wwPDB EM Validation Summary Report (i)

May 16, 2022 – 05:25 pm BST

PDB ID	:	7OOC
EMDB ID	:	EMD-11998
Title	:	Mycoplasma pneumoniae 30S subunit of ribosomes in chloramphenicol-treated cells
Authors	:	Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.
Deposited on	:	2021-05-27
Resolution	:	3.70 Å(reported)
Based on initial models	:	5MMJ, 4YBB, 3J9W

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

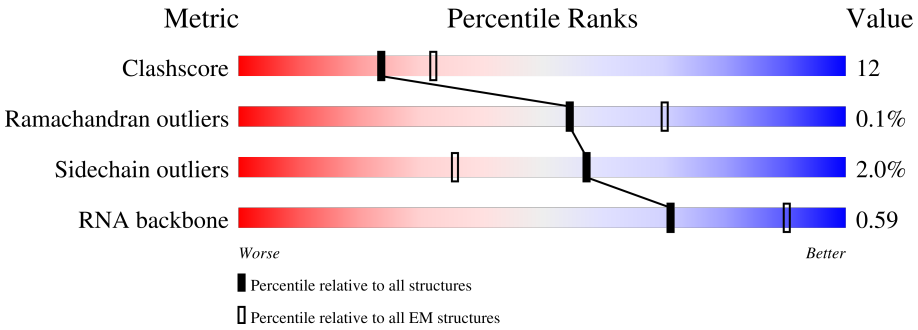
EMDB validation analysis	:	0.0.1.dev8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	273	79% 58% 20% 21%
2	D	219	70% 51% 19% 30%
3	F	155	99% 72% 28%
4	A	294	85% 57% 26% 15%
5	H	132	97% 66% 30%
6	J	121	94% 69% 25% 6%
7	C	205	99% 76% 23%

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Mol	Chain	Length	Quality of chain
8	S	87	89% 67% 21% 11%
9	O	94	93% 55% 34% 7%
10	K	139	98% 68% 29%
11	M	61	98% 62% 34%
12	I	108	94% 51% 41% 6%
13	L	124	95% 73% 21% 5%
14	N	86	97% 77% 20%
15	R	87	97% 59% 36%
16	T	60	88% 60% 25% 12%
17	G	142	99% 68% 32%
18	Q	104	62% 46% 16% 38%
19	E	215	78% 53% 25% 22%
20	P	85	98% 61% 35%
21	5	1520	98% 47% 46% 6%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 51225 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 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	215	1682	1063	308	306	5	0	0

- Molecule 2 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	153	1153	731	222	197	3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	154	1231	777	234	215	5	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	249	1917	1224	331	355	7	0	0

- Molecule 5 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	128	993	634	184	174	1	0	0

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	114	828	514	153	155	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	203	Total	C	N	O	S	0	0
			1605	1015	306	280	4		

- Molecule 8 is a protein called 30S ribosomal protein S20.

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

- Molecule 9 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	87	Total	C	N	O	S	0	0
			690	445	128	115	2		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	136	Total	C	N	O	S	0	0
			1055	667	209	177	2		

- Molecule 11 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	60	Total	C	N	O	S	0	0
			473	302	96	71	4		

- 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
			803	518	141	143	1		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	L	118	Total	C	N	O	0	0
			922	576	186	160		

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	84	Total 654	C 419	N 119	O 114	S 2	0	0

- Molecule 16 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	53	Total 439	C 275	N 93	O 70	S 1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	141	Total 1103	C 720	N 192	O 189	S 2	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	167	Total 1211	C 762	N 219	O 229	S 1	0	0

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	1493	Total 31952	C 14279	N 5792	O 10388	P 1493	0	0

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

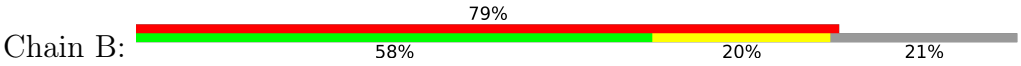
Mol	Chain	Residues	Atoms		AltConf
22	M	1	Total 1	Zn 1	0
22	Q	1	Total 1	Zn 1	0

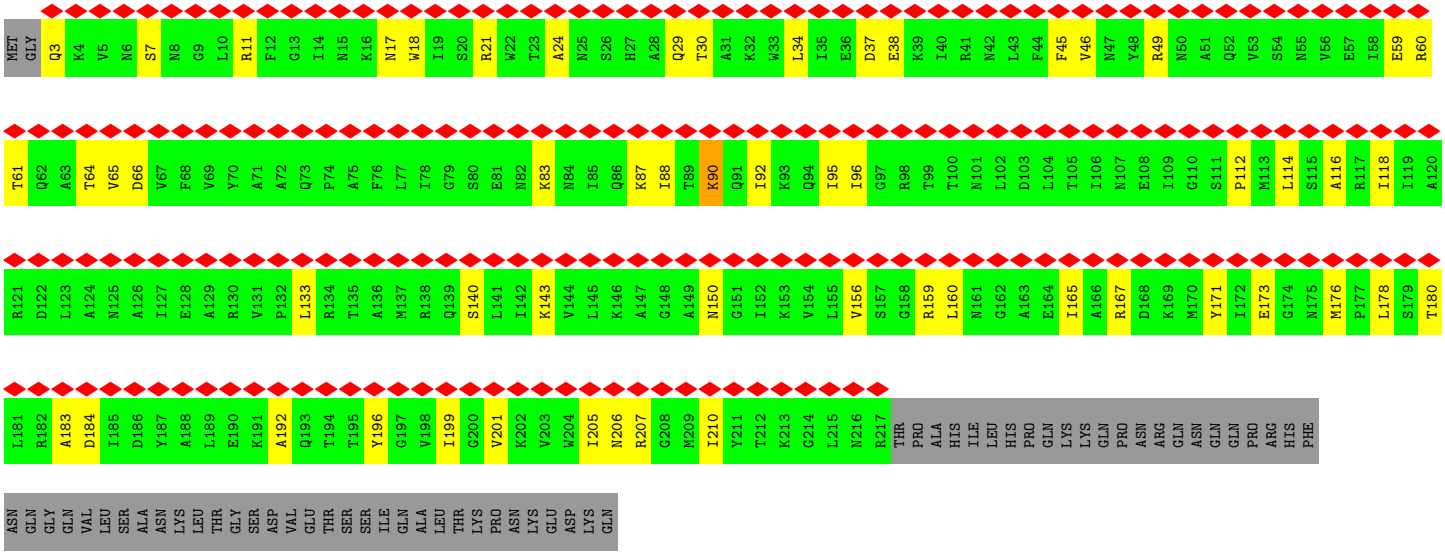
3 Residue-property plots (i)

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

• Molecule 1: 30S ribosomal protein S3

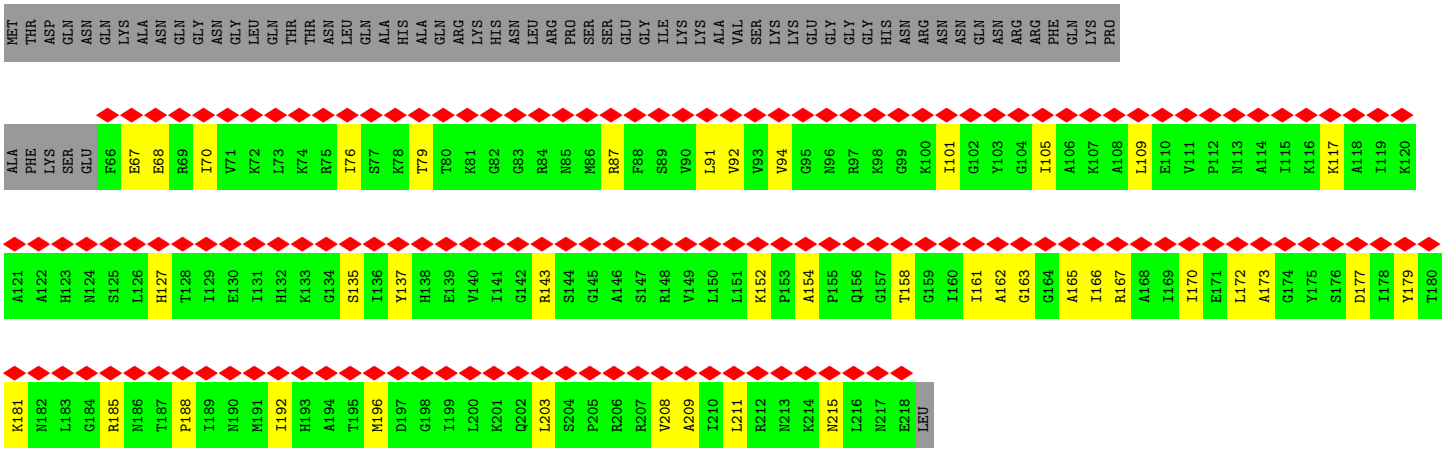
Chain B:





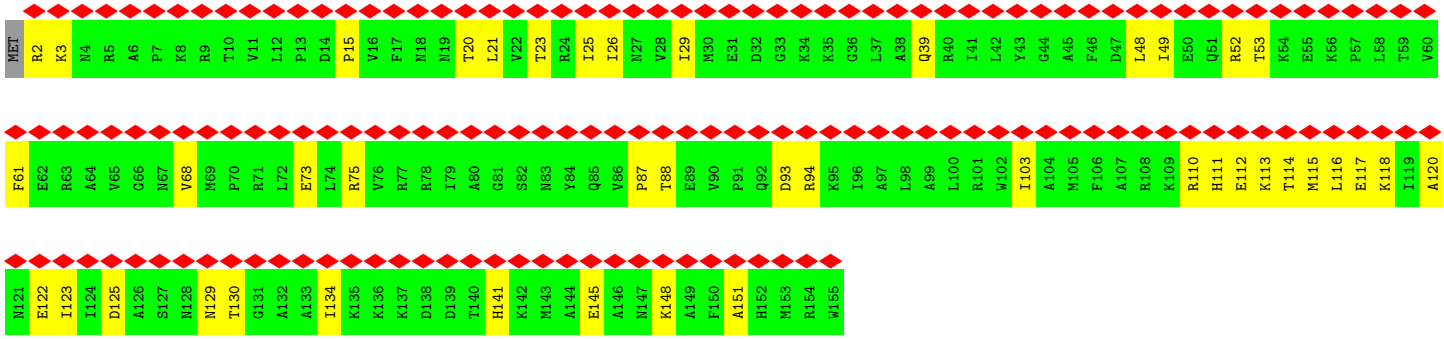
• Molecule 2: 30S ribosomal protein S5

Chain D:



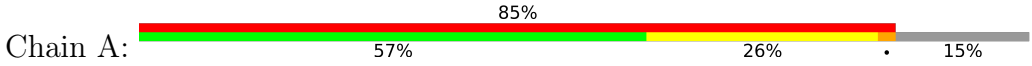
• Molecule 3: 30S ribosomal protein S7

Chain F:



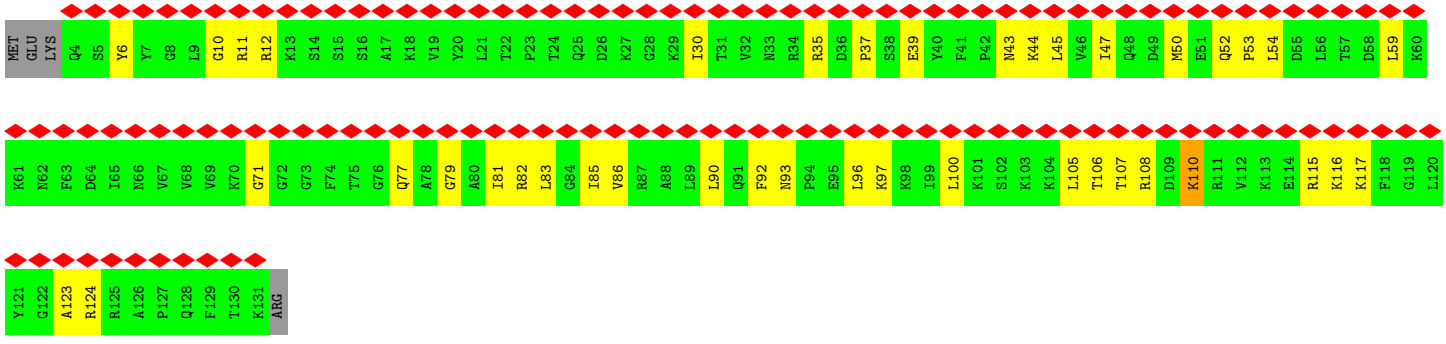
• Molecule 4: 30S ribosomal protein S2

Chain A:



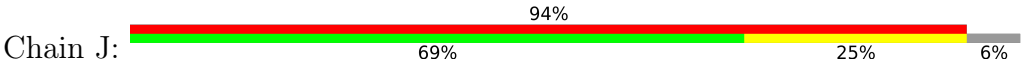
• Molecule 5: 30S ribosomal protein S9

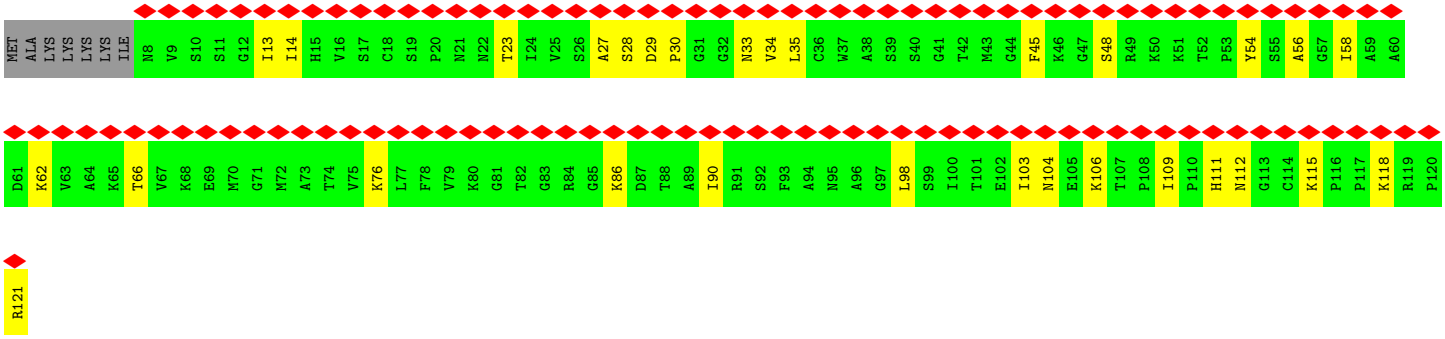
Chain H:



• Molecule 6: 30S ribosomal protein S11

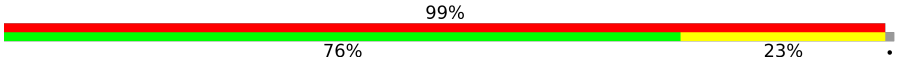
Chain J:

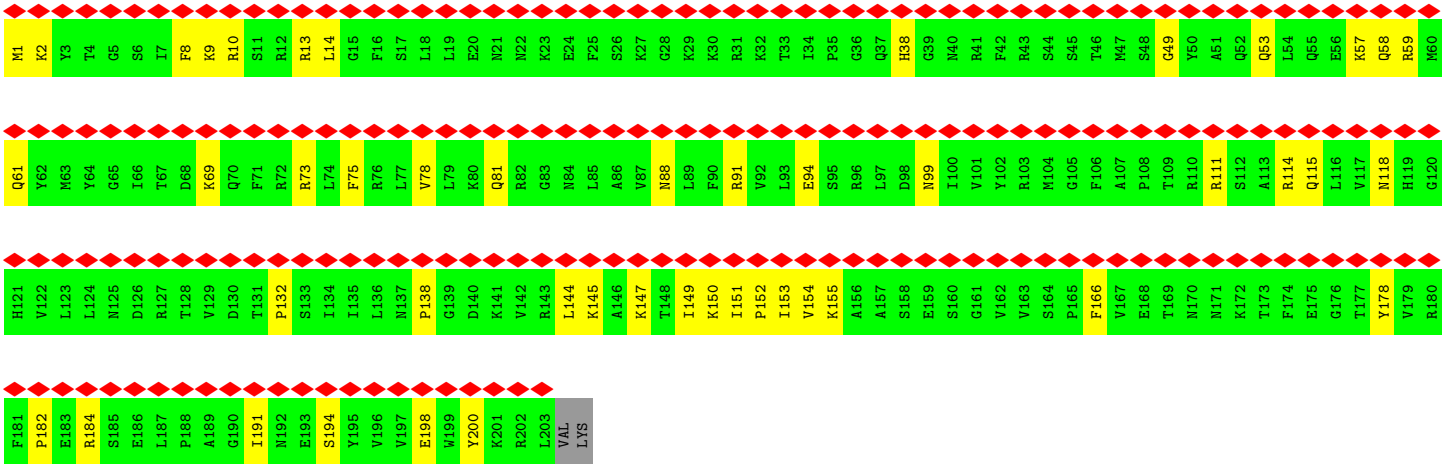




• Molecule 7: 30S ribosomal protein S4

Chain C:



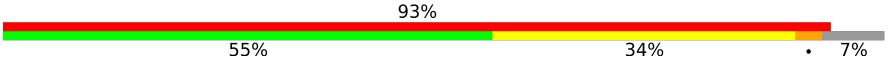


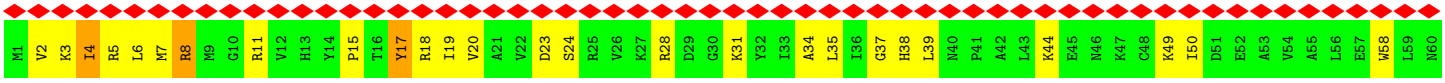
• Molecule 8: 30S ribosomal protein S20

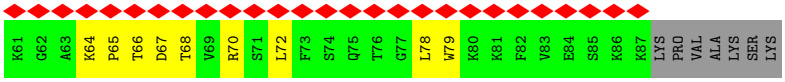
Chain S:

• Molecule 9: 30S ribosomal protein S16

Chain O:

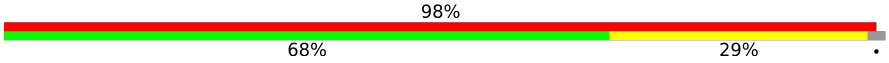


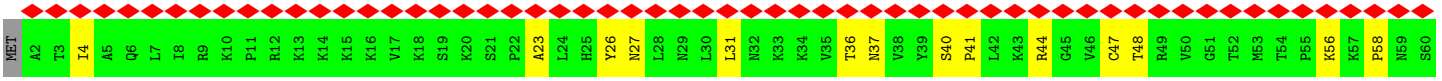


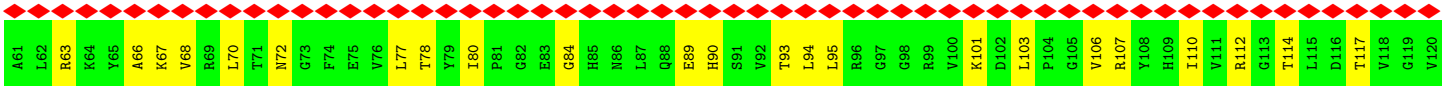


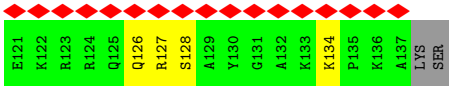
• Molecule 10: 30S ribosomal protein S12

Chain K:



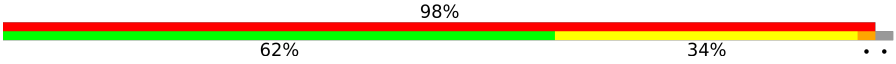


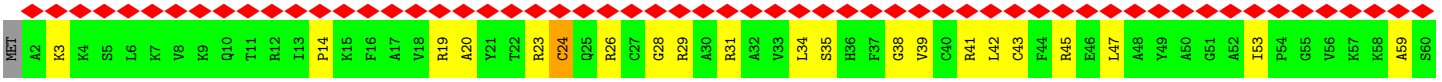




• Molecule 11: 30S ribosomal protein S14 type Z

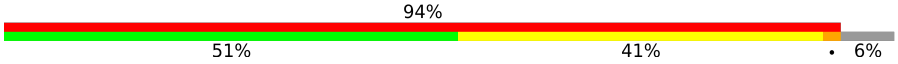
Chain M:

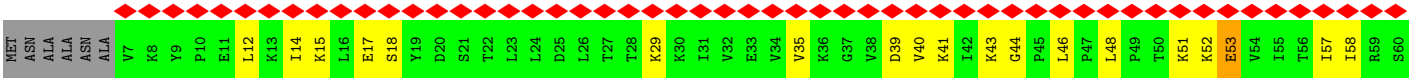


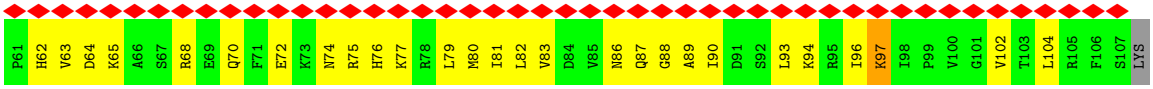


• Molecule 12: 30S ribosomal protein S10

Chain I:

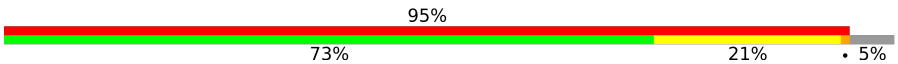


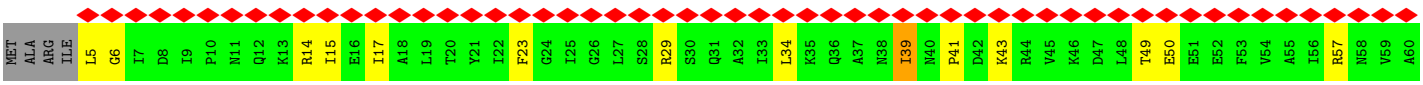


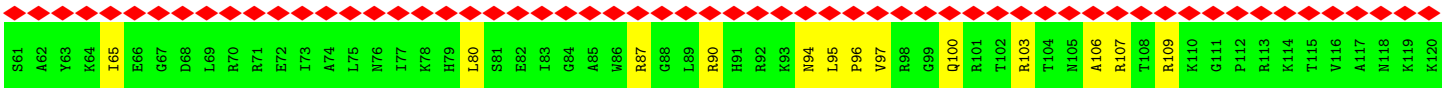


• Molecule 13: 30S ribosomal protein S13

Chain L:

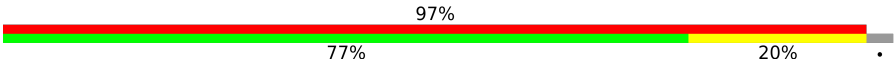


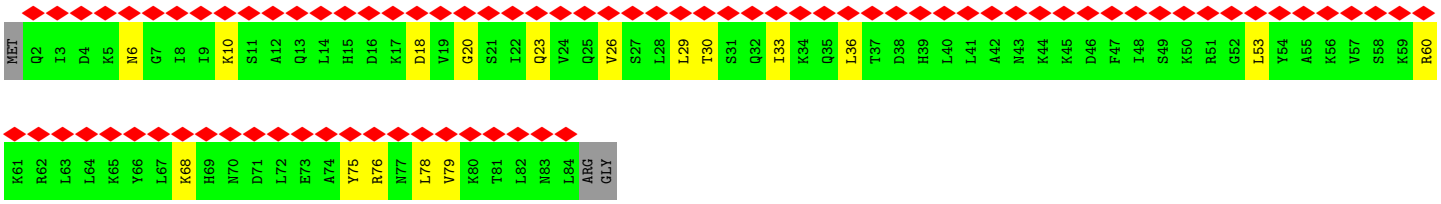




• Molecule 14: 30S ribosomal protein S15

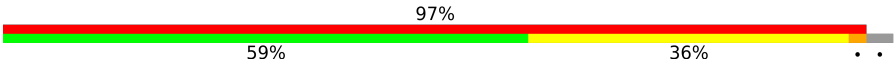
Chain N:

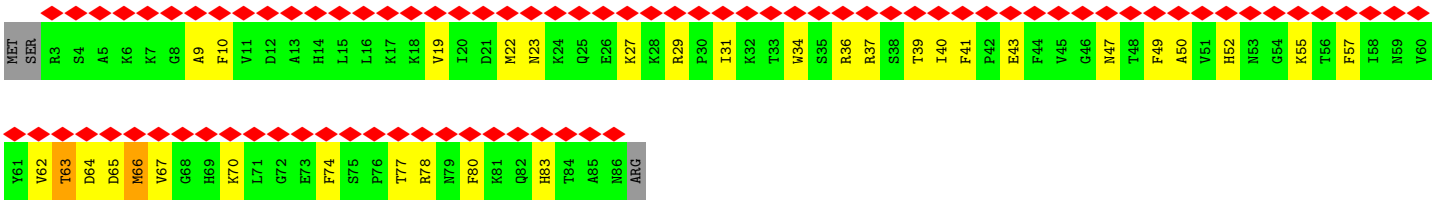




• Molecule 15: 30S ribosomal protein S19

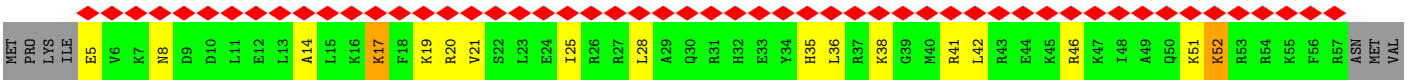
Chain R:





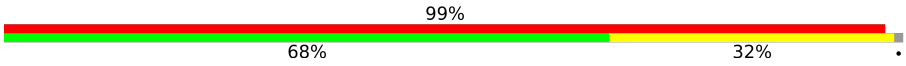
• Molecule 16: 30S ribosomal protein S21

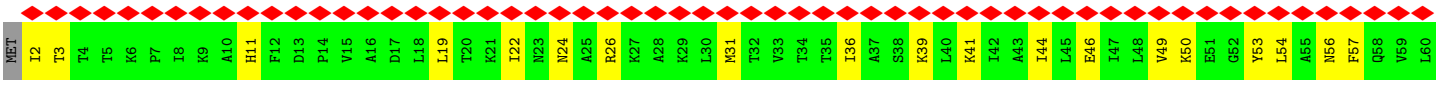
Chain T:



• Molecule 17: 30S ribosomal protein S8

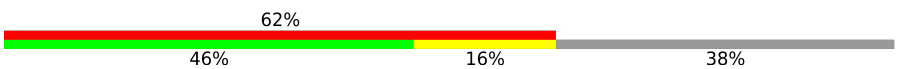
Chain G:

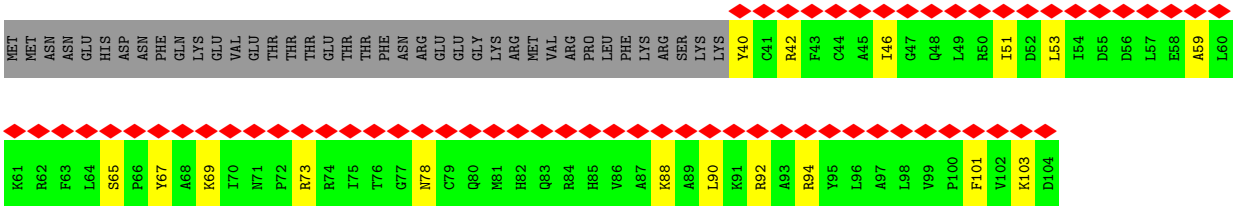




• Molecule 18: 30S ribosomal protein S18

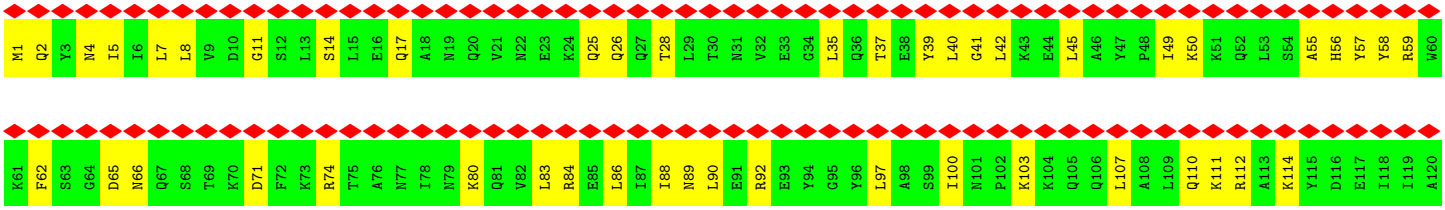
Chain Q:

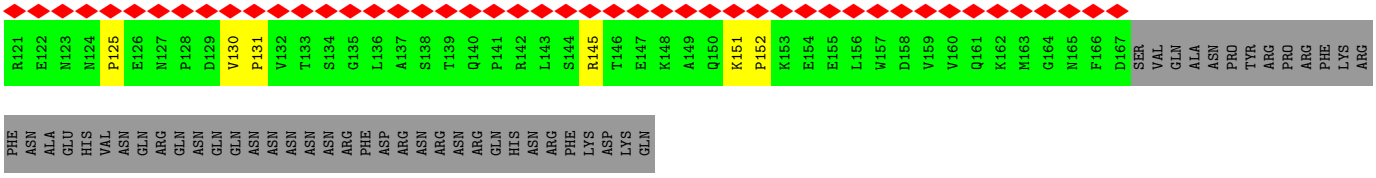




• Molecule 19: 30S ribosomal protein S6

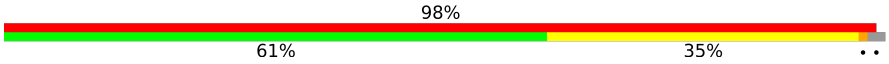
Chain E:

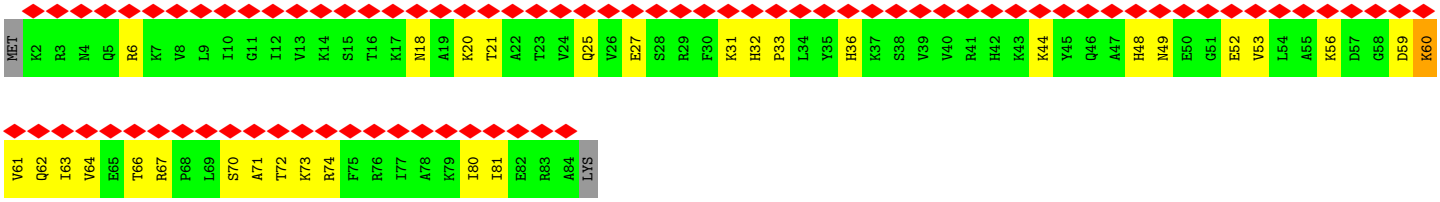




• Molecule 20: 30S ribosomal protein S17

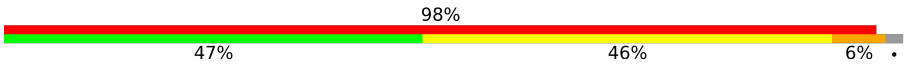
Chain P:

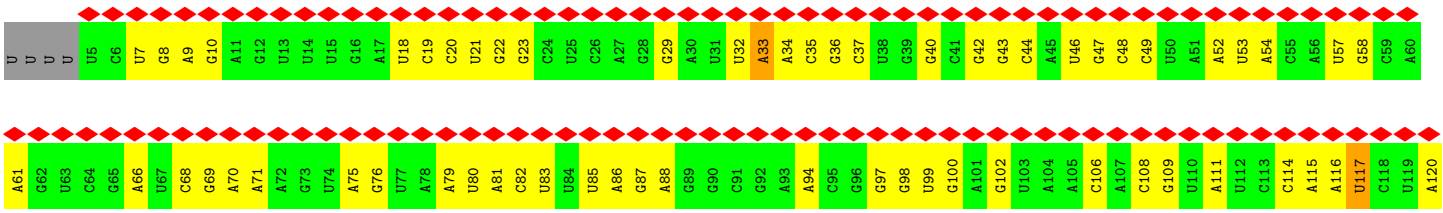


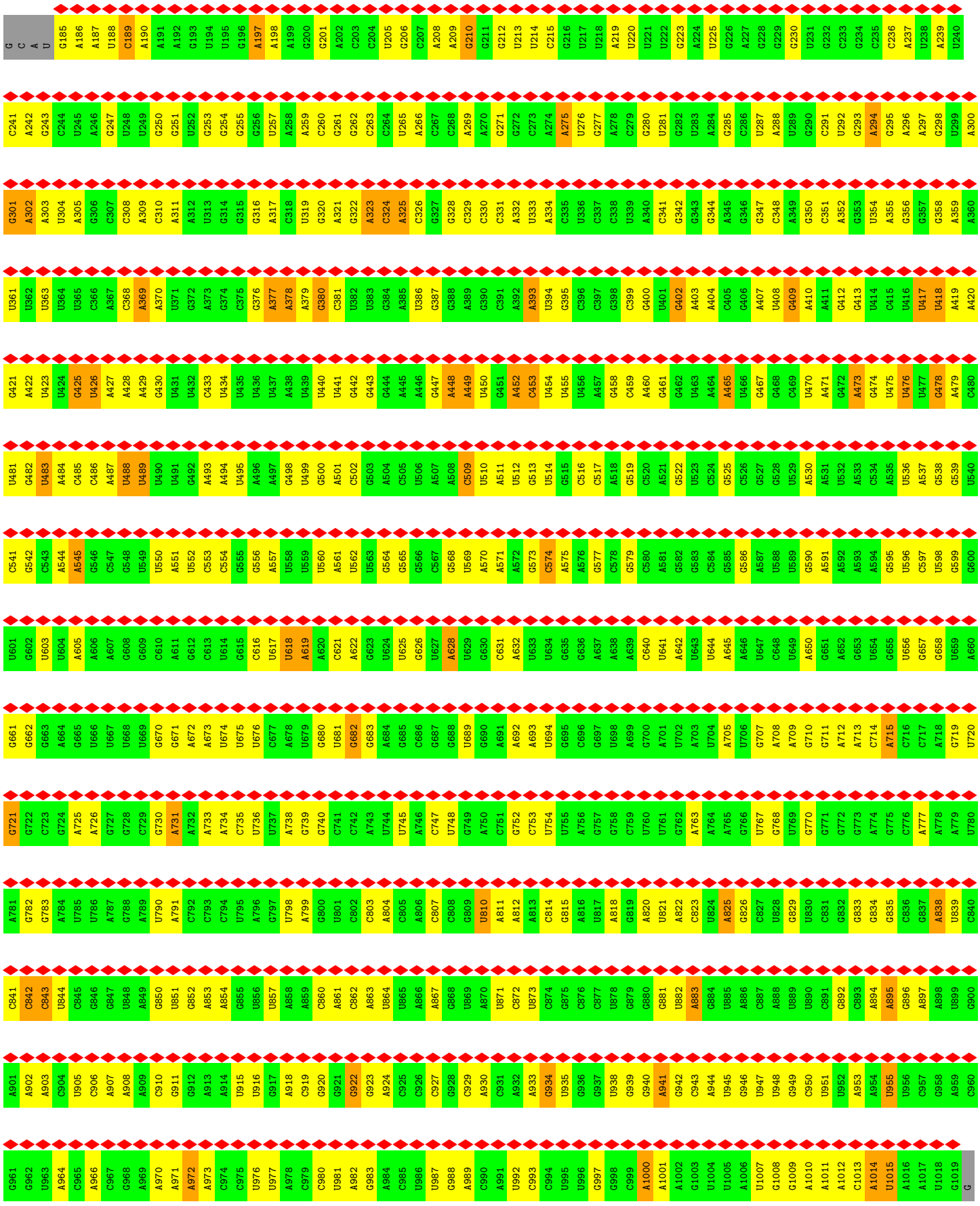


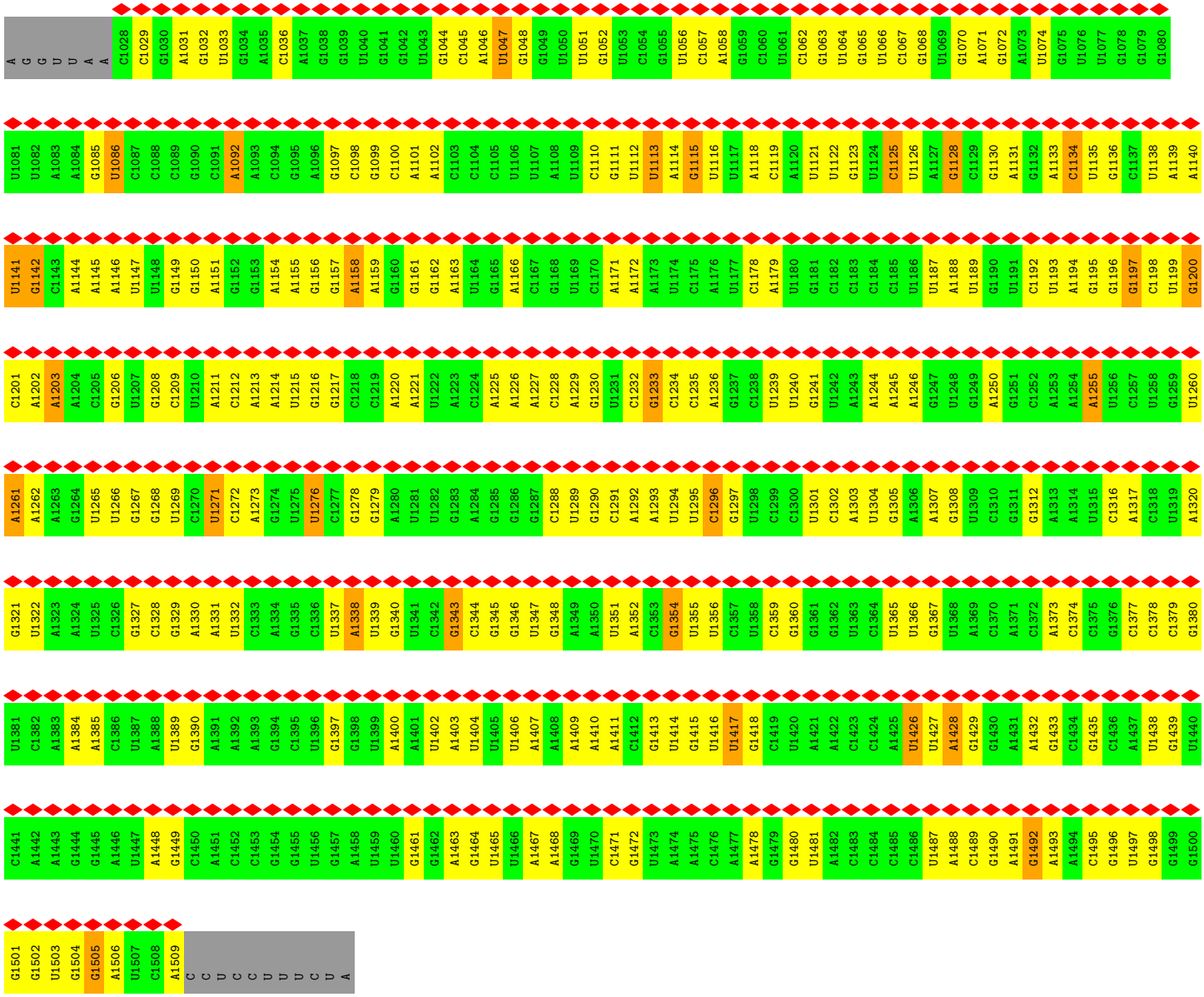
• Molecule 21: 16S rRNA

Chain 5:






G C A U
G185 A186 A187 U188 C189 A190 A191 A192 G193 U194 U195 G196 A197 A198 A199 G200 G201 A202 C203 C204 U205 G206 C207 A208 A209 G210 G211 G212 U213 U214 C215 G216 U217 U218 A219 U220 U221 U222 G223 A224 U225 G226 A227 G228 G229 G230 U231 G232 C233 G234 C235 C236 A237 U238 A239 U240
C241 A242 G243 C244 U245 A246 G247 U248 U249 G250 G251 U252 G253 G254 G255 G256 U257 A258 A259 C260 G261 G262 C263 C264 U265 A266 C267 C268 A269 A270 G271 G272 C273 A274 A275 U276 G277 A278 C279 G280 U281 G282 U283 A284 G285 C286 U287 A288 U289 G290 C291 U292 G293 A294 G295 A296 A297 G298 U299 A300
G301 A302 A303 U304 A305 G306 C307 C308 A309 C310 A311 A312 U313 G314 G315 G316 A317 C318 U319 G320 A321 G322 A323 C324 A325 C326 G327 G328 C329 C330 C331 A332 U333 A334 C335 U336 C337 C338 U339 A340 C341 G342 G343 G344 A345 G346 G347 C348 A349 G350 C351 A352 G353 U354 A355 G356 G357 G358 A359 A360
U361 U362 U363 U364 U365 C366 A367 C368 A369 A370 U371 G372 A373 G374 C375 G376 A377 A378 A379 G380 C381 U382 U383 G384 A385 U386 G387 G388 A389 G390 C391 A392 A393 U394 G395 C396 C397 G398 C399 G400 U401 G402 A403 A404 C405 G406 A407 U408 G409 A410 A411 G412 G413 U414 C415 U416 U417 U418 A419 A420
G421 A422 U423 U424 G425 U426 A427 A428 A429 G430 U431 U432 C433 U434 U435 U436 U437 A438 U439 U440 U441 G442 G443 G444 A445 A446 G447 A448 A449 U450 G451 A452 C453 U454 U455 U456 A457 G458 C459 A460 G461 G462 U463 A464 A465 U466 G467 G468 C469 U470 A471 G472 A473 G474 U475 U476 U477 G478 A479 C480
U481 G482 U483 A484 C485 C486 A487 U488 U489 U490 U491 G492 A493 A494 U495 A496 A497 G498 U499 G500 A501 C502 G503 A504 C505 U506 A507 A508 C509 U510 A511 U512 G513 U514 G515 C516 C517 A518 G519 C520 A521 G522 U523 C524 G525 C526 G527 G528 U529 A530 A531 U532 A533 C534 A535 U536 A537 G538 G539 U540
C541 G542 C543 A544 A545 G546 C547 G548 U549 U550 A551 U552 C553 C554 G555 G556 A557 U558 U559 U560 A561 U562 U563 G564 G565 G566 C567 G568 U569 A570 A571 A572 G573 C574 A575 A576 G577 G578 G579 C580 A581 G582 G583 C584 G585 C586 A587 U588 U589 G590 A591 A592 G593 A594 G595 U596 C597 U598 G599 G600
U601 G602 U603 U604 A605 A606 A607 G608 G609 C610 A611 G612 C613 U614 G615 C616 U617 U618 A619 A620 C621 A622 G623 U624 U625 G626 U627 A628 U629 G630 C631 A632 U633 U634 G635 G636 A637 A638 A639 C640 U641 A642 U643 U644 A645 A646 U647 C648 U649 A650 G651 A652 G653 U654 G655 U656 G657 G658 U659 A660
G661 G662 G663 A664 G665 U666 U667 U668 U669 G670 G671 A672 A673 U674 U675 U676 C677 A678 U679 G680 U681 G682 G683 A684 G685 C686 G687 G688 U689 G690 A691 A692 A693 U694 G695 C696 G697 U698 A699 G700 A701 U702 A703 U704 A705 U706 G707 A708 A709 G710 G711 A712 A713 C714 A715 C716 C717 A718 G719 U720
G721 G722 C723 G724 A725 A726 G727 G728 C729 G730 A731 A732 A733 A734 C735 U736 U737 A738 G739 G740 C741 C742 A743 U744 U745 A746 C747 U748 G749 A750 C751 G752 C753 U754 U755 A756 G757 G758 C759 U760 U761 G762 A763 A764 A765 G766 U767 G768 U769 G770 G771 G772 G773 A774 G775 C776 A777 A778 A779 U780
A781 G782 G783 A784 U785 U786 A787 G788 A789 U790 A791 C792 C793 C794 U795 A796 G797 U798 A799 G800 U801 C802 C803 A804 C805 A806 C807 C808 G809 U810 A811 A812 A813 C814 G815 A816 U817 A818 G819 A820 U821 A822 C823 U824 A825 G826 C827 U828 G829 U830 C831 G832 G833 G834 G835 C836 G837 A838 U839 C840
C841 C842 C843 U844 C845 G846 G847 U848 A849 G850 U851 G852 A853 A854 G855 U856 U857 A858 A859 C860 A861 C862 A863 U864 U865 A866 A867 G868 U869 A870 U871 C872 U873 C874 G875 C876 C877 U878 G879 G880 G881 U882 A883 G884 U885 A886 C887 A888 U889 U890 C891 G892 C893 A894 A895 G896 A897 A898 U899 G900
A901 A902 A903 C904 U905 C906 A907 A908 A909 C910 G911 G912 A913 A914 U915 U916 G917 A918 C919 G920 G921 G922 G923 A924 G925 C926 C927 G928 C929 A930 C931 A932 A933 G934 U935 G936 G937 U938 G939 G940 A941 G942 C943 A944 U945 G946 U947 U948 G949 C950 U951 U952 A953 A954 U955 U956 C957 G958 A959 C960
G961 G962 U963 A964 C965 A966 C967 G968 A969 A970 A971 A972 A973 C974 C975 U976 U977 A978 C979 C980 U981 A982 G983 A984 C985 U986 U987 G988 A989 C990 A991 U992 C993 C994 U995 U996 G997 G998 C999 A1000 A1001 A1002 G1003 U1004 U1005 A1006 U1007 G1008 G1009 A1010 A1011 A1012 C1013 A1014 U1015 A1016 A1017 U1018 G1019 G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U1081 U1082 A1083 A1084 G1085 U1086 C1087 C1088 C1089 G1090 C1091 A1092 A1093 C1094 G1095 A1096 G1097 C1098 G1099 C1100 A1101 A1102 C1103 C1104 C1105 U1106 U1107 A1108 U1109 C1110 G1111 U1112 U1113 A1114 G1115 U1116 U1117 A1118 C1119 A1120 U1121 U1122 G1123 U1124 C1125 U1126 A1127 G1128 C1129 G1130 A1131 G1132 A1133 C1134 U1135 G1136 C1137 U1138 A1139 A1140
U1141 G1142 C1143 A1144 A1145 A1146 U1147 U1148 G1149 G1150 A1151 G1152 G1153 A1154 A1155 G1156 G1157 A1158 A1159 G1160 G1161 G1162 A1163 U1164 G1165 A1166 C1167 G1168 U1169 C1170 A1171 A1172 A1173 U1174 C1175 A1176 U1177 C1178 A1179 U1180 G1181 C1182 C1183 C1184 C1185 U1186 U1187 A1188 U1189 G1190 U1191 C1192 U1193 A1194 G1195 G1196 G1197 C1198 U1199 G1200
C1201 A1202 A1203 A1204 C1205 G1206 U1207 G1208 C1209 U1210 A1211 C1212 A1213 A1214 U1215 G1216 G1217 C1218 C1219 A1220 A1221 U1222 A1223 C1224 A1225 A1226 A1227 C1228 A1229 G1230 U1231 C1232 G1233 C1234 C1235 A1236 G1237 C1238 U1239 U1240 G1241 U1242 A1243 A1244 A1245 A1246 G1247 U1248 G1249 A1250 G1251 C1252 A1253 A1254 A1255 U1256 C1257 U1258 G1259 U1260
A1261 A1262 A1263 G1264 U1265 U1266 G1267 G1268 U1269 C1270 U1271 C1272 A1273 G1274 U1275 U1276 C1277 G1278 G1279 A1280 U1281 U1282 G1283 A1284 G1285 G1286 G1287 C1288 U1289 G1290 C1291 A1292 A1293 U1294 U1295 C1296 G1297 U1298 C1299 C1300 U1301 C1302 A1303 U1304 G1305 A1306 A1307 G1308 U1309 C1310 G1311 G1312 A1313 A1314 U1315 C1316 A1317 C1318 U1319 A1320
G1321 U1322 A1323 A1324 U1325 C1326 G1327 C1328 G1329 A1330 A1331 U1332 C1333 A1334 G1335 C1336 U1337 A1338 U1339 G1340 U1341 C1342 G1343 C1344 G1345 G1346 U1347 G1348 A1349 A1350 U1351 A1352 C1353 G1354 U1355 U1356 C1357 U1358 C1359 G1360 G1361 G1362 U1363 C1364 U1365 U1366 G1367 U1368 A1369 C1370 A1371 C1372 A1373 C1374 C1375 G1376 C1377 C1378 C1379 G1380
U1381 C1382 A1383 A1384 A1385 C1386 U1387 A1388 U1389 G1390 A1391 A1392 A1393 G1394 C1395 U1396 G1397 G1398 U1399 A1400 A1401 U1402 A1403 U1404 U1405 U1406 A1407 A1408 A1409 A1410 A1411 C1412 G1413 U1414 G1415 U1416 U1417 G1418 C1419 U1420 A1421 A1422 C1423 C1424 A1425 U1426 U1427 A1428 G1429 G1430 A1431 A1432 G1433 C1434 G1435 C1436 A1437 U1438 G1439 U1440
C1441 A1442 A1443 G1444 G1445 A1446 U1447 A1448 G1449 C1450 A1451 C1452 C1453 G1454 G1455 U1456 G1457 A1458 U1459 U1460 G1461 G1462 A1463 G1464 U1465 U1466 A1467 A1468 G1469 U1470 C1471 G1472 U1473 A1474 A1475 C1476 A1477 A1478 G1479 G1480 U1481 A1482 C1483 C1484 C1485 C1486 U1487 A1488 C1489 G1490 A1491 G1492 A1493 A1494 C1495 G1496 U1497 G1498 G1499 G1500
G1501 G1502 U1503 G1504 G1505 A1506 U1507 C1508 A1509 C C U C C U U U C U A

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	17890	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	0.021	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0023	Depositor
Map size (Å)	323.095, 323.095, 323.095	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85025, 0.85025, 0.85025	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	B	0.25	0/1705	0.48	0/2304
2	D	0.25	0/1168	0.50	0/1568
3	F	0.25	0/1250	0.48	0/1682
4	A	0.31	0/1951	0.59	2/2652 (0.1%)
5	H	0.26	0/1009	0.53	0/1354
6	J	0.25	0/843	0.46	0/1136
7	C	0.25	0/1635	0.48	0/2202
8	S	0.24	0/631	0.46	0/838
9	O	0.32	0/703	0.64	0/945
10	K	0.27	0/1073	0.56	1/1445 (0.1%)
11	M	0.39	0/482	0.67	0/643
12	I	0.27	0/814	0.59	0/1096
13	L	0.30	0/933	0.53	0/1254
14	N	0.25	0/679	0.43	0/907
15	R	0.34	0/670	0.59	0/904
16	T	0.36	0/442	0.60	0/582
17	G	0.25	0/1119	0.53	0/1508
18	Q	0.27	0/545	0.50	0/730
19	E	0.25	0/1229	0.51	0/1670
20	P	0.24	0/684	0.50	0/913
21	5	0.21	0/35777	0.76	6/55776 (0.0%)
All	All	0.23	0/55342	0.69	9/82109 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	259	PRO	N-CA-C	-10.87	83.84	112.10
21	5	189	C	N3-C2-O2	-7.88	116.39	121.90
10	K	31	LEU	CA-CB-CG	7.05	131.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	843	C	N3-C2-O2	-6.92	117.06	121.90
21	5	843	C	C6-N1-C2	-6.05	117.88	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1682	0	1733	37	0
2	D	1153	0	1231	32	0
3	F	1231	0	1285	34	0
4	A	1917	0	1894	66	0
5	H	993	0	1023	32	0
6	J	828	0	855	23	0
7	C	1605	0	1603	43	0
8	S	629	0	681	21	0
9	O	690	0	726	37	0
10	K	1055	0	1124	28	0
11	M	473	0	505	16	0
12	I	803	0	876	33	0
13	L	922	0	957	20	0
14	N	673	0	730	12	0
15	R	654	0	629	27	0
16	T	439	0	467	11	0
17	G	1103	0	1218	33	0
18	Q	535	0	559	16	0
19	E	1211	0	1108	43	0
20	P	675	0	728	20	0
21	5	31952	0	16055	597	0
22	M	1	0	0	0	0
22	Q	1	0	0	0	0
All	All	51225	0	35987	1052	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 12.

The worst 5 of 1052 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)
21:5:1013:C:N4	21:5:1014:A:N6	2.06	1.03
21:5:1331:A:H61	21:5:1340:G:H1	1.02	0.96
21:5:242:A:H62	21:5:277:G:H21	1.13	0.94
21:5:1013:C:N4	21:5:1014:A:H62	1.65	0.94
21:5:242:A:H62	21:5:277:G:N2	1.64	0.94

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/273 (78%)	202 (95%)	11 (5%)	0	100	100
2	D	151/219 (69%)	141 (93%)	10 (7%)	0	100	100
3	F	152/155 (98%)	135 (89%)	17 (11%)	0	100	100
4	A	247/294 (84%)	227 (92%)	18 (7%)	2 (1%)	19	56
5	H	126/132 (96%)	109 (86%)	17 (14%)	0	100	100
6	J	112/121 (93%)	106 (95%)	6 (5%)	0	100	100
7	C	201/205 (98%)	186 (92%)	15 (8%)	0	100	100
8	S	75/87 (86%)	72 (96%)	3 (4%)	0	100	100
9	O	85/94 (90%)	75 (88%)	10 (12%)	0	100	100
10	K	134/139 (96%)	117 (87%)	17 (13%)	0	100	100
11	M	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
12	I	99/108 (92%)	87 (88%)	12 (12%)	0	100	100
13	L	116/124 (94%)	107 (92%)	9 (8%)	0	100	100
14	N	81/86 (94%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	R	82/87 (94%)	75 (92%)	7 (8%)	0	100 100
16	T	51/60 (85%)	45 (88%)	6 (12%)	0	100 100
17	G	139/142 (98%)	126 (91%)	13 (9%)	0	100 100
18	Q	63/104 (61%)	57 (90%)	6 (10%)	0	100 100
19	E	165/215 (77%)	146 (88%)	19 (12%)	0	100 100
20	P	81/85 (95%)	72 (89%)	9 (11%)	0	100 100
All	All	2431/2791 (87%)	2218 (91%)	211 (9%)	2 (0%)	54 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	250	PRO
4	A	254	ILE

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	B	176/232 (76%)	174 (99%)	2 (1%)	73 85
2	D	117/178 (66%)	117 (100%)	0	100 100
3	F	128/132 (97%)	128 (100%)	0	100 100
4	A	200/262 (76%)	194 (97%)	6 (3%)	41 66
5	H	101/115 (88%)	99 (98%)	2 (2%)	55 74
6	J	91/97 (94%)	91 (100%)	0	100 100
7	C	164/183 (90%)	163 (99%)	1 (1%)	86 93
8	S	70/77 (91%)	69 (99%)	1 (1%)	67 82
9	O	71/82 (87%)	63 (89%)	8 (11%)	6 28
10	K	111/120 (92%)	111 (100%)	0	100 100
11	M	47/48 (98%)	45 (96%)	2 (4%)	29 58
12	I	93/99 (94%)	90 (97%)	3 (3%)	39 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	L	92/105 (88%)	89 (97%)	3 (3%)	38 64
14	N	76/78 (97%)	76 (100%)	0	100 100
15	R	66/77 (86%)	60 (91%)	6 (9%)	9 36
16	T	43/56 (77%)	38 (88%)	5 (12%)	5 27
17	G	121/124 (98%)	121 (100%)	0	100 100
18	Q	56/94 (60%)	56 (100%)	0	100 100
19	E	107/196 (55%)	106 (99%)	1 (1%)	78 88
20	P	73/75 (97%)	72 (99%)	1 (1%)	67 82
All	All	2003/2430 (82%)	1962 (98%)	41 (2%)	57 74

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	R	63	THR
16	T	19	LYS
15	R	64	ASP
15	R	77	THR
16	T	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
17	G	23	ASN
17	G	56	ASN
20	P	62	GLN
19	E	2	GLN
7	C	38	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	5	1490/1520 (98%)	231 (15%)	5 (0%)

5 of 231 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	5	7	U

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Mol	Chain	Res	Type
21	5	10	G
21	5	32	U
21	5	33	A
21	5	40	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	5	168	A
21	5	419	A
21	5	481	U
21	5	838	A
21	5	1338	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

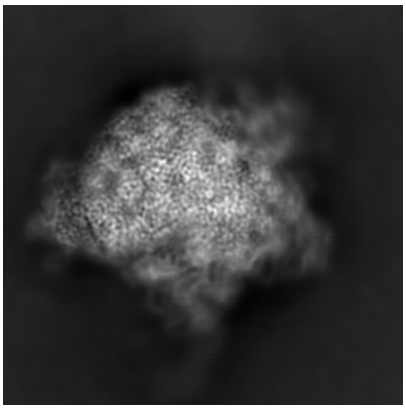
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11998. These allow visual inspection of the internal detail of the map and identification of artifacts.

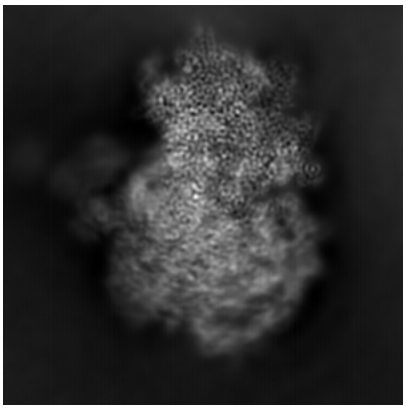
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

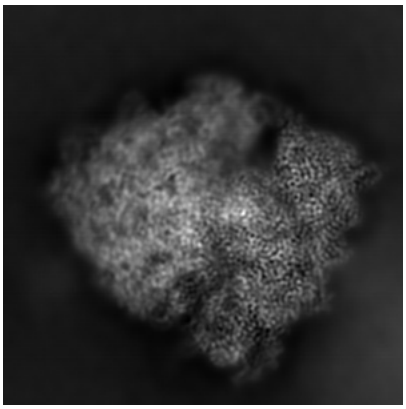
6.1.1 Primary map



X

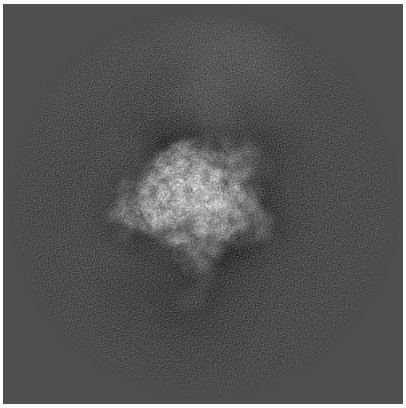


Y

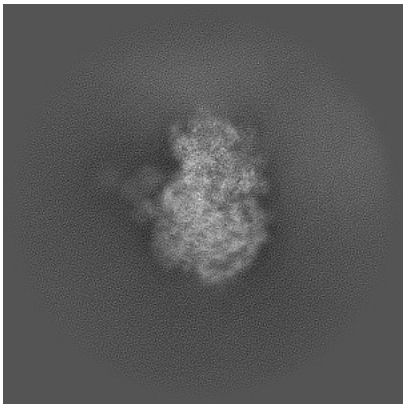


Z

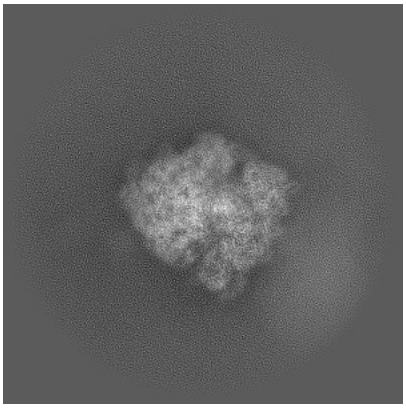
6.1.2 Raw map



X



Y

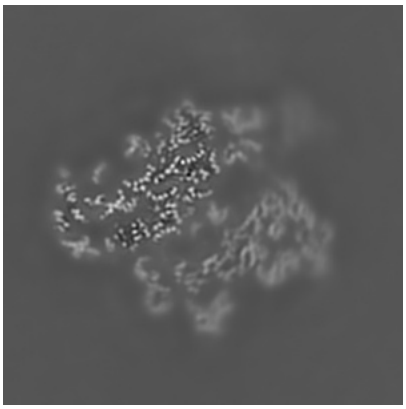


Z

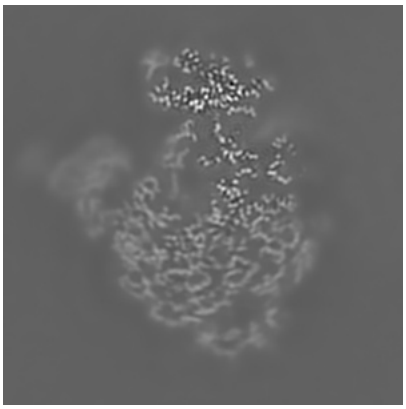
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

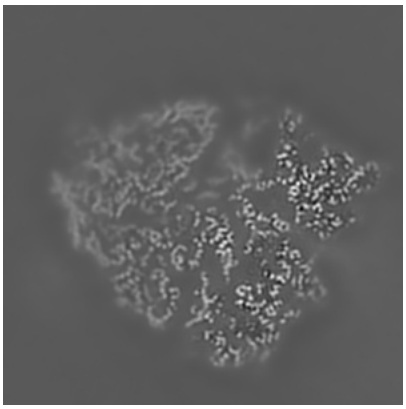
6.2.1 Primary map



X Index: 190

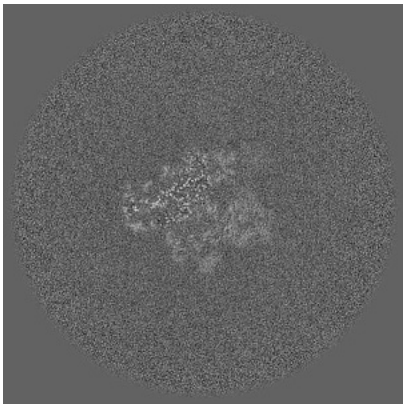


Y Index: 190

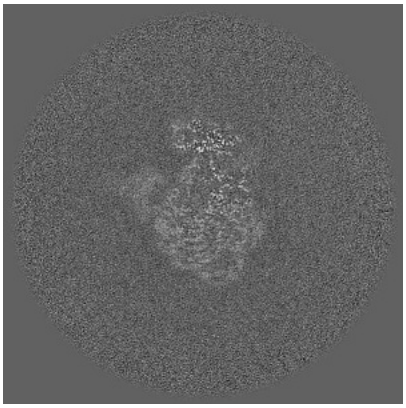


Z Index: 190

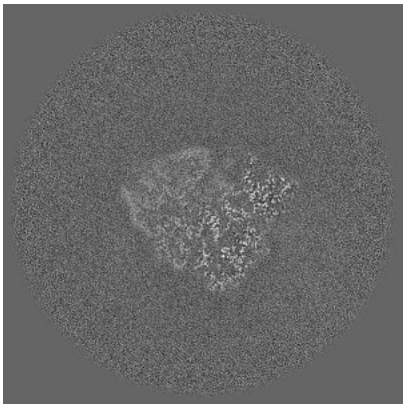
6.2.2 Raw map



X Index: 176



Y Index: 176

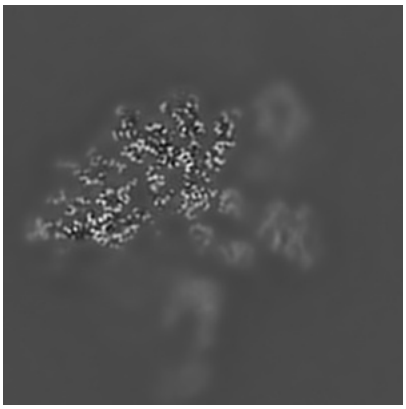


Z Index: 176

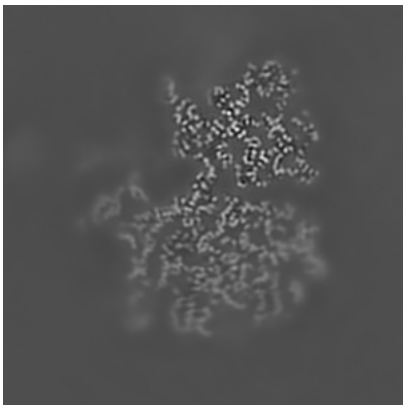
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

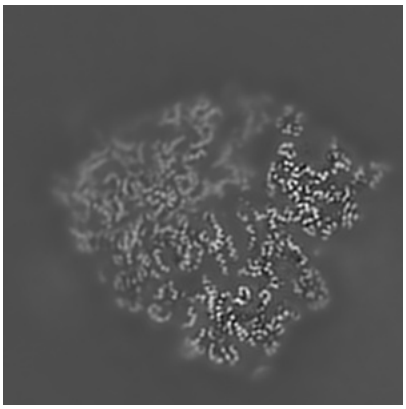
6.3.1 Primary map



X Index: 231

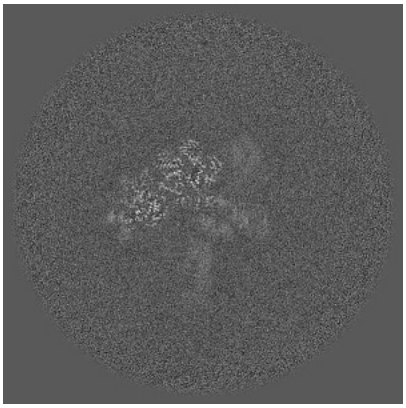


Y Index: 152

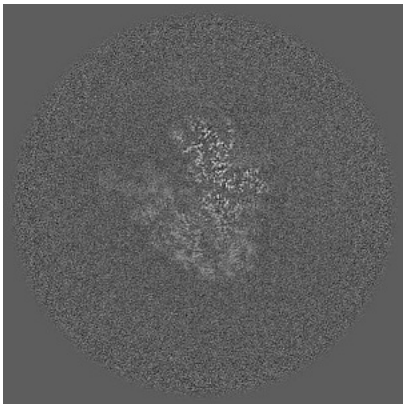


Z Index: 184

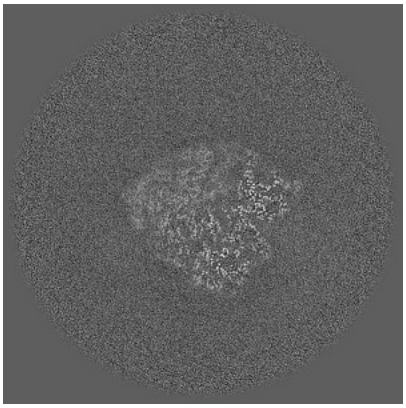
6.3.2 Raw map



X Index: 194



Y Index: 169



Z Index: 173

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

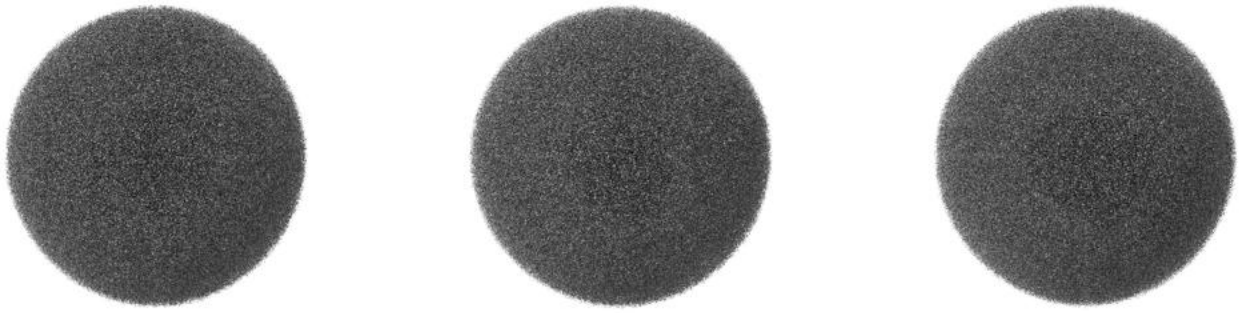
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

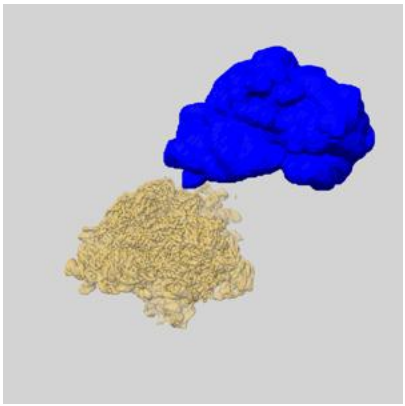
6.5 Mask visualisation (i)

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

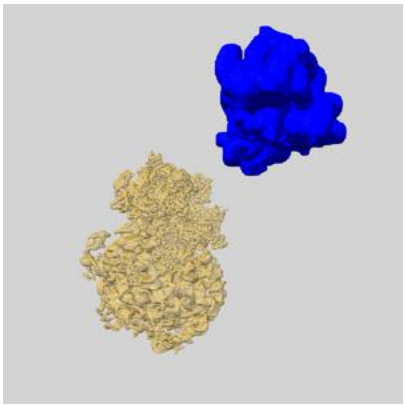
A mask typically either:

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

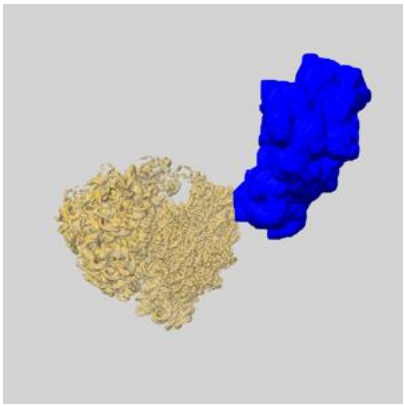
6.5.1 emd_11998_msk_1.map (i)



X



Y

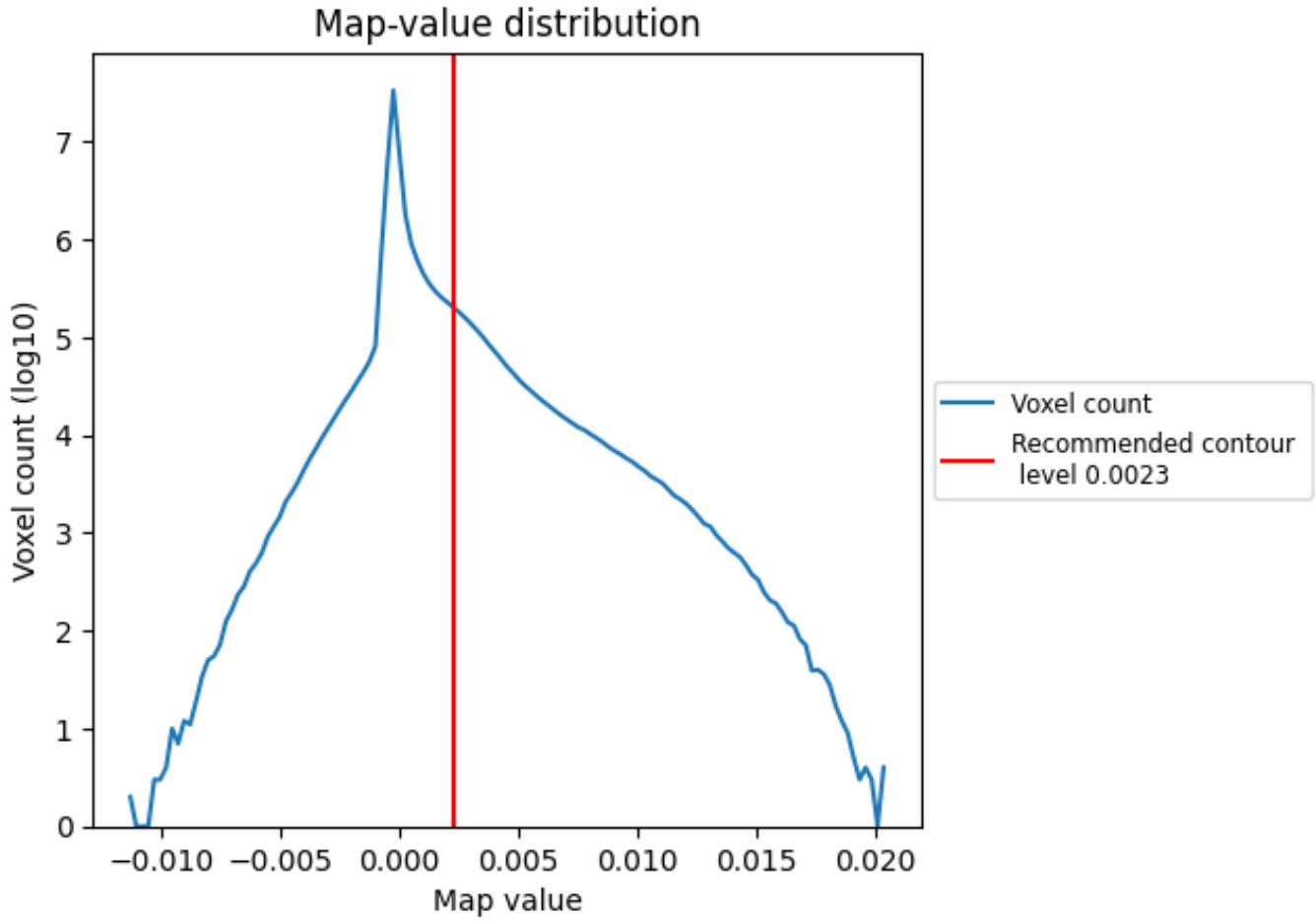


Z

7 Map analysis

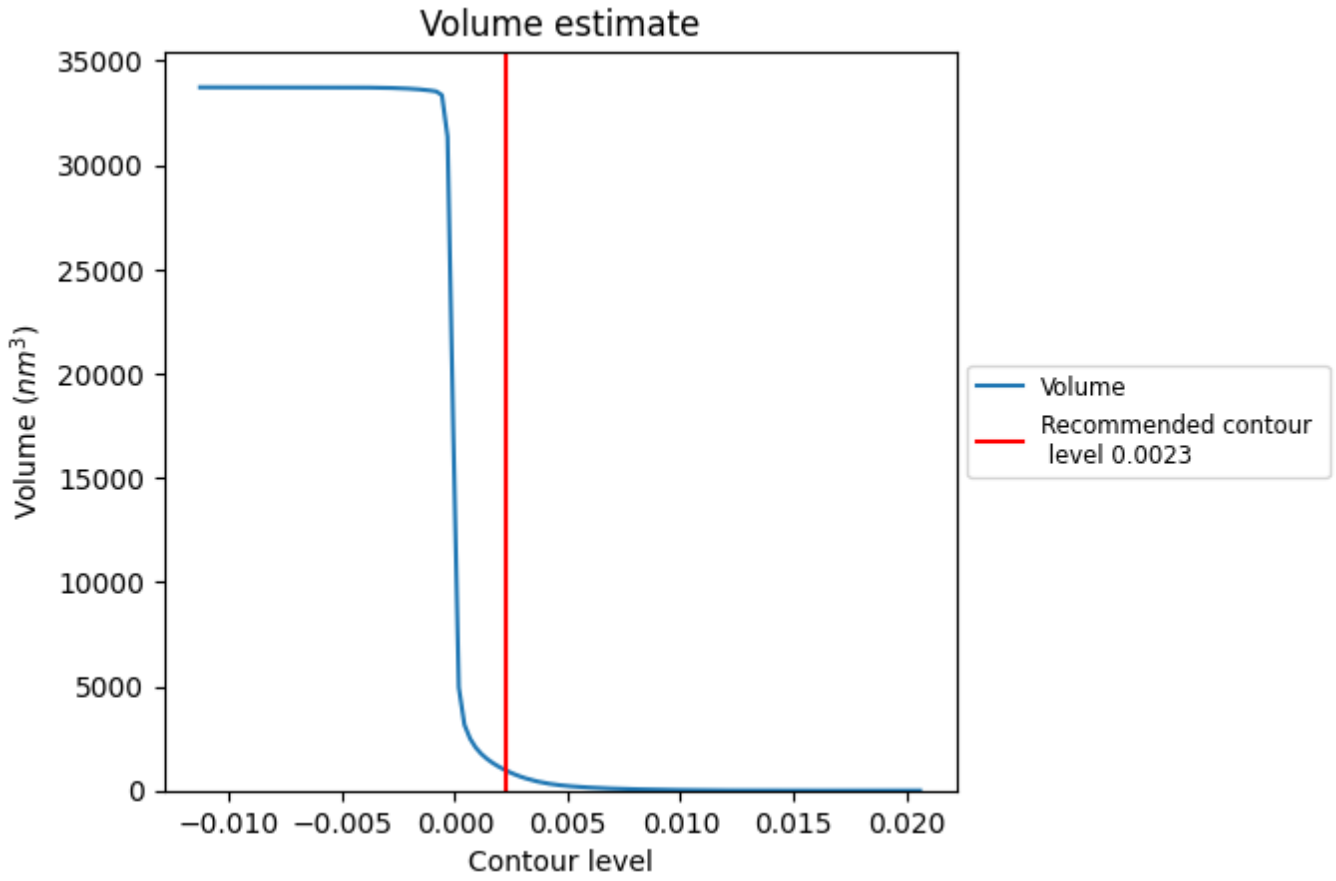
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

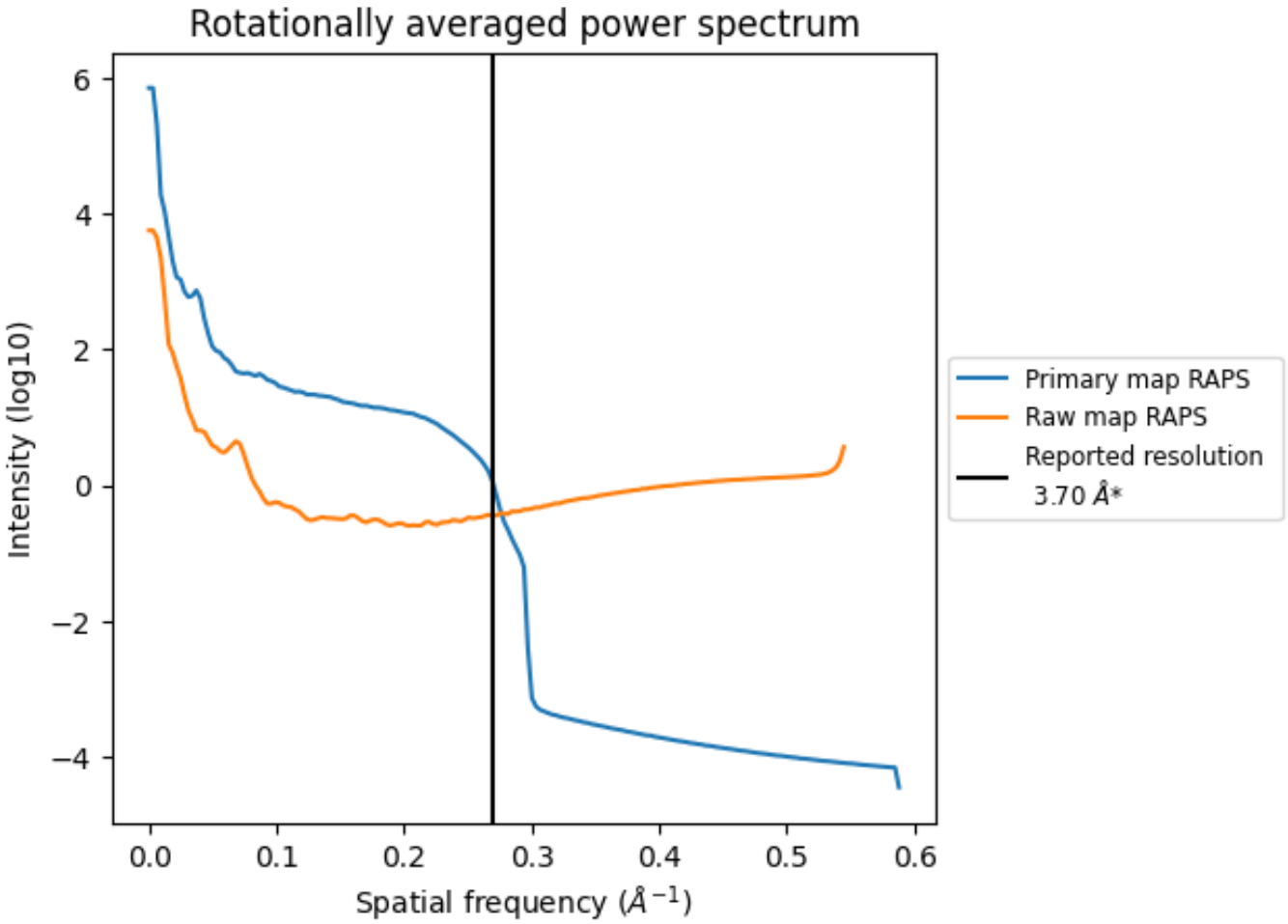
7.2 Volume estimate (i)



The volume at the recommended contour level is 952 nm^3; this corresponds to an approximate mass of 860 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

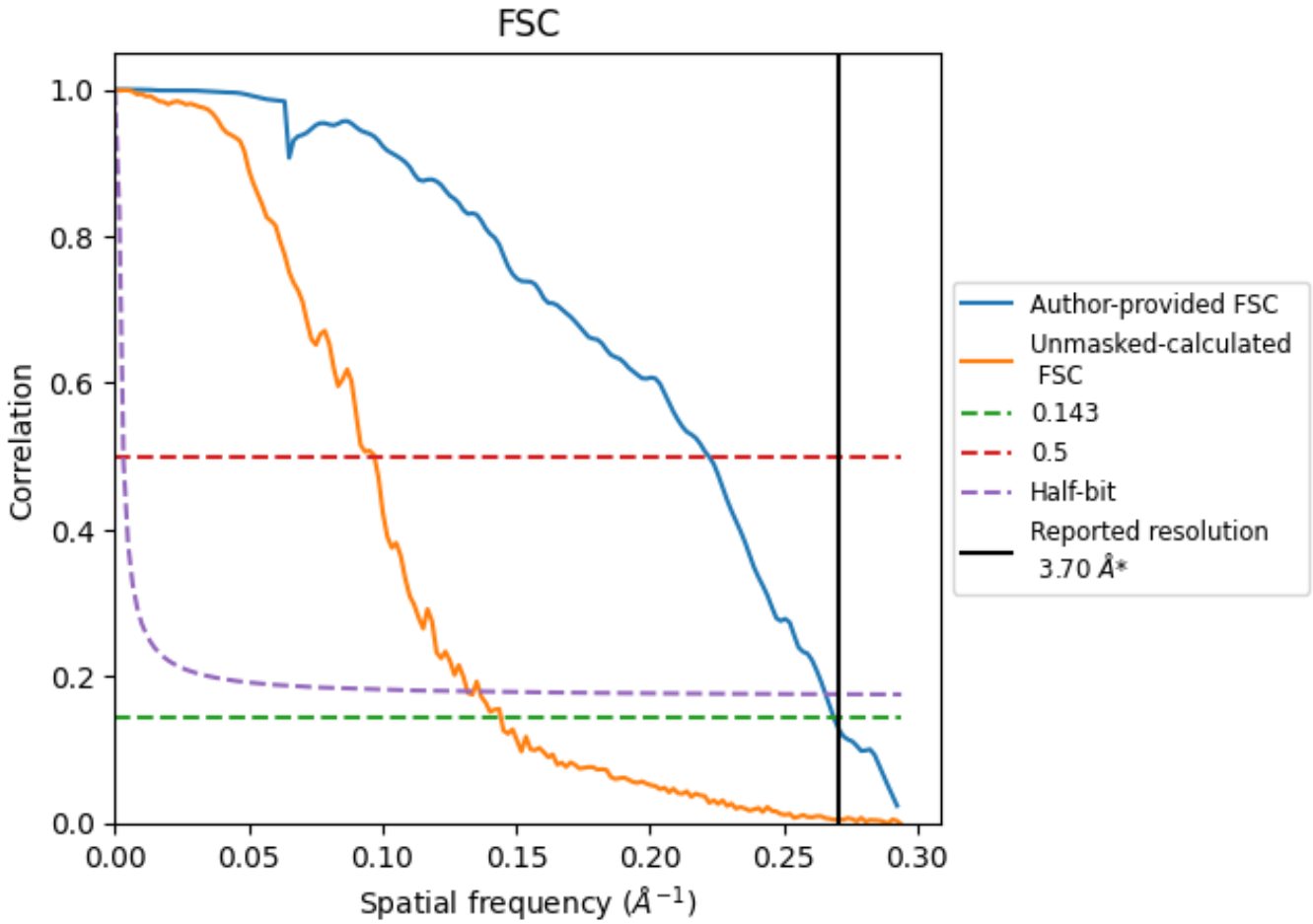


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

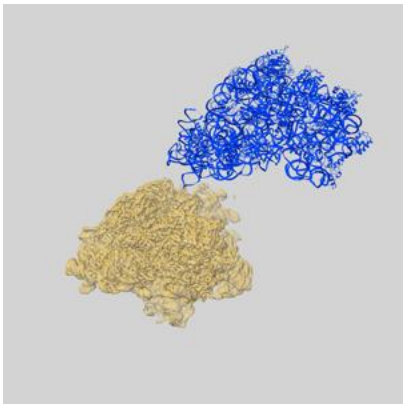
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.51	3.76
Unmasked-calculated*	6.93	10.31	7.59

*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 6.93 differs from the reported value 3.7 by more than 10 %

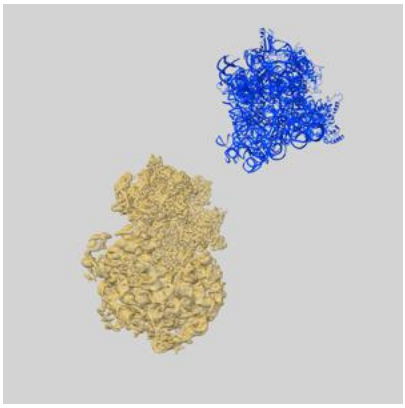
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11998 and PDB model 7OOC. Per-residue inclusion information can be found in section 3 on page 8.

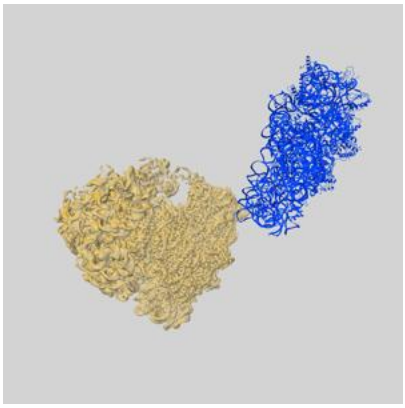
9.1 Map-model overlay



X



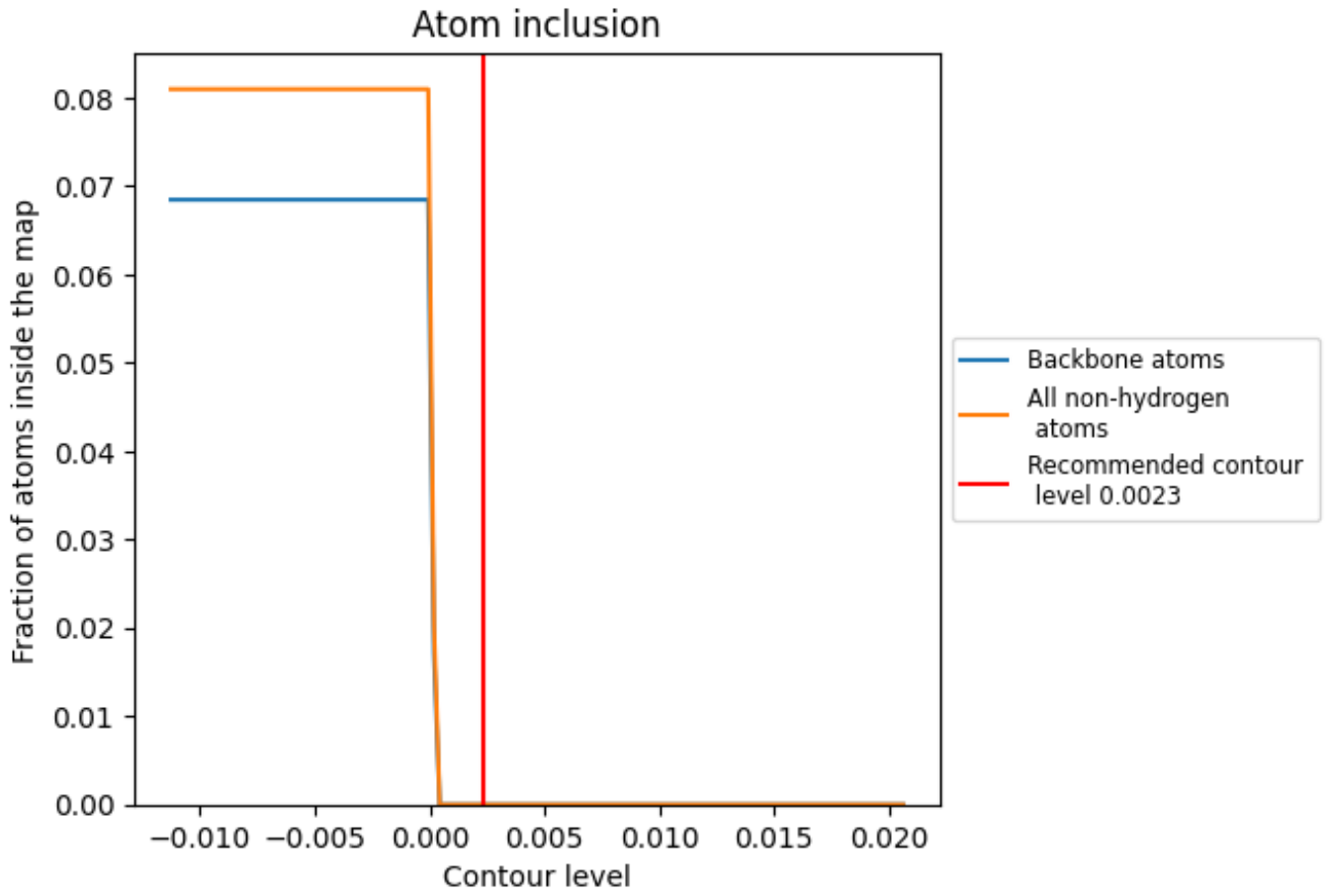
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0023 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 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.