wwPDB EM Validation Summary Report ⓘ

Nov 12, 2024 – 10:04 am GMT

PDB ID	:	8P8B
EMDB ID	:	EMD-17134
Title	:	Mycoplasma pneumoniae large ribosomal subunit in chloramphenicol-treated cells
Authors	:	Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on	:	2023-05-31
Resolution	:	2.90 Å(reported)
Based on initial models	:	7OOD, 7OOC

The following versions of software and data (see references ⓘ) were used in the production of this report:

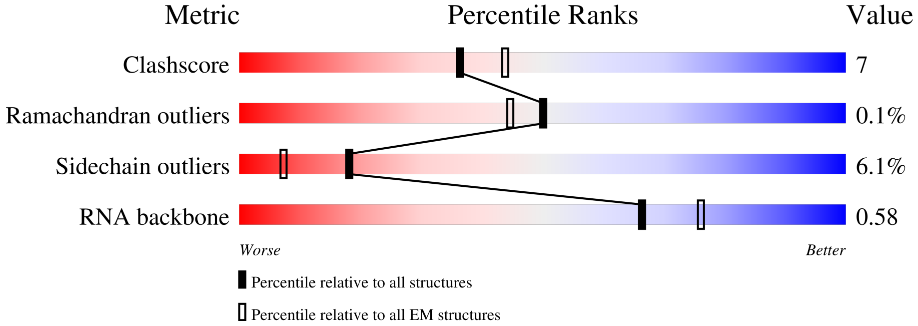
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

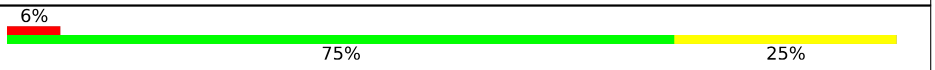
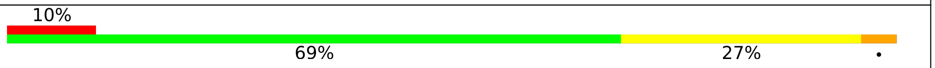
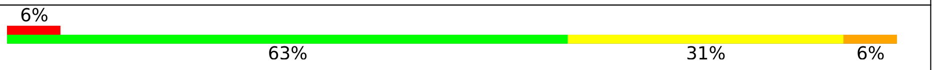
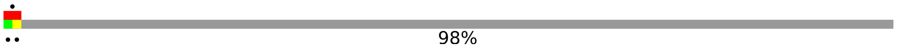
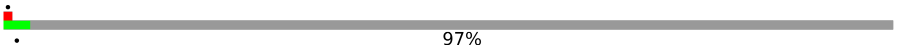
The reported resolution of this entry is 2.90 Å.

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	210492	15764
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	
2	1	59	
3	2	37	
4	3	2907	
5	4	108	
6	5	1520	
7	6	76	

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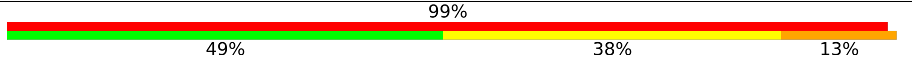
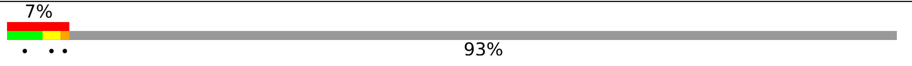
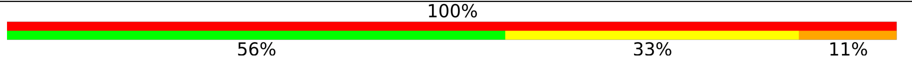
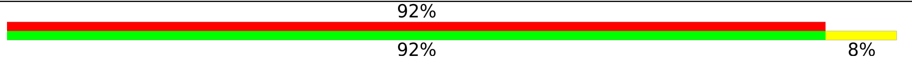
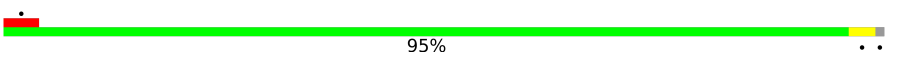
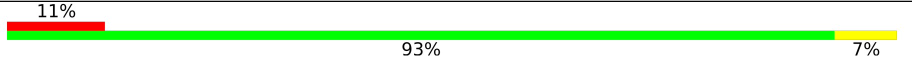
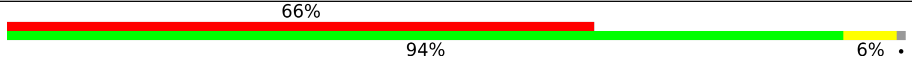
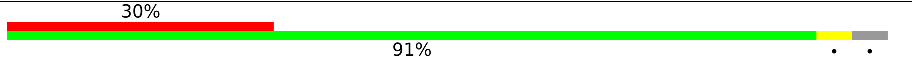
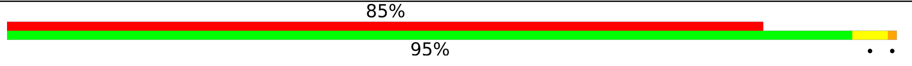
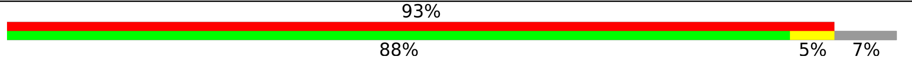
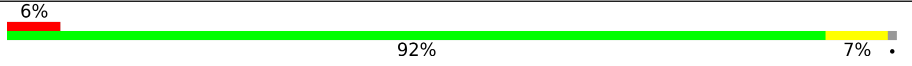
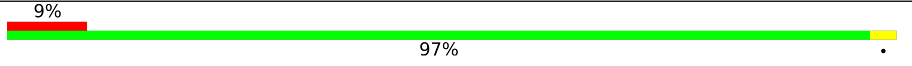
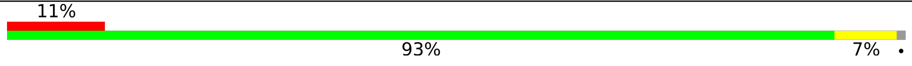
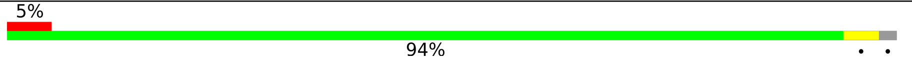
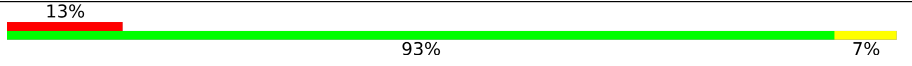
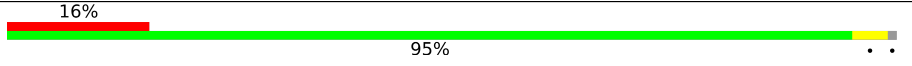
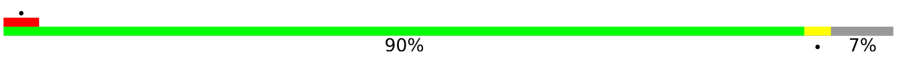
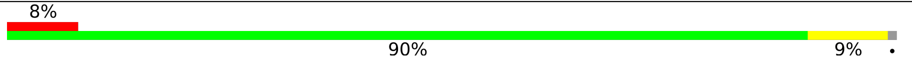
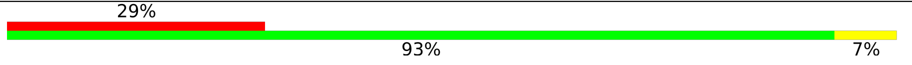
Mol	Chain	Length	Quality of chain
8	7	75	
9	8	76	
10	X	444	
11	Y	9	
12	Z	36	
13	a	287	
14	b	287	
15	c	212	
16	d	180	
17	e	184	
18	f	149	
19	g	161	
20	h	137	
21	i	146	
22	j	122	
23	k	151	
24	l	139	
25	m	124	
26	n	116	
27	o	119	
28	p	127	
29	q	100	
30	r	159	
31	s	237	
32	t	111	

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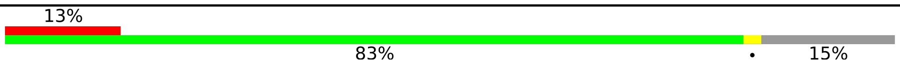
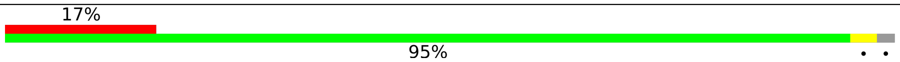
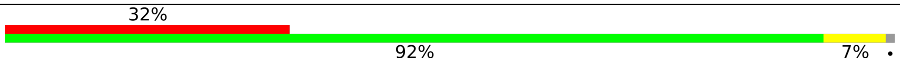
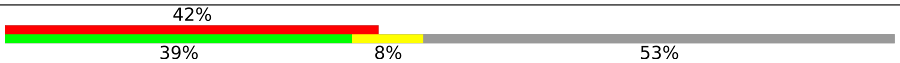
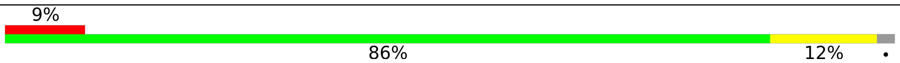
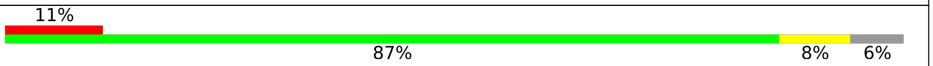
Mol	Chain	Length	Quality of chain
33	u	104	
34	v	65	
35	w	111	
36	x	97	
37	y	57	
38	z	53	

2 Entry composition (i)

There are 47 unique types of molecules in this entry. The entry contains 97182 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	48	392	242	85	63	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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	2893	61995	27704	11293	20105	2893	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	4	108	2305	1030	415	752	108	0	0

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	5	32	683	307	124	220	32	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	6	2	42	19	8	13	2	0	0

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	7	75	1599	712	279	533	75	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 9 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	8	76	1615	722	284	533	76	0	0

- Molecule 10 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	30	242	155	43	43	1	0	0

- Molecule 11 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	Y	9	195	87	38	61	9	0	0

- Molecule 12 is a protein called nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	Z	36	187	112	37	38	0	0

- Molecule 13 is a protein called 50S ribosomal protein L2.

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

- Molecule 14 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	b	231	1778	1129	320	322	7	0	0

- Molecule 15 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	c	211	1654	1053	299	299	3	0	0

- Molecule 16 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	d	179	1416	910	251	251	4	0	0

- Molecule 17 is a protein called 50S ribosomal protein L6.

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

- Molecule 18 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	f	149	1210	780	212	215	3	0	0

- Molecule 19 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	g	125	951	606	165	177	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L11.

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

- Molecule 21 is a protein called 50S ribosomal protein L13.

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

- Molecule 22 is a protein called 50S ribosomal protein L14.

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

- Molecule 23 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	k	150	1170	741	228	200	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L16.

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

- Molecule 25 is a protein called 50S ribosomal protein L17.

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

- Molecule 26 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	n	116	918	573	181	162	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	o	118	966	609	186	170	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	p	118	981	624	194	161	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L21.

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

- Molecule 30 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	r	142	1091	677	212	195	7	0	0

- Molecule 31 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	s	95	740	486	125	128	1	0	0

- Molecule 32 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	t	111	871	550	166	152	3	0	0

- Molecule 33 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	u	88	670	416	132	121	1	0	0

- Molecule 34 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	v	64	520	320	109	90	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	w	110	906	576	168	162	0	0

- Molecule 36 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	x	46	366	235	59	68	4	0	0

- Molecule 37 is a protein called 50S ribosomal protein L32.

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

- Molecule 38 is a protein called 50S ribosomal protein L33 1.

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

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
39	2	1	1	1	0
39	x	1	1	1	0
39	y	1	1	1	0

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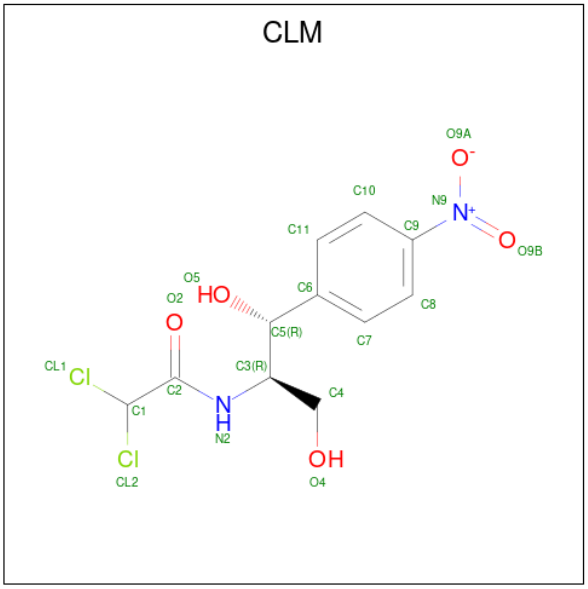
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
39	z	1	1	1	0

- Molecule 40 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
40	3	1	20	11	2	2	5	0

- Molecule 41 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
41	3	1	1	1	0

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
42	3	219	219	219	0
42	4	1	1	1	0
42	6	1	1	1	0

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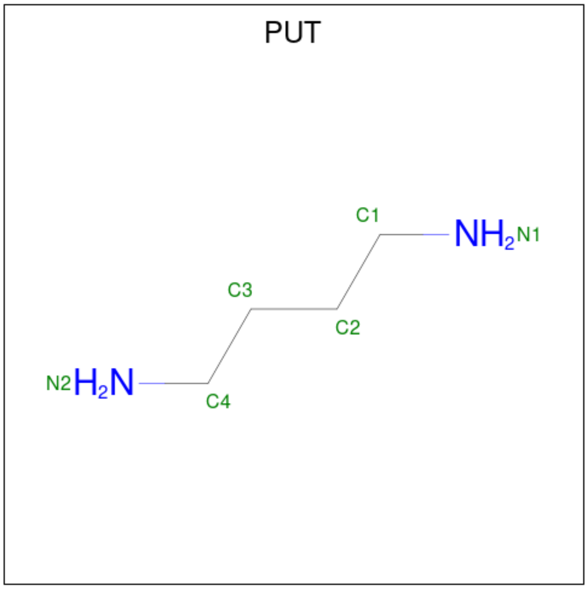
Mol	Chain	Residues	Atoms	AltConf
42	7	1	Total Mg 1 1	0
42	8	2	Total Mg 2 2	0
42	b	2	Total Mg 2 2	0
42	i	1	Total Mg 1 1	0
42	y	2	Total Mg 2 2	0

- Molecule 43 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	AltConf
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0

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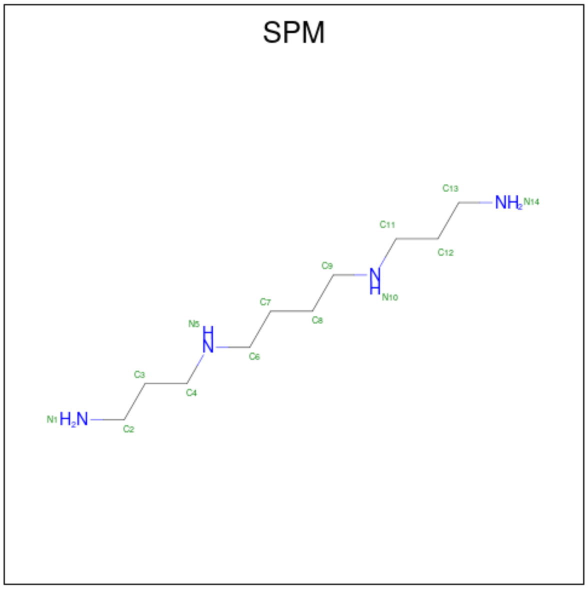
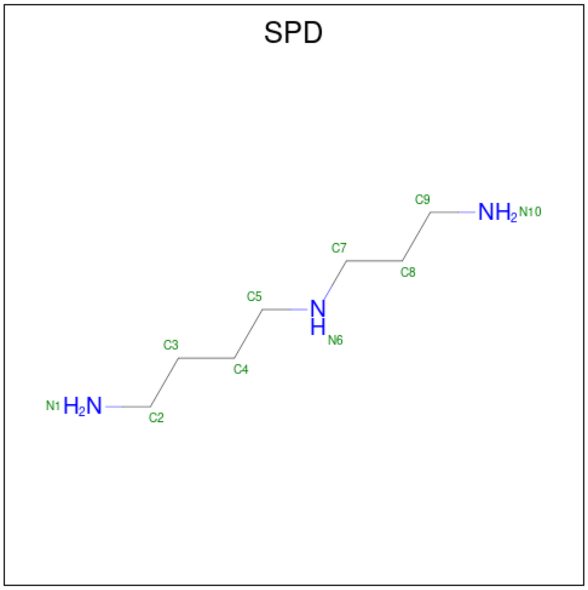
Mol	Chain	Residues	Atoms	AltConf
43	3	1	Total C N 6 4 2	0

- Molecule 44 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
44	3	1	Total C N 14 10 4	0
44	3	1	Total C N 14 10 4	0
44	3	1	Total C N 14 10 4	0
44	b	1	Total C N 14 10 4	0

- Molecule 45 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0

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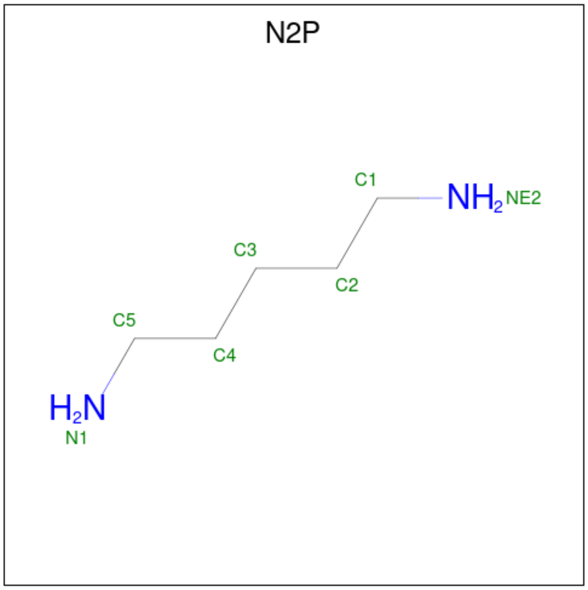
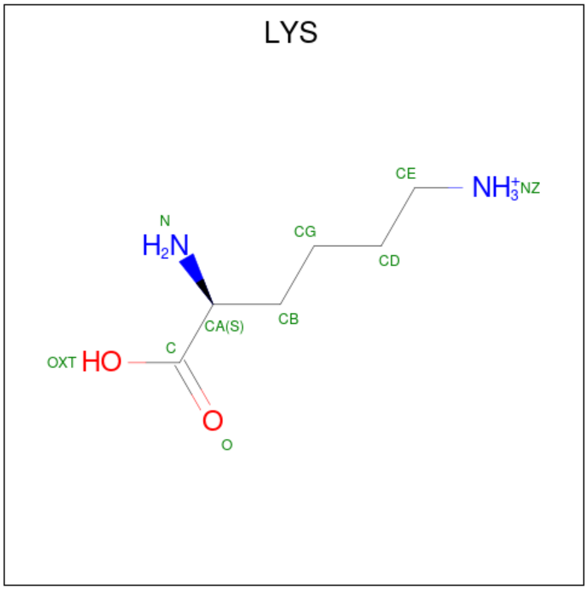
Mol	Chain	Residues	Atoms	AltConf
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0

- Molecule 46 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms	AltConf
46	3	1	Total C N 7 5 2	0
46	3	1	Total C N 7 5 2	0
46	3	1	Total C N 7 5 2	0

- Molecule 47 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



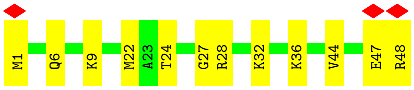
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
47	8	1	9	6	2	1	0

3 Residue-property plots

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.

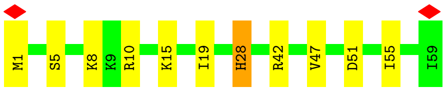
- Molecule 1: 50S ribosomal protein L34

Chain 0:



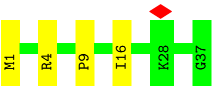
- Molecule 2: 50S ribosomal protein L35

Chain 1:



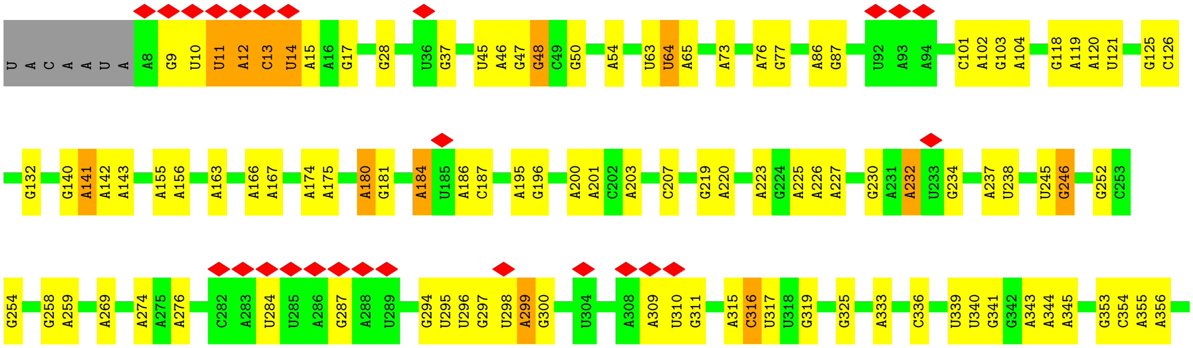
- Molecule 3: 50S ribosomal protein L36

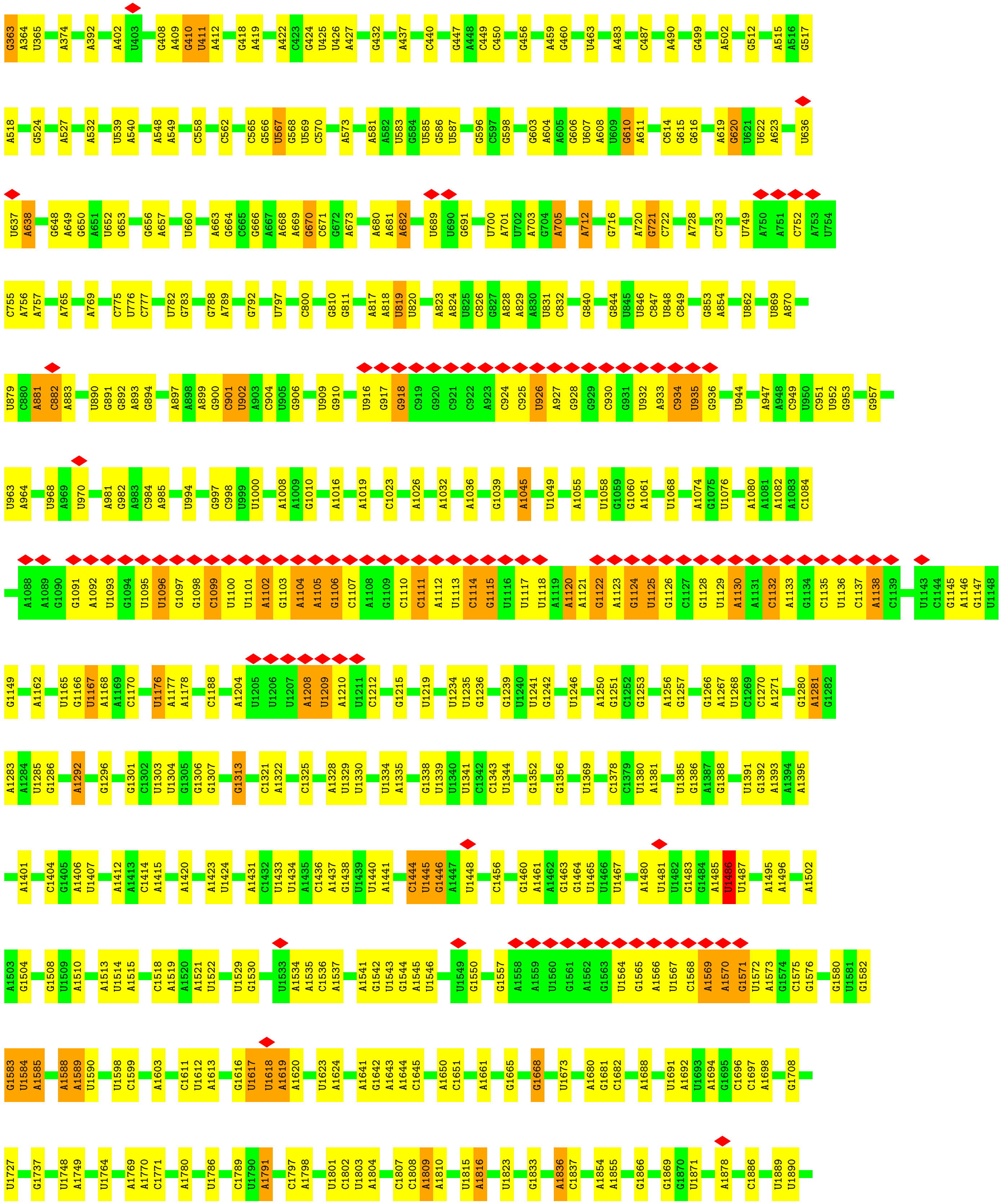
Chain 2:

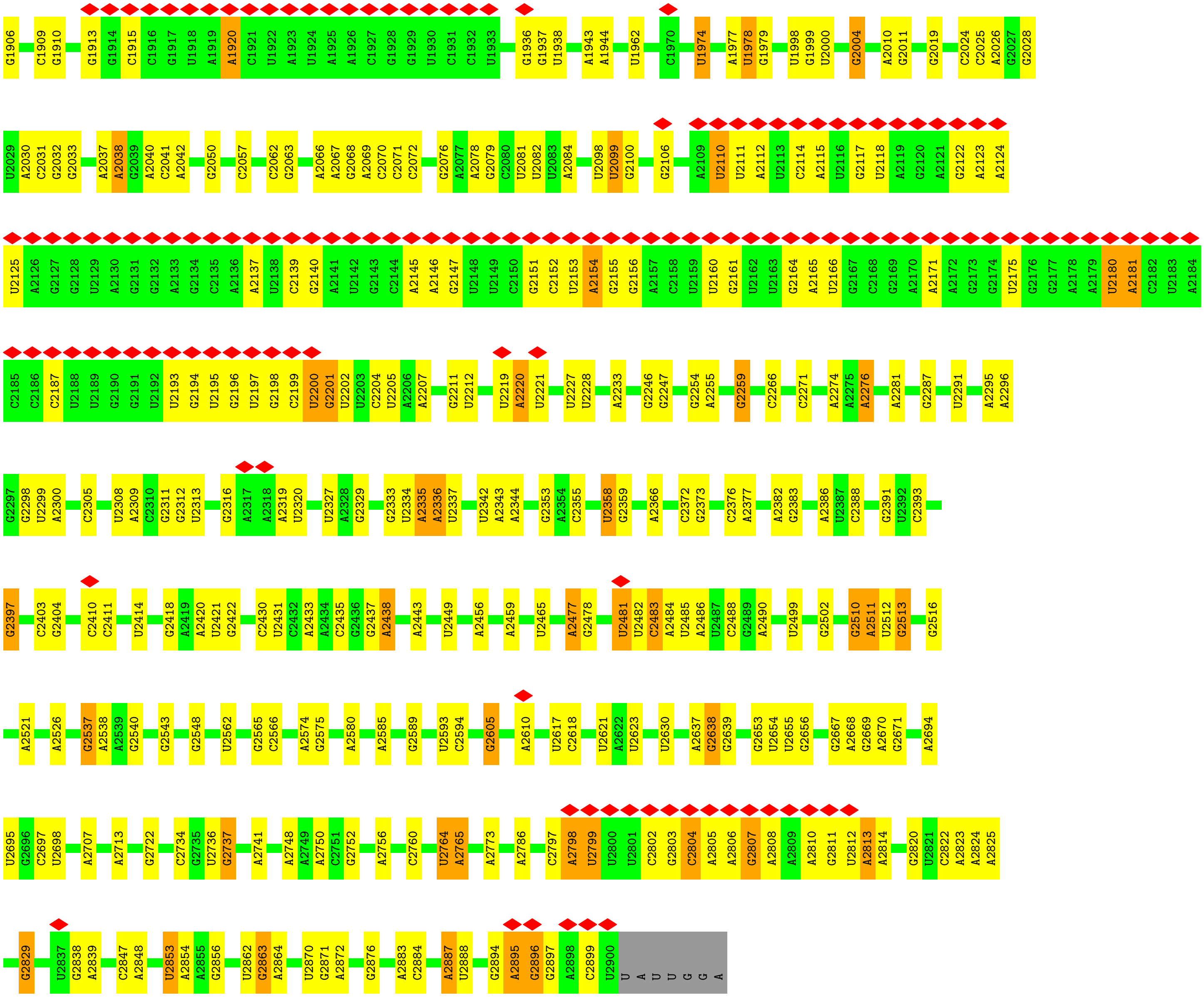


- Molecule 4: 23S ribosomal RNA

Chain 3:

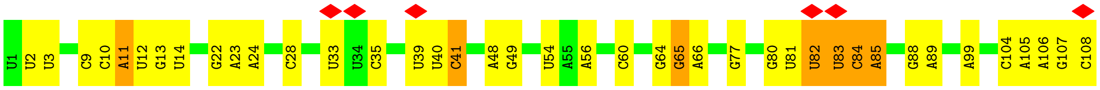



G363 A364 U365 A374 A392 A402 U403 G408 A409 G410 U411 A412 G418 A419 A422 C423 G424 U425 U426 A427 G432 A437 C440 G447 A448 C449 C450 G456 A459 G460 U463 A483 C487 A490 G499 A502 G512 A515 A516 G517
A518 G524 A527 A532 U539 A540 A548 A549 C558 C562 C565 G566 U567 G568 U569 C570 A573 A581 A582 U583 G584 U585 G586 U587 G596 C597 G598 G603 A604 A605 G606 U607 A608 U609 G610 A611 C614 G615 G616 A619 G620 U621 U622 A623 U636
U637 A638 G648 A649 G650 A651 U652 G653 G656 A657 U660 A663 G664 C665 G666 A667 A668 A669 G670 C671 G672 A673 A680 A681 A682 U689 U690 G691 U700 A701 U702 A703 G704 A705 A712 G716 A720 G721 C722 A728 C733 U749 A750 A751 C752 A753 U754
C755 A756 A757 A765 A769 C775 U776 C777 U782 G783 G788 A789 G792 U797 C800 G810 G811 A817 A818 U819 U820 A823 A824 U825 C826 G827 A828 A829 A830 U831 C832 G840 G844 U845 U846 C847 U848 C849 G853 A854 U862 U869 A870
U879 C880 A881 C882 A883 U890 G891 G892 A893 G894 A897 A898 A899 G900 C901 U902 A903 C904 U905 G906 U909 G910 U916 G917 G918 C919 G920 C921 C922 A923 C924 G925 U926 A927 G928 G929 C930 G931 U932 A933 C934 U935 G936 U944 A947 A948 C949 U950 C951 U952 G953 G957
U963 A964 U968 A969 U970 A981 G982 A983 C984 A985 U994 G997 C998 U999 U1000 A1008 A1009 G1010 A1016 A1019 C1023 A1026 A1032 A1036 G1039 A1045 U1049 A1055 U1058 G1059 G1060 A1061 U1068 A1074 G1075 U1076 A1080 A1081 A1082 A1083 C1084
A1088 A1089 G1090 G1091 A1092 U1093 G1094 U1095 U1096 G1097 G1098 C1099 U1100 U1101 A1102 G1103 A1104 A1105 G1106 C1107 A1108 G1109 C1110 C1111 A1112 U1113 C1114 G1115 U1116 U1117 U1118 A1119 A1120 A1121 G1122 A1123 G1124 U1125 G1126 C1127 G1128 U1129 A1130 A1131 C1132 A1133 G1134 C1135 U1136 C1137 A1138 C1139 U1143 C1144 G1145 A1146 G1147 U1148
G1149 A1162 U1165 G1166 U1167 A1168 A1169 C1170 U1176 A1177 A1178 C1188 A1204 U1205 U1206 U1207 A1208 U1209 A1210 U1211 C1212 G1215 U1219 U1234 U1235 G1236 G1239 U1240 U1241 G1242 U1246 A1250 G1251 C1252 G1253 A1256 G1257 G1266 A1267 U1268 C1269 C1270 A1271 G1280 A1281 G1282
A1283 A1284 U1285 G1286 A1292 G1296 G1301 C1302 U1303 U1304 G1305 G1306 G1307 G1313 C1321 A1322 C1325 A1328 U1329 U1330 U1334 A1335 G1338 U1339 U1340 U1341 C1342 C1343 U1344 G1352 G1356 U1369 C1378 C1379 U1380 A1381 U1385 G1386 A1387 G1388 U1391 G1392 A1393 A1394 A1395
A1401 C1404 G1405 A1406 U1407 A1412 A1413 C1414 A1415 A1420 A1423 U1424 A1431 C1432 U1433 U1434 A1435 C1436 A1437 G1438 U1439 U1440 A1441 C1444 U1445 G1446 A1447 U1448 C1456 G1460 A1461 A1462 G1463 G1464 U1465 U1466 U1467 A1480 U1481 U1482 G1483 G1484 A1485 U1486 U1487 A1495 A1496 A1502
A1503 G1504 G1508 U1509 A1510 A1513 U1514 A1515 C1518 A1519 A1520 A1521 U1522 U1529 G1530 U1533 A1534 A1535 C1536 A1537 A1541 G1542 U1543 G1544 A1545 U1546 U1549 G1550 G1557 A1558 A1559 U1560 G1561 A1562 G1563 U1564 G1565 A1566 U1567 C1568 A1569 A1570 G1571 U1572 A1573 G1574 C1575 G1576 G1580 U1581 G1582
G1583 U1584 A1585 A1588 A1589 U1590 U1598 C1599 A1603 C1611 U1612 A1613 G1616 U1617 U1618 A1619 A1620 U1623 A1624 A1641 G1642 A1643 A1644 C1645 A1650 C1651 A1661 G1665 G1668 U1673 A1680 G1681 C1682 A1688 U1691 A1692 U1693 A1694 G1695 C1696 C1697 A1698 G1708
U1727 G1737 U1748 A1749 U1764 A1769 A1770 C1771 A1780 U1786 C1789 U1790 A1791 C1797 A1798 U1801 C1802 U1803 A1804 C1807 C1808 A1809 A1810 U1815 A1816 U1823 G1833 A1836 C1837 A1854 A1855 G1866 G1869 G1870 U1871 A1878 C1886 U1889 U1890



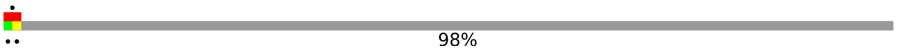
- Molecule 5: 5S ribosomal RNA

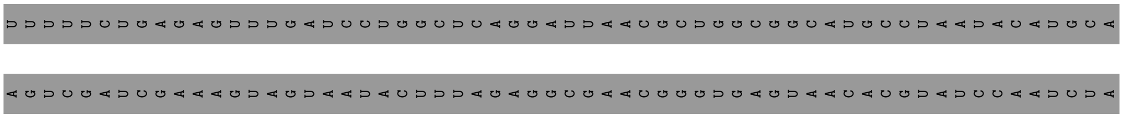
Chain 4:

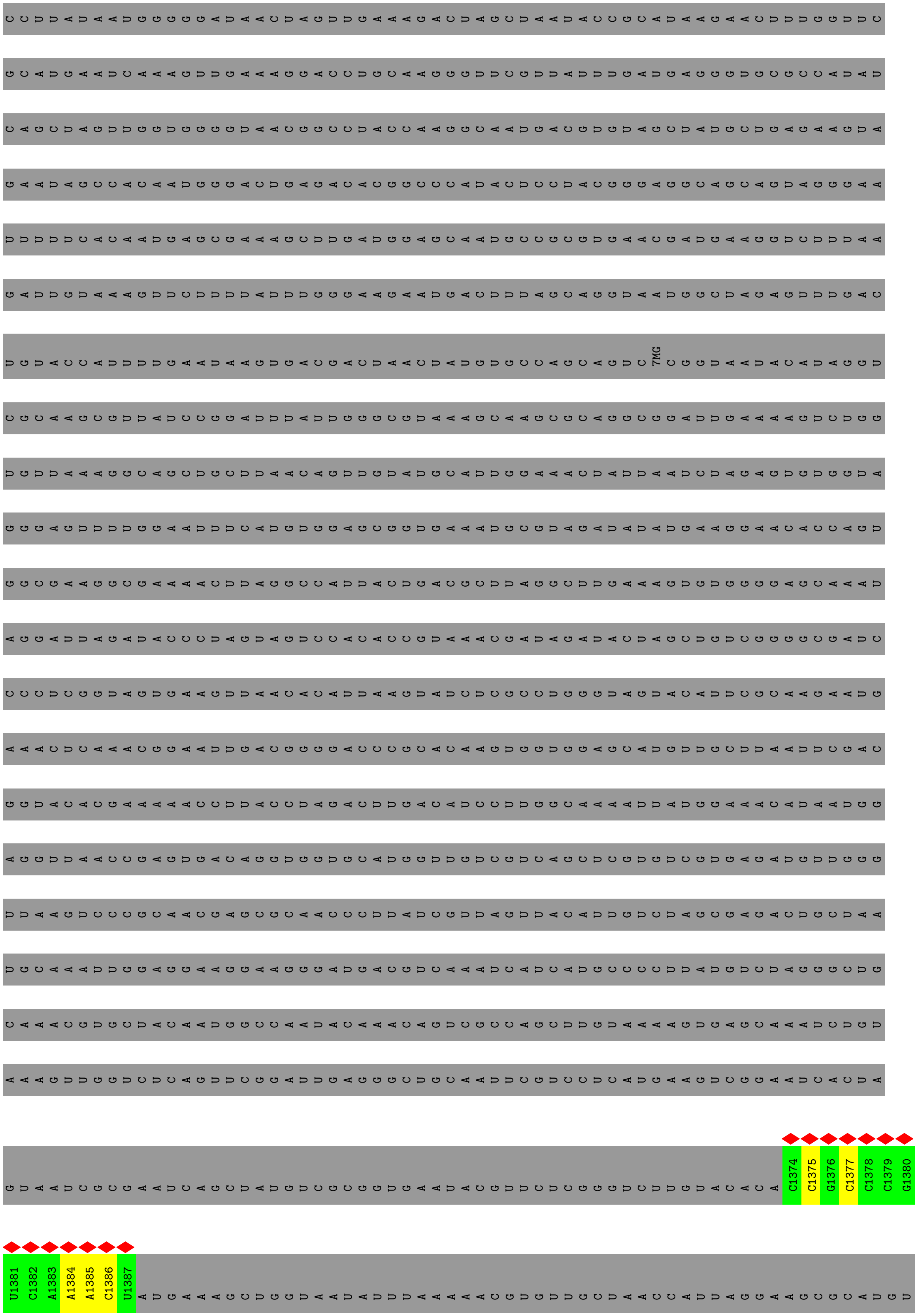


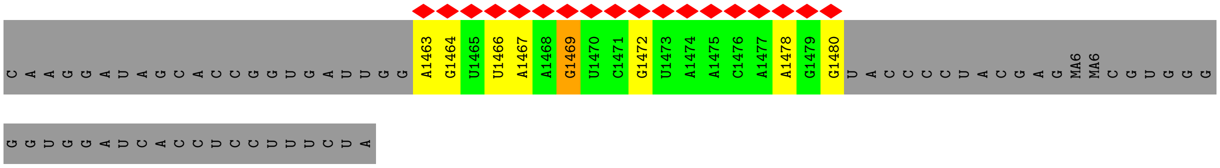
- Molecule 6: 16S ribosomal RNA

Chain 5:



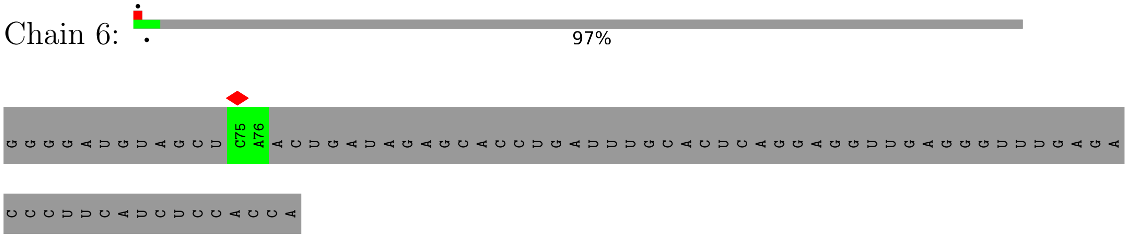



7MG
C1374
C1375
G1376
C1377
C1378
C1379
G1380
U1381
C1382
A1383
A1384
A1385
C1386
U1387



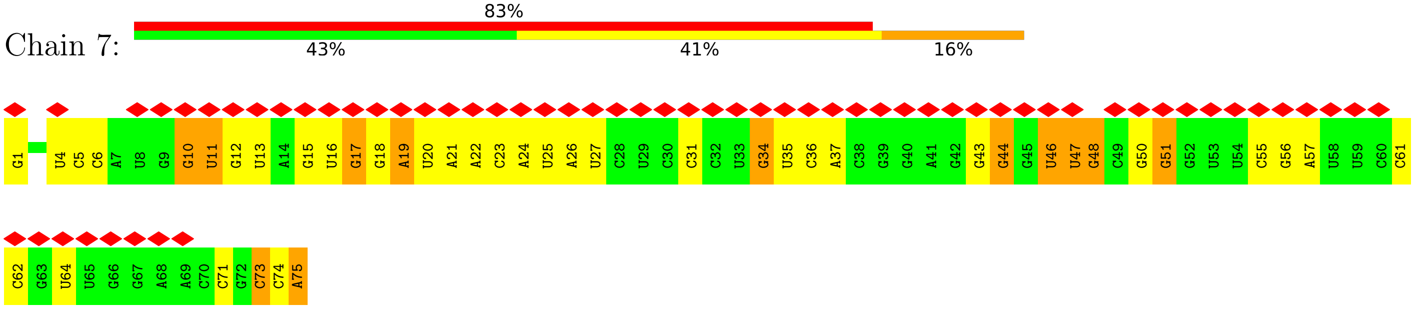
- Molecule 7: tRNA-Ala (E-site)

Chain 6:



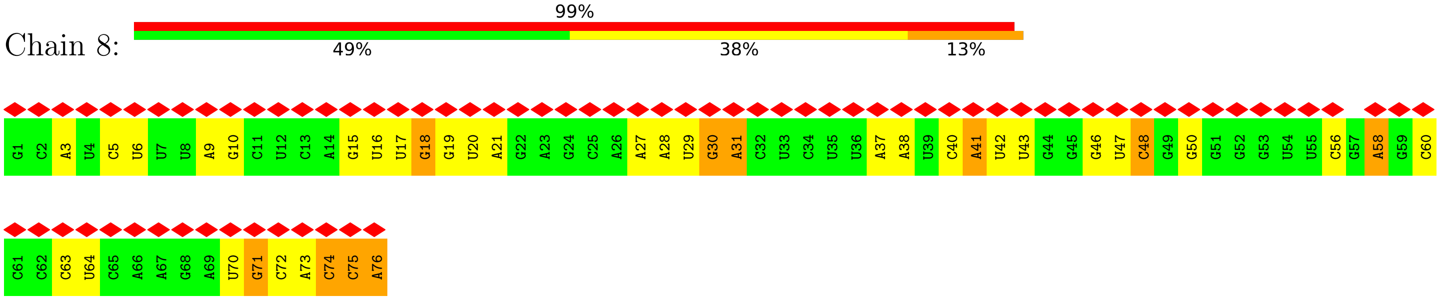
- Molecule 8: tRNA-Asp (P-site)

Chain 7:



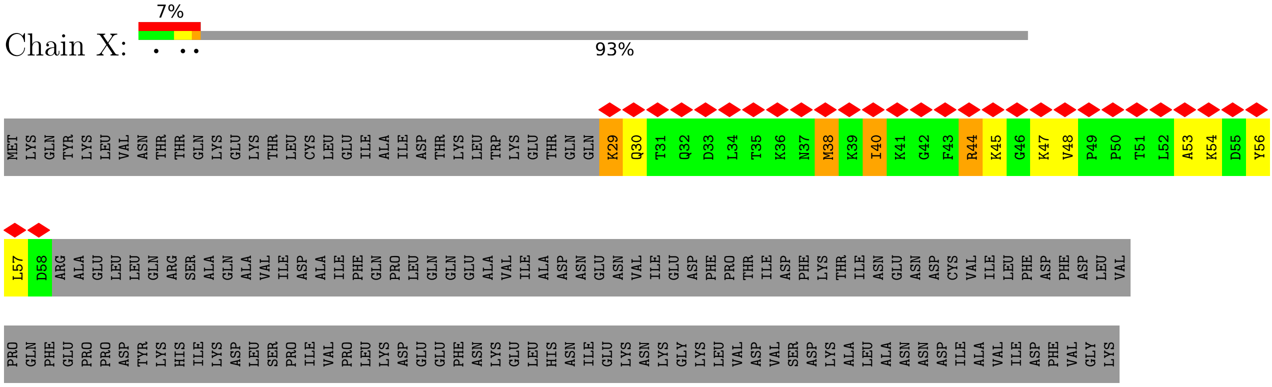
- Molecule 9: tRNA-Lys (A-site)

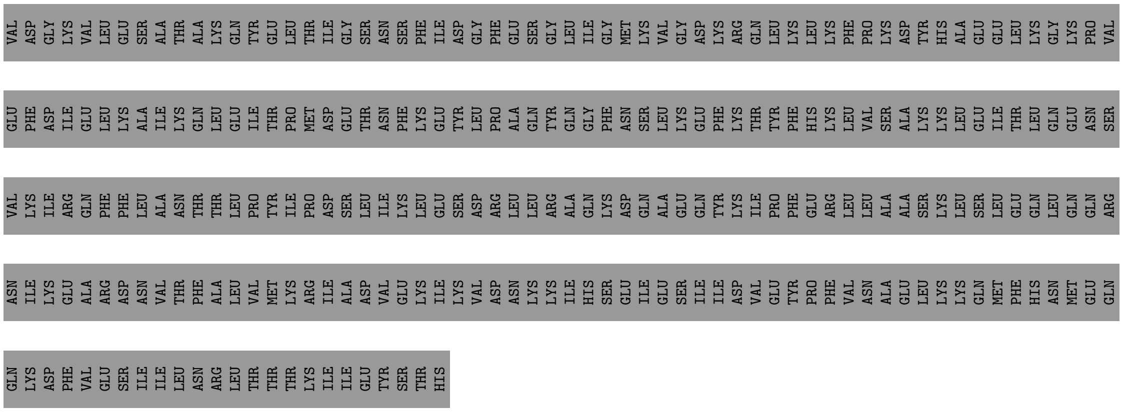
Chain 8:



- Molecule 10: Trigger factor

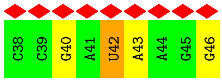
Chain X:





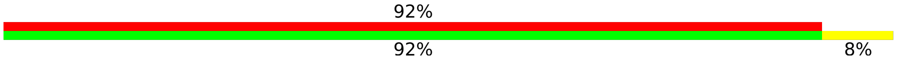
- Molecule 11: mRNA

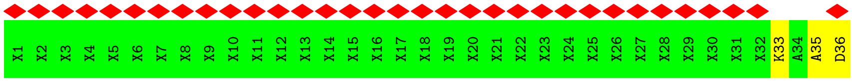
Chain Y:



- Molecule 12: nascent peptide

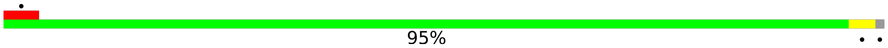
Chain Z:

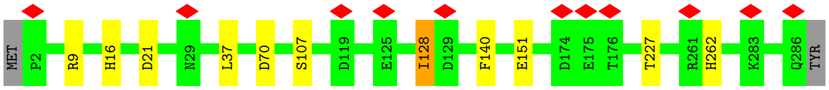




- Molecule 13: 50S ribosomal protein L2

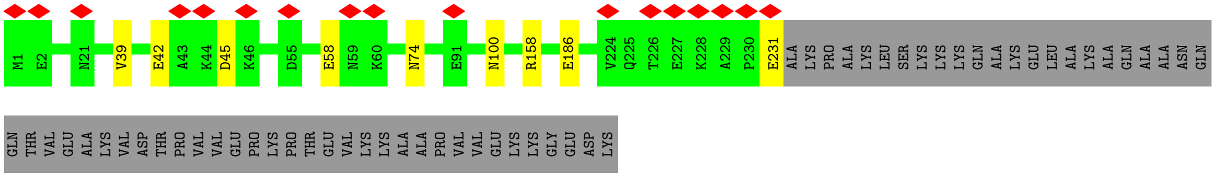
Chain a:





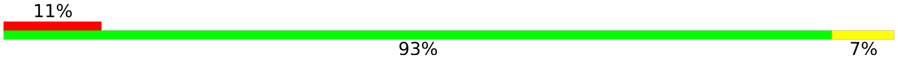
- Molecule 14: 50S ribosomal protein L3

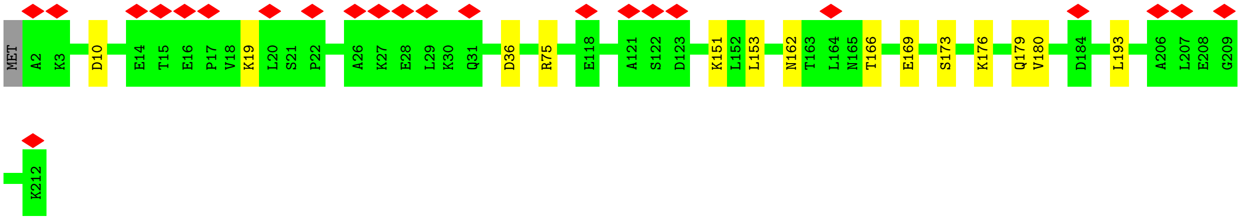
Chain b:



- Molecule 15: 50S ribosomal protein L4

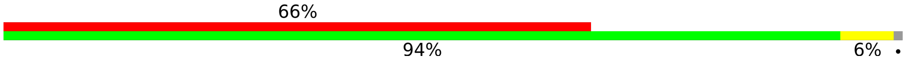
Chain c:

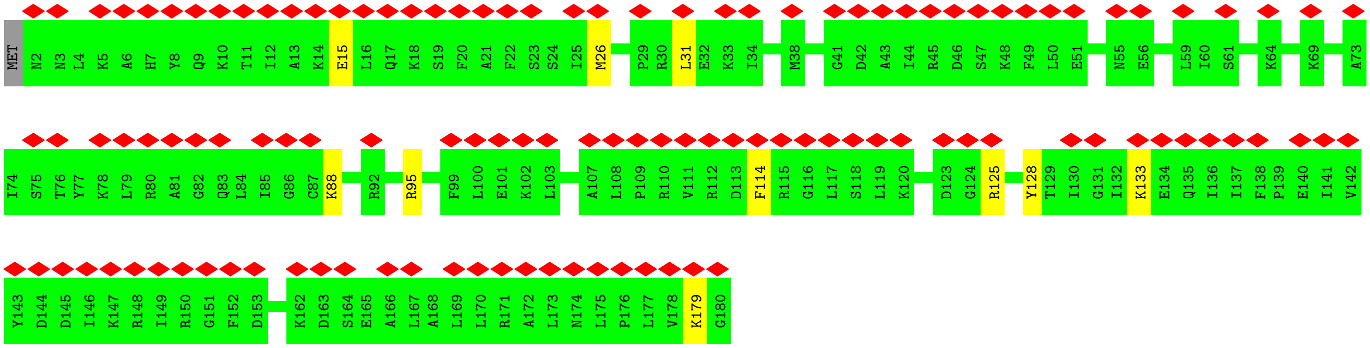




- Molecule 16: 50S ribosomal protein L5

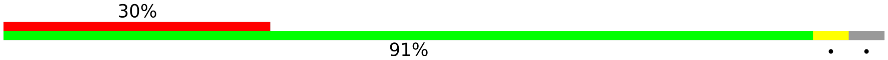
Chain d:

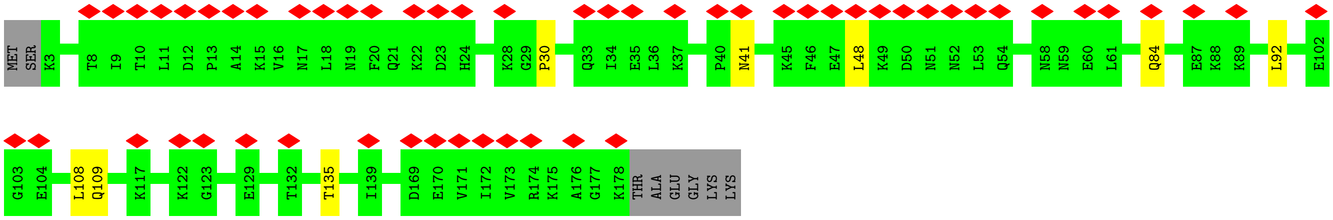




- Molecule 17: 50S ribosomal protein L6

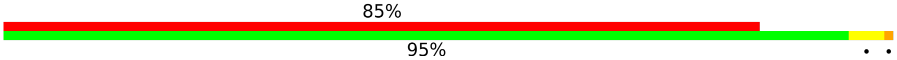
Chain e:



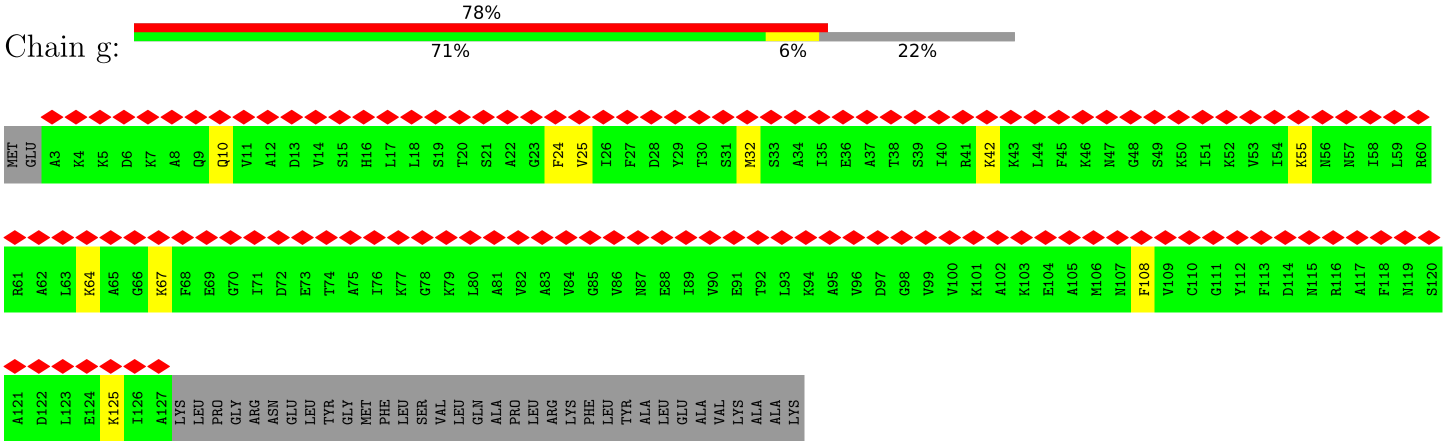


- Molecule 18: 50S ribosomal protein L9

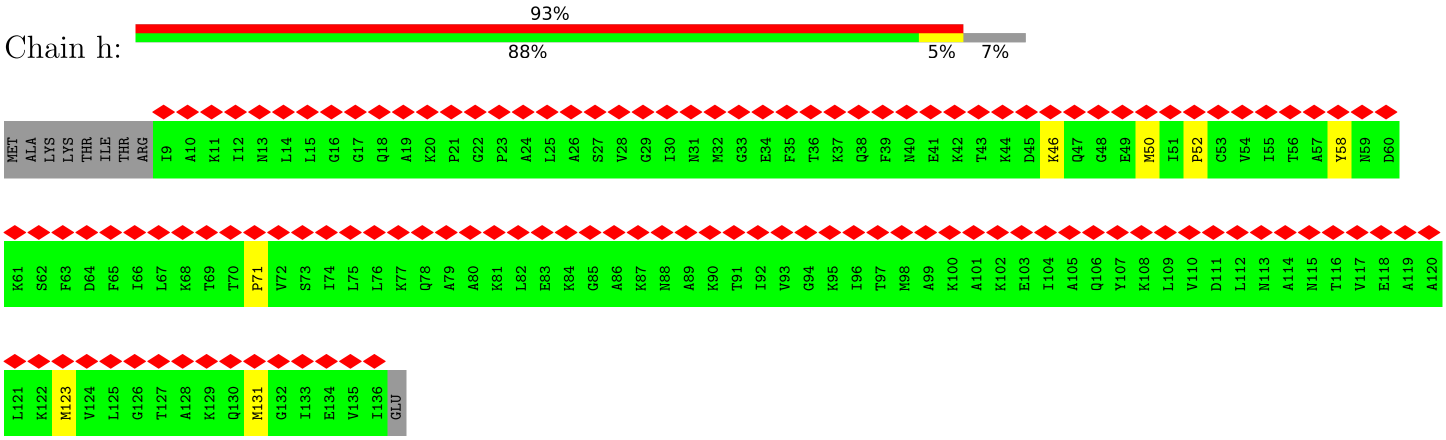
Chain f:



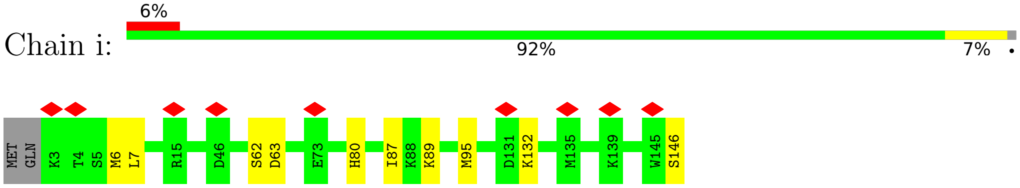
- Molecule 19: 50S ribosomal protein L10



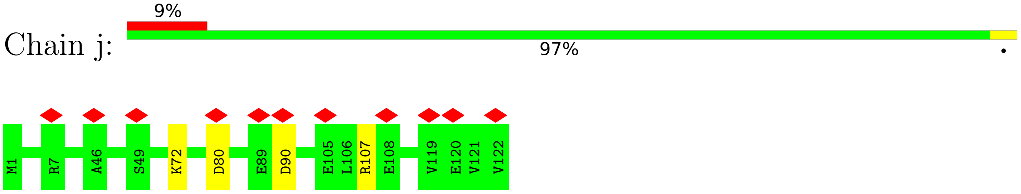
• Molecule 20: 50S ribosomal protein L11



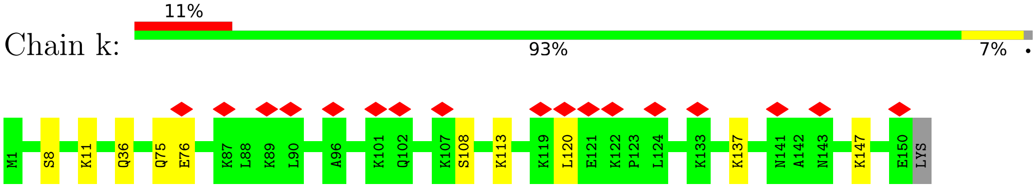
• Molecule 21: 50S ribosomal protein L13



• Molecule 22: 50S ribosomal protein L14

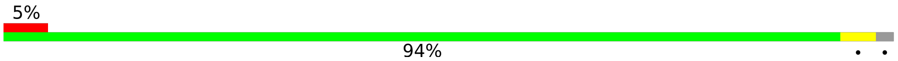


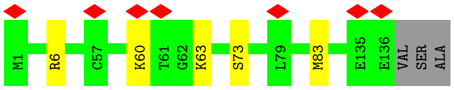
• Molecule 23: 50S ribosomal protein L15



- Molecule 24: 50S ribosomal protein L16

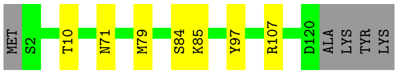
Chain l:





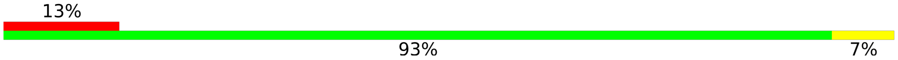
- Molecule 25: 50S ribosomal protein L17

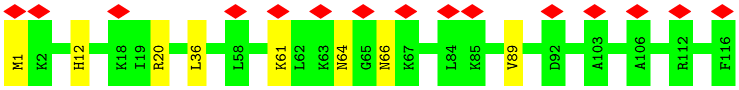
Chain m:



- Molecule 26: 50S ribosomal protein L18

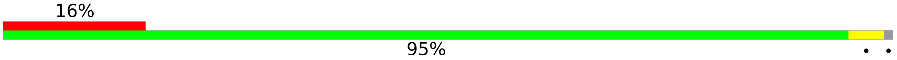
Chain n:

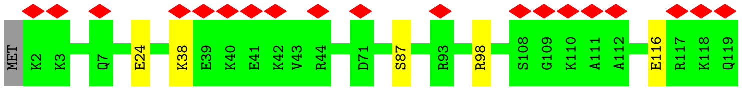




- Molecule 27: 50S ribosomal protein L19

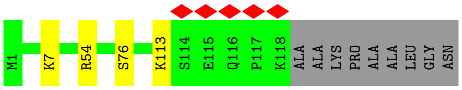
Chain o:





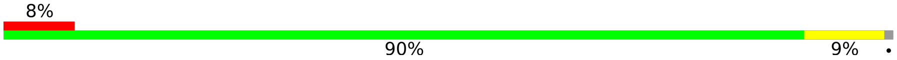
- Molecule 28: 50S ribosomal protein L20

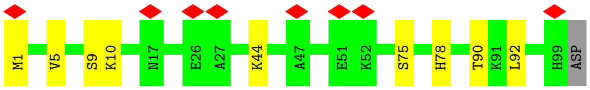
Chain p:



- Molecule 29: 50S ribosomal protein L21

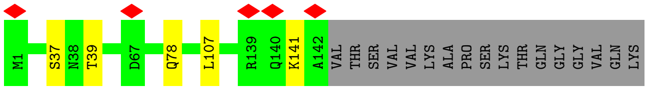
Chain q:





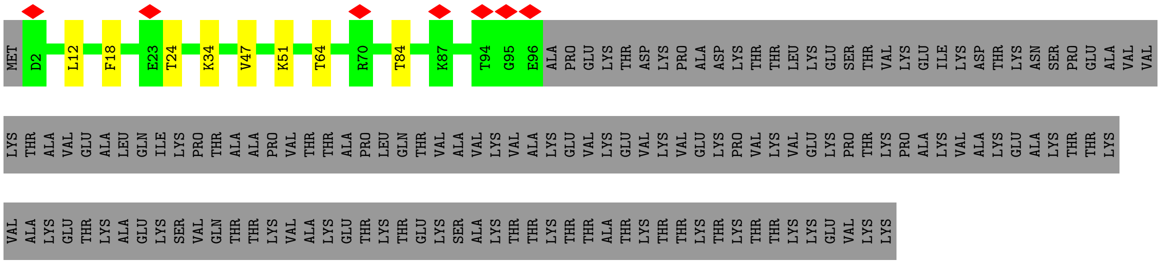
- Molecule 30: 50S ribosomal protein L22

Chain r:



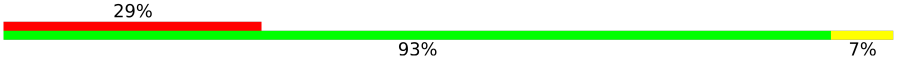
- Molecule 31: 50S ribosomal protein L23

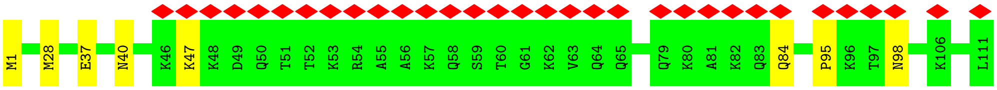
Chain s:



- Molecule 32: 50S ribosomal protein L24

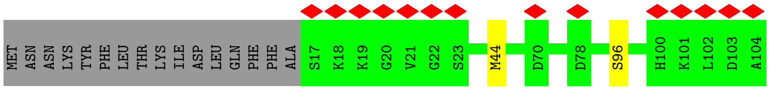
Chain t:





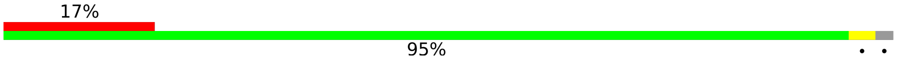
- Molecule 33: 50S ribosomal protein L27

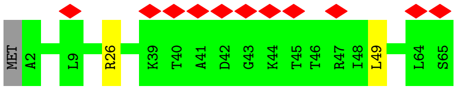
Chain u:



- Molecule 34: 50S ribosomal protein L28

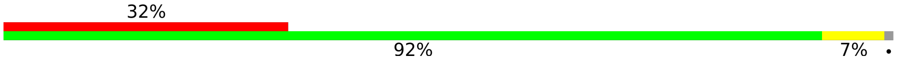
Chain v:

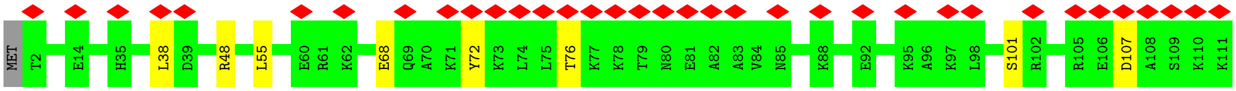




- Molecule 35: 50S ribosomal protein L29

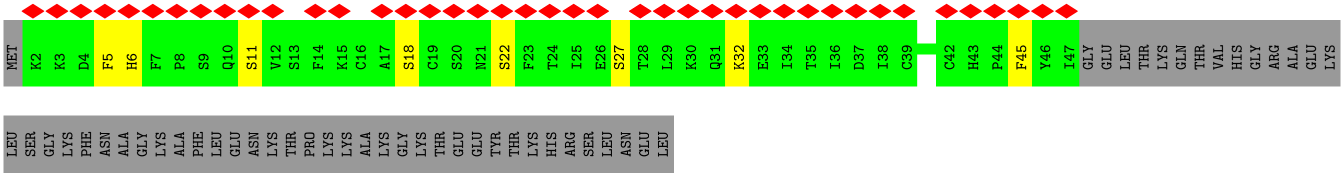
Chain w:





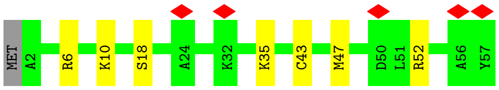
- Molecule 36: 50S ribosomal protein L31

Chain x:



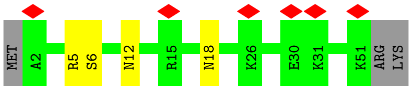
- Molecule 37: 50S ribosomal protein L32

Chain y:



- Molecule 38: 50S ribosomal protein L33 1

Chain z:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	30774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\mathring{A}^2)$	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	539.574, 539.574, 539.574	wwPDB
Map dimensions	406, 406, 406	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.329, 1.329, 1.329	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: SPD, SPM, 1MG, OMG, B8T, K, PUT, N2P, MG, ZN, 5MC, 2MA, CLM

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	0/395	0.56	0/518
2	1	0.24	0/484	0.52	0/637
3	2	0.23	0/306	0.52	0/401
4	3	0.19	0/69363	0.71	8/108161 (0.0%)
5	4	0.17	0/2578	0.72	0/4016
6	5	0.17	0/715	0.71	0/1107
7	6	0.13	0/46	0.62	0/69
8	7	0.30	1/1785 (0.1%)	0.84	2/2779 (0.1%)
9	8	0.53	6/1804 (0.3%)	0.80	0/2807
10	X	0.29	0/245	0.79	1/325 (0.3%)
11	Y	0.28	0/218	0.79	0/338
12	Z	0.75	0/26	1.33	0/33
13	a	0.37	2/2267 (0.1%)	0.60	3/3044 (0.1%)
14	b	0.29	0/1812	0.55	1/2436 (0.0%)
15	c	0.30	0/1681	0.54	1/2257 (0.0%)
16	d	0.32	0/1437	0.66	0/1931
17	e	0.49	2/1420 (0.1%)	0.94	5/1912 (0.3%)
18	f	0.40	1/1233 (0.1%)	0.62	0/1653
19	g	0.32	0/960	0.60	0/1284
20	h	0.78	4/968 (0.4%)	1.19	7/1298 (0.5%)
21	i	0.25	0/1186	0.50	0/1592
22	j	0.27	0/953	0.61	1/1275 (0.1%)
23	k	0.29	0/1187	0.60	0/1581
24	l	0.29	0/1104	0.56	0/1481
25	m	0.29	0/973	0.52	1/1309 (0.1%)
26	n	0.28	0/927	0.58	0/1239
27	o	0.31	0/976	0.59	0/1296
28	p	0.26	0/996	0.54	0/1325
29	q	0.29	0/828	0.55	0/1111
30	r	0.26	0/1100	0.50	0/1471
31	s	0.27	0/752	0.58	0/1015
32	t	0.57	1/878 (0.1%)	0.96	4/1165 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	u	0.25	0/678	0.52	0/902
34	v	0.23	0/526	0.56	0/703
35	w	0.26	0/916	0.56	0/1222
36	x	0.26	0/375	0.46	0/502
37	y	0.28	0/457	0.63	0/601
38	z	0.23	0/412	0.54	0/547
All	All	0.25	17/104967 (0.0%)	0.70	34/157343 (0.0%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	h	52	PRO	CG-CD	-15.31	1.00	1.50
32	t	95	PRO	CG-CD	-13.85	1.04	1.50
17	e	30	PRO	CB-CG	-11.82	0.90	1.50
9	8	76	A	N9-C4	10.38	1.44	1.37
20	h	52	PRO	N-CD	10.15	1.62	1.47

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	h	52	PRO	N-CD-CG	-20.95	71.77	103.20
32	t	95	PRO	N-CD-CG	-19.84	73.44	103.20
17	e	30	PRO	N-CD-CG	-19.64	73.73	103.20
17	e	30	PRO	CB-CG-CD	18.83	179.95	106.50
17	e	30	PRO	CA-CB-CG	-16.62	72.43	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	392	0	442	8	0
2	1	477	0	530	7	0
3	2	304	0	348	3	0
4	3	61995	0	31115	341	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	2305	0	1164	12	0
6	5	683	0	339	4	0
7	6	42	0	23	0	0
8	7	1599	0	805	24	0
9	8	1615	0	816	19	0
10	X	242	0	263	9	0
11	Y	195	0	99	1	0
12	Z	187	0	68	5	0
13	a	2225	0	2301	0	0
14	b	1778	0	1821	0	0
15	c	1654	0	1744	0	0
16	d	1416	0	1500	0	0
17	e	1396	0	1481	0	0
18	f	1210	0	1259	0	0
19	g	951	0	1001	0	0
20	h	959	0	1039	0	0
21	i	1164	0	1192	0	0
22	j	944	0	1019	0	0
23	k	1170	0	1274	0	0
24	l	1079	0	1134	0	0
25	m	958	0	1011	0	0
26	n	918	0	979	0	0
27	o	966	0	1042	0	0
28	p	981	0	1062	0	0
29	q	811	0	858	0	0
30	r	1091	0	1178	0	0
31	s	740	0	819	0	0
32	t	871	0	972	0	0
33	u	670	0	704	0	0
34	v	520	0	565	0	0
35	w	906	0	981	0	0
36	x	366	0	356	0	0
37	y	452	0	471	0	0
38	z	408	0	436	0	0
39	2	1	0	0	0	0
39	x	1	0	0	0	0
39	y	1	0	0	0	0
39	z	1	0	0	0	0
40	3	20	0	11	4	0
41	3	1	0	0	0	0
42	3	219	0	0	0	0
42	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	6	1	0	0	0	0
42	7	1	0	0	0	0
42	8	2	0	0	0	0
42	b	2	0	0	0	0
42	i	1	0	0	0	0
42	y	2	0	0	0	0
43	3	42	0	84	1	0
44	3	42	0	78	7	0
44	b	14	0	26	0	0
45	3	160	0	304	3	0
46	3	21	0	42	0	0
47	8	9	0	12	0	0
All	All	97182	0	64768	416	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 7.

The worst 5 of 416 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)
9:8:50:G:H1	9:8:64:U:H3	1.21	0.88
4:3:2736:U:HO2’	4:3:2737:G:H8	1.24	0.85
10:X:29:LYS:HE3	10:X:30:GLN:HG2	1.60	0.82
3:2:4:ARG:NH2	4:3:2485:U:O2	2.12	0.82
10:X:38:MET:SD	10:X:57:LEU:HD22	2.20	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
10	X	28/444 (6%)	24 (86%)	4 (14%)	0	100	100
12	Z	3/36 (8%)	3 (100%)	0	0	100	100
13	a	283/287 (99%)	268 (95%)	14 (5%)	1 (0%)	30	60
14	b	229/287 (80%)	221 (96%)	8 (4%)	0	100	100
15	c	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
16	d	177/180 (98%)	169 (96%)	8 (4%)	0	100	100
17	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
18	f	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	9	31
19	g	123/161 (76%)	116 (94%)	7 (6%)	0	100	100
20	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
21	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
22	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
23	k	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
24	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
25	m	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
26	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
27	o	116/119 (98%)	107 (92%)	9 (8%)	0	100	100
28	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
29	q	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
30	r	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
31	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
32	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
33	u	86/104 (83%)	82 (95%)	4 (5%)	0	100	100
34	v	62/65 (95%)	62 (100%)	0	0	100	100
35	w	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
36	x	44/97 (45%)	35 (80%)	8 (18%)	1 (2%)	5	20
37	y	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
38	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	3485/4359 (80%)	3310 (95%)	171 (5%)	4 (0%)	50	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	a	128	ILE
18	f	12	LEU
18	f	74	GLN
36	x	18	SER

5.3.2 Protein sidechains ⓘ

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	41/41 (100%)	39 (95%)	2 (5%)	21	53
2	1	51/51 (100%)	49 (96%)	2 (4%)	27	62
3	2	35/35 (100%)	35 (100%)	0	100	100
10	X	27/406 (7%)	22 (82%)	5 (18%)	1	4
12	Z	2/2 (100%)	2 (100%)	0	100	100
13	a	241/243 (99%)	232 (96%)	9 (4%)	29	64
14	b	188/233 (81%)	180 (96%)	8 (4%)	25	57
15	c	183/184 (100%)	170 (93%)	13 (7%)	12	36
16	d	153/154 (99%)	143 (94%)	10 (6%)	14	40
17	e	153/159 (96%)	147 (96%)	6 (4%)	27	62
18	f	134/134 (100%)	129 (96%)	5 (4%)	29	64
19	g	100/129 (78%)	90 (90%)	10 (10%)	6	20
20	h	102/110 (93%)	97 (95%)	5 (5%)	21	53
21	i	126/128 (98%)	116 (92%)	10 (8%)	10	30
22	j	103/103 (100%)	100 (97%)	3 (3%)	37	72
23	k	125/126 (99%)	115 (92%)	10 (8%)	10	30
24	l	113/115 (98%)	108 (96%)	5 (4%)	24	57
25	m	105/109 (96%)	99 (94%)	6 (6%)	17	47
26	n	99/99 (100%)	91 (92%)	8 (8%)	9	29
27	o	104/105 (99%)	99 (95%)	5 (5%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	p	104/108 (96%)	100 (96%)	4 (4%)	28	63
29	q	90/91 (99%)	81 (90%)	9 (10%)	6	20
30	r	118/132 (89%)	113 (96%)	5 (4%)	25	59
31	s	84/208 (40%)	76 (90%)	8 (10%)	7	22
32	t	96/96 (100%)	89 (93%)	7 (7%)	11	34
33	u	70/85 (82%)	68 (97%)	2 (3%)	37	72
34	v	59/60 (98%)	57 (97%)	2 (3%)	32	67
35	w	97/98 (99%)	89 (92%)	8 (8%)	9	29
36	x	44/86 (51%)	37 (84%)	7 (16%)	2	6
37	y	48/49 (98%)	41 (85%)	7 (15%)	2	8
38	z	47/50 (94%)	43 (92%)	4 (8%)	8	27
All	All	3042/3729 (82%)	2857 (94%)	185 (6%)	18	43

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	n	66	ASN
31	s	34	LYS
27	o	87	SER
29	q	44	LYS
32	t	37	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
23	k	134	GLN
26	n	64	ASN
33	u	100	HIS
28	p	71	GLN
28	p	106	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	Y	8/9 (88%)	4 (50%)	1 (12%)
4	3	2891/2907 (99%)	503 (17%)	12 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	4	107/108 (99%)	29 (27%)	0
6	5	29/1520 (1%)	6 (20%)	0
7	6	1/76 (1%)	0	0
8	7	74/75 (98%)	20 (27%)	2 (2%)
9	8	75/76 (98%)	23 (30%)	0
All	All	3185/4771 (66%)	585 (18%)	15 (0%)

5 of 585 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U
4	3	12	A
4	3	13	C
4	3	14	U
4	3	28	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	3	1583	G
8	7	46	U
4	3	1618	U
11	Y	42	U
4	3	2764	U

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	2MA	3	2511	4,42	17,25,26	2.62	5 (29%)	17,37,40	1.35	3 (17%)
6	B8T	5	1377	6	19,22,23	3.28	8 (42%)	26,31,34	0.84	1 (3%)
6	5MC	5	1375	6	18,22,23	4.07	7 (38%)	26,32,35	1.04	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	1MG	3	783	4	18,26,27	2.73	6 (33%)	19,39,42	1.50	3 (15%)
4	OMG	3	2259	8,4,42	18,26,27	2.83	7 (38%)	19,38,41	1.57	4 (21%)

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
4	2MA	3	2511	4,42	-	2/3/25/26	0/3/3/3
6	B8T	5	1377	6	-	2/7/27/28	0/2/2/2
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2
4	1MG	3	783	4	-	0/3/25/26	0/3/3/3
4	OMG	3	2259	8,4,42	-	3/5/27/28	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1375	5MC	C6-C5	9.99	1.51	1.34
4	3	2511	2MA	C2-N3	7.81	1.47	1.31
6	5	1375	5MC	C4-N3	7.53	1.46	1.34
6	5	1377	B8T	C4-N3	7.25	1.45	1.32
4	3	2259	OMG	C2-N2	7.16	1.51	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	3	783	1MG	C5-C6-N1	4.12	120.09	113.90
4	3	2259	OMG	C5-C6-N1	3.44	120.03	113.95
4	3	2511	2MA	C5-C6-N1	3.39	119.88	114.02
6	5	1375	5MC	C5-C6-N1	-3.16	120.09	123.34
4	3	2259	OMG	C2-N1-C6	-2.89	119.77	125.10

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	3	2259	OMG	O4'-C4'-C5'-O5'
4	3	2259	OMG	C3'-C4'-C5'-O5'
4	3	2259	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
6	5	1377	B8T	O4'-C4'-C5'-O5'
4	3	2511	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	2511	2MA	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 266 ligands modelled in this entry, 234 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
45	SPD	3	3245	-	9,9,9	0.32	0	8,8,8	0.89	0
45	SPD	3	3235	-	9,9,9	0.33	0	8,8,8	0.87	0
43	PUT	3	3231	-	5,5,5	0.25	0	4,4,4	0.51	0
45	SPD	3	3237	-	9,9,9	0.32	0	8,8,8	0.96	0
45	SPD	3	3246	-	9,9,9	0.33	0	8,8,8	0.82	0
45	SPD	3	3250	-	9,9,9	0.17	0	8,8,8	0.19	0
46	N2P	3	3244	-	6,6,6	0.25	0	5,5,5	0.63	0
43	PUT	3	3242	-	5,5,5	0.25	0	4,4,4	0.54	0
43	PUT	3	3224	-	5,5,5	0.25	0	4,4,4	0.54	0
45	SPD	3	3230	-	9,9,9	0.33	0	8,8,8	0.80	0
45	SPD	3	3232	-	9,9,9	0.35	0	8,8,8	0.75	0
43	PUT	3	3226	-	5,5,5	0.26	0	4,4,4	0.52	0
44	SPM	3	3249	-	13,13,13	0.35	0	12,12,12	0.87	0
45	SPD	3	3248	-	9,9,9	0.31	0	8,8,8	0.88	0
43	PUT	3	3225	-	5,5,5	0.25	0	4,4,4	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
45	SPD	3	3240	-	9,9,9	0.32	0	8,8,8	0.86	0
47	LYS	8	103	9	7,8,9	1.79	1 (14%)	3,8,10	0.37	0
44	SPM	b	303	-	13,13,13	0.16	0	12,12,12	0.32	0
45	SPD	3	3234	-	9,9,9	0.32	0	8,8,8	0.78	0
45	SPD	3	3238	-	9,9,9	0.32	0	8,8,8	0.85	0
46	N2P	3	3243	-	6,6,6	0.25	0	5,5,5	0.65	0
45	SPD	3	3239	-	9,9,9	0.32	0	8,8,8	0.88	0
43	PUT	3	3222	-	5,5,5	0.24	0	4,4,4	0.55	0
45	SPD	3	3229	-	9,9,9	0.32	0	8,8,8	0.87	0
43	PUT	3	3223	-	5,5,5	0.23	0	4,4,4	0.56	0
44	SPM	3	3227	-	13,13,13	0.35	0	12,12,12	0.90	0
46	N2P	3	3247	-	6,6,6	0.24	0	5,5,5	0.67	0
40	CLM	3	3001	-	19,20,20	0.55	1 (5%)	23,27,27	0.61	0
45	SPD	3	3228	-	9,9,9	0.32	0	8,8,8	0.87	0
44	SPM	3	3241	-	13,13,13	0.34	0	12,12,12	0.93	0
45	SPD	3	3233	-	9,9,9	0.32	0	8,8,8	0.89	0
45	SPD	3	3236	-	9,9,9	0.33	0	8,8,8	0.82	0

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
45	SPD	3	3245	-	-	0/7/7/7	-
45	SPD	3	3235	-	-	0/7/7/7	-
43	PUT	3	3231	-	-	0/3/3/3	-
45	SPD	3	3237	-	-	1/7/7/7	-
45	SPD	3	3246	-	-	1/7/7/7	-
45	SPD	3	3250	-	-	0/7/7/7	-
46	N2P	3	3244	-	-	2/4/4/4	-
43	PUT	3	3242	-	-	0/3/3/3	-
43	PUT	3	3224	-	-	0/3/3/3	-
45	SPD	3	3230	-	-	0/7/7/7	-
45	SPD	3	3232	-	-	2/7/7/7	-
43	PUT	3	3226	-	-	0/3/3/3	-
44	SPM	3	3249	-	-	1/11/11/11	-
45	SPD	3	3248	-	-	0/7/7/7	-
43	PUT	3	3225	-	-	1/3/3/3	-
45	SPD	3	3240	-	-	0/7/7/7	-
47	LYS	8	103	9	-	3/6/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	SPM	b	303	-	-	2/11/11/11	-
45	SPD	3	3234	-	-	1/7/7/7	-
45	SPD	3	3238	-	-	0/7/7/7	-
46	N2P	3	3243	-	-	1/4/4/4	-
45	SPD	3	3239	-	-	2/7/7/7	-
43	PUT	3	3222	-	-	0/3/3/3	-
45	SPD	3	3229	-	-	1/7/7/7	-
43	PUT	3	3223	-	-	0/3/3/3	-
44	SPM	3	3227	-	-	4/11/11/11	-
46	N2P	3	3247	-	-	1/4/4/4	-
40	CLM	3	3001	-	-	2/20/22/22	0/1/1/1
45	SPD	3	3228	-	-	0/7/7/7	-
44	SPM	3	3241	-	-	2/11/11/11	-
45	SPD	3	3233	-	-	0/7/7/7	-
45	SPD	3	3236	-	-	0/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	8	103	LYS	CB-CA	4.20	1.59	1.53
40	3	3001	CLM	C1-C2	-2.11	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	8	103	LYS	O-C-CA-CB
47	8	103	LYS	C-CA-CB-CG
46	3	3243	N2P	C2-C3-C4-C5
44	3	3227	SPM	C7-C8-C9-N10
40	3	3001	CLM	C5-C3-N2-C2

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	3	3231	PUT	1	0
45	3	3237	SPD	1	0
45	3	3250	SPD	1	0

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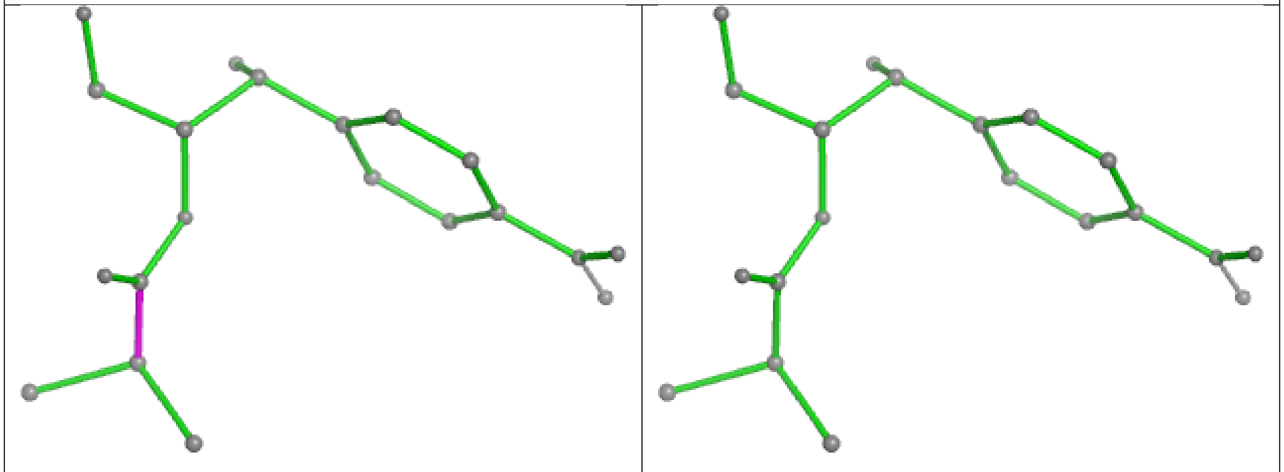
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	3	3249	SPM	2	0
45	3	3248	SPD	1	0
44	3	3227	SPM	4	0
40	3	3001	CLM	4	0
44	3	3241	SPM	1	0

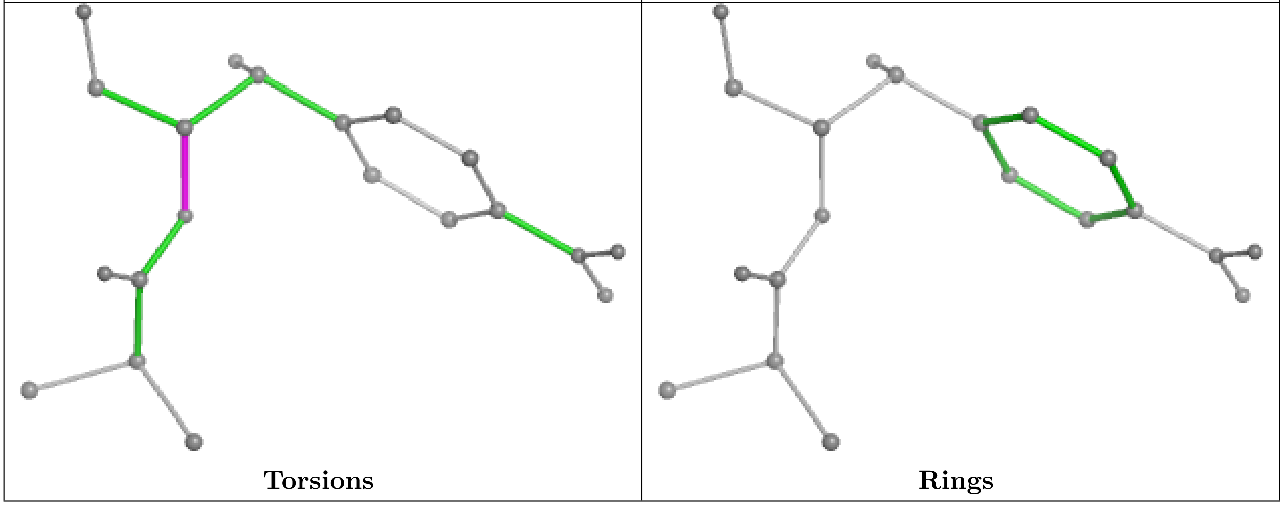
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 CLM 3 3001



Bond lengths

Bond angles



Torsions

Rings

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.

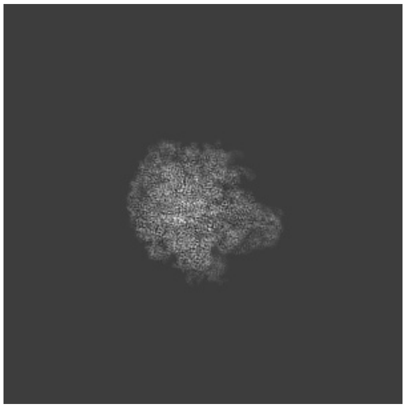
6 Map visualisation

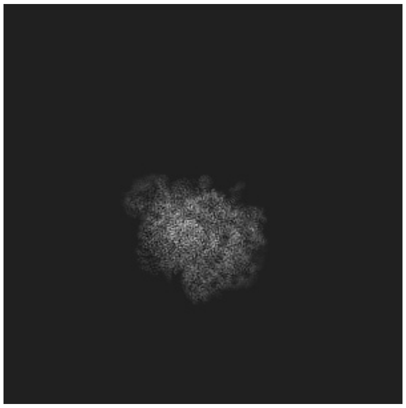
This section contains visualisations of the EMDB entry EMD-17134. These allow visual inspection of the internal detail of the map and identification of artifacts.

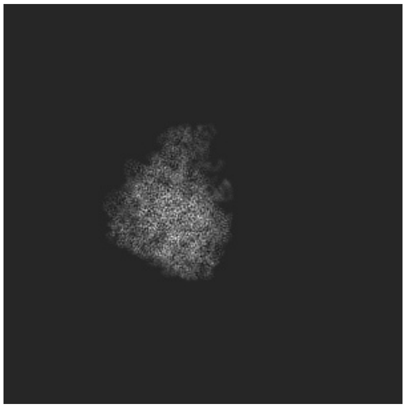
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

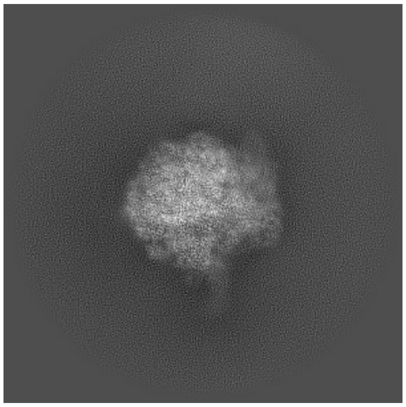
6.1.1 Primary map

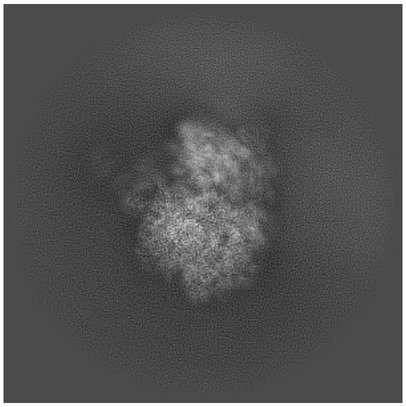

X

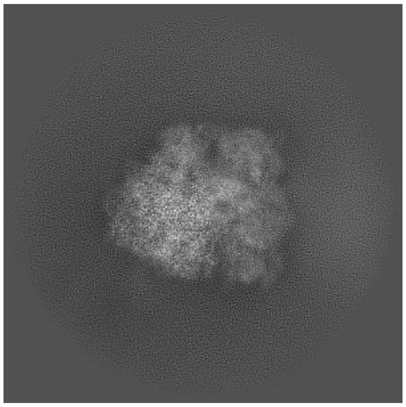

Y


Z

6.1.2 Raw map


X


Y

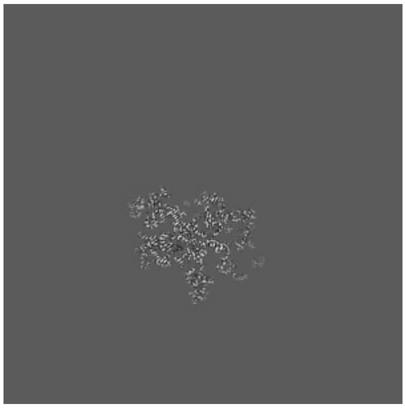

Z

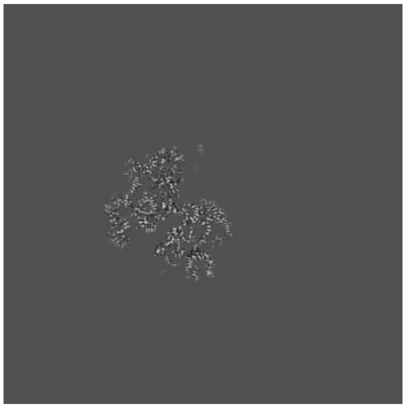
The images above show the map projected in three orthogonal directions.

6.2 Central slices

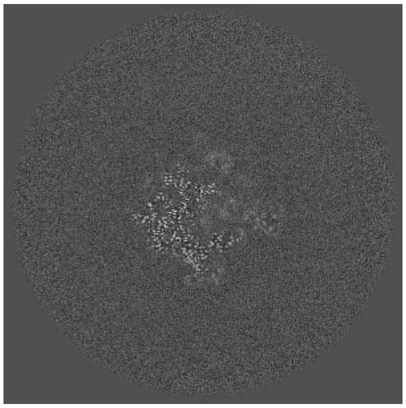
6.2.1 Primary map

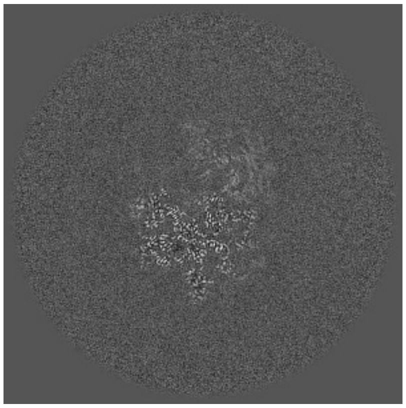

X Index: 203

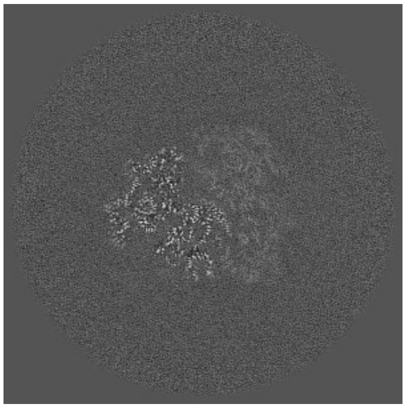

Y Index: 203


Z Index: 203

6.2.2 Raw map


X Index: 203

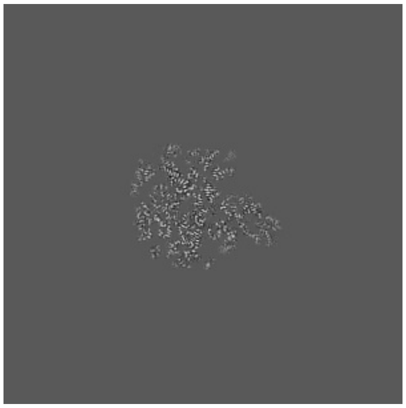

Y Index: 203


Z Index: 203

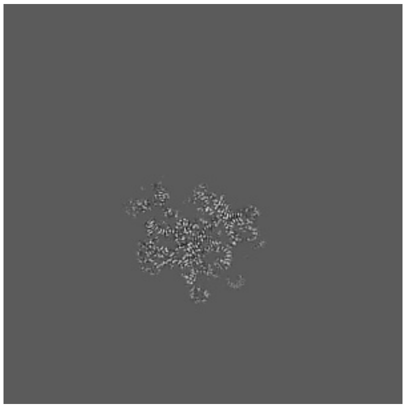
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

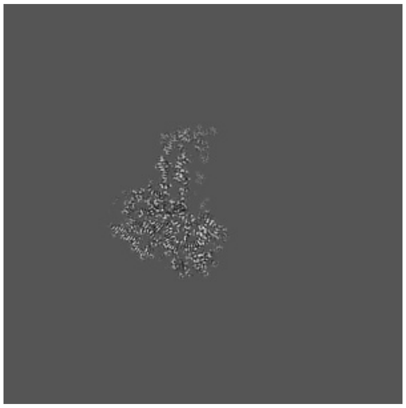
6.3.1 Primary map



X Index: 174

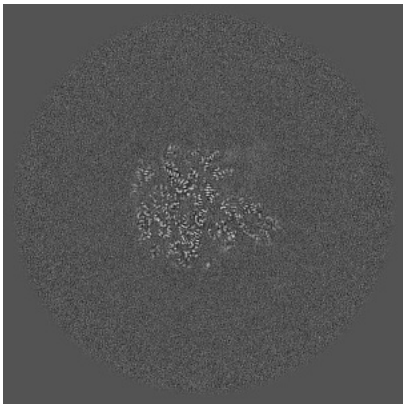


Y Index: 196

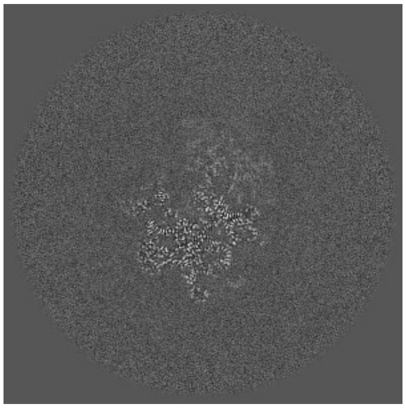


Z Index: 188

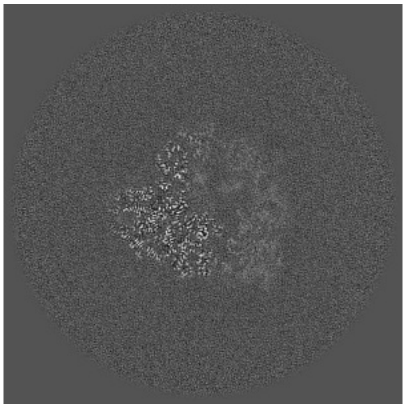
6.3.2 Raw map



X Index: 174



Y Index: 196

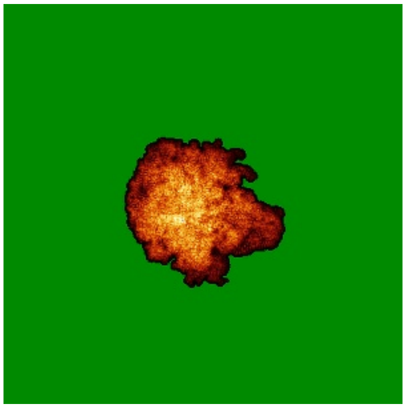


Z Index: 191

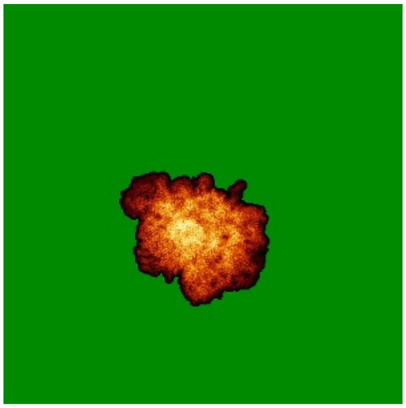
The images above show the largest variance slices of the map in three orthogonal directions.

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

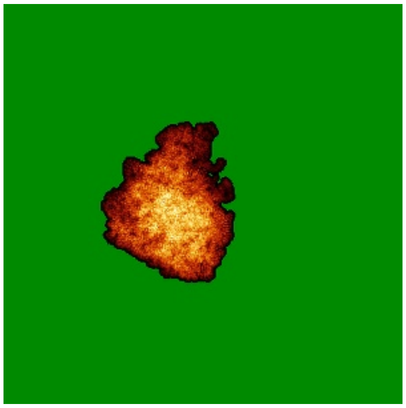
6.4.1 Primary map



X

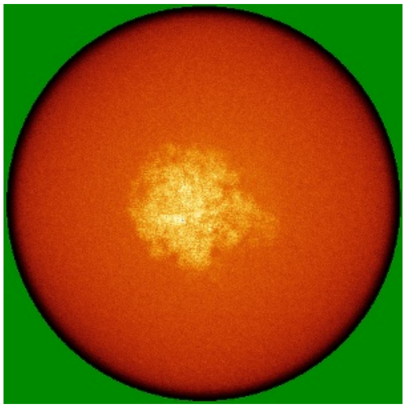


Y

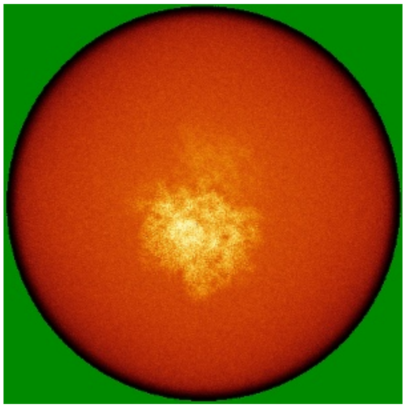


Z

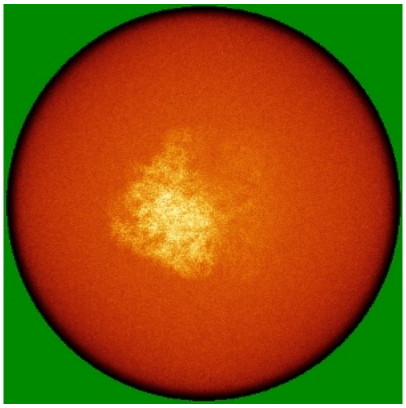
6.4.2 Raw map



X



Y



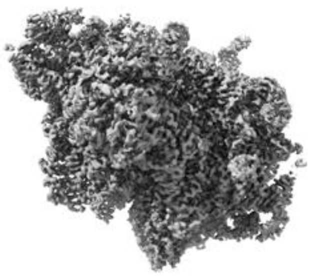
Z

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 ⓘ

6.5.1 Primary map

X

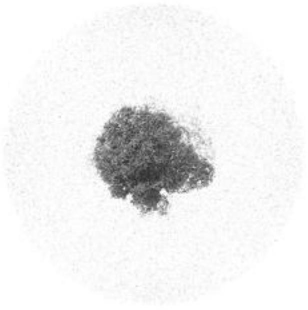


Y

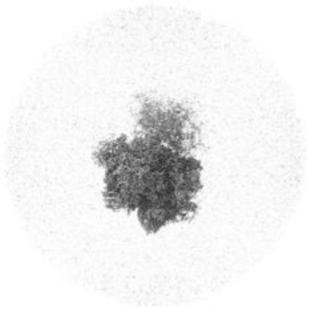
Z

The images above show the 3D surface view of the map at the recommended contour level 0.002. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

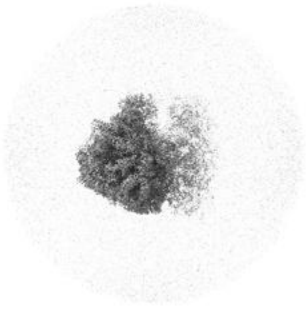
6.5.2 Raw map



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.

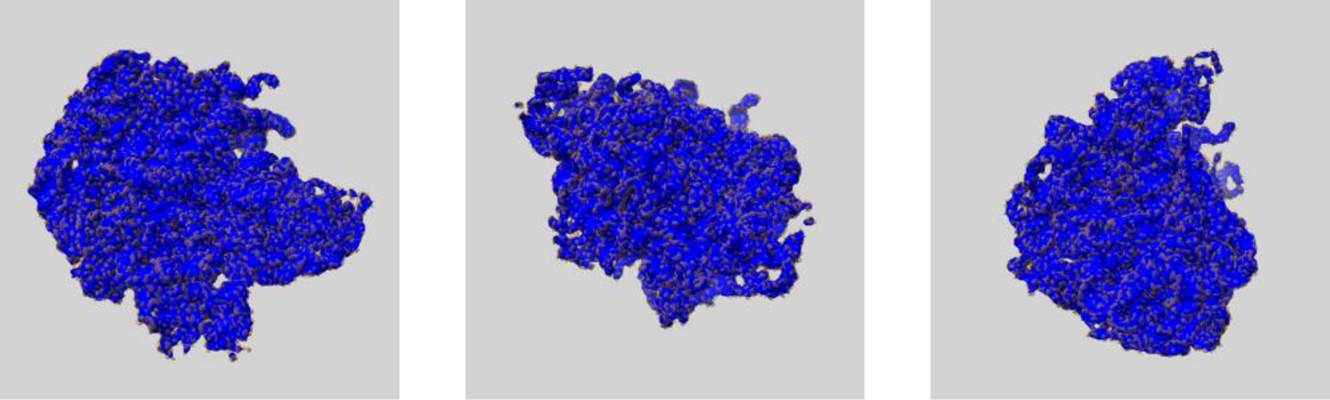
6.6 Mask visualisation ⓘ

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_17134_msk_1.map ⓘ

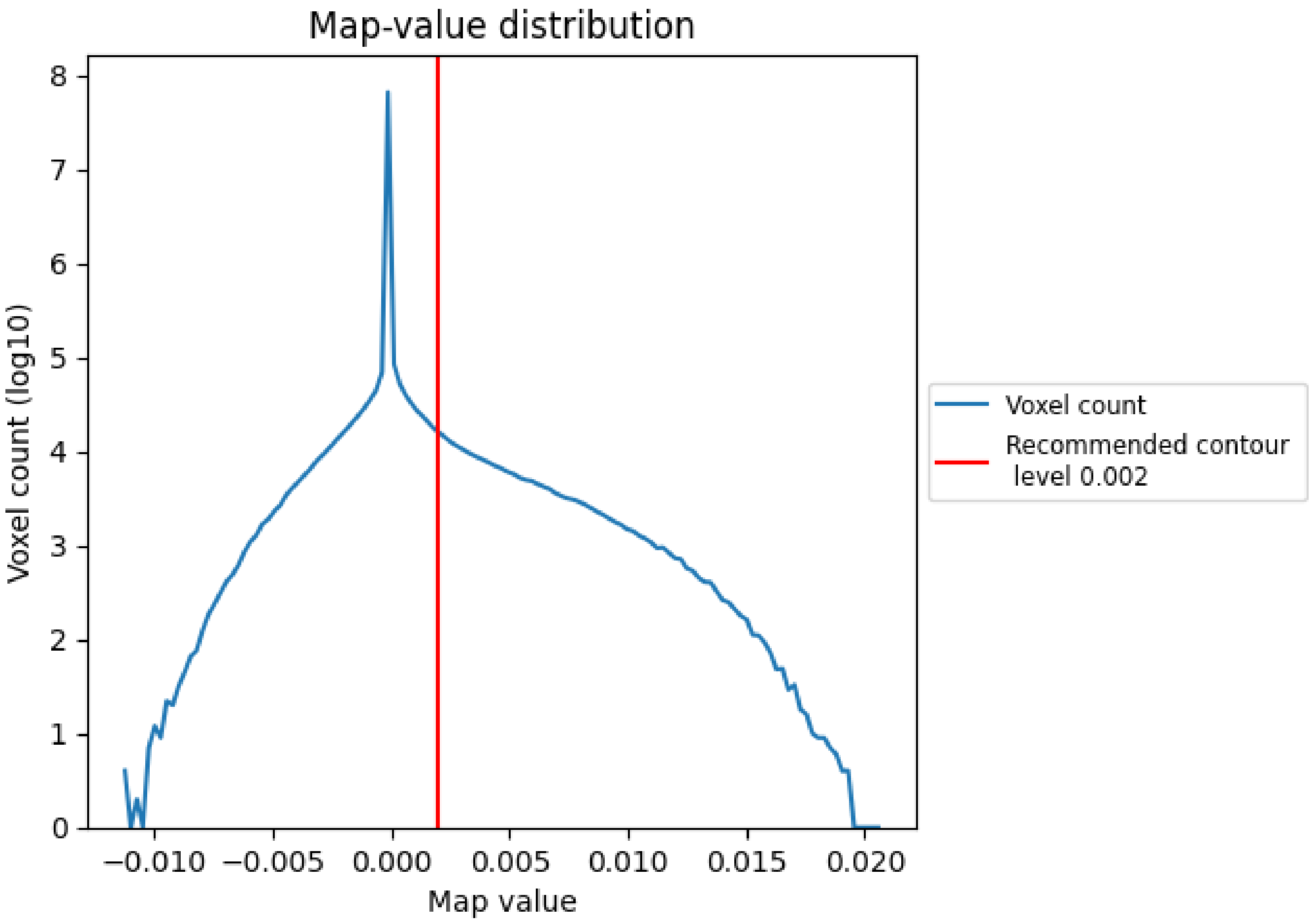


X Y Z

7 Map analysis ⓘ

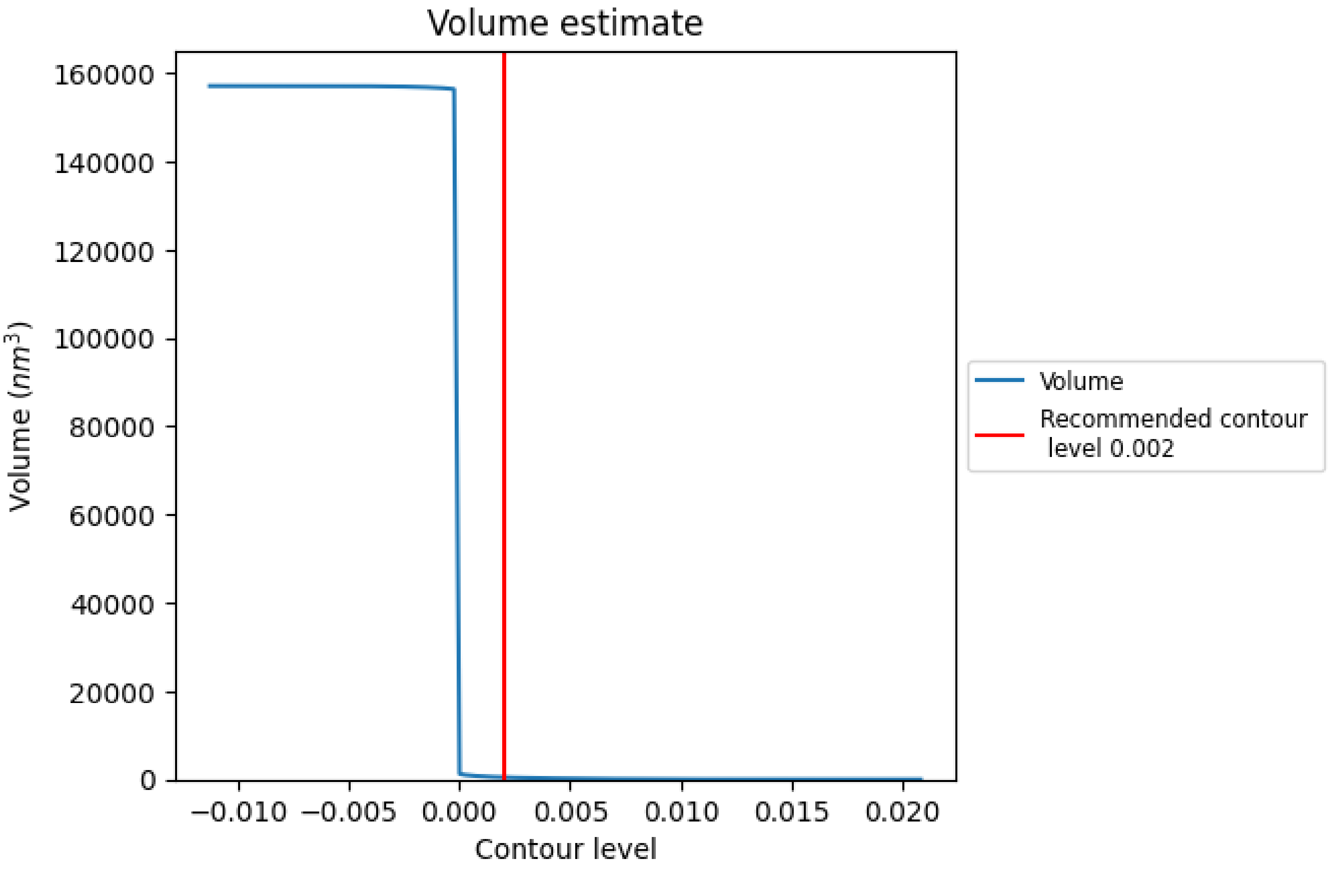
This section contains the results of statistical analysis of the map.

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.

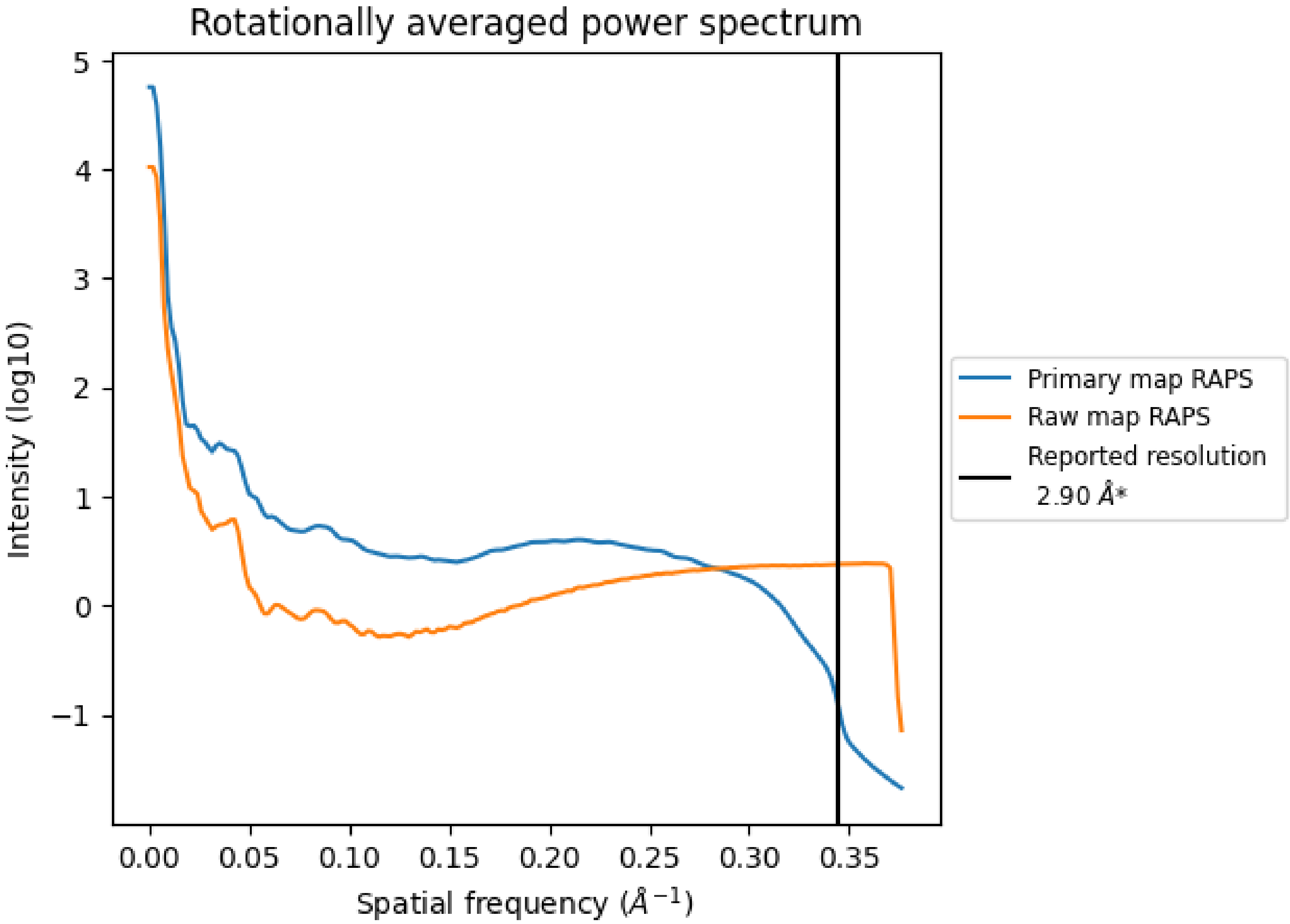
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 475 nm^3; this corresponds to an approximate mass of 429 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 ⓘ

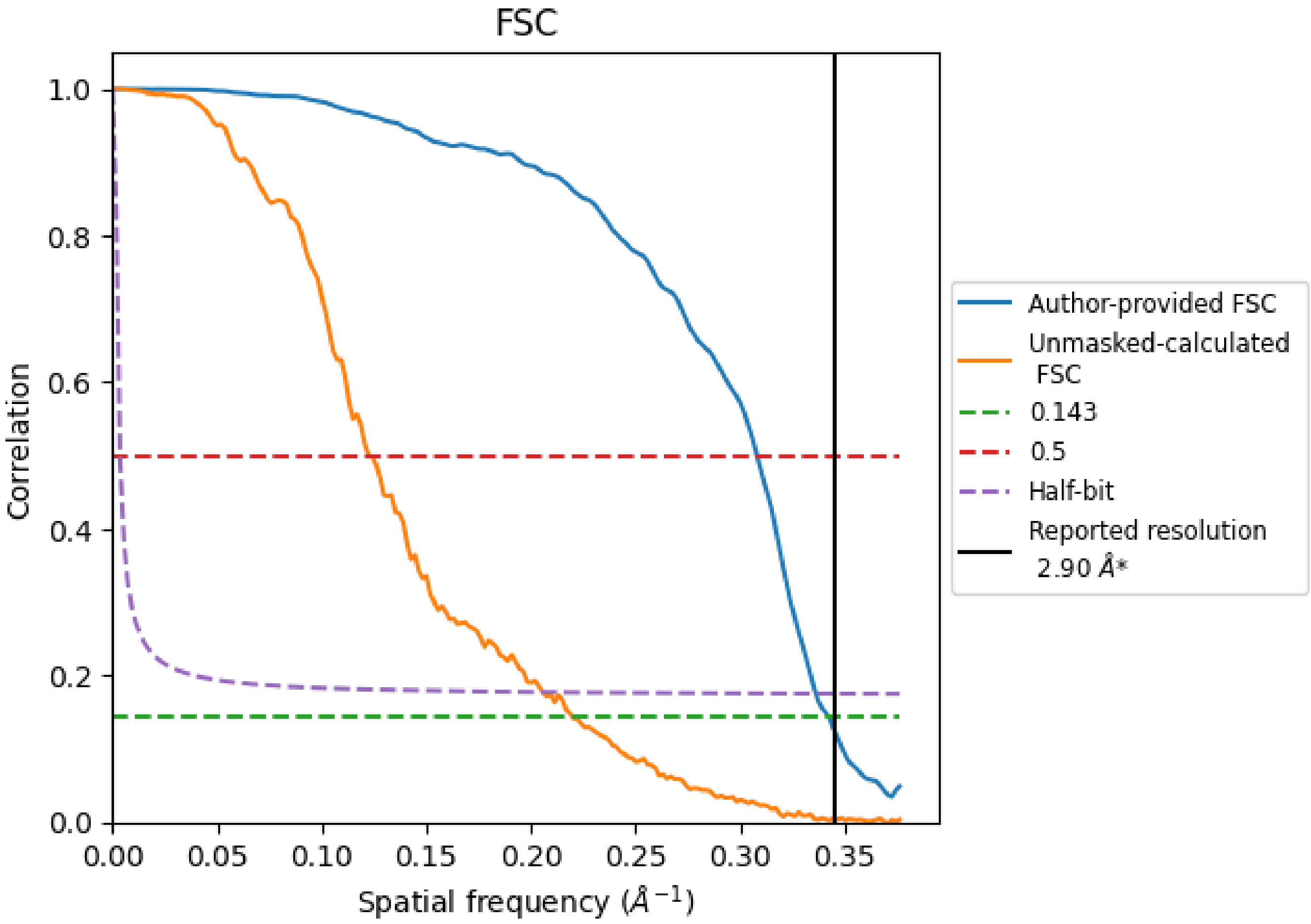


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates ⓘ

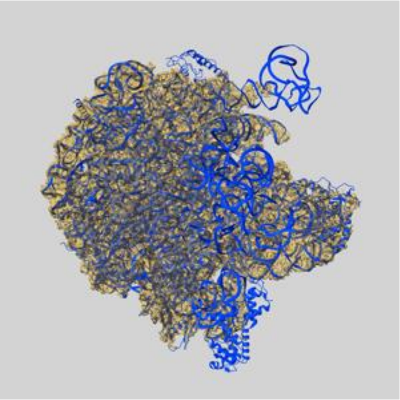
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.92	3.25	2.97
Unmasked-calculated*	4.55	8.15	4.86

*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 4.55 differs from the reported value 2.9 by more than 10 %

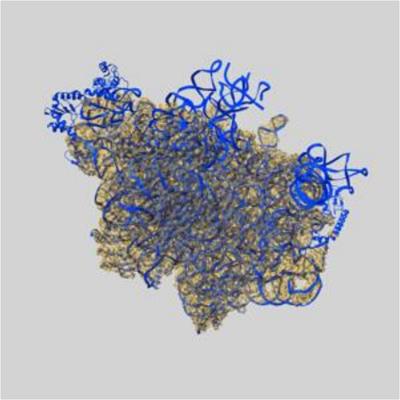
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-17134 and PDB model 8P8B. Per-residue inclusion information can be found in section 3 on page 17.

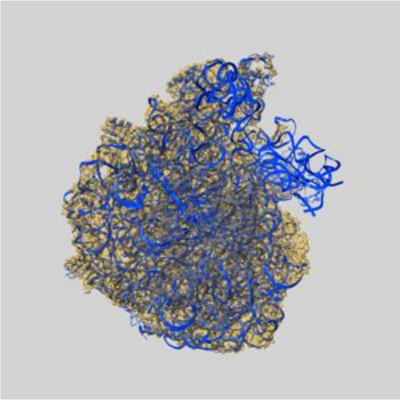
9.1 Map-model overlay ⓘ



X



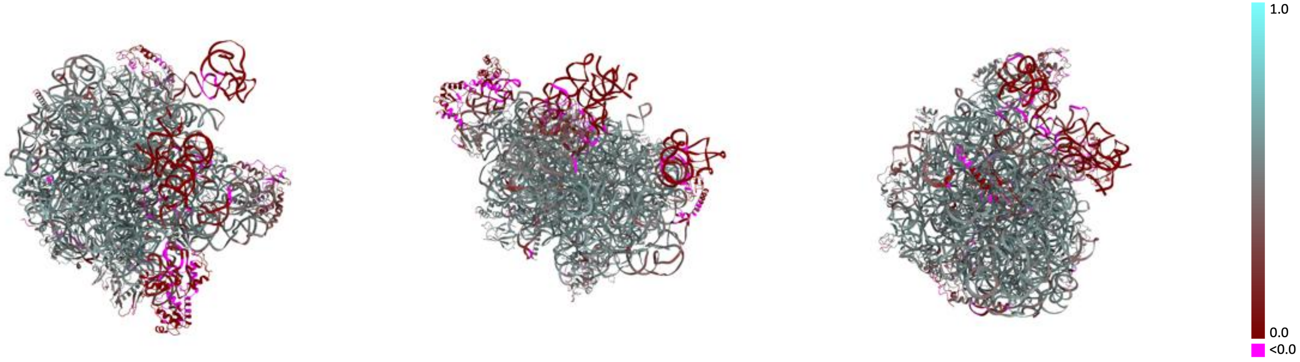
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.002 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.

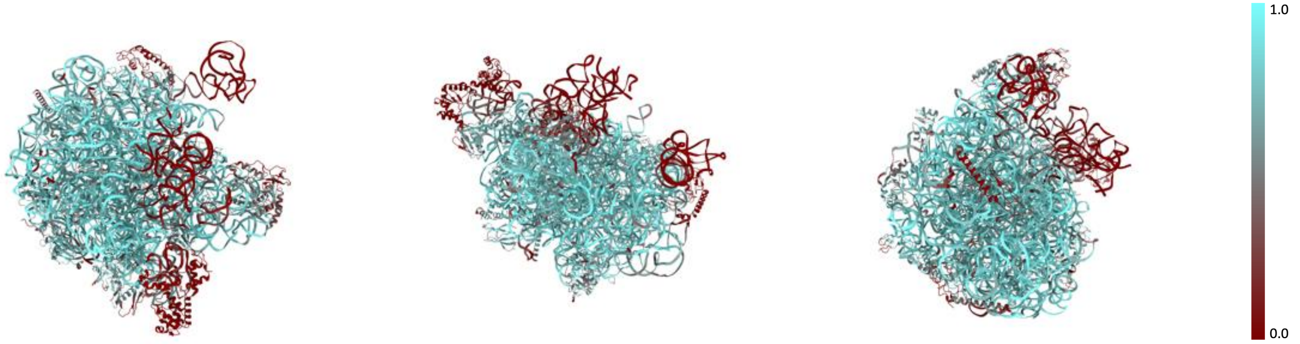
9.2 Q-score mapped to coordinate model ⓘ



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.

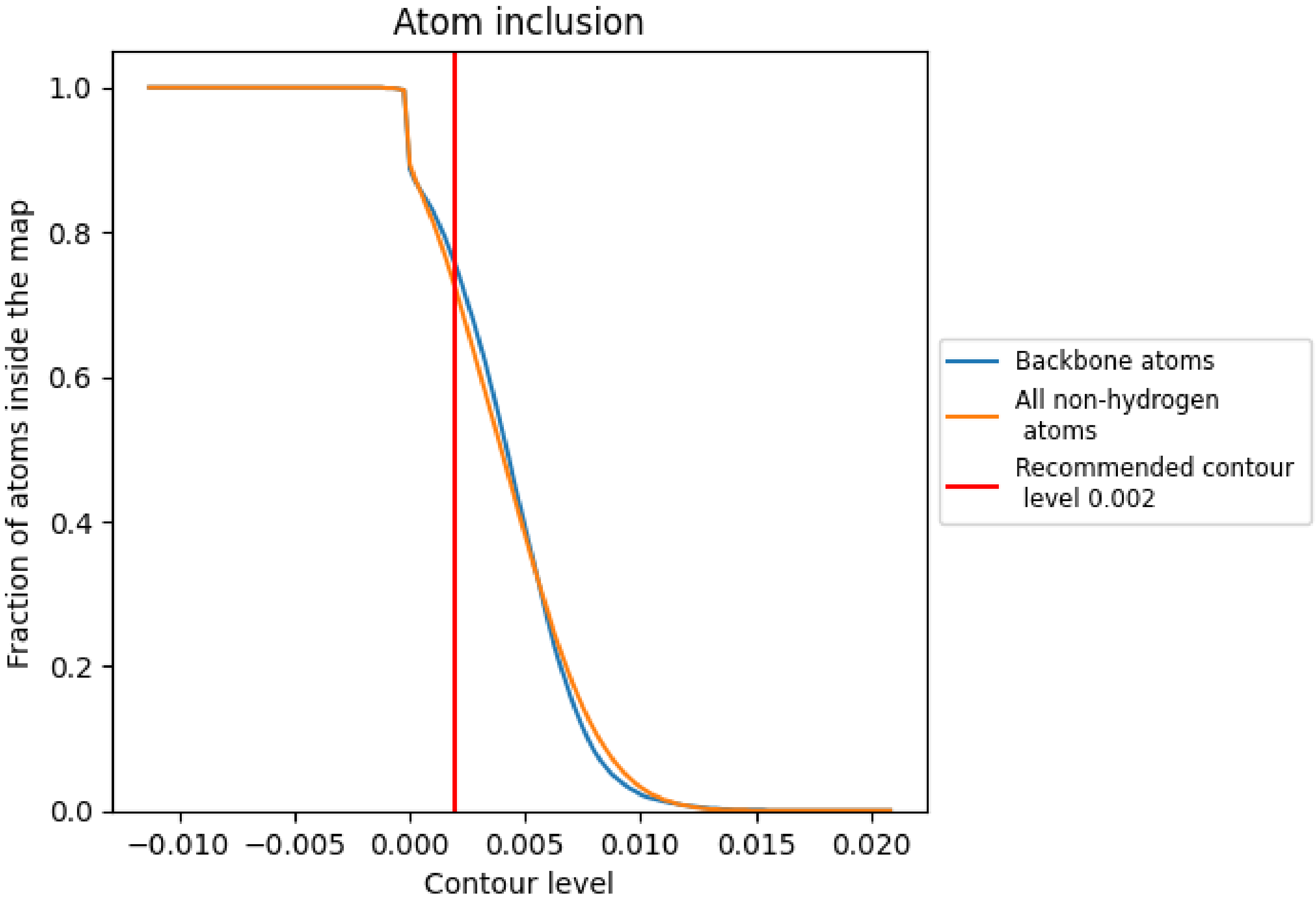
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.002).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.4660
0	0.7790	0.5500
1	0.7510	0.5530
2	0.7510	0.5370
3	0.8260	0.5100
4	0.7480	0.4430
5	0.0000	0.0000
6	0.5120	0.4240
7	0.1950	0.1240
8	0.0660	0.0710
X	0.0040	0.0520
Y	0.0000	0.0000
Z	0.1020	0.0650
a	0.7450	0.5320
b	0.7300	0.5210
c	0.6810	0.4950
d	0.3320	0.2890
e	0.4910	0.3980
f	0.1180	0.0760
g	0.0070	0.0030
h	0.0010	-0.0130
i	0.7380	0.5230
j	0.7000	0.5230
k	0.6820	0.4910
l	0.7290	0.5280
m	0.7500	0.5420
n	0.6230	0.4820
o	0.6290	0.4700
p	0.7400	0.5450
q	0.7250	0.5220
r	0.7250	0.5260
s	0.6610	0.4850
t	0.5090	0.3920
u	0.6980	0.4960
v	0.6710	0.4860

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Chain	Atom inclusion	Q-score
w	0.4970	0.4120
x	0.1310	0.1910
y	0.7480	0.5360
z	0.6760	0.5110