# wwPDB EM Validation Summary Report (i)

Mar 6, 2024 – 12:46 PM JST

| | | |
|---|---|---|
| PDB ID | : | 1XI5 |
| EMDB ID | : | EMD-5120 |
| Title | : | Clathrin D6 coat with auxilin J-domain |
| Authors | : | Fotin, A.; Cheng, Y.; Grigorieff, N.; Walz, T.; Harrison, S.C.; Kirchhausen, T. |
| Deposited on | : | 2004-09-21 |
| Resolution | : | 12.00 Å(reported) |
| Based on initial models | : | 1B89, 1BPO, 1N4C |

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:

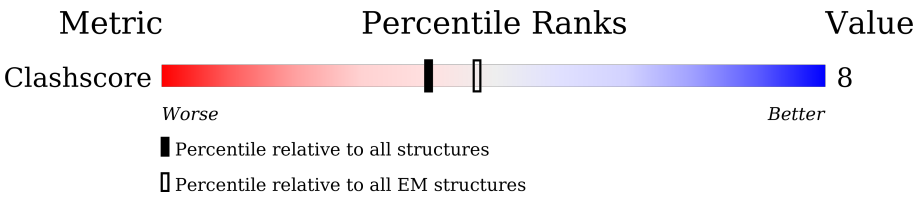
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 12.00 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 |

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 | 1630 | 32% 99% |
| 1 | B | 1630 | 39% 99% |
| 1 | C | 1630 | 34% 98% |
| 1 | D | 1630 | 36% 98% |
| 1 | E | 1630 | 28% 99% |
| 1 | F | 1630 | 38% 98% |
| 1 | G | 1630 | 41% 98% |
| 1 | H | 1630 | 33% 99% |
| 1 | I | 1630 | 47% 99% |
| 2 | J | 114 | 97% 100% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | K | 114 | 100% / 100% |
| 2 | L | 114 | 100% / 100% |
| 2 | M | 114 | 96% / 100% |
| 2 | N | 114 | 99% / 100% |
| 2 | O | 114 | 89% / 100% |
| 2 | P | 114 | 100% / 100% |
| 2 | Q | 114 | 96% / 100% |
| 2 | R | 114 | 98% / 100% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15696 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 Clathrin heavy chain.

| Mol | Chain | Residues | Atoms | | AltConf | Trace |
|---|---|---|---|---|---|---|
| | | | Total | C | | |
| 1 | A | 1630 | 1630 | 1630 | 0 | 1630 |
| 1 | B | 1630 | 1630 | 1630 | 0 | 1630 |
| 1 | C | 1630 | 1630 | 1630 | 0 | 1630 |
| 1 | D | 1630 | 1630 | 1630 | 0 | 1630 |
| 1 | E | 1630 | 1630 | 1630 | 0 | 1630 |
| 1 | F | 1630 | 1630 | 1630 | 0 | 1630 |
| 1 | G | 1630 | 1630 | 1630 | 0 | 1630 |
| 1 | H | 1630 | 1630 | 1630 | 0 | 1630 |
| 1 | I | 1630 | 1630 | 1630 | 0 | 1630 |

- Molecule 2 is a protein called Auxilin J-domain.

| Mol | Chain | Residues | Atoms | | AltConf | Trace |
|---|---|---|---|---|---|---|
| | | | Total | C | | |
| 2 | J | 114 | 114 | 114 | 0 | 114 |
| 2 | K | 114 | 114 | 114 | 0 | 114 |
| 2 | L | 114 | 114 | 114 | 0 | 114 |
| 2 | M | 114 | 114 | 114 | 0 | 114 |
| 2 | N | 114 | 114 | 114 | 0 | 114 |
| 2 | O | 114 | 114 | 114 | 0 | 114 |

*Continued on next page...*

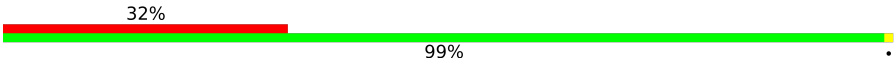
*Continued from previous page...*

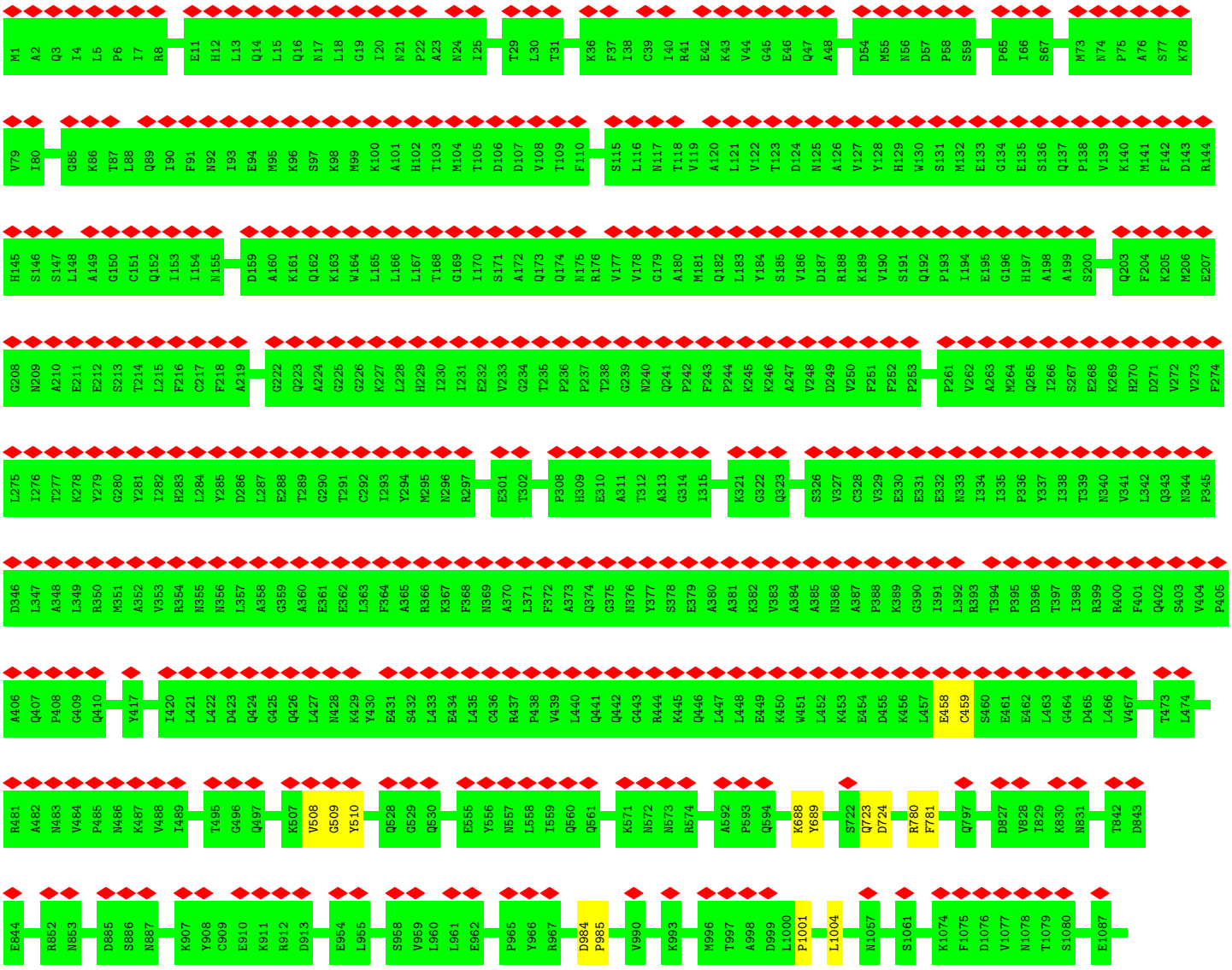
| Mol | Chain | Residues | Atoms | | AltConf | Trace |
|---|---|---|---|---|---|---|
| | | | Total | C | | |
| 2 | P | 114 | 114 | 114 | 0 | 114 |
| | | | Total | C | | |
| 2 | Q | 114 | 114 | 114 | 0 | 114 |
| | | | Total | C | | |
| 2 | R | 114 | 114 | 114 | 0 | 114 |

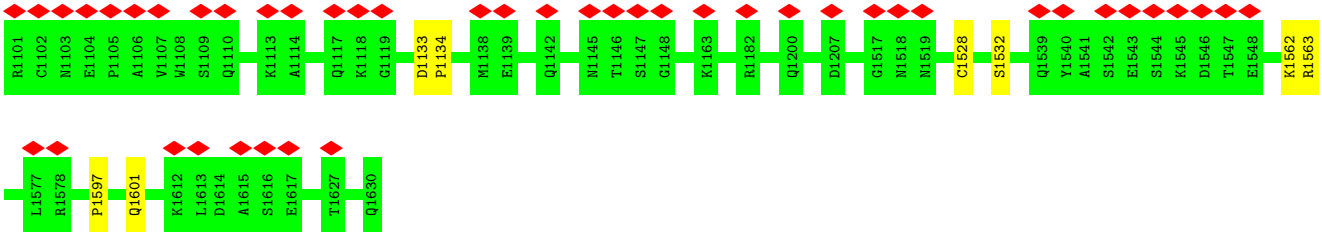
# 3 Residue-property plots (i)

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: Clathrin heavy chain

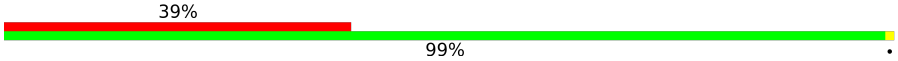
Chain A: 

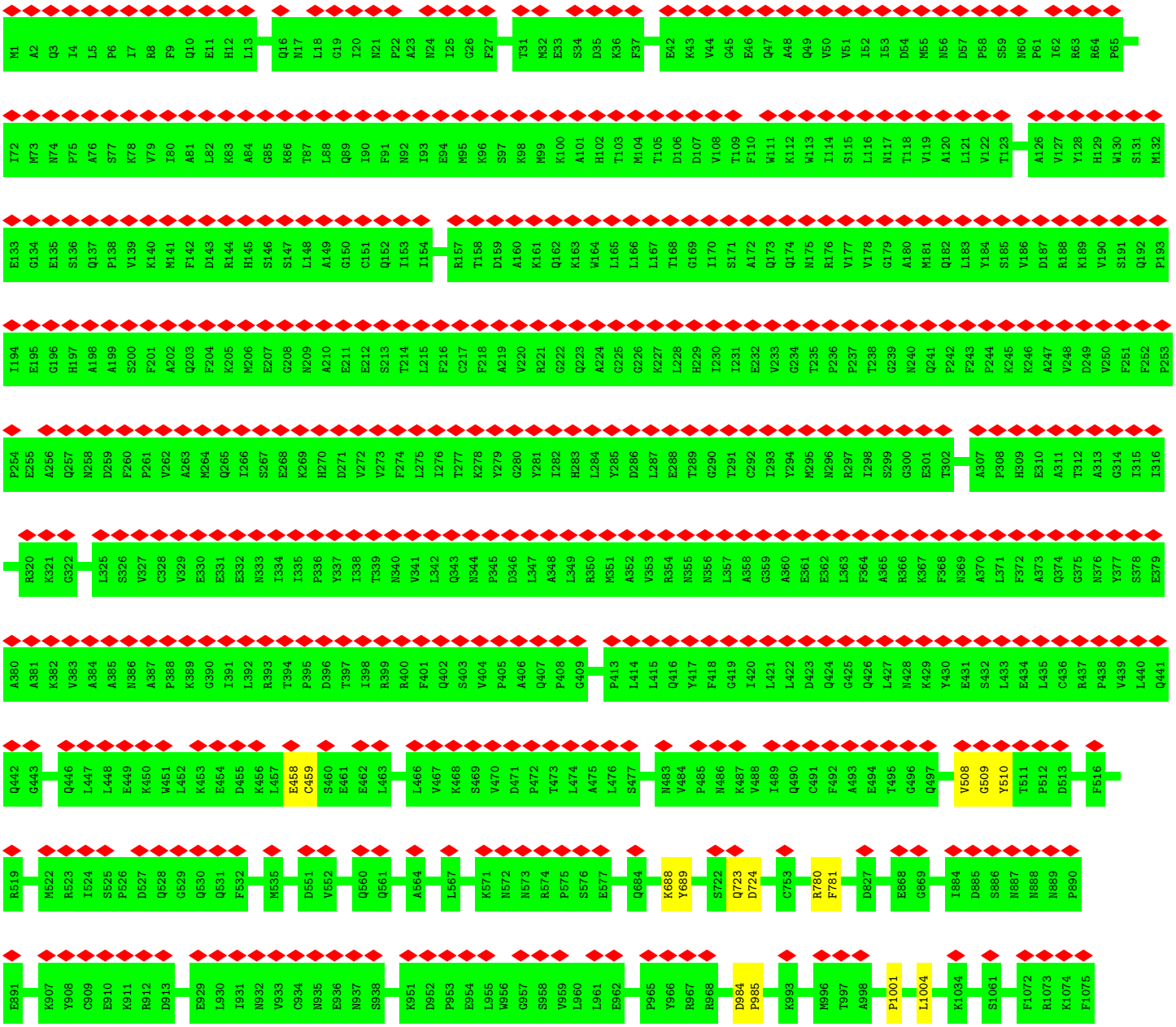



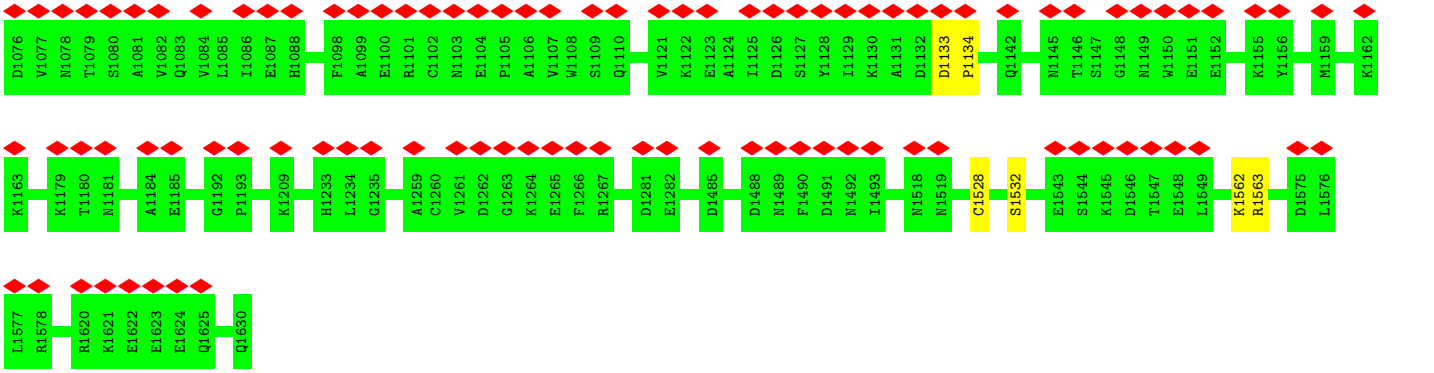



- Molecule 1: Clathrin heavy chain

Chain B:

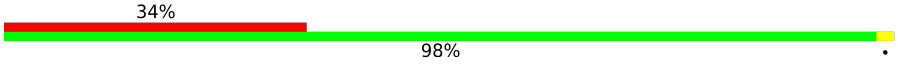


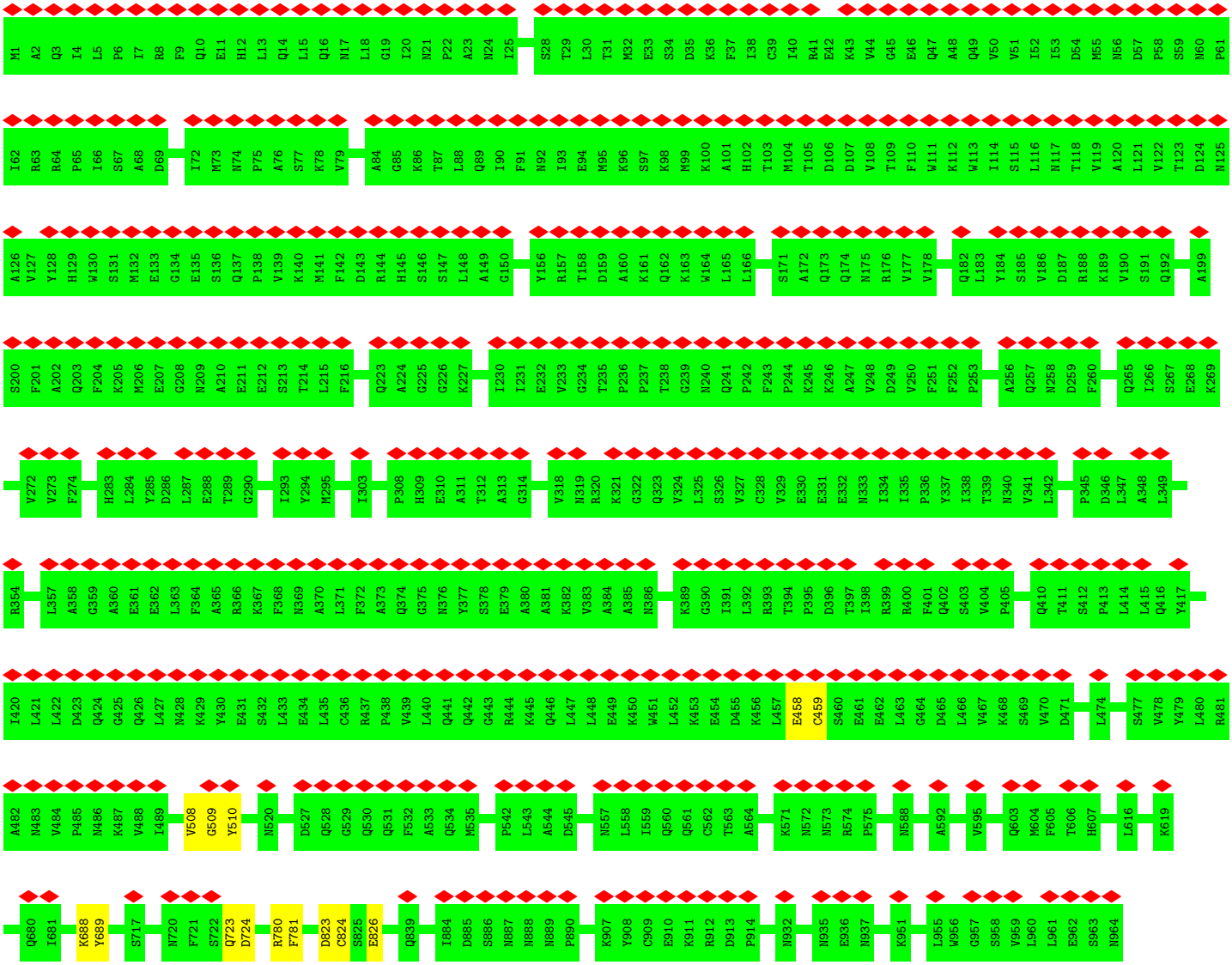






- Molecule 1: Clathrin heavy chain

Chain C:



P965 Y966 R967 R968 D984 P985 E986 E987 V990 M996 T997 A998 D999 K1034 P1053 I1060 S1061 N1062 E1063 F1075 D1076 V1077 N1078 T1079 S1080 Q1083 I1086 E1087 H1088 I1089 R1101 C1102 N1103 E1104 P1105 A1106 V1107 W1108 S1109 Q1110 L1111 A1112 K1113 A1114 Q1115 L1116 Q1117 K1118 G1119 M1120

V1121 D1133 P1134 M1138 E1139 T1146 S1147 G1148 N1149 K1254 G1273 L1274 H1275 I1276 V1277 V1278 F1471 I1472 T1473 E1474 E1475 D1476 Y1477 Q1478 A1479 L1480 R1481 T1482 S1483 I1484 D1485 A1486 E1506 C1528 S1532 Q1539 Y1540 A1541 S1542 E1543 S1544 K1545 D1546 T1547 E1548 L1549 A1550 E1551 E1552

Q1555 K1562 R1563 L1576 L1577 D1580 E1584 Q1630

- Molecule 1: Clathrin heavy chain

Chain D: 36% 98%

M1 A2 Q3 I4 L5 P6 I7 R8 F9 Q10 E11 H12 L13 Q14 L15 Q16 N17 L18 G19 I20 N21 P22 A23 N24 I25 G26 F27 S28 T29 L30 T31 M32 E33 S34 D35 K36 F37 I38 C39 I40 R41 E42 K43 V44 G45 E46 Q47 A48 Q49 V50 V51 I52 I53 D54 M55 N56 D57 P58 S59 N60

P61 I62 R63 R64 P65 I66 S67 A68 D69 S70 A71 I72 M73 N74 P75 A76 S77 K78 V79 I80 A81 L82 K83 A84 G85 K86 T87 L88 Q89 I90 F91 N92 I93 E94 M95 K96 S97 K98 M99 K100 A101 H102 T103 M104 T105 D106 D107 V108 T109 F110 W111 K112 W113 I114 S115 L116 N117 T118 V119 A120

L121 V122 T123 D124 N125 A126 V127 Y128 H129 W130 S131 M132 E133 G134 E135 S136 Q137 P138 V139 K140 M141 F142 D143 R144 H145 S146 S147 L148 A149 G150 C151 Q152 I153 I154 N155 Y156 R157 T158 D159 A160 K161 Q162 K163 W164 L165 L166 L167 T168 G169 I170 S171 A172 Q173 Q174 N175 R176 V177 V178 G179 A180

M181 Q182 L183 Y184 S185 V186 D187 R188 K189 V190 S191 Q192 P193 I194 E195 G196 H197 A198 A199 S200 F201 A202 Q203 F204 K205 M206 E207 G208 N209 A210 E211 E212 S213 T214 L215 F216 C217 F218 A219 V220 R221 G222 Q223 A224 G225 G226 K227 L228 H229 I230 I231 E232 V233 G234 T235 P236 P237 T238 G239 N240

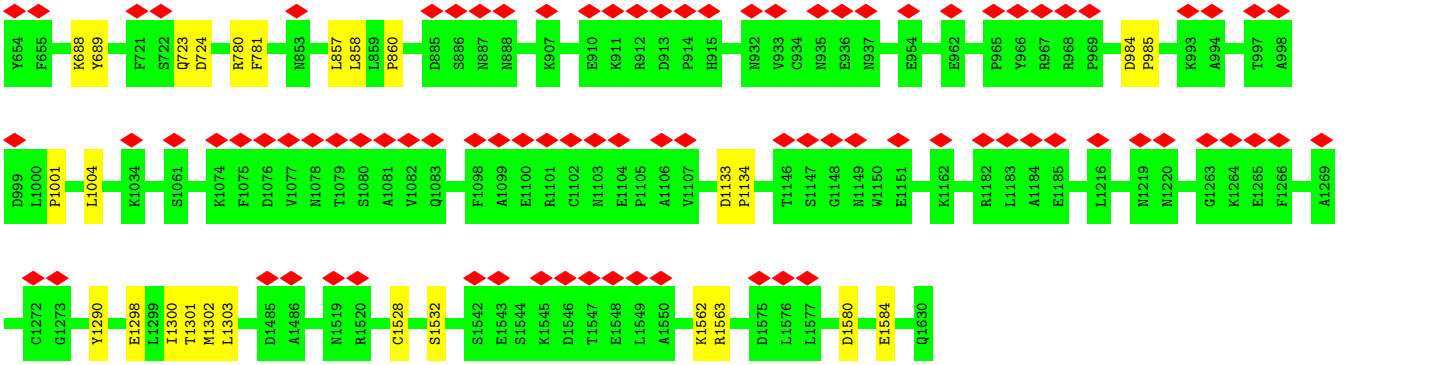
Q241 P242 F243 P244 K245 K246 A247 V248 D249 V250 F251 F252 P253 P254 E255 A256 Q257 N258 D259 F260 P261 V262 A263 M264 Q265 I266 S267 E268 K269 H270 D271 V272 V273 F274 K278 Y279 Y285 D286 L287 E288 T289 G290 T291 C292 I293 Y294 M295 N296 R297 I298 S299 G300 E301 T302 I303 F304 V305 T306

A307 P308 H309 E310 A311 T312 A313 G314 I315 I316 G317 R320 K321 G322 Q323 V324 L325 S326 V327 C328 V329 E330 E331 E332 N333 I334 I335 P336 Y337 I338 T339 N340 V341 L342 Q343 N344 P345 D346 L347 A348 L349 R350 M351 A352 N356 L357 A358 G359 A360 E361 E362 L363 R366 K367 F368 N369 A370

L371 F372 A373 Q374 G375 N376 Y377 S378 E379 K382 V383 A384 A385 N386 A387 P388 K389 G390 I391 L392 R393 T394 P395 D396 T397 I398 R399 R400 F401 Q402 S403 V404 P405 A406 Q410 T411 S412 P413 L414 L415 Q416 Y417 F418 G419 I420 L421 L422 D423 Q424 G425 Q426 L427 N428 K429 Y430 E431 S432 L433

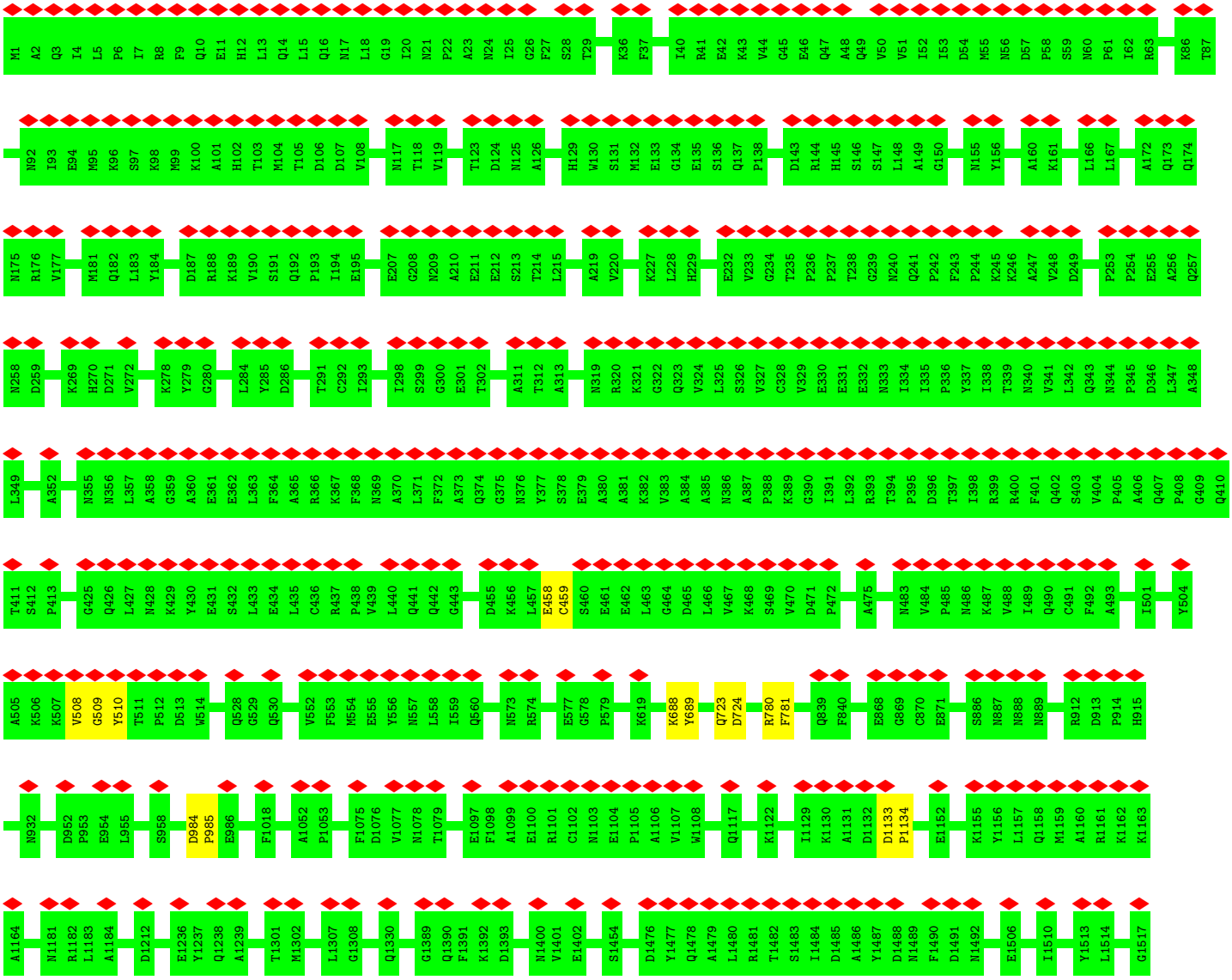
Q441 Q442 G443 R444 K445 Q446 L447 L448 E449 K450 W451 L452 K453 E454 D455 K456 L457 E458 C459 S460 E461 E462 L463 G464 D465 L466 V467 K468 S469 V470 D471 P472 T473 L474 N483 V484 P485 N486 K487 V488 T495 G496 K500 I501 V502 L503 Y504 A505 K506 K507 V508 G509 Y510 R523 I524

S525 P526 D527 Q528 G529 Q530 Q531 F532 A533 Q534 M535 Q538 E541 P542 E555 Y556 N557 L558 I559 Q560 Q561 C562 T563 A564 F565 L566 L567 D568 A569 L570 K571 N572 N573 R574 P575 S576 E577 G578 P579 Q594 V595 A598 N602 C617 A620 G621 L622 E649 W650 L651




- Molecule 1: Clathrin heavy chain

Chain E: 28% 99%



N1518 C1528 S1532 Q1539 Y1540 A1541 S1542 E1543 S1544 K1545 D1546 T1547 E1548 K1562 R1563 L1577 R1578 P1597 Q1601 K1612 Q1630

- Molecule 1: Clathrin heavy chain

Chain F: 38% 98%

M1 A2 Q3 I4 L5 P6 I7 R8 F9 Q10 E11 H12 L13 Q14 L15 N21 P22 A23 N24 T29 L30 T31 M32 E33 S34 D35 K36 F37 I38 C39 I40 R41 E42 K43 V44 G45 E46 Q47 A48 Q49 V50 V51 I52 I53 D54 M55 N56 D57 P58 S59 N60 P61 I62 R63 R64 P65 I66 S67

A68 D69 S70 A71 I72 M73 N74 P75 A76 S77 K78 V79 I80 A81 L82 K83 A84 G85 K86 T87 L88 Q89 I90 F91 N92 I93 E94 M95 K96 S97 K98 M99 K100 A101 H102 T103 M104 T105 D106 D107 V108 T109 F110 W111 K112 W113 I114 S115 L116 N117 T118 V119 A120 L121 V122 T123 D124 N125 A126 V127

Y128 H129 W130 S131 M132 E133 G134 E135 S136 Q137 P138 V139 K140 M141 F142 D143 R144 H145 S146 S147 L148 A149 G150 C151 Q152 I153 I154 N155 Y156 R157 T158 D159 A160 K161 Q162 K163 L167 T168 G169 I170 S171 A172 Q173 Q174 N175 R176 V177 V178 G179 A180 M181 Q182 L183 Y184 S185 V186 D187 R188 K189

V190 S191 Q192 P193 I194 E195 G196 H197 F201 A202 Q203 F204 K205 M206 E207 G208 N209 A210 E211 E212 S213 T214 L215 F216 C217 F218 A219 V220 R221 G222 Q223 A224 G225 G226 K227 L228 H229 I230 I231 E232 V233 G234 T235 P236 P237 T238 G239 N240 Q241 P242 F243 P244 K245 K246 A247 V248 D249 F252

P253 P254 E255 A256 Q257 N258 D259 F260 P261 V262 A263 S267 E268 K269 H270 T277 K278 Y279 E288 T289 G290 Y294 M295 A307 P308 H309 E310 A311 T312 A313 G314 I315 I316 G317 K321 G322 Q323 V324 L325 S326 V327 C328 V329 E330 E331 E332 N333 I334 I335 P336 T339 N340

Q343 N344 P345 D346 L347 A348 L349 R350 M351 A352 V353 R354 N355 N356 L357 A358 G359 A360 E361 E362 L363 F364 A365 R366 K367 F368 N369 A370 L371 F372 A373 Q374 G375 N376 Y377 S378 E379 A380 A381 K382 V383 A384 A385 N386 A387 P388 K389 G390 I391 L392 R393 T394 P395 D396 T397 I398 R399 R400 F401 Q402

S403 V404 Q407 P408 G409 Q410 T411 S412 P413 L414 L415 Q416 Y417 F418 G419 I420 L421 L422 D423 Q424 G425 Q426 L427 N428 K429 Y430 E431 S432 L433 E434 L435 C436 R437 P438 V439 L440 Q441 Q442 G443 R444 K445 Q446 L447 L448 E449 K450 W451 L452 K453 E454 D455 K456 L457 E458 C459 S460 E461 E462 L463

G464 D465 L466 T473 L474 A475 L476 S477 V478 Y479 L480 R481 A482 N483 V484 P485 G496 V508 G509 Y510 T511 P512 S525 P526 D527 Q530 Q531 F532 Q538 D539 E540 E541 P542 K571 N572 N573 R574 F575 S576 E577 K688 Y689 N720 F721 S722 Q723 D724 N752 R780

F781 Q839 F840 S841 T842 D843 E844 A847 W861 G869 A880 K881 I882 Y883 I884 D885 S886 N887 N888 N889 P890 E891 R892 F893 L894 R895 R903 V904 K907 Y908 C909 E910 K911 R912 D913 P914 H915 L916 D927 L928 E929 L930 I931 N932 V933 C934 N935 E936 N937 S938 L943

Y946 L947 V948 R949 R950 K951 D952 P953 E954 L955 W956 G957 S958 L961 E962 S963 N964 P965 Y966 R967 R968 P969 L970 I971 D984 P985 E986 E987 V988 S989 V990 K993 A994 F995 M996 T997 A998 D999 L1000 N1023 P1053 D1054 I1055 A1056 N1057 I1058 S1061 K1074 F1075 D1076 V1077 N1078

T1079 S1080 Q1083 I1086 E1087 H1088 E1100 R1101 C1102 N1103 E1104 P1105 A1106 V1107 W1108 S1109 Q1110 L1111 A1112 K1113 A1114 Q1115 L1116 Q1117 K1118 G1119 M1120 D1133 P1134 M1138 E1139 V1140 V1141 Q1142 A1143 T1146 S1147 N1181 R1182 L1286 Y1290 Q1291 D1292 R1293 E1298 L1299 I1300 K1331

E1334 H1335 L1336 E1337 K1367 K1441 P1450 N1457 H1458 Q1478 R1481 T1482 S1483 I1484 D1485 A1486 Y1487 D1488 D1491 S1494 R1498 C1528 S1532 K1535 D1536 Q1539 Y1540 A1541 S1542 E1543 S1544 K1545 D1546 T1547 K1562 R1563 L1576 L1577 R1578 K1609 K1612 L1613 D1614

A1615 S1616 E1617 R1620 Q1630

- Molecule 1: Clathrin heavy chain

Chain G: 41% 98%

M1 A2 Q3 I4 L5 P6 I7 R8 F9 Q10 E11 H12 L13 Q14 L15 Q16 N17 L18 G19 I20 N21 P22 A23 F27 S28 T31 M32 E33 S34 D35 K36 F37 I38 R41 E42 K43 V44 G45 E46 Q47 A48 Q49 V50 V51 I52 I53 D54 M55 N56 D57 P58 S59 M60 P61 I62 R63 R64

P65 I66 S67 A68 D69 S70 A71 I72 M73 N74 P75 A76 S77 K78 V79 I80 A81 L82 K83 A84 G85 K86 T87 L88 Q89 I90 F91 N92 I93 E94 M95 K96 S97 K98 M99 K100 A101 H102 T103 M104 T105 D106 K112 W113 I114 S115 L116 N117 T118 V119 A120 T123 D124 N125 A126 V127 Y128 H129

W130 S131 M132 E133 G134 E135 S136 Q137 P138 V139 K140 M141 F142 D143 R144 H145 S146 S147 L148 A149 G150 I154 N155 Y156 R157 T158 D159 A160 K161 Q162 K163 W164 L165 L166 L167 T168 Q173 Q174 A180 M181 Q182 L183 Y184 S185 V186 D187 R188 K189 V190 S191 Q192 P193 I194 E195 G196 H197 A198

A199 S200 F201 A202 Q203 F204 K205 M206 E207 G208 N209 A210 E211 E212 S213 T214 L215 F216 C217 F218 A219 G222 Q223 A224 G225 H229 I230 I231 E232 V233 G234 T235 P236 P237 T238 G239 N240 Q241 P242 F243 P244 K245 K246 A247 V248 D249 V250 F251 F252 P253 P254 E255 A256 Q257 N258 D259 F260 P261

V262 A263 M264 Q265 I266 S267 E268 K269 H270 D271 V272 V273 F274 L275 K278 Y279 H283 L284 Y285 D286 L287 E288 T289 G290 T291 C292 I293 Y294 M295 N296 R297 I298 S299 G300 E301 F304 V305 T306 A307 P308 H309 E310 A311 T312 A313 G314 I315 I316 G317 V318 N319 R320 K321 G322 Q323 S326

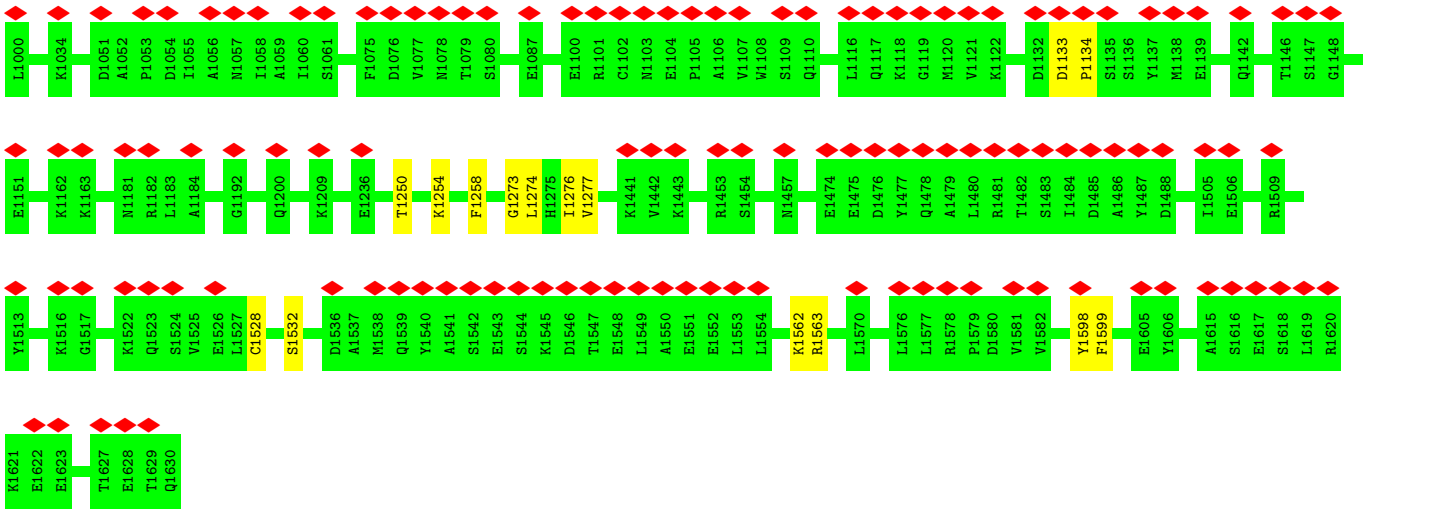
V327 C328 V329 E330 E331 E332 N333 I334 I335 P336 Y337 I338 T339 N340 V341 L342 Q343 N344 P345 D346 L347 A348 L349 R350 M351 A352 V353 R354 N355 N356 L357 A358 G359 A360 E361 E362 L363 F364 A365 R366 K367 F368 N369 A370 L371 F372 A373 Q374 G375 N376 Y377 S378 E379 A380 A381 K382 V383 A384 A385 N386

A387 P388 K389 G390 I391 L392 R393 T394 P395 D396 T397 I398 R399 R400 F401 Q402 S403 V404 P405 A406 Q407 P408 G409 Q410 T411 S412 P413 L414 L415 Q416 Y417 F418 G419 I420 L421 L422 D423 Q424 G425 Q426 L427 N428 K429 Y430 E431 S432 L433 E434 L435 C436 R437 P438 V439 L440 Q441 Q442 G443 R444 K445 Q446

L447 L448 E449 K450 W451 L452 K453 E454 D455 K456 L457 E458 C459 S460 E461 E462 L463 G464 D465 L466 V467 K468 S469 V470 D471 P472 T473 L474 A475 L476 S477 V478 Y479 L480 R481 A482 N483 V484 P485 N486 K487 V488 F492 A493 E494 T495 G496 Q497 V498 Q499 K500 K506 K507 V508 G509 Y510 N520

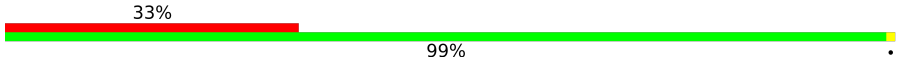
V521 I524 S525 P526 D527 Q528 G529 Q530 Q531 F532 A533 D539 E540 E541 P542 N557 L558 I559 Q560 L567 D568 A569 L570 K571 N572 N573 R574 P575 S576 E577 H591 A592 D609 W650 L651 F655 S659 V660 E661 D662 K688 Y689 S722 Q723 D724 P725 C753

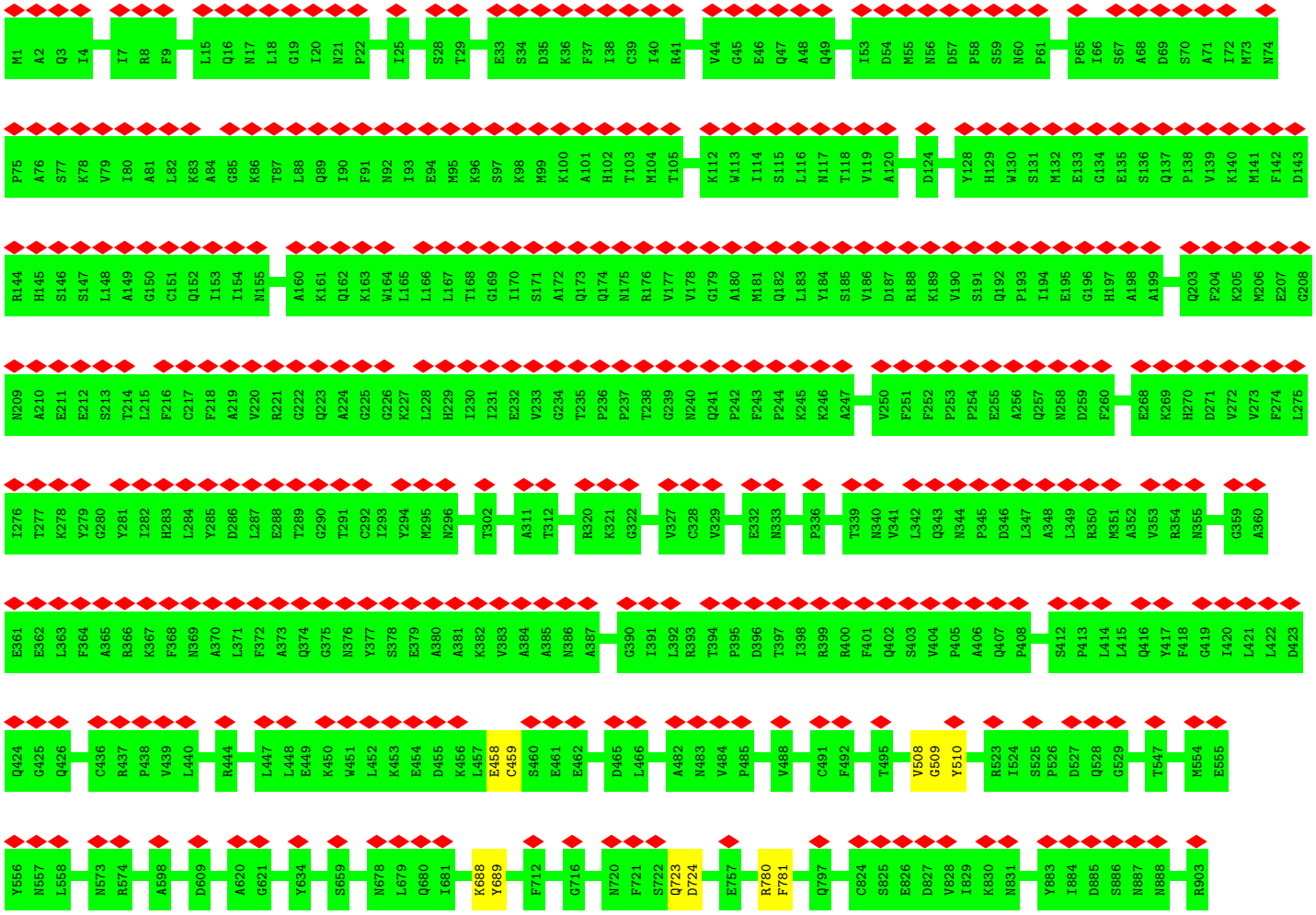
R780 F781 L820 N831 D885 S886 N887 M888 K907 Y908 C909 E910 K911 R912 D913 P914 H915 N935 E936 N937 D952 P953 E954 L955 W956 G957 S958 L961 E962 S963 N964 P965 Y966 R967 R968 P969 D984 P985 E986 E987 V988 S989 V990 T991 V992 K993 A994 F995 M996 T997 A998 D999




- Molecule 1: Clathrin heavy chain

Chain H:



K907 Y908 C909 E910 K911 R912 D913 P914 H915 L928 E929 L930 I931 N932 V933 C934 N935 E936 N937 V948 R949 R950 K951 D952 P953 E954 L955 S958 L961 E962 P965 Y966 R967 R968 D984 P985 E986 E987 V988 S989 V990 T991 V992 K993 A994 F995 M996 T997 A998 D999 L1000 P1001

H1021 R1022 K1034 A1035 P1053 D1054 N1057 F1069 A1070 I1071 F1072 R1073 K1074 F1075 D1076 V1077 N1078 T1079 S1080 A1081 V1082 Q1083 I1086 E1087 H1088 I1089 G1090 N1091 L1092 F1098 A1099 E1100 R1101 C1102 N1103 E1104 P1105 A1106 V1107 Q1110 L1111 V1121 K1122 E1123 D1133 P1134 E1139 T1146 S1147

G1148 R1161 K1162 K1163 K1179 T1180 N1181 R1182 L1183 A1184 E1188 N1191 D1207 E1208 K1331 M1332 R1333 E1334 H1335 L1336 N1457 A1486 Y1487 K1522 Q1523 C1528 S1532 S1542 E1543 S1544 K1545 D1546 T1547 E1548 L1549 A1550 E1551 K1562 R1563 L1576 L1577 R1578 P1579 T1608 K1609

V1610 D1611 K1612 L1613 L1619 E1622 Q1630

- Molecule 1: Clathrin heavy chain

Chain I: 47% 99%

M1 A2 Q3 I4 L5 P6 I7 R8 F9 Q10 E11 H12 L13 Q14 L15 Q16 N17 L18 G19 I20 N21 P22 A23 N24 I25 G26 F27 S28 T29 L30 T31 M32 E33 S34 D35 K36 F37 I38 C39 I40 R41 E42 K43 V44 G45 E46 Q47 A48 Q49 V50 V51 I52 I53 D54 M55 N56 D57 P58 S59 N60

P61 I62 R63 R64 P65 I66 S67 A68 D69 S70 A71 I72 M73 N74 P75 A76 S77 K78 V79 I80 A81 L82 K83 A84 G85 K86 T87 L88 Q89 I90 F91 N92 I93 E94 M95 K96 S97 K98 M99 K100 A101 H102 T103 M104 T105 D106 D107 V108 T109 F110 W111 K112 W113 I114 S115 L116 N117 T118 V119 A120

L121 V122 T123 D124 N125 A126 V127 Y128 H129 W130 S131 M132 E133 G134 E135 S136 Q137 P138 V139 K140 M141 F142 D143 R144 H145 S146 S147 L148 A149 G150 C151 Q152 I153 I154 N155 Y156 R157 T158 D159 A160 K161 Q162 K163 W164 L165 L166 L167 T168 G169 I170 S171 A172 Q173 Q174 N175 R176 V177 V178 G179 A180

M181 Q182 L183 Y184 S185 V186 D187 R188 K189 V190 S191 Q192 P193 I194 E195 G196 H197 A198 A199 S200 F201 A202 Q203 F204 K205 M206 E207 G208 N209 A210 E211 E212 S213 T214 L215 F216 C217 F218 A219 V220 R221 G222 Q223 A224 G225 G226 K227 L228 H229 I230 I231 E232 V233 G234 T235 P236 P237 T238 G239 N240

Q241 P242 F243 P244 K245 K246 A247 V248 D249 V250 F251 F252 P253 P254 E255 A256 Q257 N258 D259 F260 P261 M264 Q265 I266 S267 E268 K269 H270 D271 V272 V273 F274 L275 G280 Y281 I282 H283 L284 Y285 D286 L287 E288 T289 G290 T291 C292 M295 N296 R297 I298 S299 G300 E301 T302 I303 F304 V305

T306 A307 P308 H309 E310 A311 T312 A313 G314 I315 I316 G317 V318 N319 R320 K321 G322 Q323 V324 L325 S326 V327 C328 V329 G330 E331 E332 N333 I334 I335 P336 V337 I338 T339 N340 V341 L342 Q343 N344 P345 D346 L347 A348 L349 R350 M351 A352 V353 R354 N355 N356 L357 A358 G359 A360 E361 E362 L363 F364 A365

R366 K367 F368 N369 A370 L371 F372 A373 Q374 G375 N376 Y377 S378 E379 A380 A381 K382 V383 A384 A385 N386 A387 P388 K389 G390 I391 L392 R393 T394 P395 D396 T397 I398 R399 R400 F401 Q402 S403 V404 P405 A406 Q407 P408 G409 Q410 T411 S412 P413 L414 L415 Q416 Y417 F418 G419 I420 L421 L422 D423 Q424 G425

Q426 L427 N428 K429 Y430 E431 S432 L433 E434 L435 C436 R437 P438 V439 L440 Q441 Q442 G443 R444 K445 Q446 L447 L448 E449 K450 W451 L452 K453 E454 D455 K456 L457 E458 C459 S460 E461 E462 L463 G464 D465 L466 V467 K468 S469 V470 D471 P472 T473 L474 A475 L476 S477 V478 Y479 L480 R481 A482 N483 V484 P485

C491 F492 A493 E494 T495 Q499 L503 K506 K507 V508 G509 Y510 N520 V521 M522 R523 I524 S525 P526 D527 Q528 G529 Q530 Q531 F532 A533 Q534 M535 L536 V537 Q538 D539 E540 E541 P542 L543 Y556 N557 L558 Q561 C562 T563 A564 F565 L566 L567 D568 A569 L570 K571 N572 N573 R574

P575 S576 E577 G578 P593 Q594 D597 A598 G601 N602 H607 K619 A620 D635 I636 K637 E561 D662 S663 K688 Y689 S722 Q723 D724 R749 R780 F781 Q797 D827 V828 I829 K830 N831 A847 E848 K856 L857 L858 L859 L879 A880 K881 I882 Y883

I884 D885 S886 N887 N888 N889 P890 E891 R892 F893 R903 V904 V905 G906 K907 Y908 C909 E910 K911 R912 D913 P914 H915 L916 A917 C918 V919 A920 Y921 E922 Q925 C926 D927 L928 E929 L930 I931 N932 V933 C934 N935 E936 N937 K951 D952 P953 E954 L955 W956 G957 S958 V959 L960 L961 E962 S963 N964

P965 Y966 R967 R968 P969 D984 P985 E986 E987 V988 S989 V990 T991 V992 K993 A994 F995 M996 T997 A998 D999 L1000 N1015 R1022 A1052 P1053 K1074 F1075 D1076 V1077 N1078 T1079 Q1083 I1086 E1087 D1093 E1097 F1098 A1099 E1100 R1101 C1102 N1103 E1104 P1105 A1106 V1107 Q1110 G1119

M1120 V1121 K1122 E1123 D1126 I1129 K1130 A1131 D1132 D1133 P1134 T1146 S1147 G1148 N1149 W1150 E1151 E1152 K1155 Y1156 L1157 Q1158 M1159 A1160 R1161 K1162 K1163 A1164 R1165 T1180 N1181 E1187 E1188 F1189 I1190 N1191 G1192 P1193 N1194 K1209 M1210 Y1211 D1212 A1213 N1219 L1234 G1235 E1236 Y1237 Q1238 A1239

D1242 F1266 R1267 Q1270 M1271 E1334 E1337 K1441 Q1456 N1457 H1458 N1459 D1485 A1486 Y1487 D1491 S1494 G1517 N1518 N1519 R1520 W1521 K1522 E1526 L1527 C1528 S1532 S1542 E1543 S1544 K1545 D1546 T1547 E1548 L1549 A1550 E1551 E1552 L1553 L1554 Q1555 K1562 R1563 C1573

Y1574 D1575 L1576 L1577 R1578 P1579 D1580 V1581 V1582 L1583 E1584 T1585 A1586 W1587 R1588 K1609 V1610 D1611 K1612 L1613 R1620 K1621 E1622 E1623 E1624 Q1625 Q1630

- Molecule 2: Auxilin J-domain

Chain J: 97% 100%

P797 R798 T799 I800 A801 E802 M803 R804 K805 E806 E807 E811 M812 D813 P814 E815 K816 L817 K818 I819 L820 E821 W822 I823 E824 G825 K826 E827 R828 N829 I830 R831 A832 L833 L834 S835 T836 M837 H838 T839 V840 L841 W842 A843 G844 E845 T846 K847 W848 K849 P850 V851 G852 M853 A854 D855 L856 V857 T858

P859 E860 Q861 V862 K863 K864 V865 Y866 R867 K868 A869 V870 L871 V872 V873 H874 P875 D876 K877 A878 T879 G880 Q881 P882 Y883 E884 Q885 Y886 A887 K888 M889 I890 F891 M892 E893 L894 N895 D896 A897 W898 S899 E900 F901 E902 N903 Q904 G905 Q906 K907 P908 L909 Y910

- Molecule 2: Auxilin J-domain

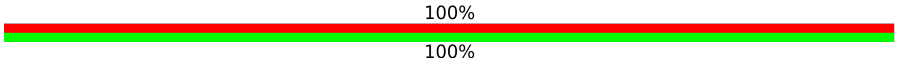
Chain K: 100% 100%

P797 R798 T799 I800 A801 E802 M803 R804 K805 E806 E807 M808 A809 K810 E811 M812 D813 P814 E815 K816 L817 K818 I819 L820 E821 W822 I823 E824 G825 K826 E827 R828 N829 I830 R831 A832 L833 L834 S835 T836 M837 H838 T839 V840 L841 W842 A843 G844 E845 T846 K847 W848 K849 P850 V851 G852 M853 A854 D855 L856

V857 T858 P859 E860 Q861 V862 K863 K864 V865 Y866 R867 K868 A869 V870 L871 V872 V873 H874 P875 D876 K877 A878 T879 G880 Q881 P882 Y883 E884 Q885 Y886 A887 K888 M889 I890 F891 M892 E893 L894 N895 D896 A897 W898 S899 E900 F901 E902 N903 Q904 G905 Q906 K907 P908 L909 Y910

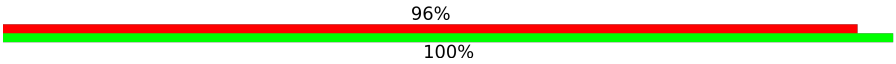
- Molecule 2: Auxilin J-domain

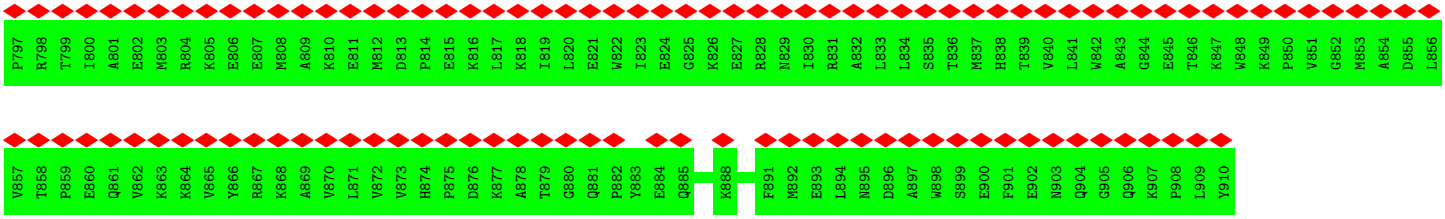
Chain L:



- Molecule 2: Auxilin J-domain

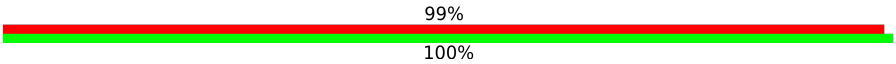
Chain M:




- Molecule 2: Auxilin J-domain

Chain N:

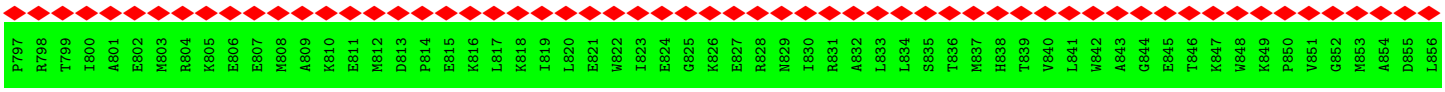


- Molecule 2: Auxilin J-domain

Chain O:

- Molecule 2: Auxilin J-domain

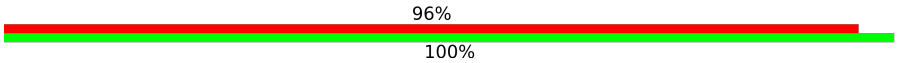
Chain P:



V857 T858 P859 E860 Q861 V862 K863 K864 V865 Y866 R867 K868 A869 V870 L871 V872 V873 H874 P875 D876 K877 A878 T879 G880 Q881 P882 Y883 E884 Q885 Y886 A887 K888 M889 I890 F891 M892 E893 L894 N895 D896 A897 W898 S899 E900 F901 E902 N903 Q904 G905 Q906 K907 P908 L909 Y910

- Molecule 2: Auxilin J-domain

Chain Q:

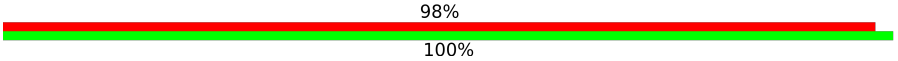



P797 R798 T799 I800 A801 E802 M803 R804 K805 E806 E807 M808 A809 K810 E811 M812 D813 P814 E815 K816 L817 K818 I819 L820 E821 W822 I823 E824 G825 K826 E827 R828 N829 I830 R831 A832 L833 L834 S835 T836 M837 H838 T839 V840 L841 W842 A843 G844 E845 T846 K847 W848 K849 P850 V851 G852 M853 A854 D855 L856

V857 T858 P859 E860 Q861 V862 K863 K864 V865 Y866 R867 K868 A869 V870 L871 V872 V873 H874 P875 D876 K877 A878 T879 G880 Q881 P882 Y883 E884 Q885 Y886 A887 K888 M889 I890 F891 M892 E893 L894 N895 D896 A897 W898 S899 E900 F901 E902 N903 Q904 G905 Q906 K907 P908 L909 Y910

- Molecule 2: Auxilin J-domain

Chain R:




P797 R798 T799 I800 A801 E802 M803 R804 K805 E806 E807 M808 A809 K810 E811 M812 D813 P814 E815 K816 L817 K818 I819 L820 E821 W822 I823 E824 G825 K826 E827 R828 N829 I830 R831 A832 L833 L834 S835 T836 M837 H838 T839 V840 L841 W842 A843 G844 E845 T846 K847 W848 K849 P850 V851 G852 M853 A854 D855 L856

V857 T858 P859 E860 Q861 V862 K863 K864 V865 Y866 R867 K868 A869 V870 L871 V872 V873 H874 P875 D876 K877 A878 T879 G880 Q881 P882 Y883 E884 Q885 Y886 A887 K888 M889 I890 F891 M892 E893 L894 N895 D896 A897 W898 S899 E900 F901 E902 N903 Q904 G905 Q906 K907 P908 L909 Y910

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, D6 | Depositor |
| Number of particles used | 900 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | CTFTILT, FREALIGN V.6.07 | Depositor |
| Microscope | FEI TECNAI F20 | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 20 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 5000 | Depositor |
| Magnification | 51160 | Depositor |
| Image detector | KODAK SO-163 FILM | Depositor |
| Maximum map value | 0.578 | Depositor |
| Minimum map value | -0.289 | Depositor |
| Average map value | 0.012 | Depositor |
| Map value standard deviation | 0.076 | Depositor |
| Recommended contour level | 0.25 | Depositor |
| Map size (Å) | 1075.2, 1075.2, 1075.2 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles (°) | 90, 90, 90 | wwPDB |
| Pixel spacing (Å) | 4.2, 4.2, 4.2 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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 | A | 1630 | 0 | 0 | 13 | 0 |
| 1 | B | 1630 | 0 | 0 | 11 | 0 |
| 1 | C | 1630 | 0 | 0 | 22 | 0 |
| 1 | D | 1630 | 0 | 0 | 23 | 0 |
| 1 | E | 1630 | 0 | 0 | 12 | 0 |
| 1 | F | 1630 | 0 | 0 | 19 | 0 |
| 1 | G | 1630 | 0 | 0 | 21 | 0 |
| 1 | H | 1630 | 0 | 0 | 11 | 0 |
| 1 | I | 1630 | 0 | 0 | 13 | 0 |
| 2 | J | 114 | 0 | 0 | 0 | 0 |
| 2 | K | 114 | 0 | 0 | 0 | 0 |
| 2 | L | 114 | 0 | 0 | 0 | 0 |
| 2 | M | 114 | 0 | 0 | 0 | 0 |
| 2 | N | 114 | 0 | 0 | 0 | 0 |
| 2 | O | 114 | 0 | 0 | 0 | 0 |
| 2 | P | 114 | 0 | 0 | 0 | 0 |
| 2 | Q | 114 | 0 | 0 | 0 | 0 |
| 2 | R | 114 | 0 | 0 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 15696 | 0 | 0 | 119 | 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 8.

The worst 5 of 119 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) |
|---|---|---|---|
| 1:F:1293:ARG:CA | 1:G:1258:PHE:CA | 1.88 | 1.50 |
| 1:C:1273:GLY:CA | 1:D:1298:GLU:CA | 1.87 | 1.49 |
| 1:F:1298:GLU:CA | 1:G:1273:GLY:CA | 1.98 | 1.42 |
| 1:C:1278:VAL:CA | 1:D:1303:LEU:CA | 2.05 | 1.33 |
| 1:F:951:LYS:CA | 1:H:951:LYS:CA | 2.07 | 1.32 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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)

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.

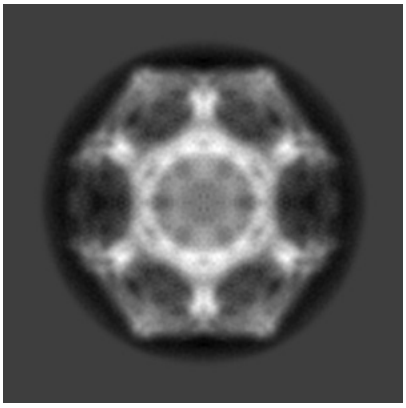
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5120. These allow visual inspection of the internal detail of the map and identification of artifacts.

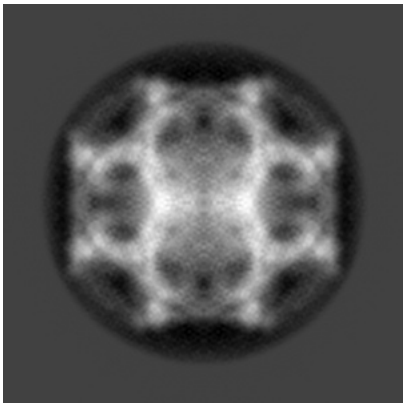
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

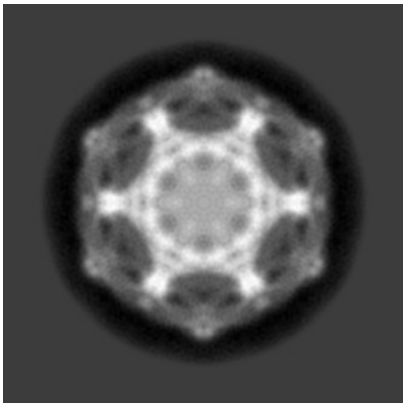
### 6.1.1 Primary map



X



Y

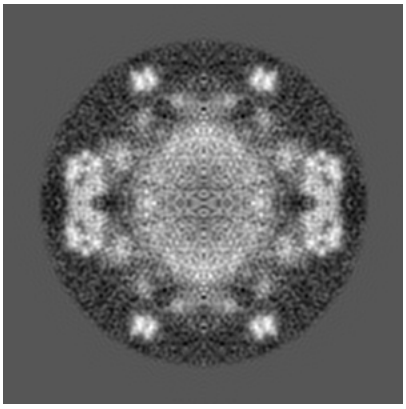


Z

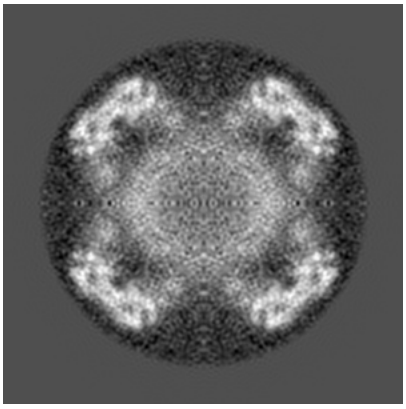
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

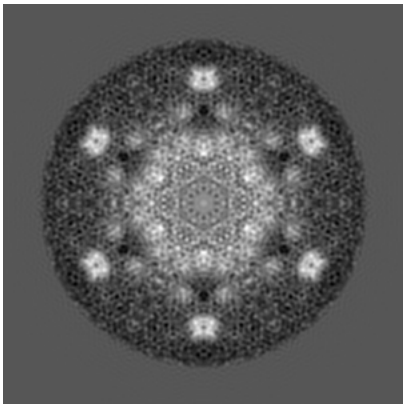
### 6.2.1 Primary map



X Index: 128



Y Index: 128

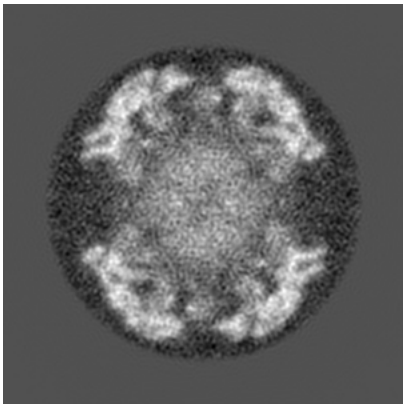


Z Index: 128

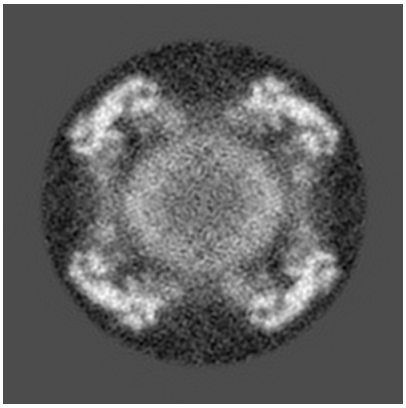
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

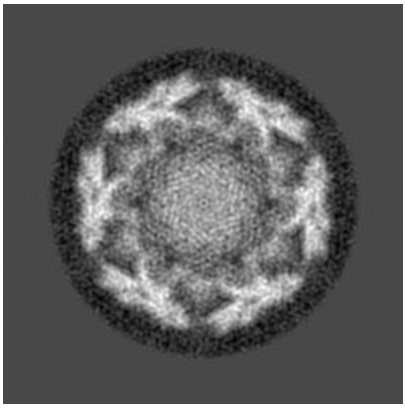
### 6.3.1 Primary map



X Index: 156



Y Index: 125

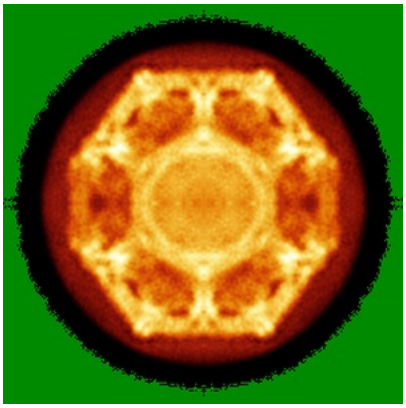


Z Index: 94

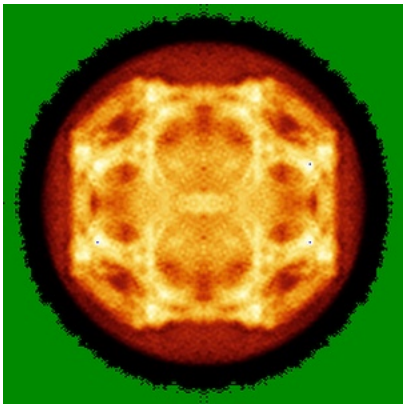
The images above show the largest variance slices of the map in three orthogonal directions.

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

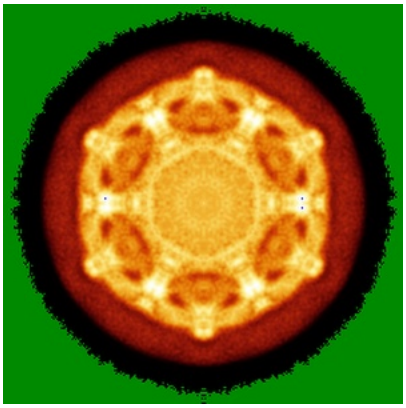
### 6.4.1 Primary map



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

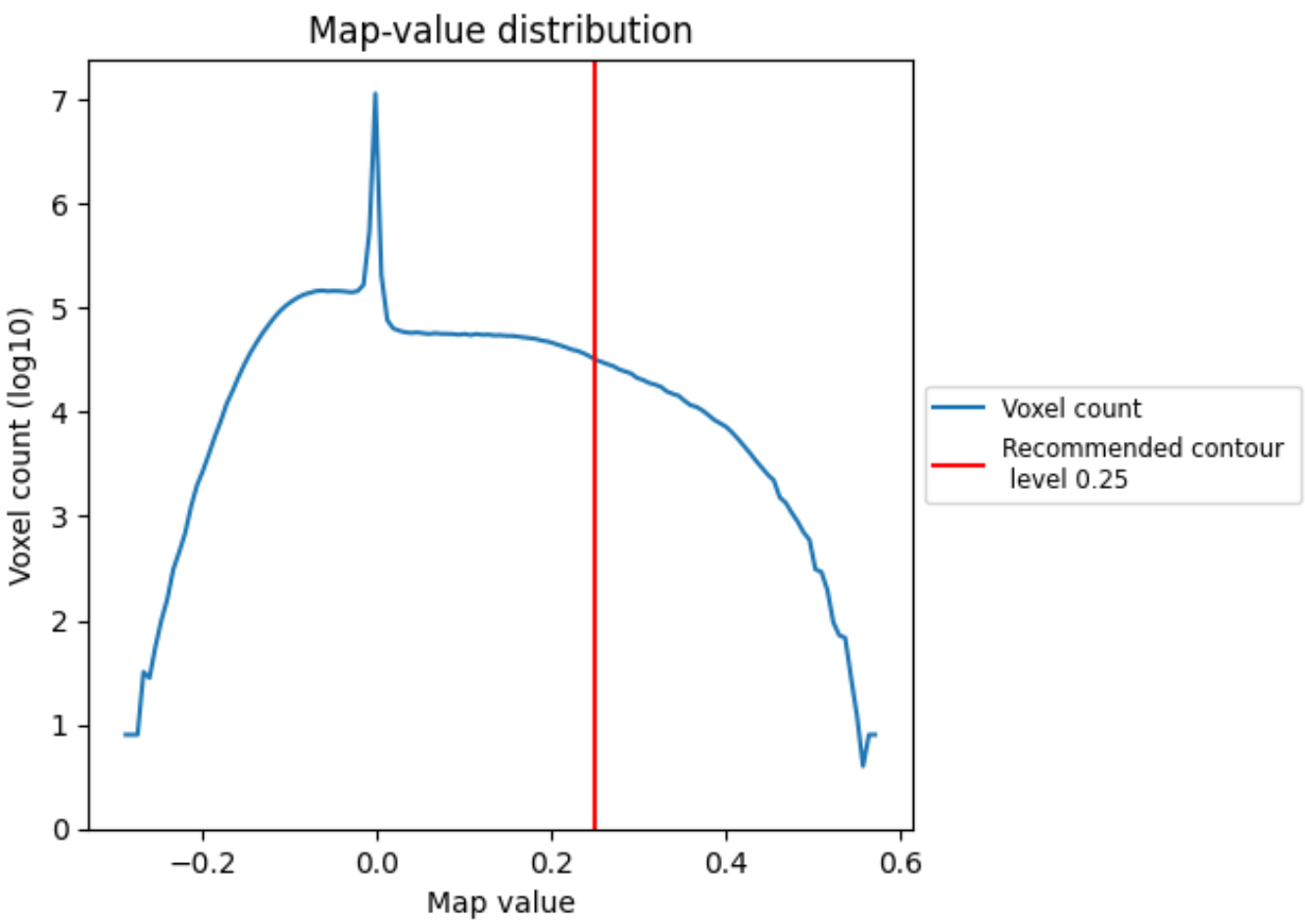
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

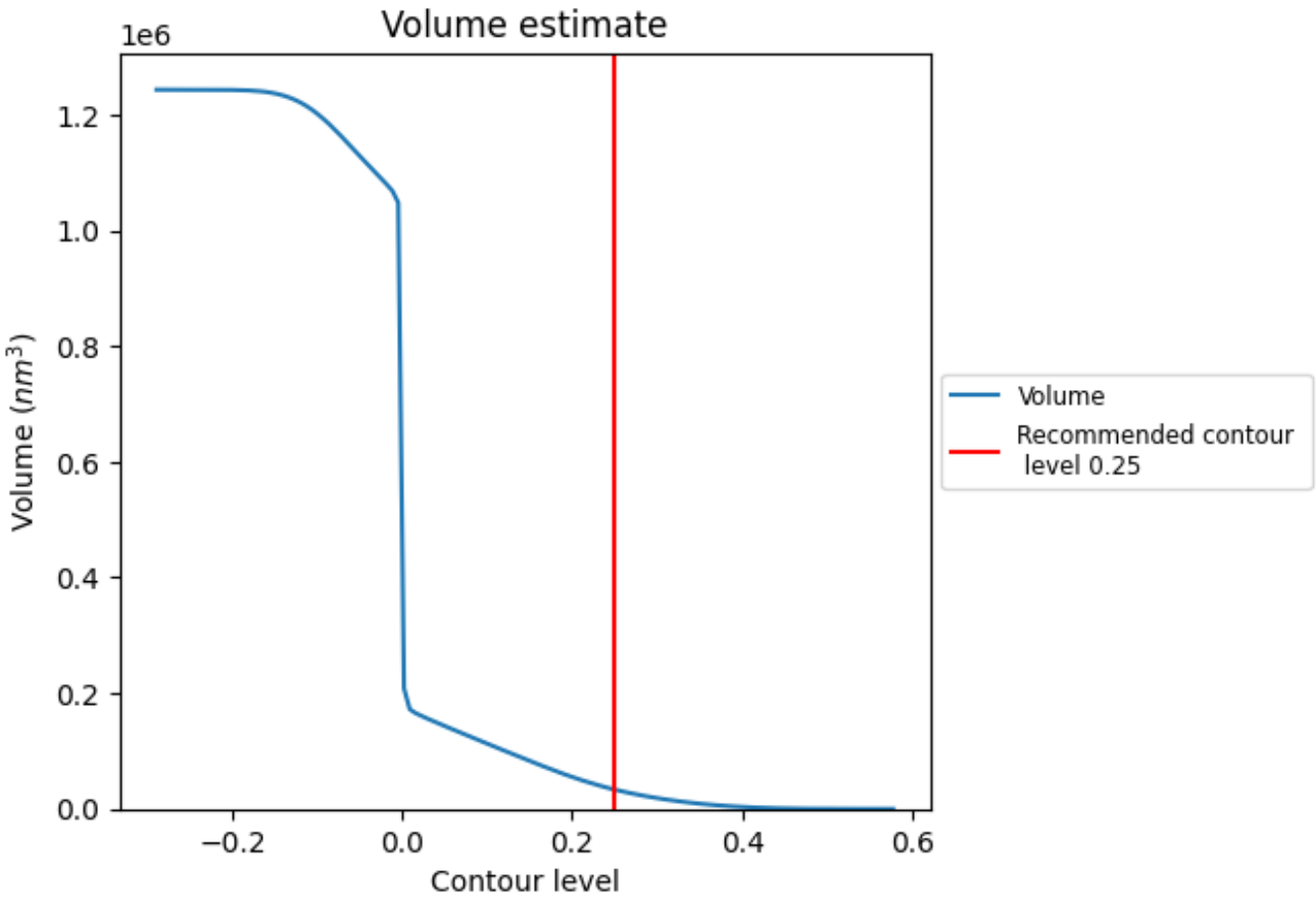
This section contains the results of statistical analysis of the map.

## 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.

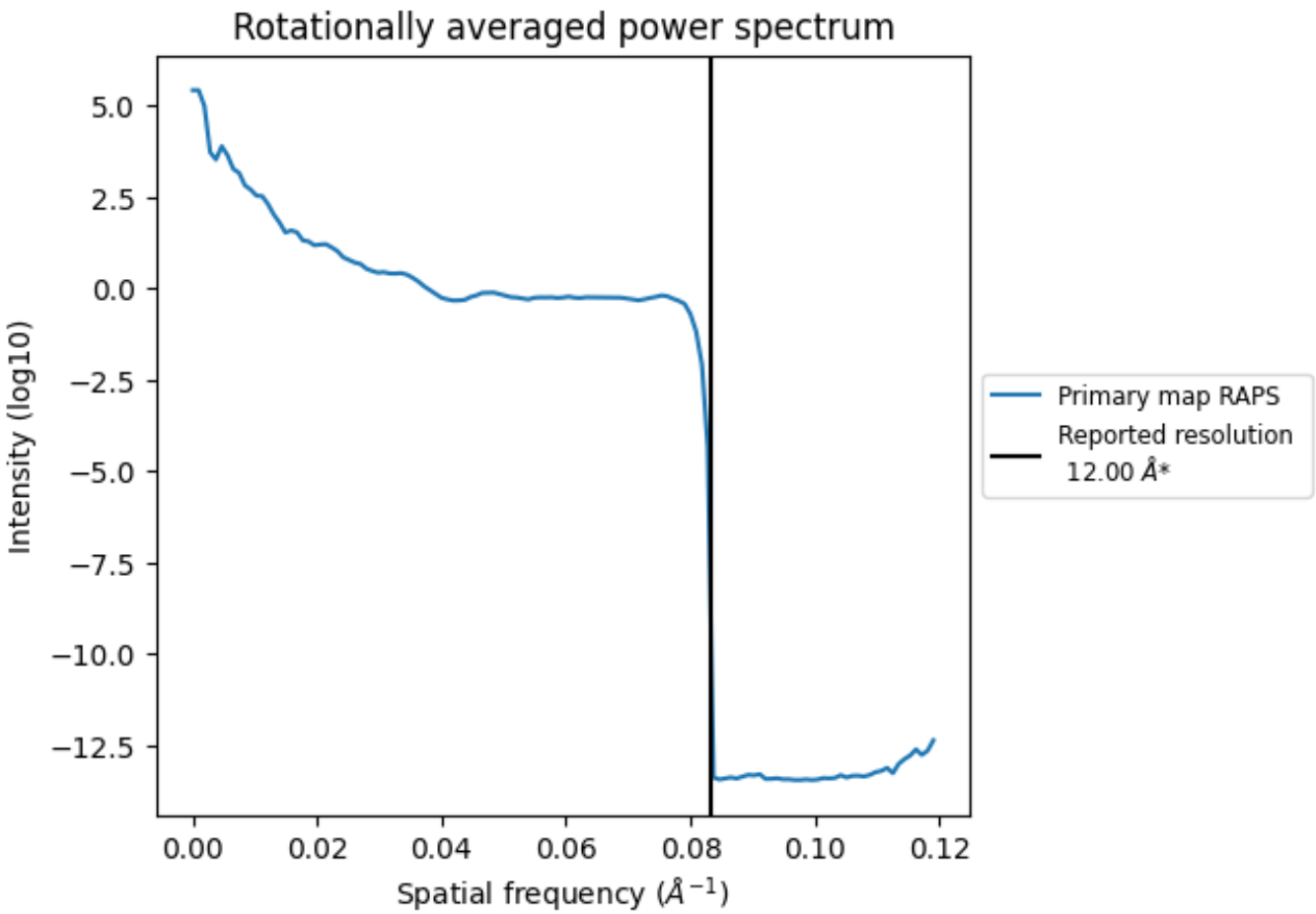
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 33428 $nm^3$; this corresponds to an approximate mass of 30197 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 0.083 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

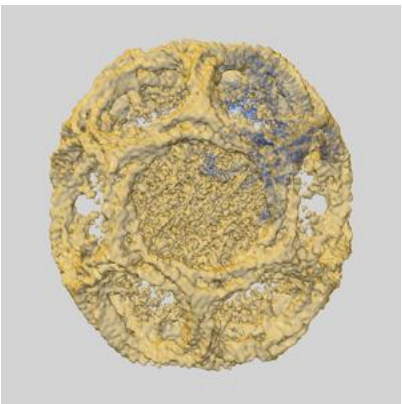
This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit (i)

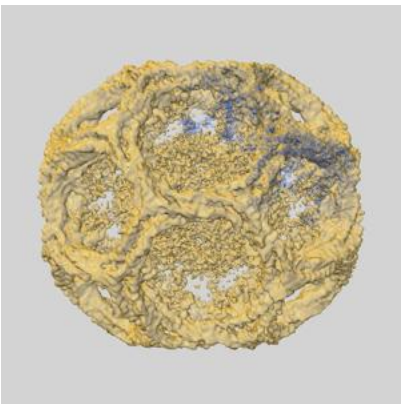
This section contains information regarding the fit between EMDB map EMD-5120 and PDB model 1XI5. Per-residue inclusion information can be found in section 3 on page 6.

## 9.1 Map-model overlays

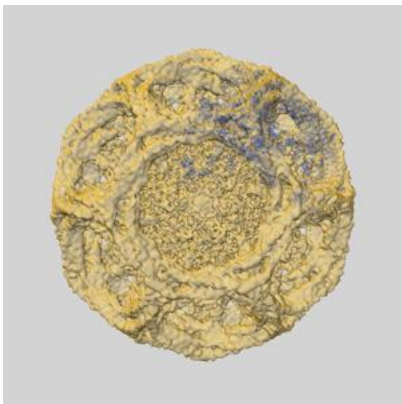
### 9.1.1 Map-model overlay (i)



X

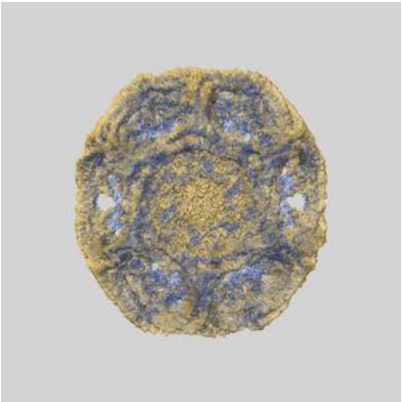


Y

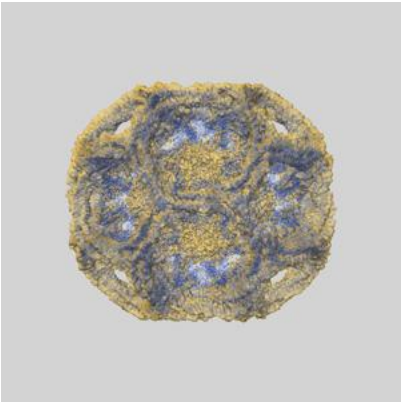


Z

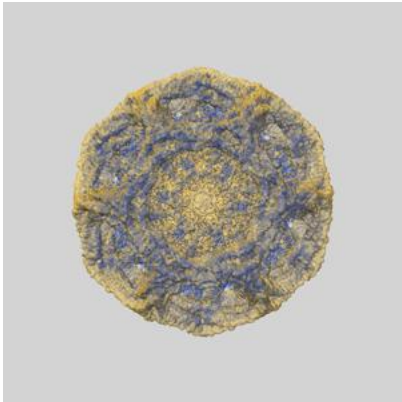
### 9.1.2 Map-model assembly overlay (i)



X



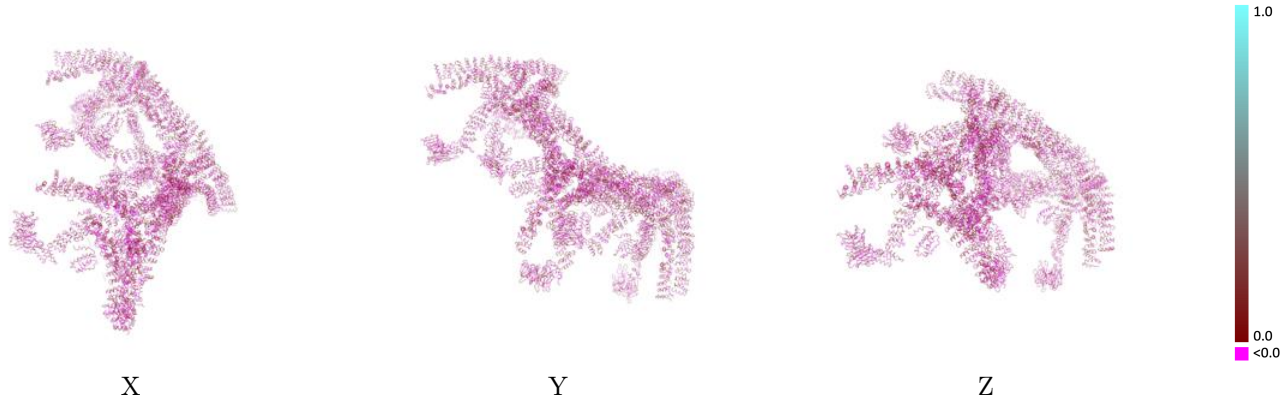
Y



Z

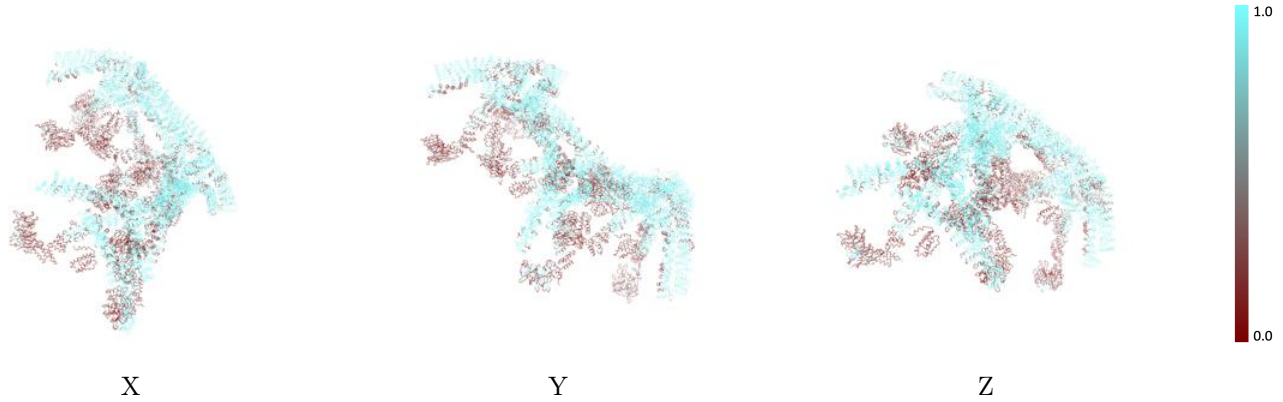
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



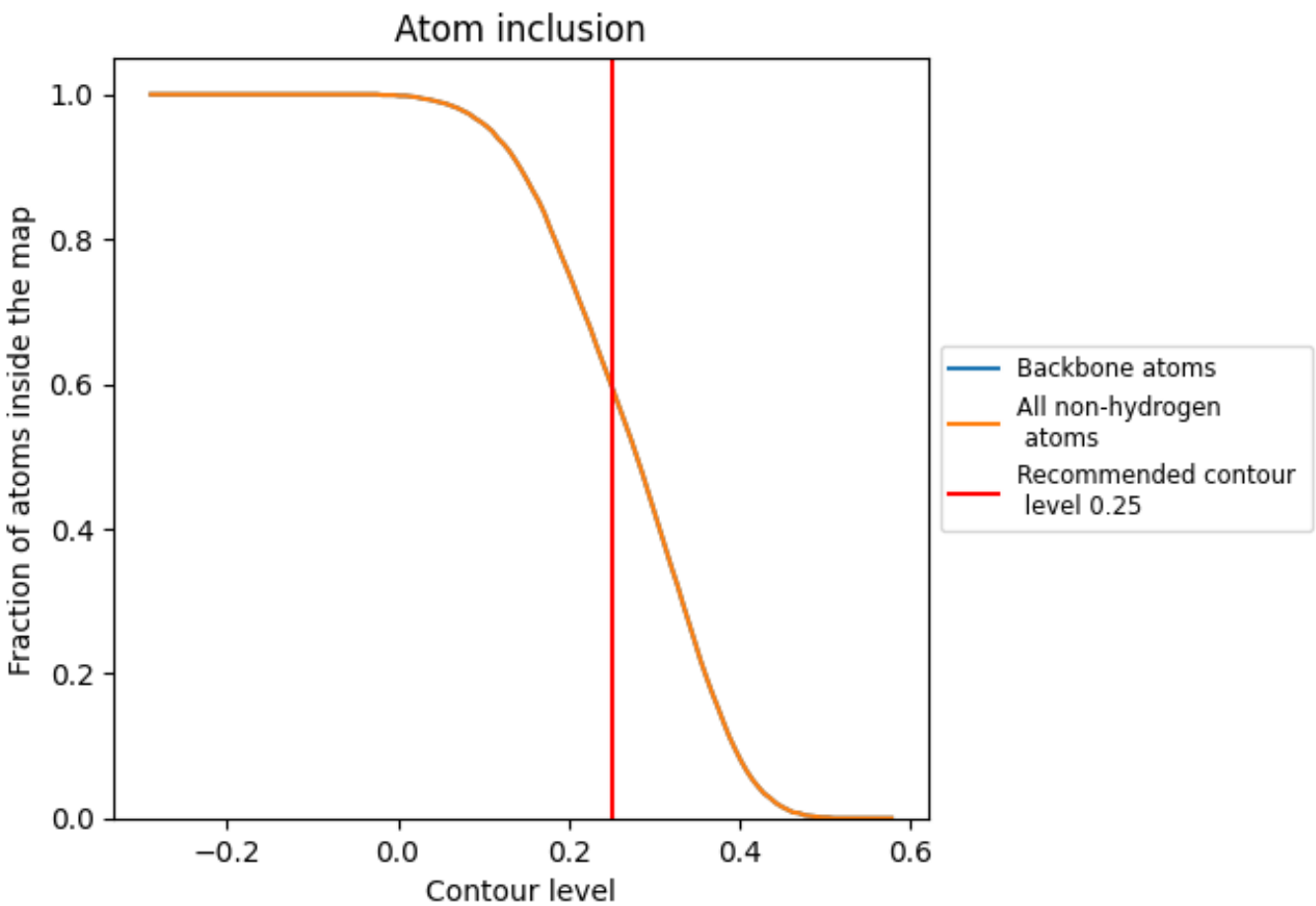

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)




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 (0.25).

## 9.4 Atom inclusion (i)




At the recommended contour level, 60% of all backbone atoms, 60% 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 (0.25) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5980 | 0.0260 |
| A | 0.6850 | 0.0210 |
| B | 0.6140 | 0.0310 |
| C | 0.6630 | 0.0340 |
| D | 0.6370 | 0.0300 |
| E | 0.7220 | 0.0320 |
| F | 0.6240 | 0.0270 |
| G | 0.5920 | 0.0250 |
| H | 0.6750 | 0.0300 |
| I | 0.5320 | 0.0250 |
| J | 0.0260 | 0.0020 |
| K | 0.0000 | -0.0010 |
| L | 0.0000 | -0.0210 |
| M | 0.0440 | -0.0100 |
| N | 0.0090 | -0.0360 |
| O | 0.1140 | -0.0010 |
| P | 0.0000 | -0.0110 |
| Q | 0.0350 | -0.0260 |
| R | 0.0180 | -0.0040 |