Full wwPDB EM Validation Report ⓘ

Feb 14, 2024 – 12:28 AM EST

PDB ID	:	3IYV
EMDB ID	:	EMD-5119
Title	:	Clathrin D6 coat as full-length Triskelions
Authors	:	Johnson, G.T.; Fotin, A.; Cheng, Y.; Sliz, P.; Grigorieff, N.; Harrison, S.C.; Kirchhausen, T.; Walz, T.
Deposited on	:	2010-06-17
Resolution	:	7.90 Å(reported)
Based on initial models	:	1BPO, 1B89

This is a Full wwPDB EM Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

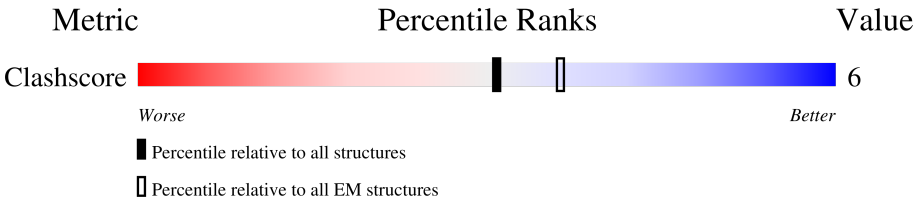
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 7.90 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	46% 99%
1	B	1630	44% 99%
1	C	1630	44% 98%
1	D	1630	46% 99%
1	E	1630	46% 99%
1	F	1630	46% 99%
1	G	1630	45% 99%
1	H	1630	46% 99%
1	I	1630	45% 99%
2	J	70	100% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	70	100% 100%
2	L	70	100% 100%
2	M	70	100% 100%
2	N	70	100% 100%
2	O	70	100% 100%
2	P	70	100% 100%
2	Q	70	100% 100%
2	R	70	100% 100%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15300 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
1	A	1630	Total C 1630 1630	0	1630
1	B	1630	Total C 1630 1630	0	1630
1	C	1630	Total C 1630 1630	0	1630
1	D	1630	Total C 1630 1630	0	1630
1	E	1630	Total C 1630 1630	0	1630
1	F	1630	Total C 1630 1630	0	1630
1	G	1630	Total C 1630 1630	0	1630
1	H	1630	Total C 1630 1630	0	1630
1	I	1630	Total C 1630 1630	0	1630

- Molecule 2 is a protein called Clathrin light chain A.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	J	70	Total C 70 70	0	70
2	K	70	Total C 70 70	0	70
2	L	70	Total C 70 70	0	70
2	M	70	Total C 70 70	0	70
2	N	70	Total C 70 70	0	70
2	O	70	Total C 70 70	0	70

Continued on next page...

Continued from previous page...

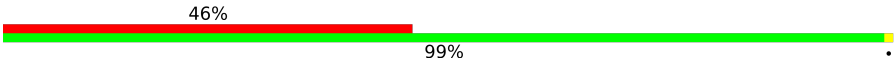
Mol	Chain	Residues	Atoms	AltConf	Trace
2	P	70	Total C 70 70	0	70
2	Q	70	Total C 70 70	0	70
2	R	70	Total C 70 70	0	70

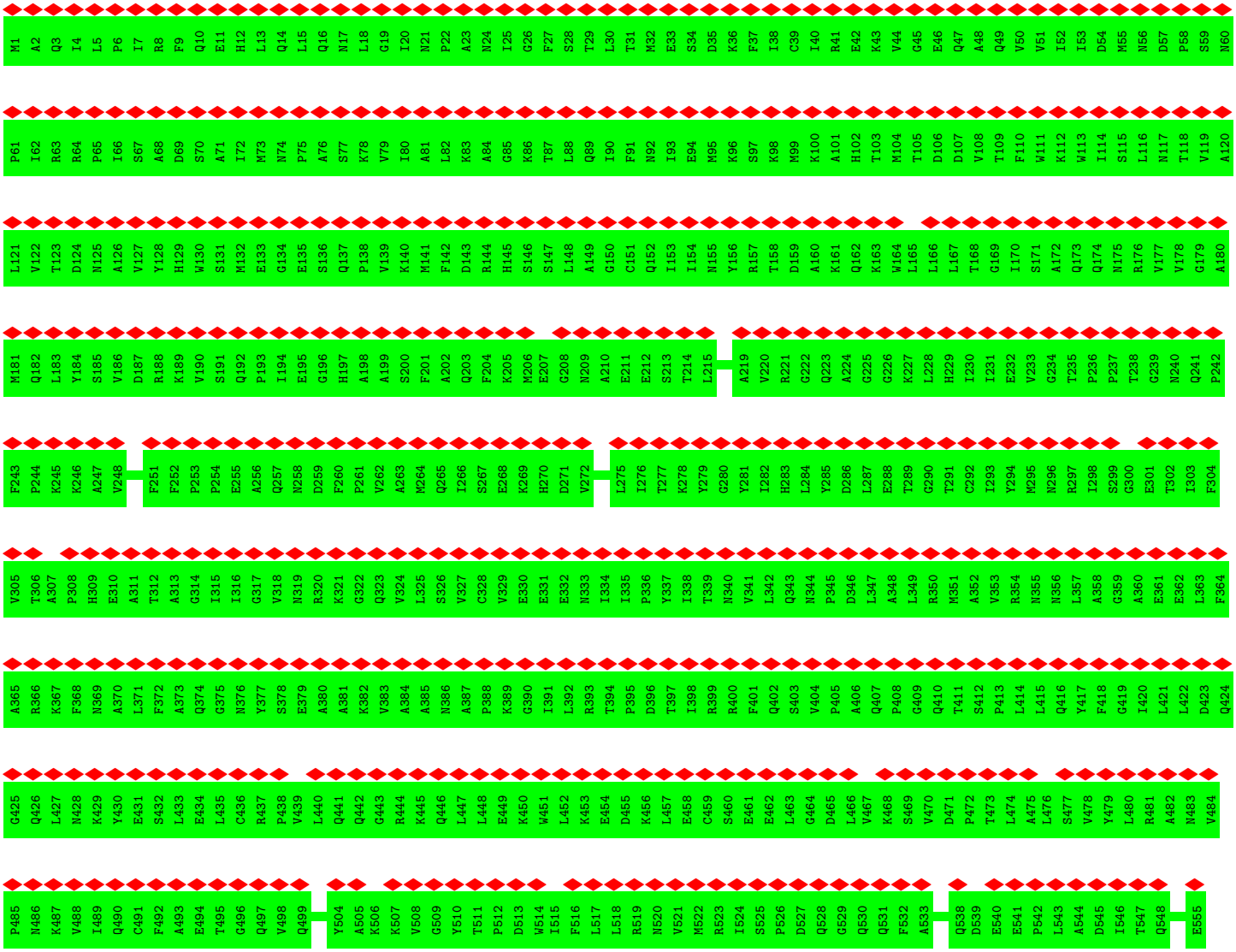
3 Residue-property plots (i)

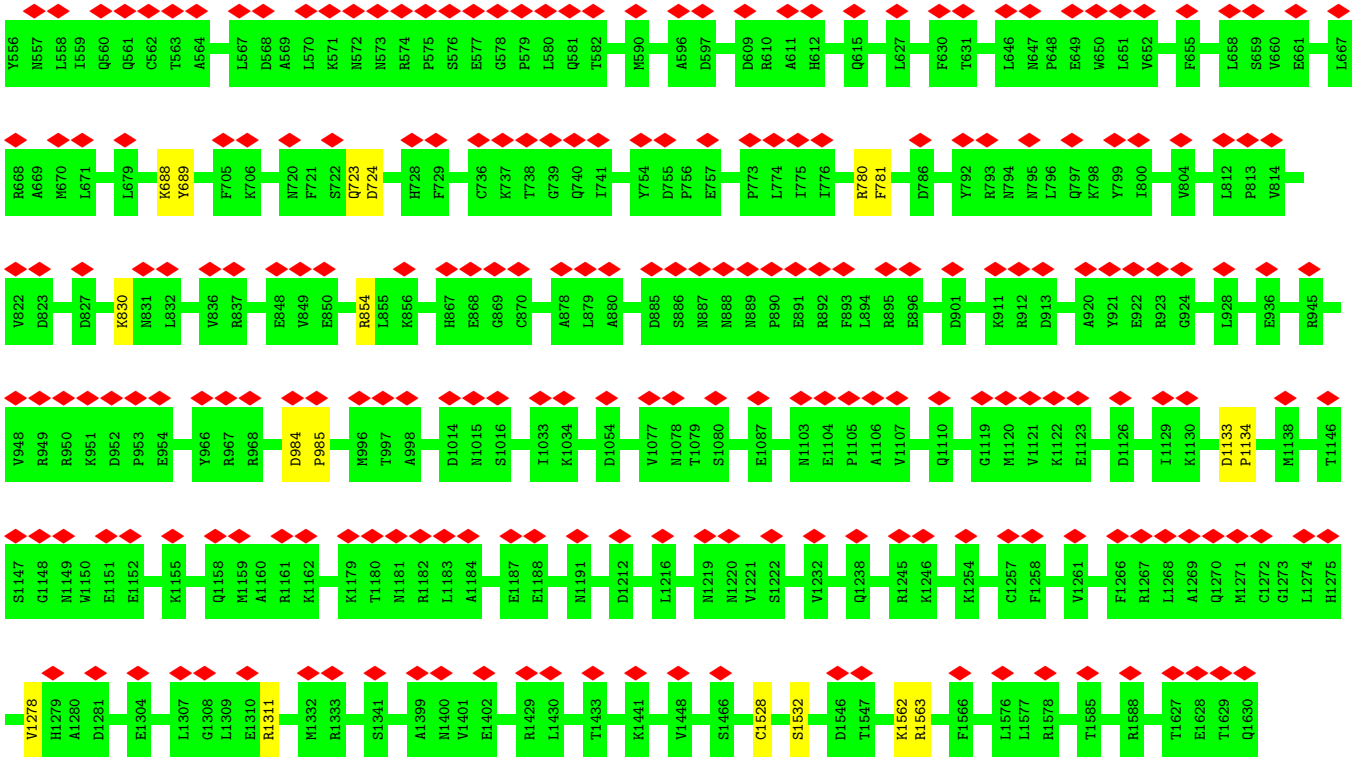
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

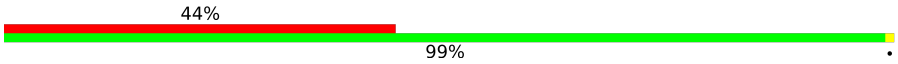


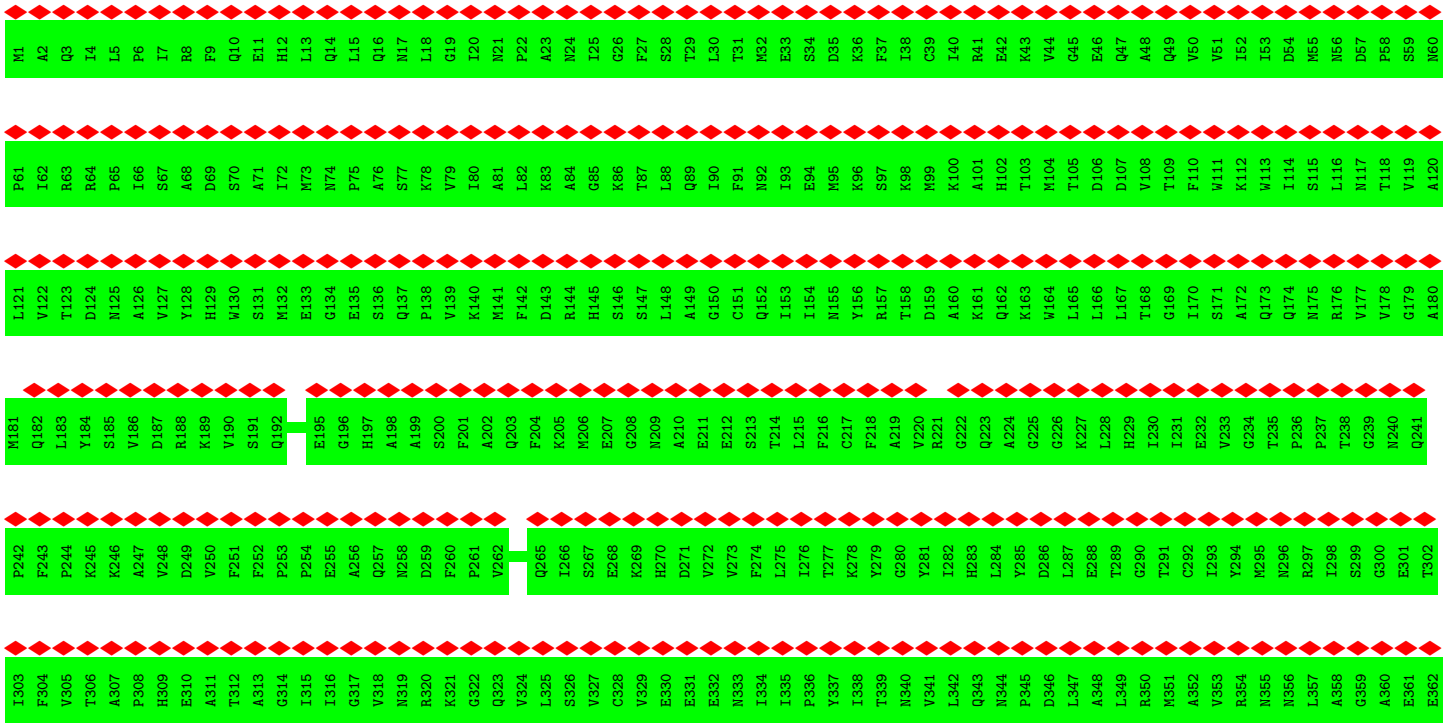


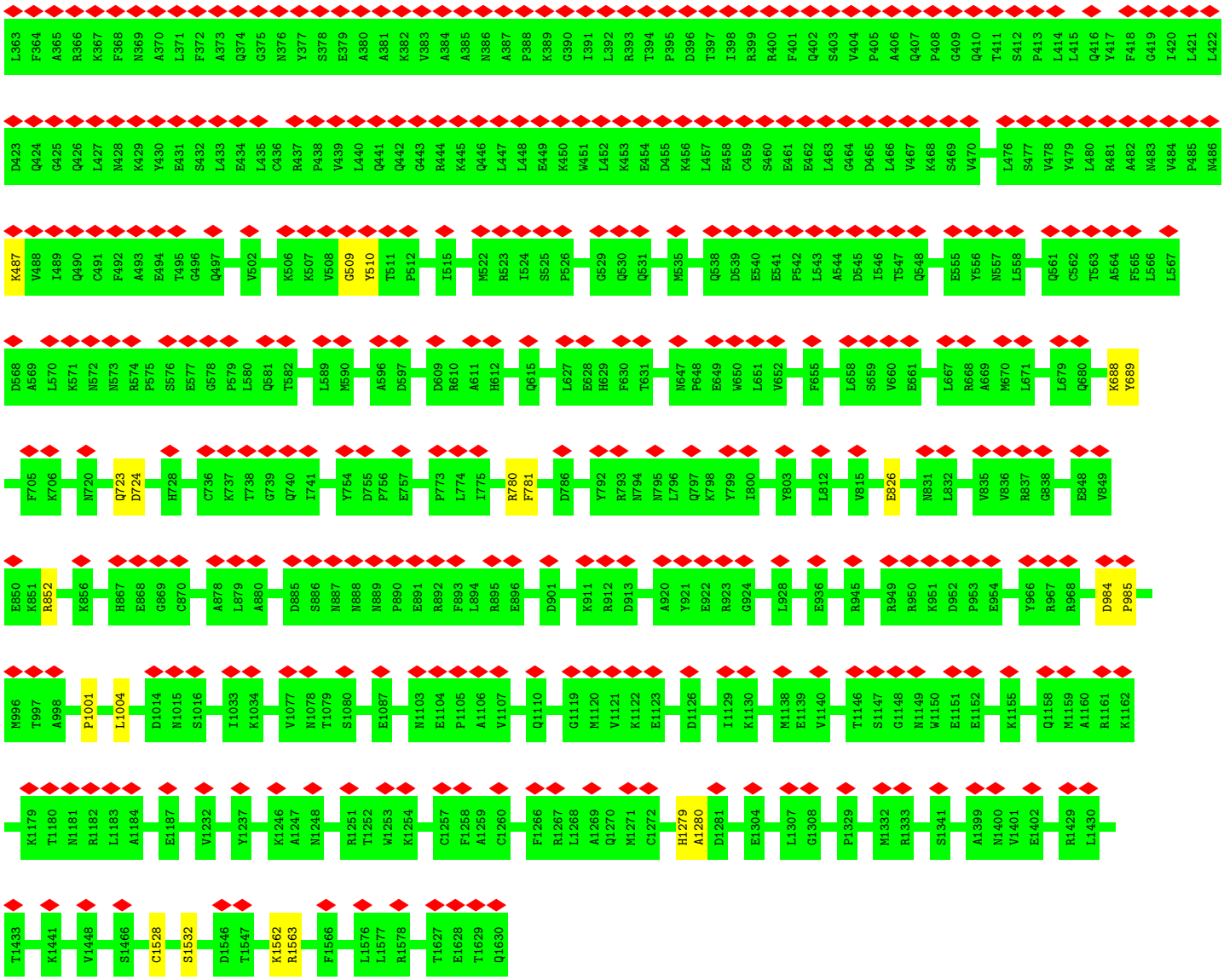


- Molecule 1: Clathrin heavy chain

Chain B:

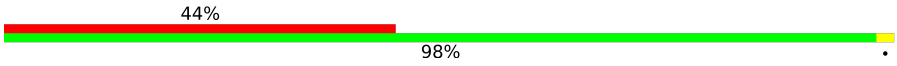


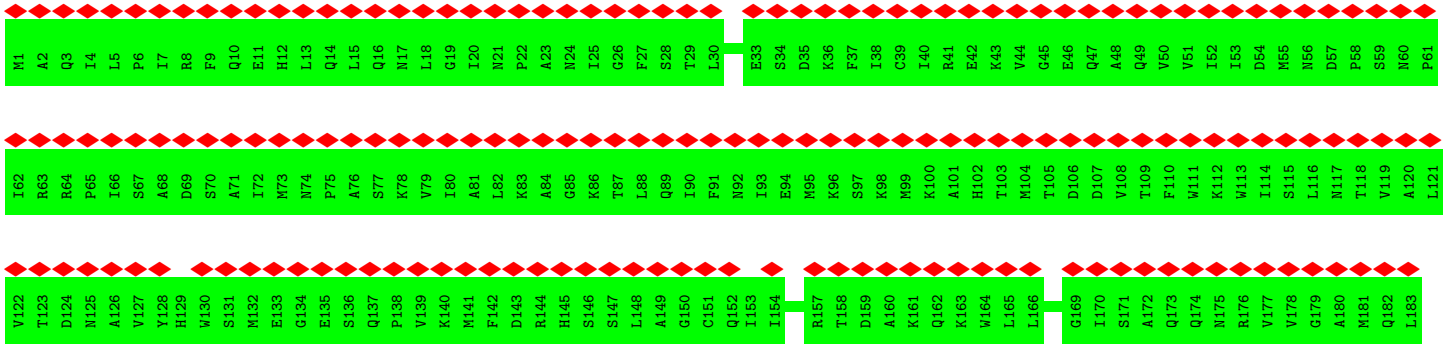


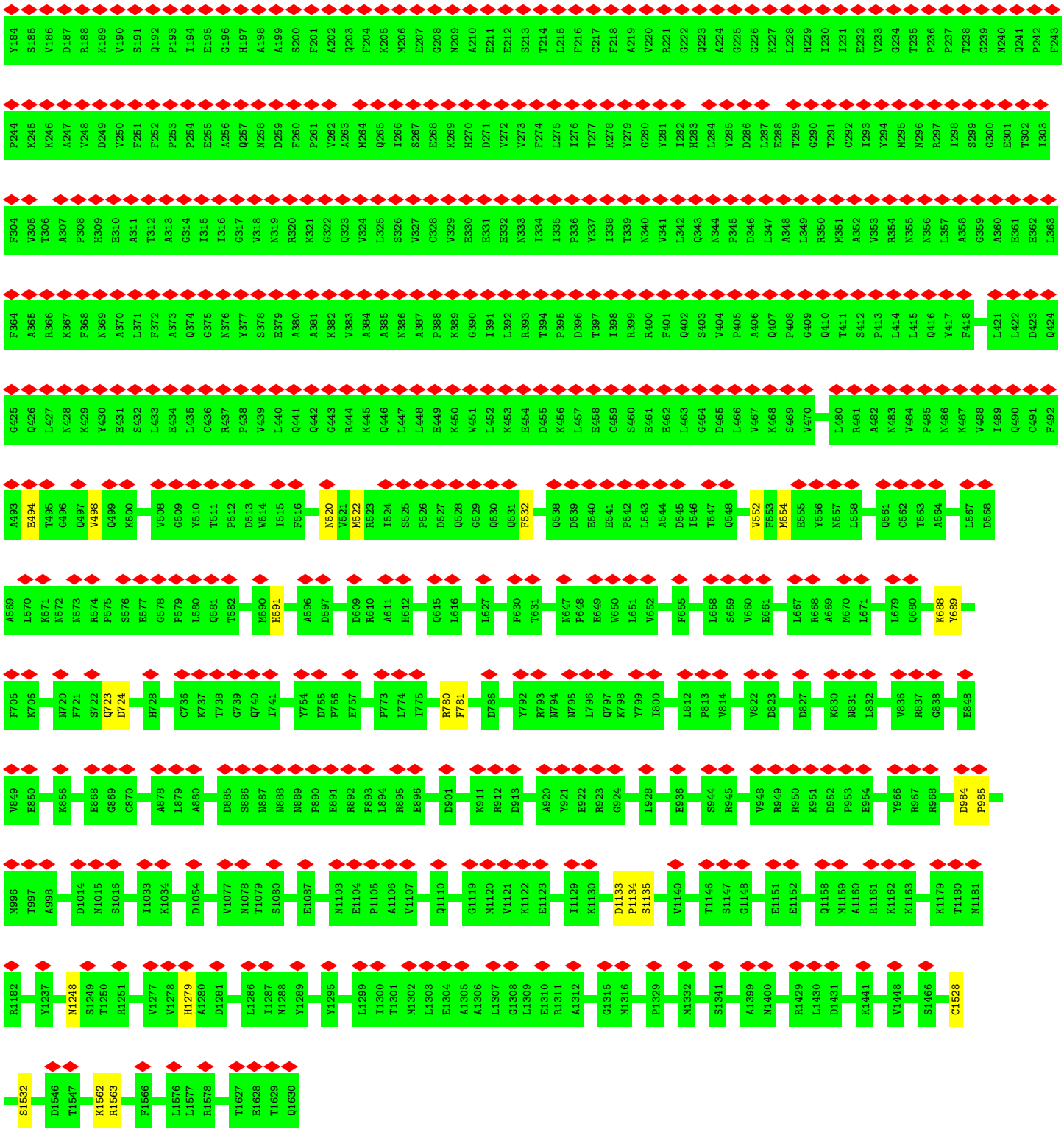


• Molecule 1: Clathrin heavy chain

Chain C:

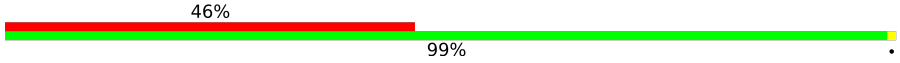


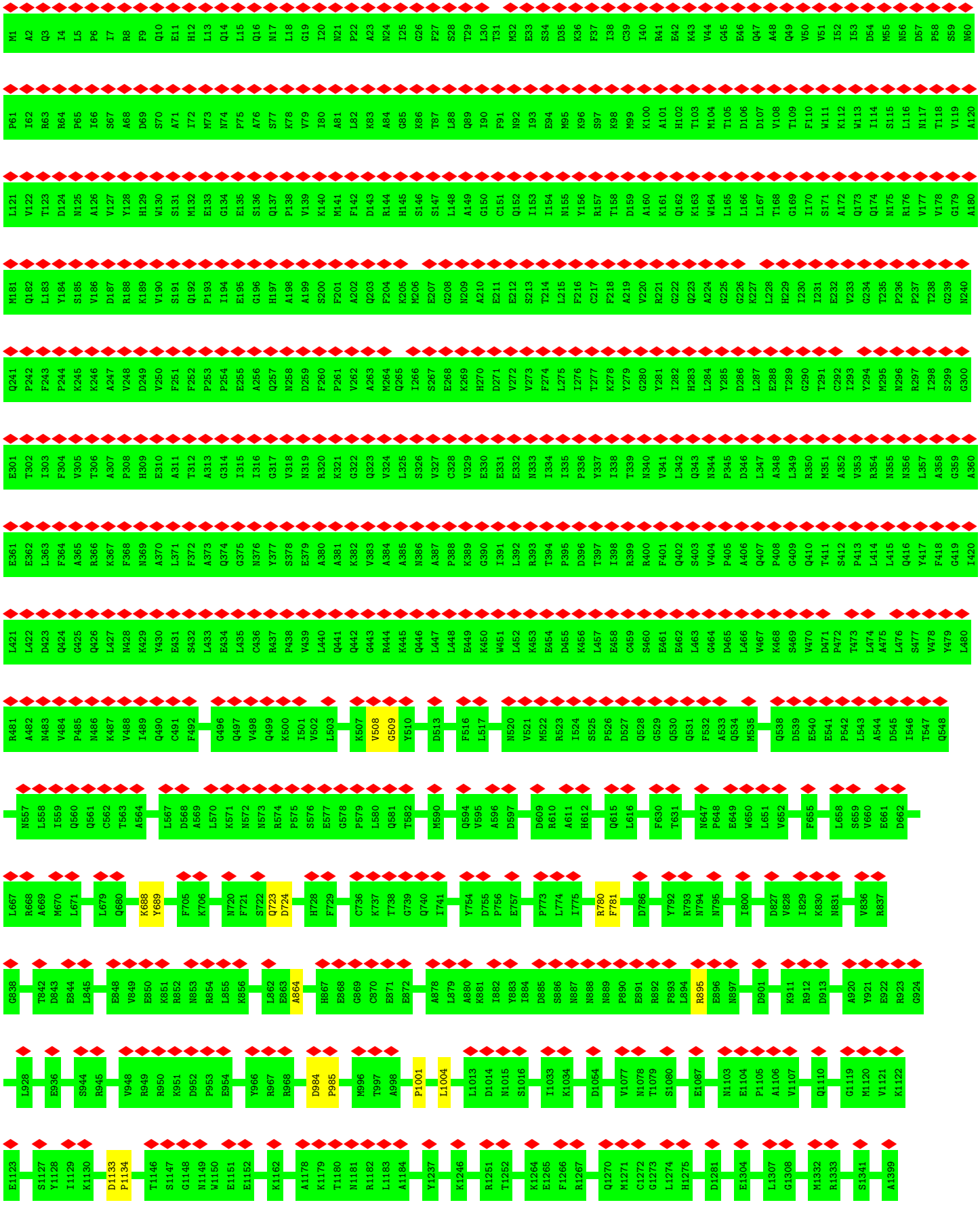


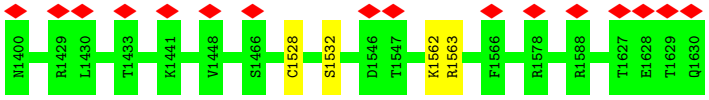


• Molecule 1: Clathrin heavy chain

Chain D:

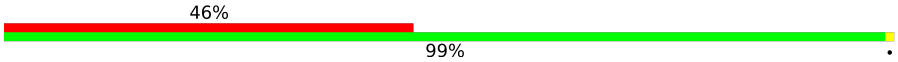


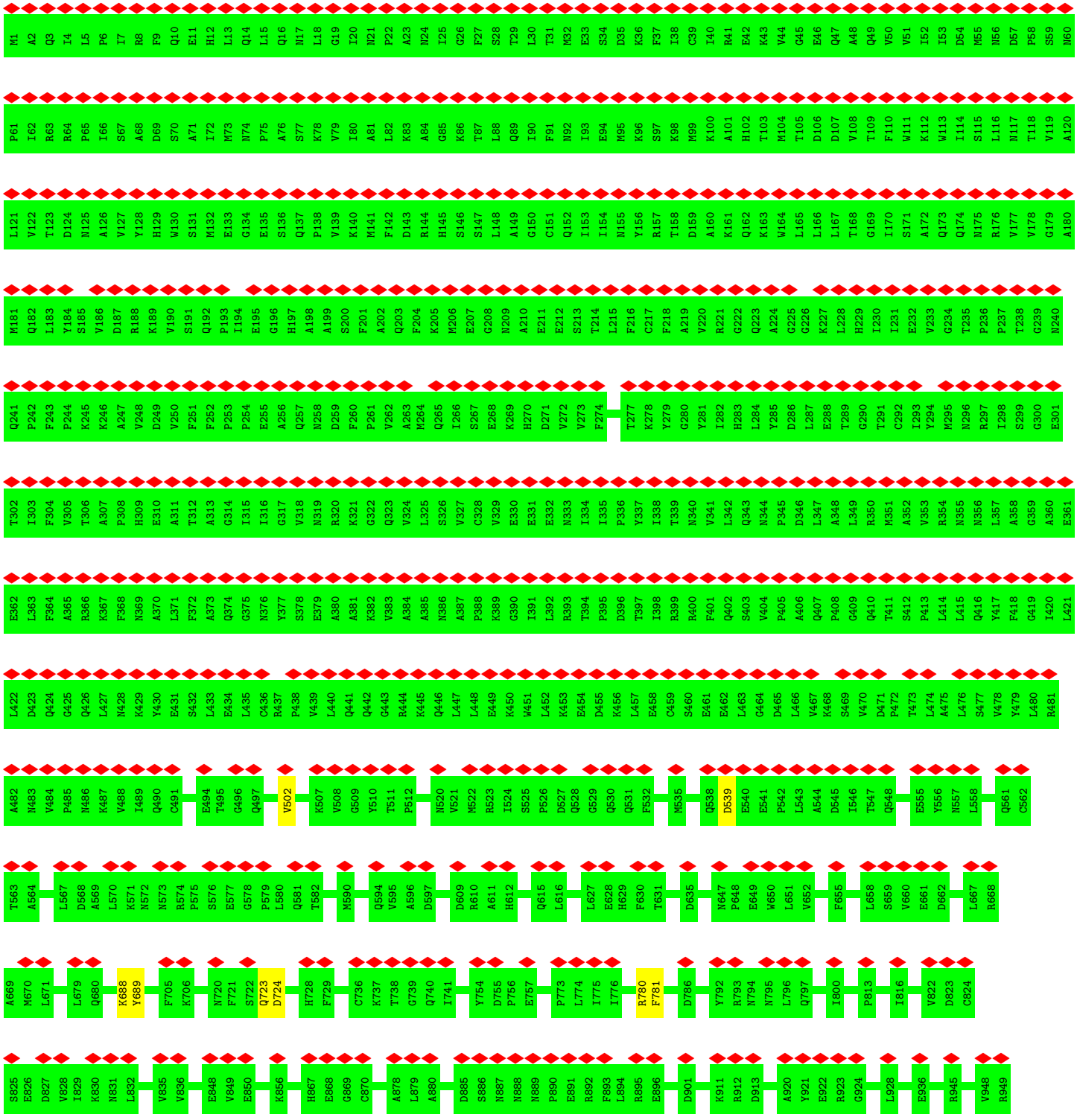

M1 A2 Q3 I4 L5 P6 I7 R8 F9 Q10 E11 H12 L13 Q14 L15 Q16 N17 L18 G19 I20 N21 P22 A23 N24 I25 G26 F27 S28 T29 L30 T31 M32 E33 S34 D35 K36 F37 I38 C39 I40 R41 E42 K43 V44 G45 E46 Q47 A48 Q49 V50 V51 I52 I53 D54 M55 N56 D57 P58 S59 N60
P61 I62 R63 R64 P65 I66 S67 A68 D69 S70 A71 I72 M73 N74 P75 A76 S77 K78 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 A139 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 L275 I276 T277 K278 Y279 G280 Y281 I282 H283 L284 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 V318 N319 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 V353 R354 N355 N356 L357 A358 G359 A360
E361 E362 L363 F364 A365 R366 K367 F368 N369 A370 L371 P372 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 I489 Q490 C491 F492 G496 Q497 V498 Q499 K500 I501 V502 L503 K507 V508 G509 Y510 D513 F516 L517 N520 V521 M522 R523 I524 S525 P526 D527 Q528 G529 Q530 Q531 F532 A533 Q534 M535 Q538 D539 E540 E541 P542 L543 A544 D545 I546 T547 Q548
N557 L558 I559 Q560 Q561 C562 T563 A564 L567 D568 A569 L570 K571 N572 N573 R574 P575 S576 E577 G578 P579 L580 Q581 T582 M590 Q594 V595 A596 D597 D609 R610 A611 H612 Q615 L616 F630 T631 N647 P648 E649 W650 L651 V652 F655 L658 S659 V660 E661 D662
L667 R668 A669 M670 L671 L679 Q680 K688 Y689 F705 K706 N720 F721 S722 Q723 D724 H728 F729 C736 K737 T738 G739 Q740 I741 Y754 D755 P756 E757 P773 L774 I775 R780 F781 D786 Y792 R793 N794 N795 I800 D827 V828 I829 K830 N831 V836 R837
G838 T842 D843 E844 L845 E848 V849 E850 K851 R852 N853 R854 L855 K856 L862 E863 A864 H867 E868 G869 C870 E871 E872 A878 L879 A880 K881 I882 Y883 I884 D885 S886 N887 N888 N889 P890 E891 R892 F893 L894 R895 E896 N897 D901 K911 R912 D913 A920 Y921 E922 R923 G924
L928 E936 S944 R945 V948 R949 R950 K951 D952 P953 E954 Y966 R967 R968 D984 P985 M996 T997 A998 P1001 L1004 L1013 D1014 N1015 S1016 I1033 K1034 D1054 V1077 N1078 T1079 S1080 E1087 N1103 E1104 P1105 A1106 V1107 Q1110 G1119 M1120 V1121 K1122
E1123 S1127 Y1128 I1129 K1130 D1133 P1134 T1146 S1147 G1148 N1149 W1150 E1151 E1152 K1162 A1178 K1179 T1180 N1181 R1182 L1183 A1184 Y1237 K1246 R1251 T1252 K1264 E1265 F1266 R1267 Q1270 M1271 C1272 G1273 L1274 H1275 D1281 E1304 L1307 G1308 M1332 R1333 S1341 A1399

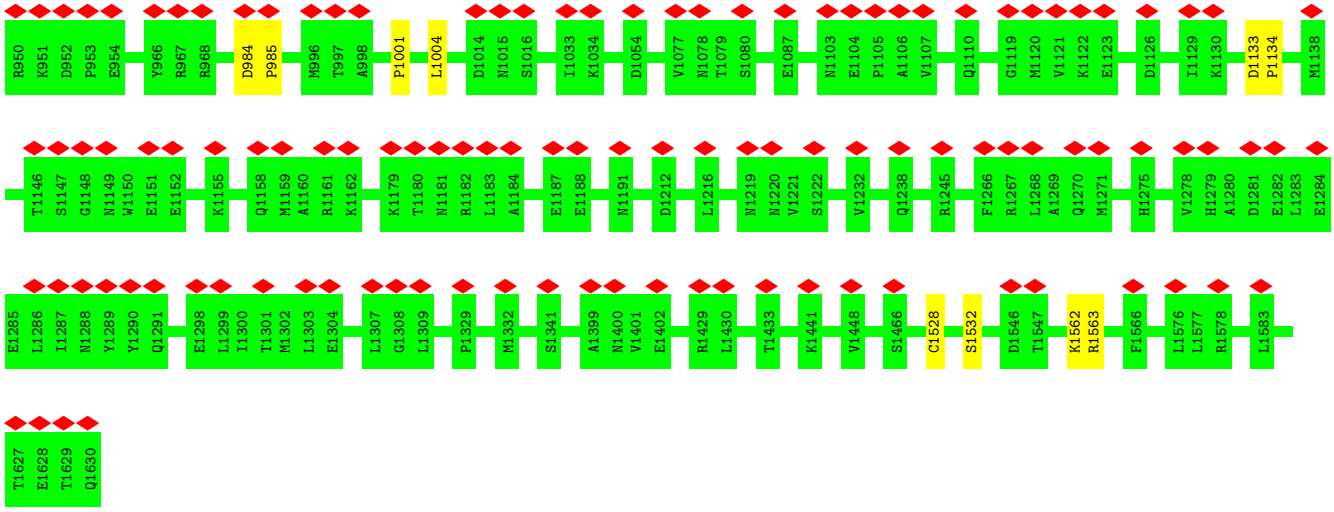


• Molecule 1: Clathrin heavy chain

Chain E:

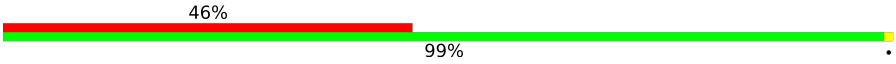


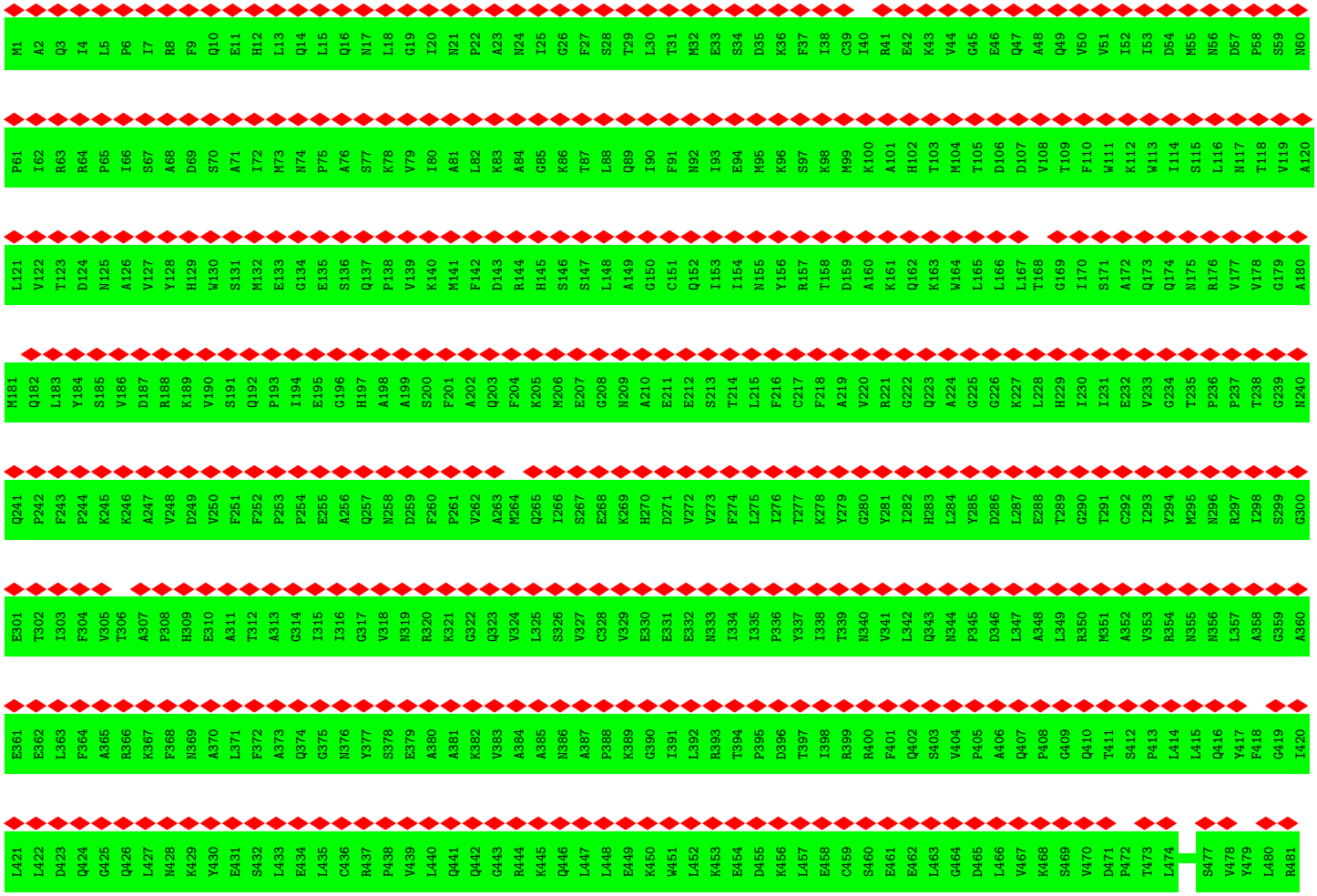


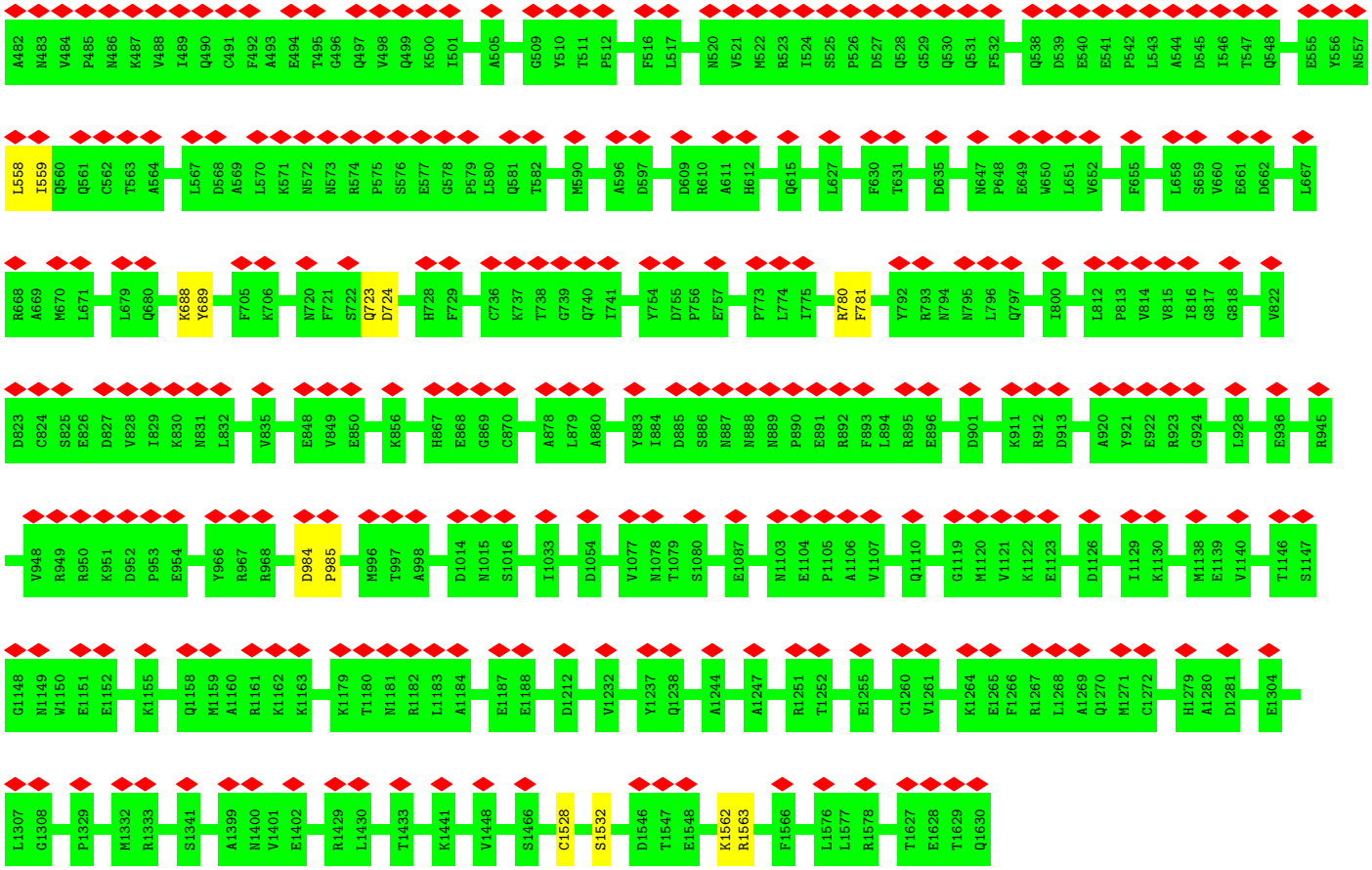


- Molecule 1: Clathrin heavy chain

Chain F:

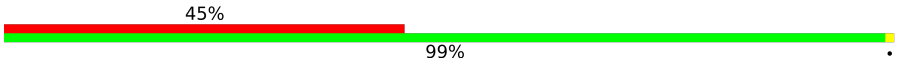


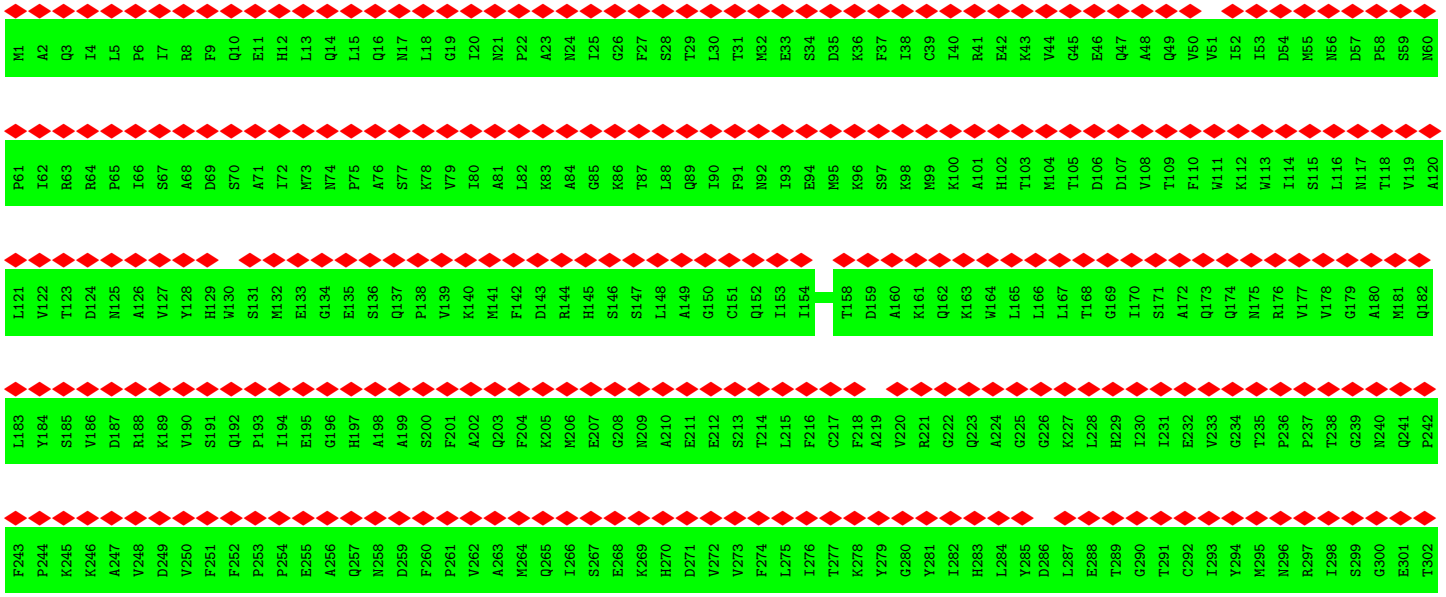


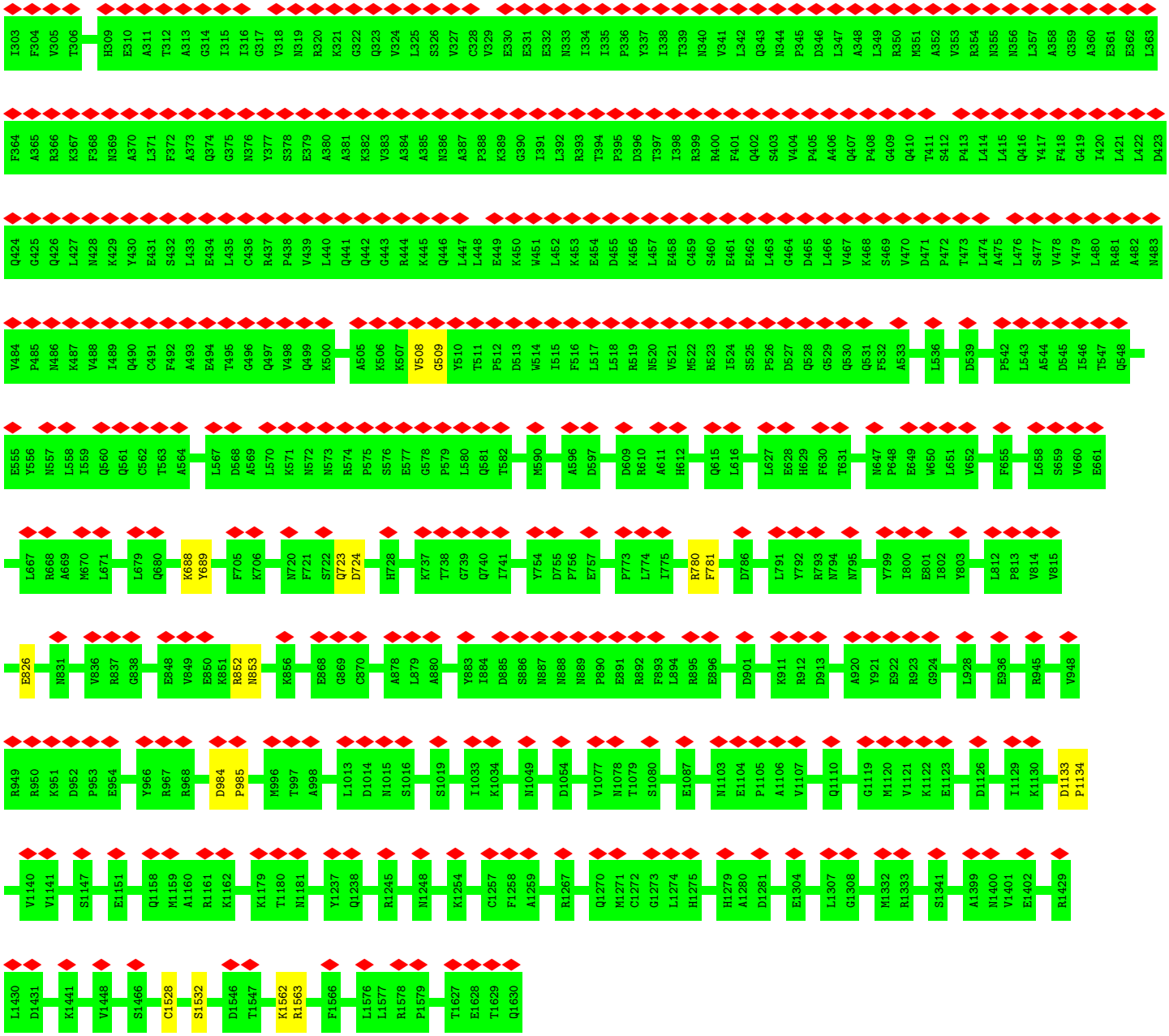


• Molecule 1: Clathrin heavy chain

Chain G:

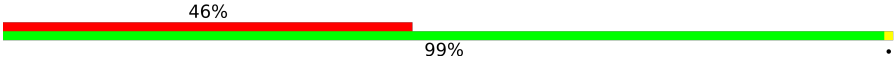


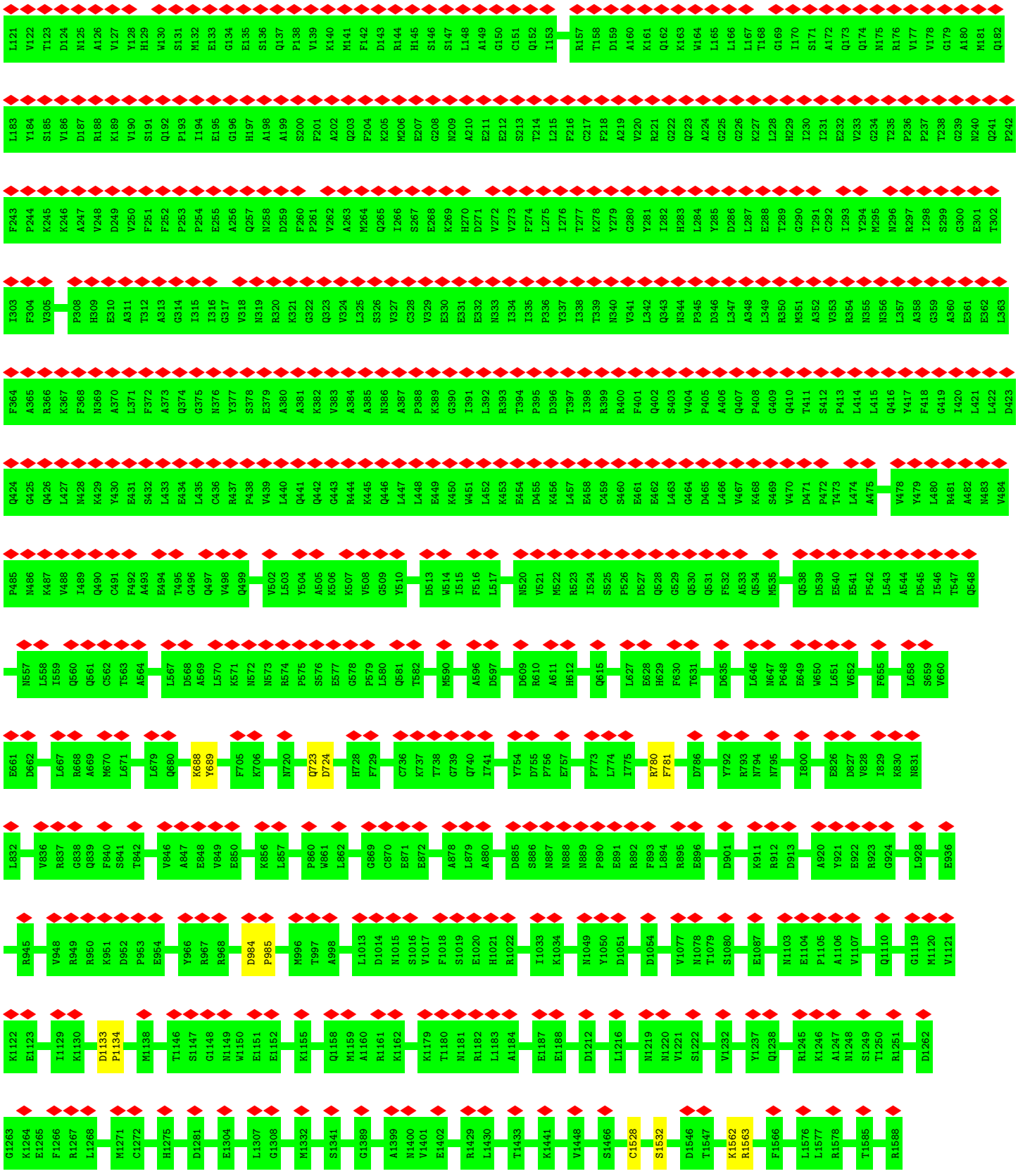


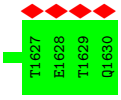


- Molecule 1: Clathrin heavy chain

Chain H:

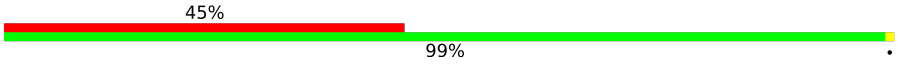


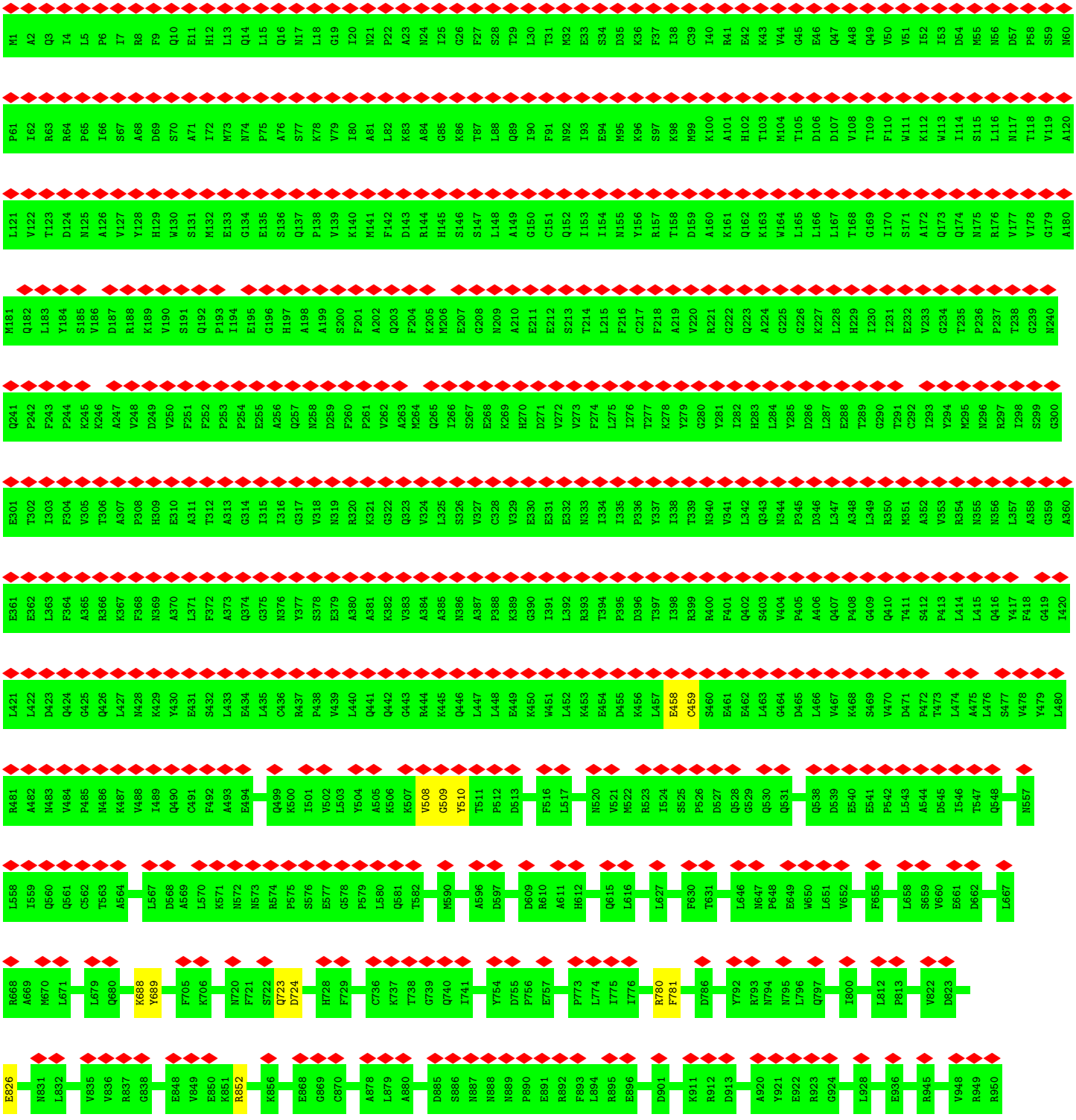

L121 V122 T123 D124 N125 A126 V127 Y128 H129 W130 S131 M132 E133 G134 E135 S136 Q137 P138 V139 K140 M141 F142 D143 R144 H145 S146 S147 L148 A149 G150 C151 Q152 I153
R157 T158 D159 A160 K161 Q162 K163 W164 L165 L166 L167 T168 G169 I170 S171 A172 Q173 Q174 N175 R176 V177 V178 G179 A180 M181 Q182
L183 Y184 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 L275 I276 T277 K278 Y279 G280 Y281 I282 H283 L284 Y285 D286 L287 E288 T289 G290 T291 C292 I293 Y294 M295 N296 R297 I298 S299 G300 E301 T302
I303 F304 V305
P308 H309 E310 A311 T312 A313 G314 I315 I316 G317 V318 N319 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 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
V478 Y479 L480 R481 A482 N483 V484
P485 N486 K487 V488 I489 Q490 C491 F492 A493 E494 T495 G496 Q497 V498 Q499
V502 L503 Y504 A505 K506 K507 V508 G509 Y510
D513 W514 I515 F516 L517
N520 V521 M522 R523 I524 S525 P526 D527 Q528 G529 Q530 Q531 F532 A533 Q534 M535
Q538 D539 E540 E541 P542 L543 A544 D545 I546 T547 Q548
N557 L558 I559 Q560 Q561 C562 T563 A564
L567 D568 A569 L570 K571 N572 N573 R574 P575 S576 E577 G578 P579 L580 Q581 T582
M590
A596 D597
D609 R610 A611 H612
Q615
L627 E628 H629 F630 T631
D635
L646 N647 P648 E649 W650 L651 V652
F655
L658 S659 V660
E661 D662
L667 R668 A669 M670 L671
L679 Q680
K688 Y689
F705 K706
N720
Q723 D724
H728 F729
C736 K737 T738 G739 Q740 I741
Y754 D755 P756 E757
P773 L774 I775
R780 F781
D786
Y792 R793 N794 N795
I800
E826 D827 V828 I829 K830 N831
L832
V836 R837 G838 Q839 F840 S841 T842
V846 A847 E848 V849 E850
K856 L857
P860 W861 L862
G869 C870 E871 E872
A878 L879 A880
D885 S886 N887 N888 N889 P890 E891 R892 F893 L894 R895 E896
D901
K911 R912 D913
A920 Y921 E922 R923 G924
L928
E936
R945
V948 R949 R950 K951 D952 P953 E954
Y966 R967 R968
D984 P985
M996 T997 A998
L1013 D1014 N1015 S1016 V1017 F1018 S1019 E1020 H1021 R1022
I1033 K1034
N1049 Y1050 D1051
D1054
V1077 N1078 T1079 S1080
E1087
N1103 E1104 P1105 A1106 V1107
Q1110
G1119 M1120 V1121
K1122 E1123
I1129 K1130
D1133 P1134
M1138
T1146 S1147 G1148 N1149 W1150 E1151 E1152
K1155
Q1158 M1159 A1160 R1161 K1162
K1179 T1180 N1181 R1182 L1183 A1184
E1187 E1188
D1212
L1216
N1219 N1220 V1221 S1222
V1232
Y1237 Q1238
R1245 K1246 A1247 N1248 S1249 T1250 R1251
D1262
G1263 K1264 E1265 F1266 R1267 L1268
M1271 C1272
H1275
D1281
E1304
L1307 G1308
M1332
S1341
G1389
A1399 N1400 V1401 E1402
R1429 L1430
T1433
K1441
V1448
S1466
C1528
S1532
D1546 T1547
K1562 R1563
F1566
L1576 L1577 R1578
T1585
R1588

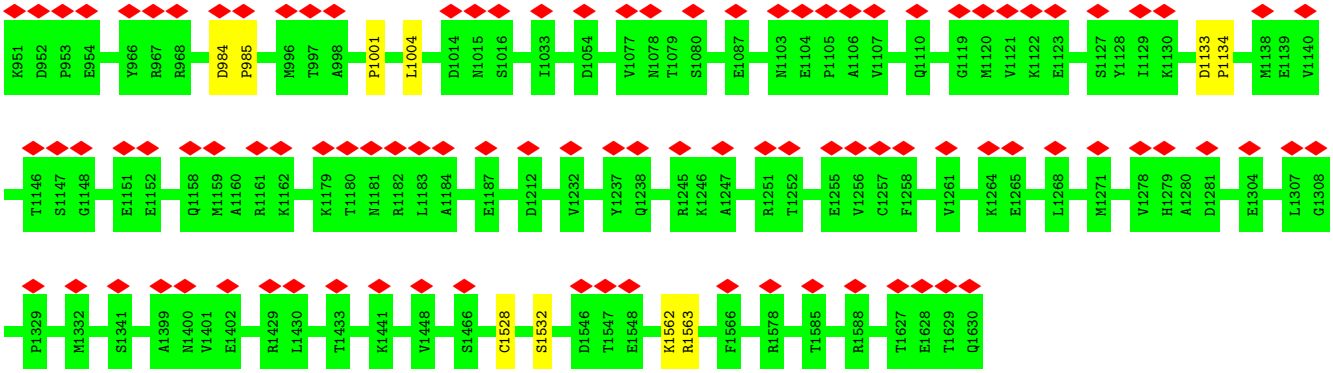


• Molecule 1: Clathrin heavy chain

Chain I:

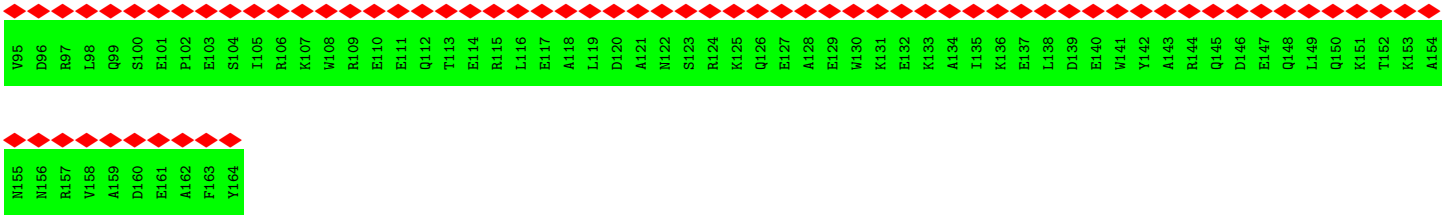






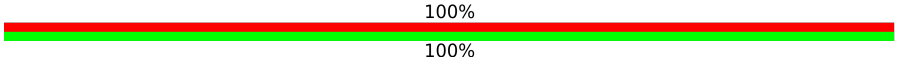
• Molecule 2: Clathrin light chain A

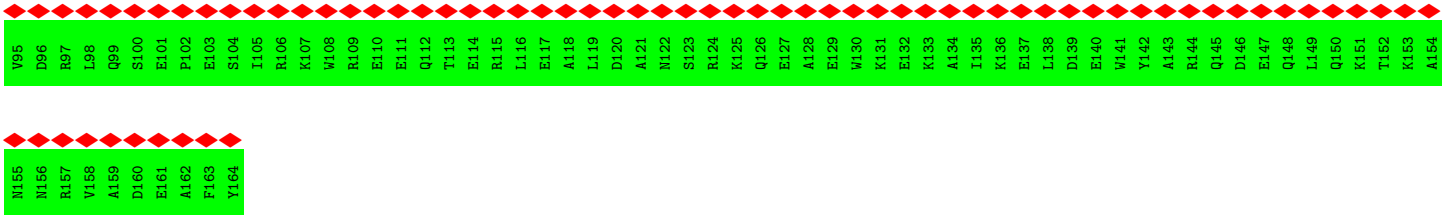
Chain J:



• Molecule 2: Clathrin light chain A

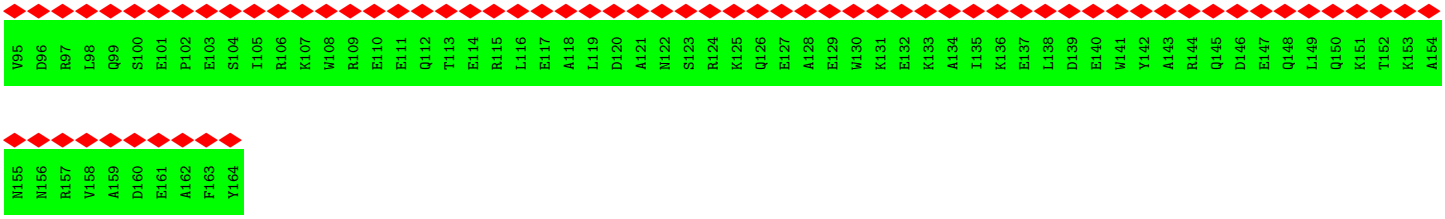
Chain K:





• Molecule 2: Clathrin light chain A

Chain L:



• Molecule 2: Clathrin light chain A

Chain M:

V95 D96 R97 L98 Q99 S100 E101 P102 E103 S104 I105 R106 K107 W108 R109 E110 E111 Q112 T113 E114 R115 L116 E117 A118 L119 D120 A121 N122 S123 R124 K125 Q126 E127 A128 E129 W130 K131 E132 K133 A134 I135 K136 E137 L138 D139 E140 W141 Y142 A143 R144 Q145 D146 E147 Q148 L149 Q150 K151 T152 K153 A154

N155 N156 R157 V158 A159 D160 E161 A162 F163 Y164

- Molecule 2: Clathrin light chain A

Chain N:

V95 D96 R97 L98 Q99 S100 E101 P102 E103 S104 I105 R106 K107 W108 R109 E110 E111 Q112 T113 E114 R115 L116 E117 A118 L119 D120 A121 N122 S123 R124 K125 Q126 E127 A128 E129 W130 K131 E132 K133 A134 I135 K136 E137 L138 D139 E140 W141 Y142 A143 R144 Q145 D146 E147 Q148 L149 Q150 K151 T152 K153 A154

N155 N156 R157 V158 A159 D160 E161 A162 F163 Y164

- Molecule 2: Clathrin light chain A

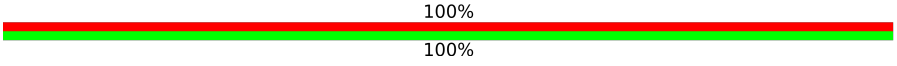
Chain O:

V95 D96 R97 L98 Q99 S100 E101 P102 E103 S104 I105 R106 K107 W108 R109 E110 E111 Q112 T113 E114 R115 L116 E117 A118 L119 D120 A121 N122 S123 R124 K125 Q126 E127 A128 E129 W130 K131 E132 K133 A134 I135 K136 E137 L138 D139 E140 W141 Y142 A143 R144 Q145 D146 E147 Q148 L149 Q150 K151 T152 K153 A154

N155 N156 R157 V158 A159 D160 E161 A162 F163 Y164

- Molecule 2: Clathrin light chain A

Chain P:



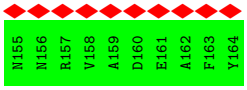
V95 D96 R97 L98 Q99 S100 E101 P102 E103 S104 I105 R106 K107 W108 R109 E110 E111 Q112 T113 E114 R115 L116 E117 A118 L119 D120 A121 N122 S123 R124 K125 Q126 E127 A128 E129 W130 K131 E132 K133 A134 I135 K136 E137 L138 D139 E140 W141 Y142 A143 R144 Q145 D146 E147 Q148 L149 Q150 K151 T152 K153 A154

N155 N156 R157 V158 A159 D160 E161 A162 F163 Y164

- Molecule 2: Clathrin light chain A

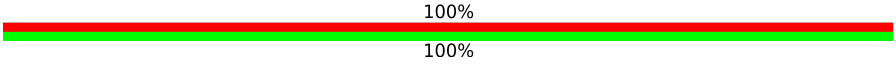
Chain Q:

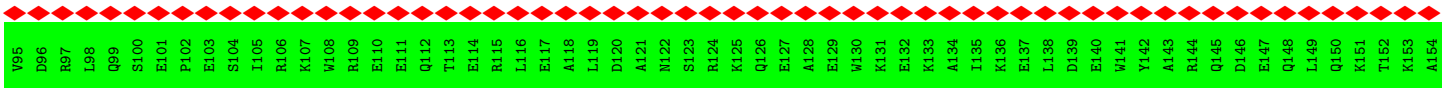
V95 D96 R97 L98 Q99 S100 E101 P102 E103 S104 I105 R106 K107 W108 R109 E110 E111 Q112 T113 E114 R115 L116 E117 A118 L119 D120 A121 N122 S123 R124 K125 Q126 E127 A128 E129 W130 K131 E132 K133 A134 I135 K136 E137 L138 D139 E140 W141 Y142 A143 R144 Q145 D146 E147 Q148 L149 Q150 K151 T152 K153 A154

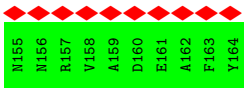


• Molecule 2: Clathrin light chain A

Chain R:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	1450	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)	2000.00	Depositor
Maximum defocus (nm)	5000.00	Depositor
Magnification	51160	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.638	Depositor
Minimum map value	-0.163	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	873.6, 873.6, 873.6	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.8, 2.8, 2.8	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).

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

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	9	0
1	B	1630	0	0	11	0
1	C	1630	0	0	14	0
1	D	1630	0	0	11	0
1	E	1630	0	0	9	0
1	F	1630	0	0	7	0
1	G	1630	0	0	10	0
1	H	1630	0	0	7	0
1	I	1630	0	0	12	0
2	J	70	0	0	0	0
2	K	70	0	0	0	0
2	L	70	0	0	0	0
2	M	70	0	0	0	0
2	N	70	0	0	0	0
2	O	70	0	0	0	0
2	P	70	0	0	0	0
2	Q	70	0	0	0	0
2	R	70	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	15300	0	0	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (88) 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:C:1134:PRO:CA	1:C:1135:SER:CA	1.84	1.53
1:G:826:GLU:CA	1:G:853:ASN:CA	1.92	1.47
1:G:723:GLN:CA	1:G:724:ASP:CA	2.24	1.16
1:C:723:GLN:CA	1:C:724:ASP:CA	2.24	1.15
1:A:723:GLN:CA	1:A:724:ASP:CA	2.24	1.15
1:B:723:GLN:CA	1:B:724:ASP:CA	2.24	1.15
1:E:723:GLN:CA	1:E:724:ASP:CA	2.24	1.15
1:F:723:GLN:CA	1:F:724:ASP:CA	2.24	1.15
1:H:723:GLN:CA	1:H:724:ASP:CA	2.24	1.15
1:D:723:GLN:CA	1:D:724:ASP:CA	2.24	1.15
1:I:723:GLN:CA	1:I:724:ASP:CA	2.24	1.13
1:G:1133:ASP:CA	1:G:1134:PRO:CA	2.27	1.13
1:H:1133:ASP:CA	1:H:1134:PRO:CA	2.27	1.13
1:A:1133:ASP:CA	1:A:1134:PRO:CA	2.27	1.12
1:C:1133:ASP:CA	1:C:1134:PRO:CA	2.27	1.12
1:E:1133:ASP:CA	1:E:1134:PRO:CA	2.27	1.12
1:D:508:VAL:CA	1:D:509:GLY:CA	2.27	1.10
1:B:984:ASP:CA	1:B:985:PRO:CA	2.30	1.10
1:H:984:ASP:CA	1:H:985:PRO:CA	2.30	1.10
1:A:984:ASP:CA	1:A:985:PRO:CA	2.30	1.09
1:C:984:ASP:CA	1:C:985:PRO:CA	2.30	1.09
1:F:984:ASP:CA	1:F:985:PRO:CA	2.30	1.08
1:D:984:ASP:CA	1:D:985:PRO:CA	2.30	1.08
1:I:984:ASP:CA	1:I:985:PRO:CA	2.30	1.08
1:E:984:ASP:CA	1:E:985:PRO:CA	2.30	1.07
1:G:984:ASP:CA	1:G:985:PRO:CA	2.30	1.07
1:A:1278:VAL:CA	1:A:1311:ARG:CA	2.38	1.01
1:H:780:ARG:CA	1:H:781:PHE:CA	2.50	0.90
1:F:780:ARG:CA	1:F:781:PHE:CA	2.50	0.90
1:A:780:ARG:CA	1:A:781:PHE:CA	2.50	0.90
1:G:780:ARG:CA	1:G:781:PHE:CA	2.50	0.90
1:C:780:ARG:CA	1:C:781:PHE:CA	2.50	0.90
1:B:780:ARG:CA	1:B:781:PHE:CA	2.50	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:ARG:CA	1:D:781:PHE:CA	2.50	0.89
1:E:780:ARG:CA	1:E:781:PHE:CA	2.50	0.89
1:I:780:ARG:CA	1:I:781:PHE:CA	2.50	0.89
1:C:494:GLU:CA	1:C:520:ASN:CA	2.53	0.86
1:G:1562:LYS:CA	1:G:1563:ARG:CA	2.56	0.84
1:H:1562:LYS:CA	1:H:1563:ARG:CA	2.56	0.84
1:A:1562:LYS:CA	1:A:1563:ARG:CA	2.56	0.83
1:B:1562:LYS:CA	1:B:1563:ARG:CA	2.56	0.83
1:D:1562:LYS:CA	1:D:1563:ARG:CA	2.56	0.83
1:I:1562:LYS:CA	1:I:1563:ARG:CA	2.56	0.82
1:C:1562:LYS:CA	1:C:1563:ARG:CA	2.56	0.82
1:E:1562:LYS:CA	1:E:1563:ARG:CA	2.56	0.82
1:F:1562:LYS:CA	1:F:1563:ARG:CA	2.56	0.82
1:B:826:GLU:CA	1:B:852:ARG:CA	2.57	0.82
1:I:1133:ASP:CA	1:I:1134:PRO:CA	2.59	0.81
1:I:509:GLY:CA	1:I:510:TYR:CA	2.60	0.80
1:D:1133:ASP:CA	1:D:1134:PRO:CA	2.64	0.76
1:G:826:GLU:CA	1:G:852:ARG:CA	2.63	0.76
1:E:502:VAL:CA	1:E:539:ASP:CA	2.67	0.72
1:C:554:MET:CA	1:C:591:HIS:CA	2.70	0.68
1:C:1248:ASN:CA	1:D:864:ALA:CA	2.75	0.64
1:B:509:GLY:CA	1:B:510:TYR:CA	2.76	0.64
1:C:498:VAL:CA	1:C:532:PHE:CA	2.77	0.63
1:G:508:VAL:CA	1:G:509:GLY:CA	2.78	0.61
1:H:688:LYS:CA	1:H:689:TYR:CA	2.80	0.60
1:A:688:LYS:CA	1:A:689:TYR:CA	2.80	0.60
1:B:688:LYS:CA	1:B:689:TYR:CA	2.80	0.60
1:G:688:LYS:CA	1:G:689:TYR:CA	2.80	0.60
1:E:688:LYS:CA	1:E:689:TYR:CA	2.80	0.60
1:F:688:LYS:CA	1:F:689:TYR:CA	2.80	0.60
1:C:688:LYS:CA	1:C:689:TYR:CA	2.80	0.59
1:D:688:LYS:CA	1:D:689:TYR:CA	2.80	0.59
1:I:826:GLU:CA	1:I:852:ARG:CA	2.81	0.59
1:I:688:LYS:CA	1:I:689:TYR:CA	2.80	0.59
1:F:558:LEU:CA	1:F:559:ILE:CA	2.81	0.58
1:A:830:LYS:CA	1:A:854:ARG:CA	2.81	0.58
1:C:1279:HIS:CA	1:D:895:ARG:CA	2.83	0.56
1:F:1528:CYS:CA	1:F:1532:SER:CA	2.84	0.56
1:H:1528:CYS:CA	1:H:1532:SER:CA	2.84	0.56
1:E:1528:CYS:CA	1:E:1532:SER:CA	2.84	0.56
1:I:1528:CYS:CA	1:I:1532:SER:CA	2.84	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1528:CYS:CA	1:B:1532:SER:CA	2.84	0.56
1:C:1528:CYS:CA	1:C:1532:SER:CA	2.84	0.56
1:A:1528:CYS:CA	1:A:1532:SER:CA	2.84	0.56
1:D:1528:CYS:CA	1:D:1532:SER:CA	2.84	0.55
1:G:1528:CYS:CA	1:G:1532:SER:CA	2.84	0.55
1:I:508:VAL:CA	1:I:510:TYR:CA	2.84	0.55
1:I:458:GLU:CA	1:I:459:CYS:CA	2.87	0.53
1:B:1279:HIS:CA	1:B:1280:ALA:CA	2.96	0.43
1:C:522:MET:CA	1:C:552:VAL:CA	2.96	0.43
1:B:487:LYS:CA	1:B:510:TYR:CA	2.98	0.41
1:I:1001:PRO:CA	1:I:1004:LEU:CA	3.00	0.40
1:B:1001:PRO:CA	1:B:1004:LEU:CA	3.00	0.40
1:D:1001:PRO:CA	1:D:1004:LEU:CA	3.00	0.40
1:E:1001:PRO:CA	1:E:1004:LEU:CA	3.00	0.40

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.

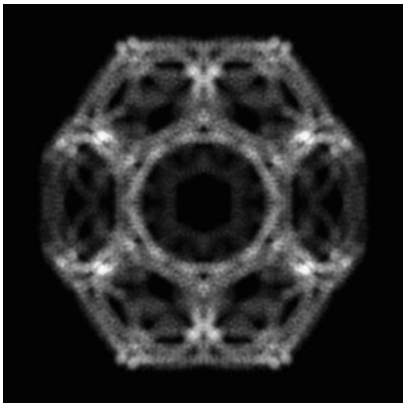
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5119. These allow visual inspection of the internal detail of the map and identification of artifacts.

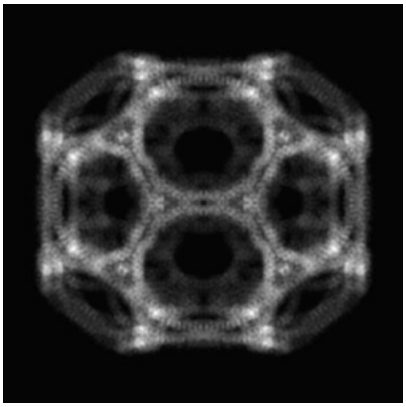
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

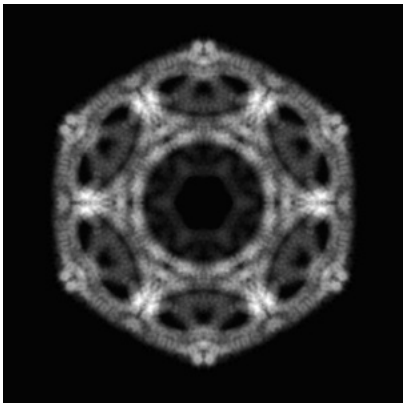
6.1.1 Primary map



X



Y

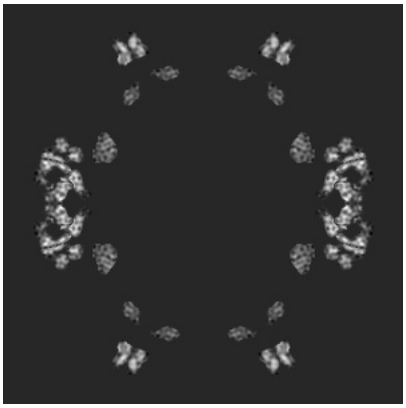


Z

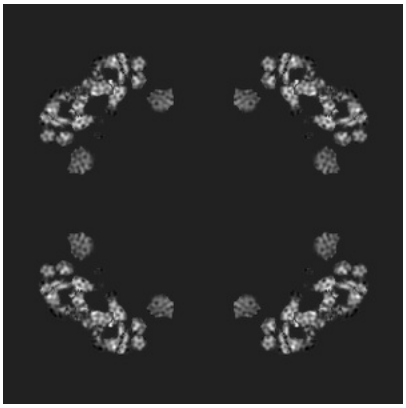
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 156



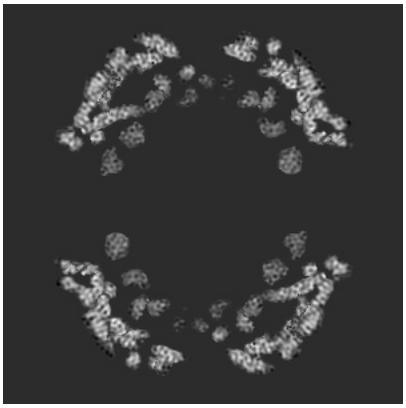
Y Index: 156

Z Index: 156

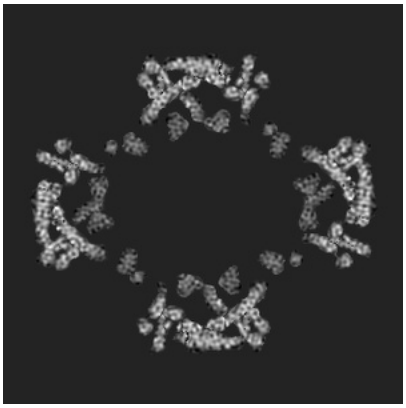
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

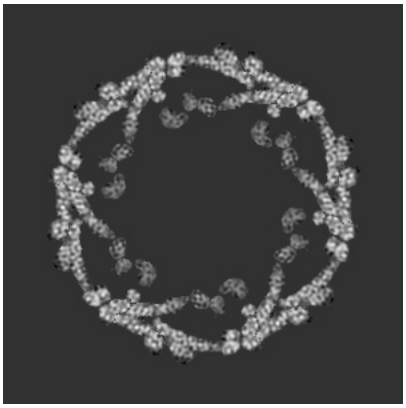
6.3.1 Primary map



X Index: 114



Y Index: 101

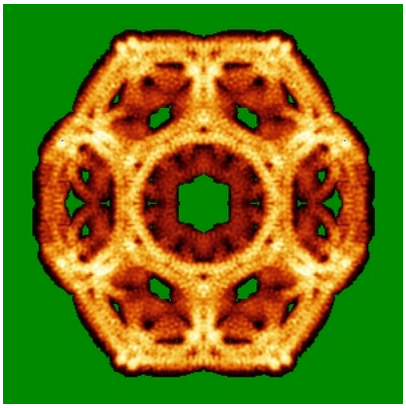


Z Index: 205

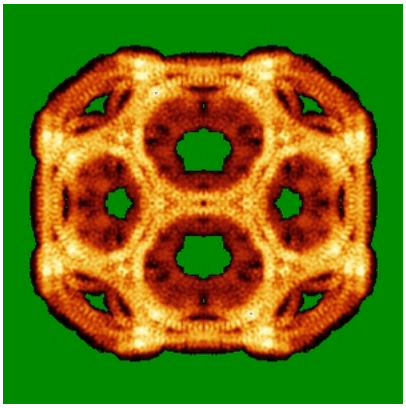
The images above show the largest variance slices of the map in three orthogonal directions.

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

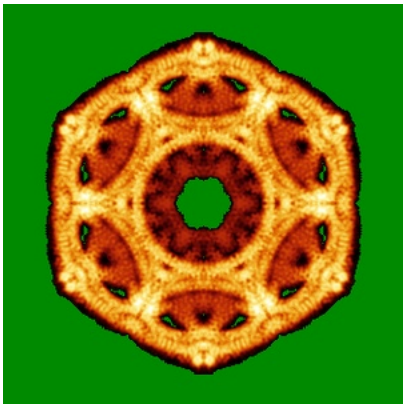
6.4.1 Primary map



X



Y

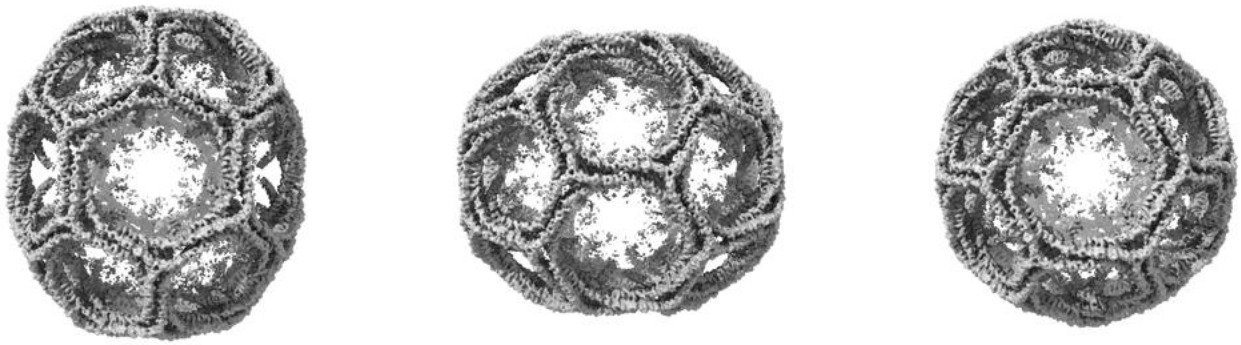


Z

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.

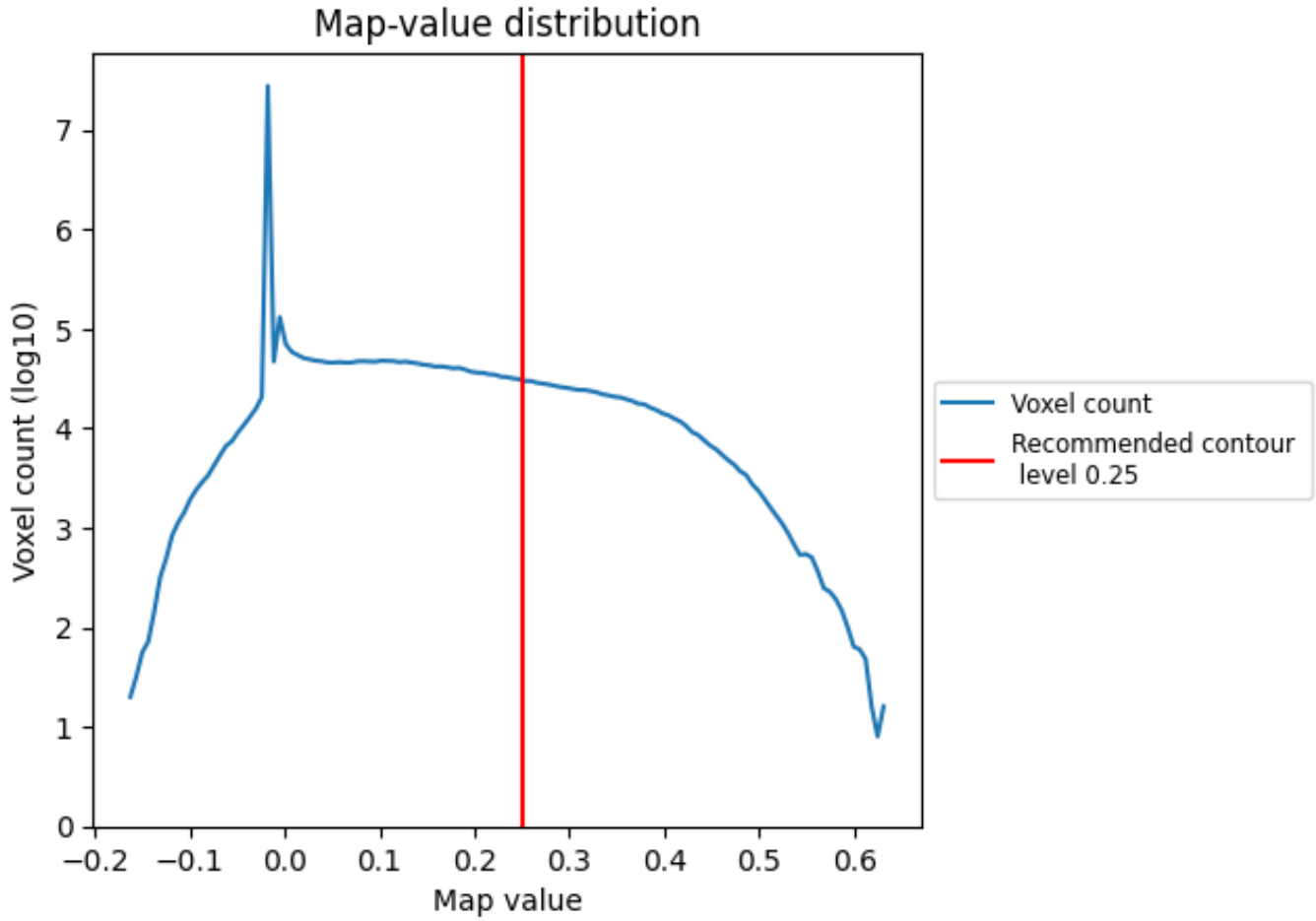
6.6 Mask visualisation (i)

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

7 Map analysis

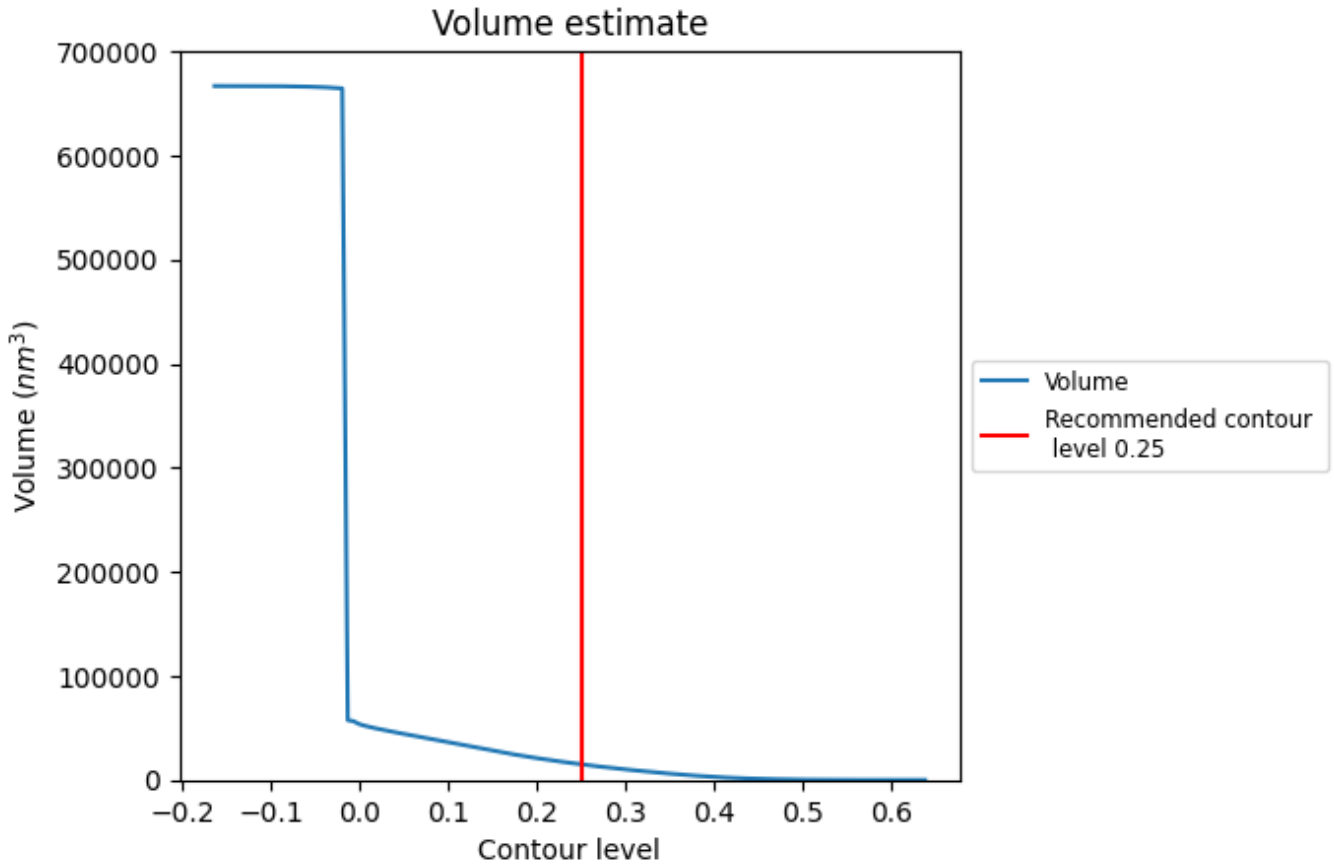
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

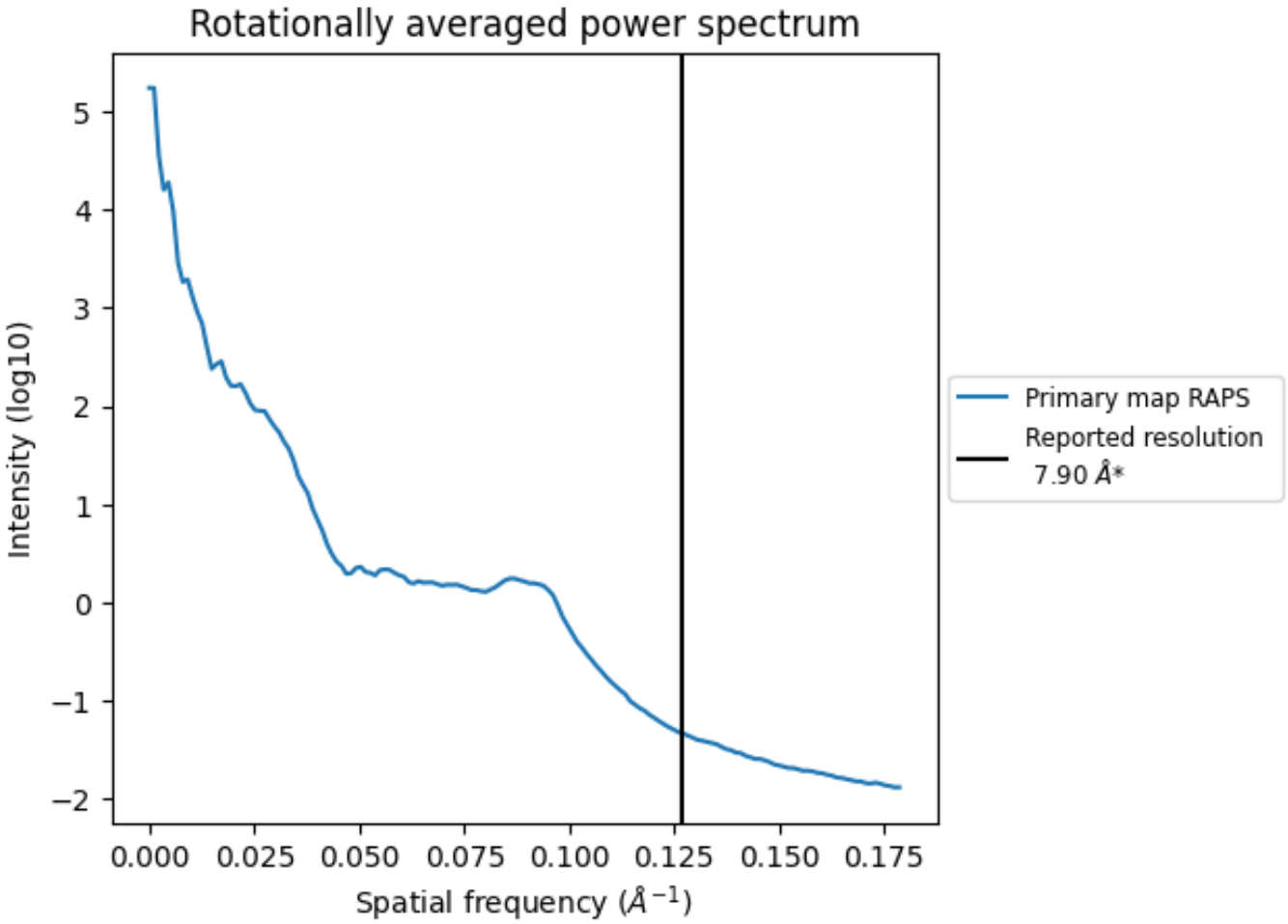
7.2 Volume estimate



The volume at the recommended contour level is 15047 nm^3; this corresponds to an approximate mass of 13592 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 0.127 Å^{-1}

8 Fourier-Shell correlation

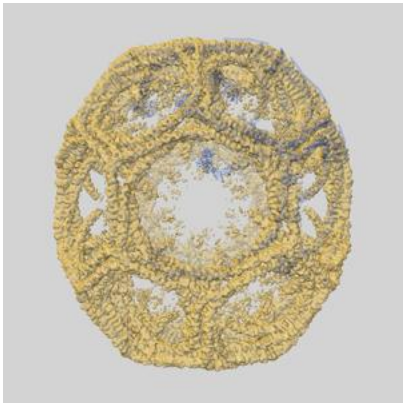
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

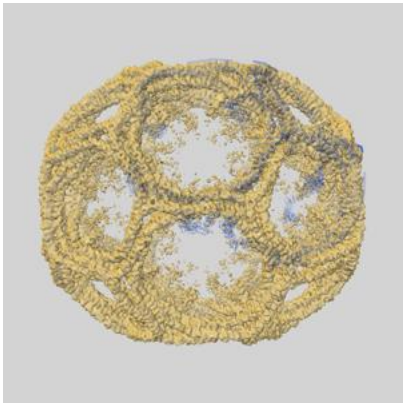
This section contains information regarding the fit between EMDB map EMD-5119 and PDB model 3IYV. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

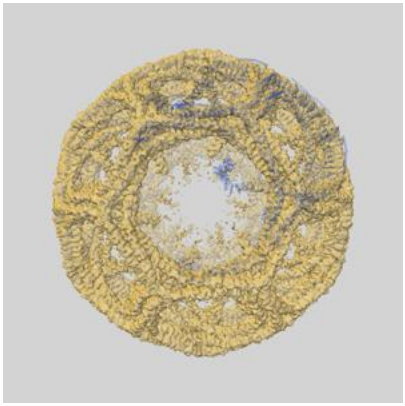
9.1.1 Map-model overlay



X

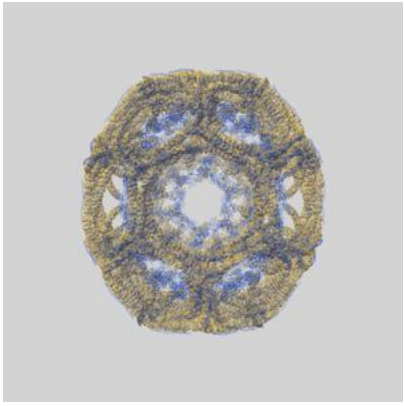


Y

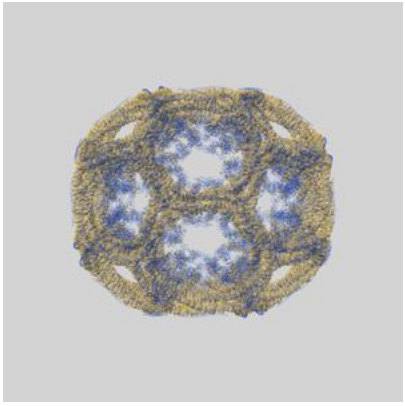


Z

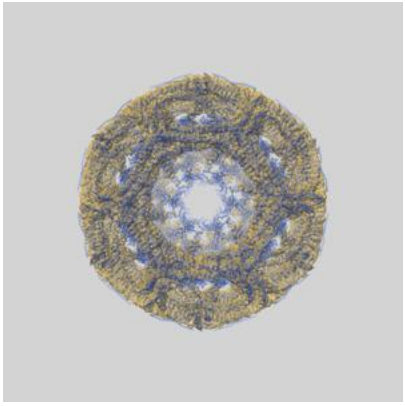
9.1.2 Map-model assembly overlay



X



Y



Z

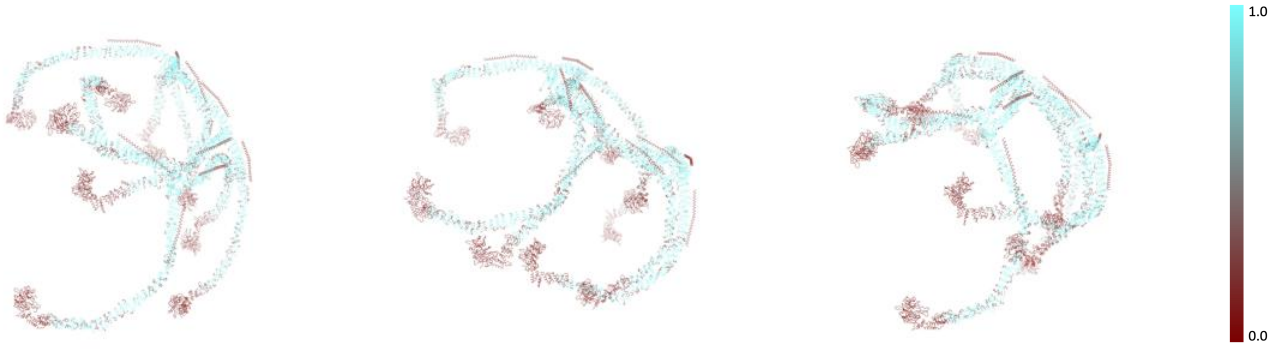
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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.

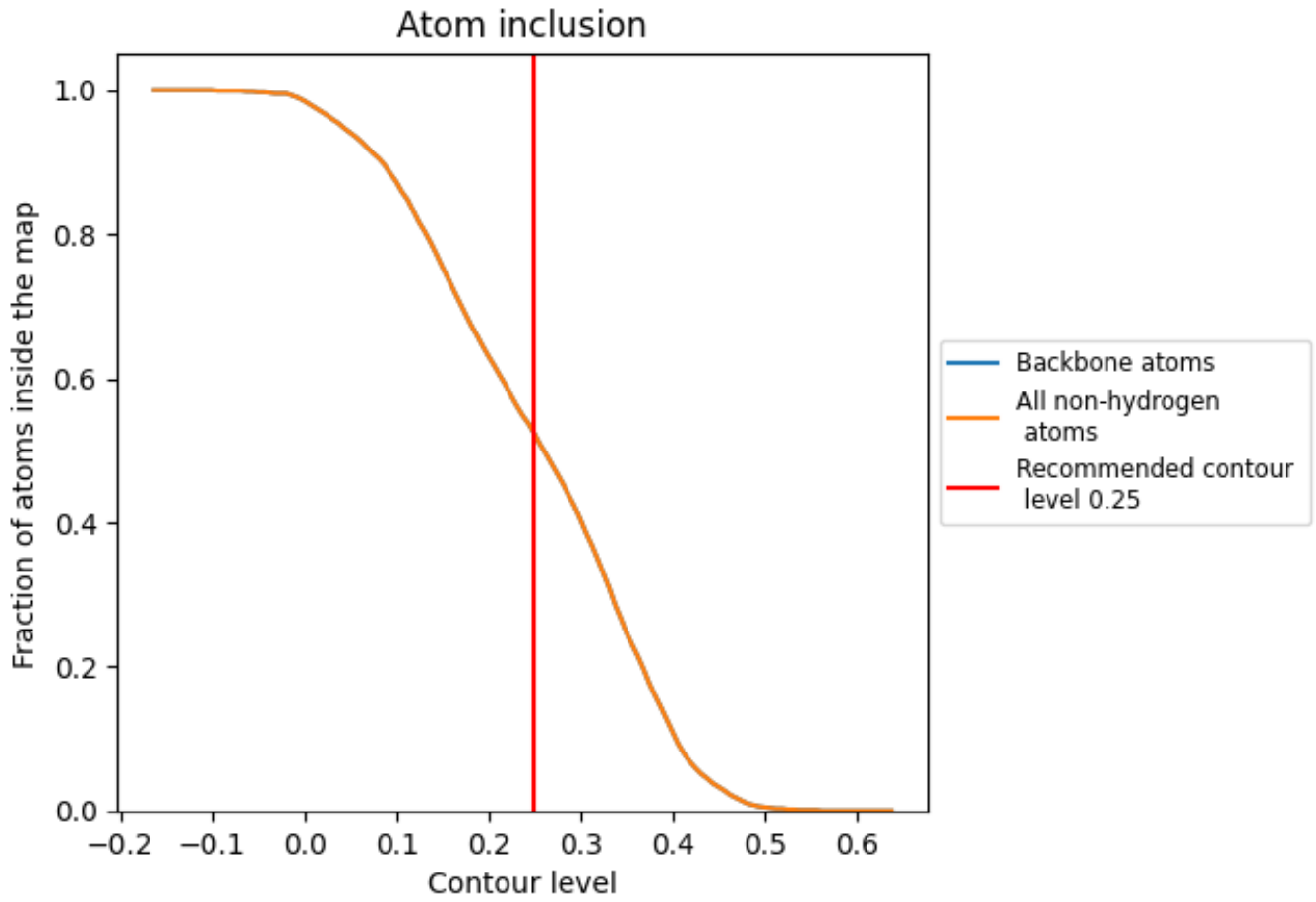
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5230	0.0550
A	0.5380	0.0530
B	0.5550	0.0610
C	0.5600	0.0620
D	0.5440	0.0580
E	0.5390	0.0570
F	0.5390	0.0580
G	0.5490	0.0630
H	0.5370	0.0530
I	0.5460	0.0590
J	0.0000	-0.0250
K	0.0000	-0.0310
L	0.0000	0.0050
M	0.0000	0.0110
N	0.0000	-0.0150
O	0.0000	-0.0380
P	0.0000	-0.0440
Q	0.0000	-0.0190
R	0.0000	-0.0300