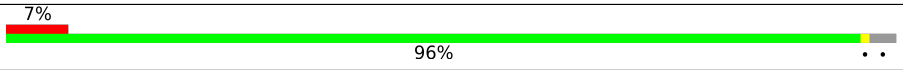
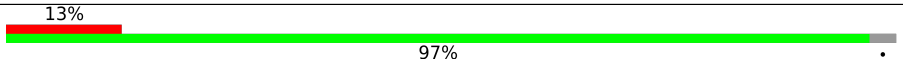
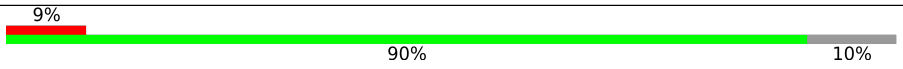
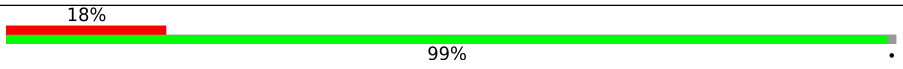
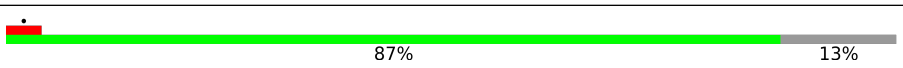
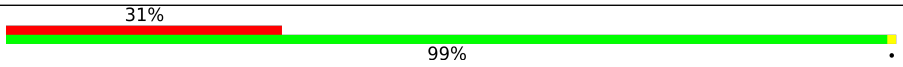
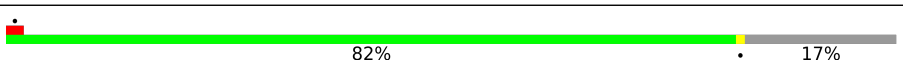
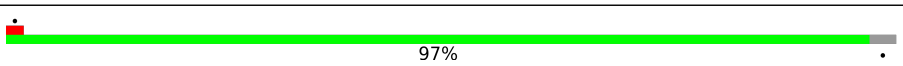
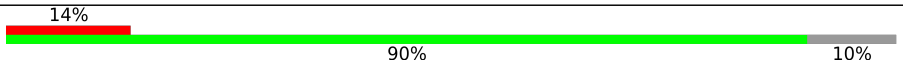
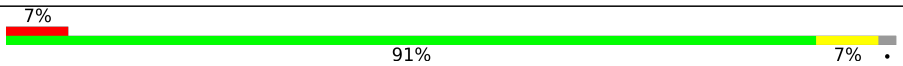
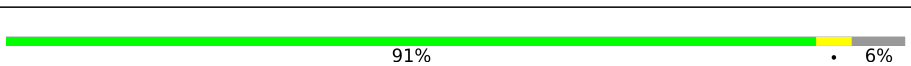
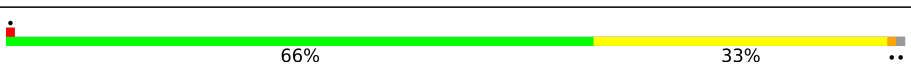
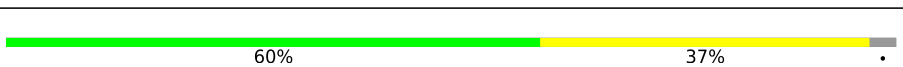
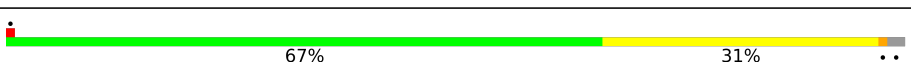
Mol	Chain	Length	Quality of chain
34	k	151	
35	l	139	
36	m	124	
37	n	116	
38	o	119	
39	p	127	
40	q	100	
41	r	159	
42	s	237	
43	t	111	
44	u	104	
45	v	65	
46	w	111	
47	x	97	
48	y	57	
49	z	53	
50	3	2907	
51	4	108	
52	5	1520	
53	8	76	

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 144440 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 L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	47	380	236	81	61	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	59	477	300	99	77	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	37	304	189	65	46	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	240	1921	1226	334	352	9	0	0

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	215	1698	1073	313	307	5	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	203	1660	1051	314	290	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	153	Total	C	N	O	S	0	0
			1173	742	226	202	3		

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	167	Total	C	N	O	S	0	0
			1362	857	240	263	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	154	Total	C	N	O	S	0	0
			1246	785	239	216	6		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	128	Total	C	N	O	S	0	0
			1028	655	191	181	1		

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	101	Total	C	N	O	S	0	0
			809	523	142	143	1		

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	136	Total	C	N	O	S	0	0
			1076	680	213	181	2		

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	L	118	Total	C	N	O	0	0
			951	594	191	166		

- Molecule 16 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	N	83	Total	C	N	O	0	0
			673	428	125	120		

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	80	Total	C	N	O	S	0	0
			646	414	119	111	2		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	P	83	Total	C	N	O	0	0
			675	425	135	115		

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	65	Total	C	N	O	S	0	0
			535	342	103	86	4		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	84	Total	C	N	O	S	0	0
			682	435	127	118	2		

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	77	Total	C	N	O	0	0
			629	383	135	111		

- Molecule 23 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	53	Total	C	N	O	S	0	0
			471	295	103	72	1		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	229	Total	C	N	O	S	0	0
			1762	1119	318	318	7		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	210	Total	C	N	O	S	0	0
			1644	1047	297	297	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1388	893	245	246	4		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	e	176	Total 1396	C 899	N 247	O 250	0	0

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	145	Total 1160	C 746	N 204	O 207	S 3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	126	Total 960	C 612	N 167	O 178	S 3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	128	Total 959	C 616	N 160	O 177	S 6	0	0

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	144	Total 1164	C 737	N 213	O 209	S 5	0	0

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	122	Total 944	C 595	N 178	O 167	S 4	0	0

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	k	148	Total 1153	C 731	N 226	O 196	0	0

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	112	Total	C	N	O	S	0	0
			889	557	175	155	2		

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	115	Total	C	N	O	S	0	0
			938	592	180	165	1		

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	114	Total	C	N	O	S	0	0
			947	603	188	154	2		

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	139	Total	C	N	O	S	0	0
			1068	663	207	191	7		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	92	Total	C	N	O	S	0	0
			720	475	122	122	1		

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	111	Total	C	N	O	S	0	0
			872	550	166	153	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	86	Total	C	N	O	S	0	0
			657	409	130	117	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	63	Total	C	N	O	S	0	0
			513	317	108	87	1		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	w	100	Total	C	N	O	0	0
			818	517	153	148		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	44	Total	C	N	O	S	0	0
			344	221	55	64	4		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 49 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 50 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	2878	Total	C	N	O	P	0	0
			61664	27558	11236	19995	2875		

- Molecule 51 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	105	Total	C	N	O	P	0	0
			2239	1003	409	724	103		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5	1493	Total	C	N	O	P	0	0
			31943	14279	5792	10382	1490		

- Molecule 53 is a RNA chain called tRNA-Phe.

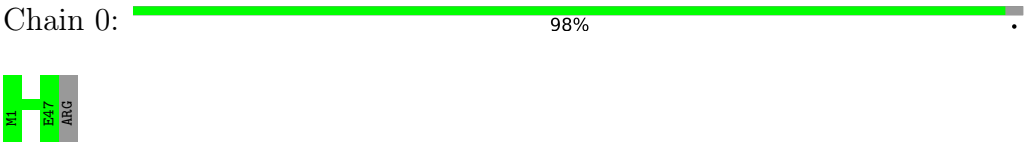
Mol	Chain	Residues	Atoms					AltConf	Trace
53	8	73	Total	C	N	O	P	0	0
			1556	695	278	511	72		

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 L34

Chain 0:



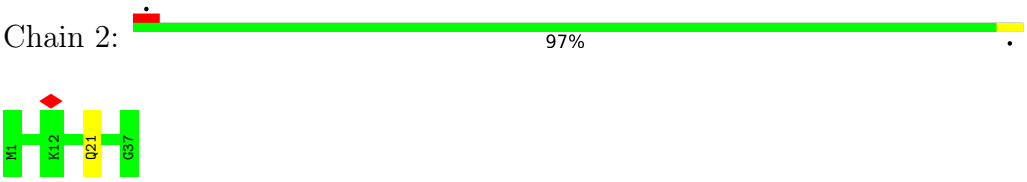
• Molecule 2: 50S ribosomal protein L35

Chain 1:

There are no outlier residues recorded for this chain.

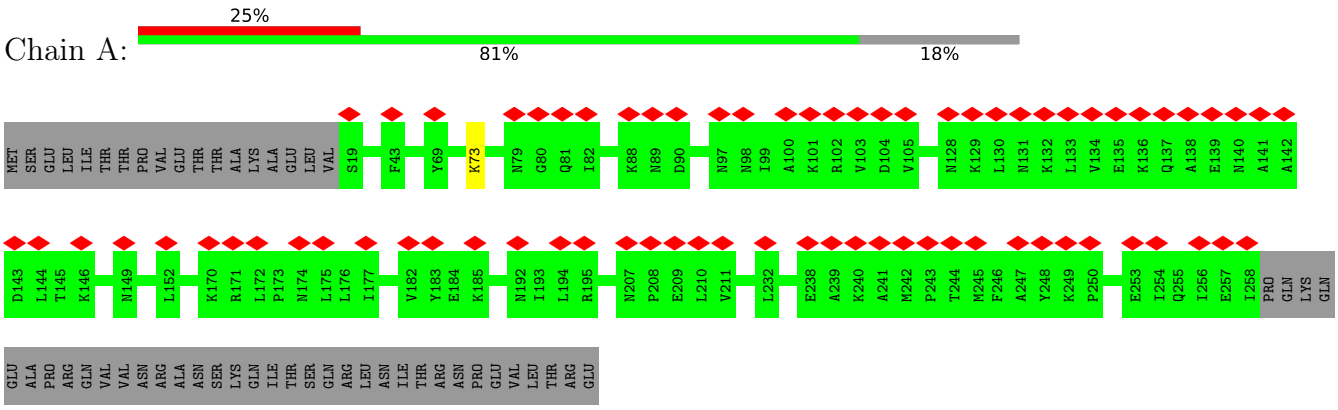
• Molecule 3: 50S ribosomal protein L36

Chain 2:



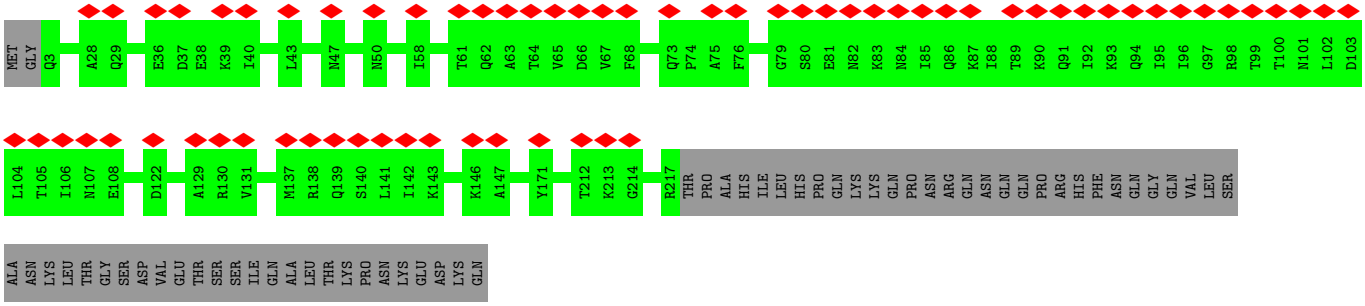
• Molecule 4: 30S ribosomal protein S2

Chain A:



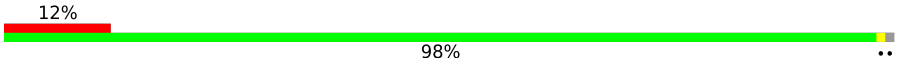
• Molecule 5: 30S ribosomal protein S3

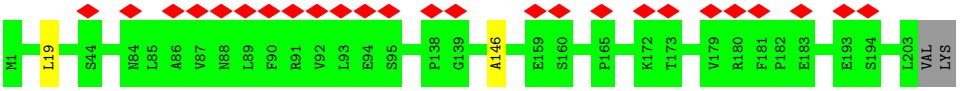
Chain B:



• Molecule 6: 30S ribosomal protein S4

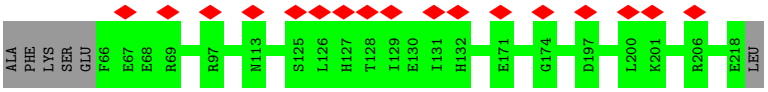
Chain C:





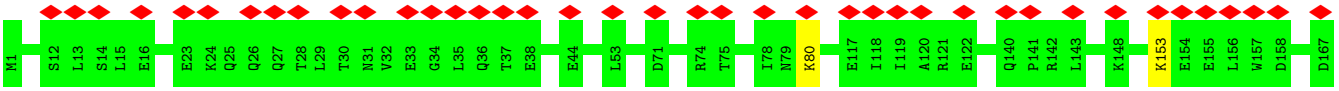
• Molecule 7: 30S ribosomal protein S5

Chain D:



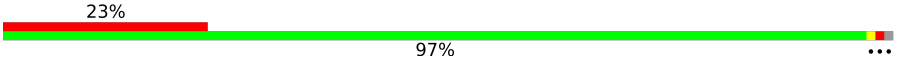
• Molecule 8: 30S ribosomal protein S6

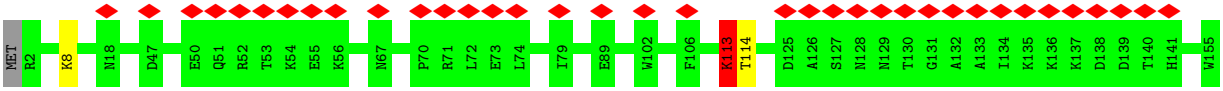
Chain E:



• Molecule 9: 30S ribosomal protein S7

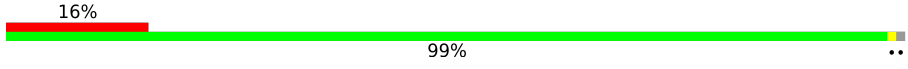
Chain F:

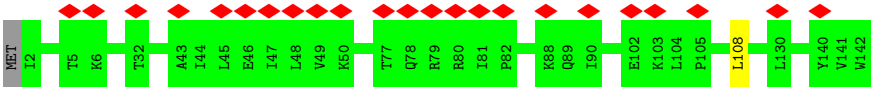




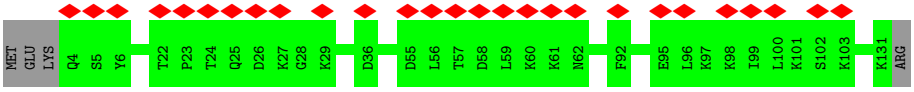
• Molecule 10: 30S ribosomal protein S8

Chain G:

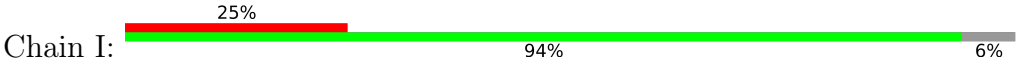


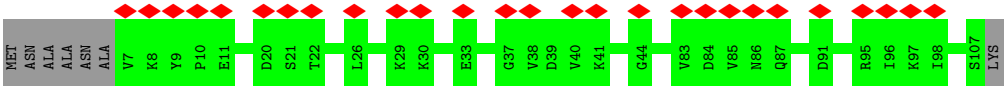


• Molecule 11: 30S ribosomal protein S9

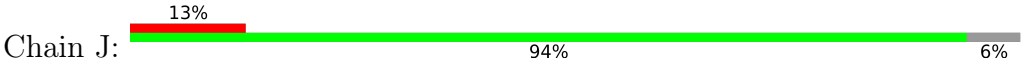


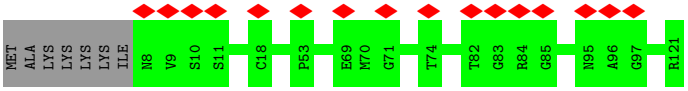
• Molecule 12: 30S ribosomal protein S10



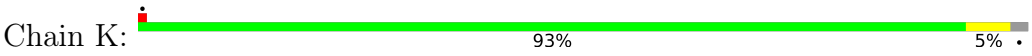


• Molecule 13: 30S ribosomal protein S11

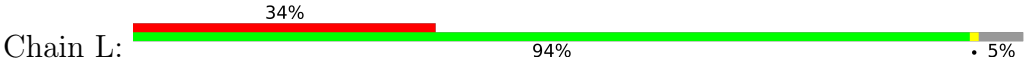


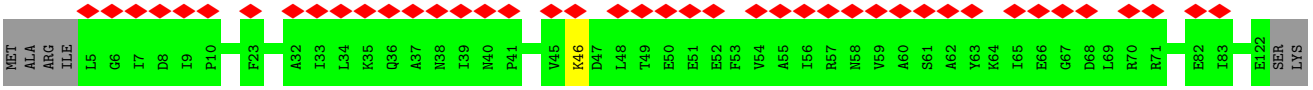


• Molecule 14: 30S ribosomal protein S12

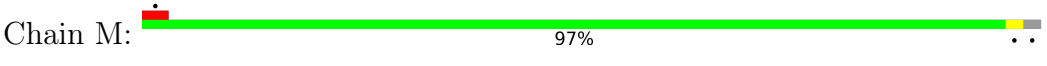


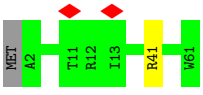
• Molecule 15: 30S ribosomal protein S13





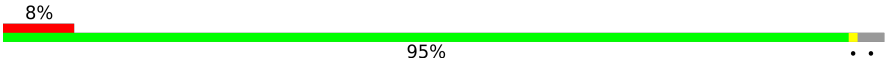
• Molecule 16: 30S ribosomal protein S14 type Z

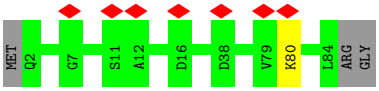




• Molecule 17: 30S ribosomal protein S15

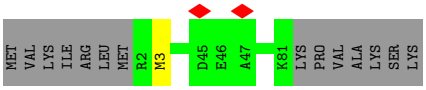
Chain N:





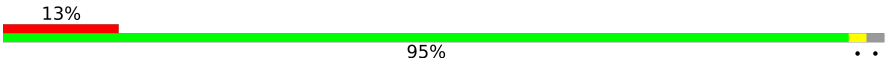
• Molecule 18: 30S ribosomal protein S16

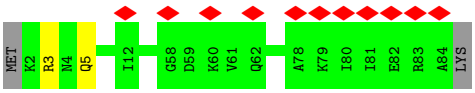
Chain O:



• Molecule 19: 30S ribosomal protein S17

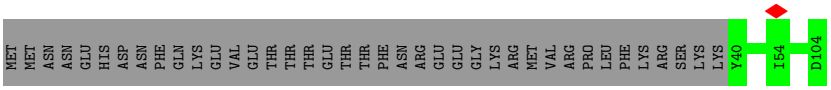
Chain P:





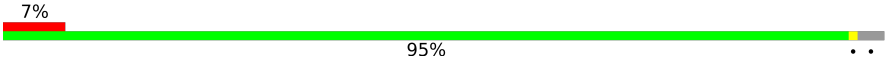
• Molecule 20: 30S ribosomal protein S18

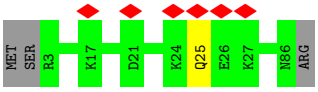
Chain Q:



• Molecule 21: 30S ribosomal protein S19

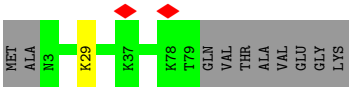
Chain R:





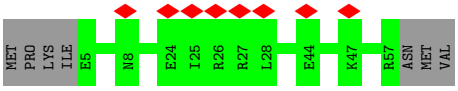
• Molecule 22: 30S ribosomal protein S20

Chain S:



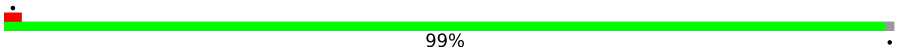
• Molecule 23: 30S ribosomal protein S21

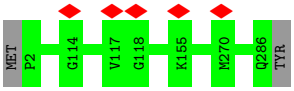
Chain T:



• Molecule 24: 50S ribosomal protein L2

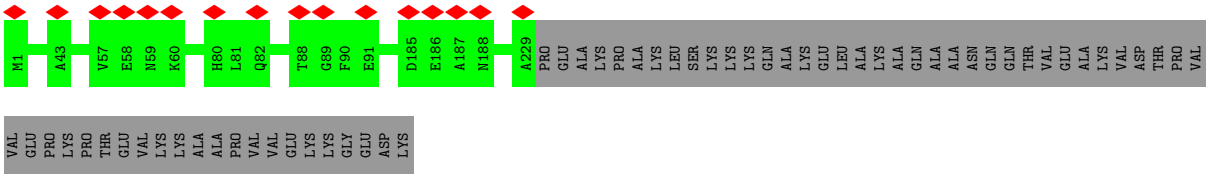
Chain a:





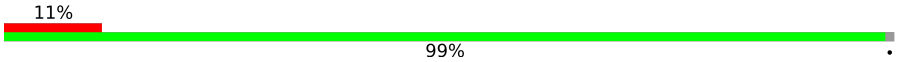
• Molecule 25: 50S ribosomal protein L3

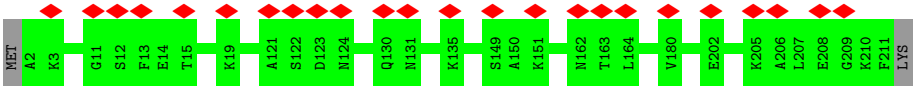
Chain b:



• Molecule 26: 50S ribosomal protein L4

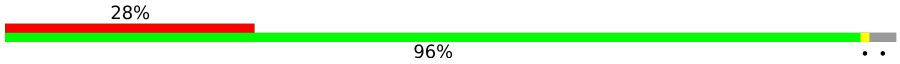
Chain c:

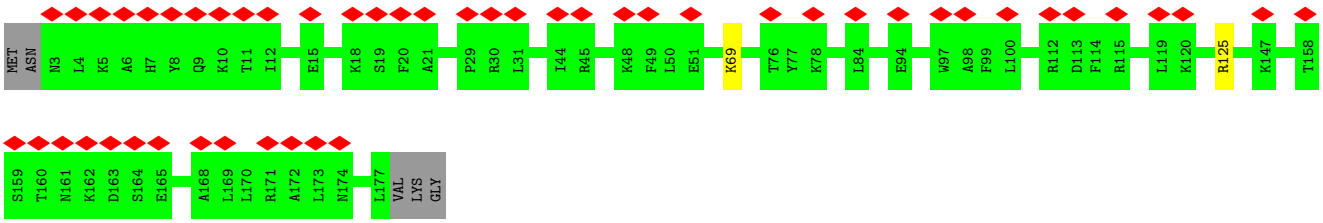




• Molecule 27: 50S ribosomal protein L5

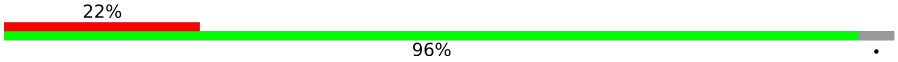
Chain d:

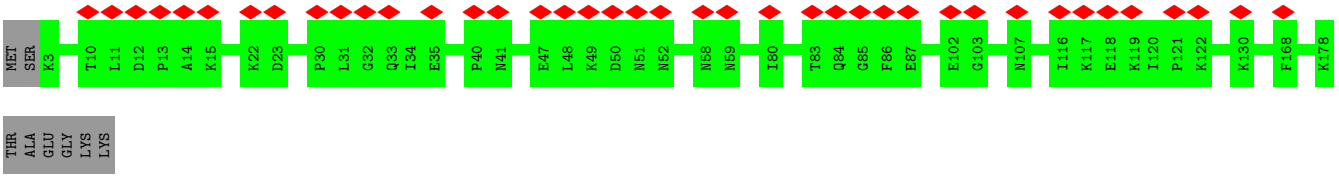




• Molecule 28: 50S ribosomal protein L6

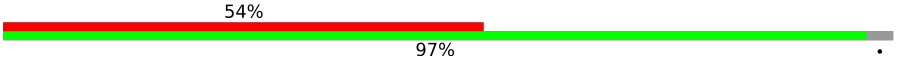
Chain e:

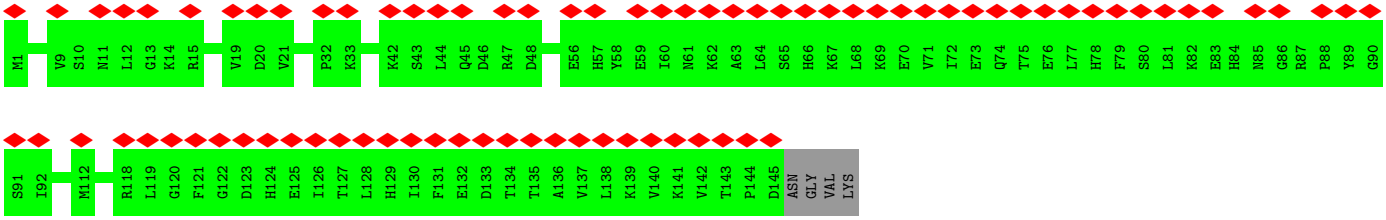




• Molecule 29: 50S ribosomal protein L9

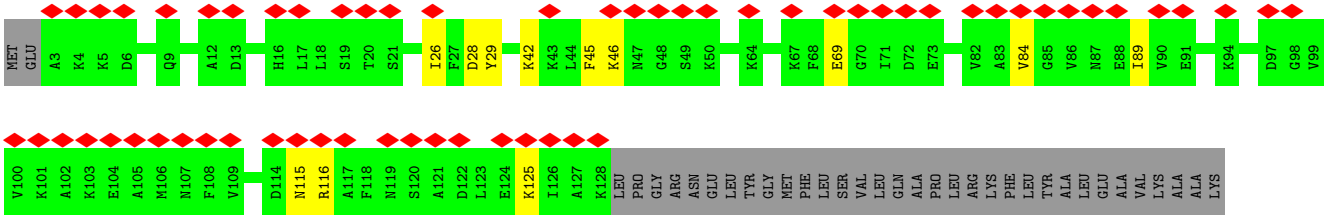
Chain f:





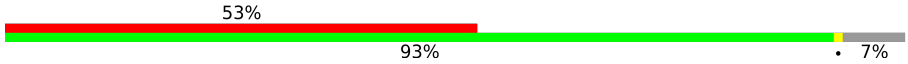
• Molecule 30: 50S ribosomal protein L10

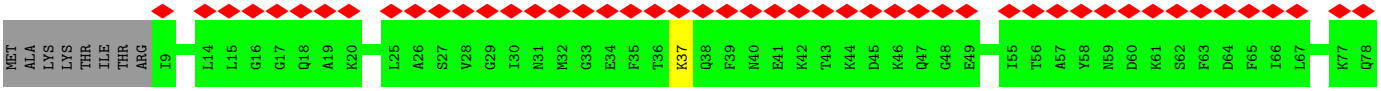
Chain g:

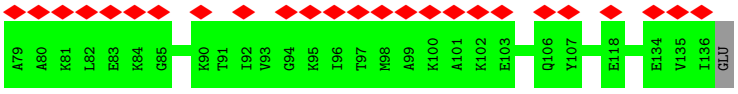


• Molecule 31: 50S ribosomal protein L11

Chain h:

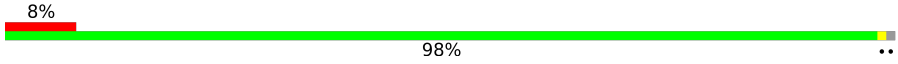


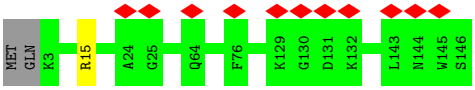




• Molecule 32: 50S ribosomal protein L13

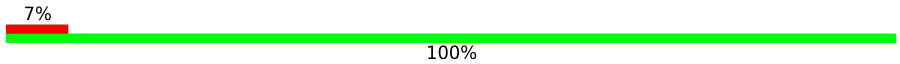
Chain i:

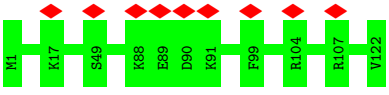




• Molecule 33: 50S ribosomal protein L14

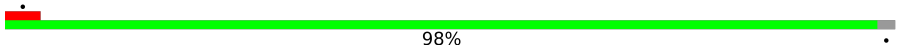
Chain j:

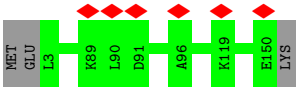




• Molecule 34: 50S ribosomal protein L15

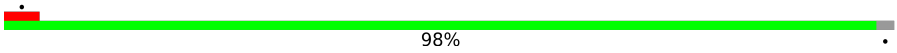
Chain k:

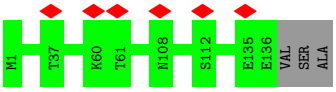




• Molecule 35: 50S ribosomal protein L16

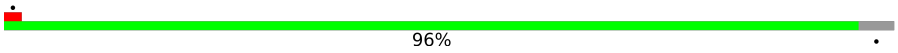
Chain l:

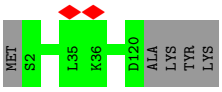




• Molecule 36: 50S ribosomal protein L17

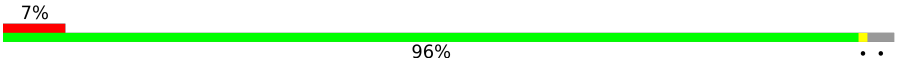
Chain m:

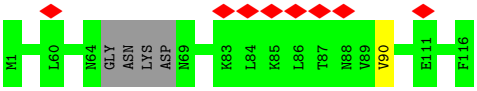




• Molecule 37: 50S ribosomal protein L18

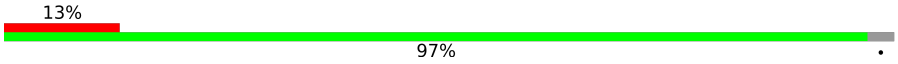
Chain n:

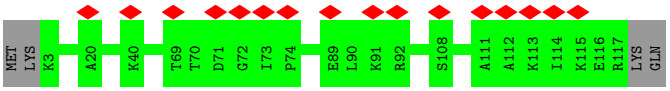




• Molecule 38: 50S ribosomal protein L19

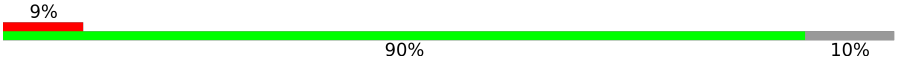
Chain o:

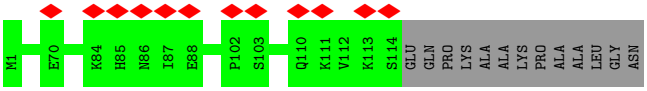




• Molecule 39: 50S ribosomal protein L20

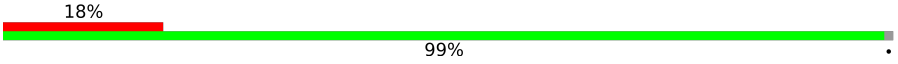
Chain p:

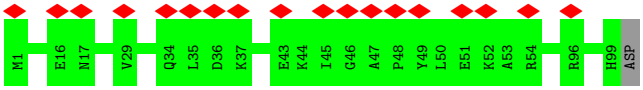




• Molecule 40: 50S ribosomal protein L21

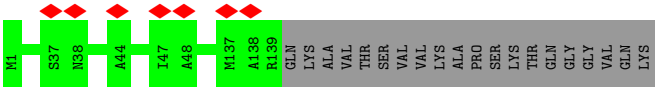
Chain q:





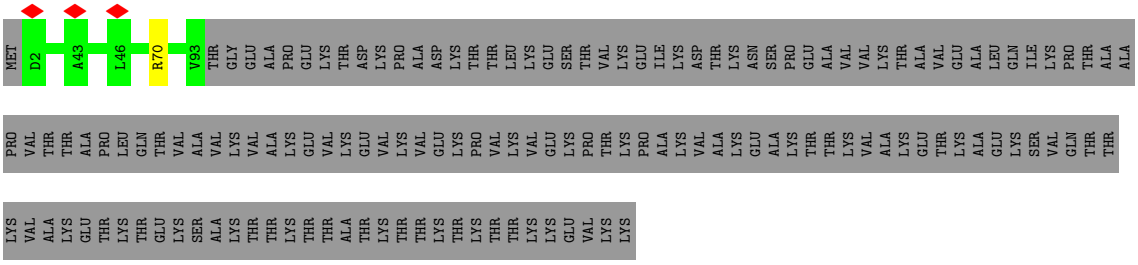
• Molecule 41: 50S ribosomal protein L22

Chain r:



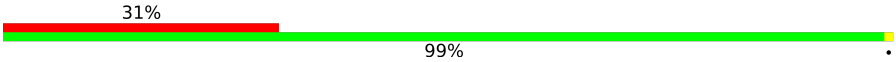
• Molecule 42: 50S ribosomal protein L23

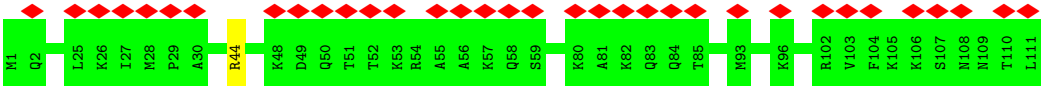
Chain s:



• Molecule 43: 50S ribosomal protein L24

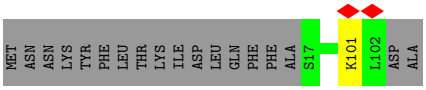
Chain t:





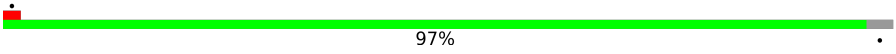
• Molecule 44: 50S ribosomal protein L27

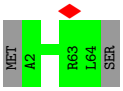
Chain u:



• Molecule 45: 50S ribosomal protein L28

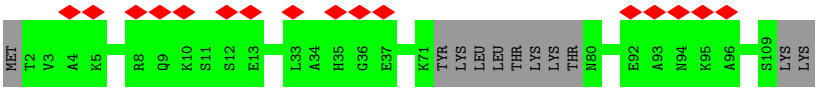
Chain v:





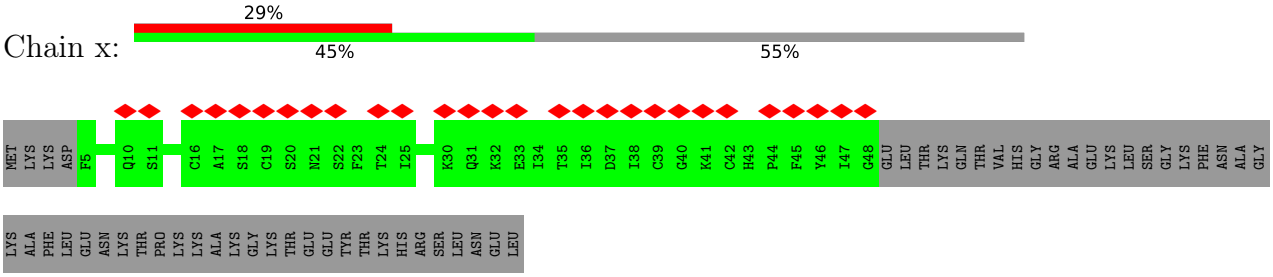
• Molecule 46: 50S ribosomal protein L29

Chain w:



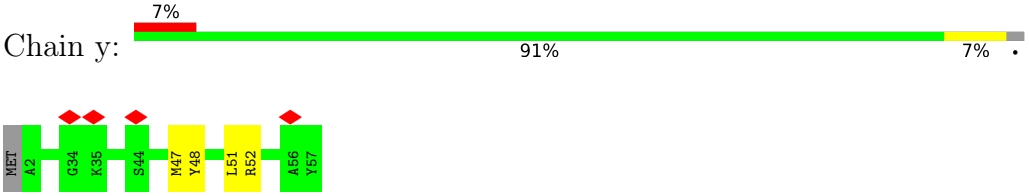
• Molecule 47: 50S ribosomal protein L31

Chain x:



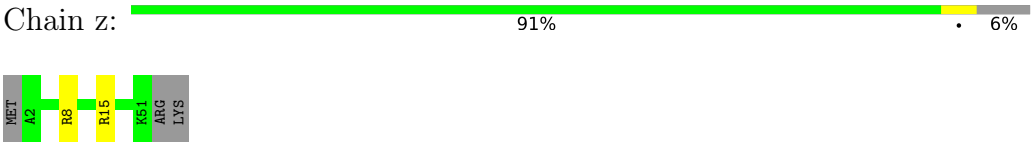
• Molecule 48: 50S ribosomal protein L32

Chain y:



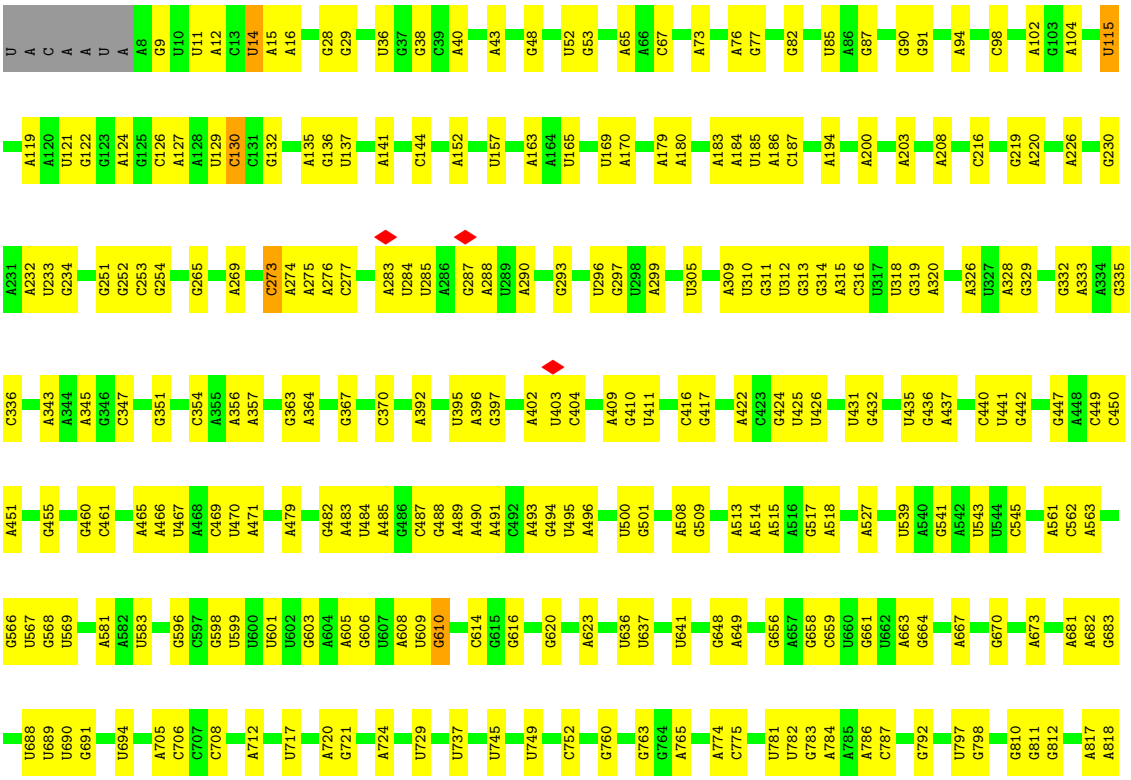
• Molecule 49: 50S ribosomal protein L33 1

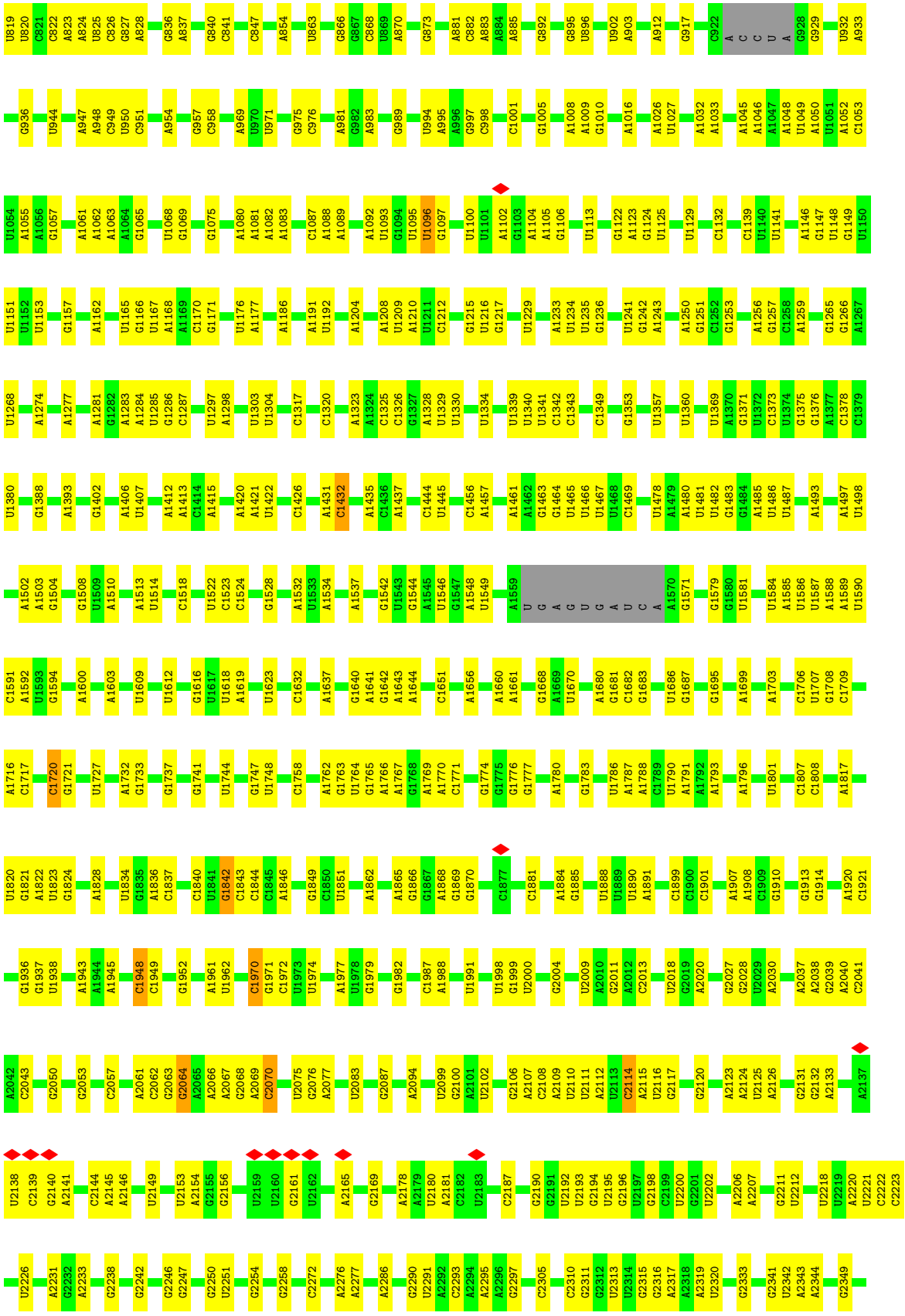
Chain z:

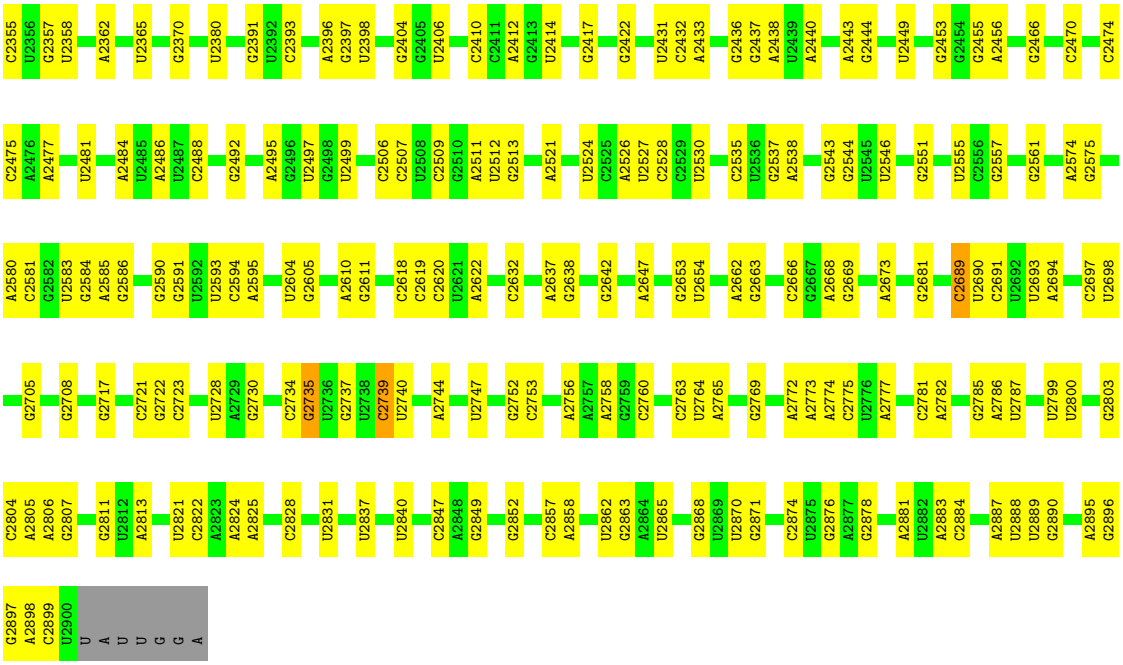


• Molecule 50: 23S ribosomal RNA

Chain 3:




U819 U820 C821 C822 A823 A824 U825 C826 G827 A828 G836 A837 G840 C841 C847 A854 U863 G866 G867 C868 U869 A870 G873 A881 C882 A883 A884 A885 G892 G895 U896 U902 A903 A912 G917 C922 A C C U A G928 G929 U932 A933
G936 U944 A947 A948 C949 U950 C951 A954 G957 C958 A969 U970 U971 G975 C976 A981 G982 A983 G989 U994 A995 A996 G997 C998 C1001 G1005 A1008 A1009 G1010 A1016 A1026 U1027 A1032 A1033 A1045 A1046 A1047 A1048 U1049 A1050 U1051 A1052 C1053
U1054 A1055 A1056 G1057 A1061 A1062 A1063 A1064 G1065 U1068 G1069 G1075 A1080 A1081 A1082 A1083 C1087 A1088 A1089 A1092 U1093 G1094 U1095 U1096 G1097 U1100 U1101 A1102 G1103 A1104 A1105 G1106 U1113 G1122 A1123 G1124 U1125 U1129 C1132 C1139 U1140 U1141 A1146 G1147 U1148 G1149 U1150
U1151 U1152 U1153 G1157 A1162 U1165 G1166 U1167 A1168 A1169 C1170 G1171 U1176 A1177 A1186 A1191 U1192 A1204 A1208 U1209 A1210 U1211 C1212 G1215 U1216 G1217 U1229 A1233 U1234 U1235 G1236 U1241 G1242 A1243 A1250 G1251 C1252 G1253 A1256 G1257 C1258 A1259 G1265 G1266 A1267
U1268 A1274 A1277 A1281 G1282 A1283 A1284 U1285 G1286 C1287 U1297 A1298 U1303 U1304 C1317 C1320 A1323 A1324 C1325 C1326 G1327 A1328 U1329 U1330 U1334 U1339 U1340 U1341 C1342 C1343 C1349 G1353 U1357 U1360 U1369 A1370 G1371 U1372 C1373 U1374 G1375 G1376 A1377 C1378 C1379
U1380 G1388 A1393 G1402 A1406 U1407 A1412 A1413 C1414 A1415 A1420 A1421 U1422 C1426 A1431 C1432 A1435 C1436 A1437 C1444 U1445 C1456 A1457 A1461 A1462 G1463 G1464 U1465 U1466 U1467 U1468 C1469 U1478 A1479 A1480 U1481 U1482 G1483 G1484 A1485 U1486 U1487 A1493 A1497 U1498
A1502 A1503 G1504 G1508 U1509 A1510 A1513 U1514 C1518 U1522 C1523 C1524 G1528 A1532 U1533 A1534 A1537 G1542 U1543 G1544 A1545 U1546 G1547 A1548 U1549 A1559 U G A G U G A U C A A1570 G1571 G1579 G1580 U1581 U1584 A1585 U1586 U1587 A1588 A1589 U1590
C1591 A1592 U1593 G1594 A1600 A1603 U1609 U1612 G1616 U1617 U1618 A1619 U1623 C1632 A1637 G1640 A1641 G1642 A1643 A1644 C1651 A1656 A1660 A1661 G1668 A1669 U1670 A1680 G1681 C1682 G1683 U1686 G1687 G1695 A1699 A1703 C1706 U1707 G1708 C1709
A1716 C1717 C1720 G1721 U1727 A1732 G1733 G1737 G1741 U1744 G1747 U1748 C1758 A1762 G1763 U1764 G1765 A1766 A1767 G1768 A1769 A1770 C1771 G1774 G1775 G1776 G1777 A1780 G1783 U1786 A1787 A1788 C1789 U1790 A1791 A1792 A1793 A1796 U1801 C1807 C1808 A1817
U1820 G1821 A1822 U1823 G1824 A1828 U1834 G1835 A1836 C1837 C1840 U1841 G1842 C1843 C1844 C1845 A1846 G1849 C1850 U1851 A1862 A1865 G1866 C1867 A1868 G1869 G1870 C1877 C1881 A1884 G1885 U1888 U1889 U1890 A1891 C1899 C1900 C1901 A1907 A1908 C1909 G1910 G1913 G1914 A1920 C1921
G1936 G1937 U1938 A1943 A1944 A1945 C1948 C1949 G1952 A1961 U1962 C1970 G1971 G1972 U1973 U1974 A1977 U1978 G1979 G1982 C1987 A1988 U1991 U1998 G1999 U2000 G2004 U2009 A2010 G2011 A2012 C2013 U2018 G2019 A2020 G2027 G2028 U2029 A2030 A2037 A2038 G2039 A2040 C2041
A2042 C2043 G2050 C2053 C2057 A2061 C2062 G2063 G2064 A2065 A2066 A2067 G2068 A2069 C2070 U2075 G2076 A2077 U2083 G2087 A2094 U2099 G2100 A2101 U2102 G2106 A2107 C2108 A2109 U2110 U2111 A2112 U2113 C2114 A2115 U2116 G2117 G2120 A2123 A2124 U2125 A2126 G2131 G2132 A2133 A2137
U2138 C2139 G2140 A2141 C2144 A2145 A2146 U2149 U2153 A2154 G2155 G2156 U2159 U2160 G2161 U2162 A2165 G2169 A2178 A2179 U2180 A2181 C2182 U2183 C2187 G2190 G2191 U2192 U2193 G2194 U2195 C2196 U2197 G2198 C2199 U2200 G2201 U2202 A2206 A2207 G2211 U2212 U2218 U2219 A2220 U2221 C2222 C2223
U2226 A2231 G2232 A2233 G2238 G2242 G2246 G2247 G2250 U2251 G2254 G2258 C2272 A2276 A2277 A2286 G2290 U2291 A2292 C2293 A2294 A2295 A2296 G2297 C2305 C2310 G2311 G2312 U2313 U2314 G2315 G2316 A2317 A2318 A2319 U2320 G2333 G2341 U2342 A2343 A2344 G2349

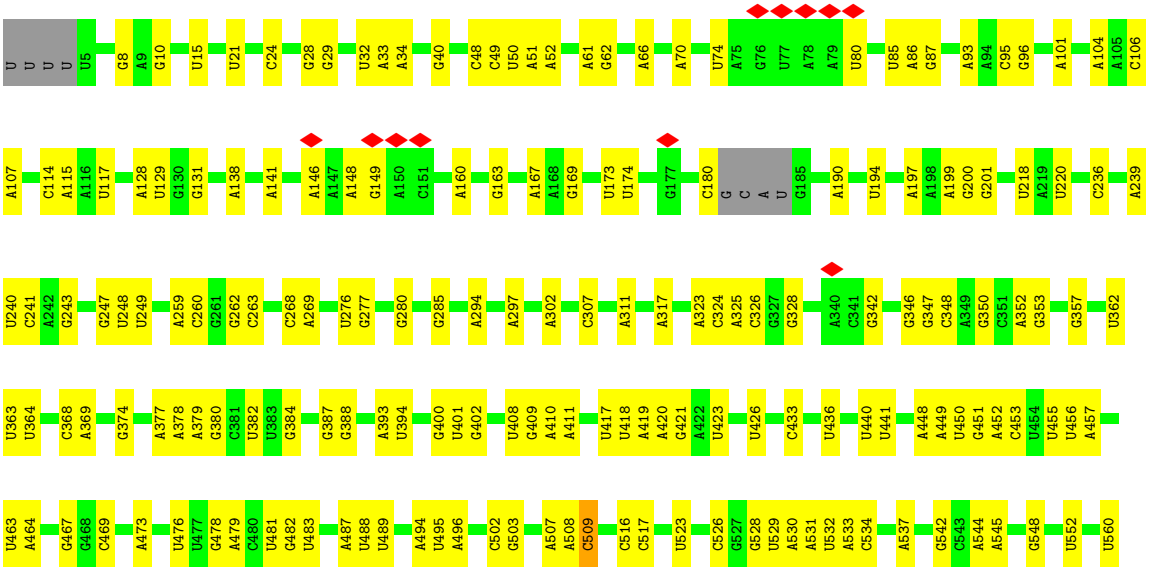


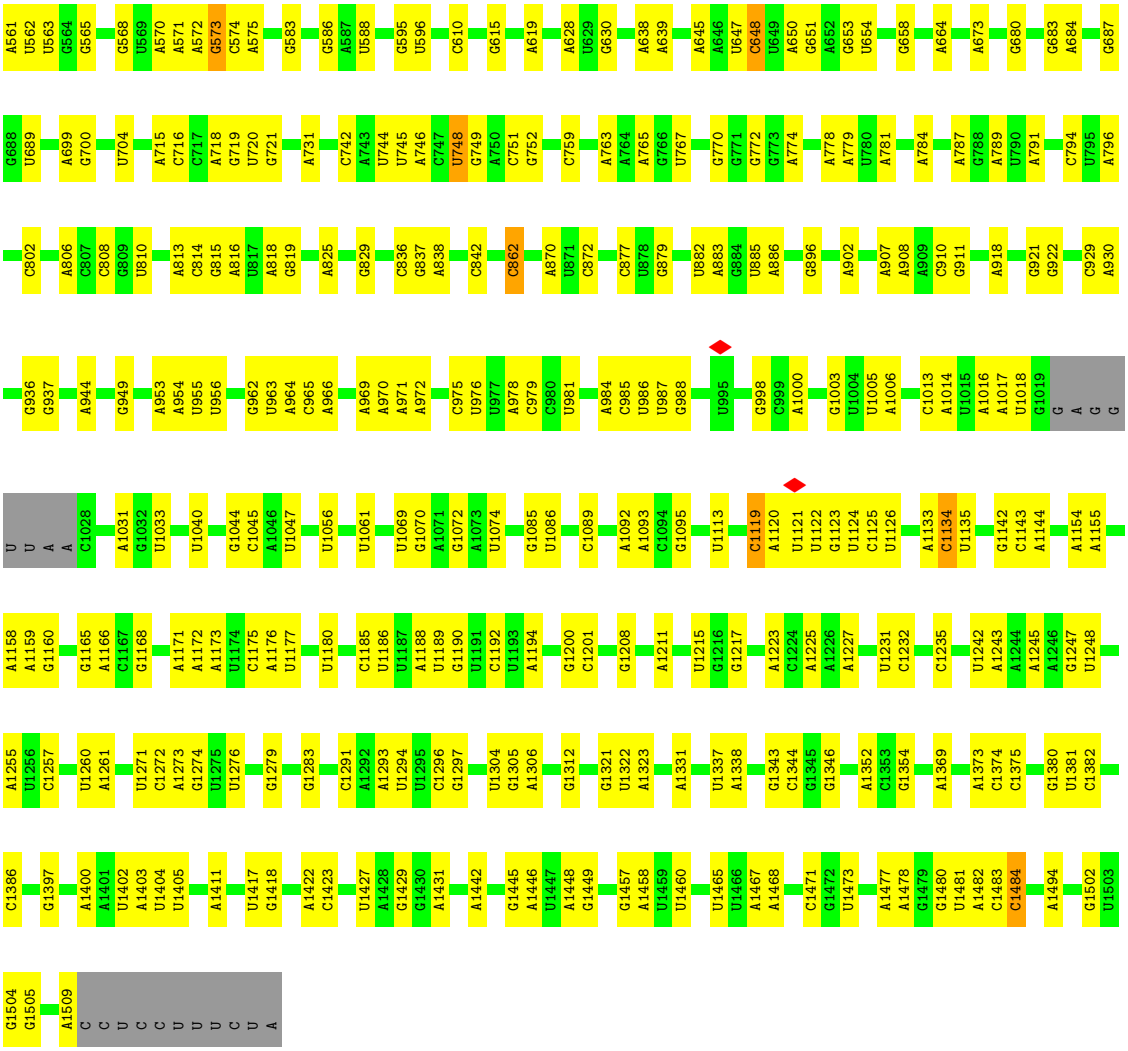
• Molecule 51: 5S ribosomal RNA

Chain 4:

• Molecule 52: 16S ribosomal RNA

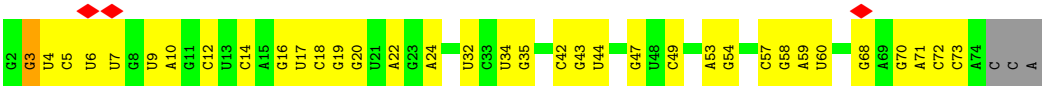
Chain 5:





• Molecule 53: tRNA-Phe

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	675	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 ($e^-/Å^2$)	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.831	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	435.328, 435.328, 435.328	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7005, 1.7005, 1.7005	Depositor

5 Model quality

5.1 Standard geometry

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	0.23	0/383	0.45	0/504
2	1	0.22	0/484	0.42	0/637
3	2	0.22	0/306	0.48	0/401
4	A	0.24	0/1954	0.44	0/2642
5	B	0.24	0/1721	0.45	0/2323
6	C	0.24	0/1691	0.42	0/2267
7	D	0.24	0/1188	0.46	0/1593
8	E	0.24	0/1384	0.47	0/1867
9	F	0.23	0/1266	0.46	0/1700
10	G	0.24	0/1126	0.50	1/1517 (0.1%)
11	H	0.26	0/1044	0.49	0/1395
12	I	0.25	0/820	0.49	0/1103
13	J	0.25	0/844	0.45	0/1136
14	K	0.28	0/1094	0.54	0/1468
15	L	0.23	0/962	0.46	0/1289
16	M	0.26	0/483	0.46	0/643
17	N	0.23	0/679	0.44	0/907
18	O	0.25	0/659	0.47	0/885
19	P	0.23	0/684	0.48	0/913
20	Q	0.24	0/545	0.43	0/730
21	R	0.25	0/698	0.49	0/936
22	S	0.23	0/631	0.40	0/838
23	T	0.22	0/475	0.40	0/621
24	a	0.24	0/2267	0.48	0/3044
25	b	0.25	0/1795	0.48	0/2412
26	c	0.24	0/1671	0.44	0/2246
27	d	0.24	0/1409	0.47	0/1894
28	e	0.25	0/1420	0.48	0/1912
29	f	0.24	0/1183	0.47	0/1587
30	g	0.40	0/969	0.63	0/1295
31	h	0.25	0/968	0.45	0/1298
32	i	0.24	0/1186	0.43	0/1592
33	j	0.24	0/953	0.48	0/1275
34	k	0.25	0/1170	0.46	0/1559

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	l	0.25	0/1104	0.44	0/1481
36	m	0.23	0/973	0.44	0/1309
37	n	0.24	0/897	0.47	0/1198
38	o	0.25	0/948	0.46	0/1262
39	p	0.23	0/961	0.38	0/1278
40	q	0.25	0/828	0.49	0/1111
41	r	0.25	0/1077	0.44	0/1441
42	s	0.24	0/732	0.48	0/988
43	t	0.25	0/879	0.49	0/1165
44	u	0.25	0/665	0.47	0/884
45	v	0.22	0/519	0.45	0/695
46	w	0.22	0/826	0.39	0/1104
47	x	0.24	0/353	0.45	0/474
48	y	0.30	0/457	0.56	0/601
49	z	0.24	0/412	0.44	0/547
50	3	0.22	0/69073	0.85	70/107710 (0.1%)
51	4	0.23	0/2505	0.84	0/3902
52	5	0.22	0/35768	0.84	28/55764 (0.1%)
53	8	0.25	0/1739	0.87	1/2710 (0.0%)
All	All	0.23	0/156828	0.76	100/234053 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	C	0	1
9	F	0	1
21	R	0	1
37	n	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	3	2620	C	N3-C2-O2	-9.45	115.28	121.90
50	3	2114	C	N3-C2-O2	-9.39	115.33	121.90
50	3	370	C	N3-C2-O2	-8.83	115.72	121.90
50	3	67	C	N1-C2-O2	8.69	124.11	118.90
50	3	2070	C	N1-C2-O2	8.33	123.90	118.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	19	LEU	Peptide
9	F	113	LYS	Peptide
21	R	25	GLN	Peptide
37	n	90	VAL	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	45/48 (94%)	41 (91%)	4 (9%)	0	100	100
2	1	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
3	2	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
4	A	238/294 (81%)	216 (91%)	22 (9%)	0	100	100
5	B	213/273 (78%)	201 (94%)	12 (6%)	0	100	100
6	C	201/205 (98%)	182 (90%)	18 (9%)	1 (0%)	25	64
7	D	151/219 (69%)	140 (93%)	11 (7%)	0	100	100
8	E	165/215 (77%)	149 (90%)	16 (10%)	0	100	100
9	F	152/155 (98%)	134 (88%)	16 (10%)	2 (1%)	10	43
10	G	139/142 (98%)	128 (92%)	11 (8%)	0	100	100
11	H	126/132 (96%)	110 (87%)	16 (13%)	0	100	100
12	I	99/108 (92%)	82 (83%)	17 (17%)	0	100	100
13	J	112/121 (93%)	107 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	K	134/139 (96%)	118 (88%)	16 (12%)	0	100	100
15	L	116/124 (94%)	107 (92%)	9 (8%)	0	100	100
16	M	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
17	N	81/86 (94%)	78 (96%)	3 (4%)	0	100	100
18	O	78/94 (83%)	70 (90%)	8 (10%)	0	100	100
19	P	81/85 (95%)	74 (91%)	7 (9%)	0	100	100
20	Q	63/104 (61%)	54 (86%)	9 (14%)	0	100	100
21	R	82/87 (94%)	72 (88%)	10 (12%)	0	100	100
22	S	75/87 (86%)	73 (97%)	2 (3%)	0	100	100
23	T	51/60 (85%)	50 (98%)	1 (2%)	0	100	100
24	a	283/287 (99%)	257 (91%)	26 (9%)	0	100	100
25	b	227/287 (79%)	203 (89%)	24 (11%)	0	100	100
26	c	208/212 (98%)	194 (93%)	14 (7%)	0	100	100
27	d	173/180 (96%)	164 (95%)	9 (5%)	0	100	100
28	e	174/184 (95%)	167 (96%)	7 (4%)	0	100	100
29	f	143/149 (96%)	127 (89%)	16 (11%)	0	100	100
30	g	124/161 (77%)	114 (92%)	10 (8%)	0	100	100
31	h	126/137 (92%)	119 (94%)	7 (6%)	0	100	100
32	i	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
33	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	k	146/151 (97%)	133 (91%)	13 (9%)	0	100	100
35	l	134/139 (96%)	126 (94%)	8 (6%)	0	100	100
36	m	117/124 (94%)	108 (92%)	9 (8%)	0	100	100
37	n	108/116 (93%)	100 (93%)	8 (7%)	0	100	100
38	o	113/119 (95%)	109 (96%)	4 (4%)	0	100	100
39	p	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
40	q	97/100 (97%)	87 (90%)	10 (10%)	0	100	100
41	r	137/159 (86%)	128 (93%)	9 (7%)	0	100	100
42	s	90/237 (38%)	83 (92%)	7 (8%)	0	100	100
43	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
44	u	84/104 (81%)	75 (89%)	9 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	v	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
46	w	96/111 (86%)	91 (95%)	5 (5%)	0	100	100
47	x	42/97 (43%)	37 (88%)	5 (12%)	0	100	100
48	y	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
49	z	48/53 (91%)	44 (92%)	4 (8%)	0	100	100
All	All	5820/6670 (87%)	5357 (92%)	460 (8%)	3 (0%)	50	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	F	113	LYS
6	C	146	ALA
9	F	114	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	40/41 (98%)	40 (100%)	0	100	100
2	1	51/51 (100%)	51 (100%)	0	100	100
3	2	35/35 (100%)	34 (97%)	1 (3%)	37	56
4	A	212/262 (81%)	211 (100%)	1 (0%)	86	89
5	B	180/232 (78%)	180 (100%)	0	100	100
6	C	181/183 (99%)	181 (100%)	0	100	100
7	D	123/178 (69%)	123 (100%)	0	100	100
8	E	150/196 (76%)	148 (99%)	2 (1%)	65	77
9	F	131/132 (99%)	129 (98%)	2 (2%)	60	75
10	G	123/124 (99%)	123 (100%)	0	100	100
11	H	111/115 (96%)	111 (100%)	0	100	100
12	I	95/99 (96%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	J	91/97 (94%)	91 (100%)	0	100 100
14	K	117/120 (98%)	110 (94%)	7 (6%)	16 37
15	L	100/105 (95%)	99 (99%)	1 (1%)	73 82
16	M	47/48 (98%)	46 (98%)	1 (2%)	48 66
17	N	76/78 (97%)	75 (99%)	1 (1%)	65 77
18	O	69/82 (84%)	68 (99%)	1 (1%)	62 75
19	P	73/75 (97%)	71 (97%)	2 (3%)	40 58
20	Q	56/94 (60%)	56 (100%)	0	100 100
21	R	74/77 (96%)	74 (100%)	0	100 100
22	S	70/77 (91%)	69 (99%)	1 (1%)	62 75
23	T	49/56 (88%)	49 (100%)	0	100 100
24	a	241/243 (99%)	241 (100%)	0	100 100
25	b	186/233 (80%)	186 (100%)	0	100 100
26	c	182/184 (99%)	182 (100%)	0	100 100
27	d	150/154 (97%)	148 (99%)	2 (1%)	65 77
28	e	153/159 (96%)	153 (100%)	0	100 100
29	f	123/134 (92%)	123 (100%)	0	100 100
30	g	101/129 (78%)	89 (88%)	12 (12%)	4 16
31	h	102/110 (93%)	101 (99%)	1 (1%)	73 82
32	i	126/128 (98%)	125 (99%)	1 (1%)	79 85
33	j	103/103 (100%)	103 (100%)	0	100 100
34	k	123/126 (98%)	123 (100%)	0	100 100
35	l	113/115 (98%)	113 (100%)	0	100 100
36	m	105/109 (96%)	105 (100%)	0	100 100
37	n	96/99 (97%)	96 (100%)	0	100 100
38	o	101/105 (96%)	101 (100%)	0	100 100
39	p	100/108 (93%)	100 (100%)	0	100 100
40	q	90/91 (99%)	90 (100%)	0	100 100
41	r	116/132 (88%)	116 (100%)	0	100 100
42	s	82/208 (39%)	81 (99%)	1 (1%)	67 78
43	t	96/96 (100%)	95 (99%)	1 (1%)	73 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	u	69/85 (81%)	68 (99%)	1 (1%)	62 75
45	v	58/60 (97%)	58 (100%)	0	100 100
46	w	87/98 (89%)	87 (100%)	0	100 100
47	x	41/86 (48%)	41 (100%)	0	100 100
48	y	48/49 (98%)	44 (92%)	4 (8%)	9 27
49	z	47/50 (94%)	45 (96%)	2 (4%)	25 46
All	All	5093/5751 (89%)	5048 (99%)	45 (1%)	74 83

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	g	69	GLU
32	i	15	ARG
30	g	84	VAL
30	g	116	ARG
43	t	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
21	R	69	HIS
36	m	59	ASN
24	a	238	HIS
40	q	85	HIS
32	i	74	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	3	2875/2907 (98%)	934 (32%)	32 (1%)
51	4	103/108 (95%)	40 (38%)	1 (0%)
52	5	1490/1520 (98%)	459 (30%)	10 (0%)
53	8	72/76 (94%)	34 (47%)	2 (2%)
All	All	4540/4611 (98%)	1467 (32%)	45 (0%)

5 of 1467 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	3	9	G
50	3	11	U
50	3	12	A
50	3	14	U
50	3	15	A

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	3	2668	A
52	5	529	U
50	3	2764	U
51	4	54	U
52	5	748	U

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

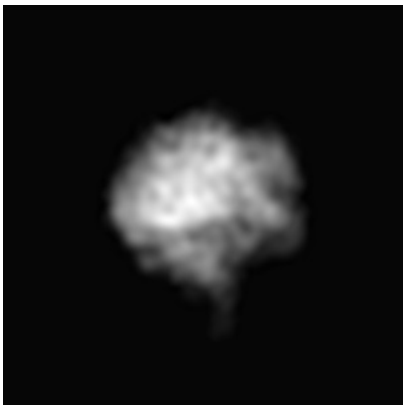
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13282. These allow visual inspection of the internal detail of the map and identification of artifacts.

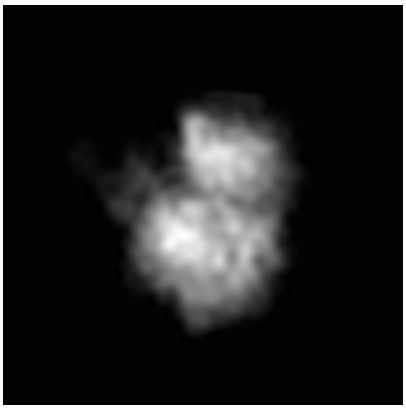
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

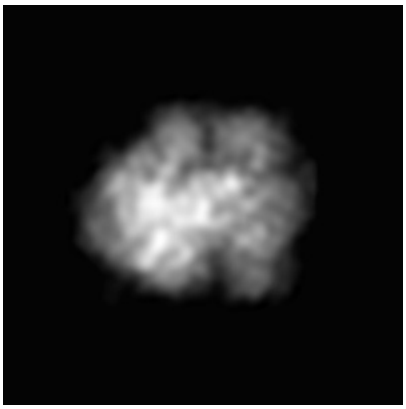
6.1.1 Primary map



X

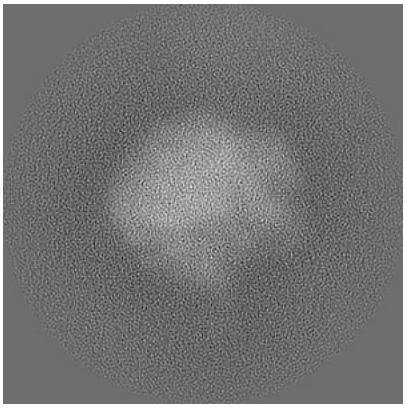


Y

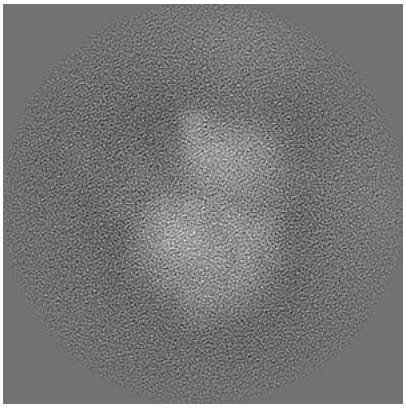


Z

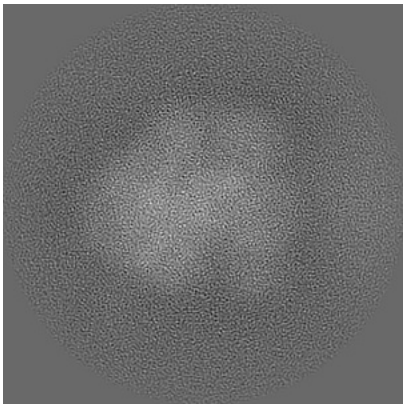
6.1.2 Raw map



X



Y

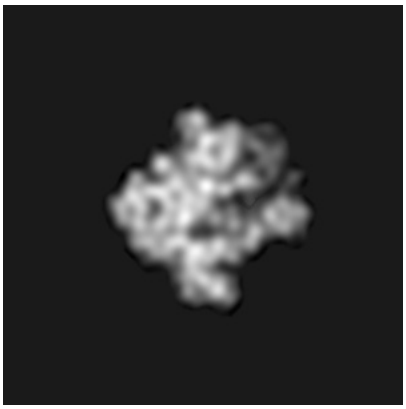


Z

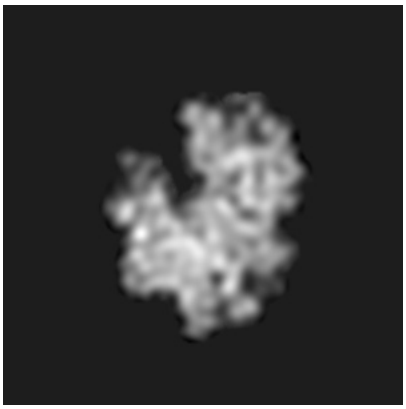
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

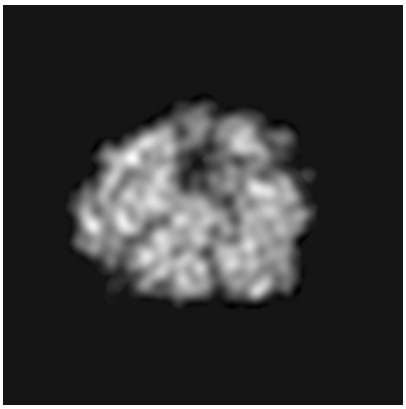
6.2.1 Primary map



X Index: 128

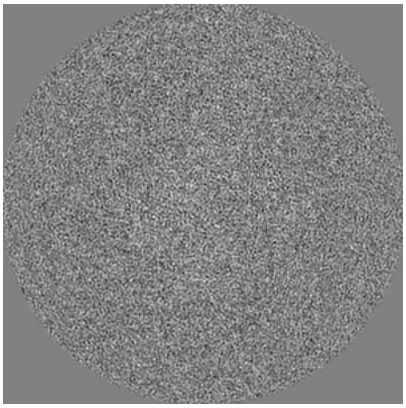


Y Index: 128

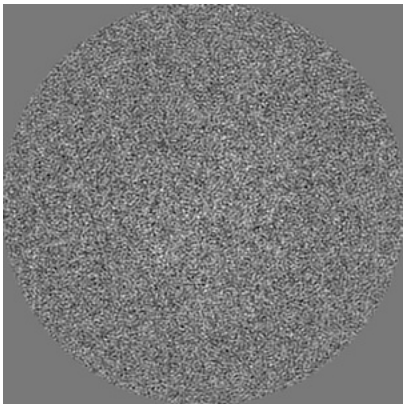


Z Index: 128

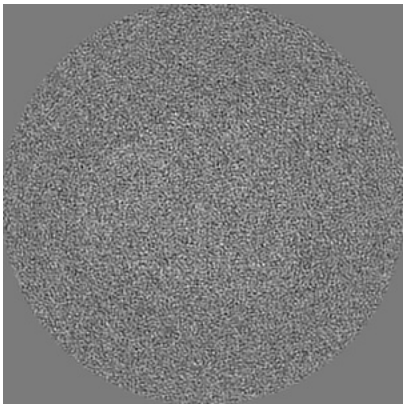
6.2.2 Raw map



X Index: 128



Y Index: 128



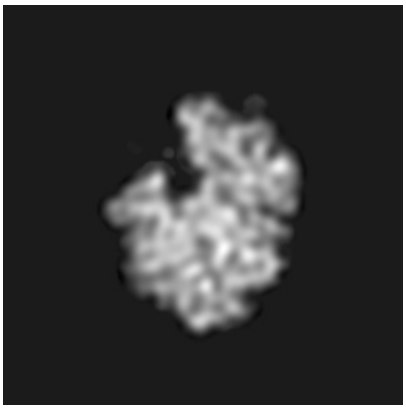
Z Index: 128

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

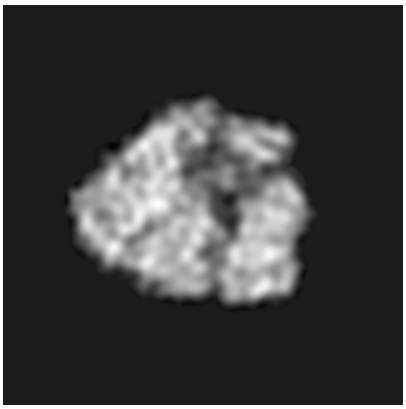
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 100

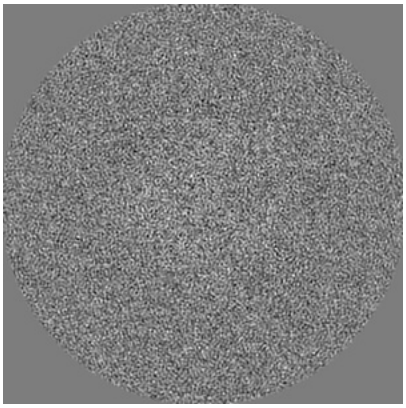


Y Index: 119

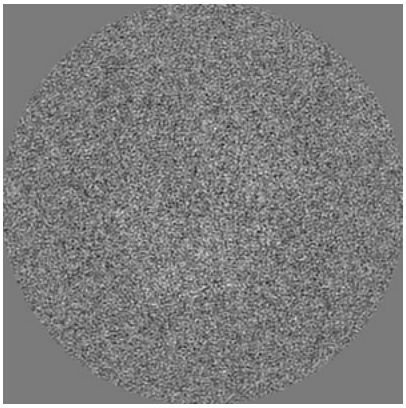


Z Index: 123

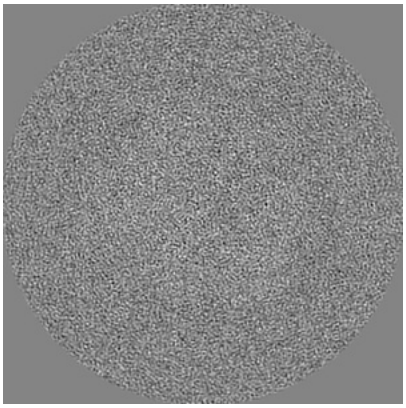
6.3.2 Raw map



X Index: 127



Y Index: 129



Z Index: 122

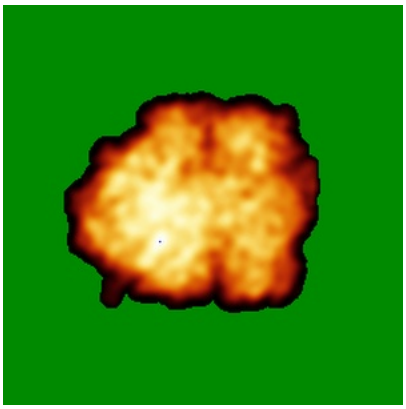
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

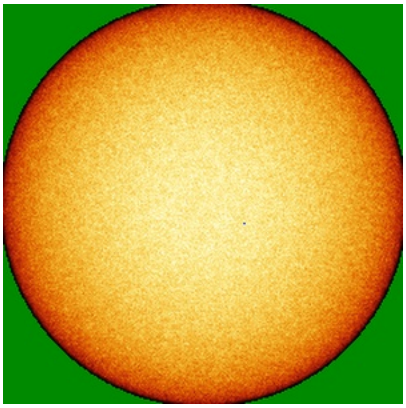
X

Y

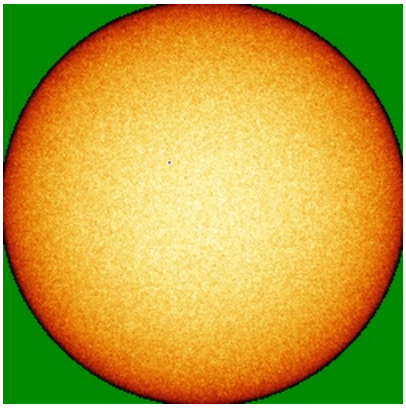


Z

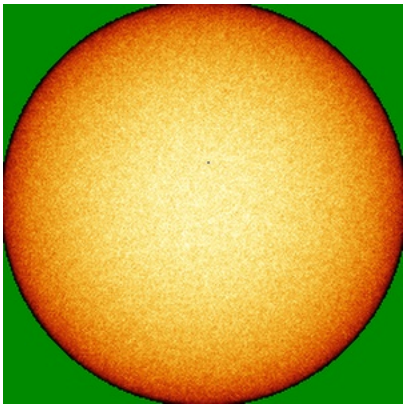
6.4.2 Raw map



X



Y

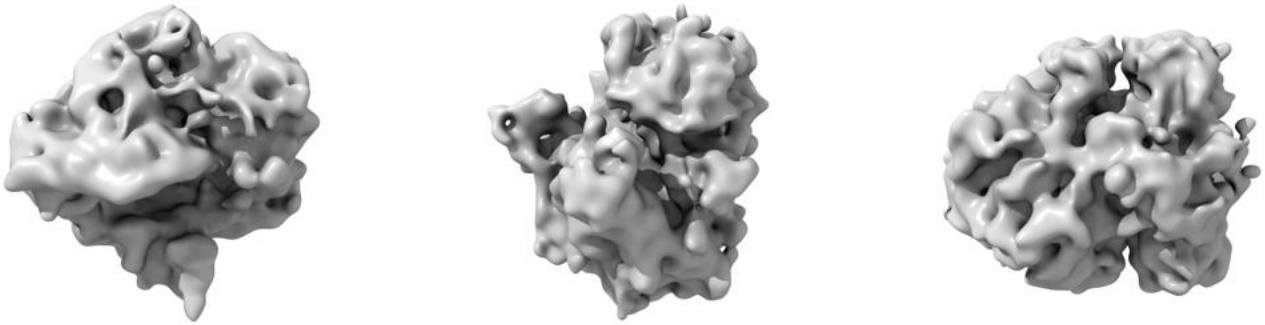


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

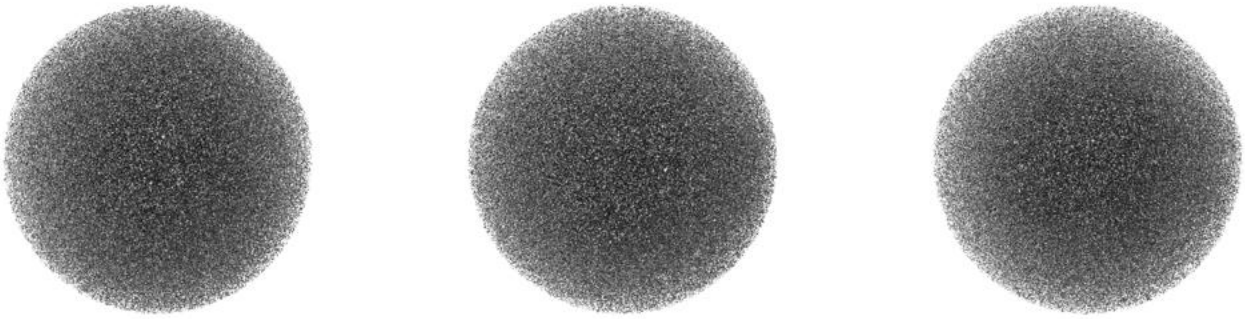
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

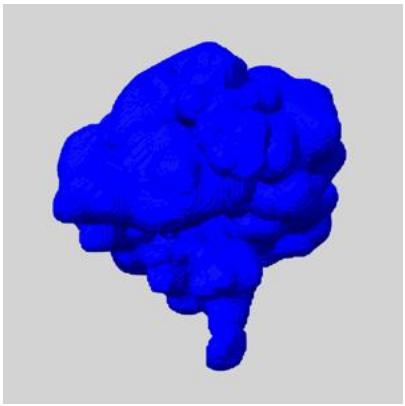
6.6 Mask visualisation

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

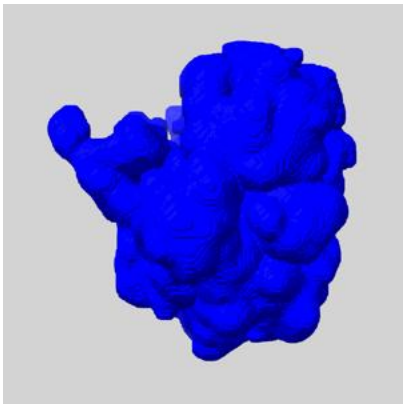
A mask typically either:

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

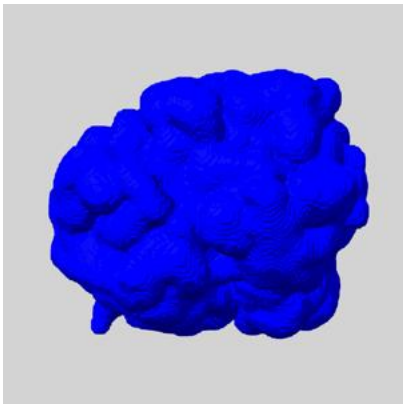
6.6.1 emd_13282_msk_1.map



X



Y

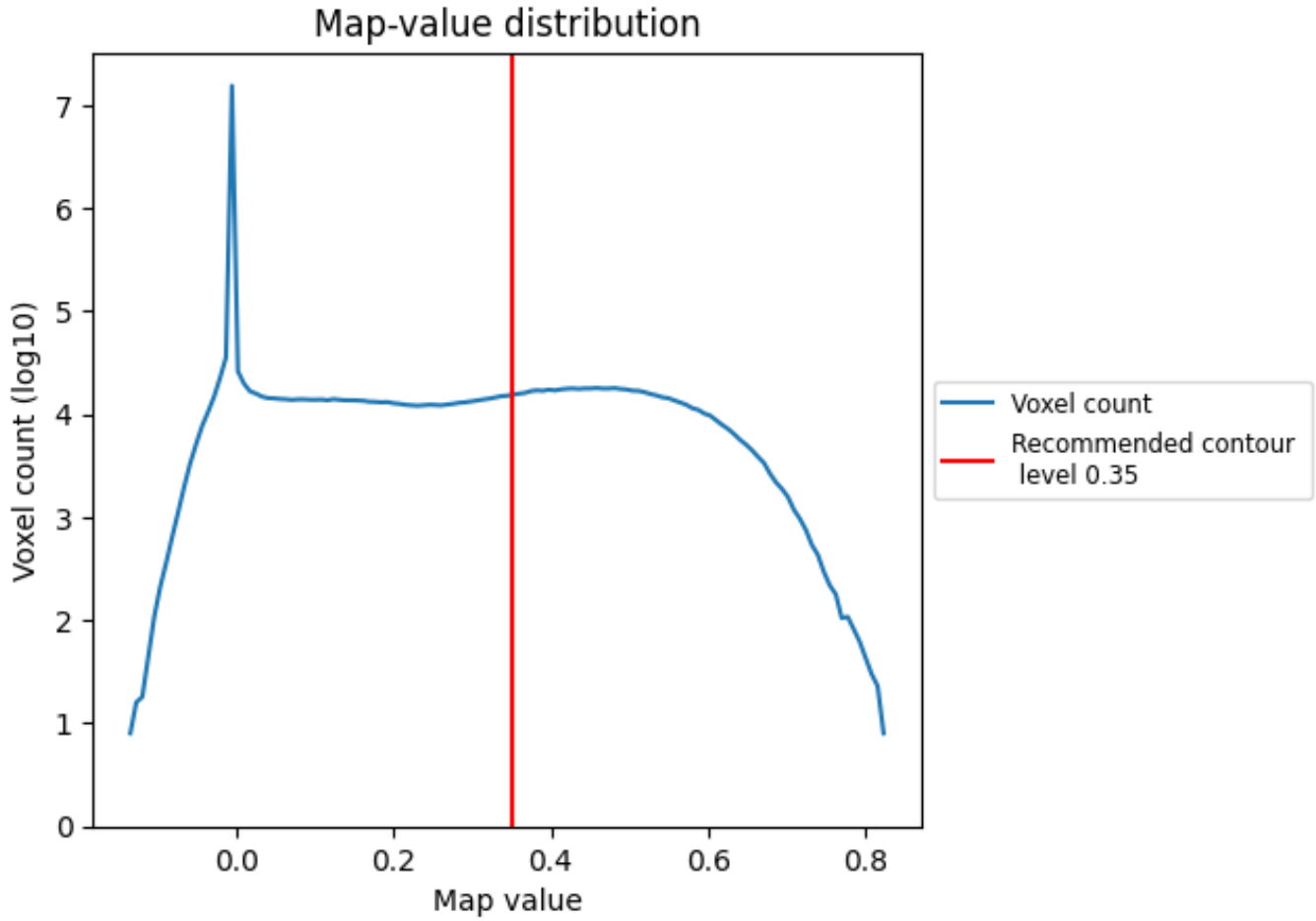


Z

7 Map analysis

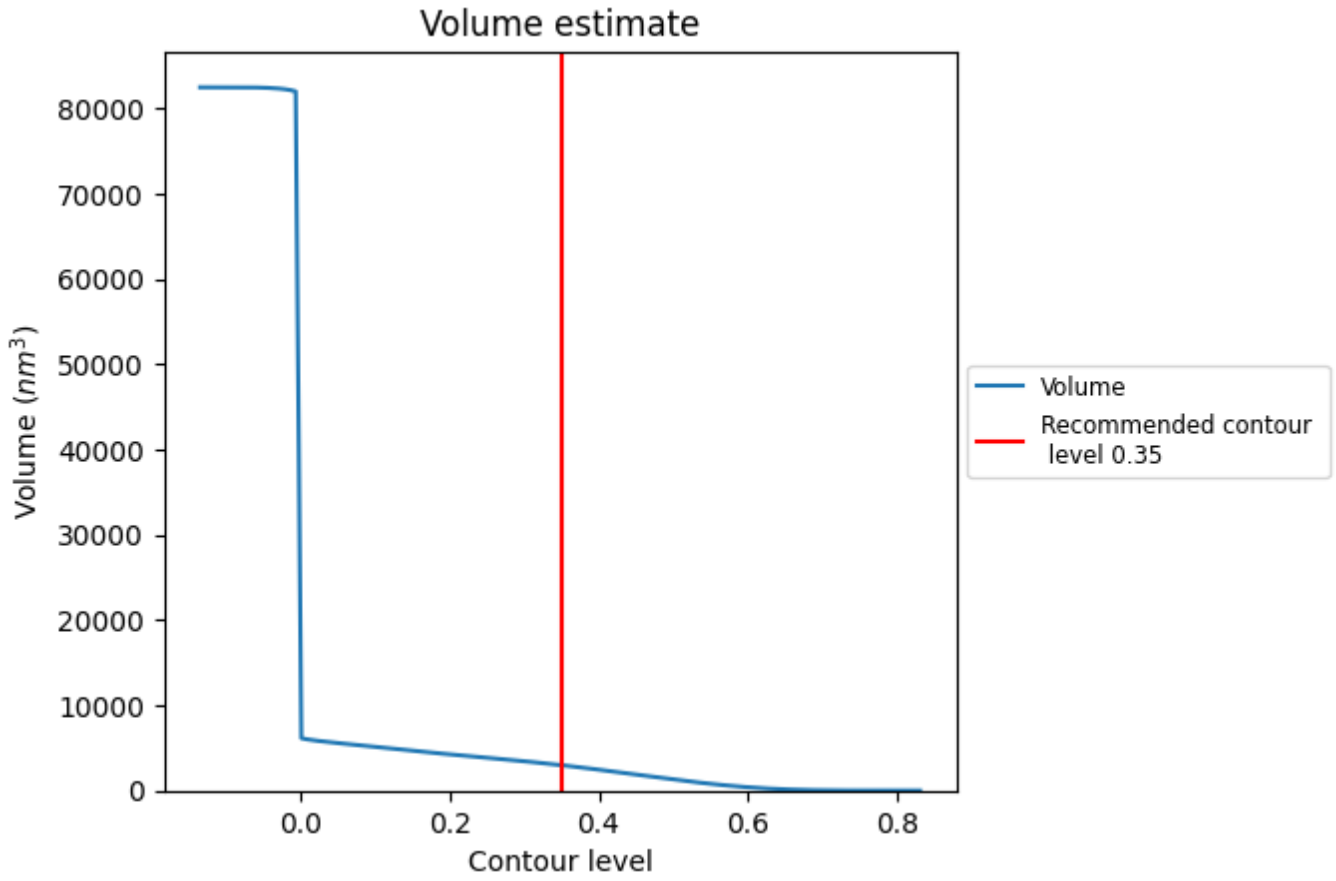
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

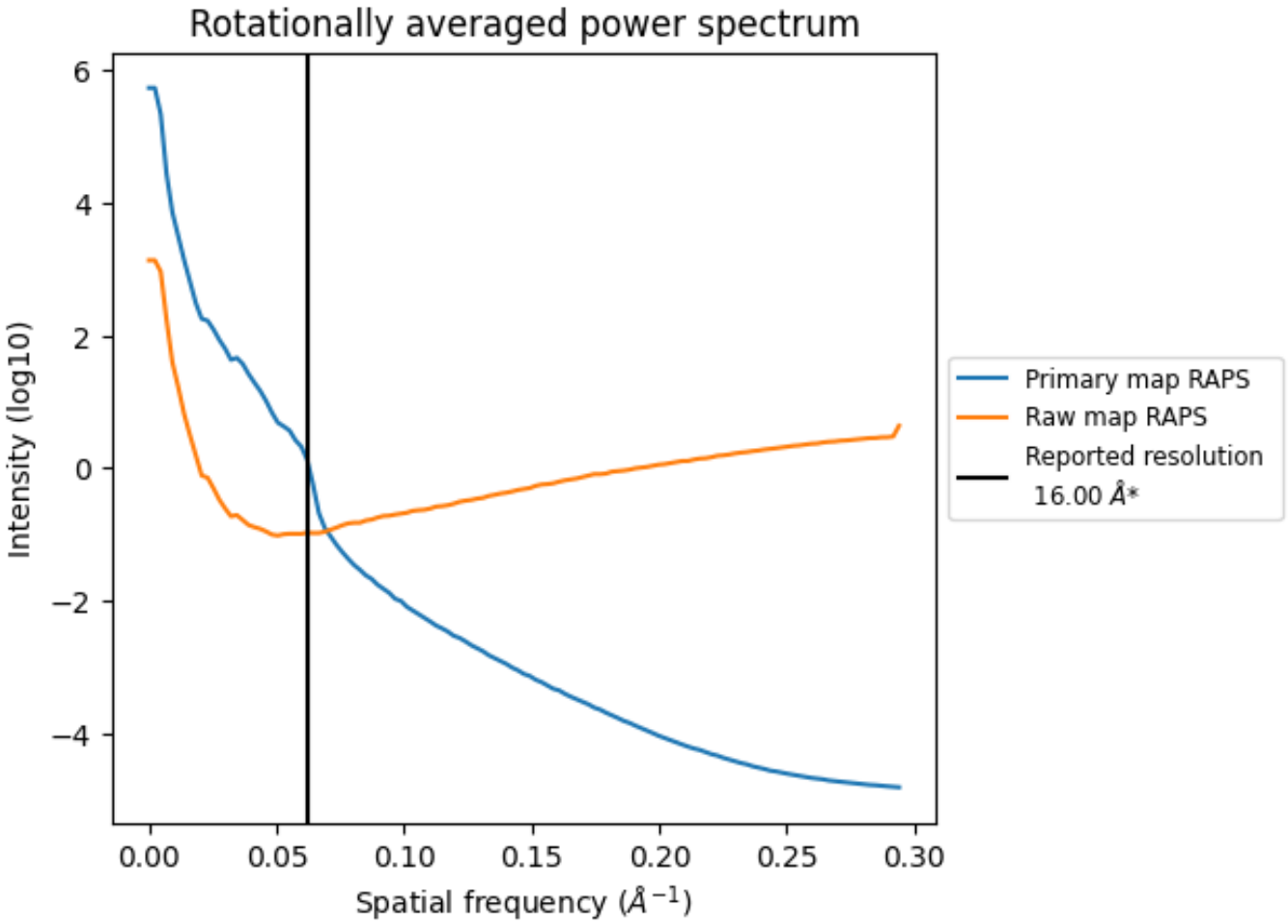
7.2 Volume estimate (i)



The volume at the recommended contour level is 2979 nm^3; this corresponds to an approximate mass of 2691 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)

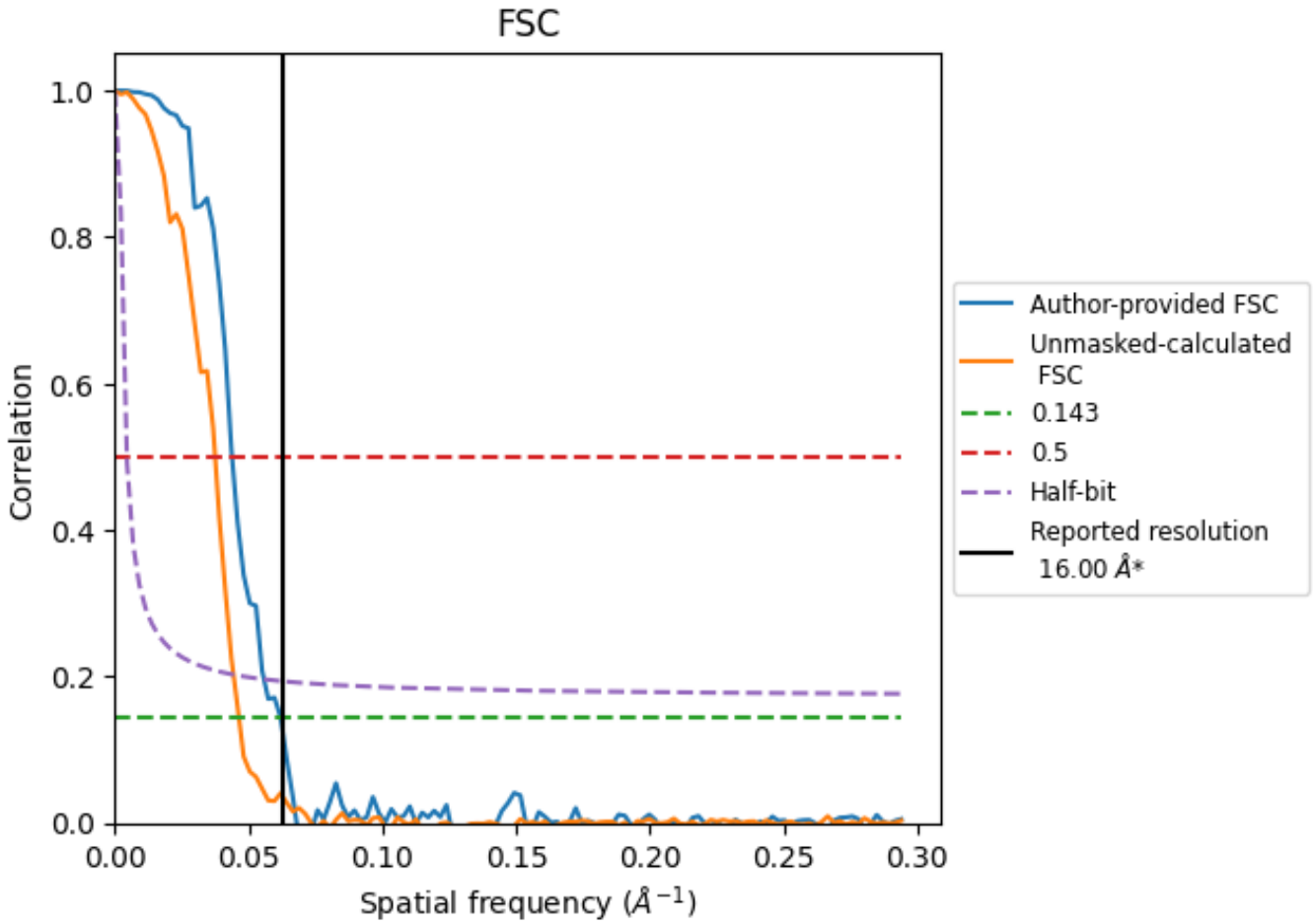


*Reported resolution corresponds to spatial frequency of 0.062 Å^{-1}

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 0.062 Å^{-1}

8.2 Resolution estimates (i)

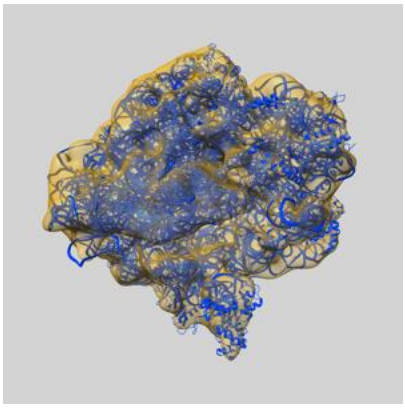
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	16.00	-	-
Author-provided FSC curve	16.10	22.78	17.89
Unmasked-calculated*	21.51	26.67	22.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 21.51 differs from the reported value 16.0 by more than 10 %

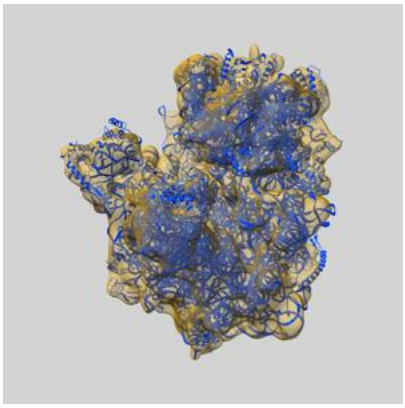
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13282 and PDB model 7PAS. Per-residue inclusion information can be found in section 3 on page 13.

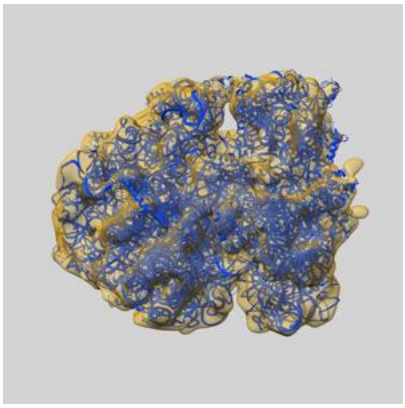
9.1 Map-model overlay



X



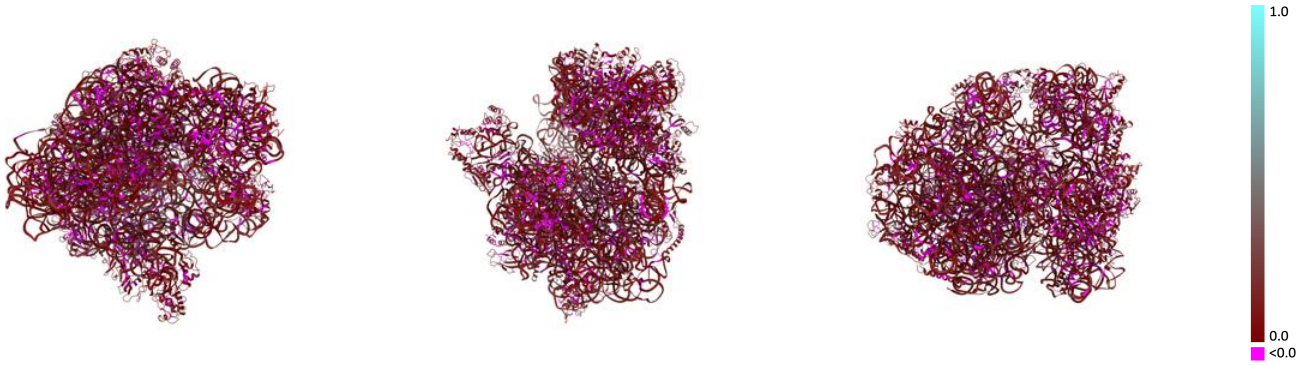
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

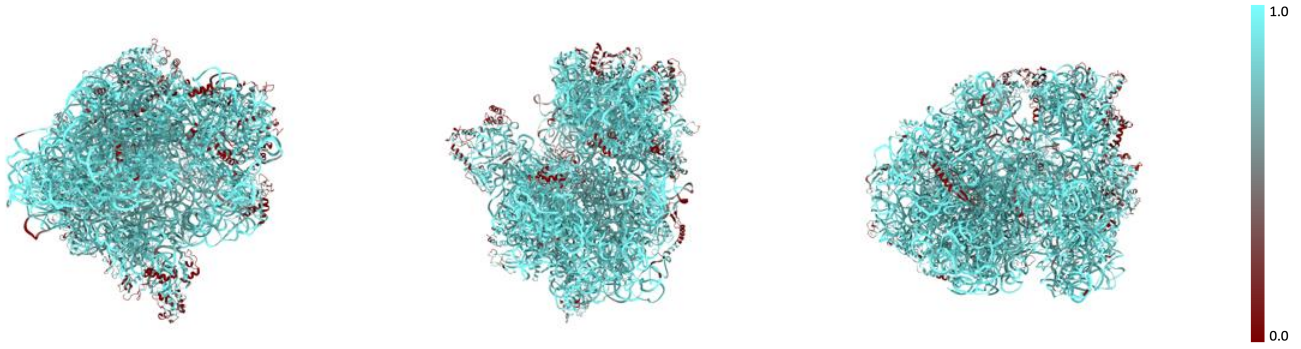
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

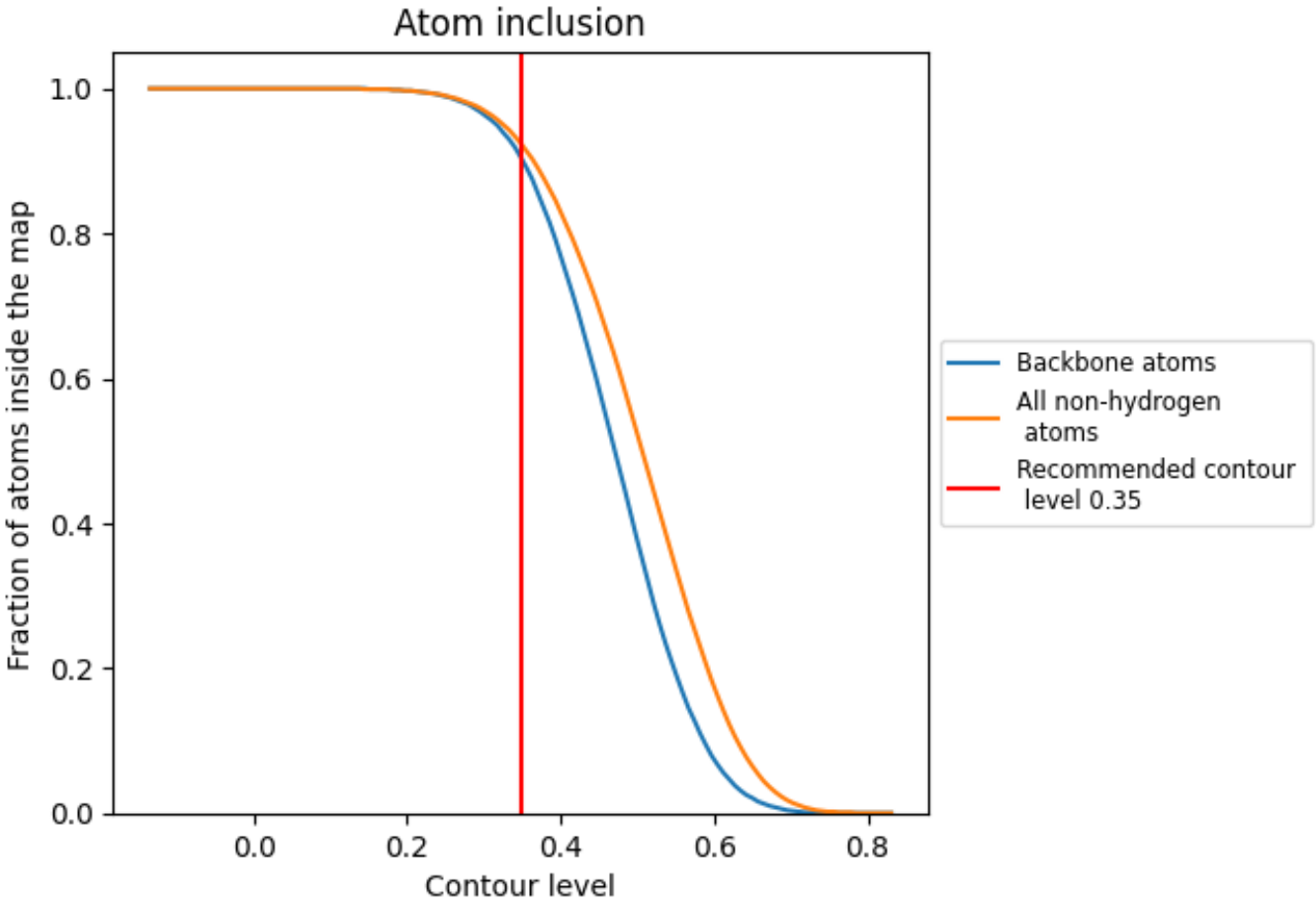
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 92% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9220	0.0690
0	1.0000	0.0170
1	0.9980	-0.0070
2	0.9760	-0.0040
3	0.9810	0.0810
4	0.9680	0.0870
5	0.9720	0.0790
8	0.9040	0.0960
A	0.6370	0.0660
B	0.6700	0.0430
C	0.8310	0.0380
D	0.8540	0.0470
E	0.7020	0.0820
F	0.7380	0.0690
G	0.7710	0.0490
H	0.7590	0.0530
I	0.6870	0.0310
J	0.8210	0.0360
K	0.9650	0.0310
L	0.6400	0.0550
M	0.9580	0.0350
N	0.8910	0.0570
O	0.9670	0.0150
P	0.8620	0.0570
Q	0.9830	0.0510
R	0.8630	0.0550
S	0.9610	0.0260
T	0.7920	0.0260
a	0.9690	0.0320
b	0.8860	0.0290
c	0.8760	0.0510
d	0.6580	0.0580
e	0.7030	0.0550
f	0.4190	0.0600
g	0.5290	0.0730

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Chain	Atom inclusion	Q-score
h	0.3770	0.0690
i	0.9090	0.0240
j	0.8900	0.0310
k	0.9350	0.0220
l	0.9450	0.0400
m	0.9630	0.0060
n	0.9020	0.0280
o	0.8260	0.0430
p	0.8800	0.0110
q	0.8010	0.0620
r	0.9420	0.0490
s	0.9630	0.0250
t	0.6280	0.0520
u	0.9700	0.0190
v	0.9620	0.0080
w	0.8000	0.0620
x	0.3940	0.1020
y	0.8890	0.0230
z	1.0000	0.0840