# wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 09:19 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 6EU1 |
| EMDB ID | : | EMD-3956 |
| Title | : | RNA Polymerase III - open DNA complex (OC-POL3). |
| Authors | : | Abascal-Palacios, G.; Ramsay, E.P.; Beuron, F.; Morris, E.; Vannini, A. |
| Deposited on | : | 2017-10-27 |
| Resolution | : | 3.40 Å(reported) |

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

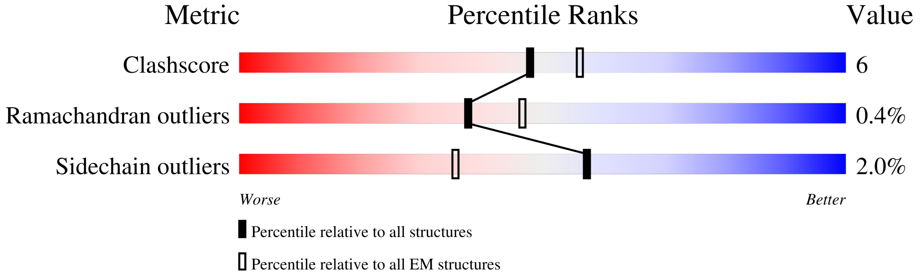
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 1 Overall quality at a glance (i)

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

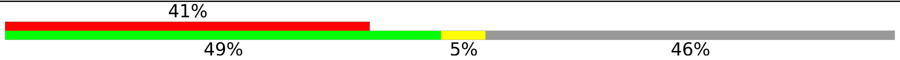
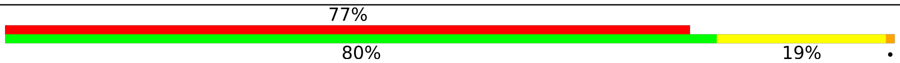
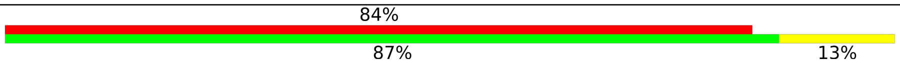
The reported resolution of this entry is 3.40 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 | A | 1460 |  |
| 2 | B | 1149 |  |
| 3 | C | 335 |  |
| 4 | D | 161 |  |
| 5 | E | 215 |  |
| 6 | F | 155 |  |
| 7 | G | 212 |  |
| 8 | H | 146 |  |

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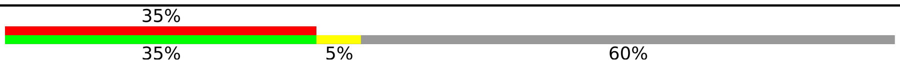
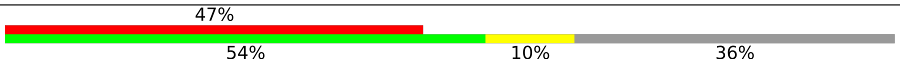
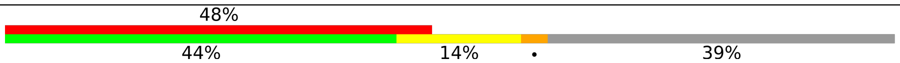
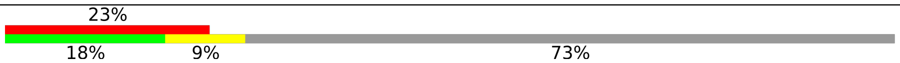
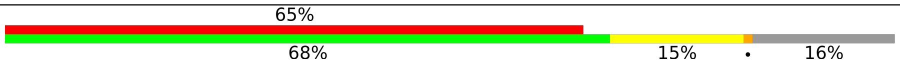
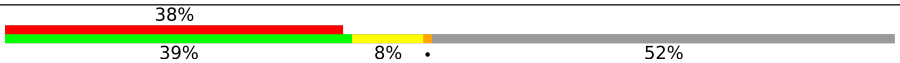
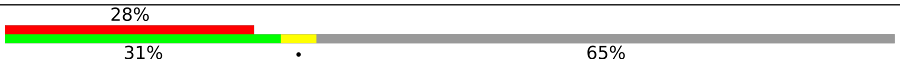
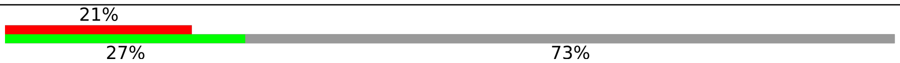
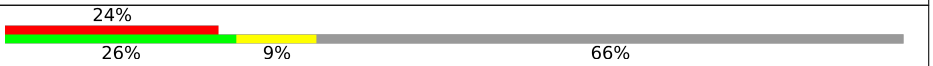
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | I | 110 |  |
| 10 | J | 70 |  |
| 11 | K | 142 |  |
| 12 | L | 70 |  |
| 13 | M | 282 |  |
| 14 | N | 422 |  |
| 15 | O | 654 |  |
| 16 | P | 317 |  |
| 17 | Q | 251 |  |
| 18 | R | 70 |  |
| 19 | S | 70 |  |

# 2 Entry composition ⓘ

There are 21 unique types of molecules in this entry. The entry contains 40547 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 DNA-directed RNA polymerase III subunit RPC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 1433 | 11187 | 7046 | 1975 | 2108 | 58 | 0 | 0 |

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 1114 | 8788 | 5558 | 1516 | 1654 | 60 | 0 | 0 |

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 335 | 2655 | 1681 | 454 | 511 | 9 | 0 | 0 |

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 138 | 1070 | 679 | 180 | 205 | 6 | 0 | 0 |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 215 | 1759 | 1116 | 310 | 321 | 12 | 0 | 0 |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 83 | 671 | 429 | 114 | 125 | 3 | 0 | 0 |

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | G | 211 | 1690 | 1093 | 275 | 316 | 6 | 0 | 0 |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | H | 146 | 1161 | 726 | 195 | 235 | 5 | 0 | 0 |

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | I | 44 | 341 | 216 | 53 | 66 | 6 | 0 | 0 |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | J | 67 | 549 | 350 | 95 | 98 | 6 | 0 | 0 |

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | K | 104 | 815 | 509 | 133 | 168 | 5 | 0 | 0 |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | L | 45 | 366 | 226 | 74 | 62 | 4 | 1 | 0 |

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | M | 172 | 1402 | 893 | 240 | 268 | 1 | 0 | 0 |

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | N | 114 | 864 | 547 | 156 | 158 | 3 | 0 | 0 |

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | O | 551 | 4426 | 2815 | 760 | 832 | 19 | 0 | 0 |

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | P | 151 | 1210 | 781 | 189 | 236 | 4 | 0 | 0 |

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | Q | 89 | 707 | 448 | 120 | 138 | 1 | 0 | 0 |

- Molecule 18 is a DNA chain called Non-Template.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 18 | R | 19 | 386 | 184 | 68 | 115 | 19 | 0 | 0 |

- Molecule 19 is a DNA chain called Template.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 19 | S | 24 | 493 | 234 | 93 | 142 | 24 | 0 | 0 |

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 20 | A | 2 | 2 | 2 | 0 |
| 20 | B | 1 | 1 | 1 | 0 |
| 20 | I | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 20 | J | 1 | Total Zn<br>1 1 | 0 |
| 20 | L | 1 | Total Zn<br>1 1 | 0 |

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

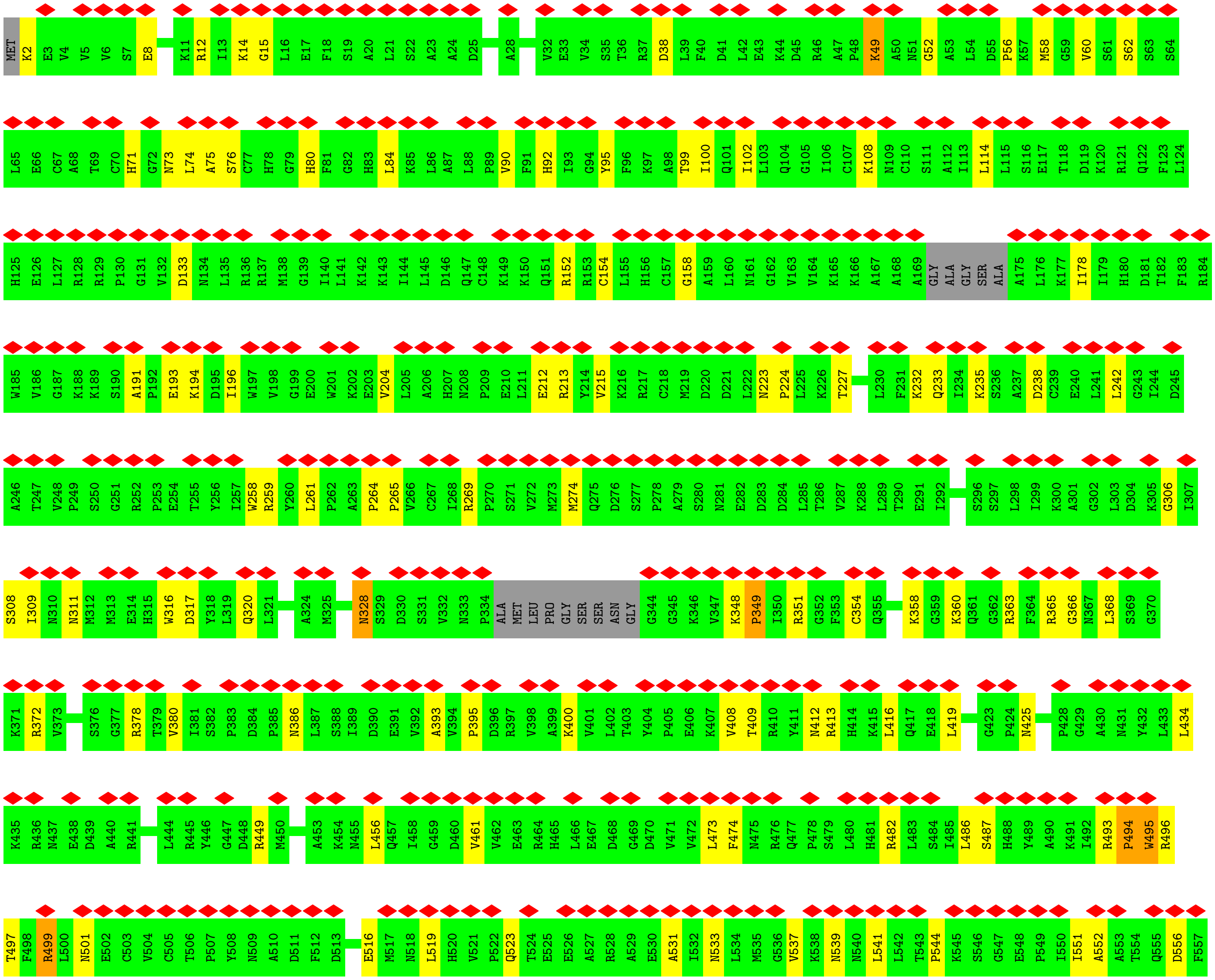
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 21 | A | 1 | Total Mg<br>1 1 | 0 |

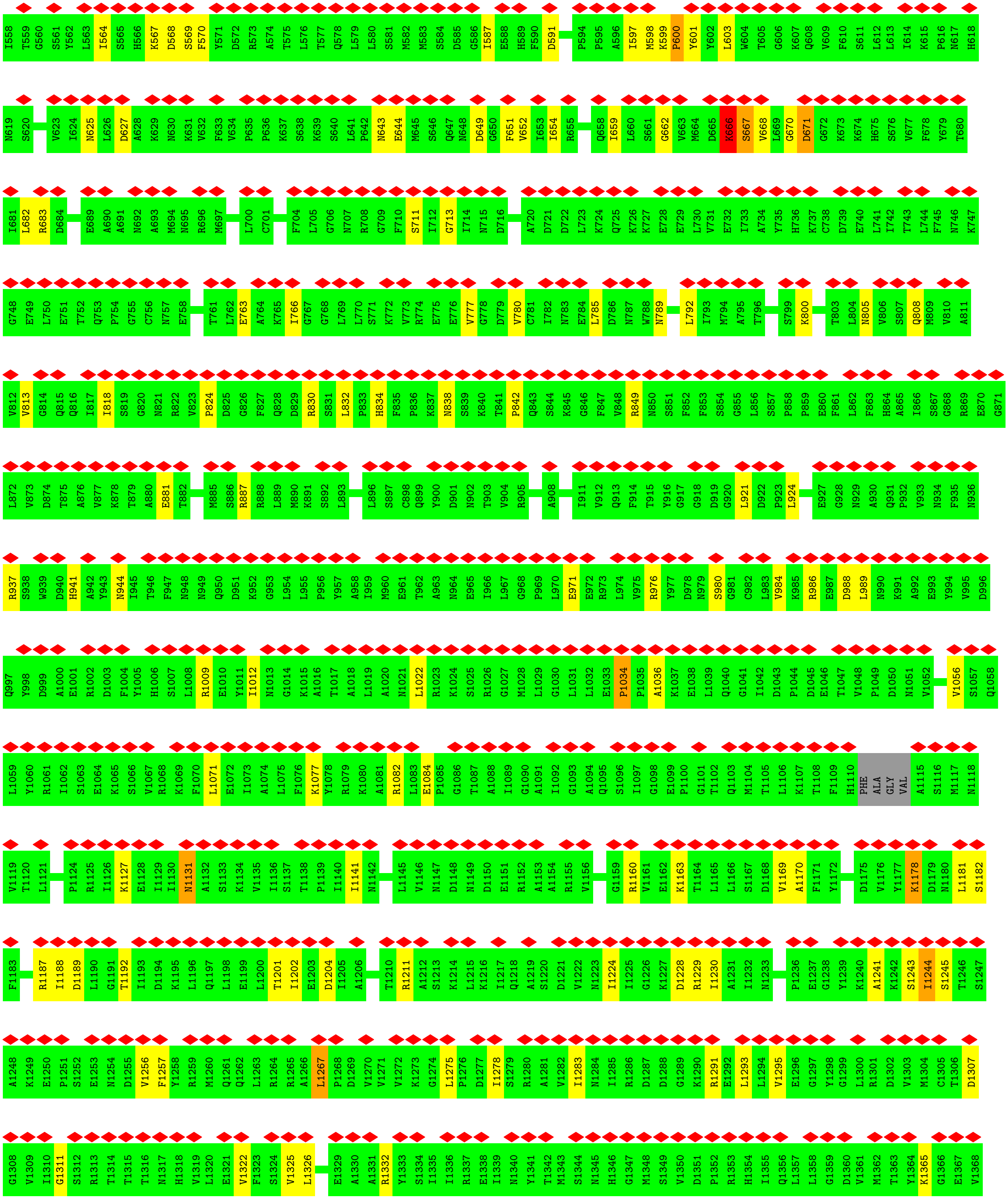
# 3 Residue-property plots ⓘ

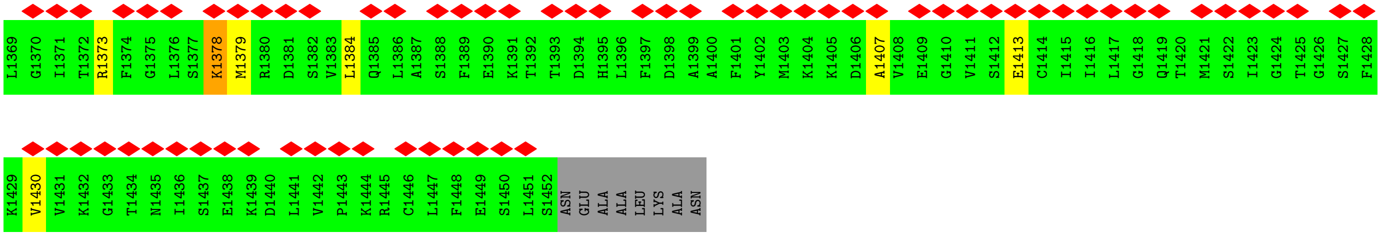
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase III subunit RPC1

Chain A:

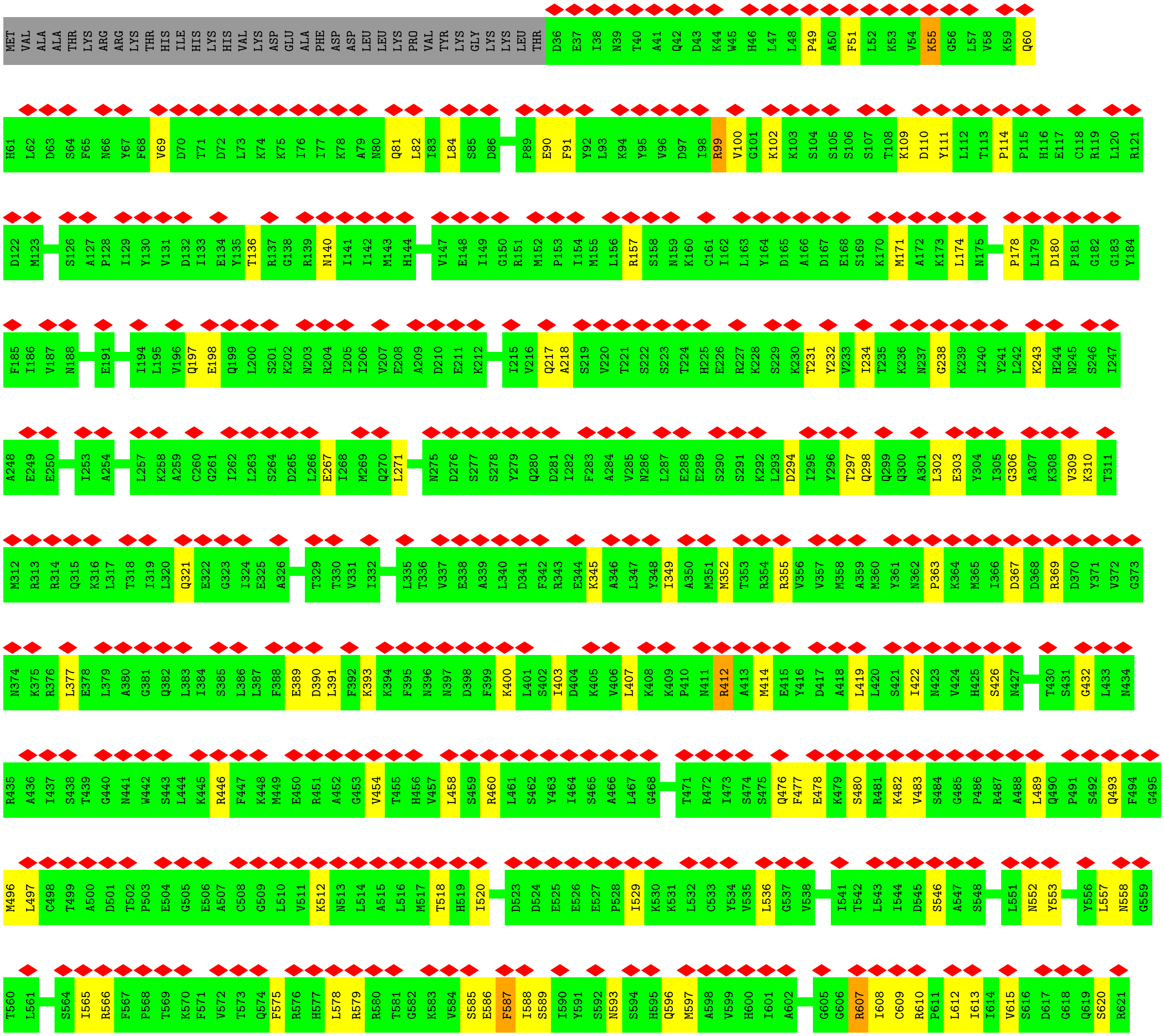


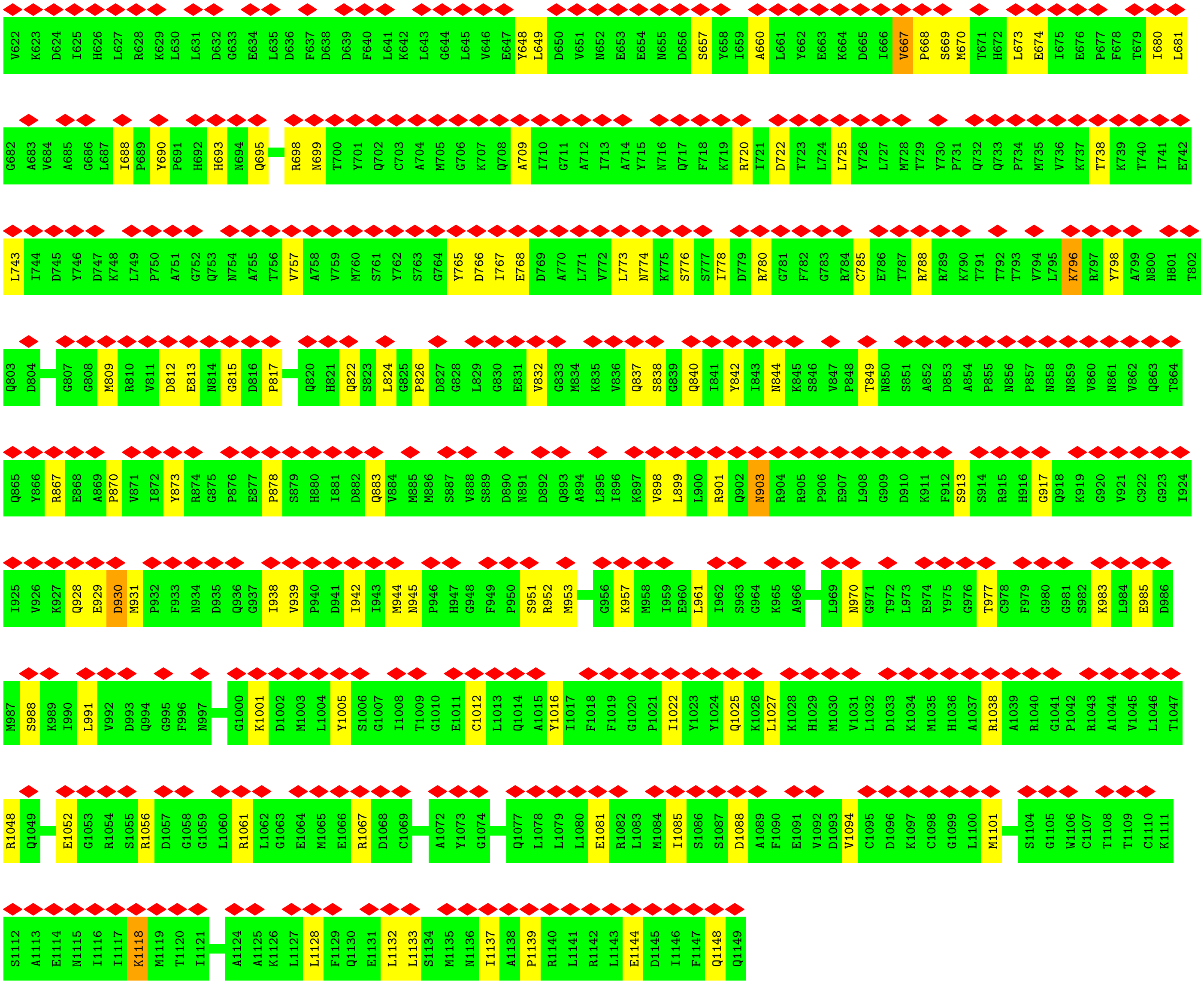

I558 T559 G560 S561 Y562 L563 I564 S565 H566 K567 D568 S569 F570 Y571 D572 R573 A574 T575 L576 T577 Q578 L579 L580 S581 M582 M583 S584 D585 G586 I587 E588 H589 F590 D591 P594 P595 A596 I597 M598 K599 P600 Y601 Y602 L603 W604 T605 G606 K607 Q608 V609 F610 S611 L612 L613 I614 K615 P616 N617 H618
N619 S620 V623 I624 N625 L626 D627 A628 K629 N630 K631 V632 F633 V634 P635 P636 K637 S638 K639 S640 L641 P642 N643 E644 M645 S646 Q647 N648 D649 G650 F651 V652 I653 I654 R655 Q658 I659 L660 S661 G662 V663 M664 D665 K666 S667 V668 L669 G670 D671 G672 K673 K674 H675 S676 V677 F678 Y679 T680
I681 L682 R683 D684 E689 A690 A691 N692 A693 M694 N695 R696 M697 L700 C701 F704 L705 G706 N707 R708 G709 F710 S711 I712 G713 I714 N715 D716 A720 D721 D722 L723 K724 Q725 K726 K727 E728 E729 L730 V731 E732 I733 A734 Y735 H736 K737 C738 D739 E740 L741 I742 T743 L744 F745 N746 K747
G748 E749 L750 E751 T752 Q753 P754 G755 C756 N757 E758 T761 L762 E763 A764 K765 I766 G767 G768 L769 L770 S771 K772 V773 R774 E775 E776 V777 G778 D779 V780 C781 I782 N783 E784 L785 D786 N787 W788 N789 L792 I793 M794 A795 T796 S799 K800 T803 L804 N805 V806 S807 Q808 M809 V810 A811
V812 V813 G814 Q815 Q816 I817 I818 S819 G820 N821 R822 V823 P824 D825 G826 F827 Q828 D829 R830 S831 L832 P833 H834 F835 P836 K837 N838 S839 K840 T841 P842 Q843 S844 K845 G846 F847 V848 R849 N850 S851 F852 F853 S854 G855 L856 S857 P858 P859 E860 F861 L862 F863 H864 A865 I866 S867 G868 R869 E870 G871
L872 V873 D874 T875 A876 V877 K878 T879 A880 E881 T882 M885 S886 R887 R888 L889 M890 K891 S892 L893 L896 S897 C898 Q899 Y900 D901 N902 T903 V904 R905 A908 I911 V912 Q913 F914 T915 Y916 G917 G918 D919 G920 L921 D922 P923 L924 E927 G928 N929 A930 Q931 P932 V933 N934 F935 N936
R937 S938 W939 D940 H941 A942 Y943 N944 I945 T946 F947 N948 N949 Q950 D951 K952 G953 L954 L955 P956 Y957 A958 I959 M960 E961 T962 A963 N964 E965 I966 L967 G968 P969 L970 E971 E972 R973 L974 V975 R976 Y977 D978 N979 S980 G981 C982 L983 V984 K985 R986 E987 D988 L989 N990 K991 A992 E993 Y994 V995 D996
Q997 Y998 D999 A1000 E1001 R1002 D1003 F1004 Y1005 H1006 S1007 L1008 R1009 E1010 Y1011 I1012 N1013 G1014 K1015 A1016 T1017 A1018 L1019 A1020 N1021 L1022 R1023 K1024 S1025 R1026 G1027 M1028 L1029 G1030 L1031 L1032 E1033 P1034 P1035 A1036 K1037 E1038 L1039 Q1040 G1041 I1042 D1043 P1044 D1045 E1046 T1047 V1048 P1049 D1050 N1051 V1052 V1056 S1057 Q1058
L1059 Y1060 R1061 I1062 S1063 E1064 K1065 S1066 V1067 R1068 K1069 F1070 L1071 E1072 I1073 A1074 L1075 F1076 K1077 Y1078 R1079 K1080 A1081 R1082 L1083 E1084 P1085 G1086 T1087 A1088 I1089 G1090 A1091 I1092 G1093 A1094 Q1095 S1096 I1097 G1098 E1099 P1100 G1101 T1102 Q1103 M1104 T1105 L1106 K1107 T1108 F1109 H1110 PHE ALA GLY VAL A1115 S1116 M1117 N1118
V1119 T1120 L1121 P1124 R1125 I1126 K1127 E1128 I1129 I1130 N1131 A1132 S1133 K1134 V1135 I1136 S1137 T1138 P1139 I1140 I1141 N1142 L1145 V1146 N1147 D1148 N1149 D1150 E1151 R1152 A1153 A1154 R1155 V1156 G1159 R1160 V1161 E1162 K1163 T1164 L1165 L1166 S1167 D1168 V1169 A1170 F1171 Y1172 D1175 V1176 Y1177 K1178 D1179 N1180 L1181 S1182
F1183 R1187 I1188 D1189 L1190 G1191 T1192 I1193 D1194 K1195 L1196 Q1197 L1198 E1199 L1200 T1201 I1202 E1203 D1204 I1205 A1206 T1210 R1211 A1212 S1213 K1214 L1215 K1216 I1217 Q1218 A1219 S1220 D1221 V1222 N1223 I1224 I1225 G1226 K1227 D1228 R1229 I1230 A1231 I1232 N1233 P1236 E1237 G1238 Y1239 K1240 A1241 K1242 S1243 I1244 S1245 T1246 S1247
A1248 K1249 E1250 P1251 S1252 E1253 N1254 D1255 V1256 F1257 Y1258 R1259 M1260 Q1261 Q1262 L1263 R1264 R1265 A1266 L1267 P1268 D1269 V1270 V1271 V1272 K1273 G1274 L1275 P1276 D1277 I1278 S1279 R1280 A1281 V1282 I1283 N1284 I1285 R1286 D1287 D1288 G1289 K1290 R1291 E1292 L1293 L1294 V1295 E1296 G1297 Y1298 G1299 L1300 R1301 D1302 V1303 M1304 C1305 T1306 D1307
G1308 V1309 I1310 G1311 S1312 R1313 T1314 T1315 T1316 N1317 H1318 V1319 L1320 E1321 V1322 F1323 S1324 V1325 L1326 E1329 A1330 A1331 R1332 Y1333 S1334 I1335 I1336 R1337 E1338 I1339 N1340 Y1341 T1342 M1343 S1344 N1345 H1346 G1347 M1348 S1349 V1350 D1351 P1352 R1353 H1354 I1355 Q1356 L1357 L1358 G1359 D1360 V1361 M1362 T1363 Y1364 K1365 G1366 E1367 V1368



- Molecule 2: DNA-directed RNA polymerase III subunit RPC2

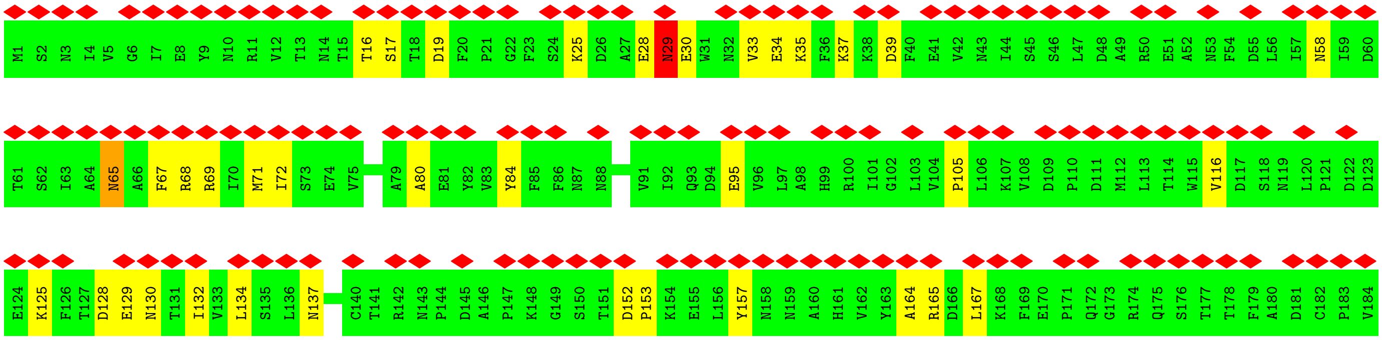
Chain B:

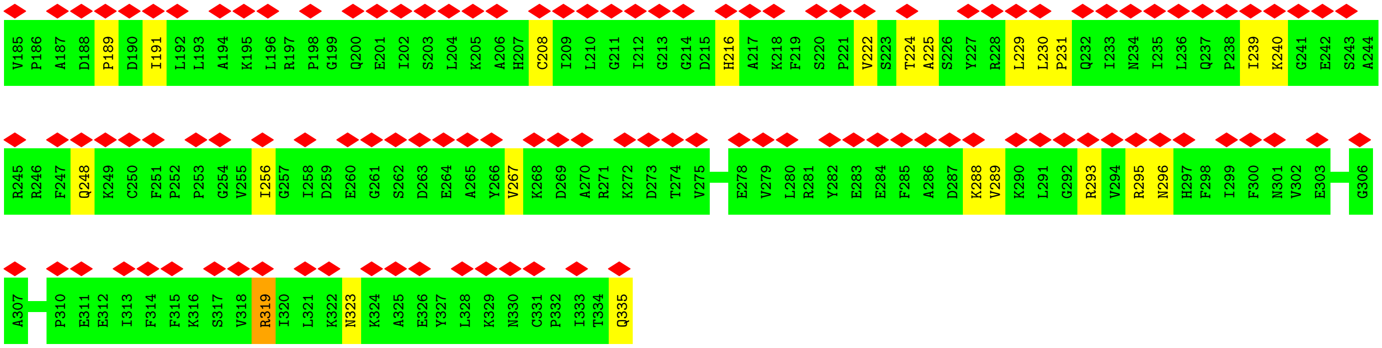




- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

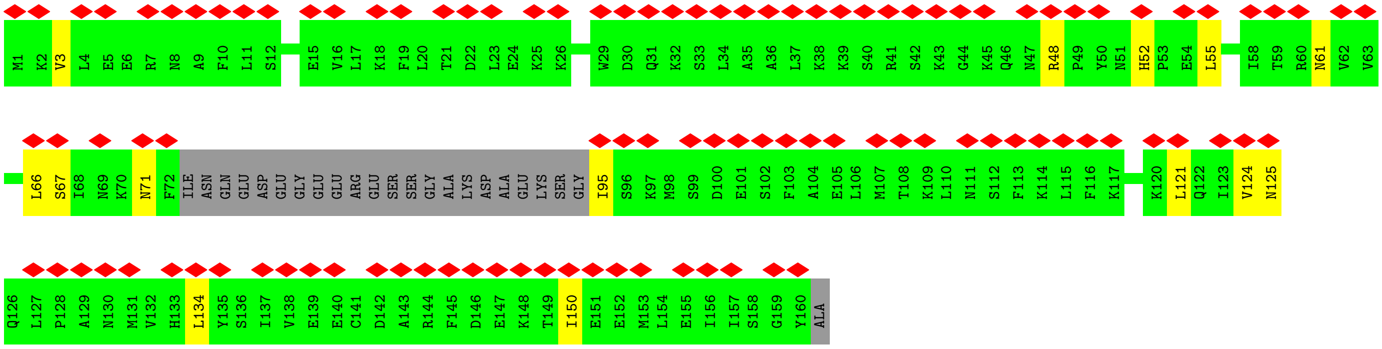
Chain C:





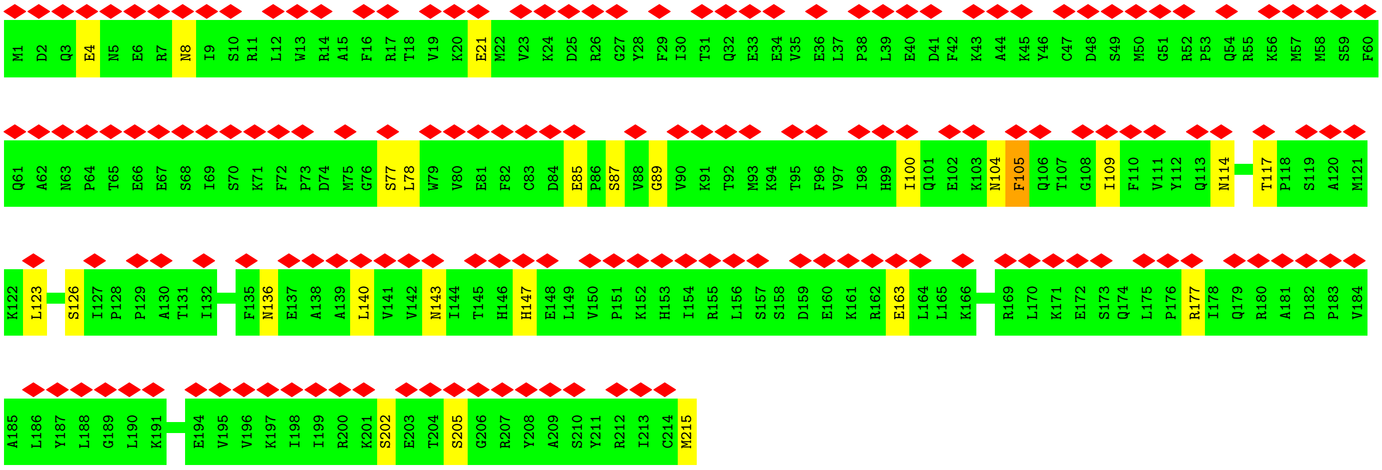
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D:



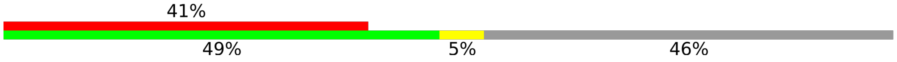
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

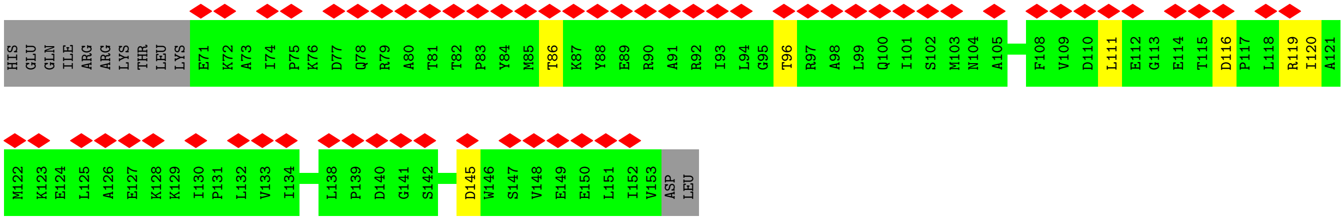
Chain E:



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

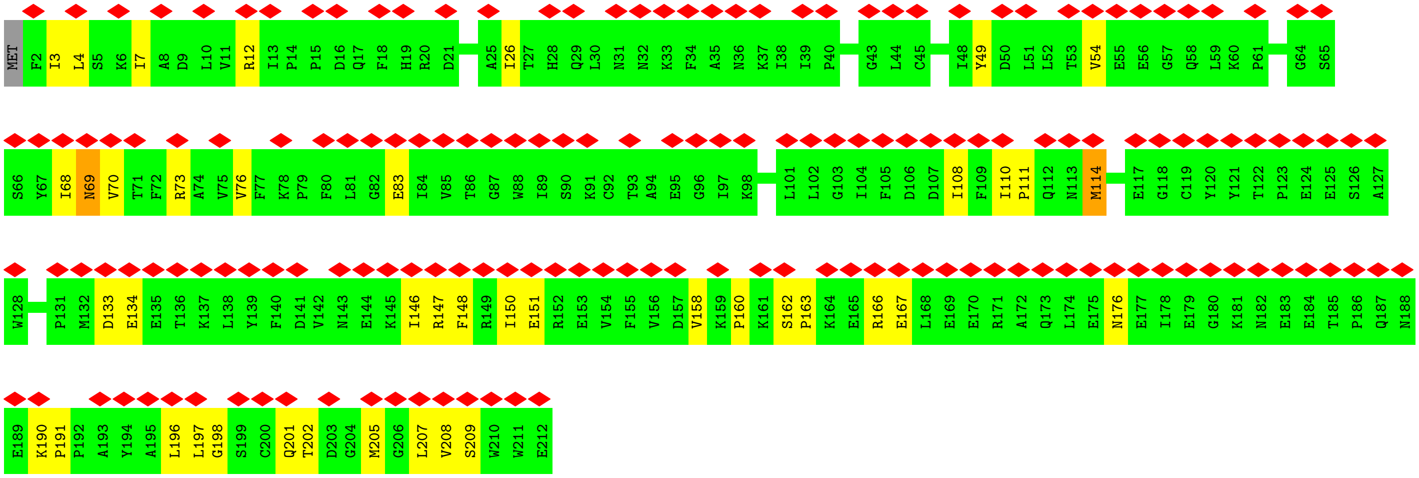
Chain F:





- Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:

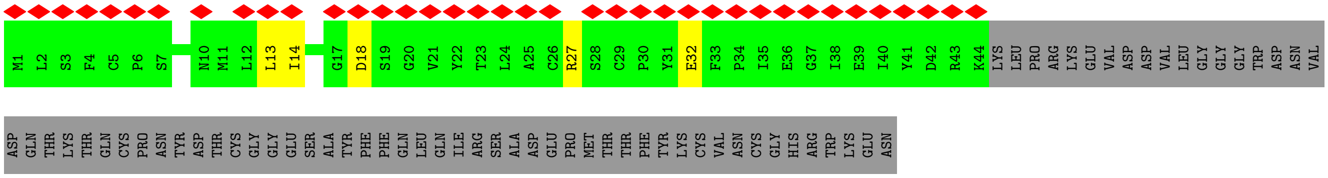


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

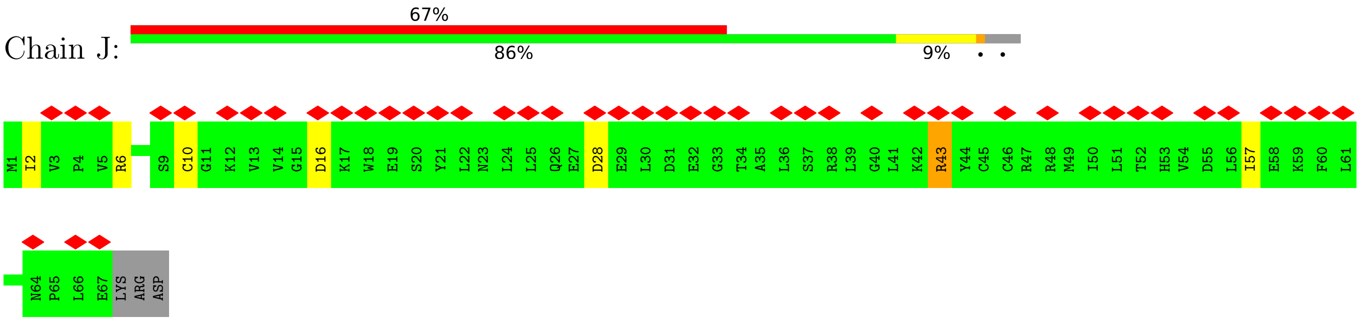
Chain H:

- Molecule 9: DNA-directed RNA polymerase III subunit RPC10

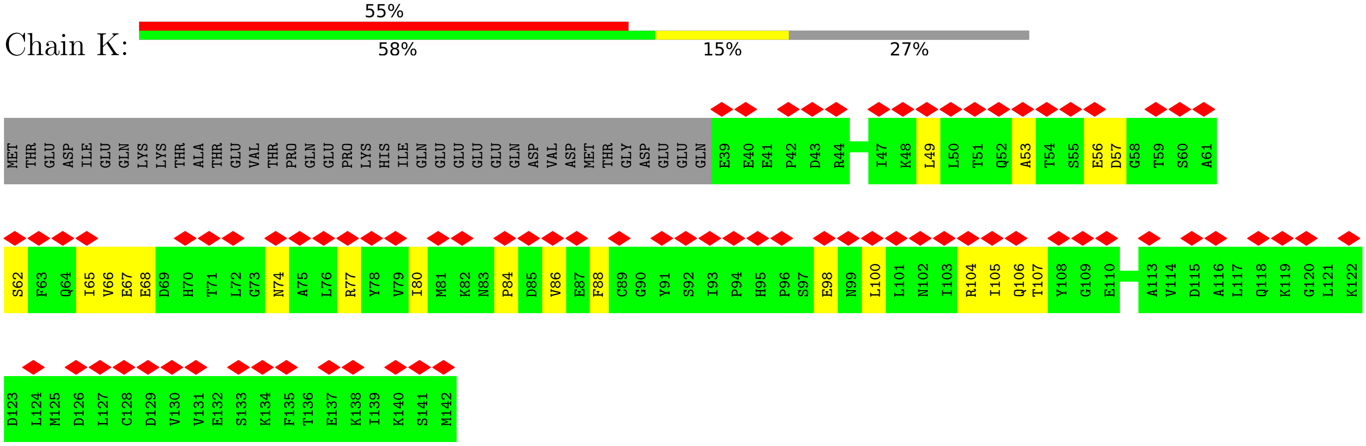
Chain I:



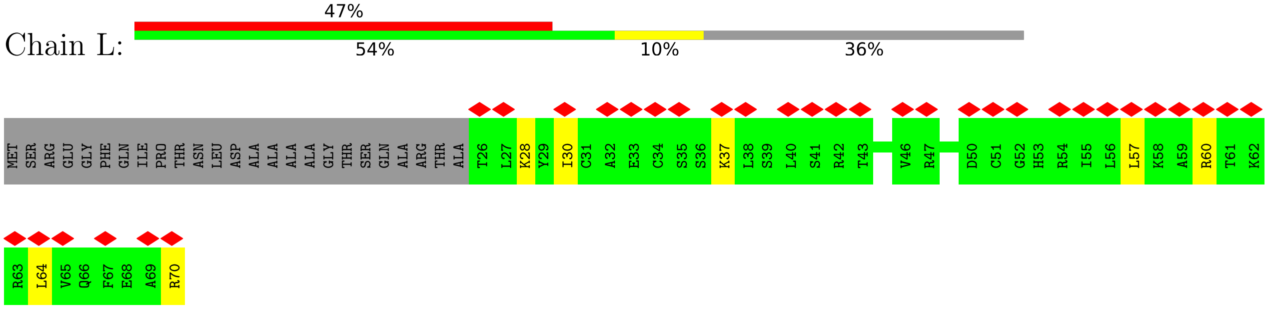
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



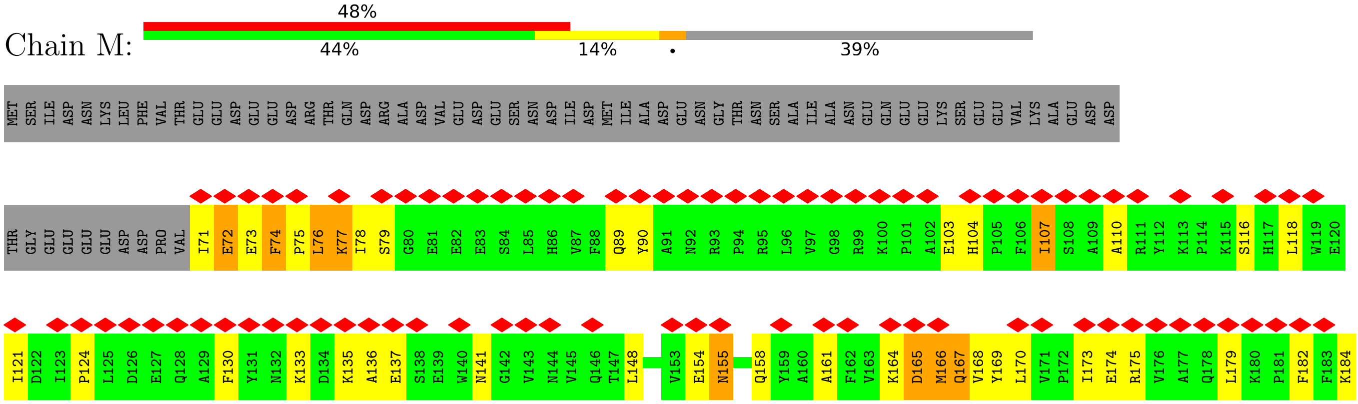
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

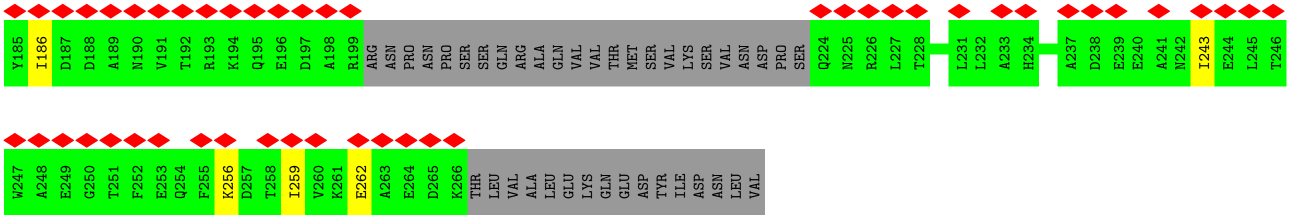


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

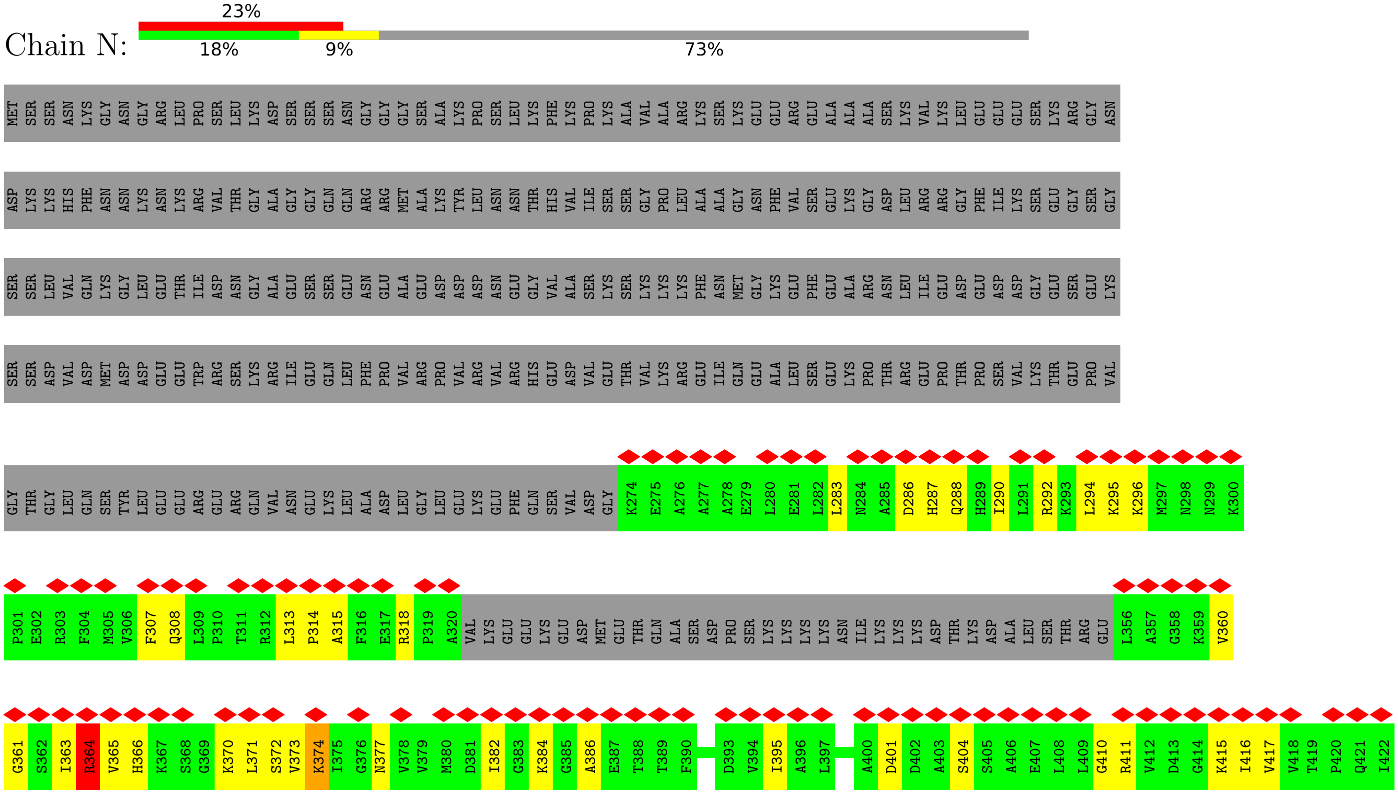


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

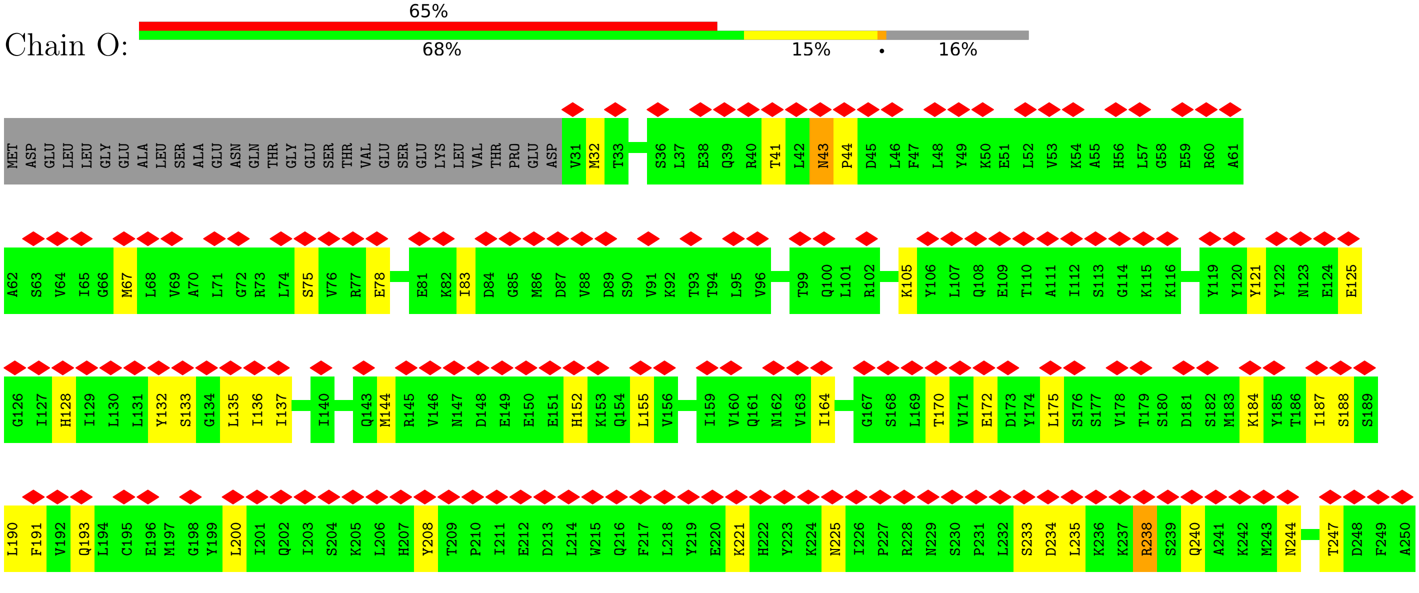


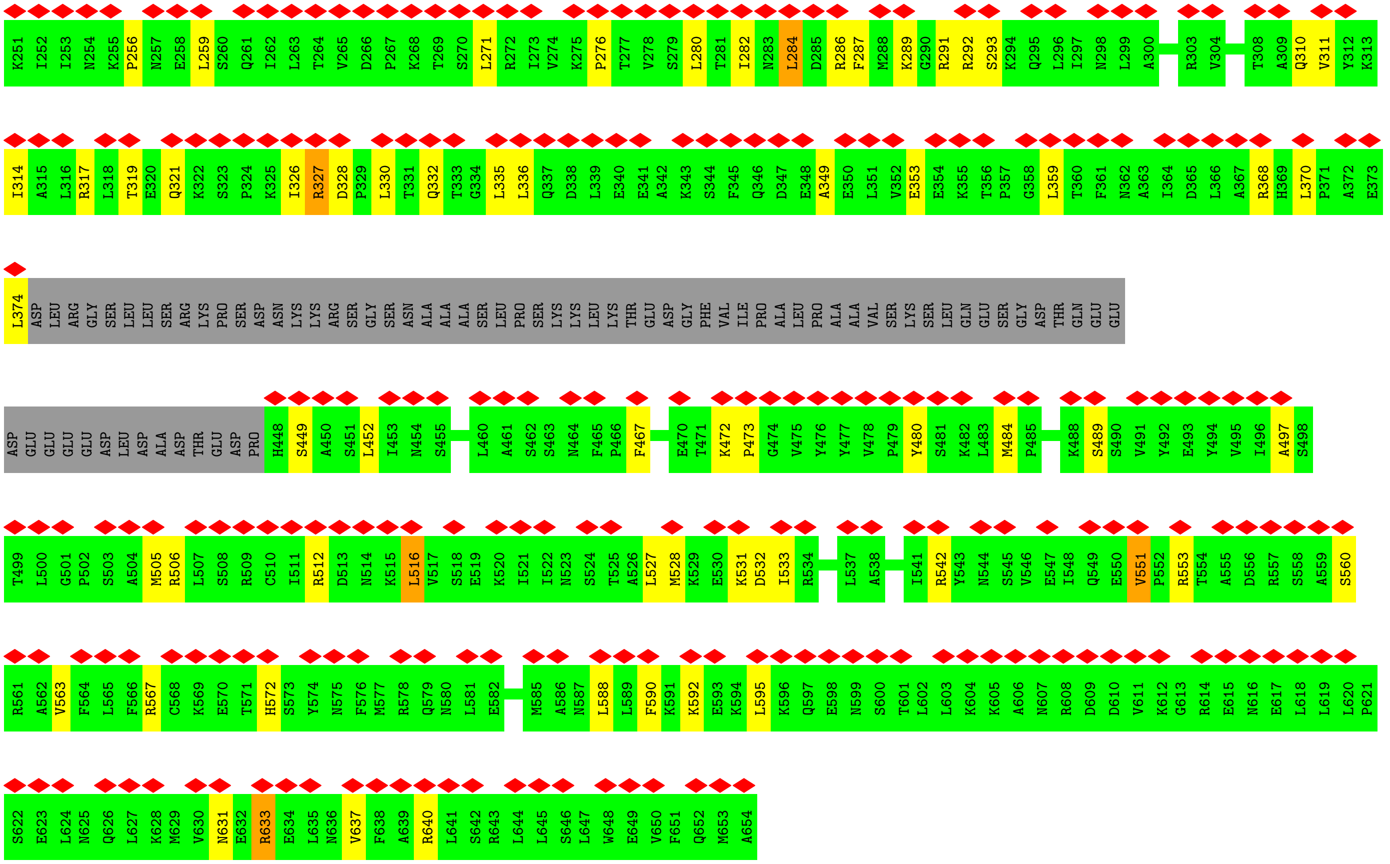


- Molecule 14: DNA-directed RNA polymerase III subunit RPC4



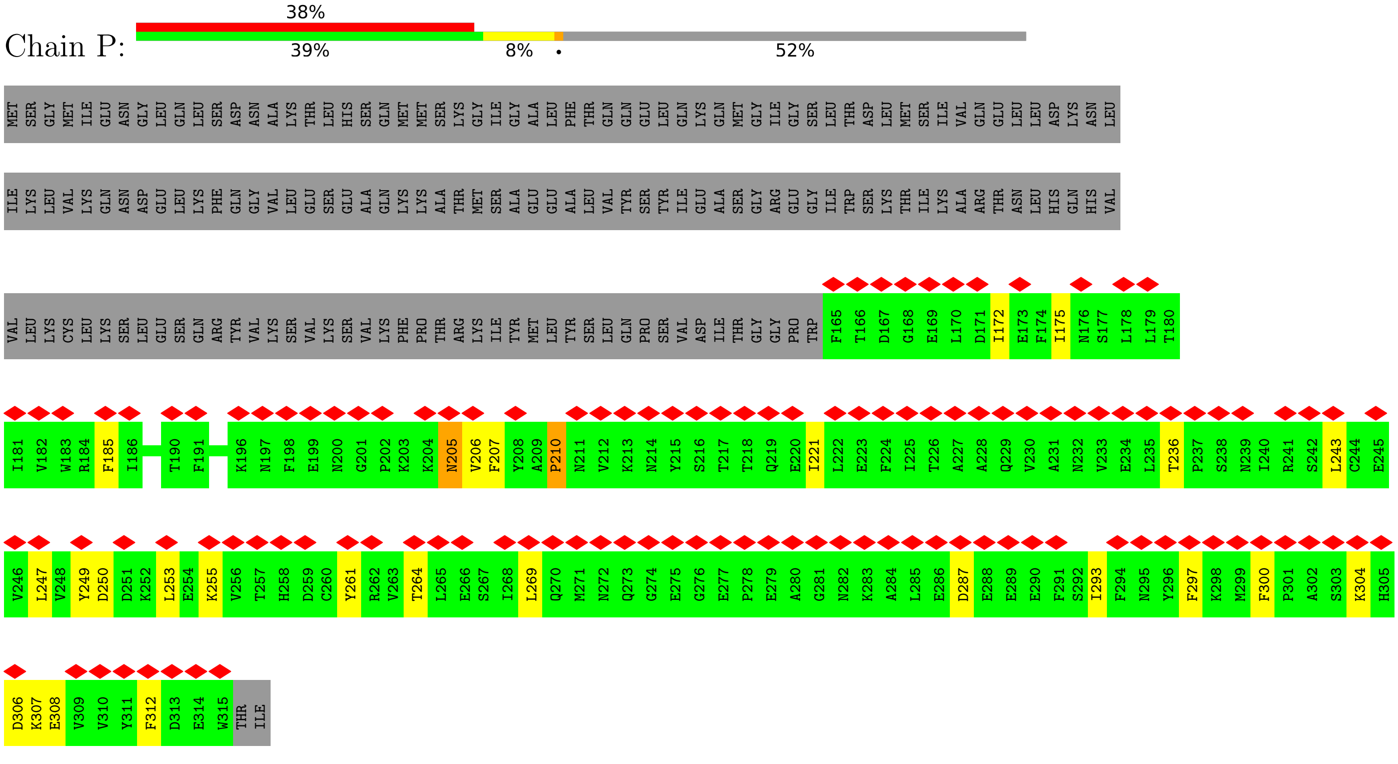
- Molecule 15: DNA-directed RNA polymerase III subunit RPC3





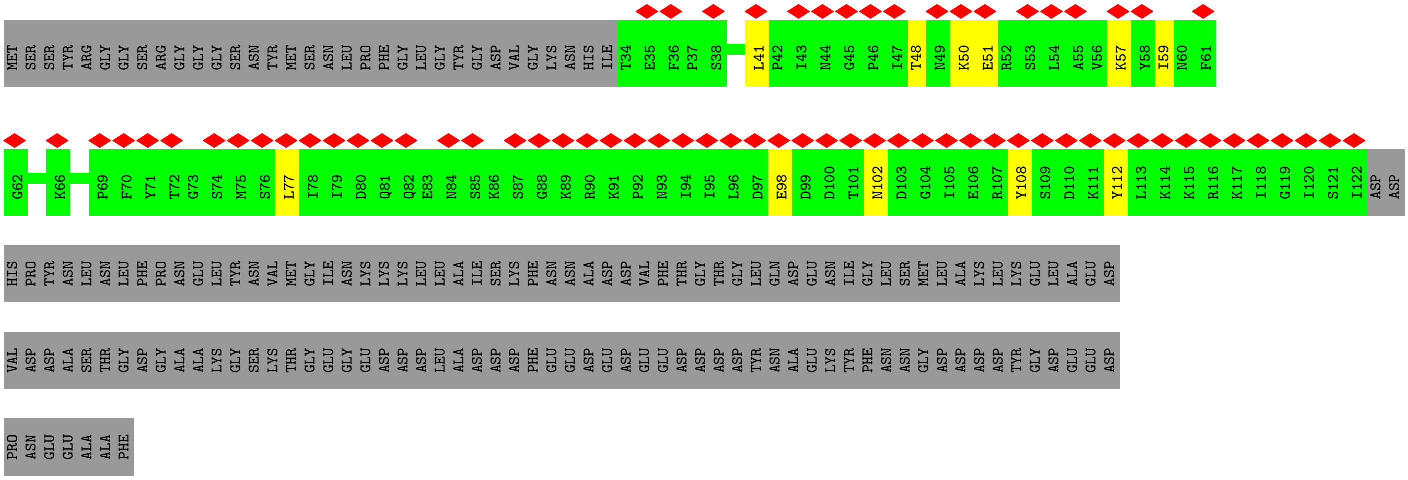
- Molecule 16: DNA-directed RNA polymerase III subunit RPC6

Chain P:



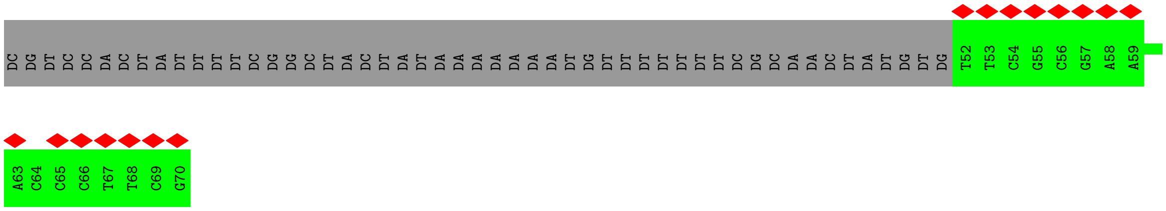
- Molecule 17: DNA-directed RNA polymerase III subunit RPC7

Chain Q:



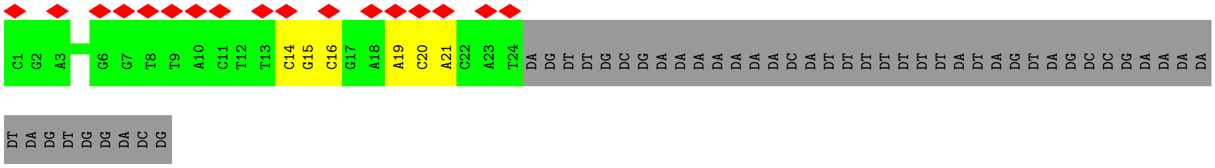
- Molecule 18: Non-Template

Chain R:



- Molecule 19: Template

Chain S:



# 4 Experimental information

| **Property** | **Value** | **Source** |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 100237 | 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 $(e^-/\text{Å}^2)$ | 40 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.396 | Depositor |
| Minimum map value | -0.249 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.009 | Depositor |
| Recommended contour level | 0.04 | Depositor |
| Map size (Å) | 323.4, 323.4, 323.4 | wwPDB |
| Map dimensions | 308, 308, 308 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.05, 1.05, 1.05 | Depositor |

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

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

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 | A | 0.30 | 0/11385 | 0.63 | 6/15382 (0.0%) |
| 2 | B | 0.29 | 0/8943 | 0.63 | 2/12068 (0.0%) |
| 3 | C | 0.29 | 0/2711 | 0.60 | 1/3676 (0.0%) |
| 4 | D | 0.25 | 0/1088 | 0.51 | 0/1455 |
| 5 | E | 0.30 | 0/1795 | 0.59 | 1/2416 (0.0%) |
| 6 | F | 0.27 | 0/683 | 0.56 | 0/923 |
| 7 | G | 0.30 | 0/1732 | 0.64 | 0/2352 |
| 8 | H | 0.29 | 0/1181 | 0.66 | 2/1602 (0.1%) |
| 9 | I | 0.29 | 0/348 | 0.62 | 0/470 |
| 10 | J | 0.31 | 0/558 | 0.70 | 1/750 (0.1%) |
| 11 | K | 0.29 | 0/826 | 0.70 | 2/1115 (0.2%) |
| 12 | L | 0.27 | 0/371 | 0.73 | 0/492 |
| 13 | M | 0.29 | 0/1433 | 0.69 | 2/1936 (0.1%) |
| 14 | N | 0.28 | 0/874 | 0.68 | 1/1175 (0.1%) |
| 15 | O | 0.31 | 0/4493 | 0.65 | 4/6062 (0.1%) |
| 16 | P | 0.30 | 0/1239 | 0.64 | 0/1682 |
| 17 | Q | 0.28 | 0/719 | 0.67 | 0/966 |
| 18 | R | 0.52 | 0/431 | 0.94 | 0/662 |
| 19 | S | 0.56 | 0/553 | 0.91 | 0/851 |
| All | All | 0.30 | 0/41363 | 0.64 | 22/56035 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 8 |
| 2 | B | 0 | 6 |
| 3 | C | 0 | 2 |
| 5 | E | 0 | 1 |

*Continued on next page...*

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 7 | G | 0 | 1 |
| 8 | H | 0 | 1 |
| 13 | M | 0 | 2 |
| 15 | O | 0 | 6 |
| 16 | P | 0 | 4 |
| 17 | Q | 0 | 1 |
| All | All | 0 | 32 |

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | M | 118 | LEU | CA-CB-CG | 8.61 | 135.11 | 115.30 |
| 11 | K | 57 | ASP | CB-CG-OD1 | 6.67 | 124.31 | 118.30 |
| 1 | A | 671 | ASP | CB-CG-OD1 | 6.57 | 124.21 | 118.30 |
| 1 | A | 1267 | LEU | CA-CB-CG | 6.44 | 130.10 | 115.30 |
| 8 | H | 135 | LEU | CA-CB-CG | 6.38 | 129.97 | 115.30 |

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 233 | GLN | Peptide |
| 1 | A | 274 | MET | Peptide |
| 1 | A | 306 | GLY | Peptide |
| 1 | A | 494 | PRO | Peptide |
| 1 | A | 600 | PRO | Peptide |

## 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 | A | 11187 | 0 | 11278 | 137 | 0 |
| 2 | B | 8788 | 0 | 8904 | 133 | 0 |
| 3 | C | 2655 | 0 | 2628 | 38 | 0 |
| 4 | D | 1070 | 0 | 1023 | 6 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 5 | E | 1759 | 0 | 1788 | 13 | 0 |
| 6 | F | 671 | 0 | 692 | 5 | 0 |
| 7 | G | 1690 | 0 | 1660 | 22 | 0 |
| 8 | H | 1161 | 0 | 1124 | 9 | 0 |
| 9 | I | 341 | 0 | 332 | 4 | 0 |
| 10 | J | 549 | 0 | 562 | 6 | 0 |
| 11 | K | 815 | 0 | 803 | 13 | 0 |
| 12 | L | 366 | 0 | 396 | 5 | 0 |
| 13 | M | 1402 | 0 | 1365 | 69 | 0 |
| 14 | N | 864 | 0 | 903 | 56 | 0 |
| 15 | O | 4426 | 0 | 4594 | 58 | 0 |
| 16 | P | 1210 | 0 | 1131 | 16 | 0 |
| 17 | Q | 707 | 0 | 724 | 6 | 0 |
| 18 | R | 386 | 0 | 215 | 0 | 0 |
| 19 | S | 493 | 0 | 270 | 5 | 0 |
| 20 | A | 2 | 0 | 0 | 0 | 0 |
| 20 | B | 1 | 0 | 0 | 0 | 0 |
| 20 | I | 1 | 0 | 0 | 0 | 0 |
| 20 | J | 1 | 0 | 0 | 0 | 0 |
| 20 | L | 1 | 0 | 0 | 0 | 0 |
| 21 | A | 1 | 0 | 0 | 0 | 0 |
| All | All | 40547 | 0 | 40392 | 513 | 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 6.

The worst 5 of 513 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) |
|---|---|---|---|
| 13:M:74:PHE:CE2 | 14:N:294:LEU:HD21 | 1.26 | 1.62 |
| 13:M:75:PRO:HG3 | 13:M:166:MET:SD | 1.39 | 1.61 |
| 13:M:74:PHE:CZ | 14:N:294:LEU:HD21 | 1.53 | 1.40 |
| 13:M:74:PHE:CE2 | 14:N:294:LEU:CD2 | 2.16 | 1.27 |
| 13:M:76:LEU:HB3 | 14:N:361:GLY:HA2 | 1.28 | 1.15 |

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 | A | 1425/1460 (98%) | 1204 (84%) | 213 (15%) | 8 (1%) | 25 | 57 |
| 2 | B | 1112/1149 (97%) | 926 (83%) | 183 (16%) | 3 (0%) | 41 | 72 |
| 3 | C | 333/335 (99%) | 285 (86%) | 47 (14%) | 1 (0%) | 41 | 72 |
| 4 | D | 134/161 (83%) | 121 (90%) | 13 (10%) | 0 | 100 | 100 |
| 5 | E | 213/215 (99%) | 184 (86%) | 29 (14%) | 0 | 100 | 100 |
| 6 | F | 81/155 (52%) | 73 (90%) | 8 (10%) | 0 | 100 | 100 |
| 7 | G | 209/212 (99%) | 156 (75%) | 53 (25%) | 0 | 100 | 100 |
| 8 | H | 144/146 (99%) | 127 (88%) | 17 (12%) | 0 | 100 | 100 |
| 9 | I | 42/110 (38%) | 37 (88%) | 5 (12%) | 0 | 100 | 100 |
| 10 | J | 65/70 (93%) | 54 (83%) | 11 (17%) | 0 | 100 | 100 |
| 11 | K | 102/142 (72%) | 91 (89%) | 11 (11%) | 0 | 100 | 100 |
| 12 | L | 44/70 (63%) | 40 (91%) | 4 (9%) | 0 | 100 | 100 |
| 13 | M | 168/282 (60%) | 116 (69%) | 50 (30%) | 2 (1%) | 13 | 41 |
| 14 | N | 110/422 (26%) | 88 (80%) | 21 (19%) | 1 (1%) | 17 | 49 |
| 15 | O | 547/654 (84%) | 464 (85%) | 82 (15%) | 1 (0%) | 47 | 78 |
| 16 | P | 149/317 (47%) | 109 (73%) | 38 (26%) | 2 (1%) | 12 | 39 |
| 17 | Q | 87/251 (35%) | 73 (84%) | 14 (16%) | 0 | 100 | 100 |
| All | All | 4965/6151 (81%) | 4148 (84%) | 799 (16%) | 18 (0%) | 38 | 67 |

5 of 18 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 348 | LYS |
| 1 | A | 349 | PRO |
| 1 | A | 1244 | ILE |
| 2 | B | 111 | TYR |
| 3 | C | 129 | GLU |

### 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 | A | 1231/1257 (98%) | 1208 (98%) | 23 (2%) | 57 | 78 |
| 2 | B | 975/1006 (97%) | 958 (98%) | 17 (2%) | 60 | 80 |
| 3 | C | 296/296 (100%) | 290 (98%) | 6 (2%) | 55 | 77 |
| 4 | D | 113/145 (78%) | 110 (97%) | 3 (3%) | 44 | 70 |
| 5 | E | 197/197 (100%) | 195 (99%) | 2 (1%) | 76 | 88 |
| 6 | F | 73/137 (53%) | 73 (100%) | 0 | 100 | 100 |
| 7 | G | 184/190 (97%) | 178 (97%) | 6 (3%) | 38 | 66 |
| 8 | H | 128/128 (100%) | 127 (99%) | 1 (1%) | 81 | 91 |
| 9 | I | 40/98 (41%) | 40 (100%) | 0 | 100 | 100 |
| 10 | J | 62/65 (95%) | 61 (98%) | 1 (2%) | 62 | 81 |
| 11 | K | 93/130 (72%) | 93 (100%) | 0 | 100 | 100 |
| 12 | L | 41/57 (72%) | 40 (98%) | 1 (2%) | 49 | 74 |
| 13 | M | 148/249 (59%) | 138 (93%) | 10 (7%) | 16 | 45 |
| 14 | N | 92/360 (26%) | 88 (96%) | 4 (4%) | 29 | 59 |
| 15 | O | 505/593 (85%) | 494 (98%) | 11 (2%) | 52 | 75 |
| 16 | P | 130/285 (46%) | 129 (99%) | 1 (1%) | 81 | 91 |
| 17 | Q | 81/212 (38%) | 80 (99%) | 1 (1%) | 71 | 85 |
| All | All | 4389/5405 (81%) | 4302 (98%) | 87 (2%) | 57 | 77 |

5 of 87 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | H | 143 | LEU |
| 14 | N | 295 | LYS |
| 12 | L | 28 | LYS |
| 13 | M | 77 | LYS |
| 15 | O | 43 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | M | 254 | GLN |
| 15 | O | 43 | ASN |
| 16 | P | 205 | ASN |
| 2 | B | 774 | ASN |
| 2 | B | 754 | ASN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

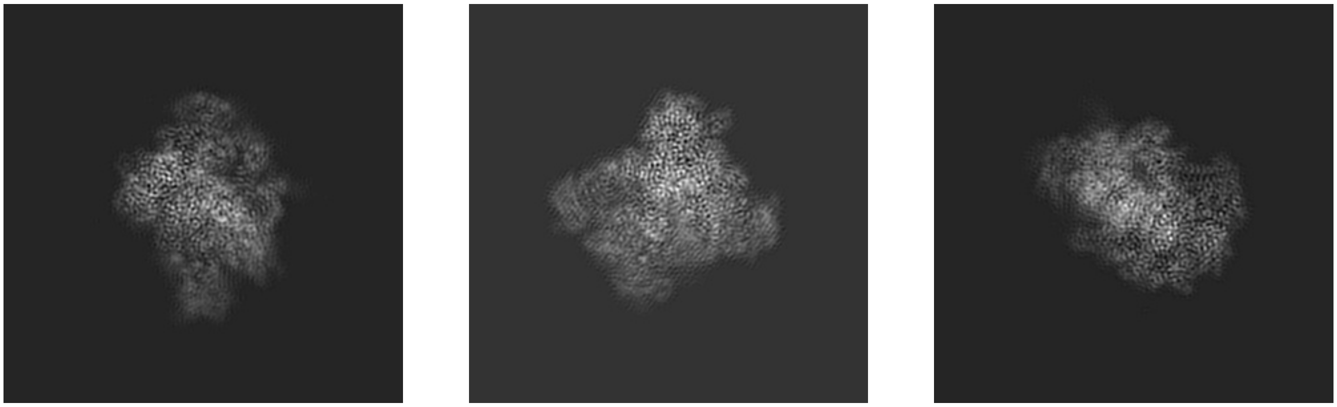
# 6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3956. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

## 6.1 Orthogonal projections ⓘ

### 6.1.1 Primary map

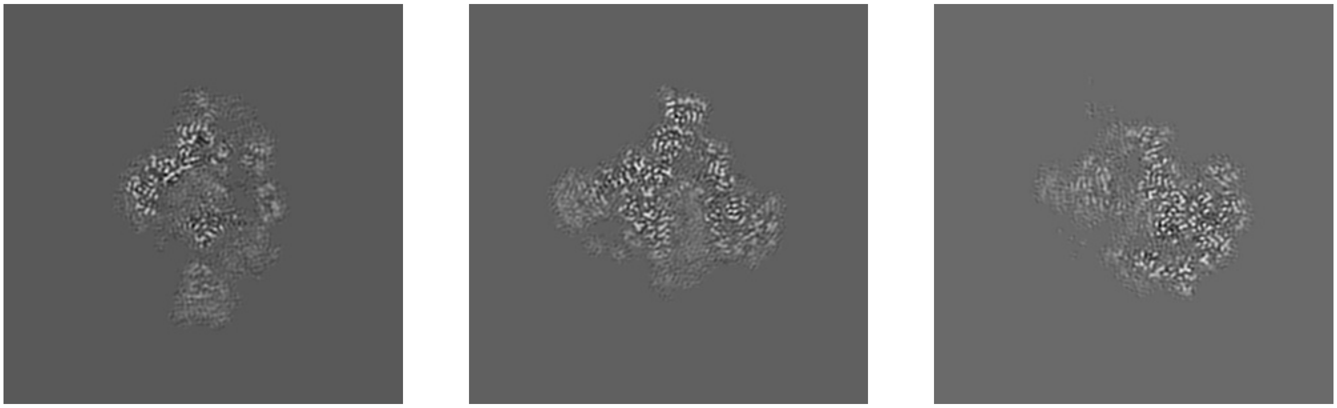


X Y Z

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

## 6.2 Central slices ⓘ

### 6.2.1 Primary map

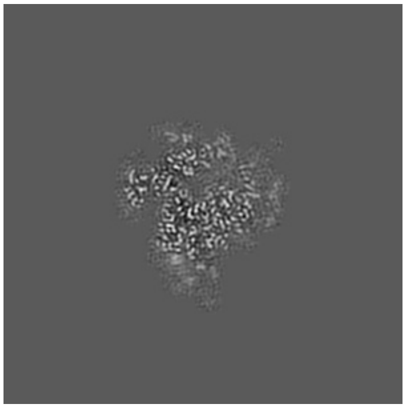


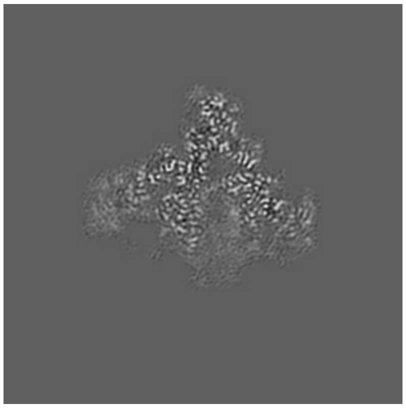
X Index: 154 Y Index: 154 Z Index: 154

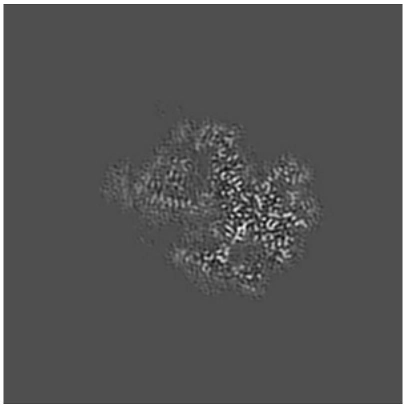
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices ⓘ

### 6.3.1 Primary map


X Index: 178


Y Index: 150


Z Index: 152

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

## 6.4 Orthogonal surface views ⓘ

### 6.4.1 Primary map


X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

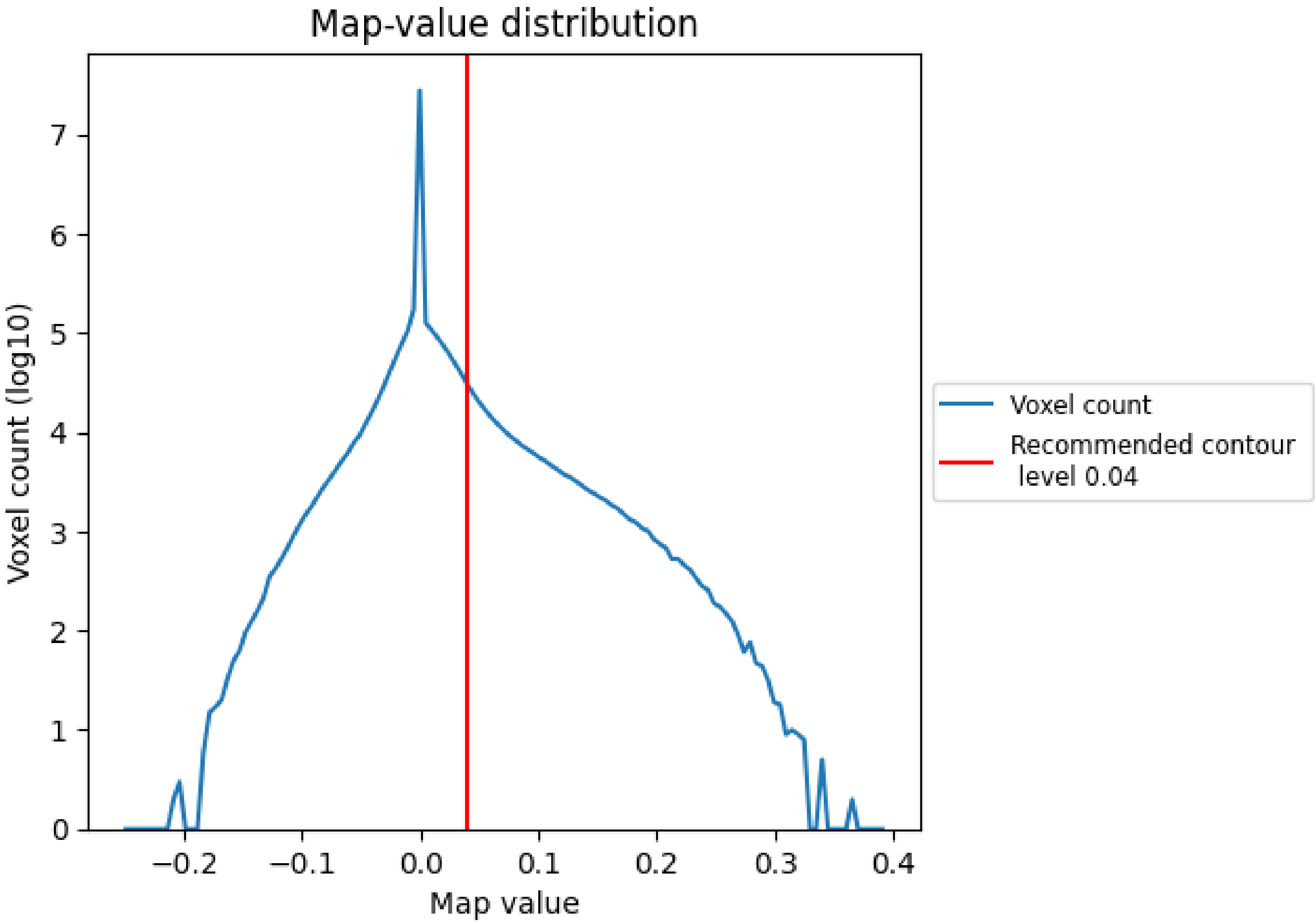
## 6.5 Mask visualisation ⓘ

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

# 7 Map analysis ⓘ

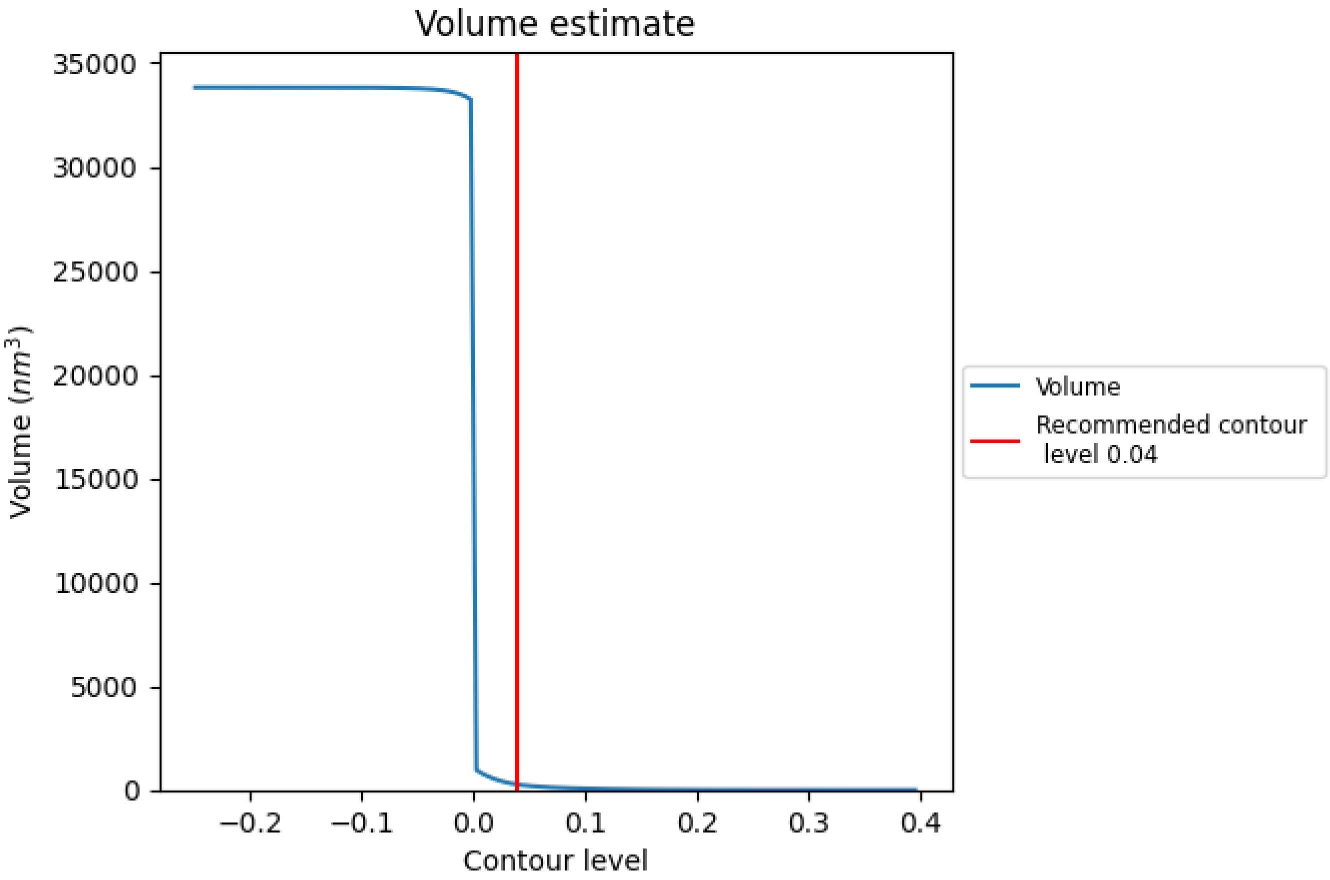
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution ⓘ



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

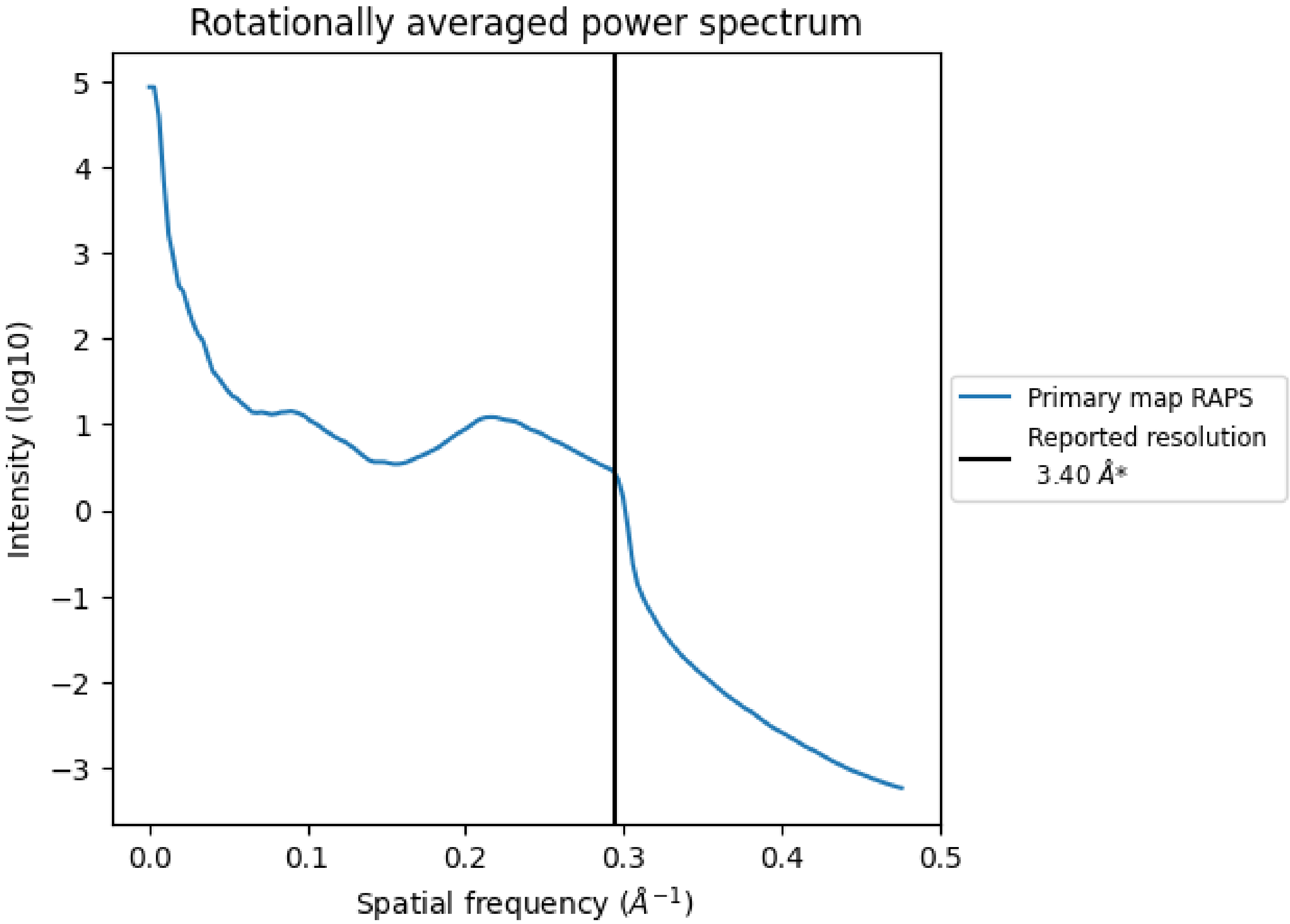
## 7.2 Volume estimate ⓘ



The volume at the recommended contour level is 261 nm$^3$; this corresponds to an approximate mass of 236 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 ⓘ

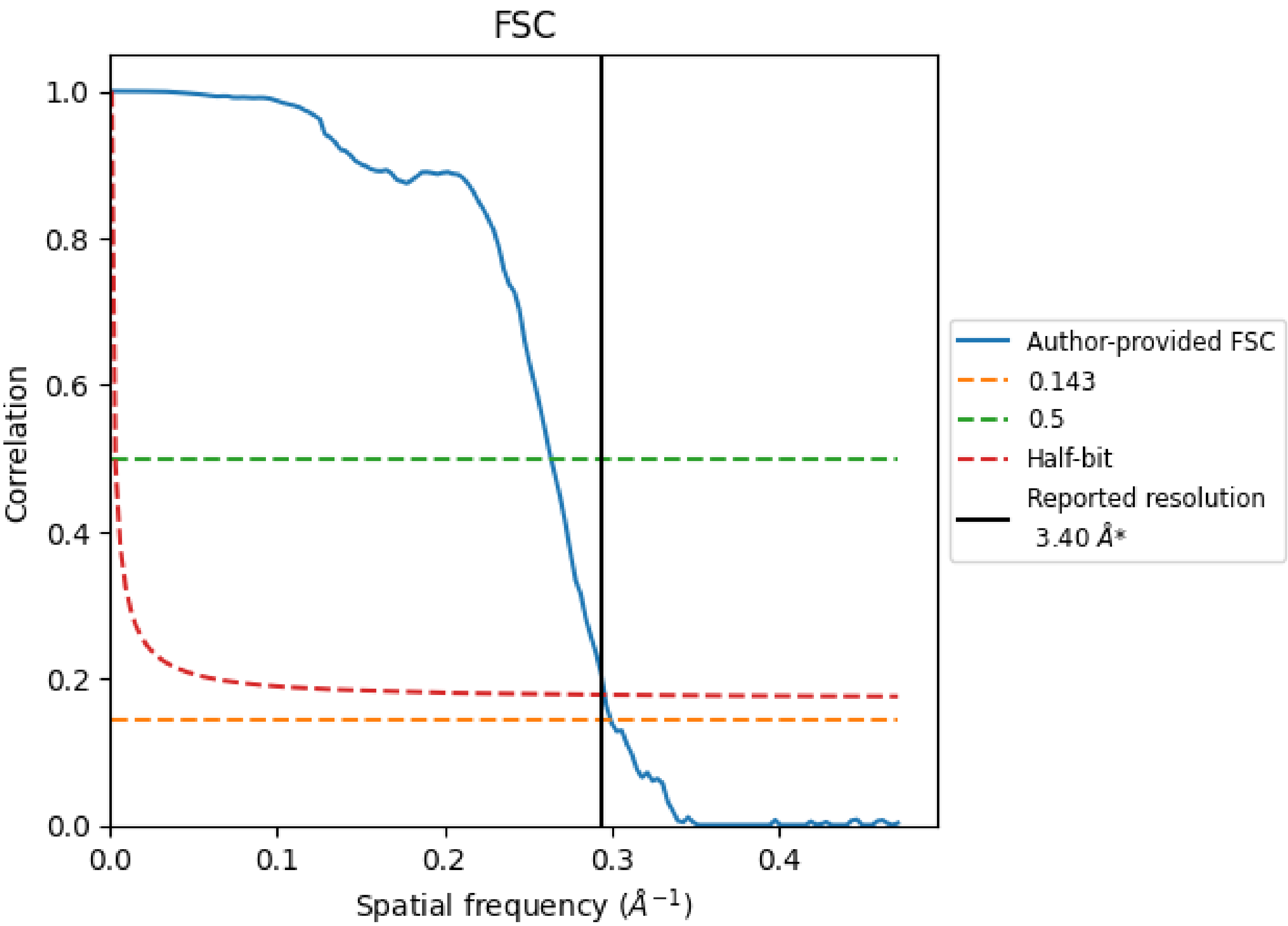


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

# 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 0.294 $Å^{-1}$

## 8.2 Resolution estimates (i)

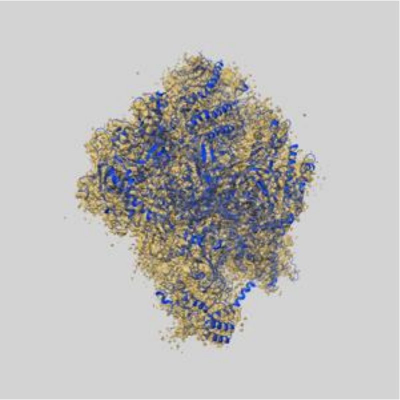
| **Resolution estimate (Å)** | **Estimation criterion (FSC cut-off)** | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.40 | - | - |
| Author-provided FSC curve | 3.34 | 3.79 | 3.38 |
| Unmasked-calculated* | - | - | - |

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

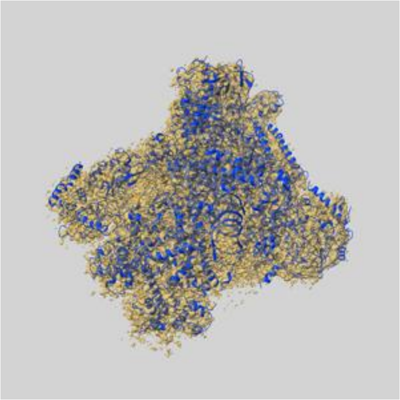
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3956 and PDB model 6EU1. Per-residue inclusion information can be found in section 3 on page 8.

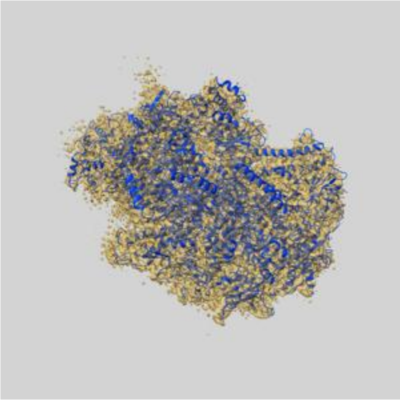
## 9.1 Map-model overlay



X



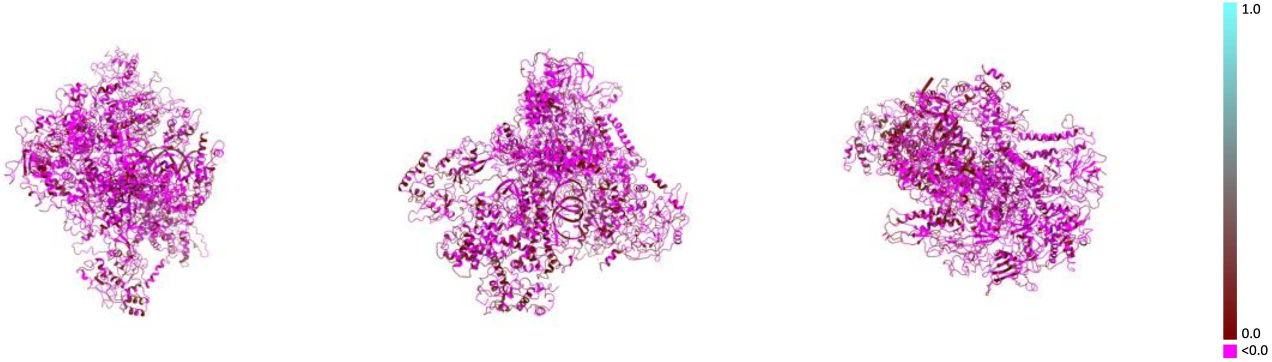
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

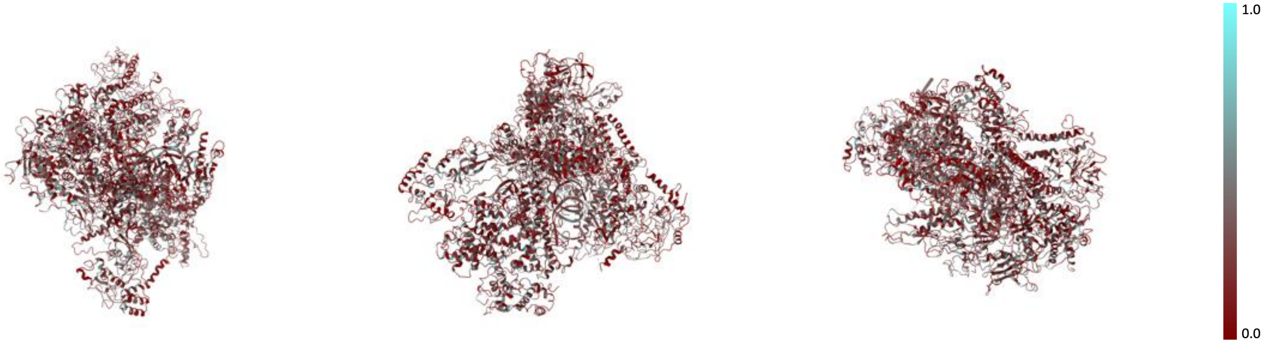
## 9.2 Q-score mapped to coordinate model ⓘ



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.

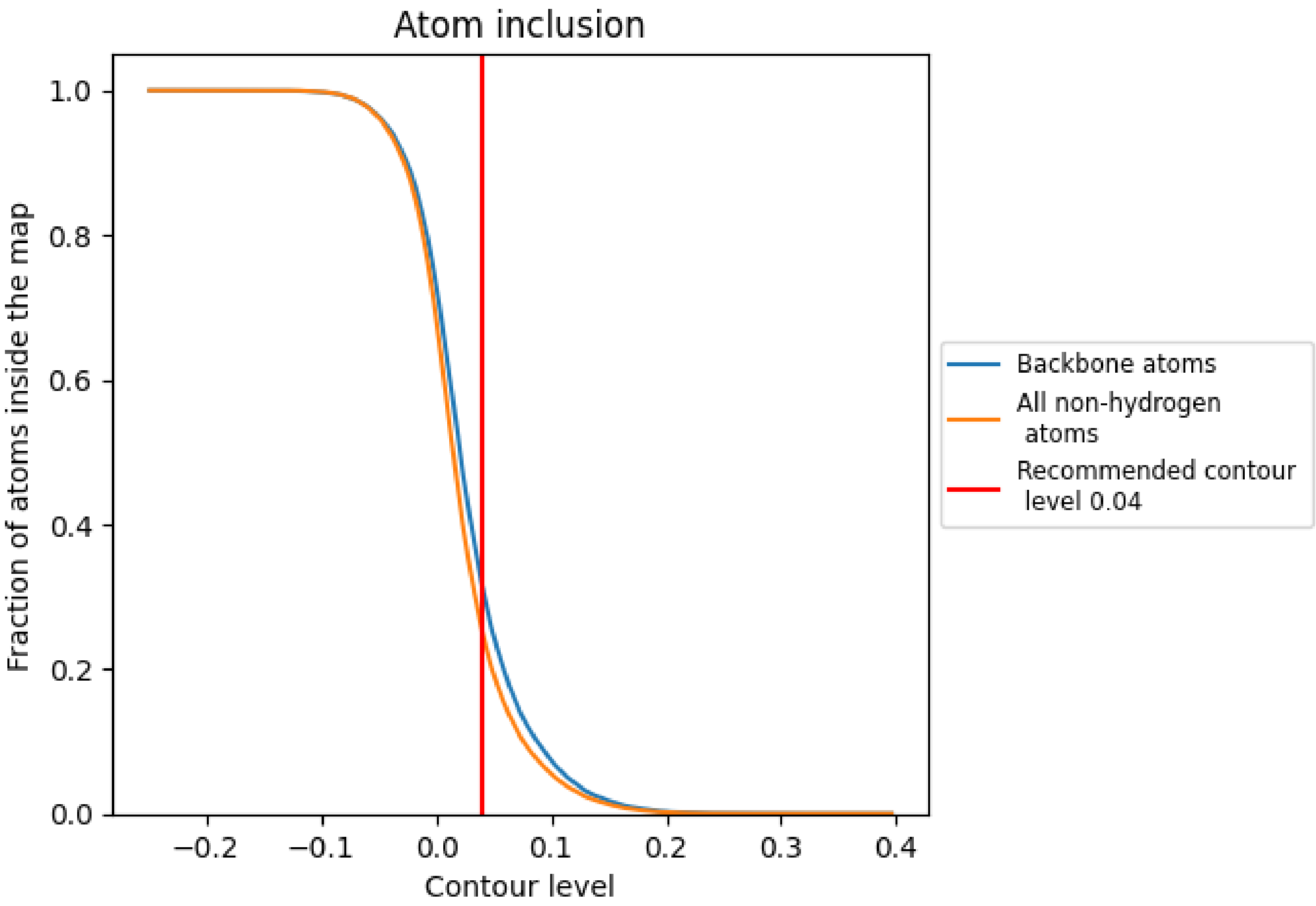
## 9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.04).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 32% of all backbone atoms, 25% 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 (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 🟥 0.2527 | 🟪 -0.0420 |
| A | 🟥 0.2485 | 🟪 -0.0590 |
| B | 🟥 0.2649 | 🟪 -0.0660 |
| C | 🟥 0.2611 | 🟪 -0.0710 |
| D | 🟥 0.2519 | 🟥 0.0570 |
| E | 🟥 0.2593 | 🟪 -0.0370 |
| F | 🟥 0.2588 | 🟪 -0.0480 |
| G | 🟥 0.2453 | 🟪 -0.0030 |
| H | 🟥 0.2074 | 🟪 -0.0950 |
| I | 🟥 0.1672 | 🟪 -0.0310 |
| J | 🟥 0.2809 | 🟪 -0.0860 |
| K | 🟥 0.2667 | 🟪 -0.0810 |
| L | 🟥 0.3121 | 🟪 -0.0520 |
| M | 🟥 0.2317 | 🟥 0.0280 |
| N | 🟥 0.1761 | 🟪 -0.0700 |
| O | 🟥 0.2594 | 🟪 -0.0070 |
| P | 🟥 0.2433 | 🟥 0.0380 |
| Q | 🟥 0.2043 | 🟥 0.0100 |
| R | 🟥 0.3083 | 🟥 0.0380 |
| S | 🟥 0.3266 | 🟥 0.0370 |