wwPDB EM Validation Summary Report

Nov 15, 2022 – 06:10 PM EST

PDB ID	:	6WCJ
EMDB ID	:	EMD-21611
Title	:	Asymmetric vertex of the clathrin minicoat cage
Authors	:	Paraan, M.; Mendez, J.; Sharum, S.; Kurtin, D.; He, H.; Stagg, S.
Deposited on	:	2020-03-30
Resolution	:	6.30 Å(reported)
Based on initial model	:	6SCT

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 ⓘ 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:

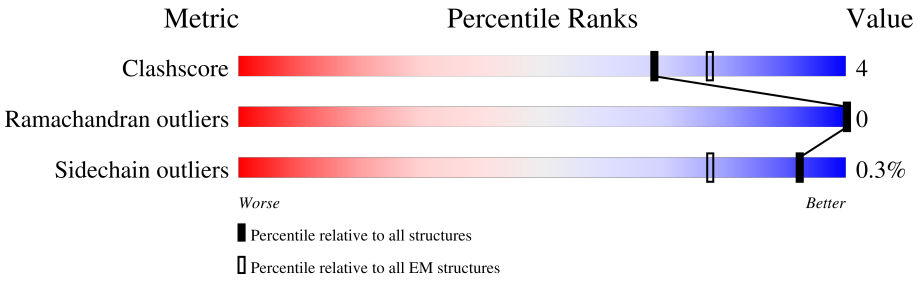
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1675	20% 76%
1	C	1675	20% 76%
1	D	1675	5% 20% 76%
1	G	1675	7% 35% 5% 60%
1	H	1675	7% 23% 74%
1	I	1675	11% 36% 60%
1	K	1675	8% 24% 74%
1	L	1675	6% 34% 5% 60%

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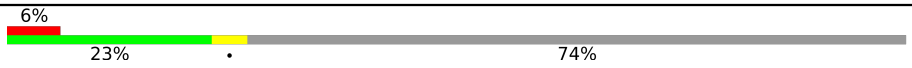
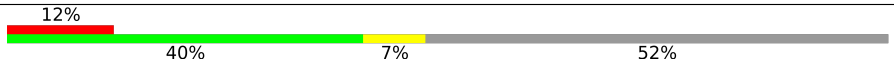
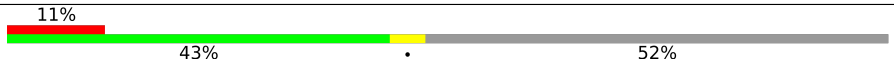
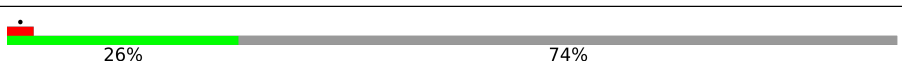
Mol	Chain	Length	Quality of chain
1	M	1675	
2	B	228	
2	E	228	
2	F	228	
2	J	228	
2	N	228	
2	O	228	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 41184 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	394	Total	C	N	O	S	0	0
			3287	2114	546	607	20		
1	C	394	Total	C	N	O	S	0	0
			3287	2114	546	607	20		
1	D	394	Total	C	N	O	S	0	0
			3287	2114	546	607	20		
1	L	666	Total	C	N	O	S	0	0
			5410	3442	927	1016	25		
1	M	441	Total	C	N	O	S	0	0
			3600	2294	615	676	15		
1	G	666	Total	C	N	O	S	0	0
			5410	3442	927	1016	25		
1	H	441	Total	C	N	O	S	0	0
			3600	2294	615	676	15		
1	I	666	Total	C	N	O	S	0	0
			5410	3442	927	1016	25		
1	K	441	Total	C	N	O	S	0	0
			3600	2294	615	676	15		

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

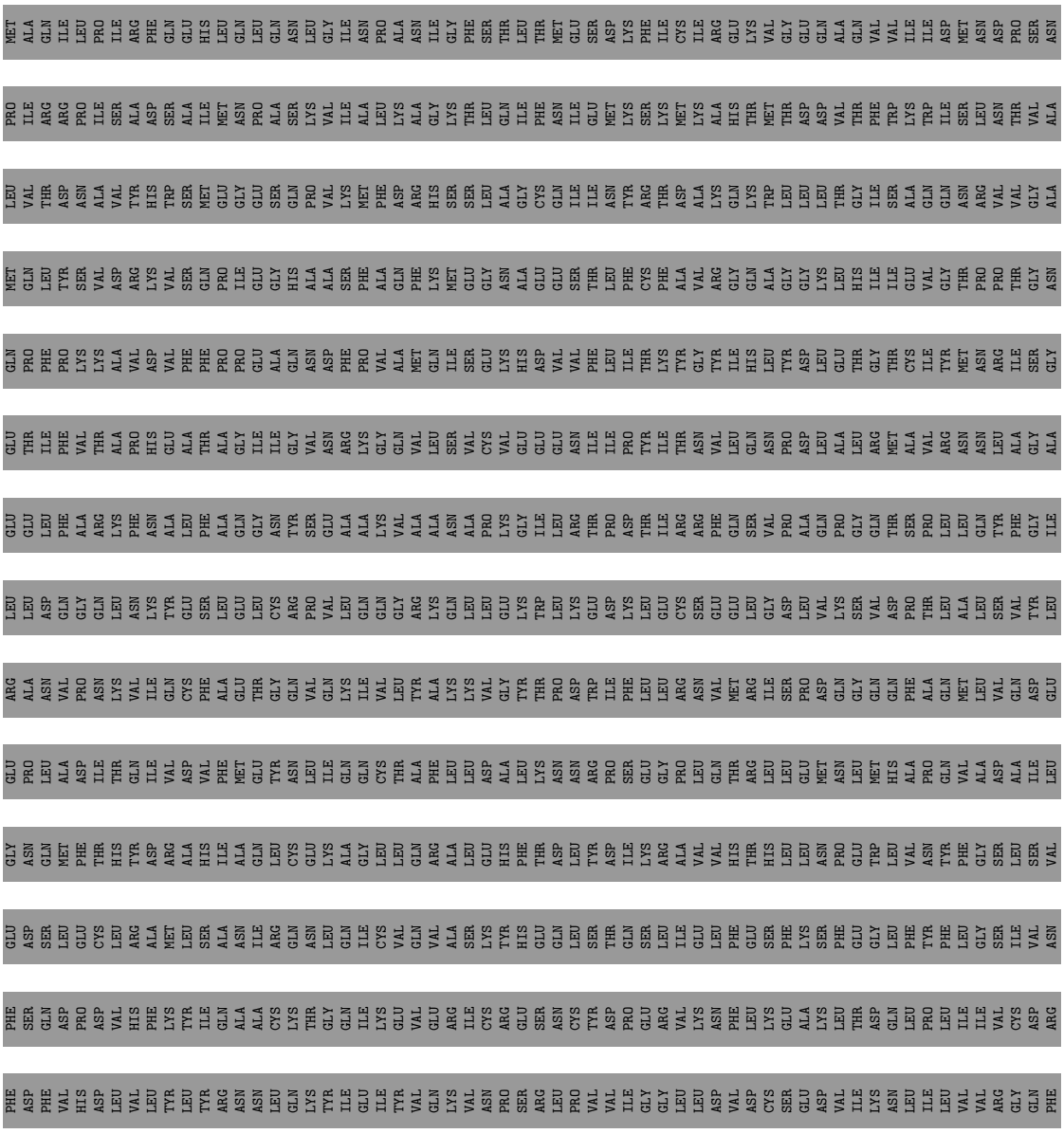
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	109	Total	C	N	O	S	0	0
			916	564	173	175	4		
2	E	109	Total	C	N	O	S	0	0
			916	564	173	175	4		
2	F	109	Total	C	N	O	S	0	0
			916	564	173	175	4		
2	O	59	Total	C	N	O	S	0	0
			515	313	101	100	1		
2	J	59	Total	C	N	O	S	0	0
			515	313	101	100	1		
2	N	59	Total	C	N	O	S	0	0
			515	313	101	100	1		

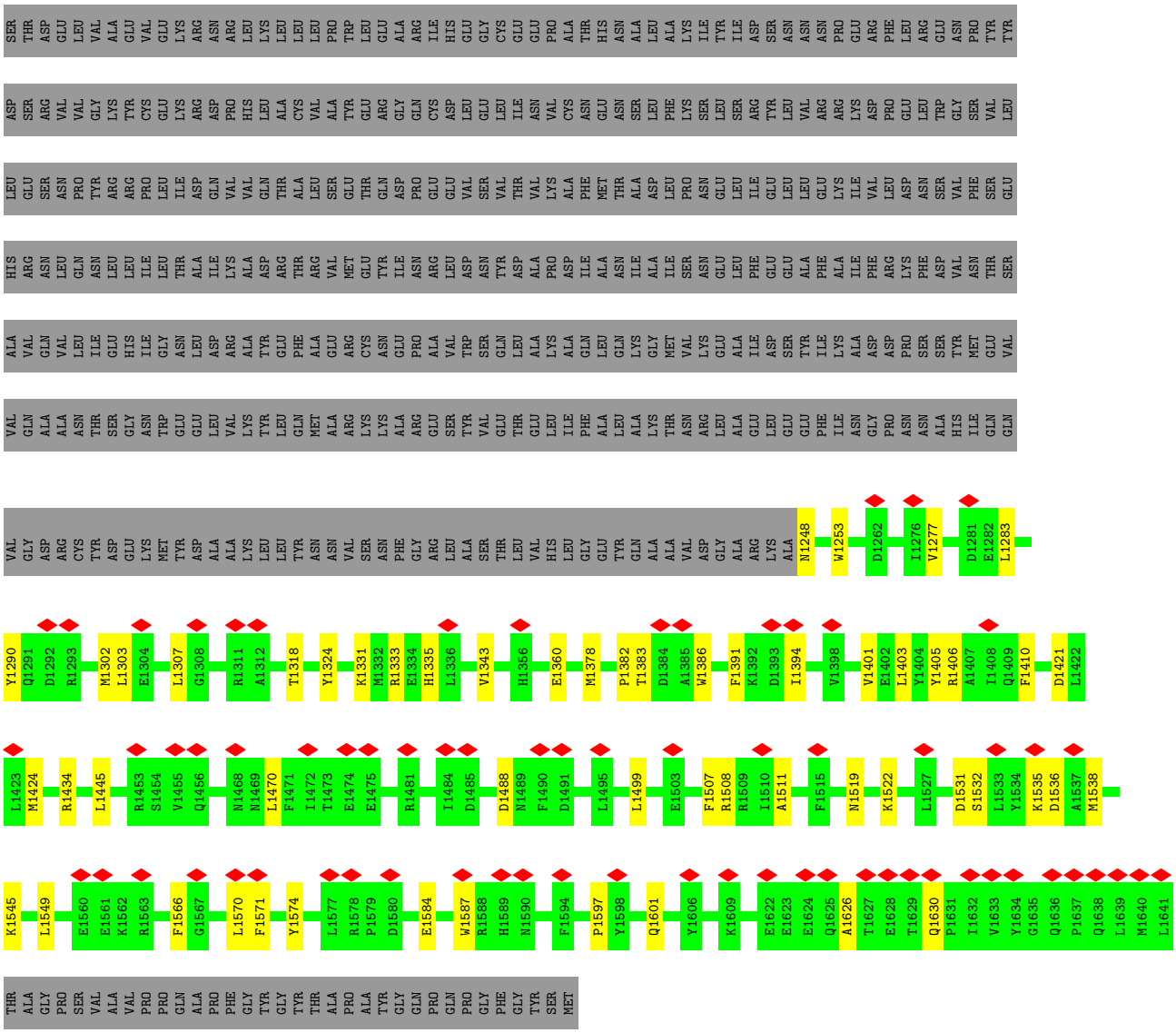
3 Residue-property plots (i)

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 1

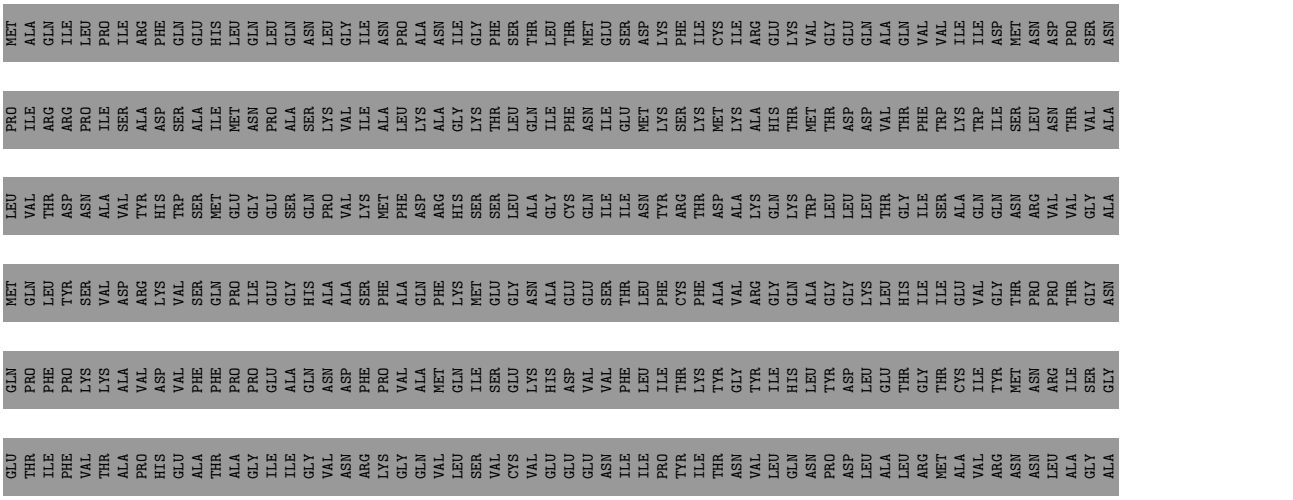
Chain A:

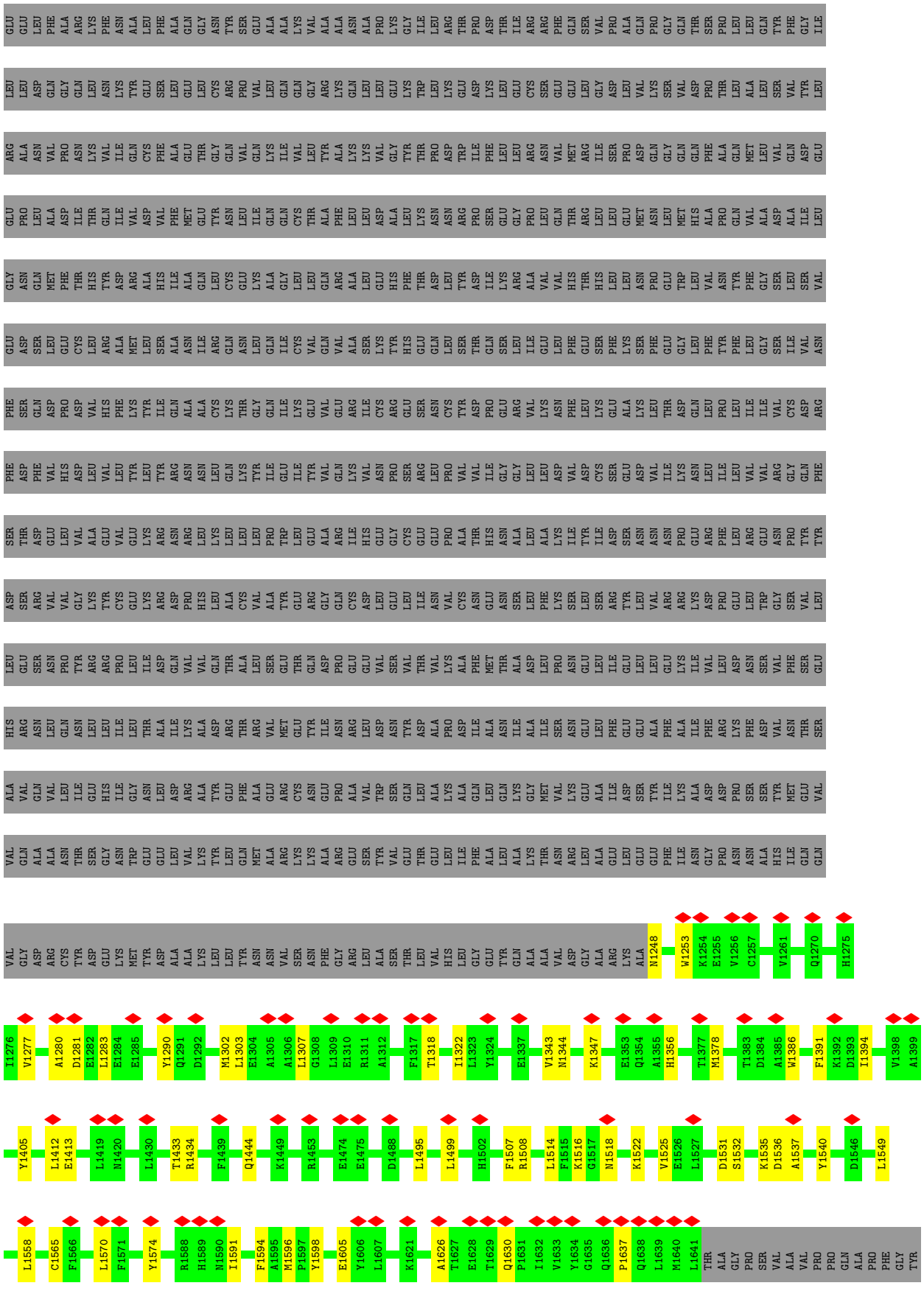




• Molecule 1: Clathrin heavy chain 1

Chain C:

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LEU LEU ASP GLN GLY GLN LEU ASN LYS TYR GLU SER LEU GLU LEU CYS ARG PRO VAL LEU GLN LEU GLN GLY ARG LYS GLN LEU LEU GLY ASP LEU VAL LYS SER VAL ASP PRO THR LEU ALA GLN MET LEU SER VAL TYR LEU
ARG ALA ASN VAL PRO ASN LYS VAL ILE GLN CYS PHE ALA GLU THR GLY GLN VAL GLN LYS ILE VAL LEU TYR ALA LYS LYS VAL GLY TYR THR PRO ASP TRP ILE PHE LEU LEU GLU ARG ASN VAL MET ARG ILE SER PRO ASP GLN GLY GLN GLN HIS PHE PRO GLN VAL ALA ASP ALA ILE LEU
GLU PRO LEU ALA ASP ILE THR GLN ILE VAL ASP VAL PHE MET GLU TYR ASN LEU ILE LYS GLN GLN CYS THR ALA PHE LEU ALA LEU ASP ASP ARG LEU LEU GLU MET ASN LEU MET HIS ALA PRO GLN VAL ALA ASP ALA ILE LEU
GLY ASN GLN MET PHE THR HIS TYR ASP ARG ALA ALA HIS ILE ALA ALA GLY LEU LEU GLN ARG ALA LEU GLU GLU HIS PHE THR ASP LEU TYR ASP ILE LYS ARG ALA VAL VAL HIS THR HIS LEU LEU ASN PRO GLU TRP THR LEU VAL ASN TYR PHE GLY SER LEU SER VAL
GLU ASP SER LEU GLU CYS LEU ARG ALA MET LEU SER ALA ASN ILE ARG GLN LEU ASN LEU GLN VAL ALA LEU GLN CYS GLU LYS ALA GLY LEU LEU LEU GLN VAL ALA ILE GLN GLN LEU ILE CYS VAL GLN VAL ALA ALA LEU GLU HIS TYR THR ASP LEU TYR ASP SER LEU LEU GLU LEU ILE GLU LEU PHE GLU SER PHE LYS SER PHE GLU GLY LEU PHE TYR PHE LEU GLY SER ILE VAL ASN
PHE SER GLN ASP PRO ASP VAL HIS PHE LYS TYR ILE GLN ALA ALA CYS LYS THR GLY GLN ILE LYS GLU VAL GLU ARG ILE CYS ARG GLU SER ASN CYS TYR ASP PRO GLU ARG VAL LYS ASN PHE LEU LYS GLU ALA LYS LEU THR ASP GLN LEU PRO LEU ILE LEU VAL CYS ASP ASP ARG
PHE ASP PHE VAL HIS ASP LEU VAL LEU TYR LEU TYR ARG ASN ASN LEU GLN LYS TYR ILE GLU ILE TYR VAL GLN LYS VAL ASN PRO SER ARG LEU PRO VAL VAL ILE GLY GLY LEU LEU ASP VAL ASN PHE LEU LYS ASP CYS SER GLU ASP VAL ILE LYS ASN LEU PRO ILE LEU VAL ARG GLY GLN PHE
SER THR ASP GLU LEU VAL ALA GLU VAL GLU LYS ARG ASN ARG LEU LYS LEU LEU LEU PRO TRP LEU GLU GLU ALA ARG ILE HIS GLU GLY CYS GLU GLU PRO ALA THR HIS ASN ALA LEU ALA LYS ILE TYR ILE ASP SER ASN ASN ASN PRO GLU PHE LEU ARG GLU GLU ASN PRO SER TYR TYR
ASP SER ARG VAL VAL GLY LYS TYR CYS GLU LYS ARG ASP PRO HIS LEU ALA CYS VAL ALA TYR GLU ARG GLY GLN CYS ASP LEU GLU GLU LEU ILE ASN VAL CYS ASN GLU ASN SER LEU PHE LYS SER LEU SER ARG TYR LEU VAL ARG LYS ASP PRO GLU LEU TRP GLY SER VAL LEU
LEU GLU SER ASN PRO TYR ARG ARG PRO LEU ILE ASP GLN VAL VAL GLN THR ALA LEU SER GLU THR GLN ASP PRO GLU GLU VAL SER VAL THR VAL LYS ILE PRO GLU LEU ILE GLU LEU LEU GLU LYS ILE VAL LEU ASP ASP ASN SER GLU
HIS ARG ASN LEU GLN ASN LEU LEU ILE LEU THR ALA ILE LYS ALA ASP ARG THR ARG VAL MET GLU TYR ILE ASN ARG LEU ASP ASN TYR ASP ALA PRO ASP ILE ALA ASN ILE ALA ILE SER ASN GLU LEU PHE GLU GLU ALA PHE ALA ILE PHE ARG LYS PHE ASP VAL ASN THR SER
ALA VAL GLN VAL LEU ILE GLY ASN LEU ILE GLU HIS GLU ARG CYS ASN GLU PRO ALA VAL TRP SER GLN LEU ALA LYS GLU LEU ILE ASP SER TYR ILE LYS ASN GLU LEU ALA ILE ASP GLU LEU GLU GLU PHE ILE LYS ALA ASP PRO PRO SER SER TYR MET GLU VAL
VAL GLN ALA ALA ASN THR SER GLY ASN GLY LYS TYR LEU GLN MET ALA ALA ARG LYS LYS ALA ARG GLU SER ARG GLU LEU VAL LYS GLU GLU THR LEU GLU THR VAL GLU LEU GLU LEU ILE PHE ALA LEU ALA LYS THR ASN ARG LEU ALA GLU LEU GLU GLU PHE ILE ASN ASN GLY PRO ASN ASN ALA HIS ILE GLN GLN
VAL GLY ASP ARG CYS TYR MET TYR ASP GLU LEU GLU LYS ASN VAL ASN PHE GLY ARG LEU ALA SER ASN THR LEU VAL HIS LEU GLU GLY GLU TYR GLN ALA ALA VAL ASP GLY ALA ARG LYS ALA N1248 W1253 K1254 E1255 V1256 C1257 V1261 Q1270 H1275
I1276 V1277 A1280 D1281 E1282 L1283 E1284 E1285 Y1290 Q1291 D1292 M1302 L1303 E1304 A1305 A1306 L1307 G1308 L1309 E1310 R1311 A1312 F1317 T1318 I1322 L1323 Y1324 E1337 V1343 N1344 K1347 E1353 Q1354 A1355 H1356 T1377 M1378 T1383 D1384 A1385 W1386 F1391 K1392 D1393 I1394 V1398 A1399
Y1405 L1412 E1413 L1419 N1420 L1430 T1433 R1434 F1439 Q1444 K1449 R1453 E1474 E1475 D1488 L1495 L1499 H1502 F1507 R1508 L1514 F1515 K1516 G1517 N1518 K1522 V1525 E1526 L1527 D1531 S1532 K1535 D1536 A1537 Y1540 D1546 L1549
L1558 C1565 F1566 L1570 F1571 Y1574 R1588 H1589 N1590 I1591 F1594 A1595 M1596 P1597 Y1598 E1605 Y1606 L1607 K1621 A1626 T1627 E1628 T1629 Q1630 P1631 I1632 V1633 Y1634 G1635 Q1636 P1637 Q1638 L1639 M1640 L1641 THR ALA GLY PRO SER VAL ALA VAL PRO PRO GLN ALA PRO PHE GLY TYR

GLY TYR THR ALA PRO ALA TYR GLY GLN PRO GLN PRO GLY PHE GLY TYR SER MET

• Molecule 1: Clathrin heavy chain 1

Chain D: 5% 20% 76%

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

PRO ILE ARG ARG PRO ILE SER ALA ASP SER ALA ILE MET ASN PRO ALA SER LYS VAL ILE ALA LEU LYS ALA GLY LYS THR LEU GLN ILE PHE ASN ILE GLU MET LYS SER LYS MET THR ASP VAL THR PHE TRP LYS TRP ILE SER LEU ASN THR VAL ALA

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

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

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

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

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

LEU LEU ASP GLN GLY GLN LEU ASN LYS TYR GLU SER LEU GLU LEU CYS ARG PRO VAL LEU GLN LEU LEU GLU LYS TRP LEU LYS GLU ASP LYS LEU GLU CYS SER GLU GLU LEU GLY ASP LEU VAL LYS SER VAL ASP PRO THR LEU ALA LEU SER VAL TYR LEU

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

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

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

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

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

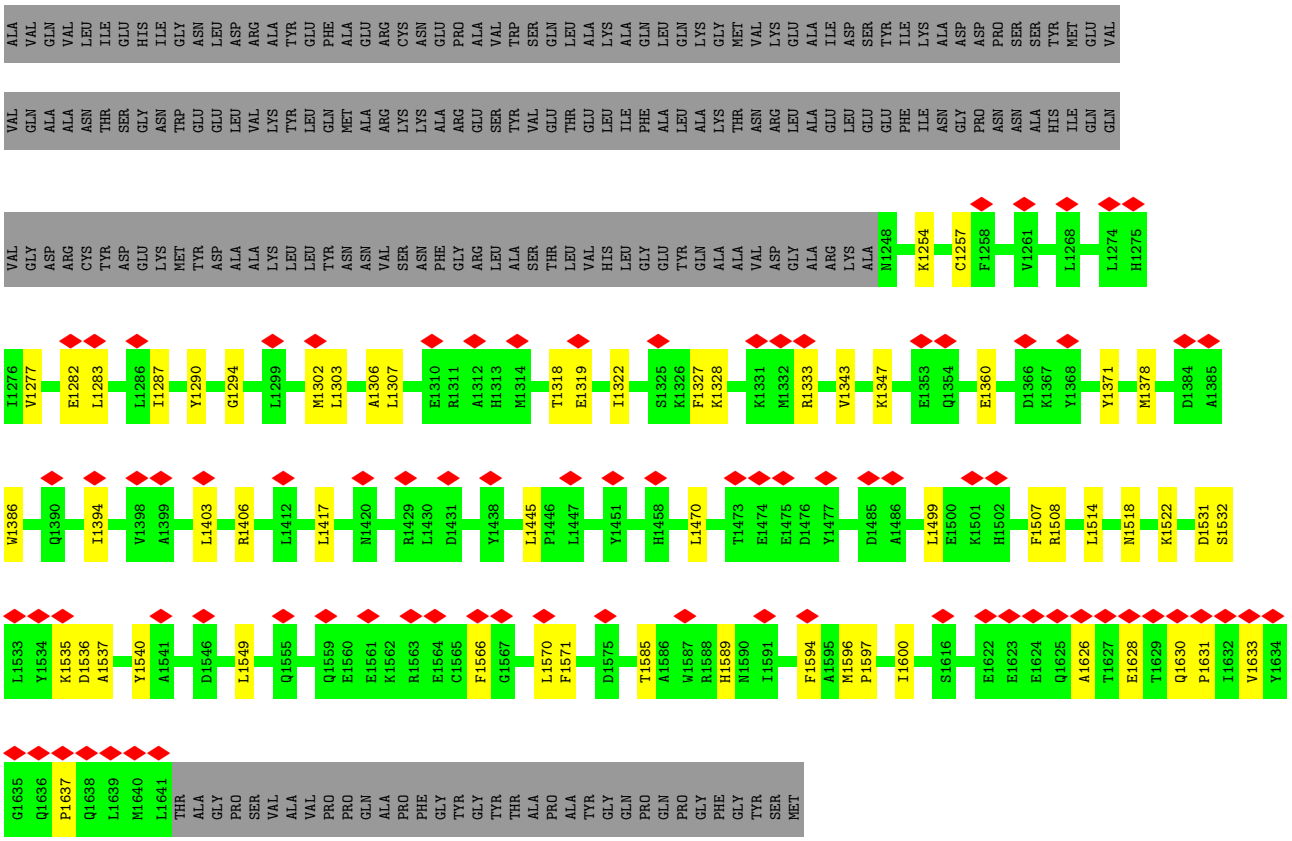
PHE ASP PHE VAL HIS ASP LEU TYR LEU TYR ARG ASN ASN LEU GLN LYS TYR ILE GLU ILE TYR VAL GLN LYS VAL ASN PRO SER ARG LEU PRO VAL VAL ILE GLY GLY LEU LEU ASP VAL ASP CYS SER GLU ASP VAL ILE LYS ASN ASP LEU LEU ILE LEU VAL VAL ARG GLY GLN PHE

SER THR ASP GLU LEU VAL ALA GLU VAL LYS ARG ASN ARG LEU LYS LEU LEU LEU PRO TRP LEU GLU GLU ALA ARG ILE HIS GLU GLY CYS GLU GLU PRO ALA THR HIS ASN ALA LEU ALA LYS ILE TYR ILE ASP SER ASN ASN PRO GLU ARG PHE LEU ARG GLU ASP PRO GLU

ASP SER ARG VAL VAL LYS TYR CYS GLU LYS ARG ASP PRO HIS HIS LEU ALA CYS VAL ALA TYR GLU ARG GLY GLN CYS ASP LEU GLU GLU LEU ILE ASN VAL CYS ASN GLU ILE ASN SER LEU PHE LYS SER LEU SER ARG TYR LEU VAL ARG ARG LYS ILE VAL ASP PRO GLU LEU GLY SER VAL LEU

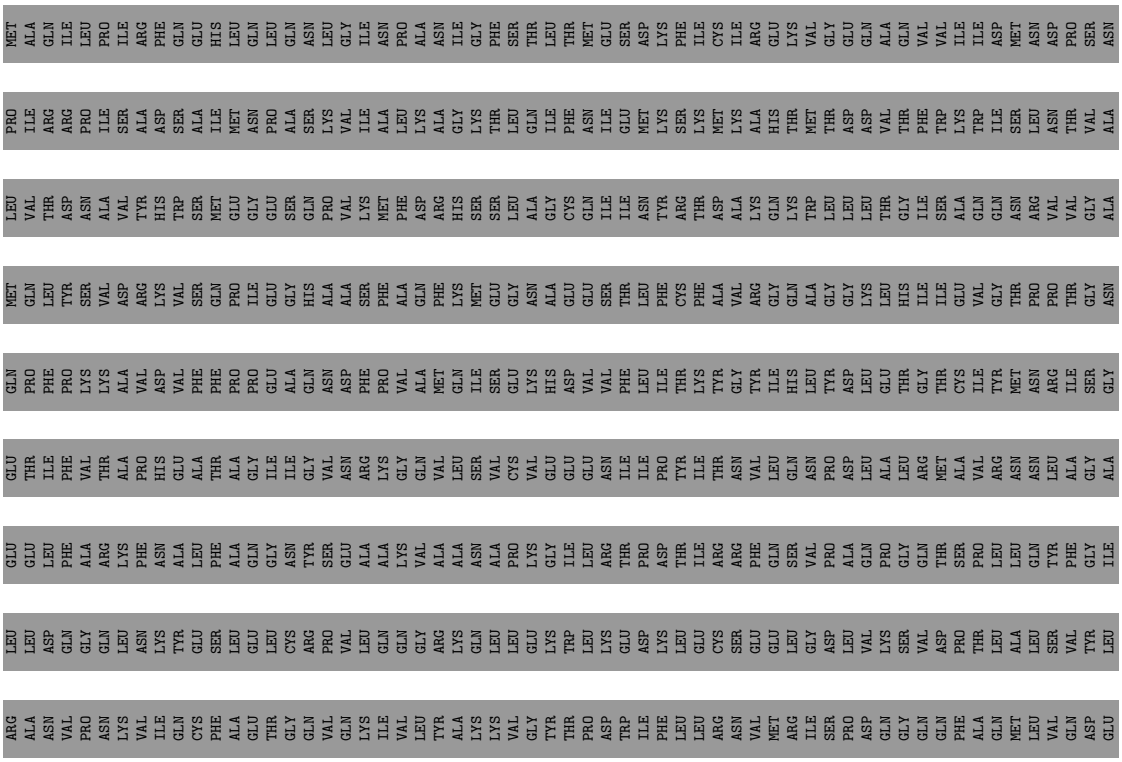
LEU GLU SER ASN PRO TYR ARG ARG PRO GLU LEU ILE ASP GLN VAL VAL GLN THR ALA LEU SER GLU THR GLN ASP PRO GLU GLU VAL SER VAL THR VAL LYS ALA PHE MET THR ALA ASP LEU PRO ASN GLU LEU ILE LEU GLU GLU LEU LEU GLU GLU LYS ILE LEU VAL LEU GLU ASP ASN SER VAL PHE SER GLU

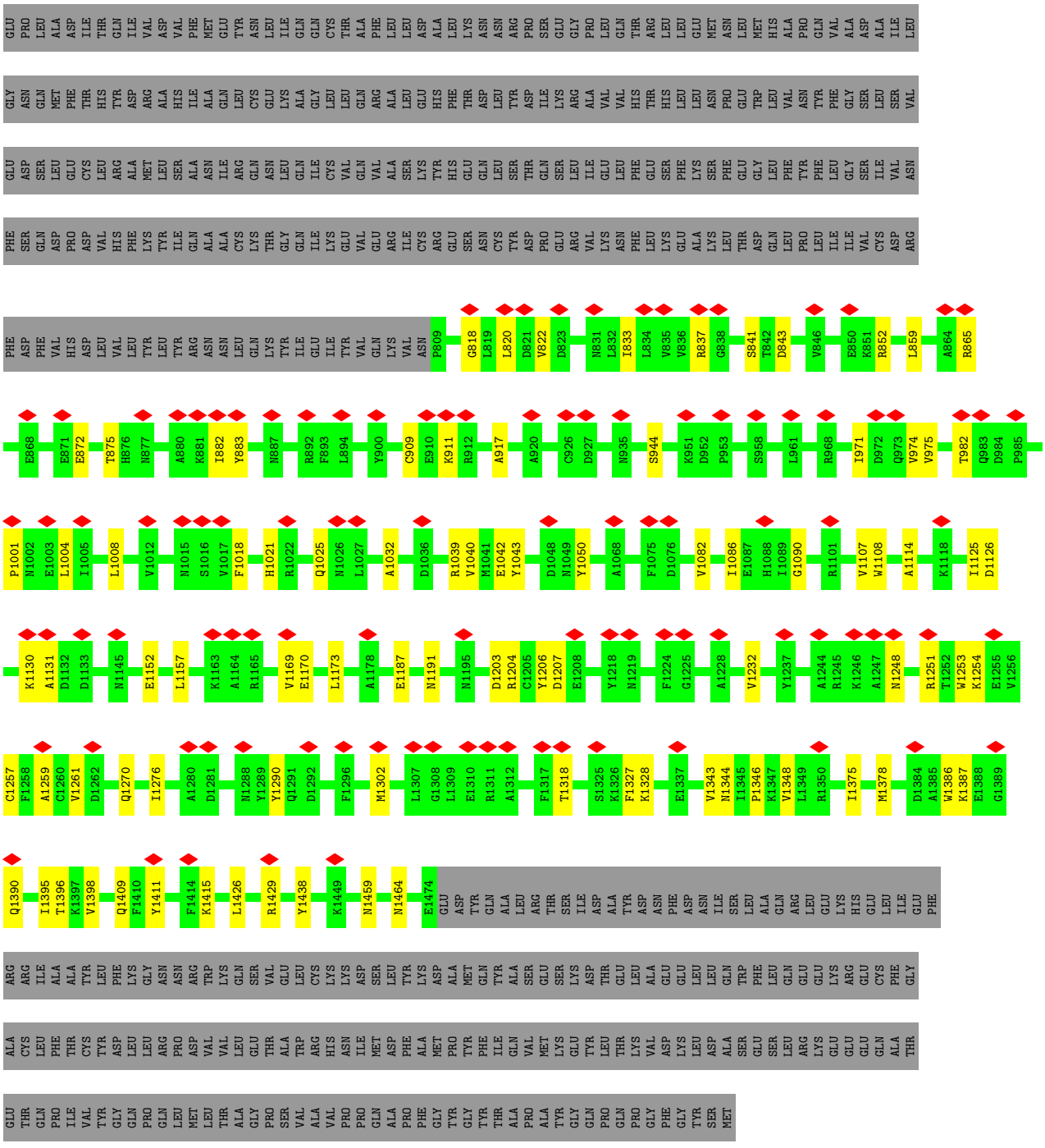
HIS ARG ASN LEU GLN ASN LEU LEU ILE LEU THR ALA ILE LYS ALA ASP ARG THR ARG VAL MET GLU TYR ILE ASN ARG LEU ASP ASN TYR ASP ALA PRO ASP ILE ALA ASN ILE ALA ILE SER ASN GLU LEU PHE GLU GLU ALA PHE ALA ILE PHE ARG LYS PHE ASP VAL ASN THR SER



• Molecule 1: Clathrin heavy chain 1

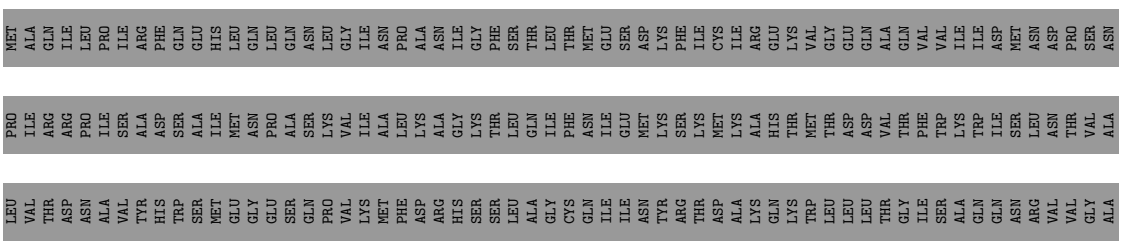
Chain L:

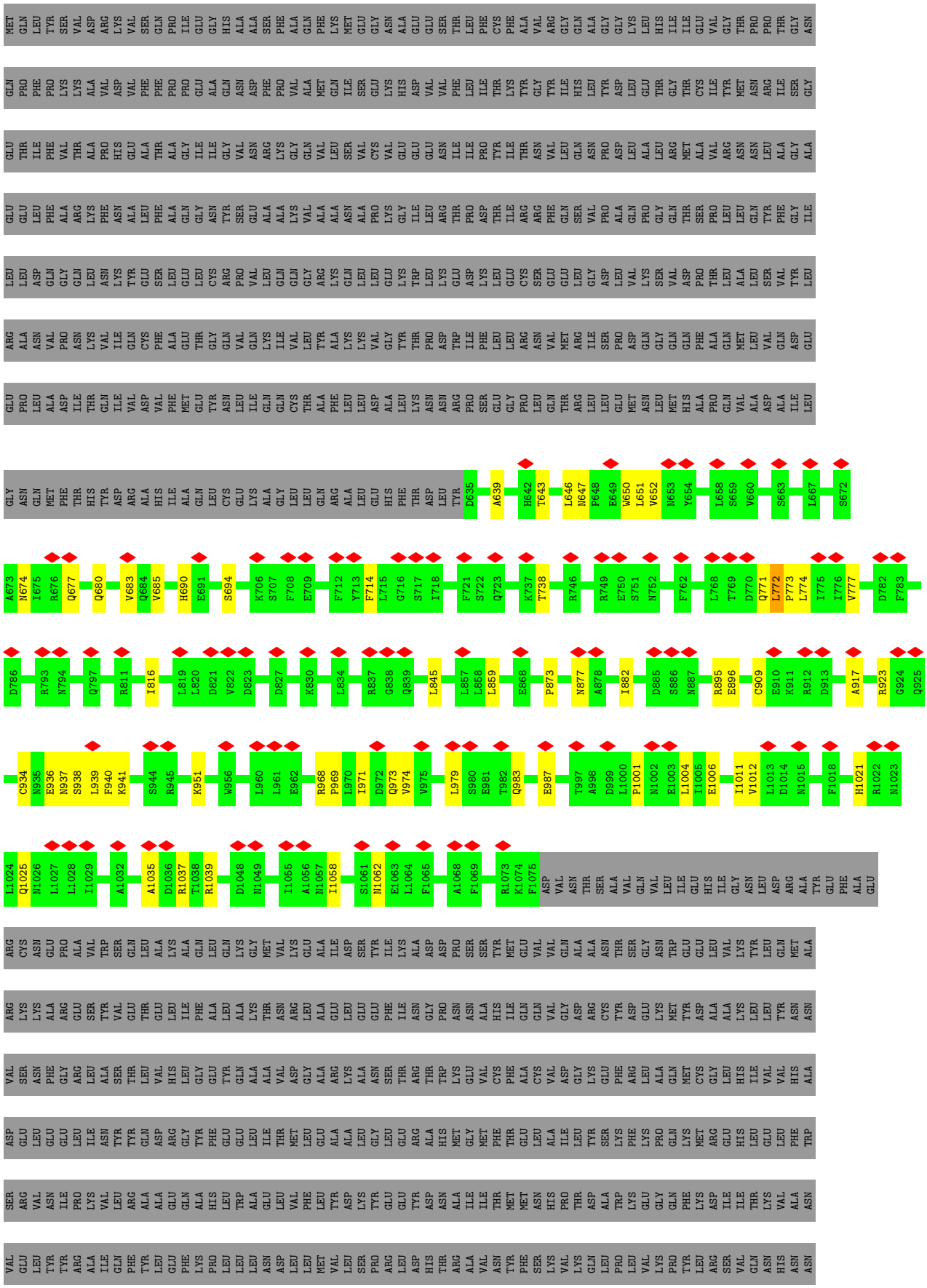


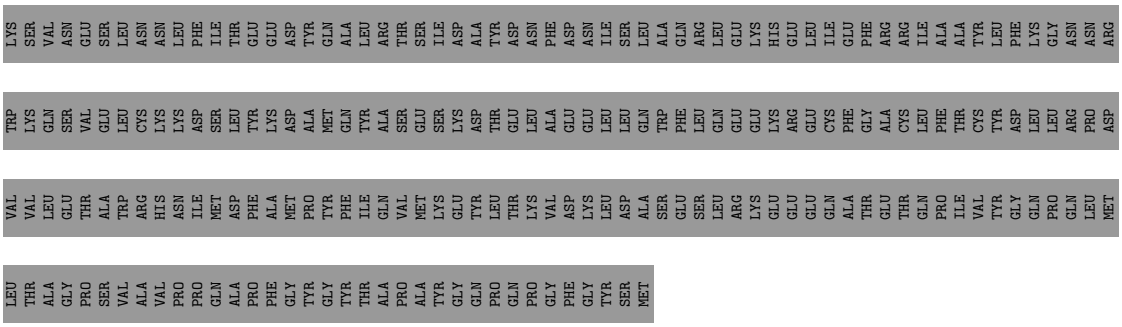


• Molecule 1: Clathrin heavy chain 1

Chain M:

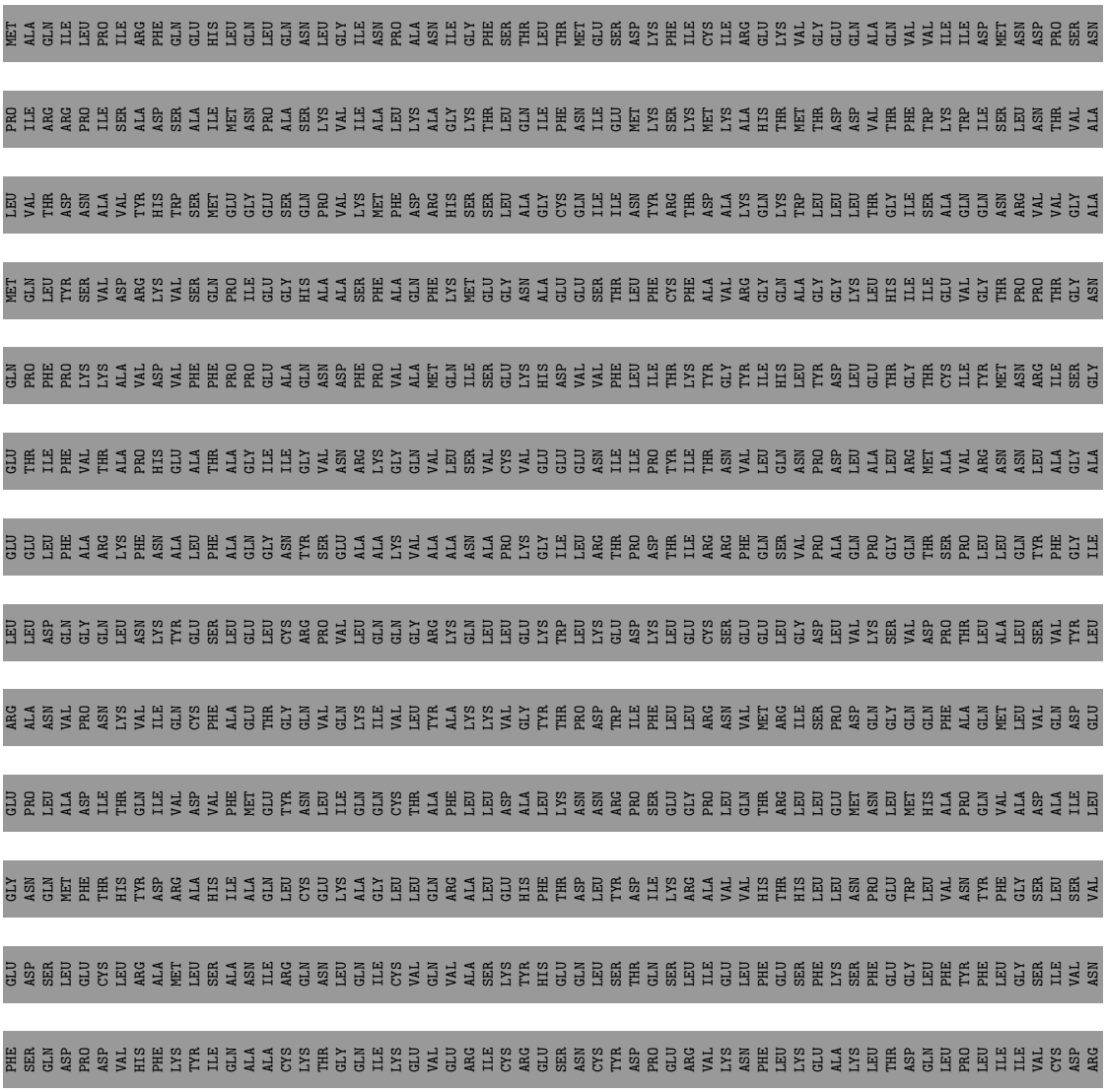


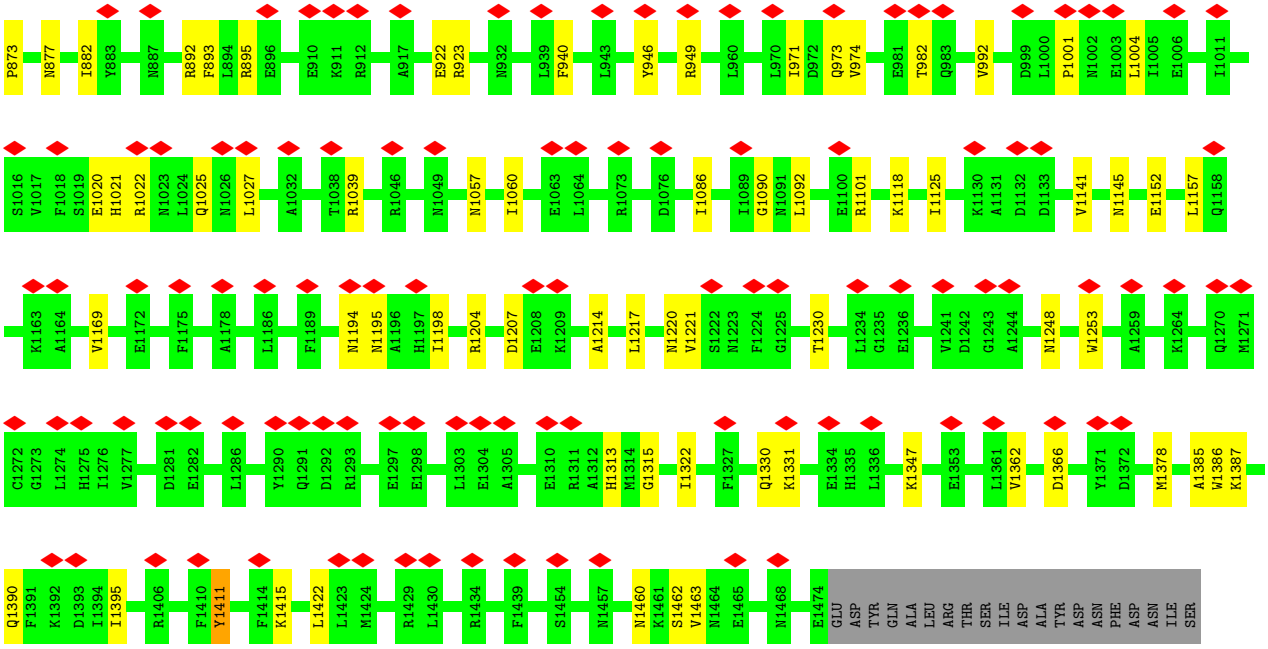

MET GLN LEU TYR SER VAL ASP ARG LYS VAL SER GLN PRO ILE GLU GLY HIS ALA ALA SER PHE ALA GLN PHE LYS MET GLU GLY ASN ALA GLU GLU SER THR LEU PHE CYS PHE ALA VAL ARG GLY GLN ALA GLY GLY LYS LEU HIS ILE ILE GLU VAL GLY THR PRO PRO THR GLY ASN
GLN PRO PHE PRO LYS LYS ALA VAL ASP VAL PHE PHE PRO PRO GLU ALA GLN ASN ASP PHE PRO VAL ALA MET GLN ILE SER GLU LYS HIS ASP VAL VAL PHE LEU ILE THR LYS TYR GLY TYR ILE HIS LEU TYR ASP LEU GLU THR GLY THR CYS ILE TYR MET ASN ARG ILE SER GLY
GLU THR ILE PHE VAL THR ALA PRO HIS GLU ALA THR ALA GLY ILE ILE GLY VAL ASN ARG LYS GLY GLN VAL LEU GLU GLU GLU ASN ILE ILE PRO TYR ILE THR ASN VAL LEU GLN ASN PRO ASP LEU ALA LEU ARG MET ALA VAL ILE TYR ASN ARG ILE ALA GLY GLY
GLU GLU LEU PHE ALA ARG LYS PHE ASN ALA LEU PHE ASP ALA GLN GLY ASN TYR SER GLU ALA ALA ALA LYS VAL ALA ALA ASN ALA PRO LYS GLY ILE LEU ARG THR PRO ASP THR ILE ARG ARG PHE GLN SER VAL PRO ALA GLN PRO GLY GLN THR SER PRO LEU LEU LEU GLN TYR PHE GLY ILE
LEU LEU ASP GLN GLY GLN LEU ASN LYS TYR GLU SER LEU GLU GLU LEU CYS ARG PRO VAL LEU GLN LYS LYS ALA GLN LEU GLY LEU LEU GLU LYS TRP LEU LYS GLU ASP LYS LEU GLU CYS SER GLU GLU LEU GLY ASP LEU VAL LYS SER VAL ASP PRO THR LEU ALA LEU SER VAL TYR LEU
ARG ALA ASN VAL PRO ASN LYS VAL LEU ILE GLN CYS PHE ALA GLU THR GLY GLN VAL GLN LYS ILE VAL LEU TYR ALA LYS LYS VAL GLY TYR THR PRO ASP TRP ILE PHE LEU GLN ASN VAL MET ARG ILE SER PRO VAL ASP GLN GLY GLN GLN PHE PRO ALA ALA GLN MET LEU VAL GLN LYS GLU
GLU PRO LEU ALA ASP ILE THR GLN ILE VAL ALA PHE MET GLU TYR ASN LEU ILE GLN GLN CYS THR ALA PHE LEU LEU ASP ALA LEU LYS ASN ASN ARG PRO SER GLU GLY PRO LEU GLN THR ARG LEU LEU MET ASN LEU MET HIS ALA PRO GLN VAL ALA ASP ALA ILE LEU
GLY ASN GLN MET PHE THR HIS TYR ASP ARG ALA HIS ILE ALA GLN LEU CYS GLU LYS ALA GLY LEU LEU GLN ARG ALA LEU GLU HIS PHE THR ASP LEU TYR D635 A639 H642 T643 L646 N647 P648 E649 W650 L651 V652 N653 Y654 L658 S659 V660 S663 L667 S672
A673 N674 I675 R676 Q677 Q680 V683 Q684 V685 H690 E691 S694 K706 S707 F708 E709 F712 Y713 F714 L715 G716 S717 I718 F721 S722 Q723 K737 T738 R746 R749 E750 S751 N752 F762 L768 T769 D770 Q771 L772 P773 L774 I775 I776 V777 D782 F783
D786 R793 N794 Q797 R811 I816 L819 L820 D821 V822 D823 D827 K830 L834 R837 G838 Q839 L845 L857 L858 L859 E868 P873 N877 A878 I882 D885 S886 N887 R895 E896 C909 E910 K911 R912 D913 A917 R923 G924 Q925
C934 N935 E936 N937 S938 L939 F940 K941 S944 R945 K951 W956 L960 L961 E962 R968 P969 L970 I971 D972 Q973 V974 V975 L979 S980 E981 T982 Q983 E987 T997 A998 D999 L1000 P1001 N1002 E1003 L1004 I1005 E1006 I1011 V1012 L1013 D1014 N1015 F1018 H1021 R1022 N1023
L1024 Q1025 N1026 L1027 L1028 I1029 A1032 A1035 D1036 R1037 T1038 R1039 D1048 N1049 I1055 A1056 N1057 I1058 S1061 N1062 E1063 L1064 F1065 A1068 F1069 R1073 K1074 F1075 ASP VAL ASN THR SER ALA VAL GLN VAL LEU ILE GLU HIS ILE GLY ASN LEU ASP ARG ALA TYR GLU PHE ALA GLU
ARG CYS ASN GLU PRO ALA VAL TRP SER GLN LEU ALA LYS ALA GLN LEU GLN LYS GLY MET VAL LYS GLU ALA ILE ASP SER TYR ILE LYS ALA ASP ASP PRO SER SER SER TYR MET GLU VAL VAL GLN ALA ALA ASN THR SER GLY ASN TRP GLU GLU LEU VAL LYS TYR LEU GLN MET ALA
ARG LYS LYS ALA ARG GLU SER TYR VAL GLU THR GLU LEU ILE PHE ALA LEU LYS THR ASN ARG LEU GLU LEU GLU GLU PHE ILE ASN GLY PRO ASN ASN ALA HIS ILE GLN GLN VAL GLY ASP ARG CYS TYR ASP GLU LYS MET TYR ASP ALA ALA LYS LEU LEU LEU TYR ASN ASN
VAL SER ASN PHE GLY ARG LEU ALA SER THR LEU VAL HIS LEU GLY GLU TYR GLN ALA ALA ALA VAL ASP GLY ALA ARG LYS ALA ASN SER THR ARG THR TRP LYS GLU VAL CYS PHE ALA CYS VAL ASP GLY LYS GLU PHE ARG LEU ALA GLN MET CYS GLY LEU HIS ILE VAL HIS ALA
ASP GLU LEU GLU LEU ILE ASN TYR TYR GLN ASP ARG GLY TYR PHE GLU GLU LEU ILE THR MET LEU GLU ALA LEU GLY LEU GLU ARG ALA HIS MET GLY MET PHE THR GLU LEU ALA ILE LEU TYR SER LYS PHE LYS PRO GLN LYS MET ARG GLU HIS LEU GLU LEU PHE TRP
SER ARG VAL ASN ILE PRO LYS VAL LEU ARG ALA ALA GLU GLN ALA HIS LEU TRP ALA GLU LEU VAL PHE LEU TYR ASP LYS TYR GLU GLU TYR ASP ASN ALA ILE THR MET MET ASN HIS PRO THR ASP ALA TRP LYS GLU GLY GLN PHE LYS ASP ILE ILE THR LYS VAL ALA ASN
VAL GLU LEU TYR TYR ARG ALA ILE GLN PHE TYR LEU GLU PHE LYS PRO LEU LEU LEU ASN ASP LEU LEU MET VAL LEU SER PRO ARG LEU ASP HIS THR ARG ALA VAL ASN TYR PHE SER LYS VAL LYS GLN LEU PRO LEU VAL LYS PRO TYR LEU ARG SER VAL GLN ASN HIS ASN ASN



- Molecule 1: Clathrin heavy chain 1

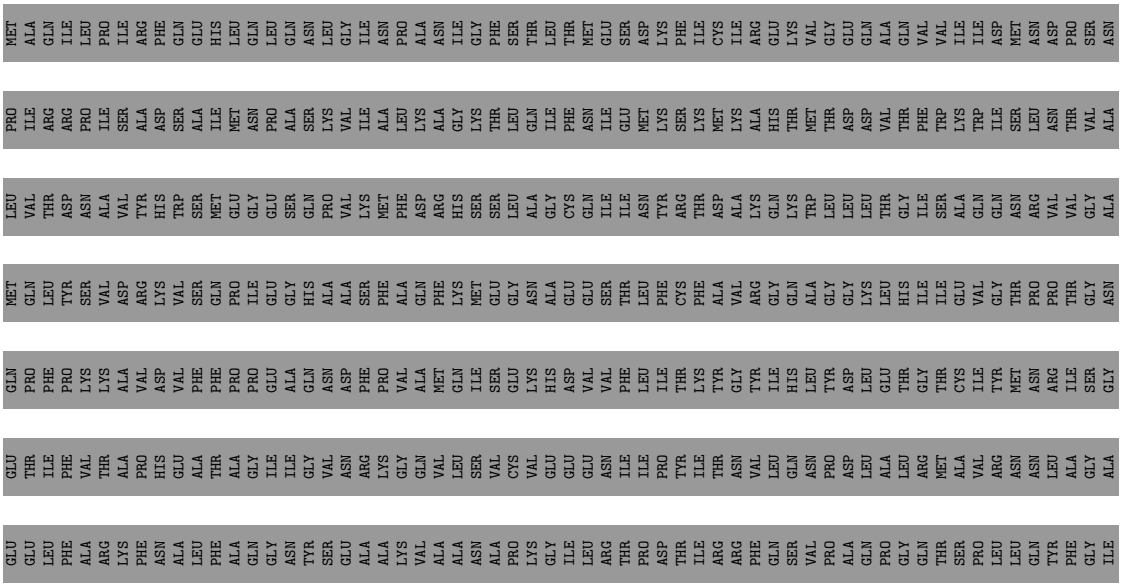
Chain G:

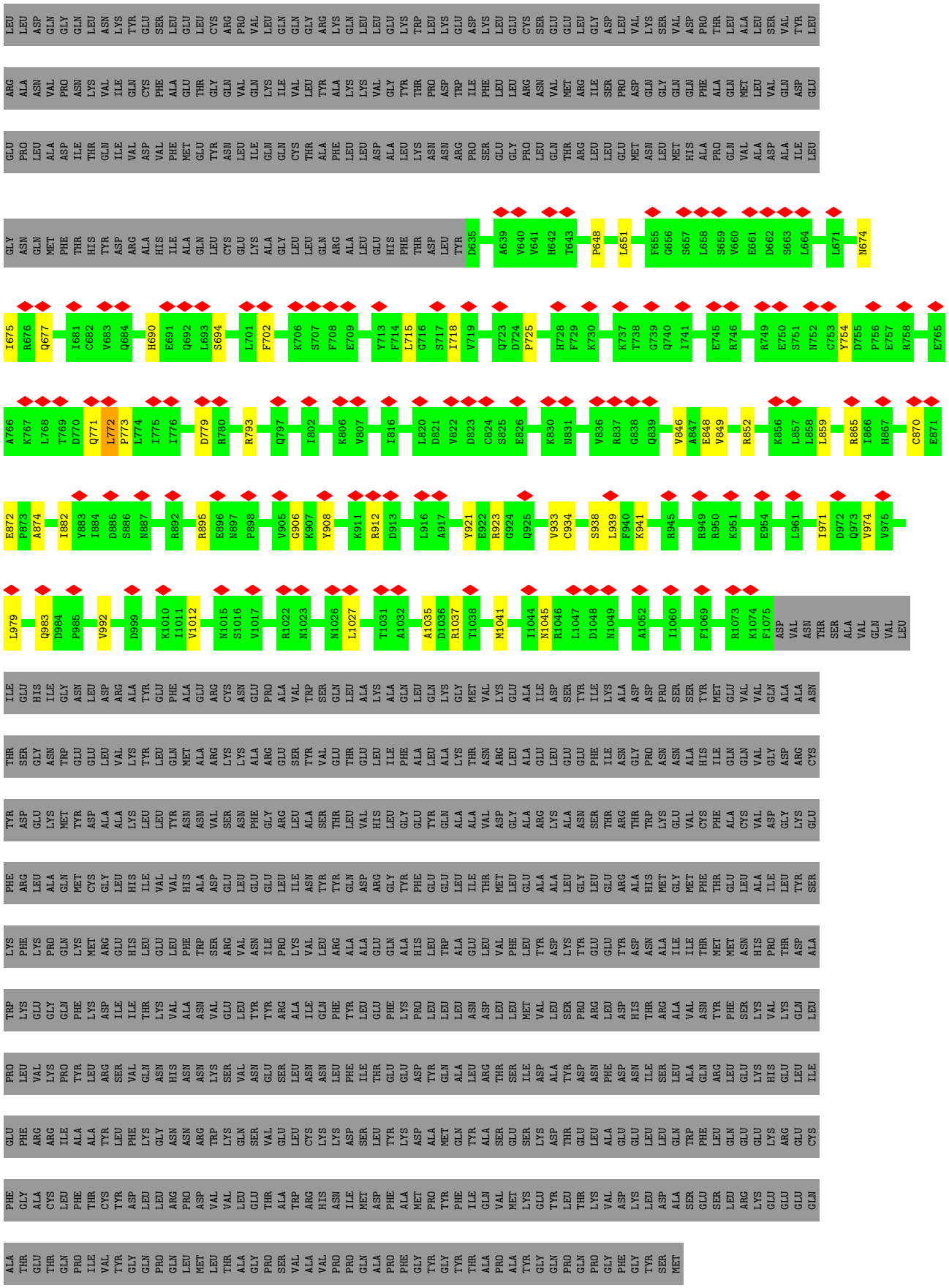




• Molecule 1: Clathrin heavy chain 1

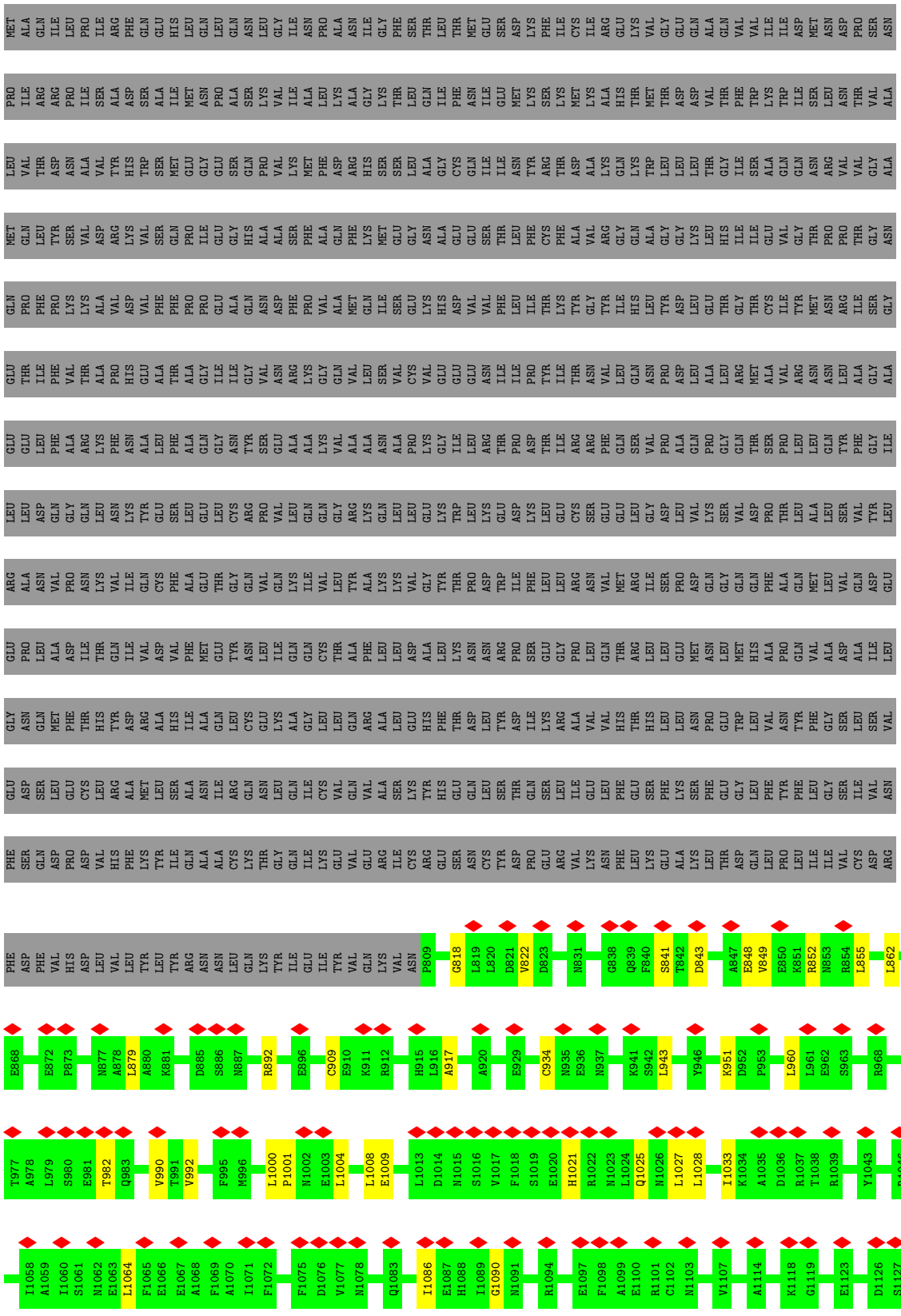
Chain H:

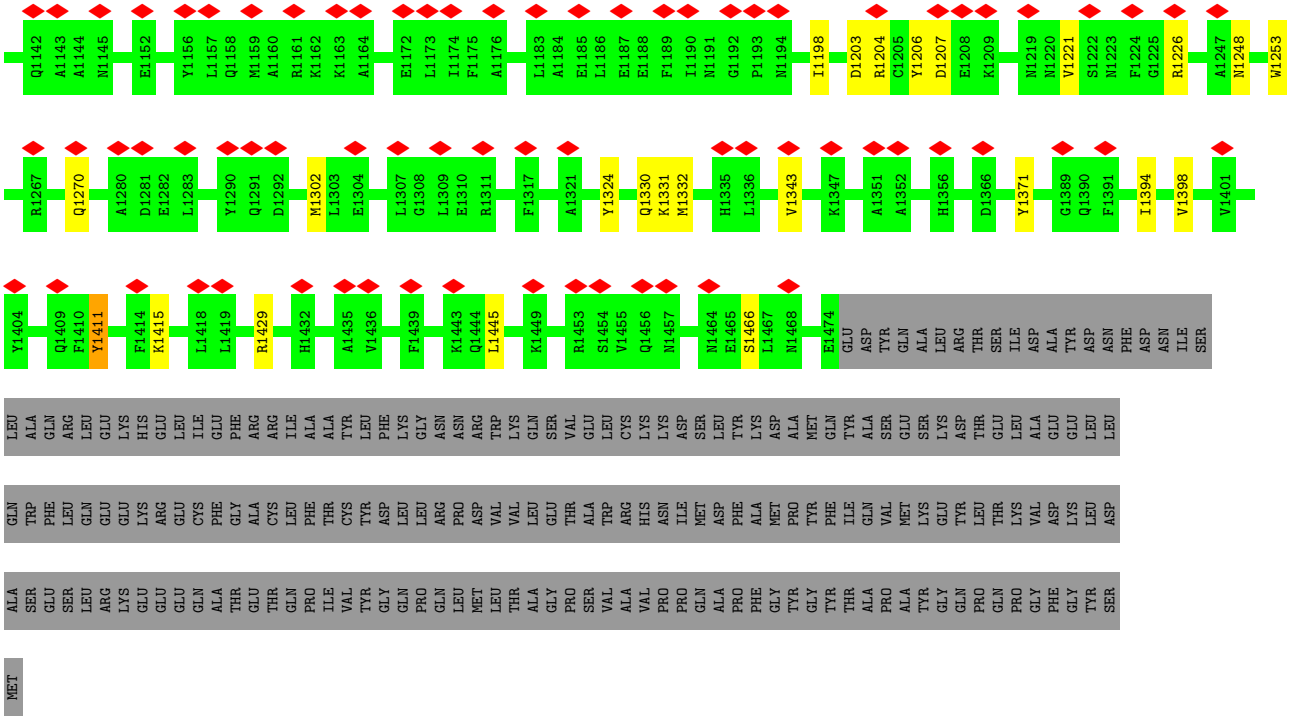



LEU LEU ASP GLN GLY GLN LEU ASN LYS TYR GLU SER LEU GLU LEU CYS ARG PRO VAL LEU GLN GLN GLY ARG LYS GLN LEU LEU GLU LYS TRP LEU LYS GLU ASP LYS LEU GLU CYS SER GLU GLU LEU GLY ASP LEU VAL LYS SER VAL ASP PRO THR LEU ALA LEU SER VAL TYR LEU
ARG ALA ASN VAL PRO ASN LYS VAL ILE GLN CYS PHE ALA GLU GLU THR GLY GLN VAL GLN LYS ILE VAL LEU TYR ALA LYS LYS VAL GLY TYR THR PRO ASP TRP ILE PHE LEU GLU ARG ASN VAL MET ARG ILE SER PRO ASP GLN GLY GLN GLN PHE ALA GLN MET LEU VAL ALA GLN ASP GLU
GLU PRO LEU ALA ASP ILE THR GLN ILE VAL ASP VAL PHE MET GLU TYR ASN LEU ILE GLN GLN CYS THR ALA PHE LEU LEU LEU ASP ALA LEU LYS ASN ASN ARG PRO SER GLU GLY PRO LEU GLN THR ARG LEU LEU GLU MET ASN LEU MET HIS ALA PRO GLN VAL ALA ASP ALA ILE LEU
GLY ASN GLN MET PHE THR HIS TYR ASP ARG ALA HIS ILE ALA GLN LEU CYS GLU LYS ALA GLY LEU LEU GLN ARG ALA LEU GLU HIS PHE THR ASP LEU TYR D636 A639 V640 V641 H642 T643 P648 L651 F655 G656 S657 L658 S659 V660 E661 D662 S663 L664 L671 N674
I675 R676 Q677 I681 C682 V683 Q684 H690 E691 Q692 L693 S694 L701 F702 K706 S707 F708 E709 Y713 F714 L715 G716 S717 I718 V719 Q723 D724 P725 H728 F729 K730 K737 T738 G739 Q740 I741 E745 R746 R749 E750 S751 N752 C753 Y754 D755 P756 E757 R758 E765
A766 K767 L768 T769 D770 Q771 L772 P773 L774 I775 I776 D779 R780 R793 Q797 I802 K806 V807 I816 L820 D821 V822 D823 C824 S825 E826 K830 N831 V836 R837 G838 Q839 V846 A847 E848 V849 R852 K856 L857 L858 L859 R865 I866 H867 C870 E871
E872 P873 A874 I882 Y883 I884 D885 S886 N887 R892 R895 E896 N897 P898 V905 G906 K907 Y908 K911 R912 D913 L916 A917 Y921 E922 R923 G924 Q925 V933 C934 S938 L939 F940 K941 R945 R949 R950 K951 E954 L961 I971 D972 Q973 V974 V975
L979 Q983 D984 P985 V992 D999 K1010 I1011 V1012 N1015 S1016 V1017 R1022 N1023 N1026 L1027 T1031 A1032 A1035 D1036 R1037 T1038 M1041 I1044 N1045 R1046 L1047 D1048 N1049 A1052 I1060 F1069 R1073 K1074 F1075 ASP VAL ASN THR SER ALA VAL GLN VAL LEU
ILE GLU HIS ILE GLY ASN LEU ASP ARG ALA TYR GLU PHE ALA GLU ARG CYS ASN GLU PRO ALA VAL TRP SER GLN LEU ALA LYS ALA GLN LEU GLN LYS GLY MET VAL LYS GLU ALA ILE ASP SER TYR ILE LYS ALA ASP ASP PRO SER SER TYR MET GLU VAL VAL GLN ALA ALA ASN
THR SER GLY ASN TRP GLU GLU LEU VAL LYS TYR LEU GLN MET ALA ARG LYS LYS ALA ARG GLU SER TYR VAL GLU THR GLU LEU ILE PHE ALA LEU GLN LEU ALA LYS THR ASN ARG LEU ALA GLU LEU GLU GLU PHE ILE ASN GLY PRO ASN ASN ALA HIS ILE GLN GLN VAL GLY ASP ARG CYS
TYR ASP GLU LYS MET TYR ASP ALA ALA LYS LEU LEU LEU TYR ASN ASN VAL SER ASN PHE GLY ARG LEU ALA SER THR LEU VAL HIS LEU GLY GLU TYR GLN ALA ALA VAL ASP GLY ALA ARG LYS ALA ASN SER THR ARG THR TRP LYS GLU VAL CYS PHE ALA CYS VAL ASP GLY LYS GLU
PHE ARG LEU ALA GLN MET CYS GLY LEU HIS ILE VAL VAL HIS ALA ASP GLU LEU GLU LEU LEU ILE VAL HIS ALA ASP GLU LEU GLU LEU LEU ILE THR MET LEU GLU ILE ASN TYR TYR GLN ASP ARG GLY TYR PHE GLU LEU GLU ILE THR MET LEU GLU ILE ALA LEU GLY LEU GLU MET PHE THR GLU LEU ALA ILE LEU TYR SER
LYS PHE LYS PRO GLN LYS MET ARG GLU HIS LEU GLU LEU PHE TRP SER ARG VAL ASN ILE PRO LYS VAL LEU ARG ALA ALA GLU GLN ALA HIS LEU LEU TRP ALA GLU LEU VAL PHE LEU TYR ASP LYS TYR GLU GLU TYR ASP ASN ALA ILE ILE THR MET MET ASN HIS PRO THR ASP ALA
TRP LYS GLU GLY GLN PHE LYS ASP ILE ILE THR LYS VAL ALA ASN VAL GLU LEU TYR TYR ARG ALA ILE GLN PHE TYR LEU GLU GLU PHE LYS PRO LEU LEU LEU LEU ASN ASP LEU LEU MET VAL LEU SER PRO ARG LEU ASP HIS THR ARG ALA ILE VAL ASN TYR PHE SER LYS VAL LYS GLN LEU
PRO LEU VAL LYS PRO TYR LEU ARG SER VAL GLN ASN HIS ASN ASN LYS SER VAL ASN GLU SER LEU ASN ASN ASN LEU PHE ILE THR GLU GLU GLU ASP TYR GLN ALA LEU ARG THR SER ILE ASP ALA TYR ASP ASN PHE ASP ASN ILE SER LEU LEU ALA GLN ARG LEU GLU LYS HIS GLU LEU ILE
GLU PHE ARG ARG ILE ALA TYR LEU PHE LYS GLY ASN ASN ARG TRP LYS GLN SER VAL GLU LEU CYS LYS LYS ASP SER LEU TYR LYS ASP ALA MET GLN TYR ALA SER GLU SER LYS ASP THR GLU LEU ALA GLU GLU LEU LEU GLN TRP PHE LEU GLN GLU GLU LYS LYS ARG GLU CYS
PHE GLY ALA CYS LEU PHE THR CYS TYR ASP LEU LEU PHE LYS VAL VAL LEU GLU THR ALA TRP ARG HIS ASN ILE MET ASP PHE ALA MET PRO PRO TYR PHE ILE GLN VAL MET PRO ARG ASP VAL ARG LEU THR LYS VAL ASP ALA SER GLU SER LEU GLU ARG LYS GLU GLU
ALA THR GLU THR GLN PRO ILE VAL TYR GLY GLN PRO GLN LEU MET LEU THR ALA GLY PRO PRO GLN ALA ALA VAL PRO PRO GLY PHE GLY TYR GLY TYR THR ALA PRO ALA TYR GLY GLN PRO GLN PRO GLY PHE GLY TYR SER MET

• Molecule 1: Clathrin heavy chain 1

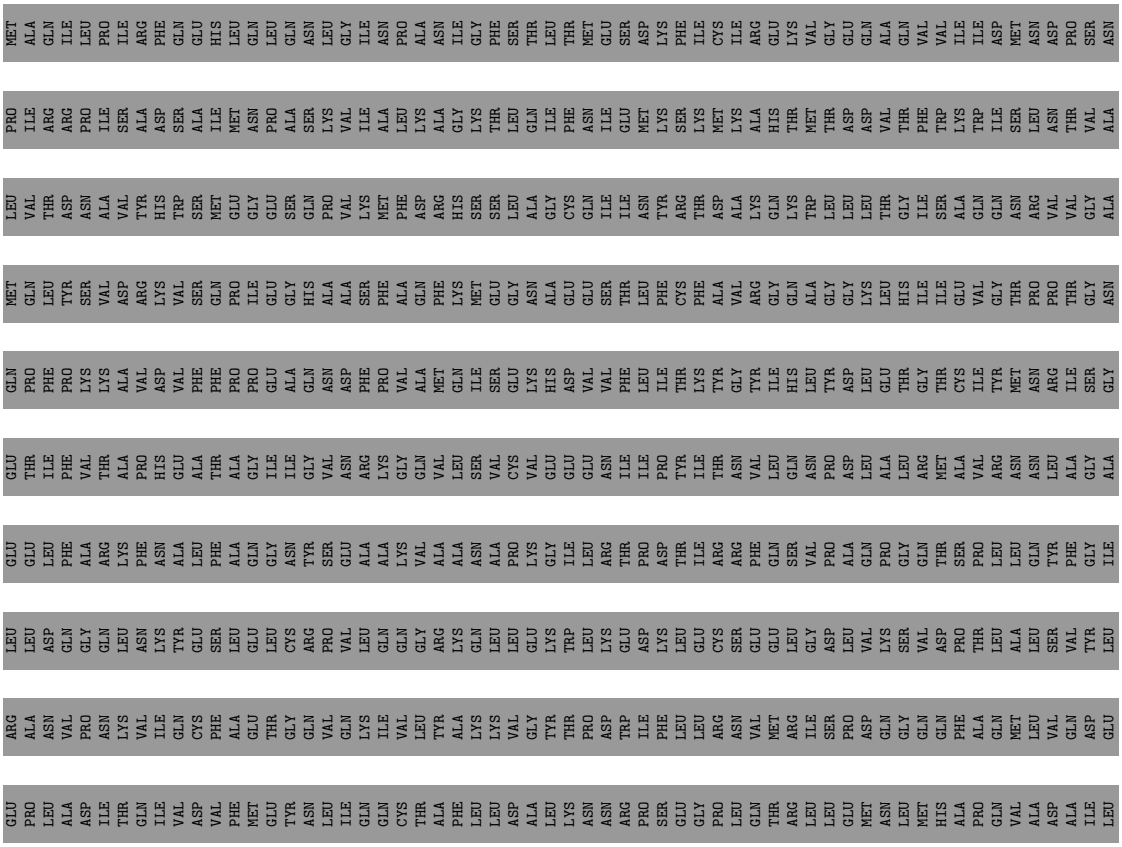
Chain I:

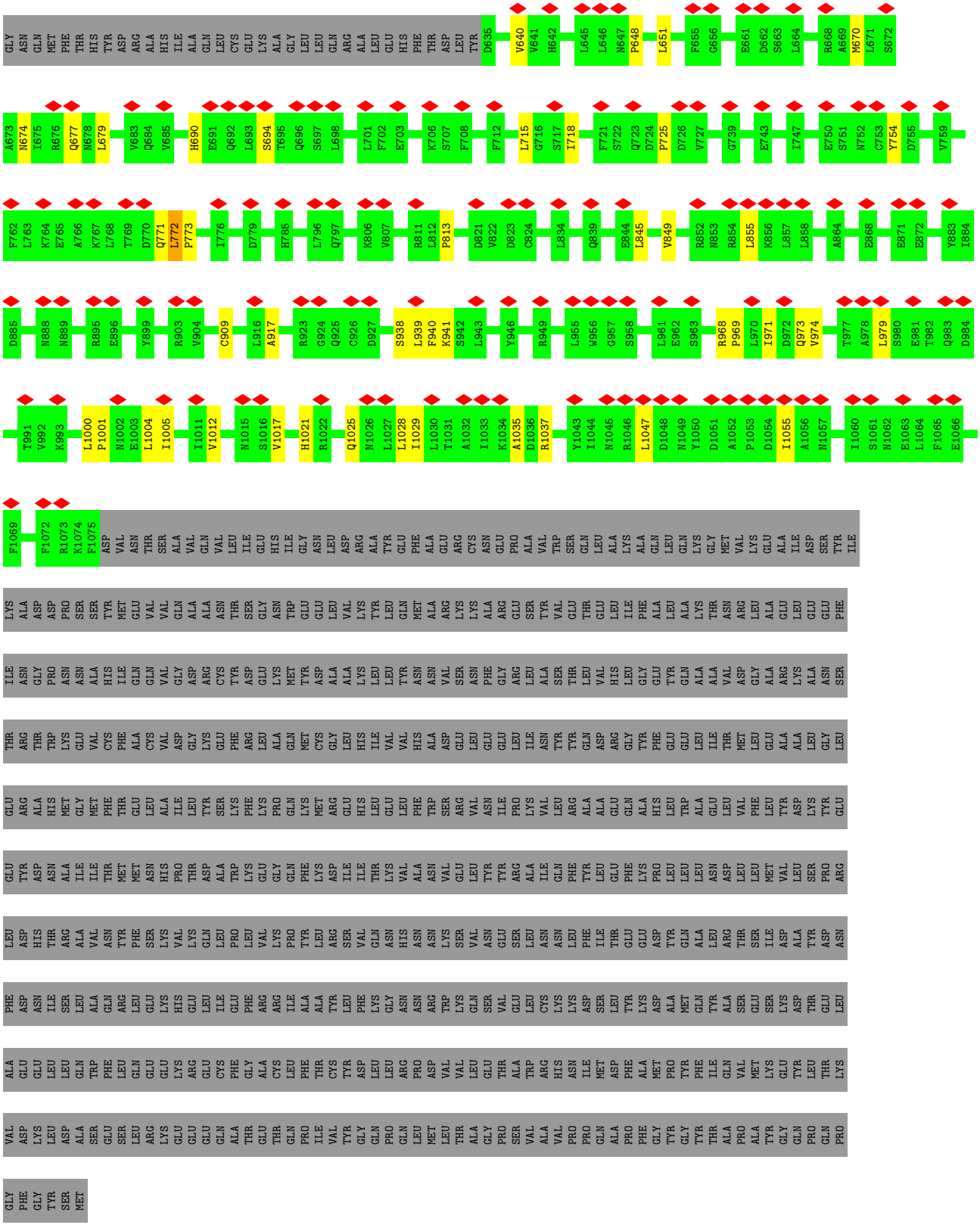




- Molecule 1: Clathrin heavy chain 1

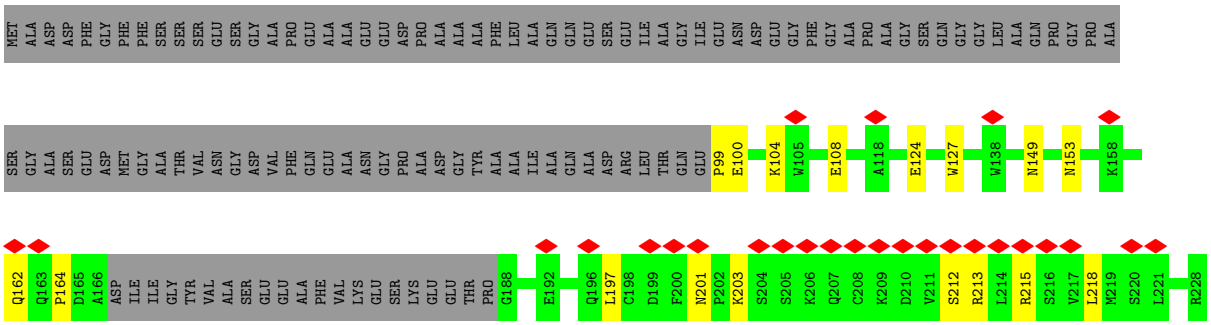
Chain K:



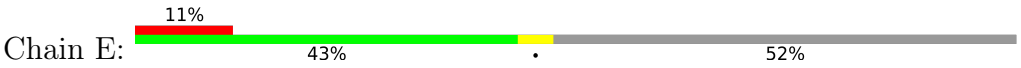


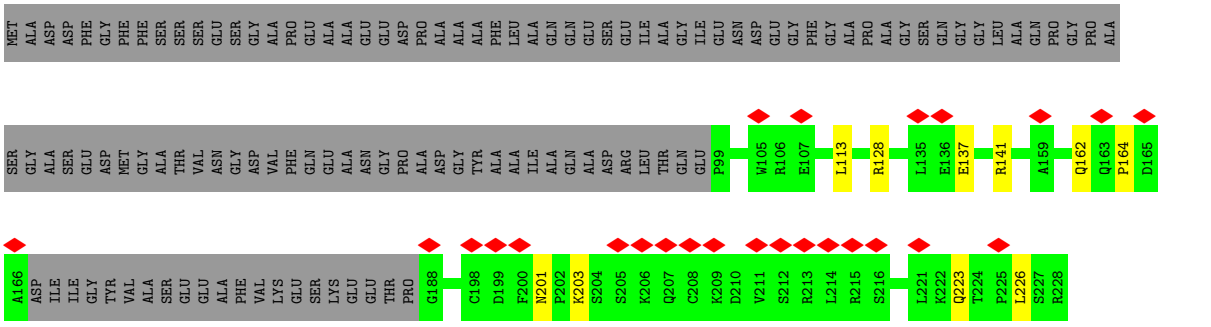
• Molecule 2: Clathrin light chain B

Chain B:

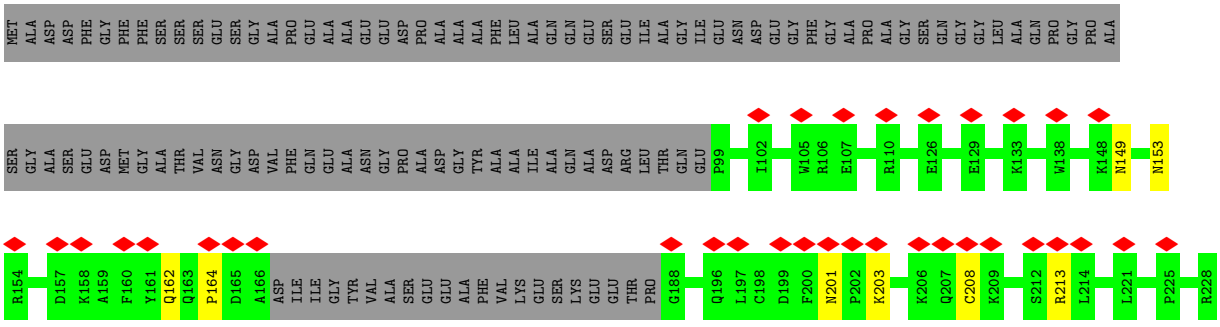


• Molecule 2: Clathrin light chain B

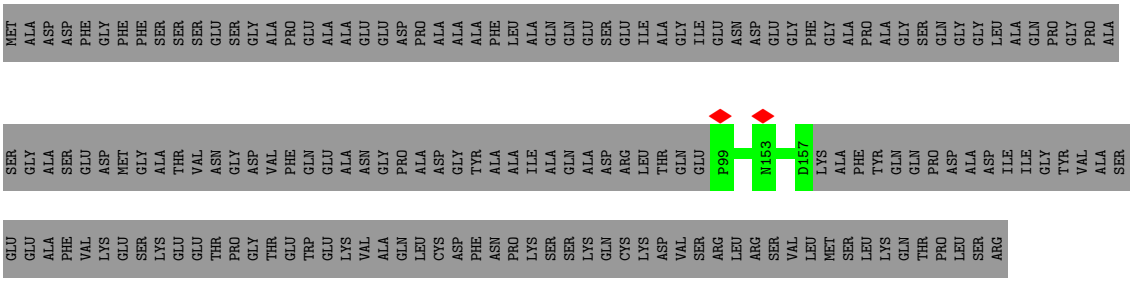




• Molecule 2: Clathrin light chain B

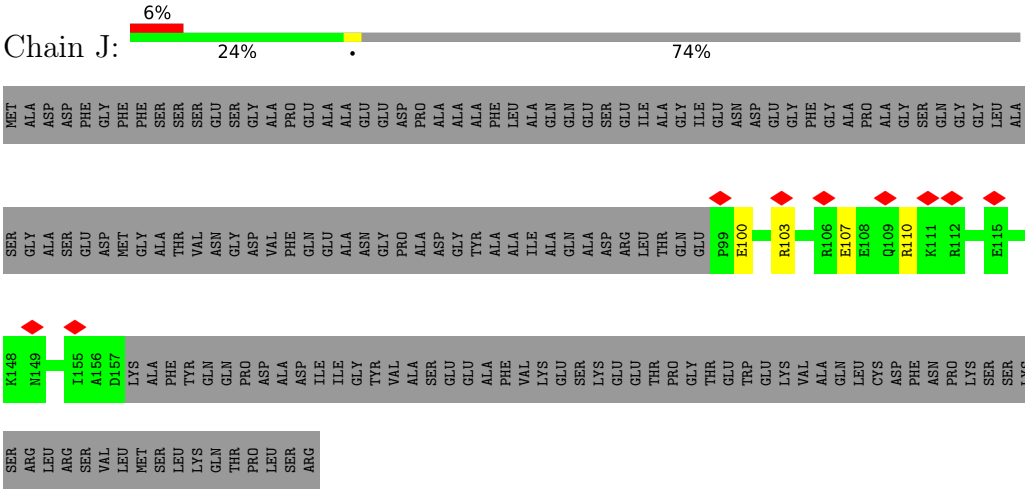


• Molecule 2: Clathrin light chain B



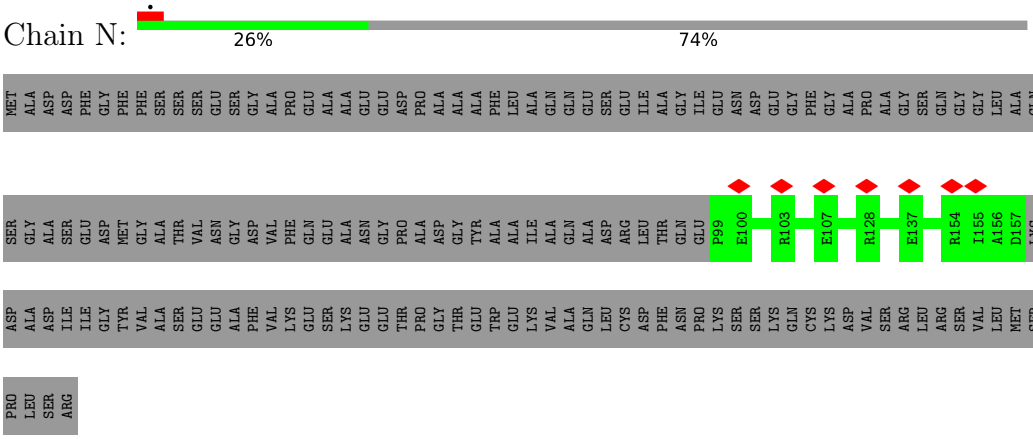
• Molecule 2: Clathrin light chain B

Chain J:



• Molecule 2: Clathrin light chain B

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	305413	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	35000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	19.387	Depositor
Minimum map value	-9.134	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.238	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	793.8, 793.8, 793.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.323, 1.323, 1.323	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.23	0/3362	0.36	0/4543
1	C	0.23	0/3362	0.36	0/4543
1	D	0.23	0/3362	0.35	0/4543
1	G	0.23	0/5518	0.36	0/7475
1	H	0.23	0/3669	0.36	0/4973
1	I	0.23	0/5518	0.36	0/7475
1	K	0.23	0/3669	0.36	0/4973
1	L	0.23	0/5518	0.36	0/7475
1	M	0.23	0/3669	0.36	0/4973
2	B	0.22	0/929	0.32	0/1239
2	E	0.22	0/929	0.32	0/1239
2	F	0.22	0/929	0.31	0/1239
2	J	0.21	0/521	0.31	0/692
2	N	0.21	0/521	0.30	0/692
2	O	0.21	0/521	0.30	0/692
All	All	0.23	0/41997	0.36	0/56766

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	3287	0	3239	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3287	0	3239	31	0
1	D	3287	0	3239	35	0
1	G	5410	0	5373	46	0
1	H	3600	0	3597	28	0
1	I	5410	0	5373	31	0
1	K	3600	0	3597	25	0
1	L	5410	0	5373	52	0
1	M	3600	0	3597	34	0
2	B	916	0	917	12	0
2	E	916	0	917	7	0
2	F	916	0	917	4	0
2	J	515	0	510	2	0
2	N	515	0	510	0	0
2	O	515	0	510	0	0
All	All	41184	0	40908	314	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 4.

The worst 5 of 314 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:1558:LEU:HD22	1:C:1591:ILE:HG21	1.76	0.66
1:H:934:CYS:HA	1:H:938:SER:HB3	1.78	0.65
1:M:983:GLN:HE22	1:G:892:ARG:HB2	1.61	0.65
1:C:1514:LEU:O	1:C:1518:ASN:ND2	2.30	0.63
1:L:975:VAL:HA	1:L:1008:LEU:HD13	1.81	0.63

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/1675 (23%)	390 (100%)	2 (0%)	0	100	100
1	C	392/1675 (23%)	387 (99%)	5 (1%)	0	100	100
1	D	392/1675 (23%)	388 (99%)	4 (1%)	0	100	100
1	G	664/1675 (40%)	654 (98%)	10 (2%)	0	100	100
1	H	439/1675 (26%)	420 (96%)	19 (4%)	0	100	100
1	I	664/1675 (40%)	647 (97%)	17 (3%)	0	100	100
1	K	439/1675 (26%)	418 (95%)	21 (5%)	0	100	100
1	L	664/1675 (40%)	652 (98%)	12 (2%)	0	100	100
1	M	439/1675 (26%)	420 (96%)	19 (4%)	0	100	100
2	B	105/228 (46%)	104 (99%)	1 (1%)	0	100	100
2	E	105/228 (46%)	103 (98%)	2 (2%)	0	100	100
2	F	105/228 (46%)	104 (99%)	1 (1%)	0	100	100
2	J	57/228 (25%)	57 (100%)	0	0	100	100
2	N	57/228 (25%)	57 (100%)	0	0	100	100
2	O	57/228 (25%)	57 (100%)	0	0	100	100
All	All	4971/16443 (30%)	4858 (98%)	113 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	356/1470 (24%)	355 (100%)	1 (0%)	92	95
1	C	356/1470 (24%)	356 (100%)	0	100	100
1	D	356/1470 (24%)	355 (100%)	1 (0%)	92	95
1	G	589/1470 (40%)	587 (100%)	2 (0%)	92	95
1	H	406/1470 (28%)	404 (100%)	2 (0%)	88	93
1	I	589/1470 (40%)	586 (100%)	3 (0%)	88	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	406/1470 (28%)	404 (100%)	2 (0%)	88 93
1	L	589/1470 (40%)	589 (100%)	0	100 100
1	M	406/1470 (28%)	404 (100%)	2 (0%)	88 93
2	B	101/182 (56%)	101 (100%)	0	100 100
2	E	101/182 (56%)	101 (100%)	0	100 100
2	F	101/182 (56%)	101 (100%)	0	100 100
2	J	55/182 (30%)	55 (100%)	0	100 100
2	N	55/182 (30%)	55 (100%)	0	100 100
2	O	55/182 (30%)	55 (100%)	0	100 100
All	All	4521/14322 (32%)	4508 (100%)	13 (0%)	92 95

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	772	LEU
1	I	982	THR
1	K	772	LEU
1	I	1411	TYR
1	K	771	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	642	HIS
1	I	853	ASN
2	J	152	ASN
1	K	674	ASN
1	G	1460	ASN

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.

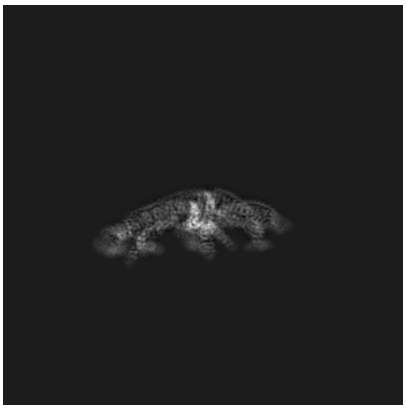
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21611. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

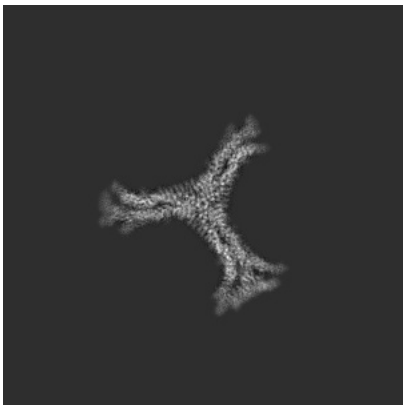
6.1 Orthogonal projections

6.1.1 Primary map



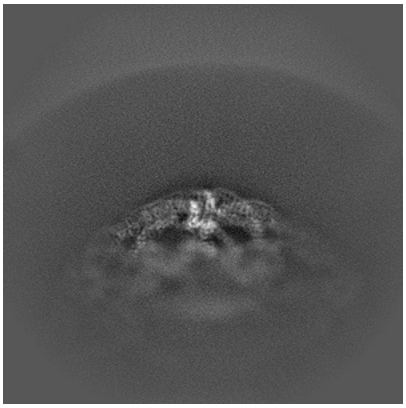
X

Y

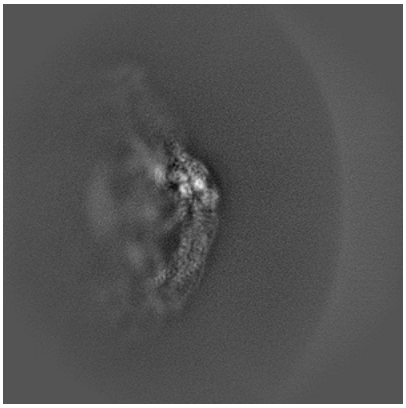


Z

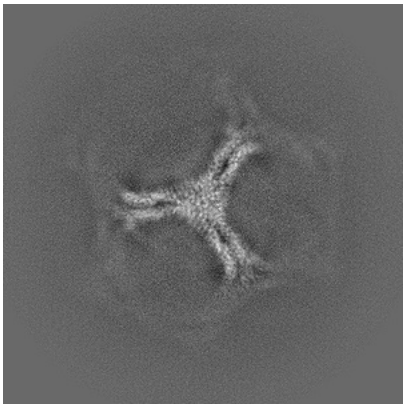
6.1.2 Raw map



X



Y



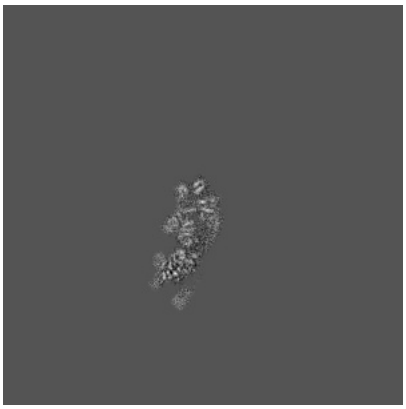
Z

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

6.2 Central slices (i)

6.2.1 Primary map

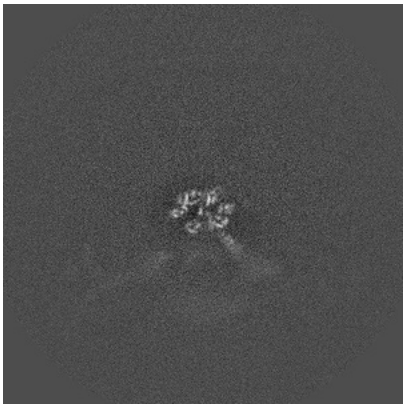
X Index: 300



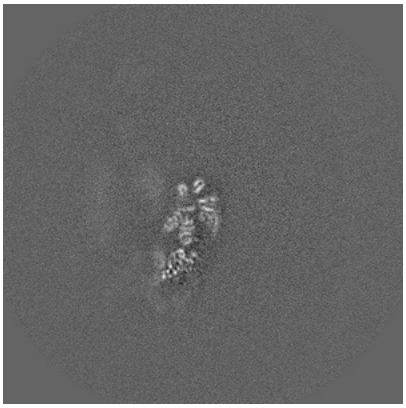
Y Index: 300

Z Index: 300

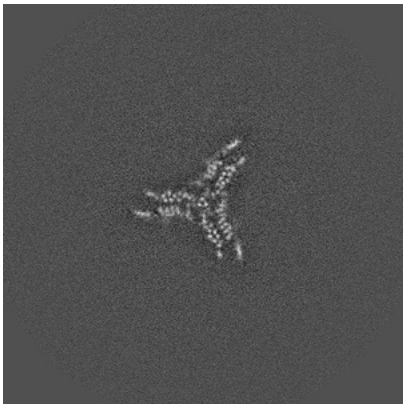
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

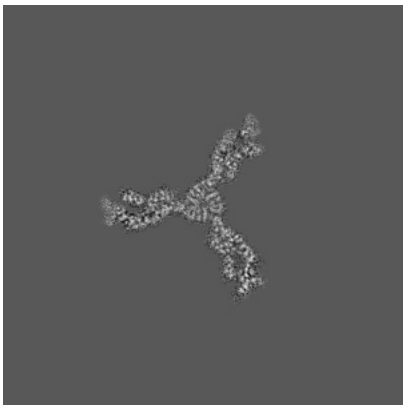
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

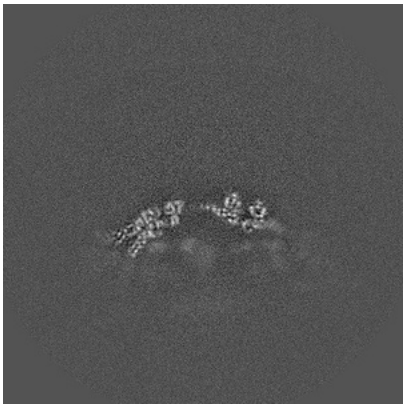
X Index: 337

Y Index: 308



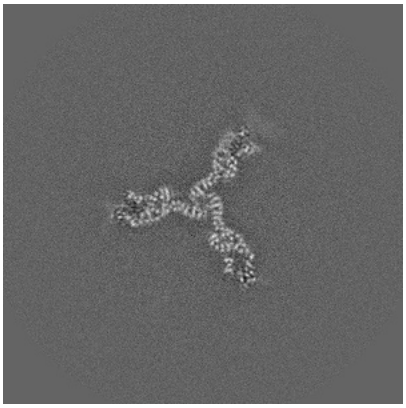
Z Index: 270

6.3.2 Raw map



X Index: 337

Y Index: 308



Z Index: 272

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

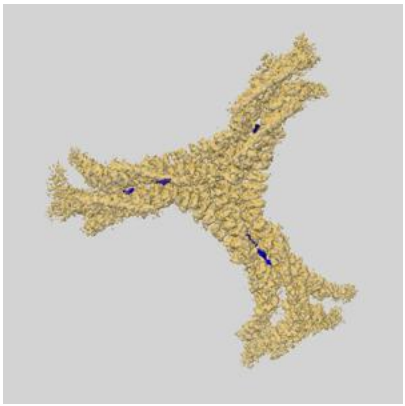
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_21611_msk_1.map (i)

X

Y

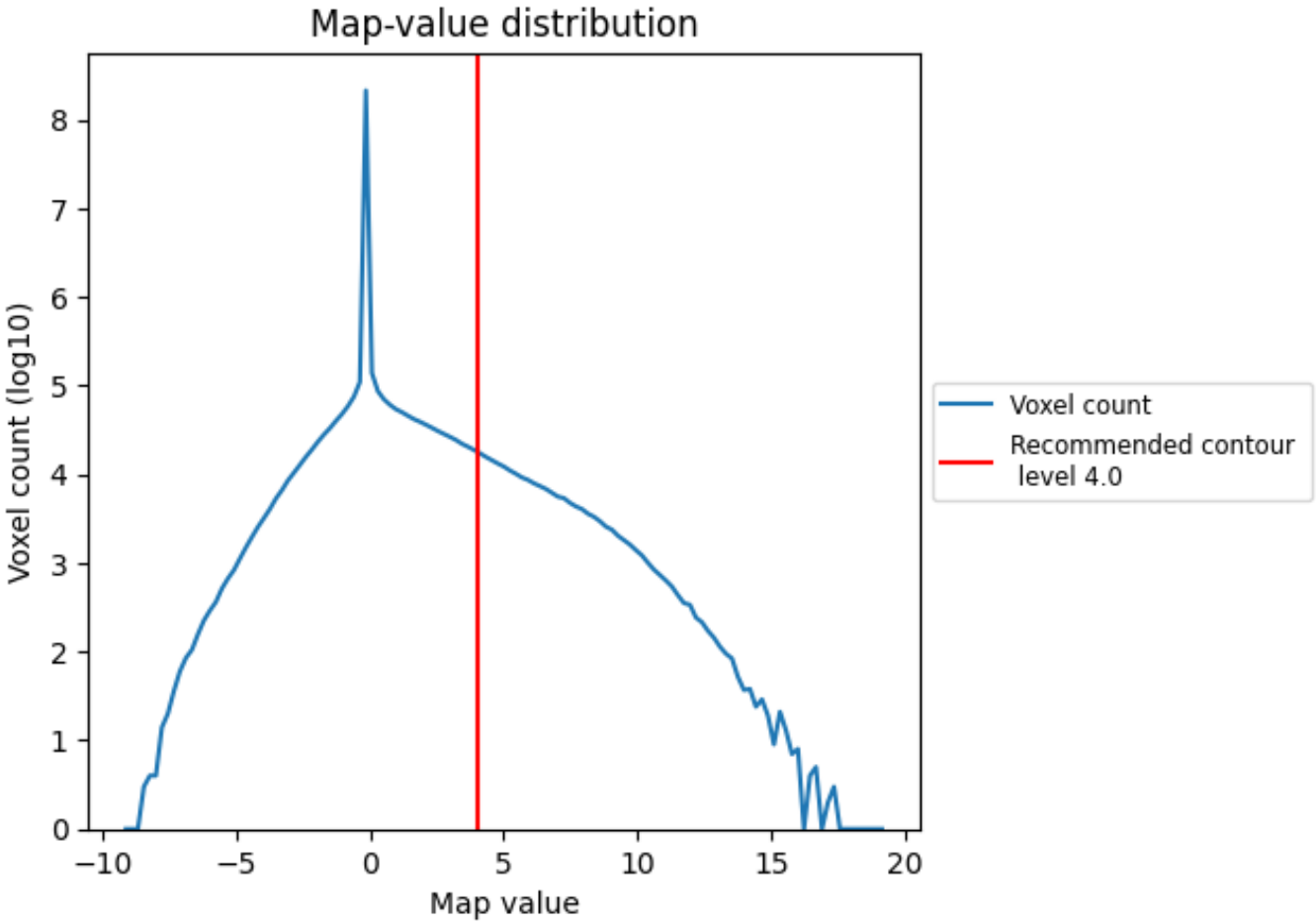


Z

7 Map analysis

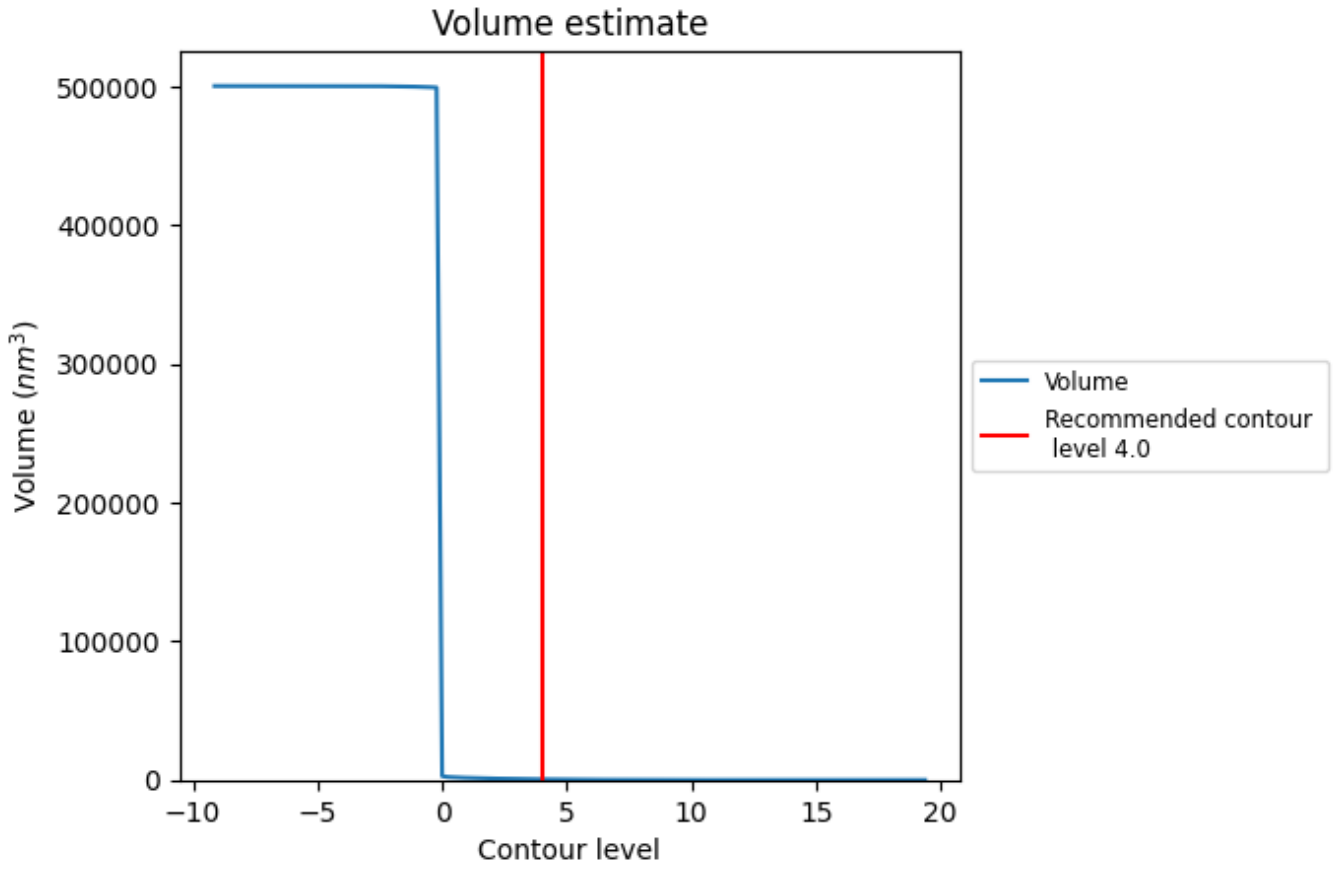
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

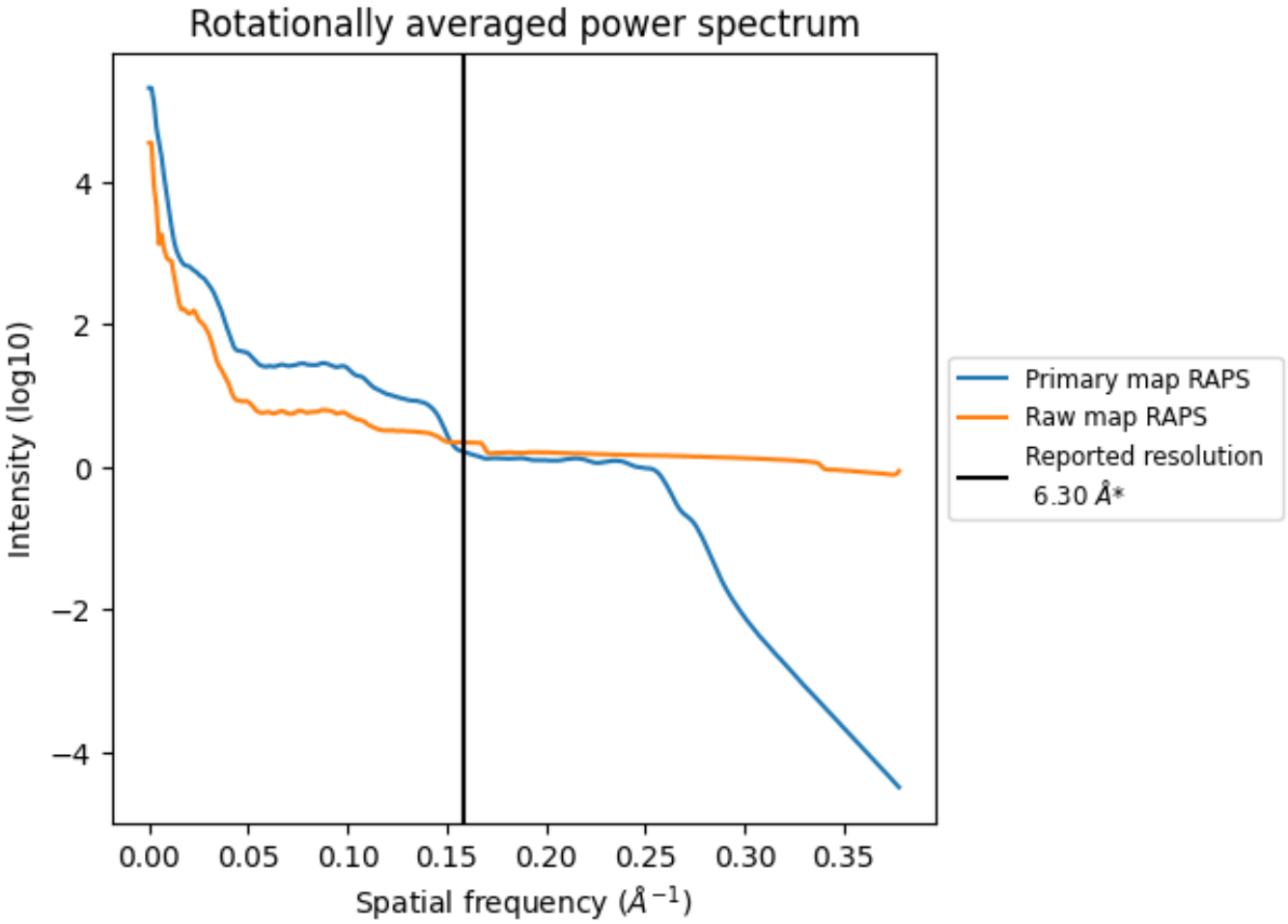
7.2 Volume estimate (i)



The volume at the recommended contour level is 471 nm^3; this corresponds to an approximate mass of 426 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)

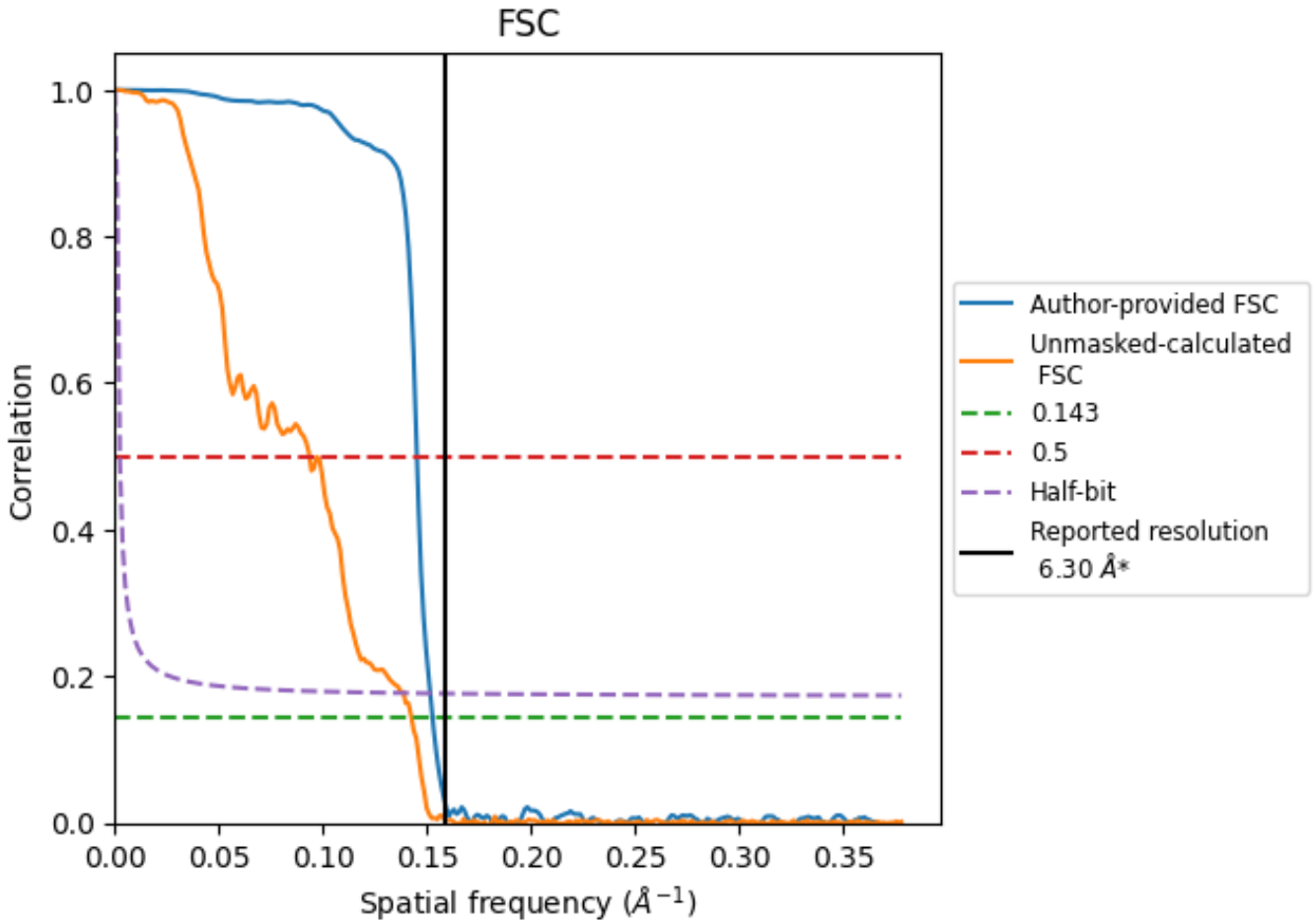


*Reported resolution corresponds to spatial frequency of 0.159 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.159 Å^{-1}

8.2 Resolution estimates (i)

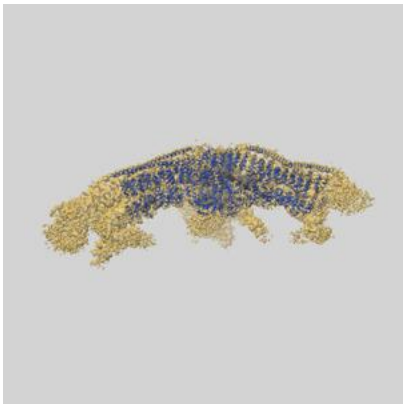
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.55	6.89	6.60
Unmasked-calculated*	7.02	10.70	7.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.02 differs from the reported value 6.3 by more than 10 %

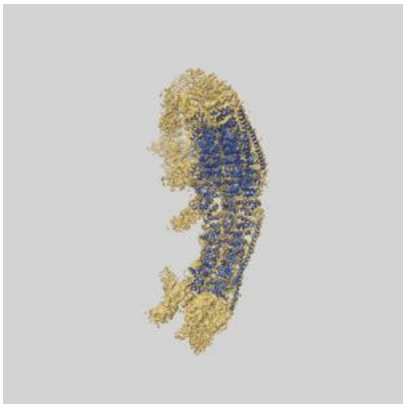
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21611 and PDB model 6WCJ. Per-residue inclusion information can be found in section 3 on page 5.

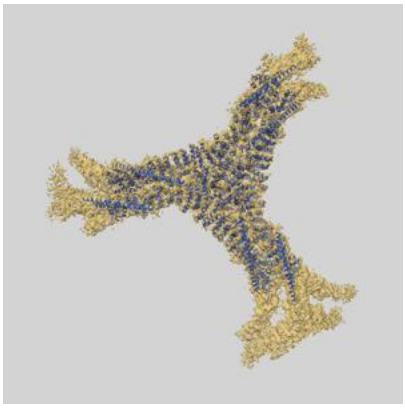
9.1 Map-model overlay



X



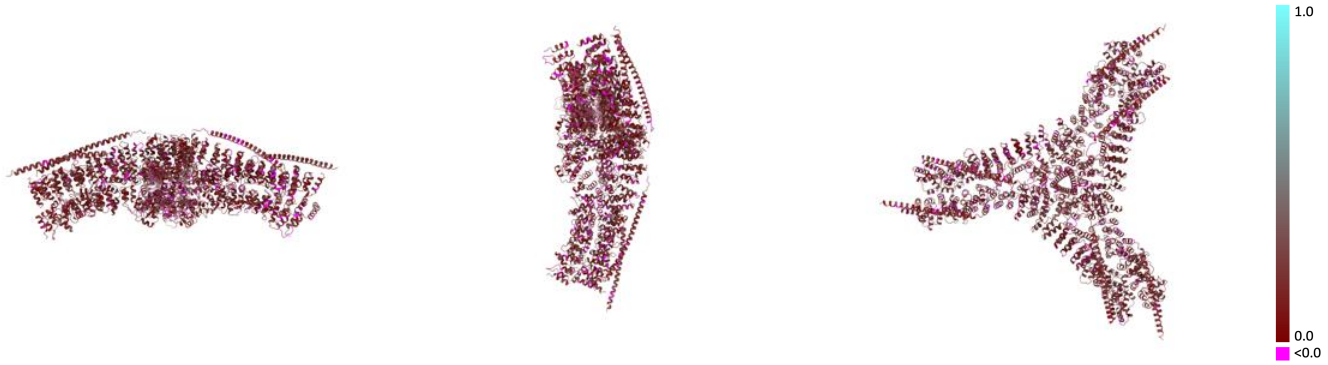
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

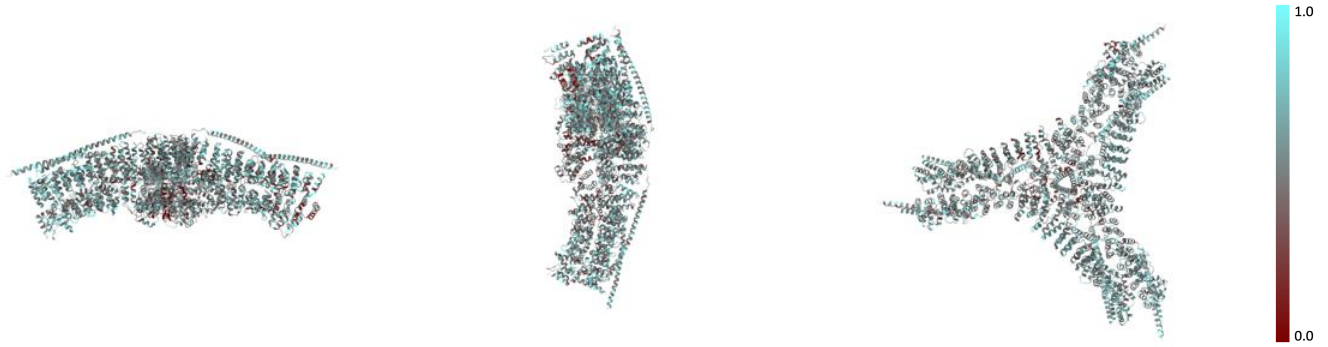
9.2 Q-score mapped to coordinate model (i)



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.

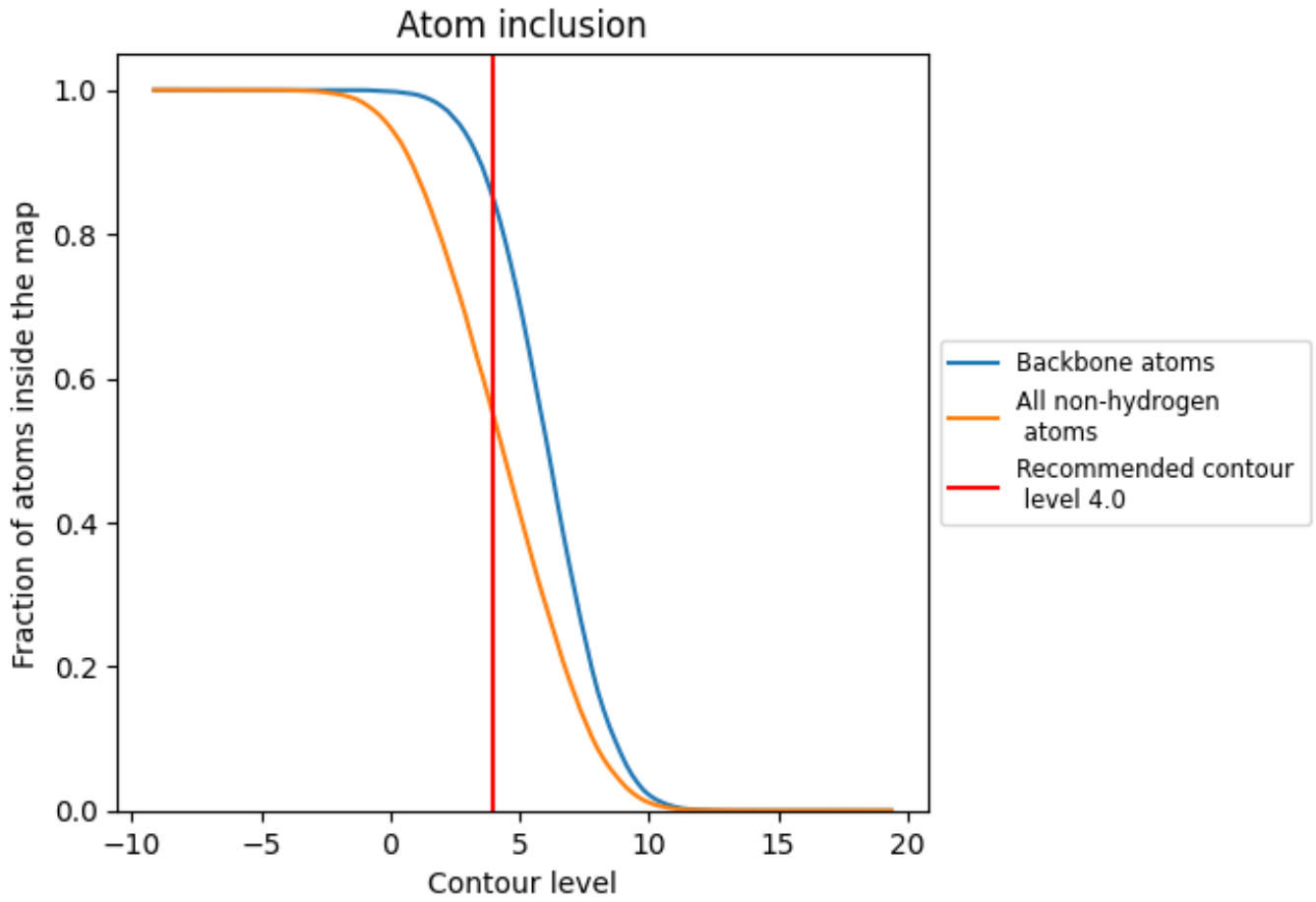
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 55% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5467	0.1630
A	0.5586	0.1750
B	0.5376	0.1830
C	0.5673	0.1550
D	0.5474	0.1590
E	0.5320	0.1420
F	0.5062	0.1500
G	0.5680	0.1680
H	0.5194	0.1620
I	0.5312	0.1470
J	0.5723	0.1590
K	0.5038	0.1600
L	0.5706	0.1700
M	0.5390	0.1700
N	0.5984	0.1770
O	0.6084	0.1950