# wwPDB EM Validation Summary Report

Jan 1, 2025 – 07:45 PM EST

| | | |
|---|---|---|
| PDB ID | : | 8ZJL |
| EMDB ID | : | EMD-60149 |
| Title | : | Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 4) |
| Authors | : | Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Mishima-Tsumagari, C.; Yonemochi, M.; Inoue, M.; Nakagawa, R.; Kaushik, R.; Zhang, K.Y.J.; Shirouzu, M. |
| Deposited on | : | 2024-05-15 |
| Resolution | : | 4.31 Å(reported) |
| Based on initial model | : | 7DPA |

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

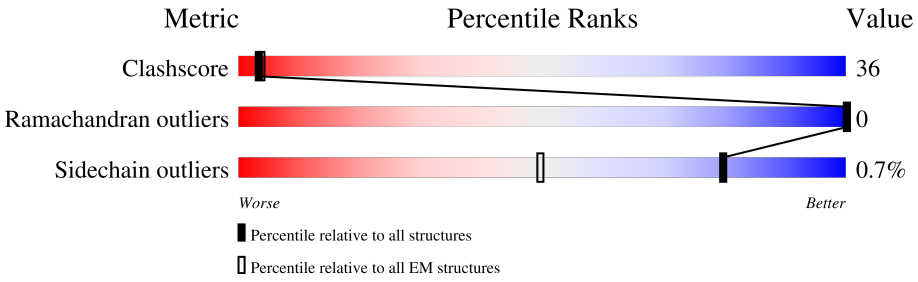
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.40 |

# 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 4.31 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 |

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 | 733 | 11% 16% 73% |
| 1 | D | 733 | 11% 15% 73% |
| 2 | B | 1648 | 7% 39% 60% |
| 2 | E | 1648 | 7% 38% 61% |
| 3 | C | 184 | 40% 56% |
| 3 | F | 184 | 38% 58% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 32858 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 Engulfment and cell motility protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1608 | 1018 | 277 | 303 | 10 | | |
| 1 | D | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1608 | 1018 | 277 | 303 | 10 | | |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -5 | GLY | - | expression tag | UNP Q92556 |
| A | -4 | GLY | - | expression tag | UNP Q92556 |
| A | -3 | SER | - | expression tag | UNP Q92556 |
| A | -2 | GLY | - | expression tag | UNP Q92556 |
| A | -1 | GLY | - | expression tag | UNP Q92556 |
| A | 0 | SER | - | expression tag | UNP Q92556 |
| D | -5 | GLY | - | expression tag | UNP Q92556 |
| D | -4 | GLY | - | expression tag | UNP Q92556 |
| D | -3 | SER | - | expression tag | UNP Q92556 |
| D | -2 | GLY | - | expression tag | UNP Q92556 |
| D | -1 | GLY | - | expression tag | UNP Q92556 |
| D | 0 | SER | - | expression tag | UNP Q92556 |

- Molecule 2 is a protein called Dedicator of cytokinesis protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 1642 | Total | C | N | O | S | 0 | 0 |
| | | | 13436 | 8618 | 2264 | 2484 | 70 | | |
| 2 | E | 1642 | Total | C | N | O | S | 0 | 0 |
| | | | 13436 | 8618 | 2264 | 2484 | 70 | | |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -5 | GLY | - | expression tag | UNP Q9H7D0 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -4 | GLY | - | expression tag | UNP Q9H7D0 |
| B | -3 | SER | - | expression tag | UNP Q9H7D0 |
| B | -2 | GLY | - | expression tag | UNP Q9H7D0 |
| B | -1 | GLY | - | expression tag | UNP Q9H7D0 |
| B | 0 | SER | - | expression tag | UNP Q9H7D0 |
| B | 1285 | ARG | LYS | variant | UNP Q9H7D0 |
| E | -5 | GLY | - | expression tag | UNP Q9H7D0 |
| E | -4 | GLY | - | expression tag | UNP Q9H7D0 |
| E | -3 | SER | - | expression tag | UNP Q9H7D0 |
| E | -2 | GLY | - | expression tag | UNP Q9H7D0 |
| E | -1 | GLY | - | expression tag | UNP Q9H7D0 |
| E | 0 | SER | - | expression tag | UNP Q9H7D0 |
| E | 1285 | ARG | LYS | variant | UNP Q9H7D0 |

- Molecule 3 is a protein called Ras-related C3 botulinum toxin substrate 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1385 | 890 | 228 | 259 | 8 | | |
| 3 | F | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1385 | 890 | 228 | 259 | 8 | | |

There are 16 discrepancies between the modelled and reference sequences:

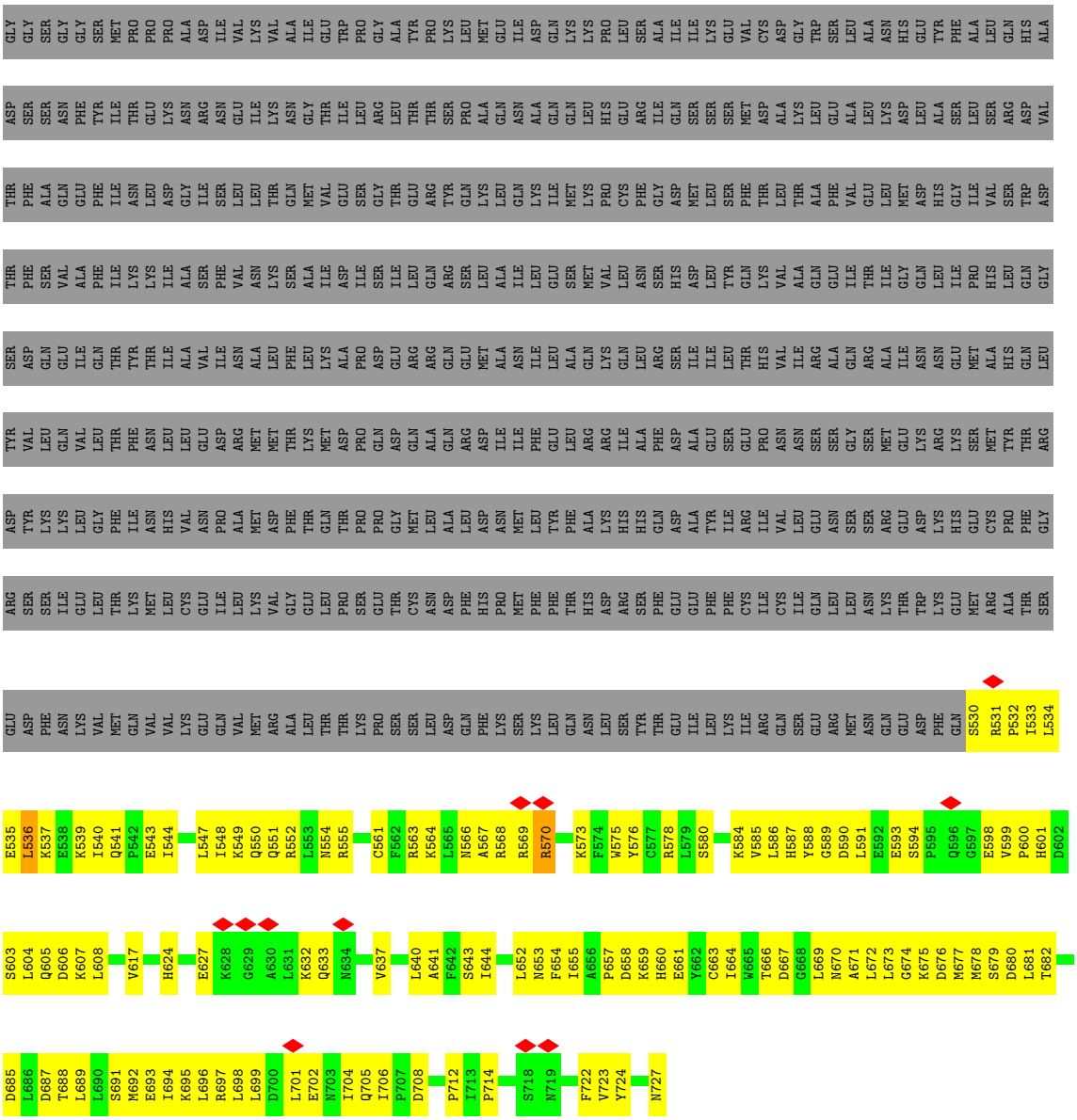
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | -6 | GLY | - | expression tag | UNP P63000 |
| C | -5 | SER | - | expression tag | UNP P63000 |
| C | -4 | SER | - | expression tag | UNP P63000 |
| C | -3 | GLY | - | expression tag | UNP P63000 |
| C | -2 | SER | - | expression tag | UNP P63000 |
| C | -1 | SER | - | expression tag | UNP P63000 |
| C | 0 | GLY | - | expression tag | UNP P63000 |
| C | 15 | ALA | GLY | engineered mutation | UNP P63000 |
| F | -6 | GLY | - | expression tag | UNP P63000 |
| F | -5 | SER | - | expression tag | UNP P63000 |
| F | -4 | SER | - | expression tag | UNP P63000 |
| F | -3 | GLY | - | expression tag | UNP P63000 |
| F | -2 | SER | - | expression tag | UNP P63000 |
| F | -1 | SER | - | expression tag | UNP P63000 |
| F | 0 | GLY | - | expression tag | UNP P63000 |
| F | 15 | ALA | GLY | engineered mutation | UNP P63000 |

# 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.

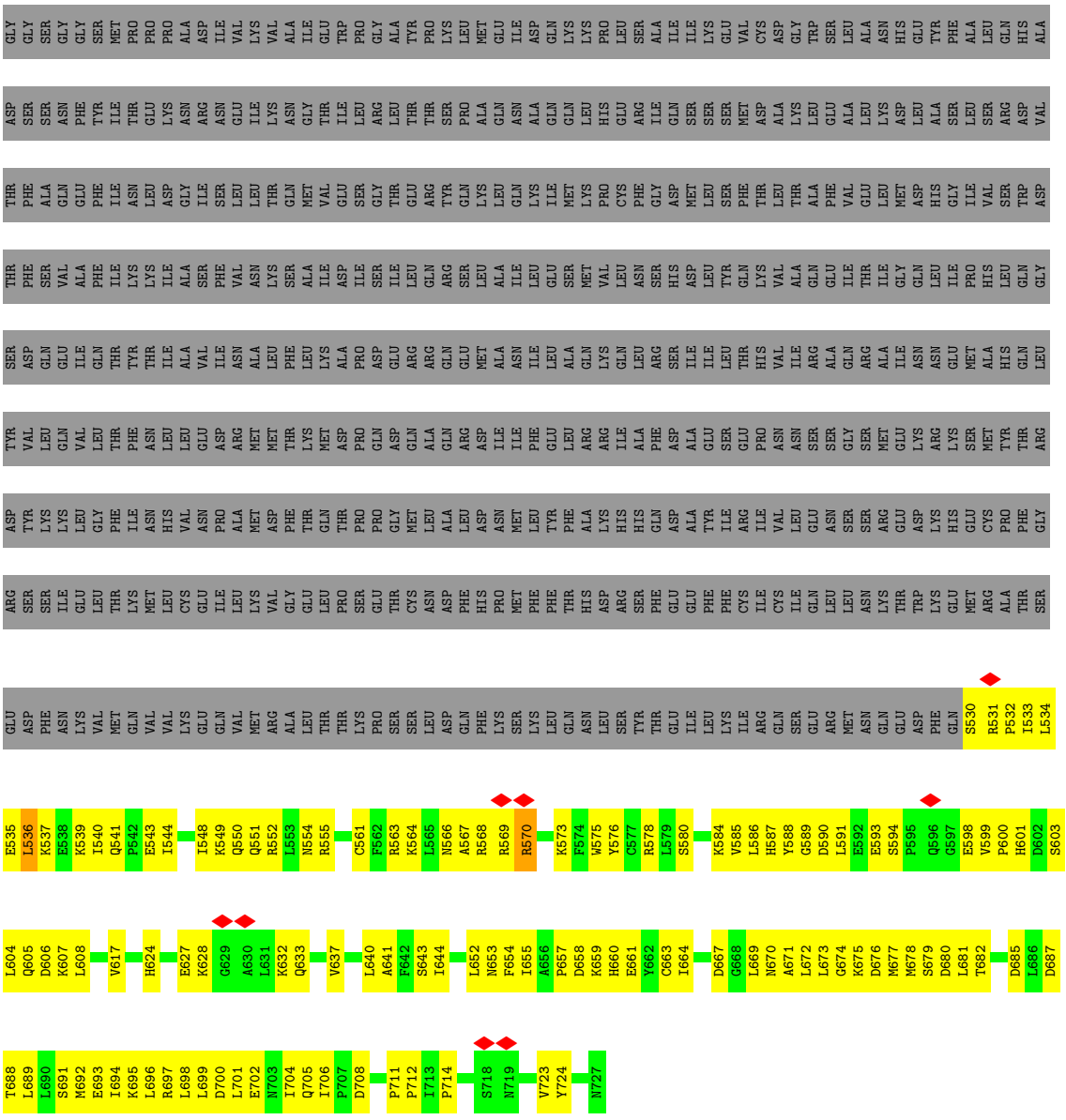
- Molecule 1: Engulfment and cell motility protein 1

Chain A:



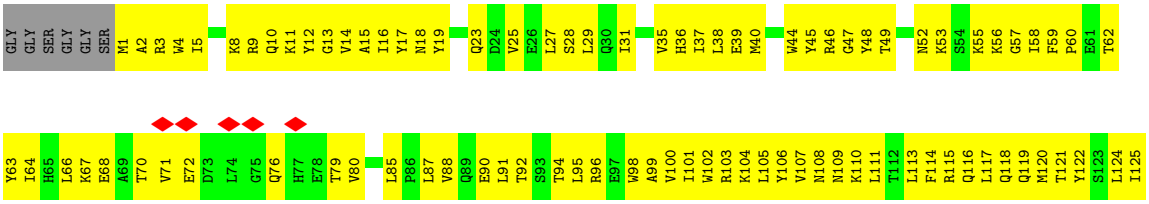
• Molecule 1: Engulfment and cell motility protein 1

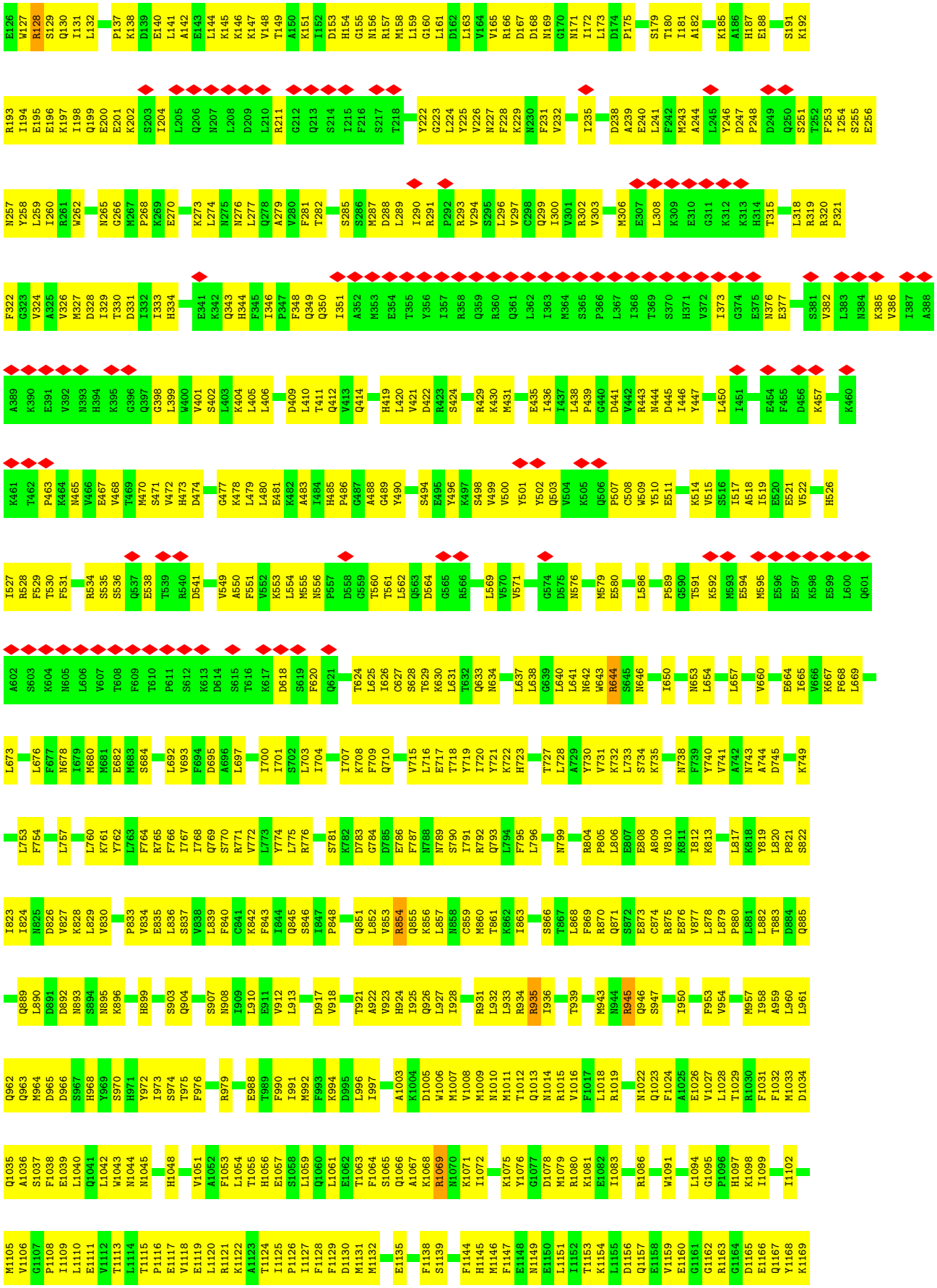
Chain D:

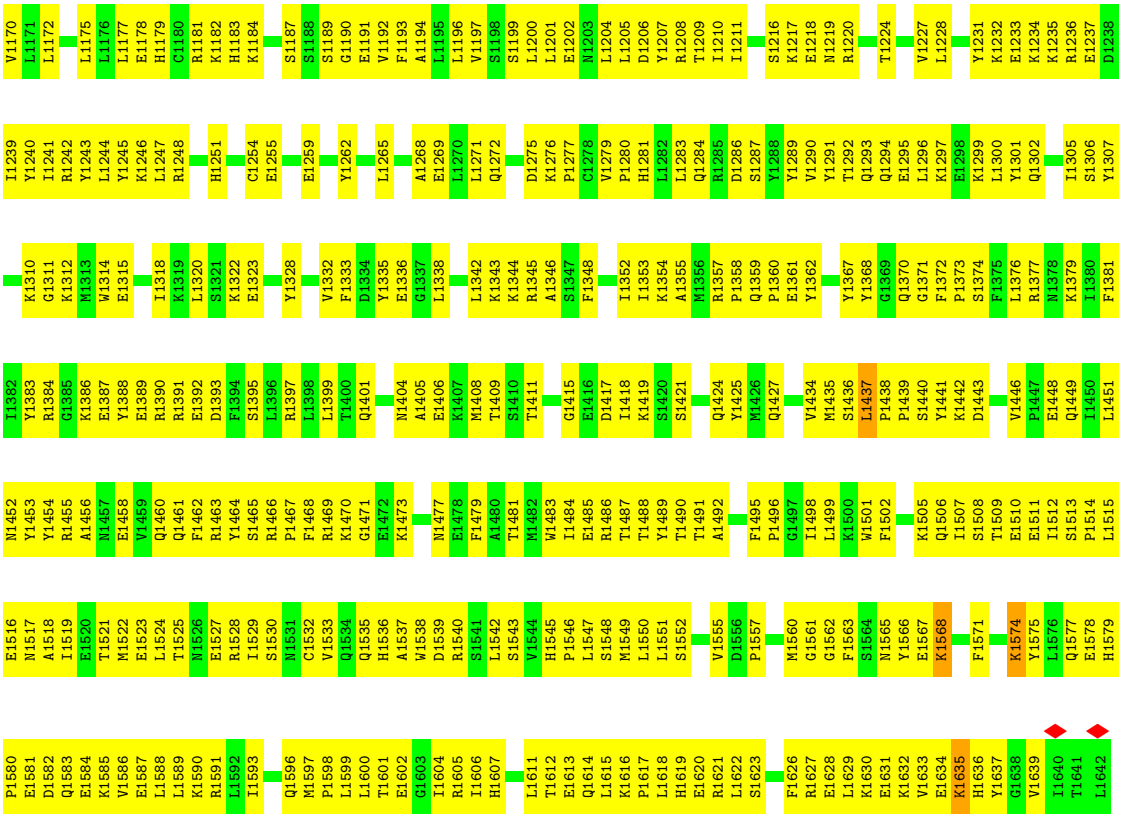



• Molecule 2: Dedicator of cytokinesis protein 5

Chain B:

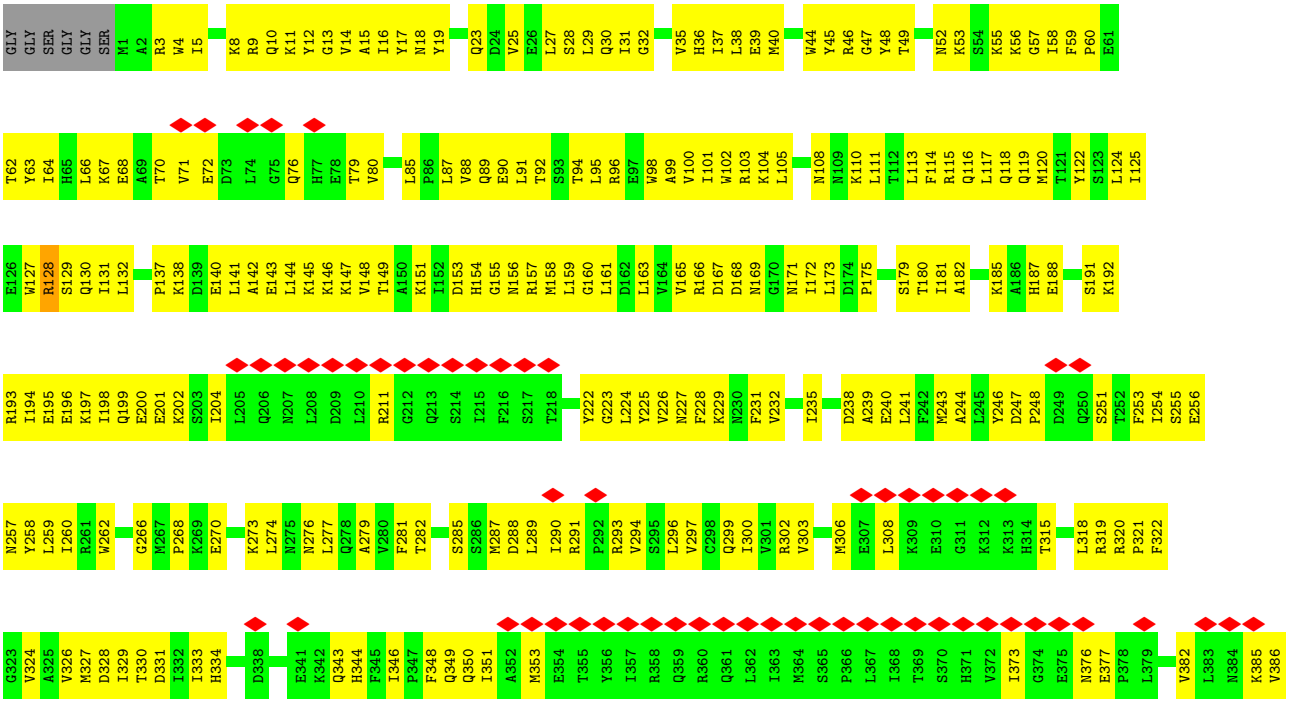


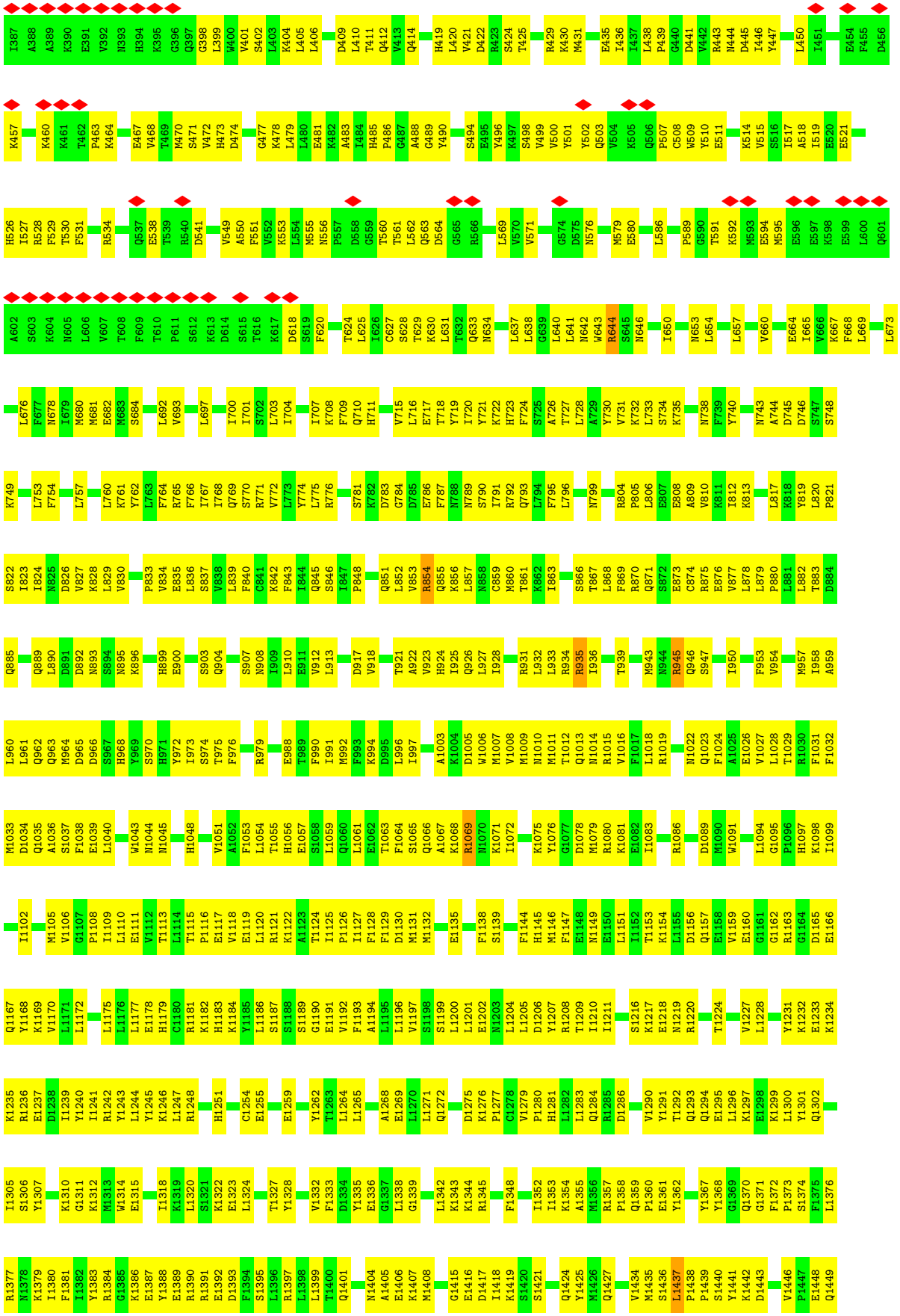


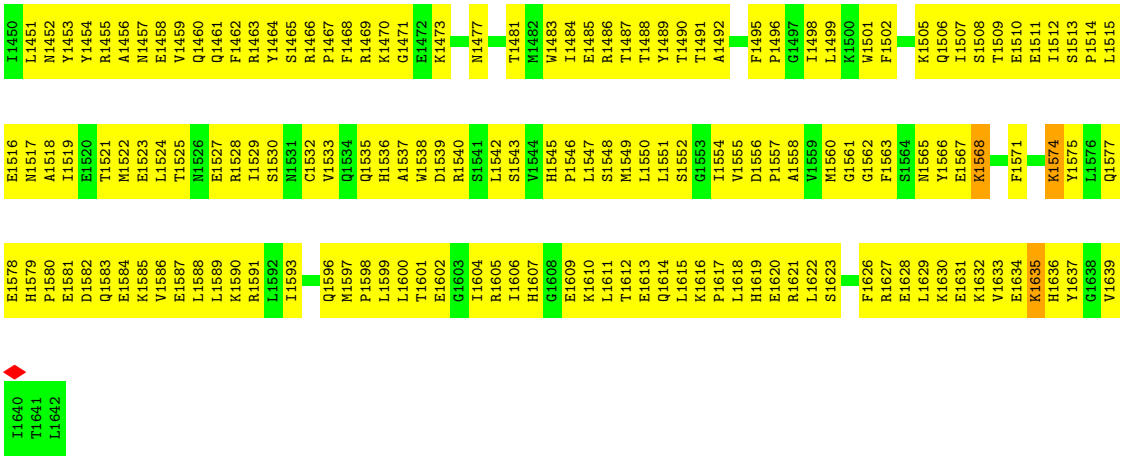


• Molecule 2: Dedicator of cytokinesis protein 5

Chain E:

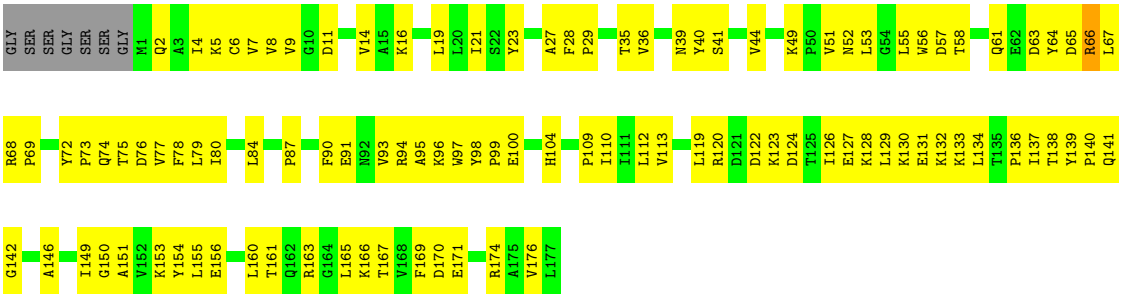



I387 A388 A389 K390 E391 V392 N393 H394 K395 G396 Q397 G398 L399 W400 V401 S402 L403 K404 L405 L406 D409 L410 T411 Q412 V413 Q414 H419 L420 V421 D422 R423 S424 T425 R429 K430 M431 E435 I436 I437 L438 P439 G440 D441 V442 R443 N444 D445 I446 Y447 L450 I451 E454 F455 D456
K457 K460 K461 T462 P463 K464 E467 V468 T469 M470 S471 V472 H473 D474 G477 K478 L479 L480 E481 K482 A483 T484 H485 P486 G487 A488 G489 Y490 S494 E495 Y496 K497 S498 V499 V500 Y501 Y502 Q503 V504 K505 Q506 P507 C508 W509 Y510 E511 K514 V515 S516 I517 A518 I519 E520 E521
H526 I527 R528 F529 T530 F531 R534 Q537 E538 T539 R540 D541 V549 A550 F551 V552 K553 L554 M555 N556 P557 D558 G559 T560 T561 L562 Q563 D564 G565 R566 L569 V570 V571 G574 D575 N576 M579 E580 L586 P589 G590 T591 K592 M593 E594 M595 E596 E597 K598 E599 L600 Q601
A602 S603 K604 N605 L606 V607 T608 F609 T610 P611 S612 K613 D614 S615 T616 K617 D618 S619 F620 T624 L625 I626 C627 S628 T629 K630 L631 T632 Q633 N634 L637 L638 G639 L640 L641 N642 W643 R644 S645 N646 I650 N653 L654 L657 V660 E664 I665 V666 K667 F668 L669 L673
L676 F677 N678 I679 M680 M681 E682 M683 S684 L692 V693 L697 I700 I701 S702 L703 I704 I707 K708 F709 Q710 H711 V715 L716 E717 T718 Y719 I720 Y721 K722 H723 F724 S725 A726 T727 L728 A729 Y730 V731 K732 L733 S734 K735 N738 F739 Y740 N743 A744 D745 D746 S747 S748
K749 L753 F754 L757 L760 K761 Y762 L763 F764 R765 F766 I767 I768 Q769 S770 R771 V772 L773 Y774 L775 R776 S781 K782 D783 G784 D785 E786 F787 N788 N789 S790 I791 R792 Q793 L794 F795 L796 N799 R804 P805 L806 E807 E808 A809 V810 K811 I812 K813 L817 K818 Y819 L820 P821
S822 I823 I824 N825 D826 V827 K828 L829 V830 P833 V834 E835 L836 S837 V838 L839 F840 C841 K842 F843 I844 Q845 S846 I847 P848 Q851 L852 V853 R854 Q855 K856 L857 N858 C859 M860 T861 K862 I863 S866 T867 L868 F869 R870 Q871 S872 E873 C874 R875 E876 V877 L878 L879 P880 L881 L882 T883 D884
Q886 Q889 L890 D891 D892 N893 S894 N895 K896 H899 E900 S903 Q904 S907 N908 I909 L910 E911 V912 L913 D917 V918 T921 A922 V923 H924 I925 Q926 L927 I928 R931 L932 L933 R934 R935 I936 T939 M943 N944 R945 Q946 S947 I950 F953 V964 M957 I958 A959
L960 L961 Q962 Q963 M964 D965 D966 S967 H968 Y969 S970 H971 Y972 I973 S974 T975 F976 R979 E988 T989 F990 I991 M992 F993 K994 D995 L996 I997 A1003 K1004 D1005 W1006 M1007 V1008 M1009 N1010 M1011 T1012 Q1013 N1014 R1015 V1016 F1017 L1018 R1019 N1022 Q1023 F1024 A1025 E1026 V1027 L1028 T1029 R1030 F1031 F1032
M1033 D1034 Q1035 A1036 S1037 F1038 E1039 L1040 W1043 N1044 N1045 H1048 V1051 A1052 F1053 L1054 T1055 H1056 E1057 S1058 L1059 Q1060 L1061 E1062 T1063 F1064 S1065 Q1066 A1067 K1068 R1069 N1070 K1071 I1072 K1075 Y1076 G1077 D1078 M1079 R1080 K1081 E1082 I1083 R1086 D1089 M1090 W1091 L1094 G1095 P1096 H1097 K1098 I1099
I1102 M1105 V1106 G1107 P1108 I1109 L1110 E1111 V1112 T1113 L1114 T1115 P1116 E1117 V1118 E1119 L1120 R1121 K1122 A1123 T1124 I1125 P1126 I1127 F1128 F1129 D1130 M1131 M1132 E1135 F1138 S1139 F1144 H1145 M1146 F1147 E1148 N1149 E1150 L1151 I1152 T1153 K1154 L1155 D1156 Q1157 E1158 V1159 E1160 G1161 G1162 R1163 G1164 D1165 E1166
Q1167 Y1168 K1169 V1170 L1171 L1172 L1175 L1176 L1177 E1178 H1179 C1180 R1181 K1182 H1183 K1184 Y1185 L1186 S1187 S1188 S1189 G1190 E1191 V1192 F1193 A1194 L1195 L1196 S1199 L1200 L1201 E1202 N1203 L1204 L1205 D1206 Y1207 R1208 T1209 I1210 I1211 S1216 K1217 E1218 N1219 R1220 T1224 V1227 L1228 Y1231 K1232 E1233 K1234
K1235 R1236 E1237 D1238 I1239 Y1240 I1241 R1242 Y1243 L1244 Y1245 K1246 L1247 R1248 H1251 C1254 E1255 E1259 Y1262 T1263 L1264 L1265 A1268 E1269 L1270 Q1271 Q1272 D1275 K1276 P1277 C1278 Y1279 P1280 H1281 L1282 L1283 Q1284 R1285 D1286 V1290 Y1291 T1292 Q1293 Q1294 E1295 L1296 K1297 E1298 K1299 L1300 Y1301 Q1302
I1305 S1306 Y1307 K1310 G1311 K1312 M1313 W1314 E1315 I1318 K1319 L1320 S1321 K1322 E1323 L1324 T1327 Y1328 V1332 F1333 D1334 Y1335 E1336 G1337 L1338 G1339 L1342 K1343 K1344 R1345 F1348 I1352 I1353 K1354 A1355 M1356 R1357 P1358 D1359 P1360 E1361 Y1362 Y1367 Y1368 G1369 Q1370 G1371 F1372 P1373 S1374 F1375 L1376
R1377 N1378 K1379 I1380 F1381 I1382 Y1383 R1384 G1385 K1386 E1387 Y1388 E1389 R1390 R1391 E1392 D1393 F1394 S1395 L1396 R1397 L1398 L1399 T1400 Q1401 N1404 A1405 E1406 K1407 M1408 G1415 E1416 D1417 I1418 K1419 S1420 S1421 Q1424 Y1425 M1426 Q1427 V1434 M1435 S1436 L1437 P1438 P1439 S1440 Y1441 K1442 D1443 V1446 P1447 E1448 Q1449



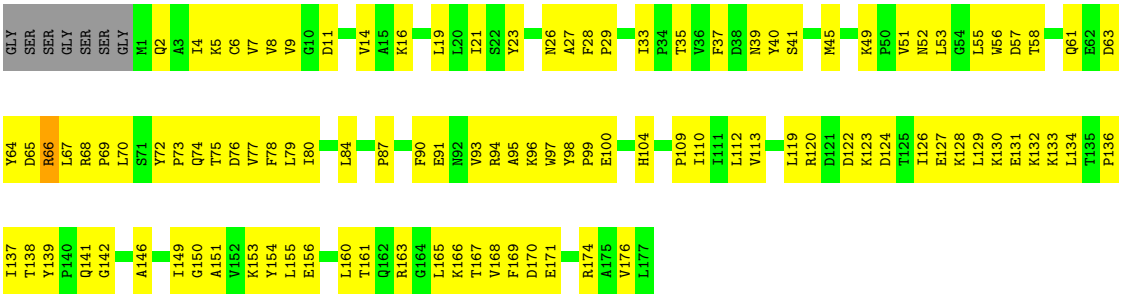

• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain C:




• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain F:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 123816 | 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 ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | 64000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.058 | Depositor |
| Minimum map value | -0.017 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.01 | Depositor |
| Map size (Å) | 452.2, 452.2, 452.2 | wwPDB |
| Map dimensions | 340, 340, 340 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.33, 1.33, 1.33 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.29 | 0/1641 | 0.52 | 1/2218 (0.0%) |
| 1 | D | 0.29 | 0/1641 | 0.52 | 1/2218 (0.0%) |
| 2 | B | 0.34 | 0/13722 | 0.51 | 1/18514 (0.0%) |
| 2 | E | 0.33 | 0/13722 | 0.51 | 1/18514 (0.0%) |
| 3 | C | 0.33 | 0/1415 | 0.49 | 0/1924 |
| 3 | F | 0.33 | 0/1415 | 0.49 | 0/1924 |
| All | All | 0.33 | 0/33556 | 0.51 | 4/45312 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 536 | LEU | CB-CG-CD2 | -5.42 | 101.79 | 111.00 |
| 1 | A | 536 | LEU | CB-CG-CD2 | -5.40 | 101.81 | 111.00 |
| 2 | E | 1437 | LEU | CA-CB-CG | 5.25 | 127.36 | 115.30 |
| 2 | B | 1437 | LEU | CA-CB-CG | 5.24 | 127.35 | 115.30 |

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 | A | 1608 | 0 | 1617 | 127 | 0 |
| 1 | D | 1608 | 0 | 1617 | 123 | 0 |
| 2 | B | 13436 | 0 | 13516 | 987 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | E | 13436 | 0 | 13516 | 1003 | 0 |
| 3 | C | 1385 | 0 | 1407 | 106 | 0 |
| 3 | F | 1385 | 0 | 1407 | 111 | 0 |
| All | All | 32858 | 0 | 33080 | 2381 | 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 36.

The worst 5 of 2381 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) |
|---|---|---|---|
| 2:E:1217:LYS:HA | 2:E:1220:ARG:HE | 1.30 | 0.96 |
| 2:B:1217:LYS:HA | 2:B:1220:ARG:HE | 1.30 | 0.95 |
| 2:B:46:ARG:HB3 | 2:B:58:ILE:HG13 | 1.54 | 0.89 |
| 2:E:4:TRP:HB3 | 2:E:39:GLU:HB3 | 1.55 | 0.88 |
| 3:F:9:VAL:HG22 | 3:F:78:PHE:HZ | 1.39 | 0.88 |

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 | A | 196/733 (27%) | 174 (89%) | 22 (11%) | 0 | 100 | 100 |
| 1 | D | 196/733 (27%) | 174 (89%) | 22 (11%) | 0 | 100 | 100 |
| 2 | B | 1640/1648 (100%) | 1493 (91%) | 147 (9%) | 0 | 100 | 100 |
| 2 | E | 1640/1648 (100%) | 1493 (91%) | 147 (9%) | 0 | 100 | 100 |
| 3 | C | 175/184 (95%) | 164 (94%) | 11 (6%) | 0 | 100 | 100 |
| 3 | F | 175/184 (95%) | 164 (94%) | 11 (6%) | 0 | 100 | 100 |
| All | All | 4022/5130 (78%) | 3662 (91%) | 360 (9%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 183/664 (28%) | 181 (99%) | 2 (1%) | 70 | 80 |
| 1 | D | 183/664 (28%) | 181 (99%) | 2 (1%) | 70 | 80 |
| 2 | B | 1495/1497 (100%) | 1486 (99%) | 9 (1%) | 84 | 88 |
| 2 | E | 1495/1497 (100%) | 1486 (99%) | 9 (1%) | 84 | 88 |
| 3 | C | 153/157 (98%) | 151 (99%) | 2 (1%) | 65 | 77 |
| 3 | F | 153/157 (98%) | 151 (99%) | 2 (1%) | 65 | 77 |
| All | All | 3662/4636 (79%) | 3636 (99%) | 26 (1%) | 80 | 87 |

5 of 26 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 570 | ARG |
| 2 | E | 854 | ARG |
| 3 | F | 66 | ARG |
| 2 | E | 644 | ARG |
| 2 | E | 935 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 1359 | GLN |
| 2 | E | 1401 | GLN |
| 3 | F | 2 | GLN |
| 2 | B | 1401 | GLN |
| 2 | B | 1359 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 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.

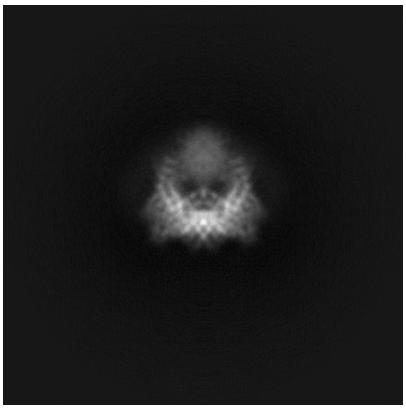
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60149. These allow visual inspection of the internal detail of the map and identification of artifacts.

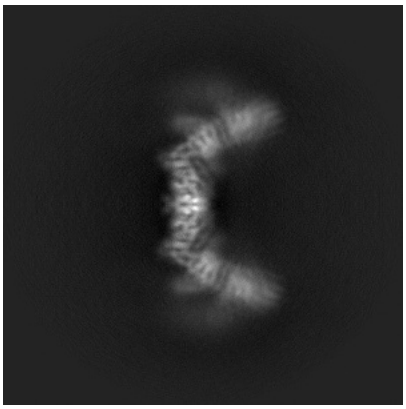
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

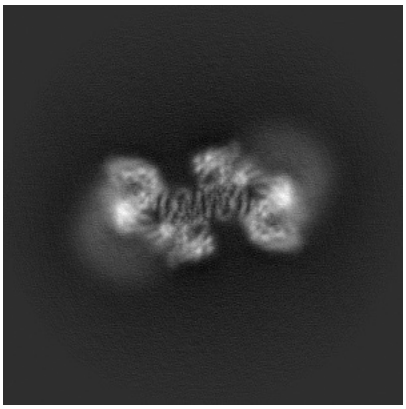
### 6.1.1 Primary map



X

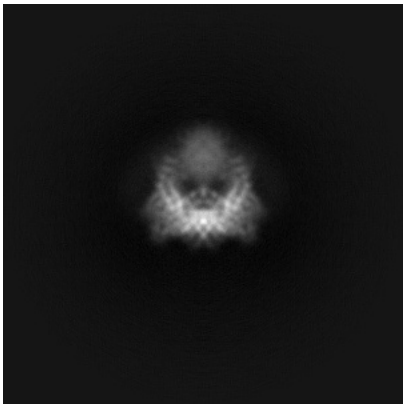


Y

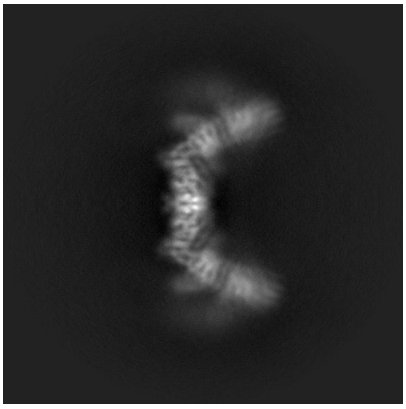


Z

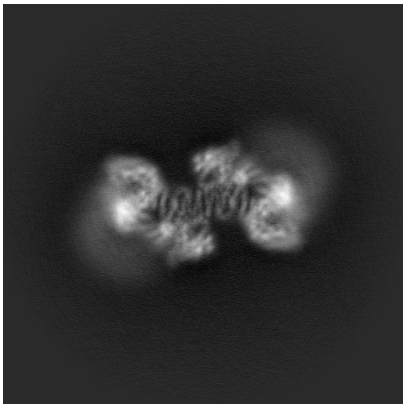
### 6.1.2 Raw map



X



Y

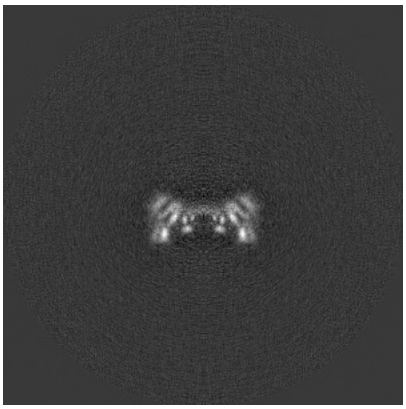


Z

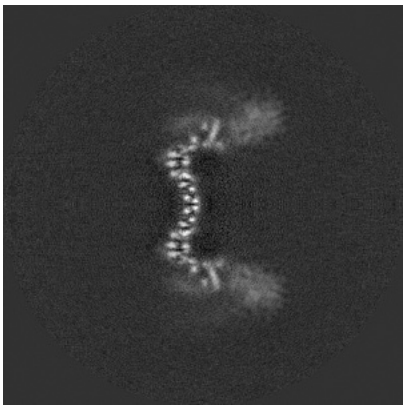
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

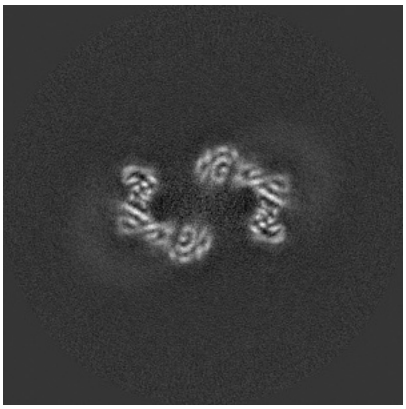
### 6.2.1 Primary map



X Index: 170

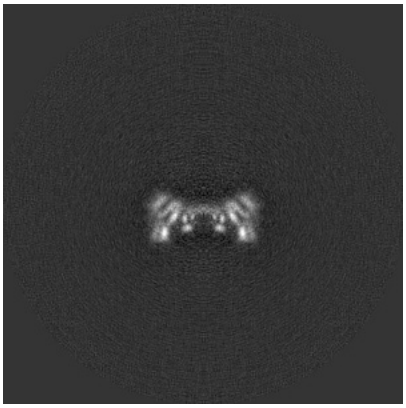


Y Index: 170

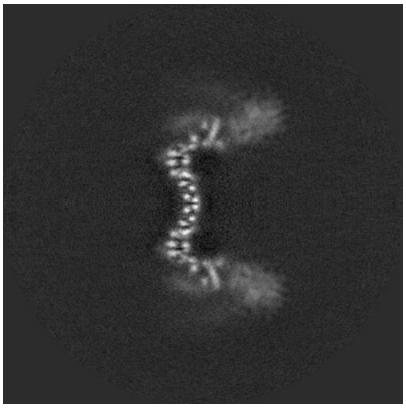


Z Index: 170

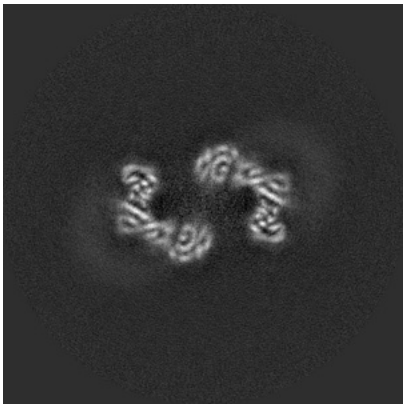
### 6.2.2 Raw map



X Index: 170



Y Index: 170

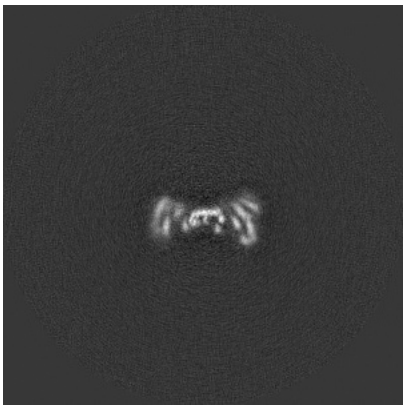


Z Index: 170

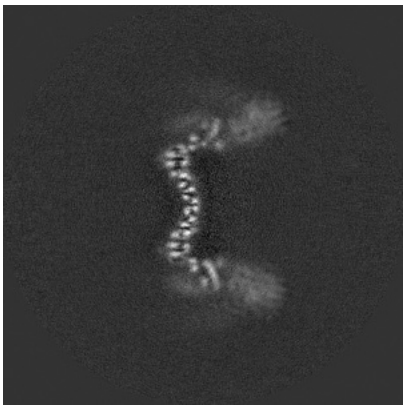
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

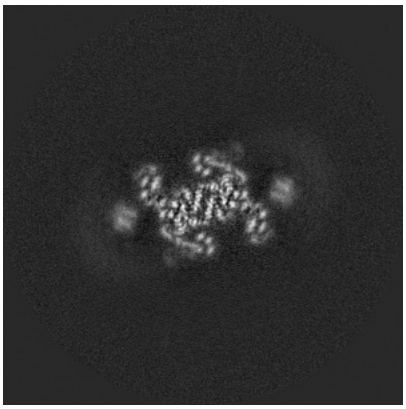
### 6.3.1 Primary map



X Index: 173

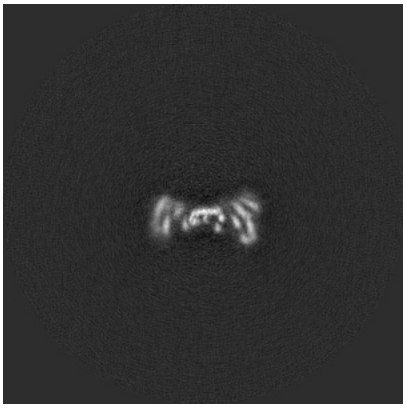


Y Index: 169

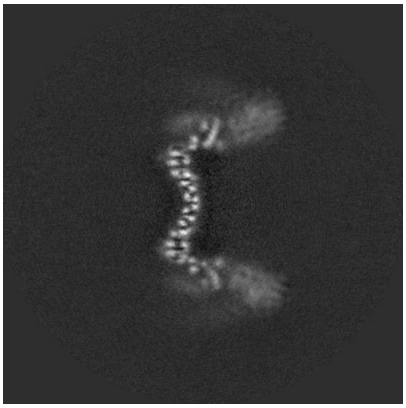


Z Index: 155

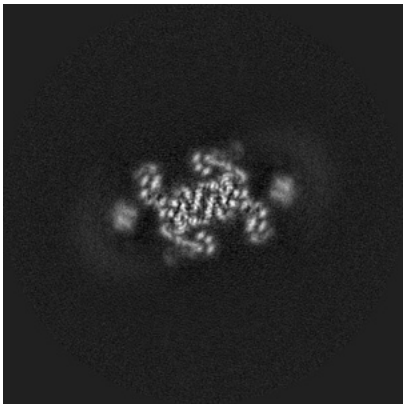
### 6.3.2 Raw map



X Index: 173



Y Index: 171

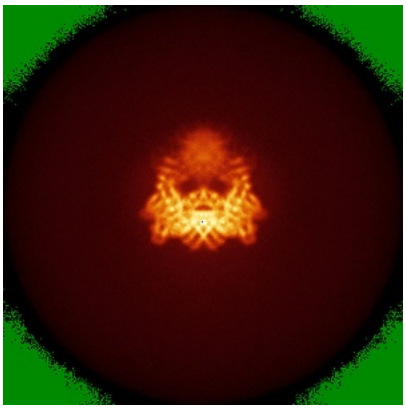


Z Index: 155

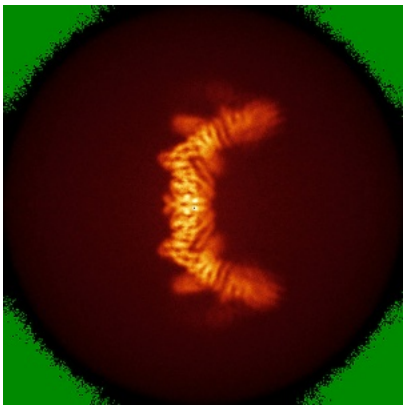
The images above show the largest variance slices of the map in three orthogonal directions.

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

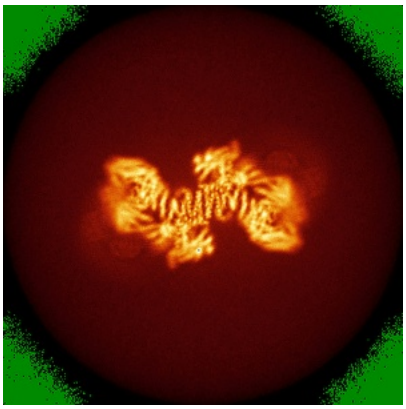
### 6.4.1 Primary map



X



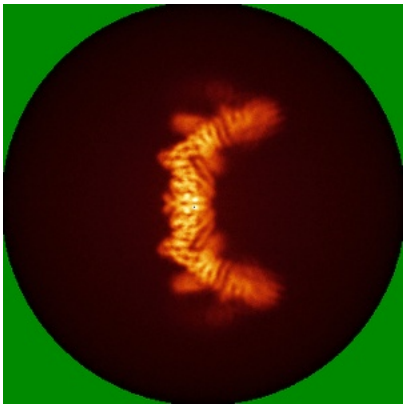
Y



Z

### 6.4.2 Raw map

X



Y

Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

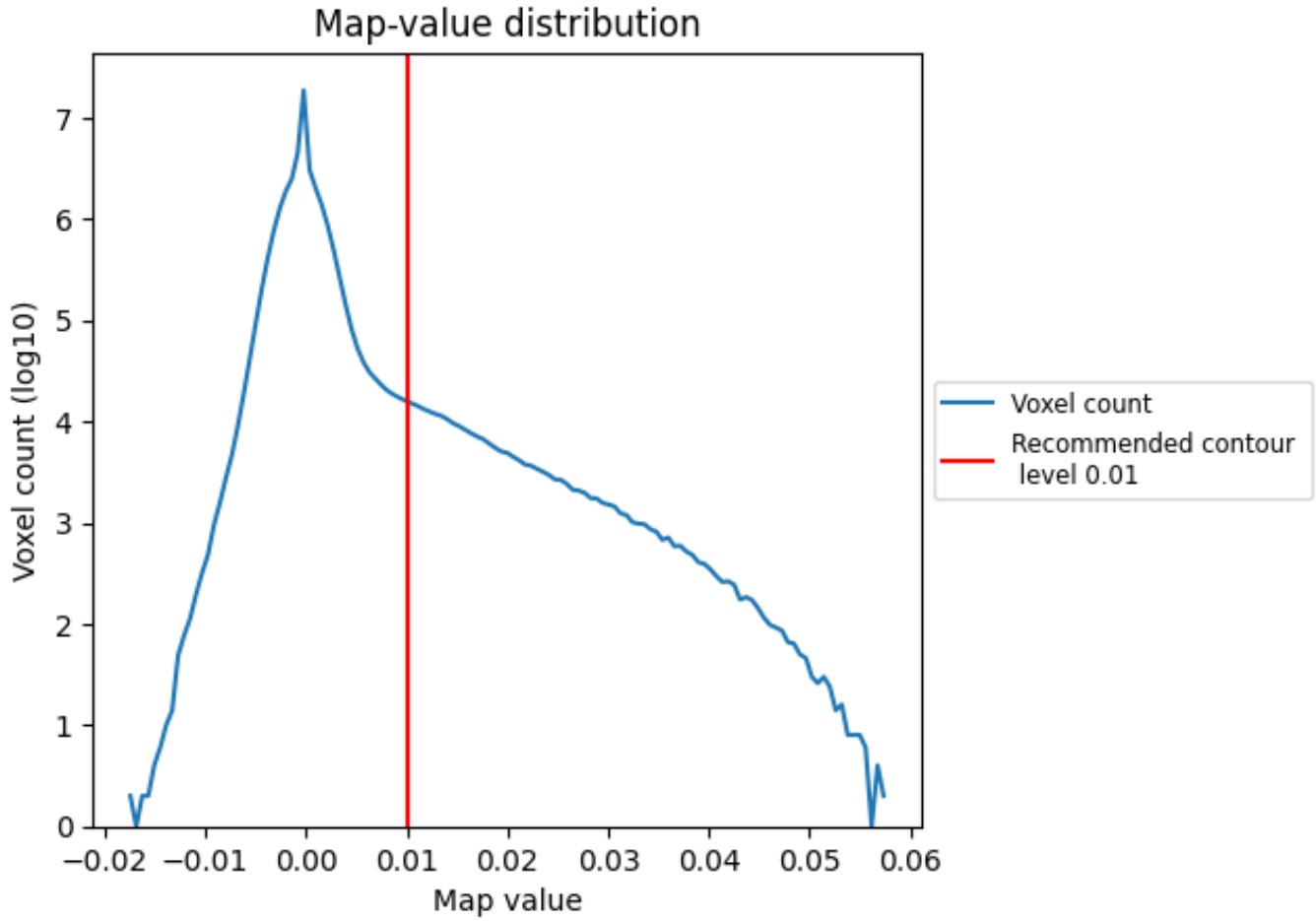
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

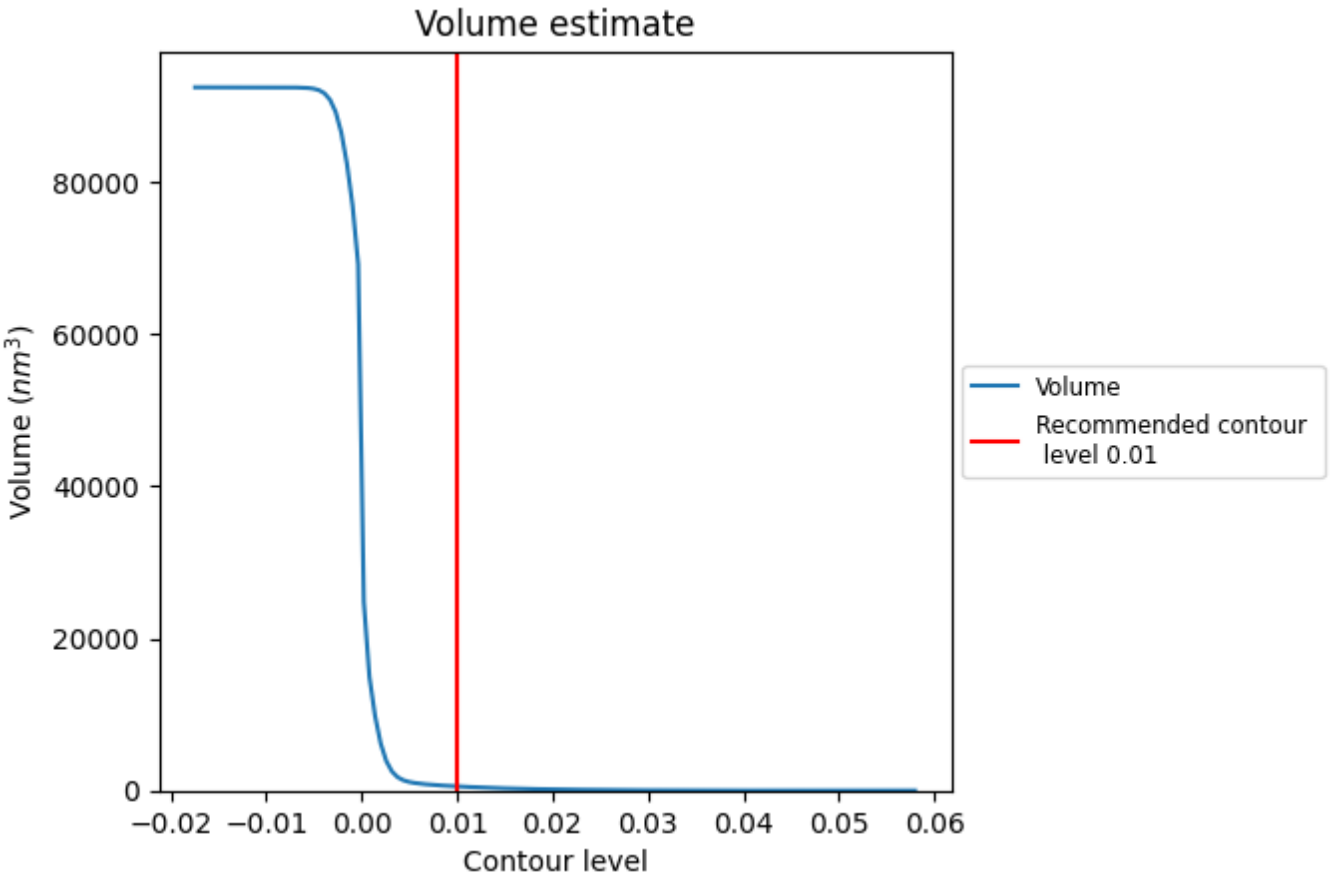
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

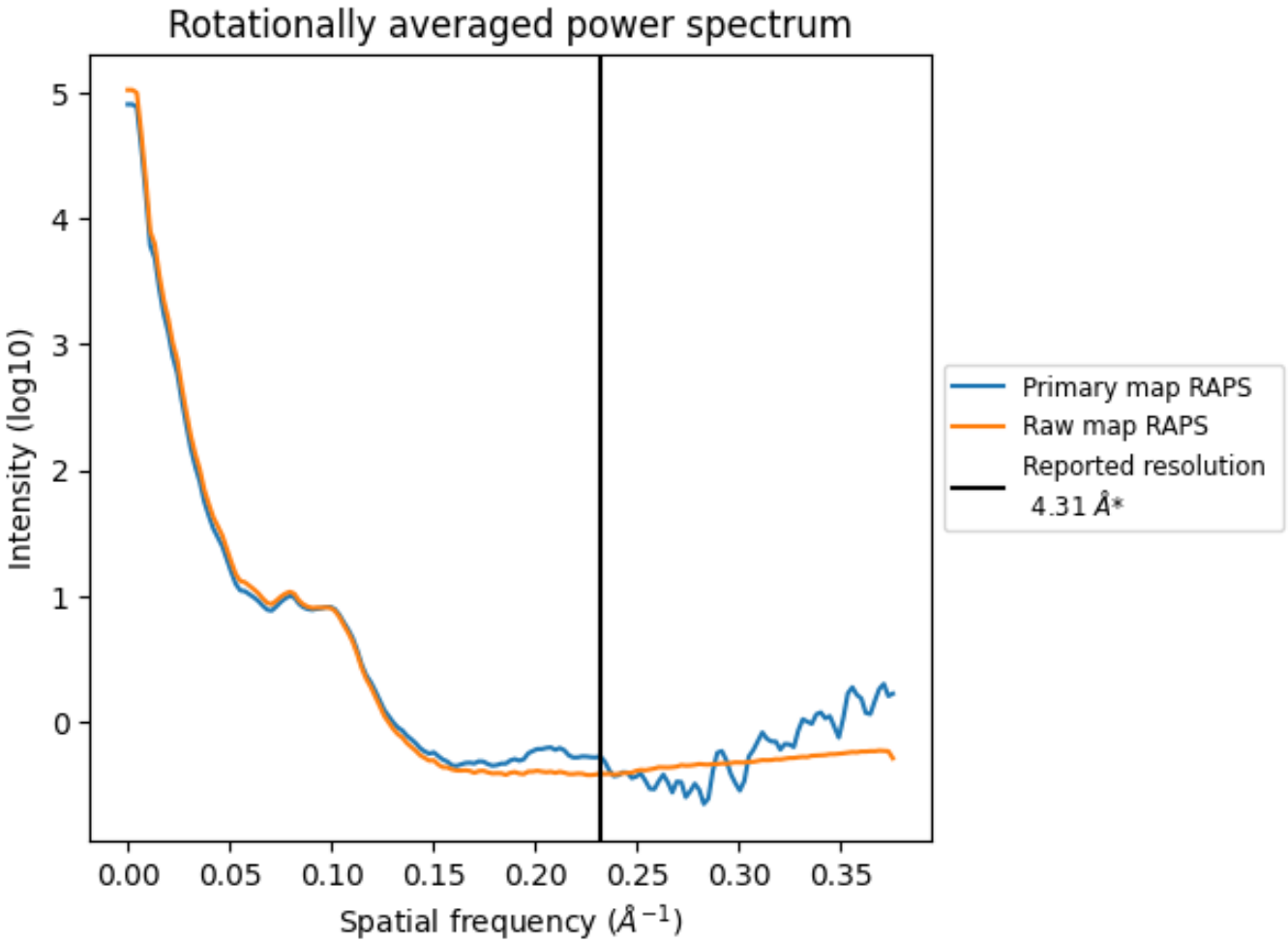
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 550 $nm^3$; this corresponds to an approximate mass of 497 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)

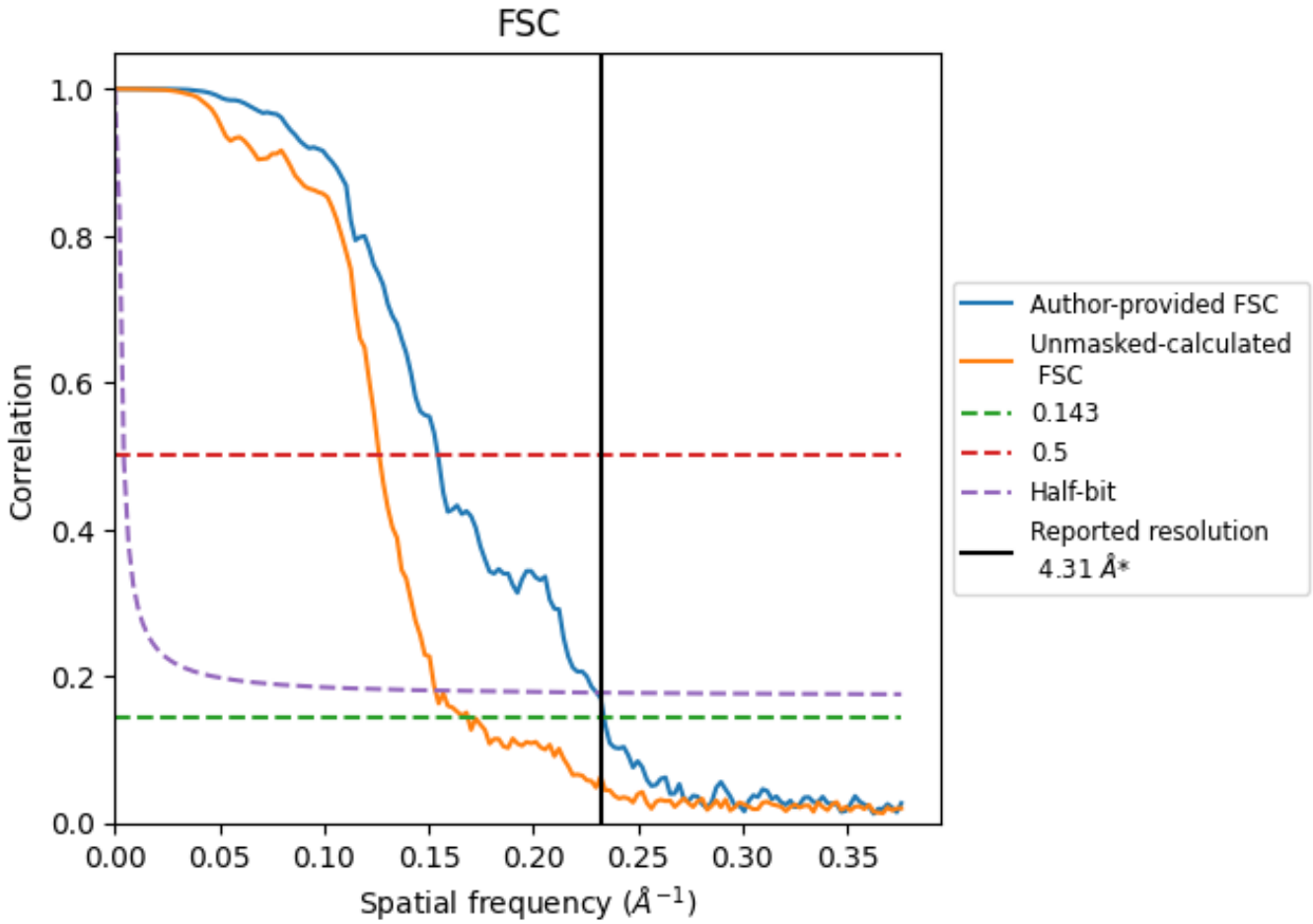



*Reported resolution corresponds to spatial frequency of 0.232 Å$^{-1}$

# 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 0.232 Å$^{-1}$

## 8.2 Resolution estimates (i)

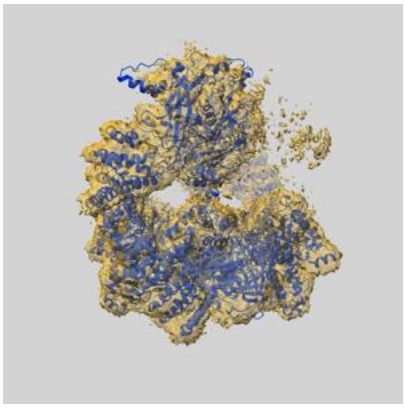
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.31 | - | - |
| Author-provided FSC curve | 4.28 | 6.47 | 4.34 |
| Unmasked-calculated* | 5.93 | 7.91 | 6.53 |

*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 5.93 differs from the reported value 4.31 by more than 10 %

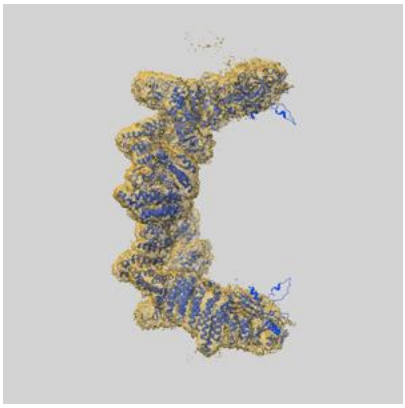
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60149 and PDB model 8ZJL. Per-residue inclusion information can be found in section 3 on page 5.

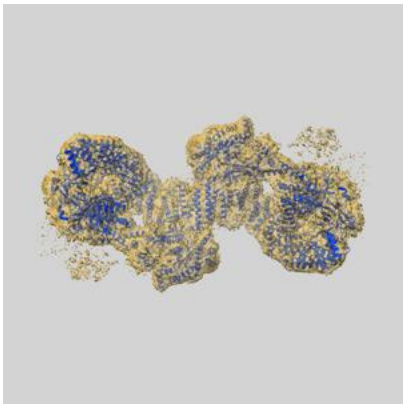
## 9.1 Map-model overlay



X



Y



Z

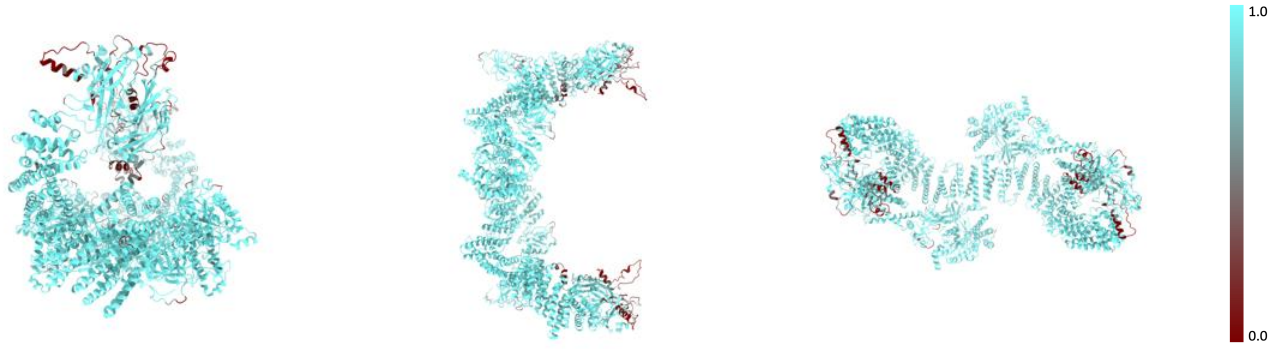
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

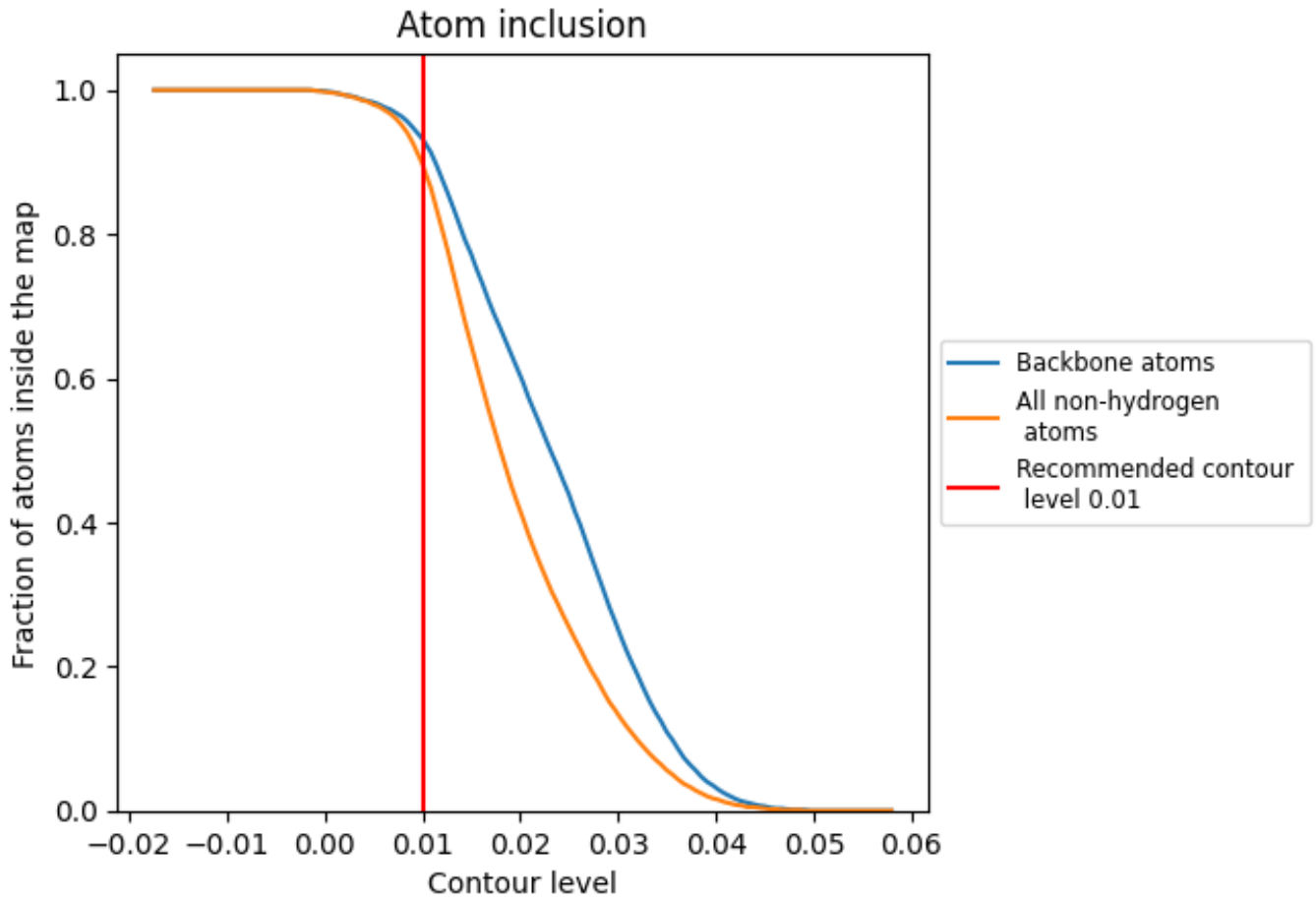
## 9.3 Atom inclusion mapped to coordinate model




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 (0.01).

## 9.4 Atom inclusion (i)




At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8970 | 0.2110 |
| A | 0.9040 | 0.1550 |
| B | 0.8860 | 0.2130 |
| C | 0.9740 | 0.2670 |
| D | 0.9080 | 0.1620 |
| E | 0.8890 | 0.2090 |
| F | 0.9750 | 0.2690 |