# wwPDB EM Validation Summary Report (i)

May 12, 2024 – 12:36 am BST

| | | |
|---|---|---|
| PDB ID | : | 6RQT |
| EMDB ID | : | EMD-4985 |
| Title | : | RNA Polymerase I-tWH-Rrn3-DNA |
| Authors | : | Mueller, C.W.; Sadian, Y.; Tafur, L. |
| Deposited on | : | 2019-05-16 |
| Resolution | : | 4.00 Å(reported) |

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.

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

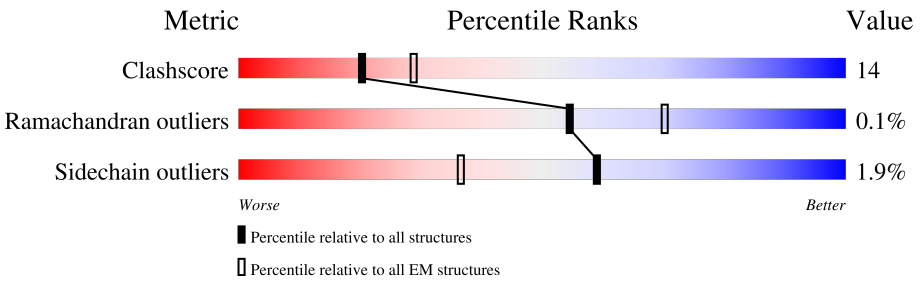
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 4.00 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| 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 | T | 70 | 13% 13% 13% 74% |
| 2 | U | 70 | 11% • 16% 80% |
| 3 | A | 1664 | 17% 62% 25% • 12% |
| 4 | B | 1203 | 16% 64% 32% • • |
| 5 | C | 335 | 14% 62% 29% 9% |
| 6 | D | 137 | 25% 28% 15% 57% |
| 7 | E | 215 | 24% 74% 25% |
| 8 | F | 155 | 12% 47% 17% • 35% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | G | 326 | 32% 45% 17% 38% |
| 10 | H | 146 | 16% 68% 23% 8% |
| 11 | I | 125 | 18% 41% 10% 49% |
| 12 | J | 70 | 17% 60% 37% |
| 13 | K | 142 | 13% 49% 20% 30% |
| 14 | L | 70 | 20% 43% 19% 39% |
| 15 | M | 415 | 66% 69% 25% 6% |
| 16 | N | 233 | 18% 38% 20% 42% |
| 17 | O | 627 | 73% 60% 14% 26% |

# 2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 39820 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 DNA chain called Template strand.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | T | 18 | 364 | 175 | 59 | 112 | 18 | 0 | 0 |

- Molecule 2 is a DNA chain called Nontemplate strand.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | U | 14 | 293 | 139 | 59 | 81 | 14 | 0 | 0 |

- Molecule 3 is a protein called DNA-directed RNA polymerase I subunit RPA190.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | A | 1466 | 11571 | 7309 | 2012 | 2188 | 62 | 0 | 0 |

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA135.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | B | 1170 | 9301 | 5888 | 1625 | 1737 | 51 | 0 | 0 |

- Molecule 5 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | C | 304 | 2418 | 1536 | 414 | 460 | 8 | 0 | 0 |

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA14.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 6 | D | 59 | 467 | 293 | 80 | 94 | 0 | 0 |

- Molecule 7 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 | | |
| 7 | E | 214 | 1751 | 1111 | 309 | 320 | 11 | 0 | 0 |

- Molecule 8 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 | | |
| 8 | F | 100 | 823 | 522 | 144 | 154 | 3 | 0 | 0 |

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | G | 202 | 1600 | 1026 | 276 | 293 | 5 | 0 | 0 |

- Molecule 10 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 | | |
| 10 | H | 134 | 1075 | 677 | 182 | 212 | 4 | 0 | 0 |

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | I | 64 | 472 | 295 | 78 | 95 | 4 | 0 | 0 |

- Molecule 12 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 | | |
| 12 | J | 69 | 569 | 362 | 101 | 100 | 6 | 0 | 0 |

- Molecule 13 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | K | 100 | 785 | 491 | 129 | 160 | 5 | 0 | 0 |

- Molecule 14 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 | | |
| 14 | L | 43 | 344 | 211 | 69 | 60 | 4 | 0 | 0 |

- Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA49.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | M | 392 | 3100 | 1978 | 526 | 592 | 4 | 0 | 0 |

- Molecule 16 is a protein called DNA-directed RNA polymerase I subunit RPA34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | N | 135 | 1070 | 685 | 175 | 206 | 4 | 0 | 0 |

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | O | 463 | 3811 | 2473 | 623 | 694 | 21 | 0 | 0 |

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

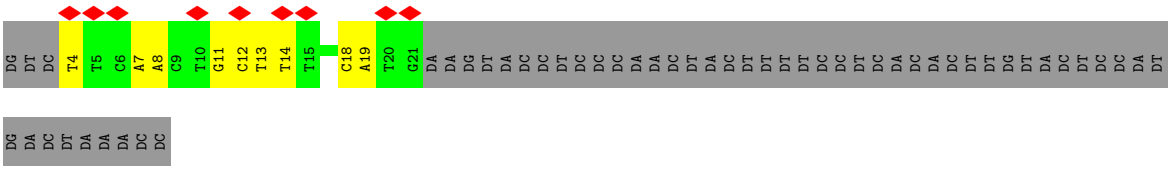
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 18 | A | 2 | 2 | 2 | 0 |
| 18 | B | 1 | 1 | 1 | 0 |
| 18 | I | 1 | 1 | 1 | 0 |
| 18 | J | 1 | 1 | 1 | 0 |
| 18 | L | 1 | 1 | 1 | 0 |

# 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.

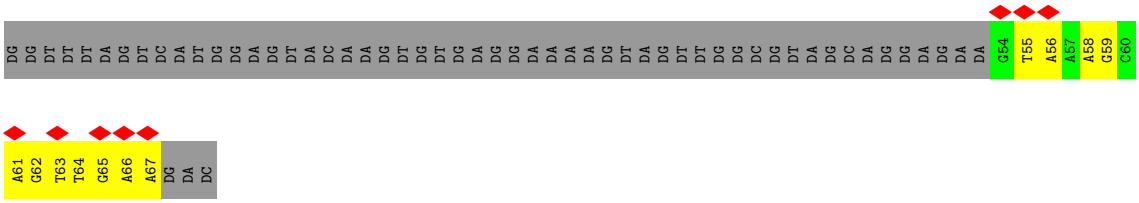
- Molecule 1: Template strand

Chain T: 13% 13% 13% 74%



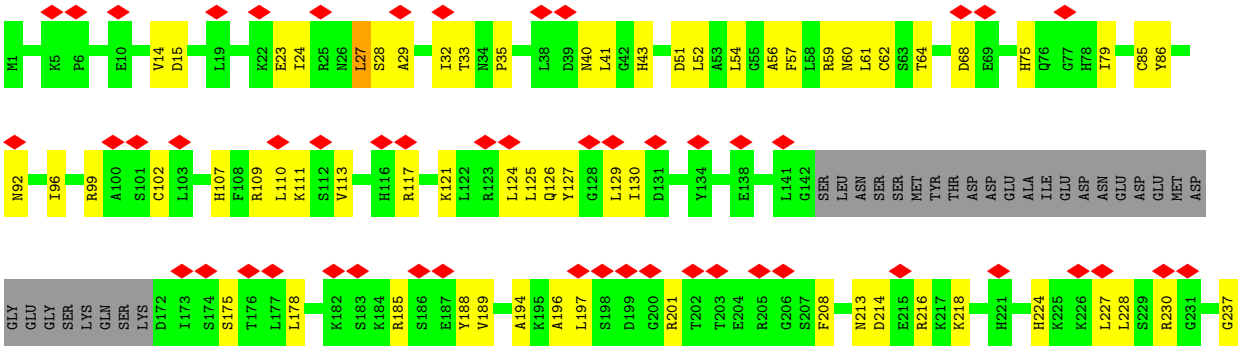

- Molecule 2: Nontemplate strand

Chain U: 11% • 16% 80%




- Molecule 3: DNA-directed RNA polymerase I subunit RPA190

Chain A: 17% 62% 25% • 12%



M238 K242 F243 R244 K245 D246 T249 K250 I251 F252 E253 T254 A255 L256 N257 E258 K259 N263 N264 R265 V266 K267 G268 F269 I270 ARG GLN ASP MET ILE LYS LYS GLN LYS GLN ALA LYS LYS LEU ASP GLY SER ASN GLU ALA SER ALA ASN ASP GLU GLU SER PHE ASP VAL GLY ARG

ASN PRO THR THR ARG PRO LYS THR GLY S312 T313 Y314 I315 L316 S317 T318 N322 D325 R329 K330 E331 Q332 C333 V334 L335 V338 F339 H340 P343 R347 V350 K351 A352 D353 S354 F355 F356 M357 D358 V359 L360 R368 L369 P370 S371 K372 L373 G374 E375 E376 V377 H378

E379 N380 S381 Q382 N383 Q384 L385 L386 S387 L394 L395 I396 R397 D398 L399 N400 D401 D402 L403 S404 K405 L406 GLN LYS ASP LYS VAL SER LEU GLU ASP ARG R417 V418 I419 F420 S421 R422 L423 M424 N425 A426 F427 Q431 N432 D433 V434 N435 A436 F437 I438 D439 S440 T441 K442 A443 Q444 G445

R446 T447 S448 G449 K450 V451 P452 I453 V456 K457 Q458 A459 L460 E461 K462 K463 E464 G465 L466 F467 R468 K469 H470 M471 K474 A480 R481 S482 V483 D487 P488 N489 I490 E491 E494 I495 G496 P499 A502 T506 T512 A513 Y514 N515 I516 A517 E518 L519 R520 W530

P531 G532 I536 Q537 N538 E539 D540 G541 S542 L543 V551 R554 K555 N559 Q560 L561 L562 T563 P564 S565 S566 N567 V568 S569 T570 H571 T572 K575 K576 V577 H580 N583 R584 D585 V586 V587 L588 Q592 M600 M601 G602 V605 R606 V607 L608 T613 L614 R615

Y618 A626 D629 G630 N634 M635 Q639 N642 E646 A647 L648 N649 L650 A651 N652 T653 D654 S655 Q656 R667 G668 L669 I670 Q671 D672 H673 T681 S682 K683 F686 F687 Y692 R701 P702 E703 T708 R709 S710 L715 F720 K721 P722 Y723 P724 L725 W726

T727 G728 K729 Q730 I731 I732 L736 T740 D743 H744 P745 N748 L749 N757 E758 Y759 K762 G763 S764 L765 E766 N767 F771 K772 D773 G774 L777 L781 D782 K783 Y786 G787 A788 S789 K790 Y791 G792 I793 V794 H795 V809 L810 S811 V812 L813 G814 R815 L816 F817

T818 N819 Y820 I821 T827 C828 G829 G830 D831 D832 L833 R834 L835 T836 A837 E838 G839 N840 K841 W842 R843 T844 D845 E856 T862 M863 L864 D865 K866 D867 T868 D871 D872 P873 E874 L875 L876 K877 R878 L879 Q880 E881 I882 L883 R884 D885 K888 S889 G890 I891 L892 D893 A894 V895 T896

S897 S898 A902 V908 C911 V912 P913 D914 G915 K919 N923 Q926 L930 S931 G932 A933 K934 G935 S936 N937 V938 N939 V940 S941 Q942 I943 L946 L947 G948 Q949 Q950 G954 M960 Y972 D975 Y981 R985 F986 Y987 I990 Y995 E1004 G1005

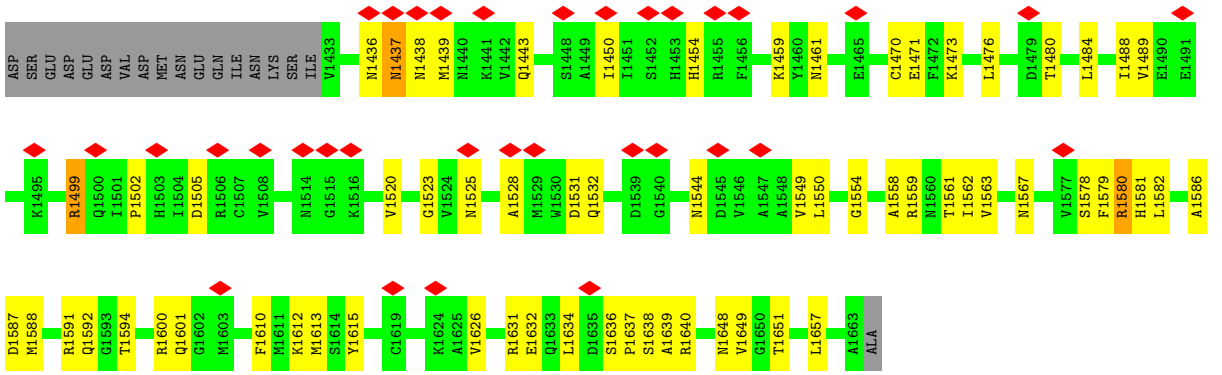
L1006 I1007 A1010 V1011 K1012 T1013 S1014 R1015 Y1018 L1019 Q1020 R1021 T1024 K1025 Q1026 L1027 E1028 G1029 V1030 H1031 V1032 I1038 R1039 D1040 A1041 D1042 G1043 T1044 L1045 V1046 Q1047 Y1050 D1053 A1054 I1055 D1056 I1057 T1058 S1061 H1062 M1063 F1068 C1069 N1072 Y1073 Y1074 A1075 L1076 Y1080

L1085 I1086 E1087 H1088 L1089 D1090 V1091 A1094 Y1097 S1098 K1099 K1100 K1103 Y1104 R1105 K1106 K1110 H1113 Y1114 K1115 Q1116 K1119 Y1120 D1121 A1125 K1126 Y1127 N1128 P1129 A1130 K1131 Y1132 L1133 S1137 E1138 K1143 L1148 D1149 K1150 K1153 LEU PHE LYS SER SER ASP G1160 Q1171

L1172 K1173 Y1174 M1175 R1176 S1177 L1178 I1179 N1180 P1181 G1182 G1186 A1189 V1193 S1197 T1198 Q1199 M1200 T1201 L1202 N1203 T1204 F1205 HIS PHE ALA GLY HIS GLY ALA ALA N1214 R1221 L1222 R1223 E1224 T1228 A1231 A1232 I1233 P1236 Q1237 Q1250 A1251 D1252 T1253 F1254 C1255 K1256 K1260

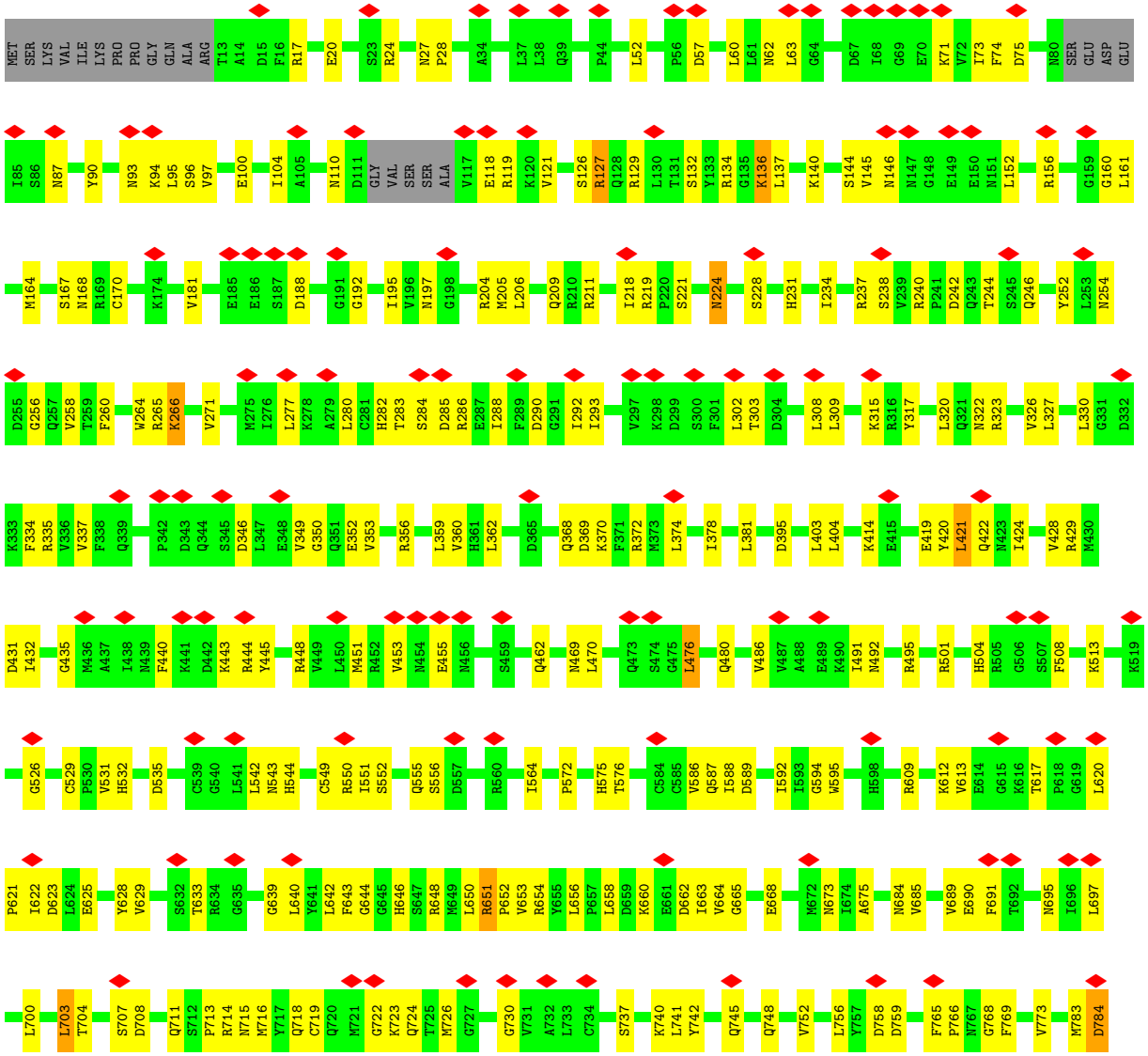
V1261 L1262 D1268 K1269 V1270 E1274 T1275 T1276 G1277 THR SER ASN THR ALA GLY GLY ASN ALA A1287 R1288 M1294 D1298 E1301 E1304 E1305 Y1306 D1307 E1311 E1332 I1333 K1334 K1335 Q1336 K1337 R1338 THR THR GLY PRO ASP ILE GLY VAL ALA VAL PRO ARG LEU GLN THR ASP VAL

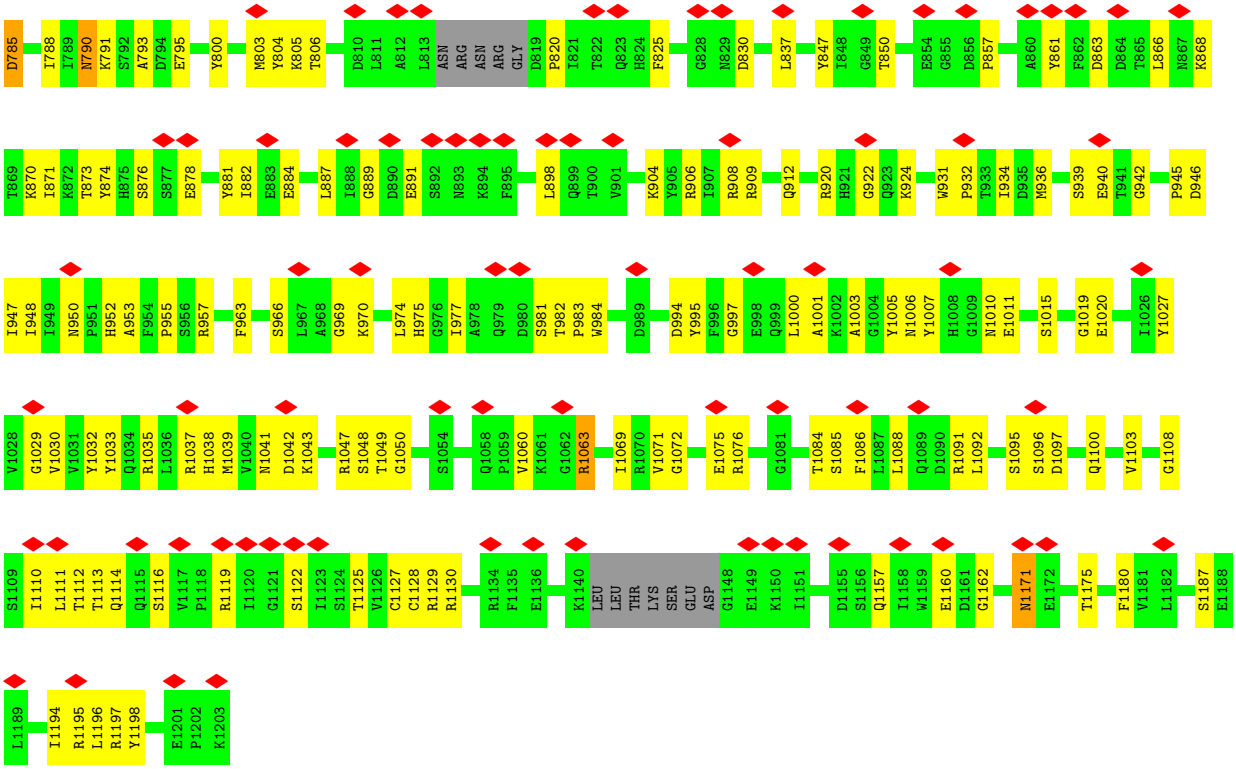
ALA ASN SER SER SER ASN SER LYS ARG LEU GLU GLU ASP ASN ASP GLU GLU GLN SER HIS LYS LYS THR LYS GLN ALA VAL SER TYR ASP GLU PRO ASP GLU ASP GLU ILE GLU THR MET ARG GLU ALA GLU LYS SER SER ASP GLU GLU GLY ILE ASP SER ASP LYS GLU PRO SER ASP SER




- Molecule 4: DNA-directed RNA polymerase I subunit RPA135

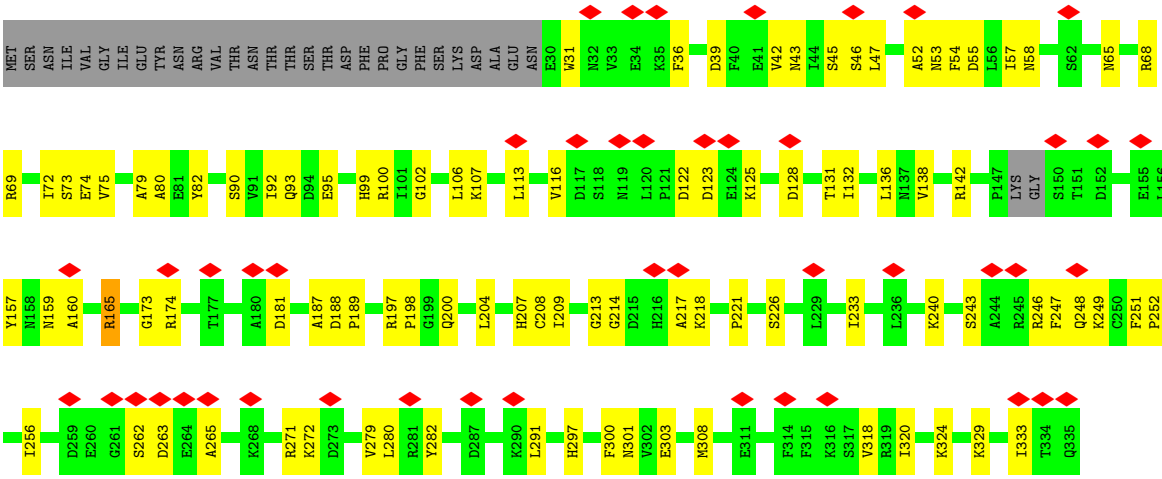
Chain B:





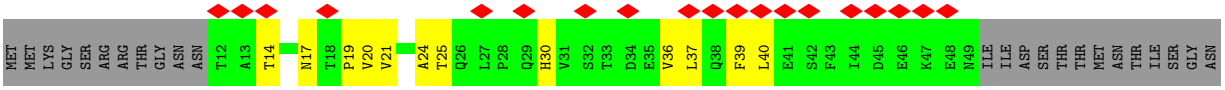

- Molecule 5: DNA-directed RNA polymerases I and III subunit RPAC1

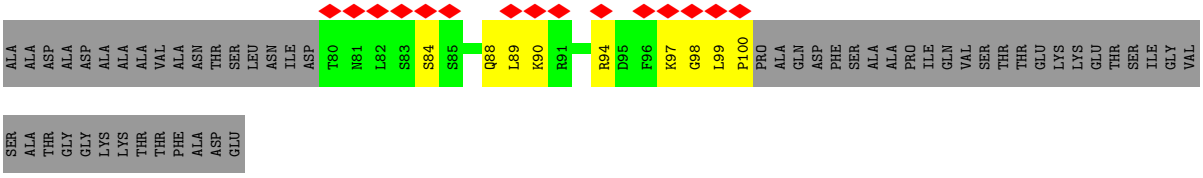
Chain C:




- Molecule 6: DNA-directed RNA polymerase I subunit RPA14

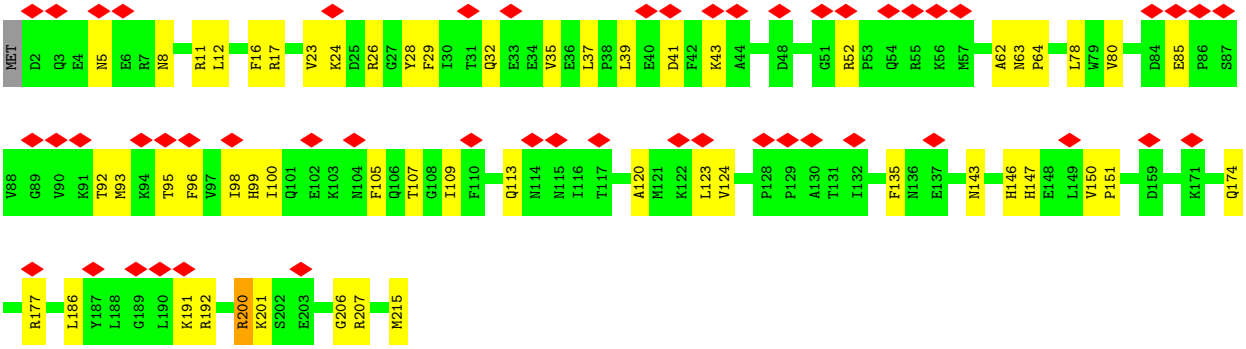
Chain D:





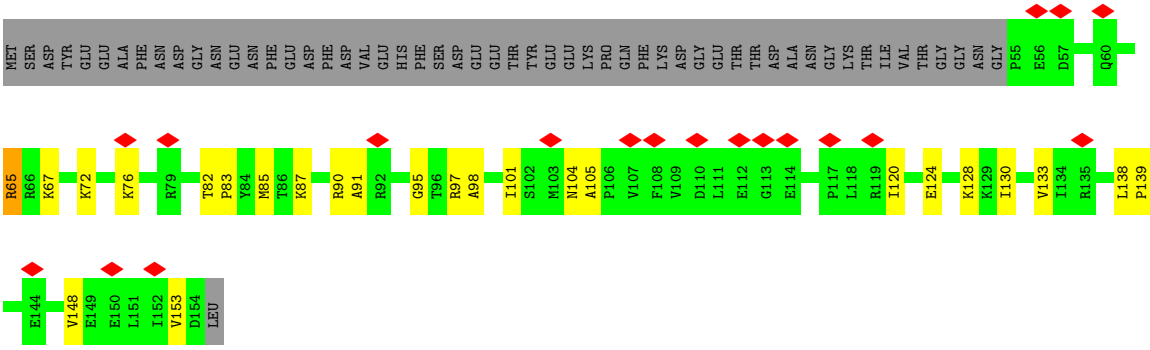

• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



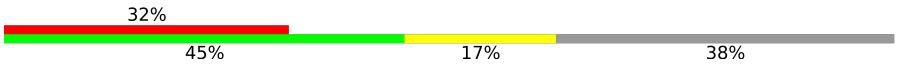

• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

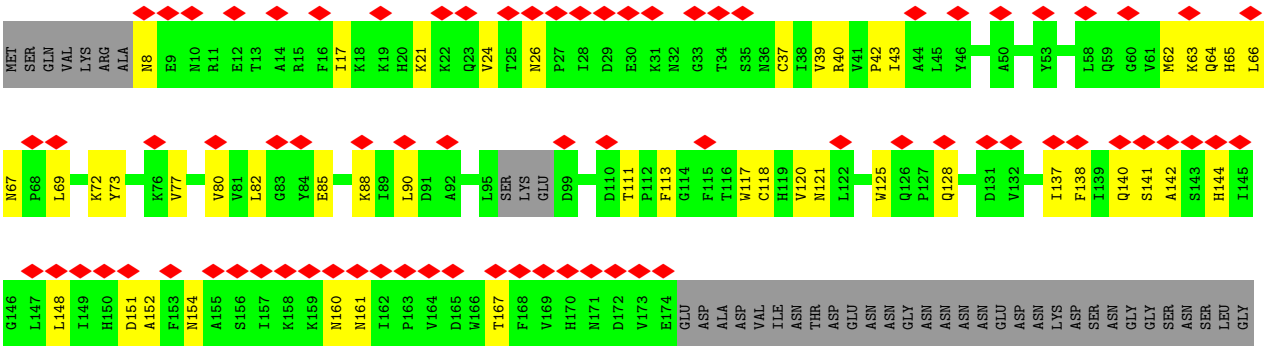
Chain F:

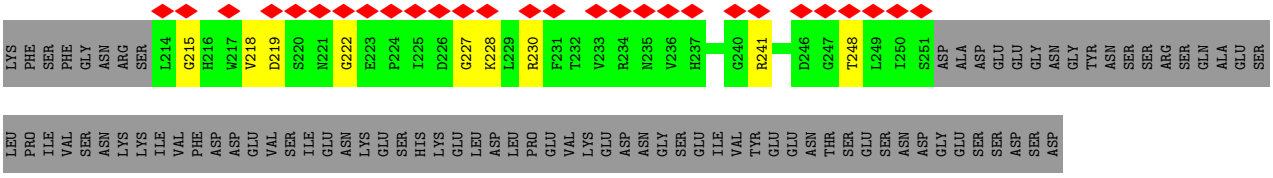



• Molecule 9: DNA-directed RNA polymerase I subunit RPA43

Chain G:

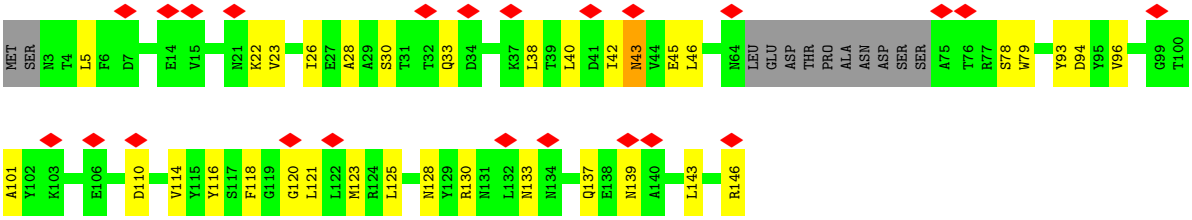




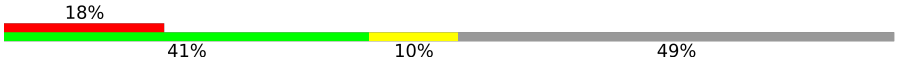

• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

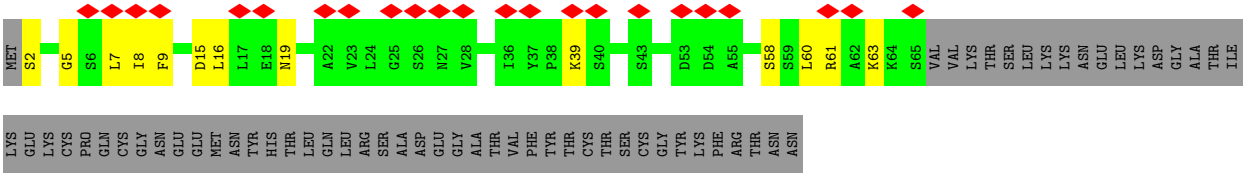
Chain H:




• Molecule 11: DNA-directed RNA polymerase I subunit RPA12

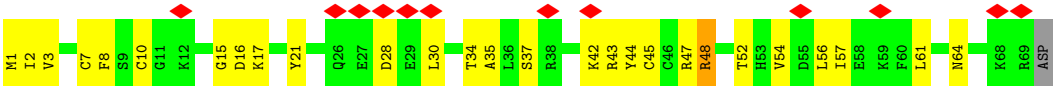
Chain I:



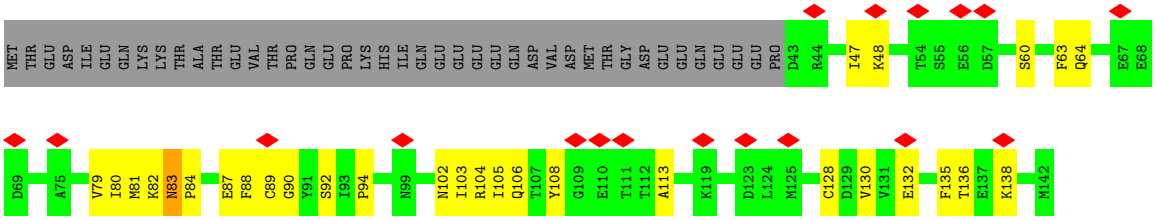

• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



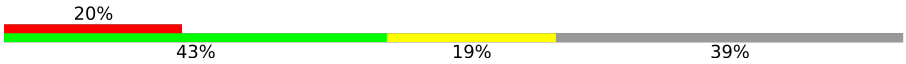

• Molecule 13: DNA-directed RNA polymerases I and III subunit RPAC2

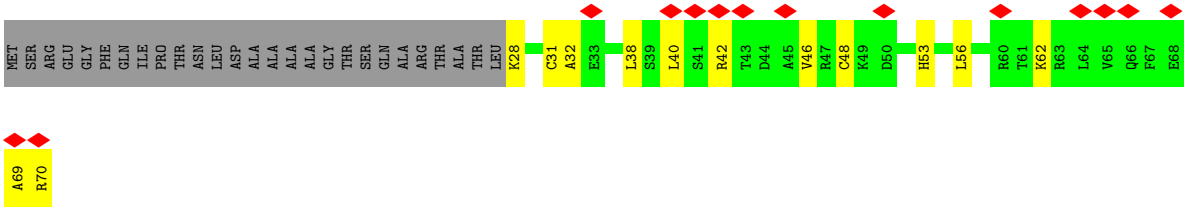
Chain K:




• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC4

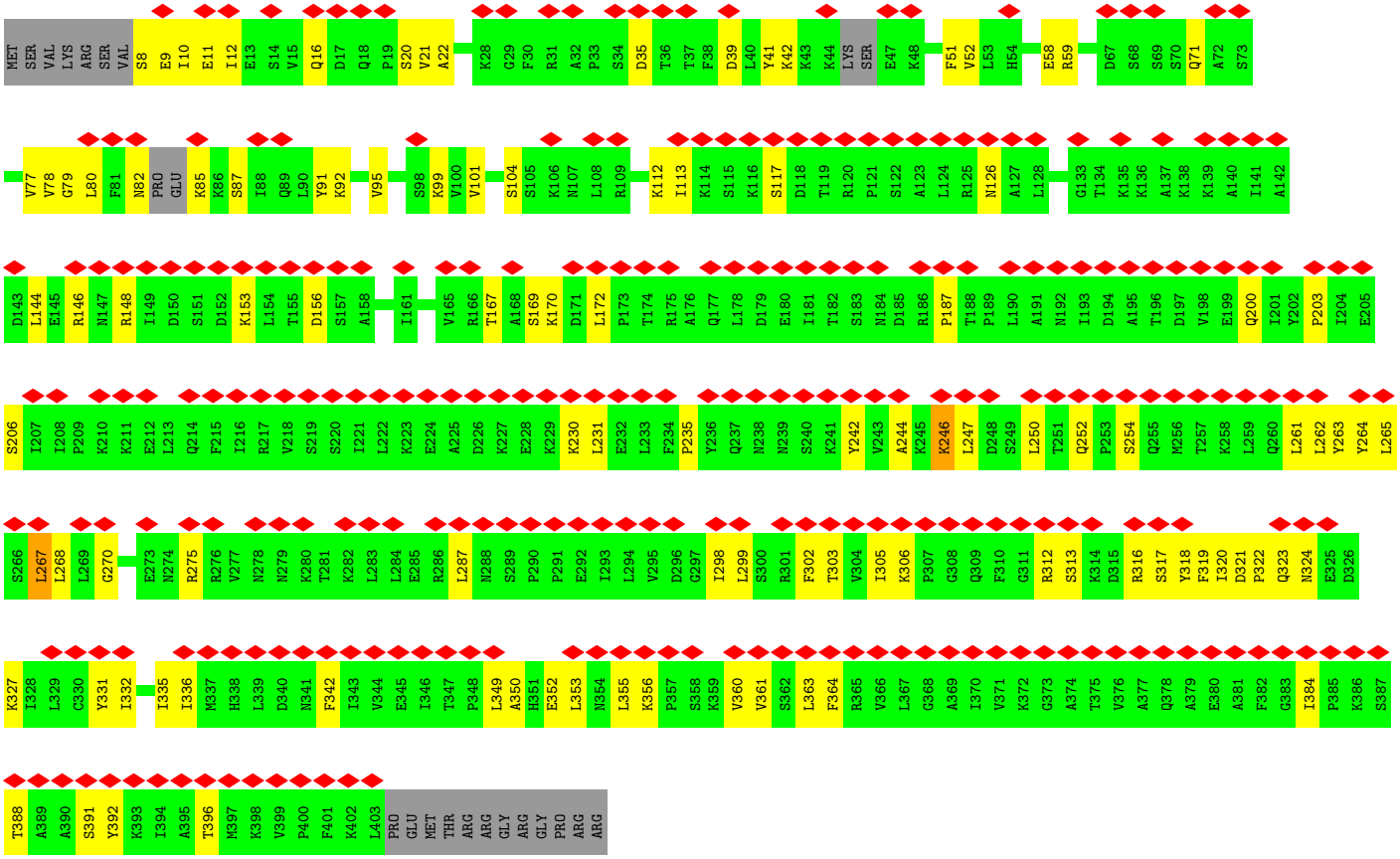
Chain L:





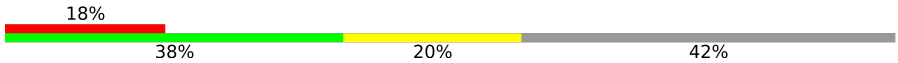

• Molecule 15: DNA-directed RNA polymerase I subunit RPA49

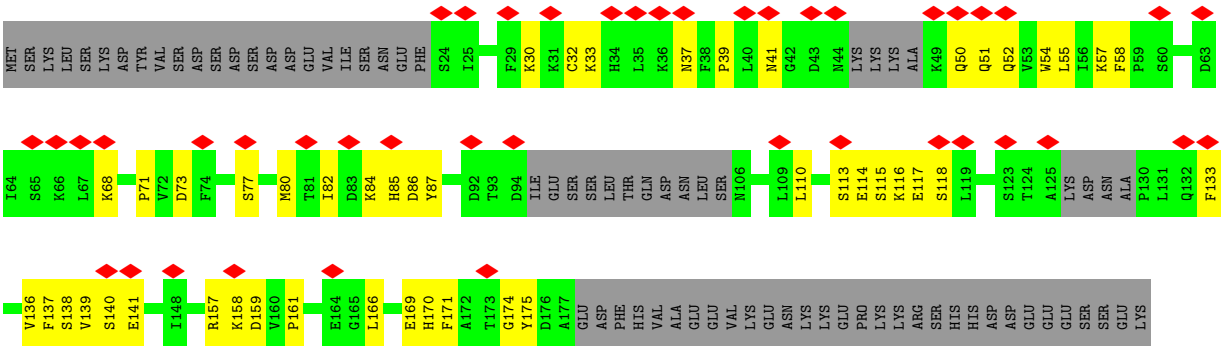
Chain M:




• Molecule 16: DNA-directed RNA polymerase I subunit RPA34

Chain N:



LYS LYS LYS LYS LYS GLU LYS LYS ARG GLU LYS ARG GLU LYS LYS ASP LYS LYS ASP LYS LYS LYS LYS HIS ARG ASP

- Molecule 17: RNA polymerase I-specific transcription initiation factor RRN3

Chain O: 73% 60% 14% 26%

MET MET ALA PHE GLU ASN THR SER LYS ARG PRO PRO GLN ASP PHE VAL ALA PRO ILE ASP GLN LYS LYS ARG LYS VAL GLN PHE SER ASP SER THR GLY LEU VAL THR LEU GLN PRO GLU GLU ILE LYS ASP GLU VAL PHE S48 A49 A50 M51 Y52 S53 B54 F55 V56 K57 S58 A59 L60

D61 D62 L63 D64 K65 N66 D67 S68 T69 Q70 I71 G72 I73 I74 A75 N76 Q77 V78 A79 L80 P81 S82 K83 N84 P85 E86 R87 I88 N89 D90 K91 N92 L93 N94 I95 L96 L97 D98 I99 L100 S101 S102 N103 I104 N105 R106 I107 E108 S109 S110 R111 G112 T113 F114 L115 I116 Q117 S118 I119 I120

N121 F122 E123 K124 W125 W126 E127 L128 P129 P130 H131 T132 L133 S134 K135 Y136 I137 Y138 F139 I140 K141 I142 L143 C144 S145 S146 I147 P148 K149 W150 W151 Q152 D153 V154 S155 M156 I157 L158 V159 S160 C161 F162 I163 L164 P165 I166 K167 Q168 T169 V170 C171 H172 H173 D174 M175 L176 K177 Y178 F179 L180

R181 M182 I183 P184 S185 S186 M187 G188 F189 I190 D191 T192 Y193 L194 A195 K196 F197 F198 P199 N200 K201 N202 D203 T204 R205 R206 K207 L208 V209 N210 Y211 T212 S213 N214 L215 L216 K217 L218 R219 G220 Y221 C222 S223 E224 L225 G226 F227 Q228 I229 W230 S231 L232 L233 I234 E235 K236 I237 I238 S239 I240

D241 V242 E243 L244 Q245 N246 E247 L248 ASP GLU LEU ASP ASP ASP VAL ASP ASP ASP ASP LEU GLU GLU GLU VAL ASP LEU GLU ASP ASP ASP ASP LEU ASP ASP ASP SER GLY ASP ASP ASP ASP GLU ASN CYS GLY ASN SER ASN GLU GLU LEU ARG SER GLY ALA ALA ASP GLY SER GLN SER

ASP SER GLU ASP MET ASP ILE ILE GLU GLY MET ASP GLY THR GLU GLU TYR ASN VAL GLU LEU THR GLN G324 I325 K326 E327 L328 S329 T330 K331 L332 D333 S334 I335 L336 T337 L338 V339 S340 T341 H342 V343 E344 E345 Q346 V347 T348 P349 E350 S351 L352 E353 S354 G355 E356 G357 V358 G359 V360

F361 N362 T363 L364 T365 T366 L367 F368 K369 T370 H371 V372 L373 P374 T375 Y376 Y377 T378 R379 S380 I381 Q382 Y383 I384 M385 F386 H387 V388 S389 Q390 Q391 Q392 L393 E394 L395 M396 D397 S398 F399 L400 V401 T402 L403 I404 D405 I406 S407 F408 A409 V410 N411 E412 A413 A414 E415 K416 K417 I418 K419 S420

L421 Q422 Y423 L424 G425 S426 Y427 I428 A429 R430 A431 K432 K433 L434 S435 R436 T437 Q438 I439 I440 F441 V442 A443 S444 Y445 L446 T447 S448 W449 L450 N451 R452 Y453 V454 I455 E456 R457 E458 E459 E460 V461 D462 Q463 R464 G465 M467 E468 R469 F470 K471 H472 F473 Y474 A475 A476 F477 Q478 A479 L480

C481 Y482 I483 F484 C485 F486 R487 H488 N489 I490 F491 R492 D493 T494 D495 G496 N497 W498 E499 C500 E501 L502 D503 K504 F505 F506 Q507 R508 M509 V510 I511 S512 K513 F514 N515 P516 L517 K518 F519 C520 N521 E522 N523 V524 M525 L526 M527 F528 A529 R530 I531 A532 Q533 Q534 E535 S536 V537 A538 Y539 C540

F541 S542 I543 I544 E545 N546 N547 N548 N549 E550 R551 LEU ARG GLY ILE ILE GLY LYS ALA ASP SER ASP LYS LYS GLU ASN SER ALA GLN ALA ASN THR THR SER SER SER TRP SER LEU ALA T581 R582 Q583 Q584 F585 I586 C587 D587 L588 Q589 S590 Y591 F592 P593 Y594 D595 P596 L597 F598 L599 K600

N601 Y602 K603 I604 L605 M606 K607 E608 Y609 Y610 I611 E612 W613 S614 GLU ALA SER GLY GLU TYR GLU SER ASP GLY SER ASP ASP

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 9789 | 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 ($e^-/Å^2$) | 1.57175 | 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 | 0.286 | Depositor |
| Minimum map value | -0.181 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.014 | Depositor |
| Recommended contour level | 0.05 | Depositor |
| Map size (Å) | 233.5168, 233.5168, 233.5168 | wwPDB |
| Map dimensions | 176, 176, 176 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.3268, 1.3268, 1.3268 | 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 | T | 0.54 | 0/405 | 0.93 | 1/622 (0.2%) |
| 2 | U | 0.46 | 0/330 | 0.71 | 0/508 |
| 3 | A | 0.40 | 0/11782 | 0.67 | 0/15913 |
| 4 | B | 0.44 | 1/9506 (0.0%) | 0.69 | 0/12847 |
| 5 | C | 0.39 | 0/2469 | 0.66 | 0/3347 |
| 6 | D | 0.31 | 0/473 | 0.62 | 0/641 |
| 7 | E | 0.40 | 0/1787 | 0.63 | 0/2406 |
| 8 | F | 0.38 | 0/838 | 0.64 | 0/1129 |
| 9 | G | 0.34 | 0/1637 | 0.62 | 0/2226 |
| 10 | H | 0.41 | 0/1093 | 0.66 | 0/1480 |
| 11 | I | 0.36 | 0/478 | 0.72 | 0/647 |
| 12 | J | 0.48 | 0/578 | 0.76 | 0/775 |
| 13 | K | 0.38 | 0/795 | 0.63 | 0/1072 |
| 14 | L | 0.33 | 0/346 | 0.67 | 0/457 |
| 15 | M | 0.33 | 0/3150 | 0.65 | 0/4247 |
| 16 | N | 0.38 | 0/1090 | 0.71 | 0/1466 |
| 17 | O | 0.28 | 0/3897 | 0.55 | 0/5268 |
| All | All | 0.39 | 1/40654 (0.0%) | 0.66 | 1/55051 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | B | 121 | VAL | C-N | -5.01 | 1.22 | 1.34 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | T | 11 | DG | P-O3'-C3' | 5.31 | 126.07 | 119.70 |

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 | T | 364 | 0 | 206 | 17 | 0 |
| 2 | U | 293 | 0 | 158 | 15 | 0 |
| 3 | A | 11571 | 0 | 11653 | 369 | 0 |
| 4 | B | 9301 | 0 | 9193 | 343 | 0 |
| 5 | C | 2418 | 0 | 2401 | 74 | 0 |
| 6 | D | 467 | 0 | 468 | 16 | 0 |
| 7 | E | 1751 | 0 | 1776 | 36 | 0 |
| 8 | F | 823 | 0 | 841 | 16 | 0 |
| 9 | G | 1600 | 0 | 1600 | 38 | 0 |
| 10 | H | 1075 | 0 | 1046 | 24 | 0 |
| 11 | I | 472 | 0 | 474 | 7 | 0 |
| 12 | J | 569 | 0 | 587 | 23 | 0 |
| 13 | K | 785 | 0 | 782 | 23 | 0 |
| 14 | L | 344 | 0 | 365 | 8 | 0 |
| 15 | M | 3100 | 0 | 3210 | 109 | 0 |
| 16 | N | 1070 | 0 | 1085 | 61 | 0 |
| 17 | O | 3811 | 0 | 3804 | 53 | 0 |
| 18 | A | 2 | 0 | 0 | 0 | 0 |
| 18 | B | 1 | 0 | 0 | 0 | 0 |
| 18 | I | 1 | 0 | 0 | 0 | 0 |
| 18 | J | 1 | 0 | 0 | 0 | 0 |
| 18 | L | 1 | 0 | 0 | 0 | 0 |
| All | All | 39820 | 0 | 39649 | 1077 | 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 14.

The worst 5 of 1077 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) |
|---|---|---|---|
| 3:A:912:VAL:HG22 | 3:A:913:PRO:CD | 1.52 | 1.37 |
| 4:B:1005:TYR:HE1 | 16:N:171:PHE:CZ | 1.54 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:618:TYR:CD1 | 4:B:783:MET:HE1 | 1.70 | 1.25 |
| 3:A:41:LEU:HD12 | 3:A:43:HIS:ND1 | 1.53 | 1.21 |
| 4:B:1005:TYR:OH | 16:N:169:GLU:HG3 | 1.39 | 1.21 |

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 | |
|---|---|---|---|---|---|---|---|
| 3 | A | 1450/1664 (87%) | 1234 (85%) | 212 (15%) | 4 (0%) | 41 | 75 |
| 4 | B | 1160/1203 (96%) | 980 (84%) | 177 (15%) | 3 (0%) | 41 | 75 |
| 5 | C | 300/335 (90%) | 269 (90%) | 31 (10%) | 0 | 100 | 100 |
| 6 | D | 55/137 (40%) | 50 (91%) | 5 (9%) | 0 | 100 | 100 |
| 7 | E | 212/215 (99%) | 192 (91%) | 20 (9%) | 0 | 100 | 100 |
| 8 | F | 98/155 (63%) | 87 (89%) | 11 (11%) | 0 | 100 | 100 |
| 9 | G | 196/326 (60%) | 168 (86%) | 28 (14%) | 0 | 100 | 100 |
| 10 | H | 130/146 (89%) | 112 (86%) | 18 (14%) | 0 | 100 | 100 |
| 11 | I | 62/125 (50%) | 49 (79%) | 13 (21%) | 0 | 100 | 100 |
| 12 | J | 67/70 (96%) | 59 (88%) | 8 (12%) | 0 | 100 | 100 |
| 13 | K | 98/142 (69%) | 87 (89%) | 11 (11%) | 0 | 100 | 100 |
| 14 | L | 41/70 (59%) | 36 (88%) | 5 (12%) | 0 | 100 | 100 |
| 15 | M | 386/415 (93%) | 303 (78%) | 83 (22%) | 0 | 100 | 100 |
| 16 | N | 127/233 (54%) | 96 (76%) | 31 (24%) | 0 | 100 | 100 |
| 17 | O | 457/627 (73%) | 392 (86%) | 65 (14%) | 0 | 100 | 100 |
| All | All | 4839/5863 (82%) | 4114 (85%) | 718 (15%) | 7 (0%) | 54 | 84 |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 913 | PRO |
| 3 | A | 757 | ASN |
| 4 | B | 784 | ASP |
| 4 | B | 684 | ASN |
| 3 | A | 530 | TRP |

### 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 | |
|---|---|---|---|---|---|---|
| 3 | A | 1293/1465 (88%) | 1263 (98%) | 30 (2%) | 50 | 70 |
| 4 | B | 1025/1053 (97%) | 1008 (98%) | 17 (2%) | 60 | 78 |
| 5 | C | 269/296 (91%) | 265 (98%) | 4 (2%) | 65 | 80 |
| 6 | D | 56/116 (48%) | 55 (98%) | 1 (2%) | 59 | 77 |
| 7 | E | 196/197 (100%) | 190 (97%) | 6 (3%) | 40 | 63 |
| 8 | F | 90/137 (66%) | 86 (96%) | 4 (4%) | 28 | 55 |
| 9 | G | 180/291 (62%) | 177 (98%) | 3 (2%) | 60 | 78 |
| 10 | H | 117/128 (91%) | 114 (97%) | 3 (3%) | 46 | 67 |
| 11 | I | 56/110 (51%) | 53 (95%) | 3 (5%) | 22 | 50 |
| 12 | J | 64/65 (98%) | 63 (98%) | 1 (2%) | 62 | 79 |
| 13 | K | 90/130 (69%) | 88 (98%) | 2 (2%) | 52 | 71 |
| 14 | L | 38/57 (67%) | 35 (92%) | 3 (8%) | 12 | 39 |
| 15 | M | 350/371 (94%) | 344 (98%) | 6 (2%) | 60 | 78 |
| 16 | N | 125/220 (57%) | 123 (98%) | 2 (2%) | 62 | 79 |
| 17 | O | 427/576 (74%) | 427 (100%) | 0 | 100 | 100 |
| All | All | 4376/5212 (84%) | 4291 (98%) | 85 (2%) | 59 | 75 |

5 of 85 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | E | 215 | MET |
| 12 | J | 48 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | F | 67 | LYS |
| 10 | H | 43 | ASN |
| 14 | L | 42 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | E | 153 | HIS |
| 15 | M | 351 | HIS |
| 9 | G | 8 | ASN |
| 10 | H | 43 | ASN |
| 16 | N | 52 | GLN |

#### 5.3.3 RNA (i)

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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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.

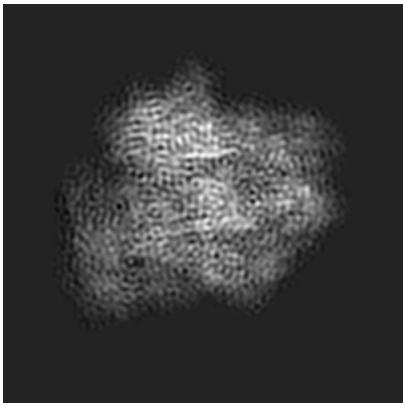
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4985. These allow visual inspection of the internal detail of the map and identification of artifacts.

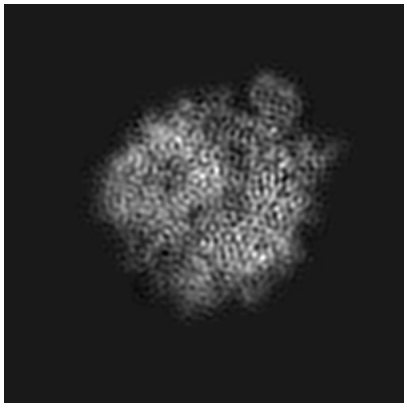
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

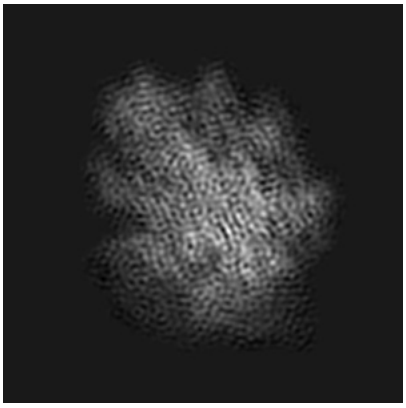
### 6.1.1 Primary map



X



Y

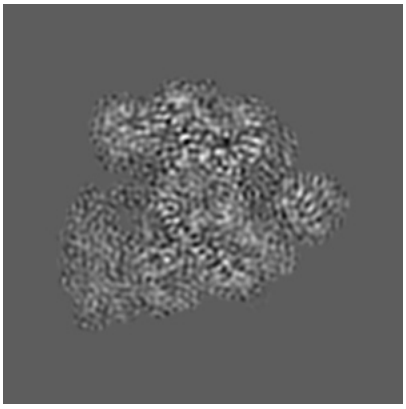


Z

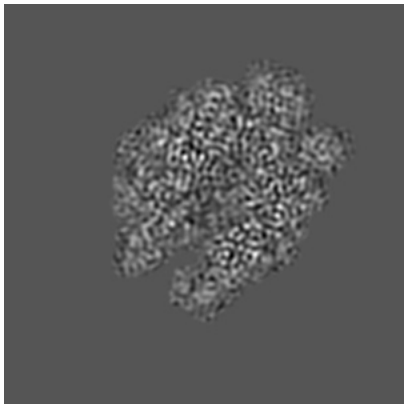
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

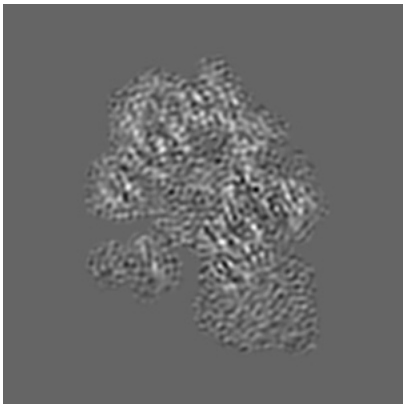
### 6.2.1 Primary map



X Index: 88



Y Index: 88

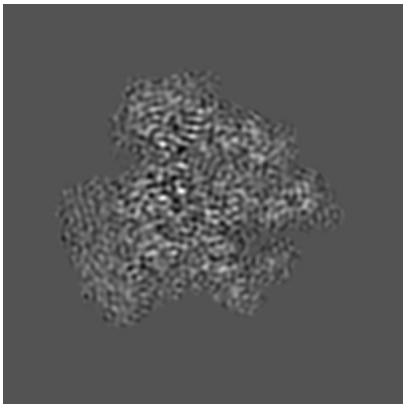


Z Index: 88

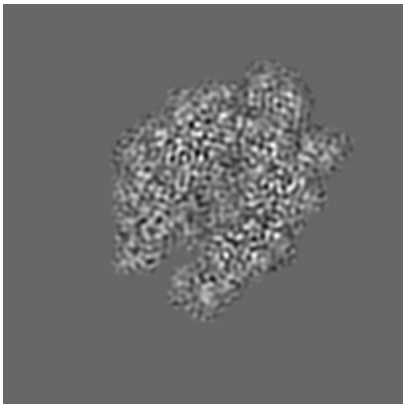
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

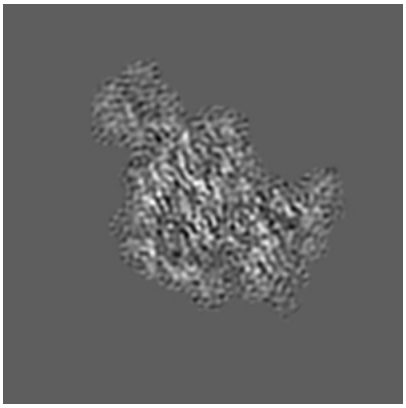
### 6.3.1 Primary map



X Index: 101



Y Index: 89

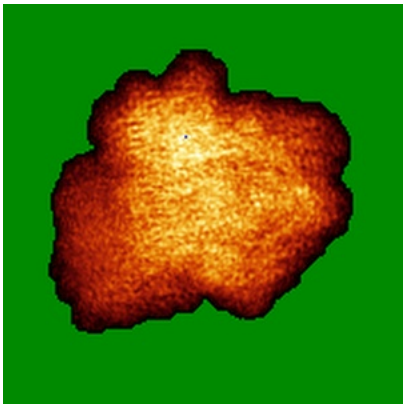


Z Index: 110

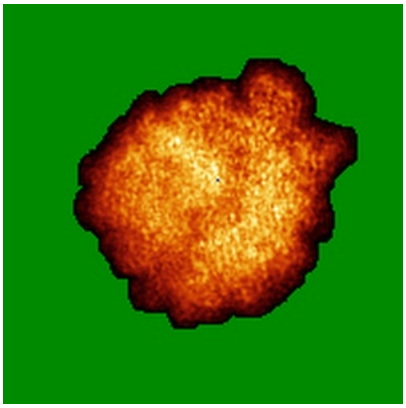
The images above show the largest variance slices of the map in three orthogonal directions.

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

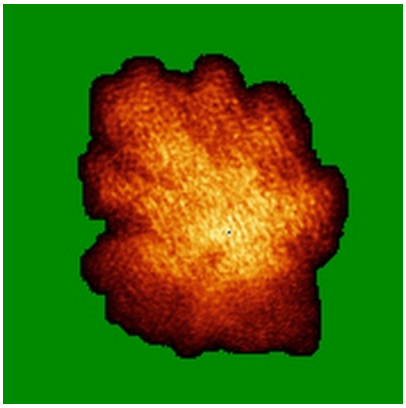
### 6.4.1 Primary map



X



Y

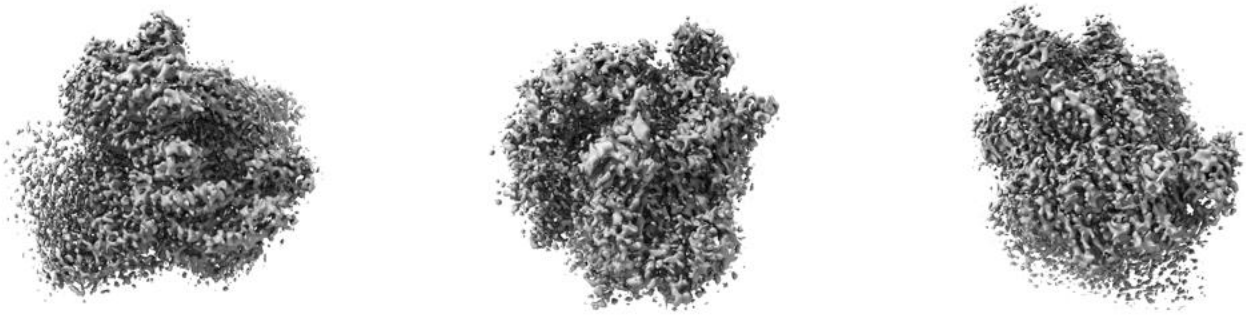


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

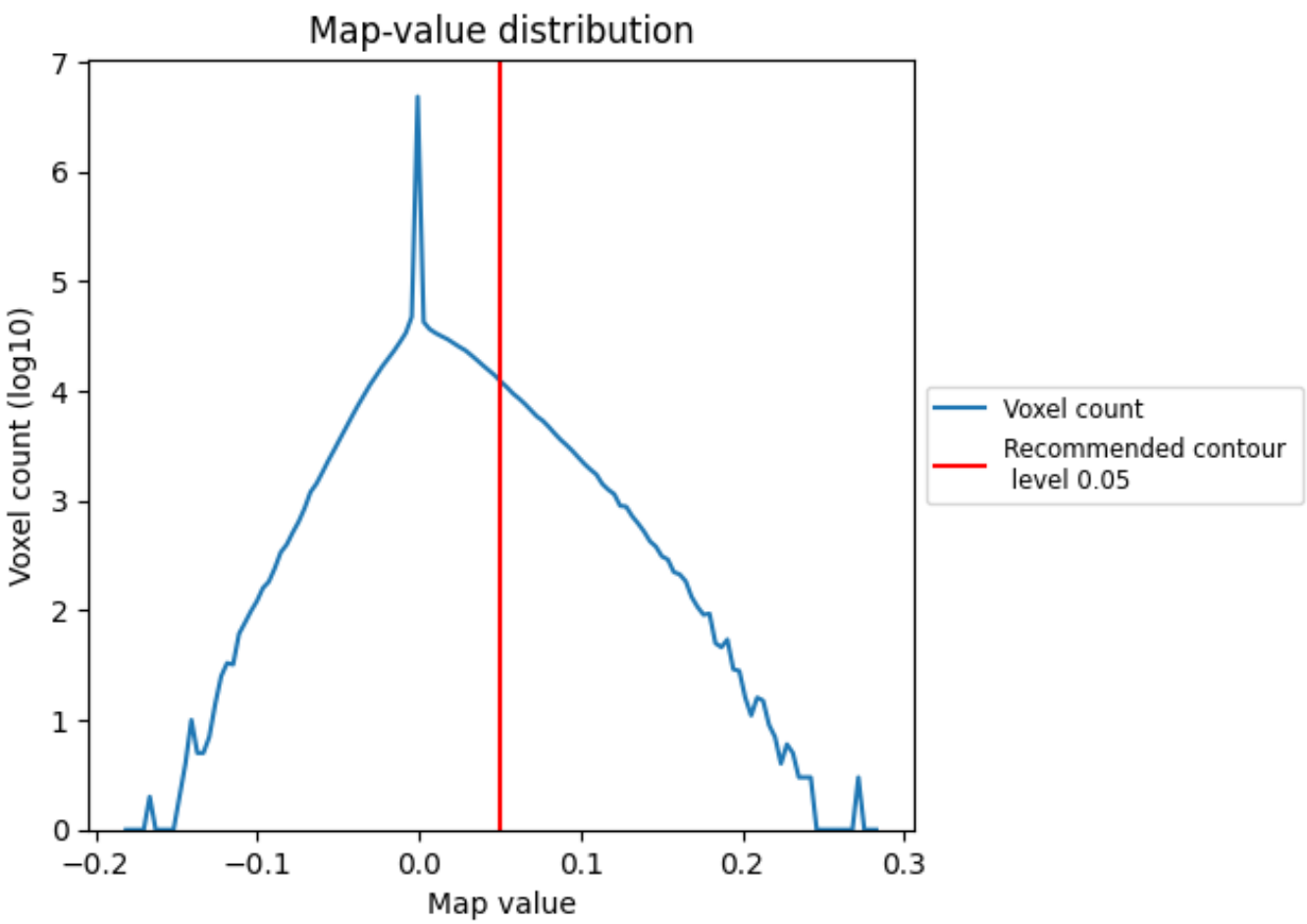
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

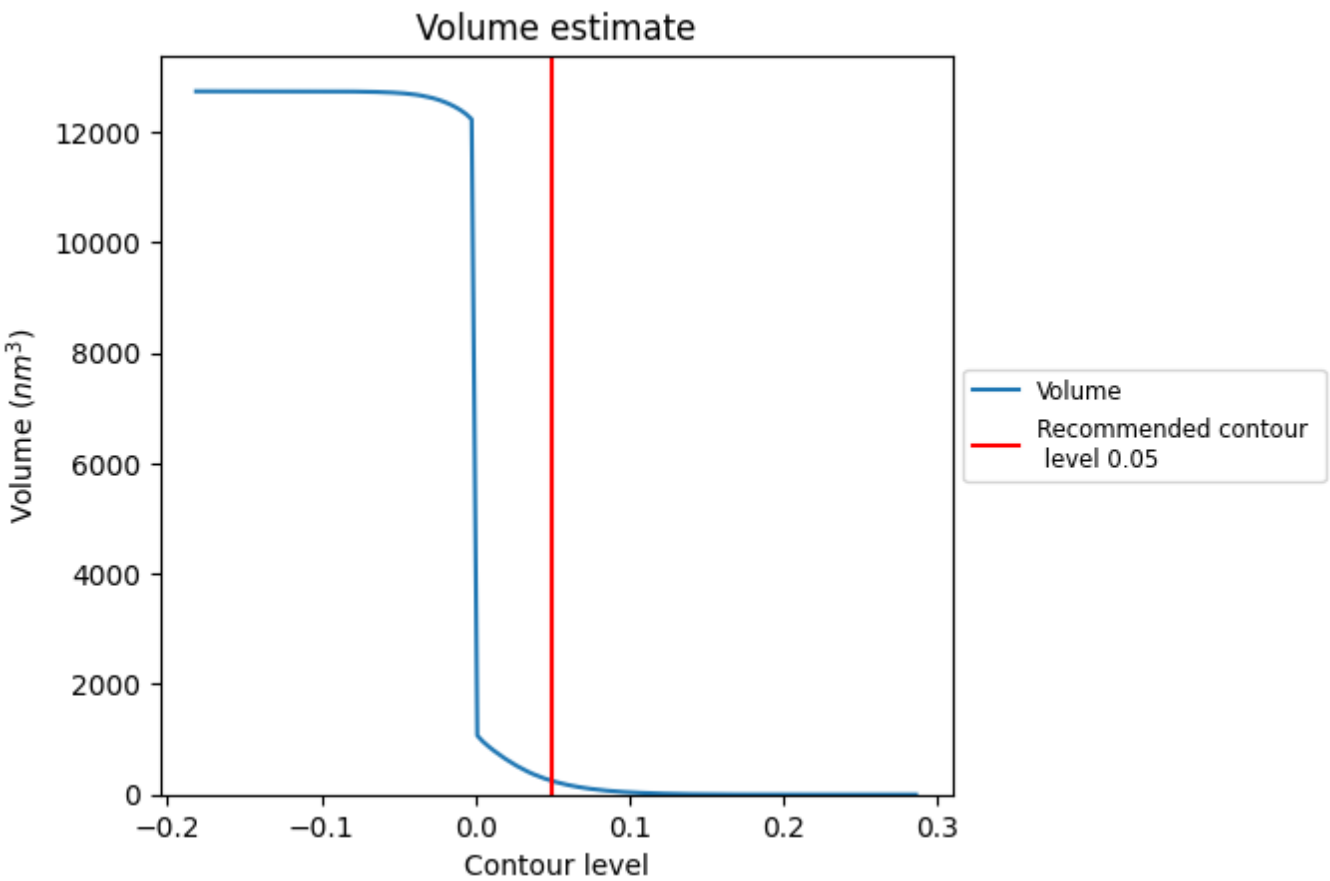
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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.

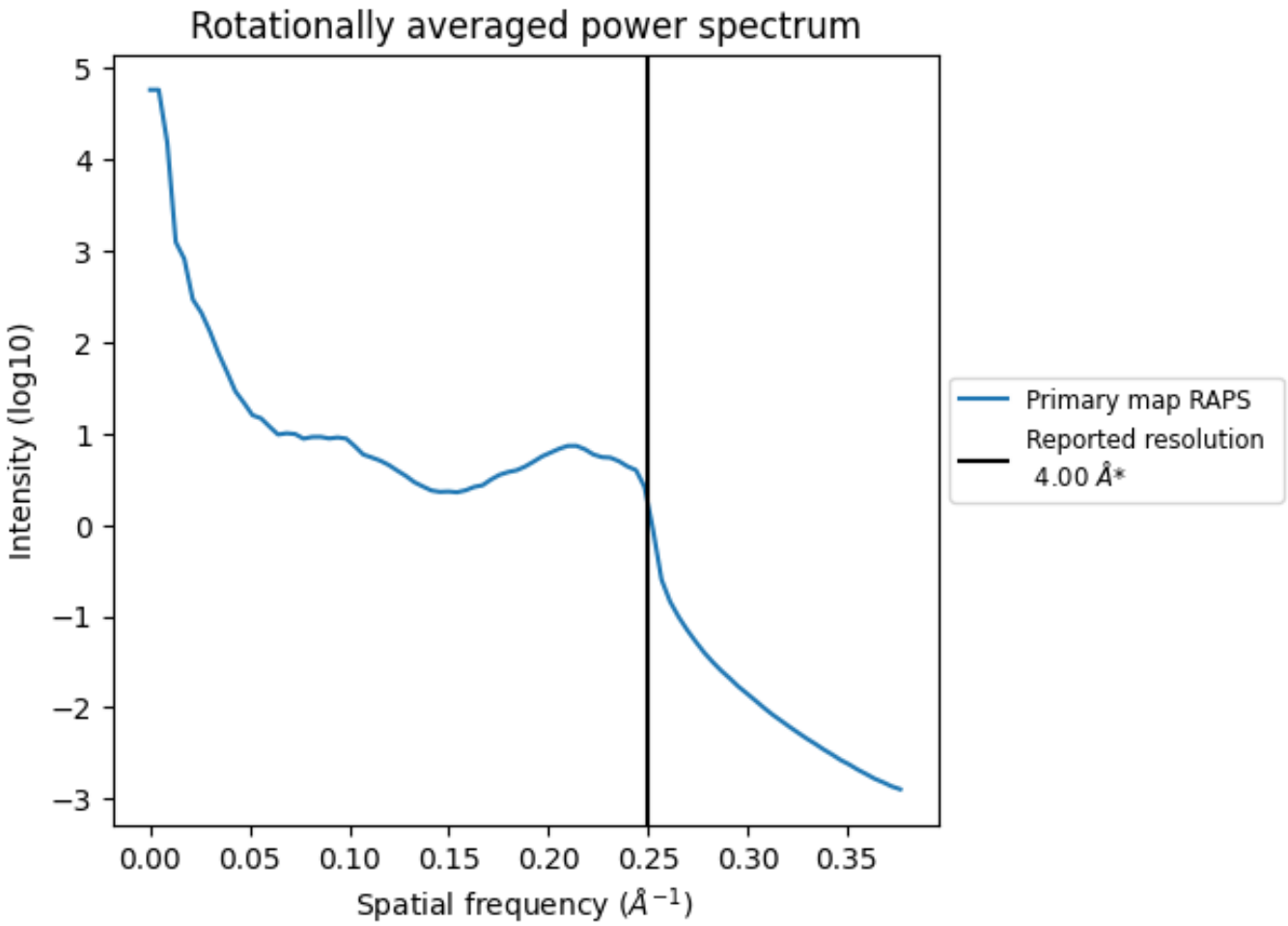
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 247 $nm^3$; this corresponds to an approximate mass of 223 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 0.250 Å$^{-1}$

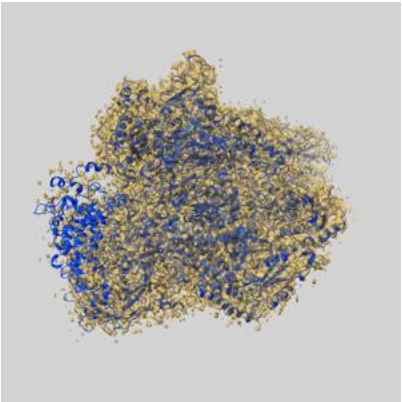
# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

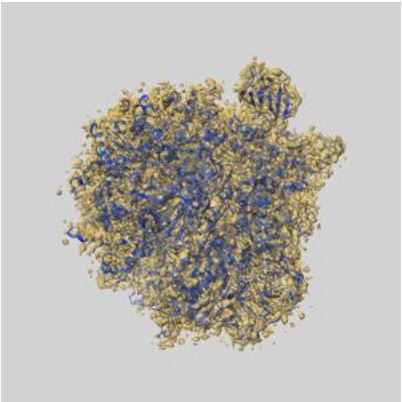
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4985 and PDB model 6RQT. Per-residue inclusion information can be found in section 3 on page 7.

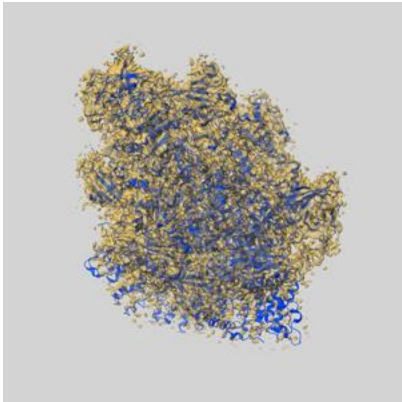
## 9.1 Map-model overlay (i)



X



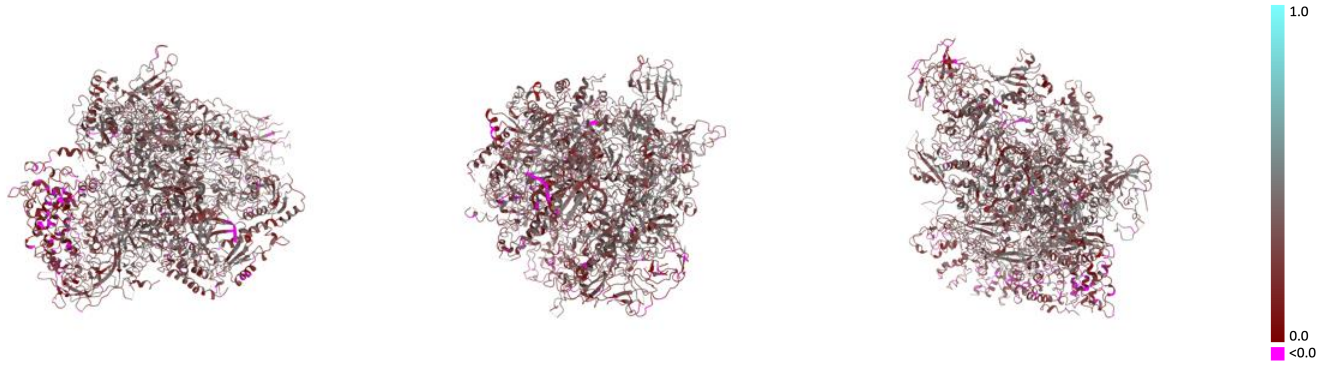
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

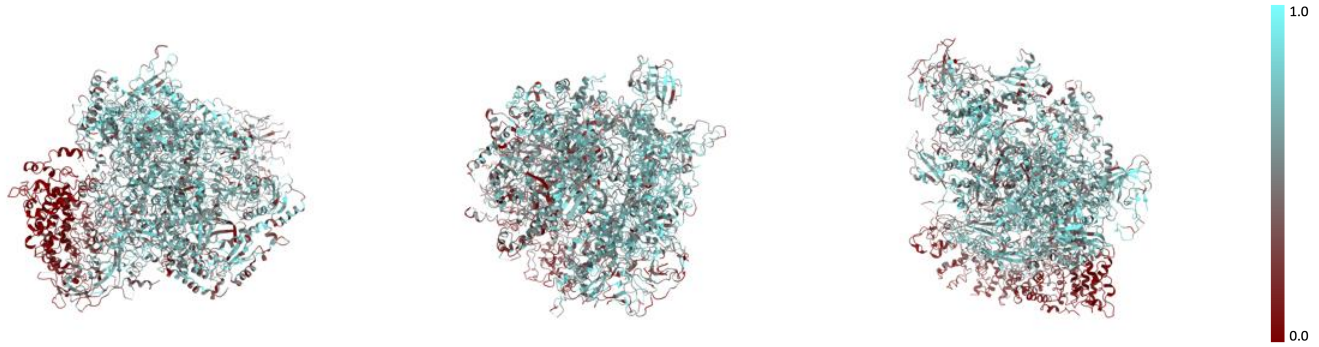
## 9.2 Q-score mapped to coordinate model (i)




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.

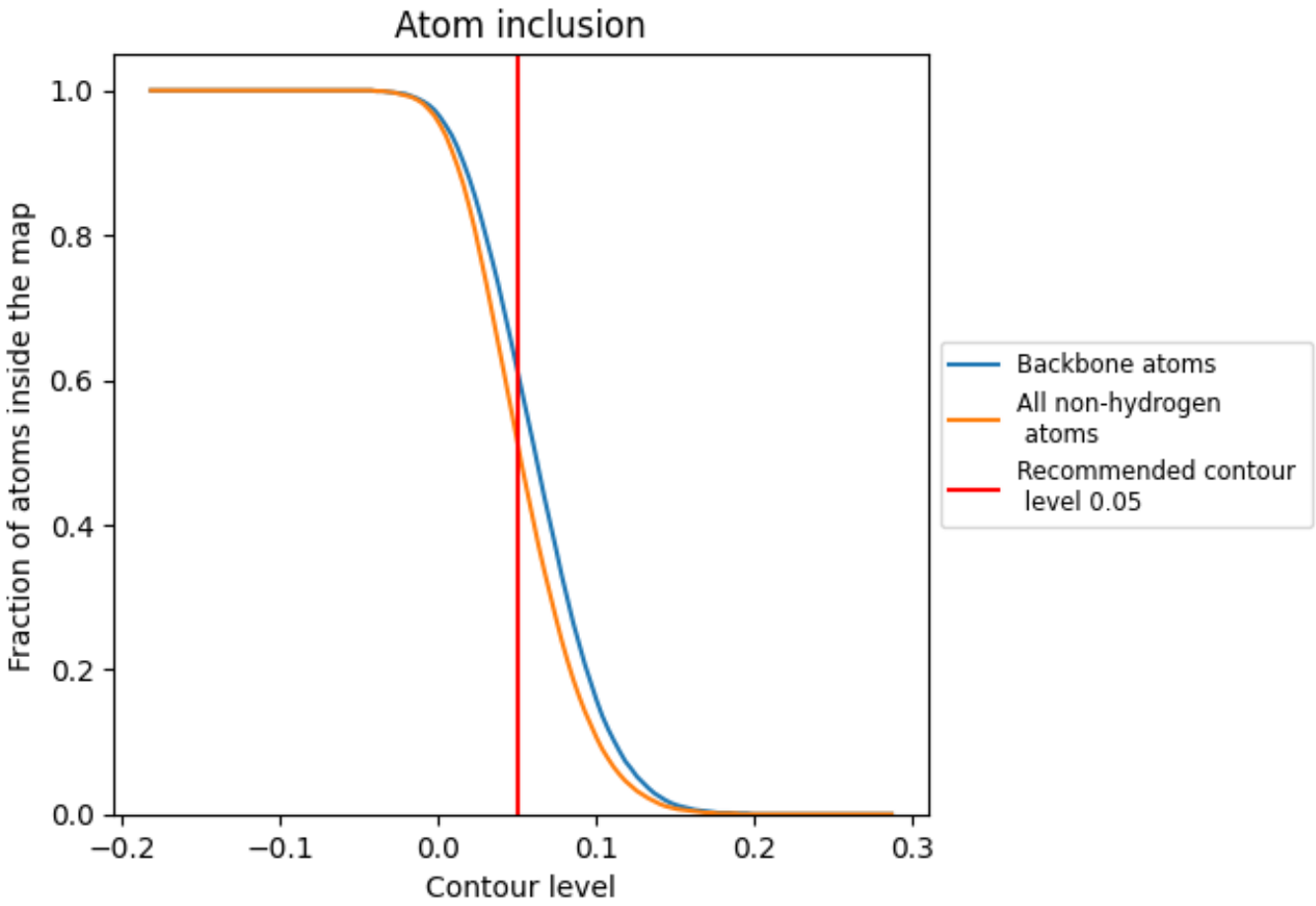
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.05).

## 9.4 Atom inclusion (i)




At the recommended contour level, 62% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5160 | 0.2950 |
| A | 0.6030 | 0.3270 |
| B | 0.6300 | 0.3340 |
| C | 0.6380 | 0.3400 |
| D | 0.4040 | 0.2660 |
| E | 0.5860 | 0.3040 |
| F | 0.6120 | 0.3580 |
| G | 0.4050 | 0.2720 |
| H | 0.6290 | 0.3260 |
| I | 0.5130 | 0.3020 |
| J | 0.6740 | 0.3220 |
| K | 0.6130 | 0.3220 |
| L | 0.5270 | 0.2890 |
| M | 0.2760 | 0.2050 |
| N | 0.4870 | 0.2550 |
| O | 0.0590 | 0.1670 |
| T | 0.3820 | 0.1360 |
| U | 0.3480 | 0.1270 |