



# wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 05:57 PM 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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 2.31.3

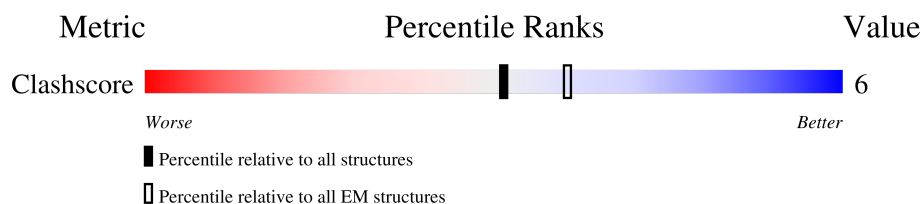
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

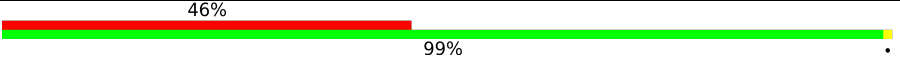
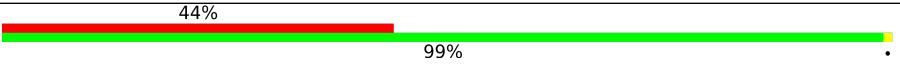
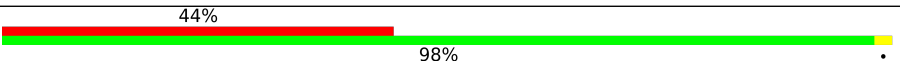
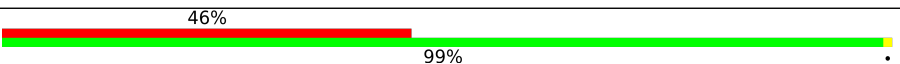
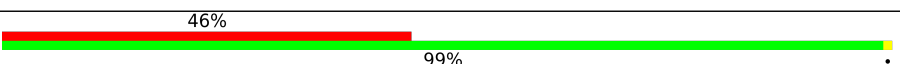
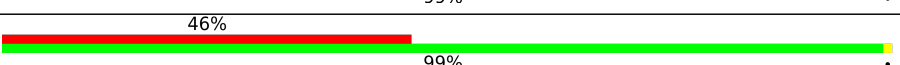
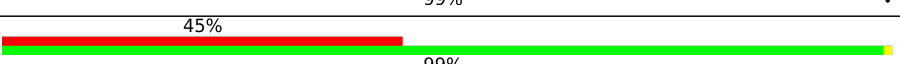
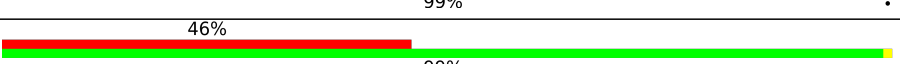
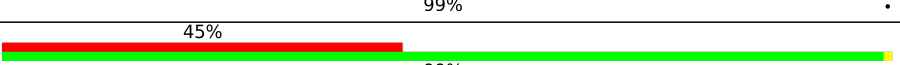
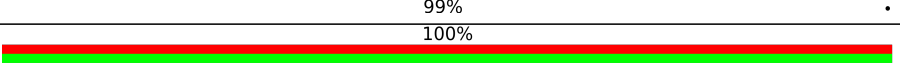
The reported resolution of this entry is 7.90 Å.

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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	1630	
1	C	1630	
1	D	1630	
1	E	1630	
1	F	1630	
1	G	1630	
1	H	1630	
1	I	1630	
2	J	70	

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

## 2 Entry composition

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

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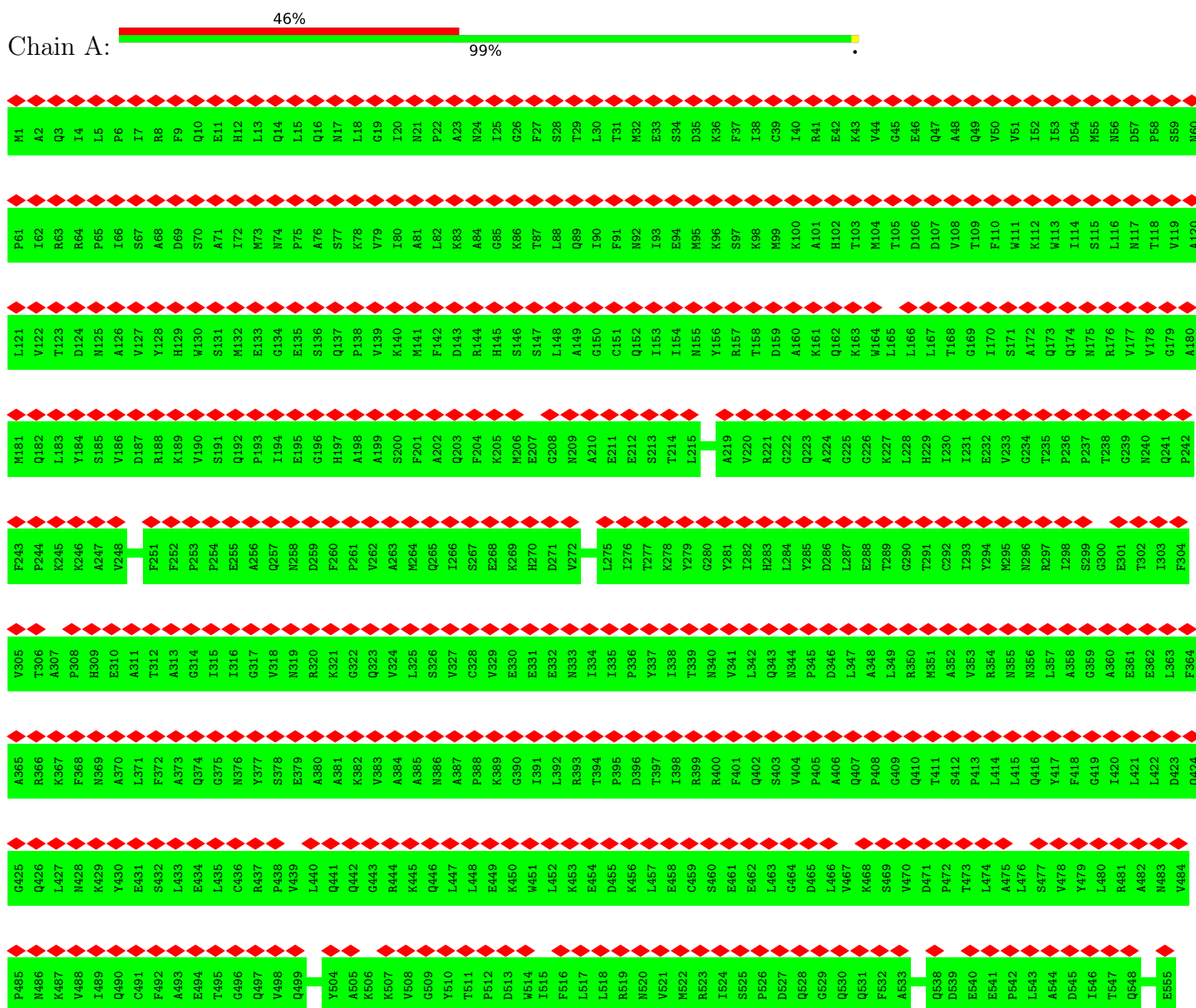
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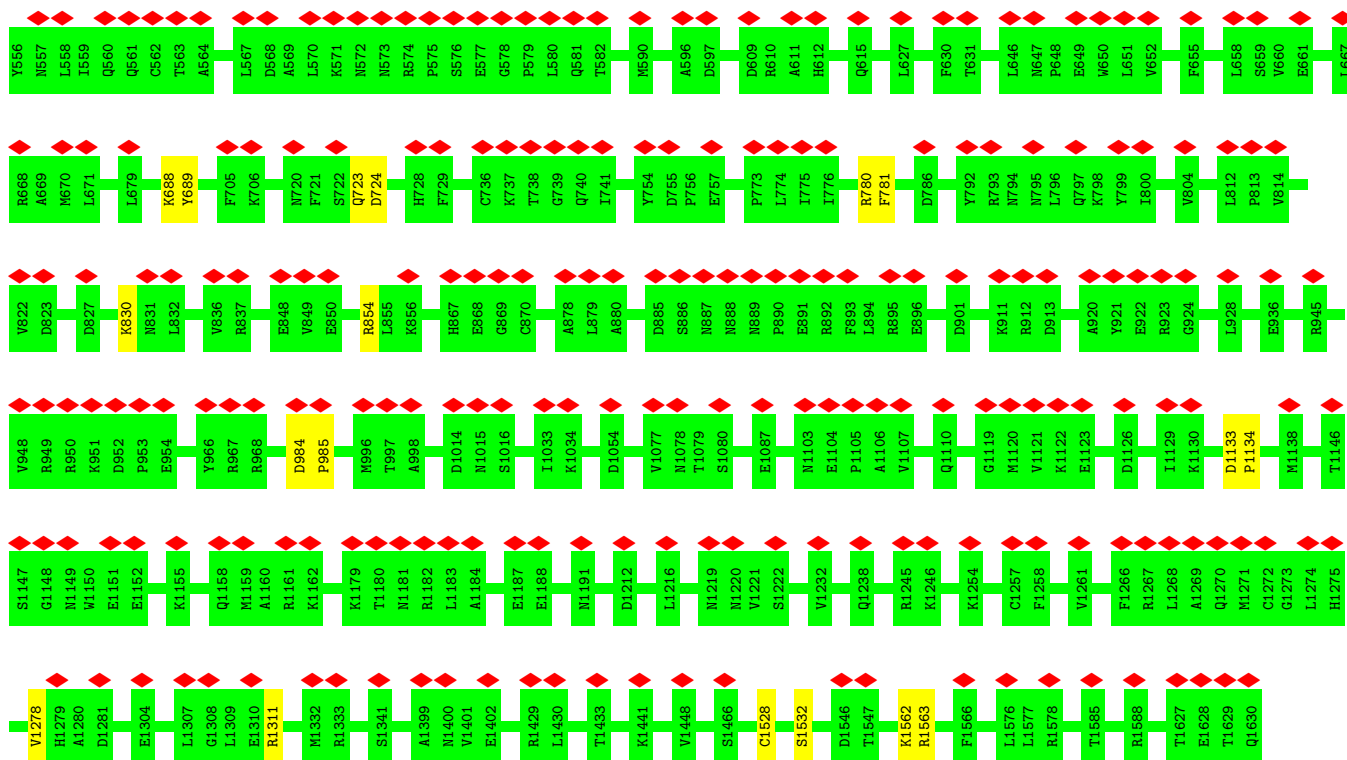
Mol	Chain	Residues	Atoms		AltConf	Trace
2	P	70	Total 70	C 70	0	70
2	Q	70	Total 70	C 70	0	70
2	R	70	Total 70	C 70	0	70

### 3 Residue-property plots

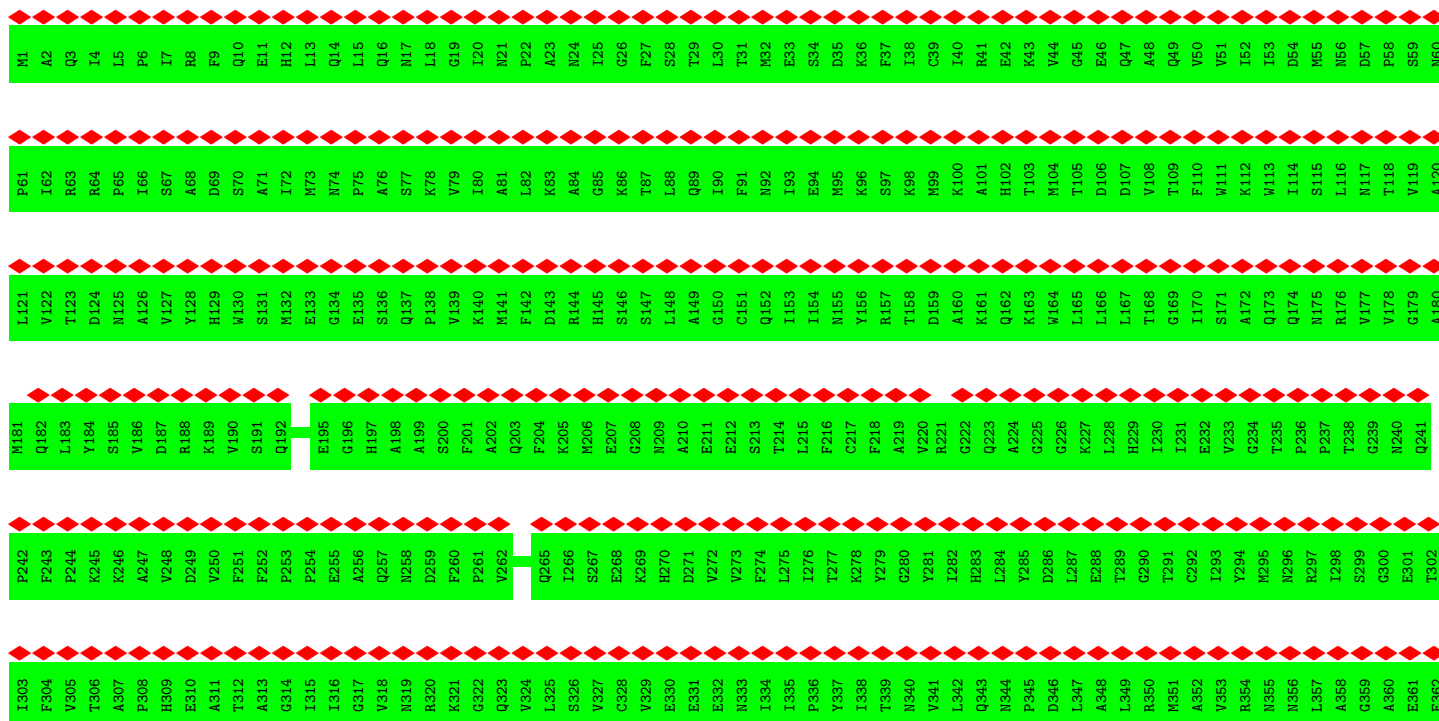
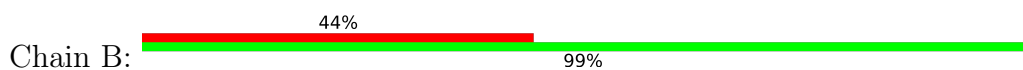
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

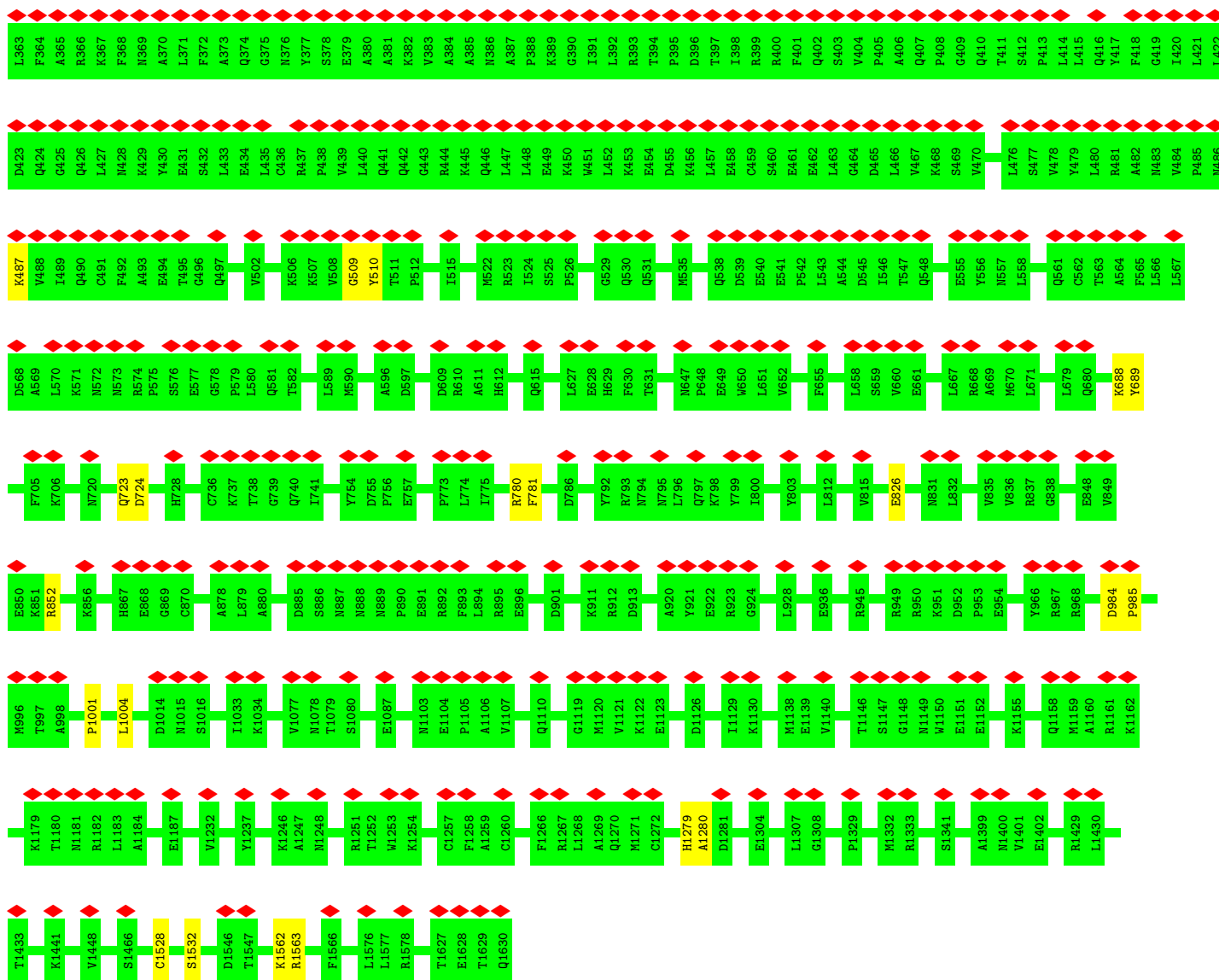
#### • Molecule 1: Clathrin heavy chain



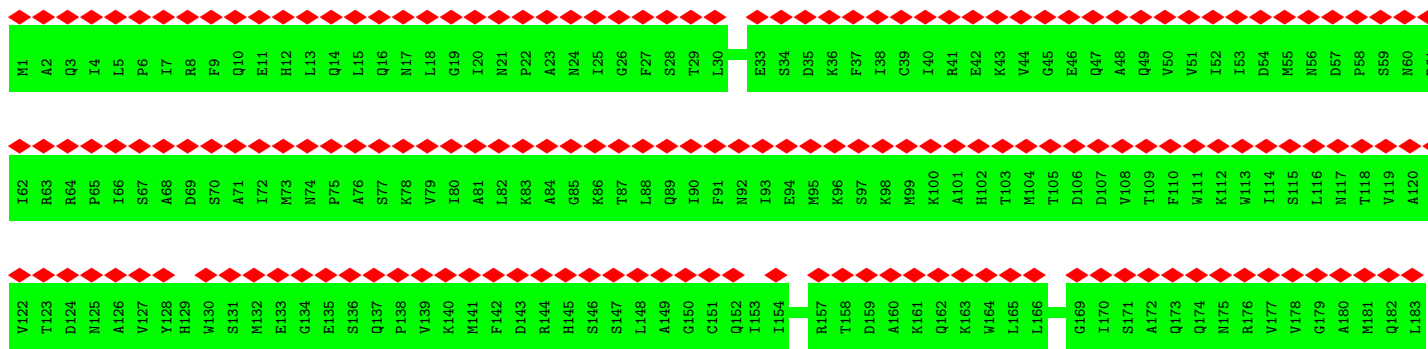
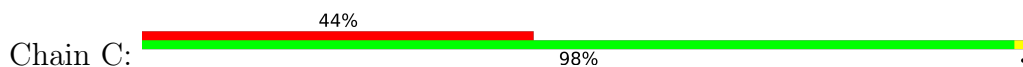


• Molecule 1: Clathrin heavy chain

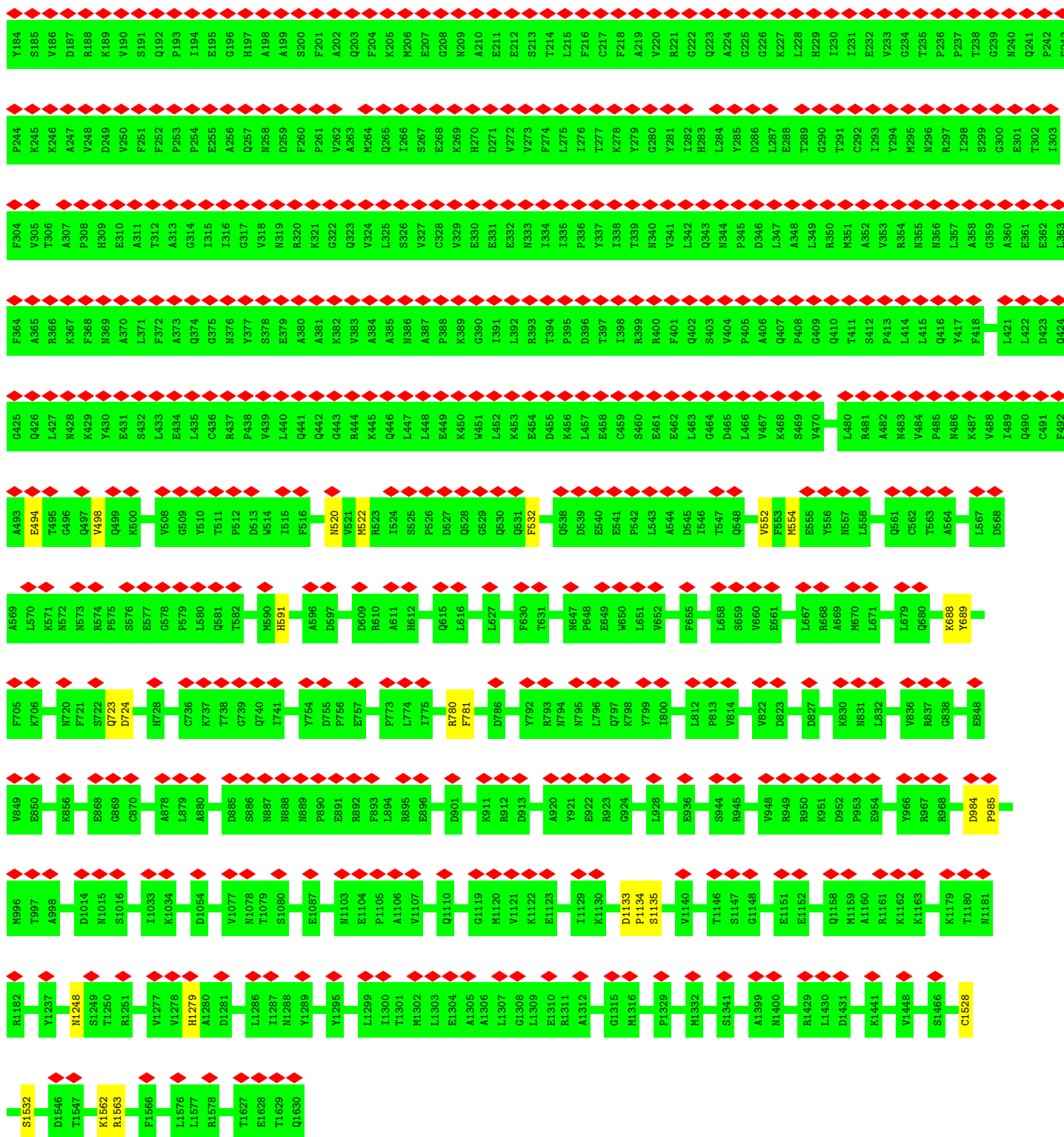




• Molecule 1: Clathrin heavy chain



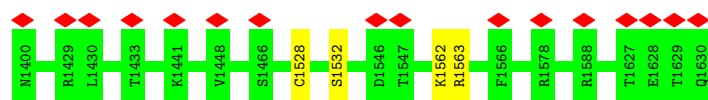




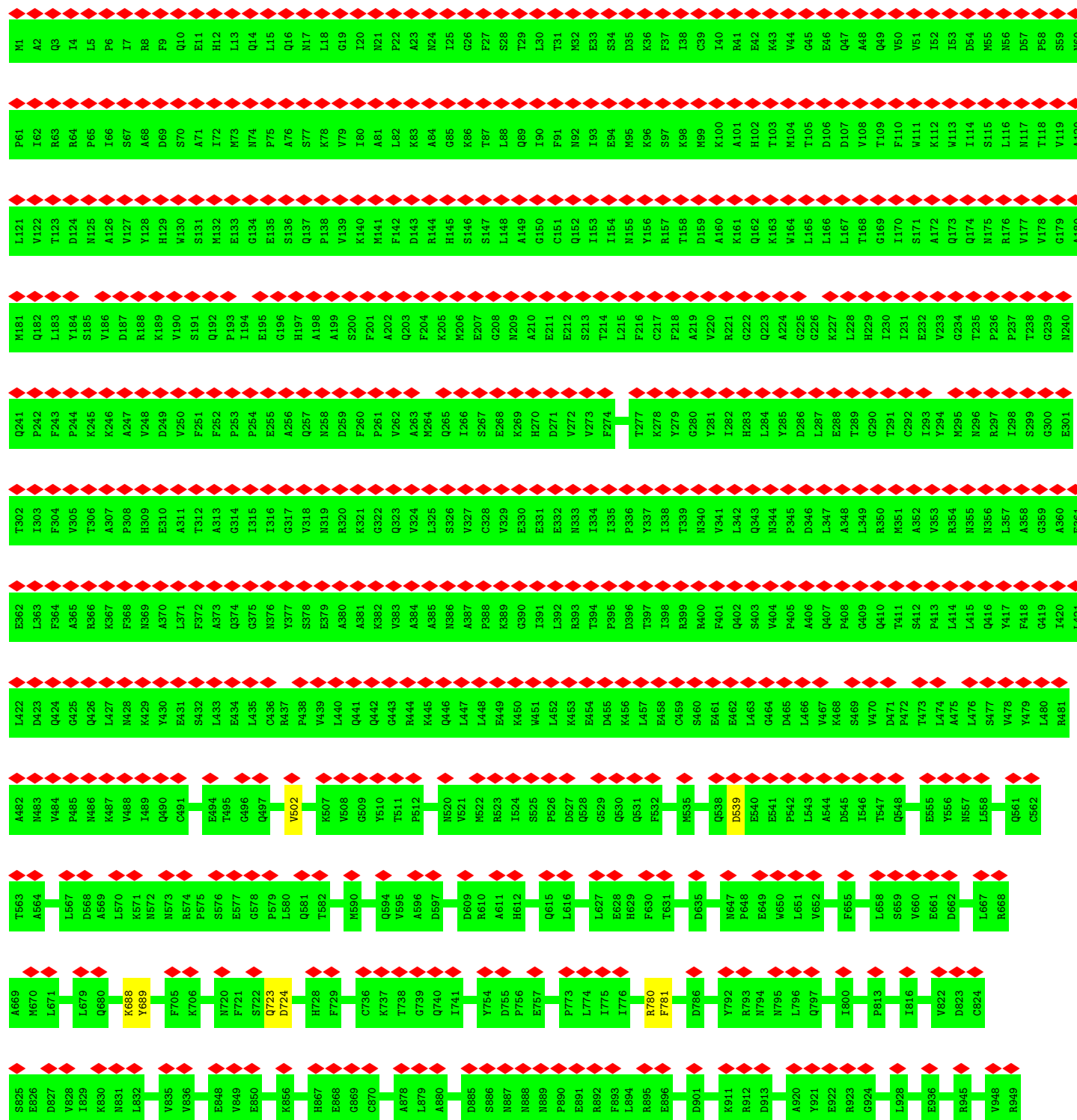
• Molecule 1: Clathrin heavy chain

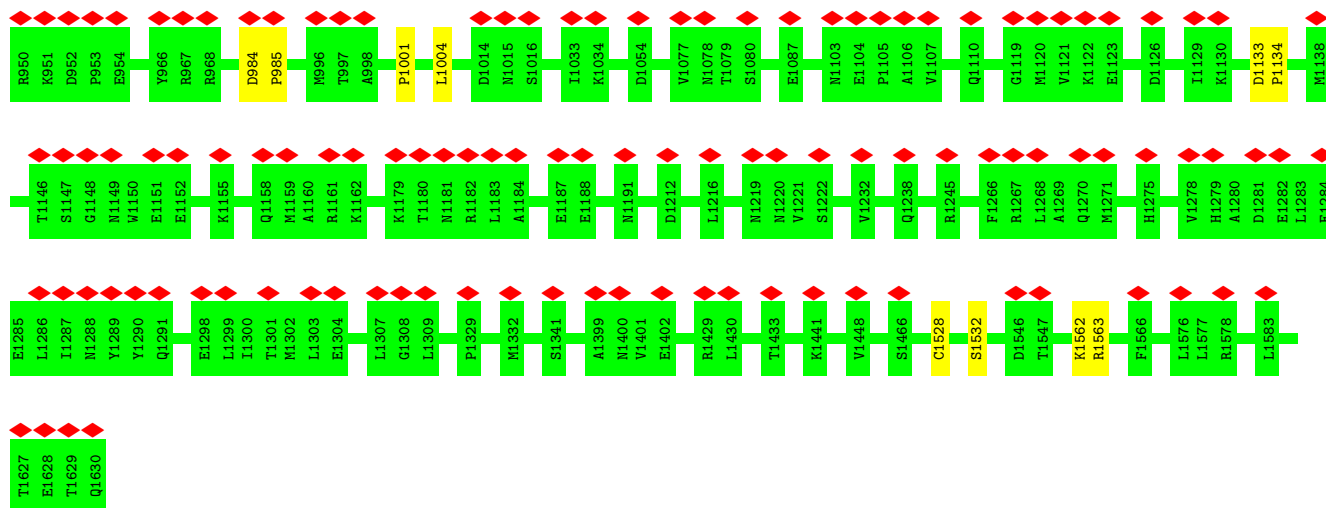


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P61	I62	R63	R64	P65	T66	S67	A68	D69	S70	A71	T72	M73	N74	P75	A76	S77	K78	V79	T80	A81	L82	K83	A84	G85	K86	T87	L88	Q89	T90	I91	N92	I93	E94	N95	K96	S97	T98	D99	I100	A101	H102	T103	M104	L105	T106	D107	V108	T109	F110	W111	K112	W113	Q114	S115	L116	N117	T118	V119	A120	
L121	V122	T123	D124	M125	A126	V127	Y128	H129	W130	S131	M132	E133	G134	E135	S136	I137	P138	V139	K140	M141	F142	D143	R144	H145	S146	S147	L148	A149	G150	C151	Q152	I153	T154	M155	Y156	R157	T158	D159	I160	K161	Q162	K163	W164	L165	L166	L167	T168	G169	I170	S171	A172	Q173	Q174	M175	L176	V177	T178	G179	A180	
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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	L266	S267	E268	K269	H270	D271	V272	V273	F274	L275	T276	T277	I278	A279	G280	Y281	L282	H283	L284	Y285	D286	L287	E288	T289	G290	N291	C292	I293	Y294	M295	N296	R297	L298	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	G328	V329	E330	E331	E332	N333	I334	I335	P336	Y337	I338	T339	N340	V341	L342	Q343	N344	P345	D346	L347	A348	L349	R350	N351	A352	V353	R354	N355	N356	L357	F358	G359	A360	
E361	E362	L363	F364	A365	R366	K367	F368	N369	A370	L371	F372	A373	Q374	G375	N376	Y377	E378	A379	A380	A381	K382	V383	A384	A385	N386	A387	P388	K389	K390	E391	L392	R393	T394	P395	D396	Y397	I398	R399	R400	F401	Q402	S403	V404	P405	A406	Q407	P408	Q409	Q410	T411	S412	P413	L414	L415	Q416	Y417	G418	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	A444	K445	Q446	L447	L448	A449	K450	W451	L452	K453	E454	D455	K456	L457	E458	D459	S460	E461	L462	L463	G464	D465	L466	V467	K468	S469	V470	D471	P472	T473	L474	A475	D476	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							
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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	D885	S886	N887	N888	N889	P890	E891	R892	F893	L894	R895	E896	N897	D901	K911	R912	D913	A920	Y921	E922	R923	G924										
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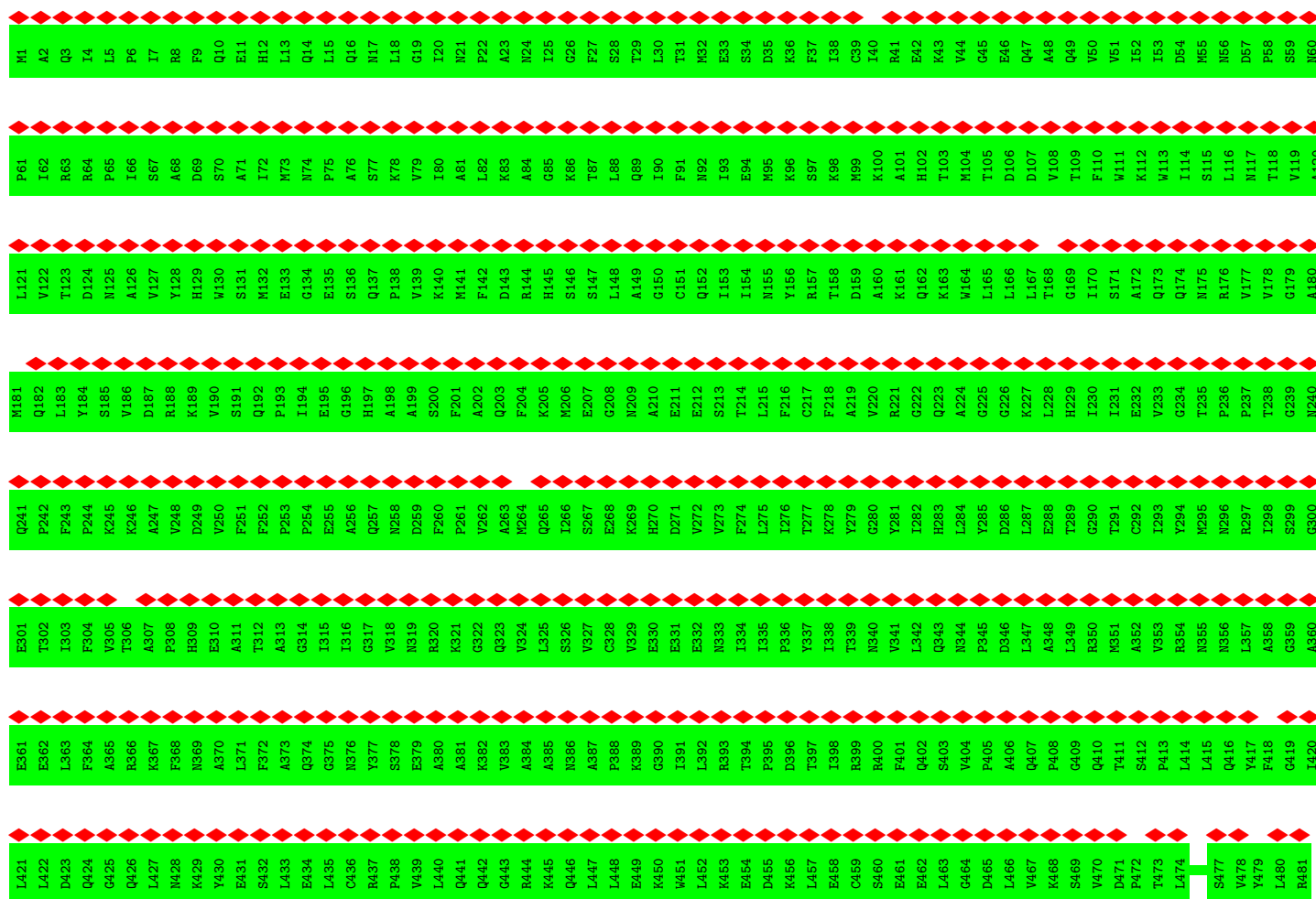


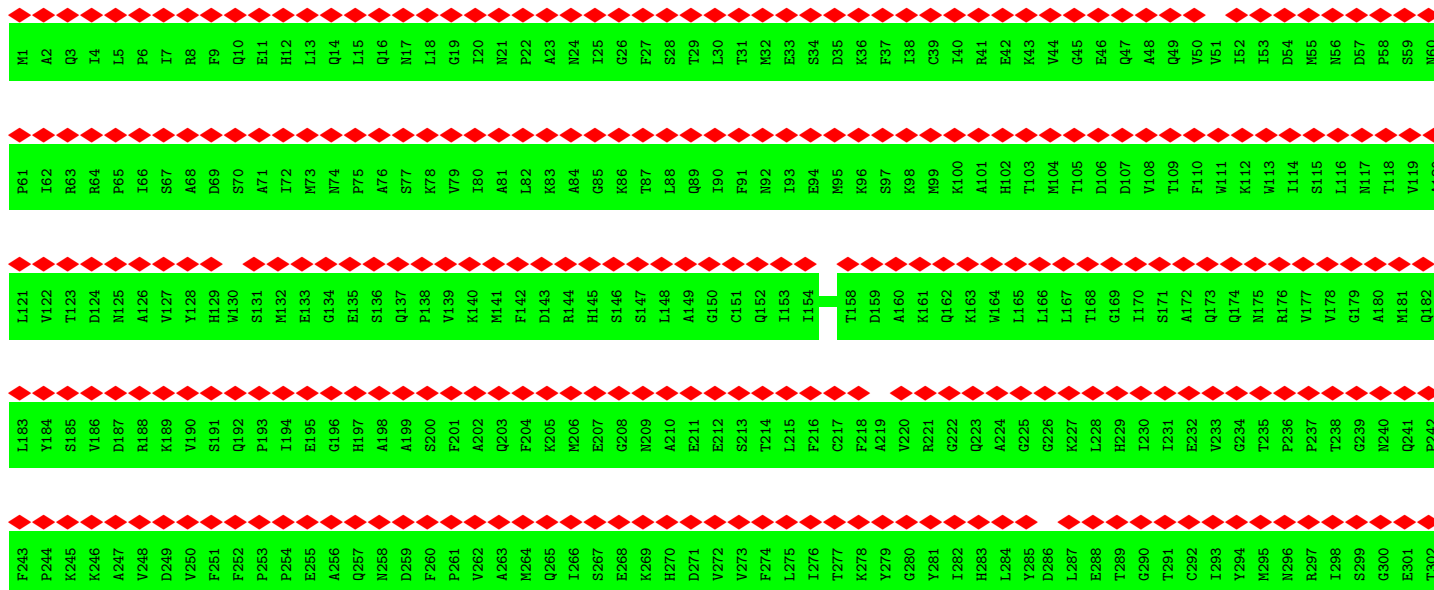
● Molecule 1: Clathrin heavy chain

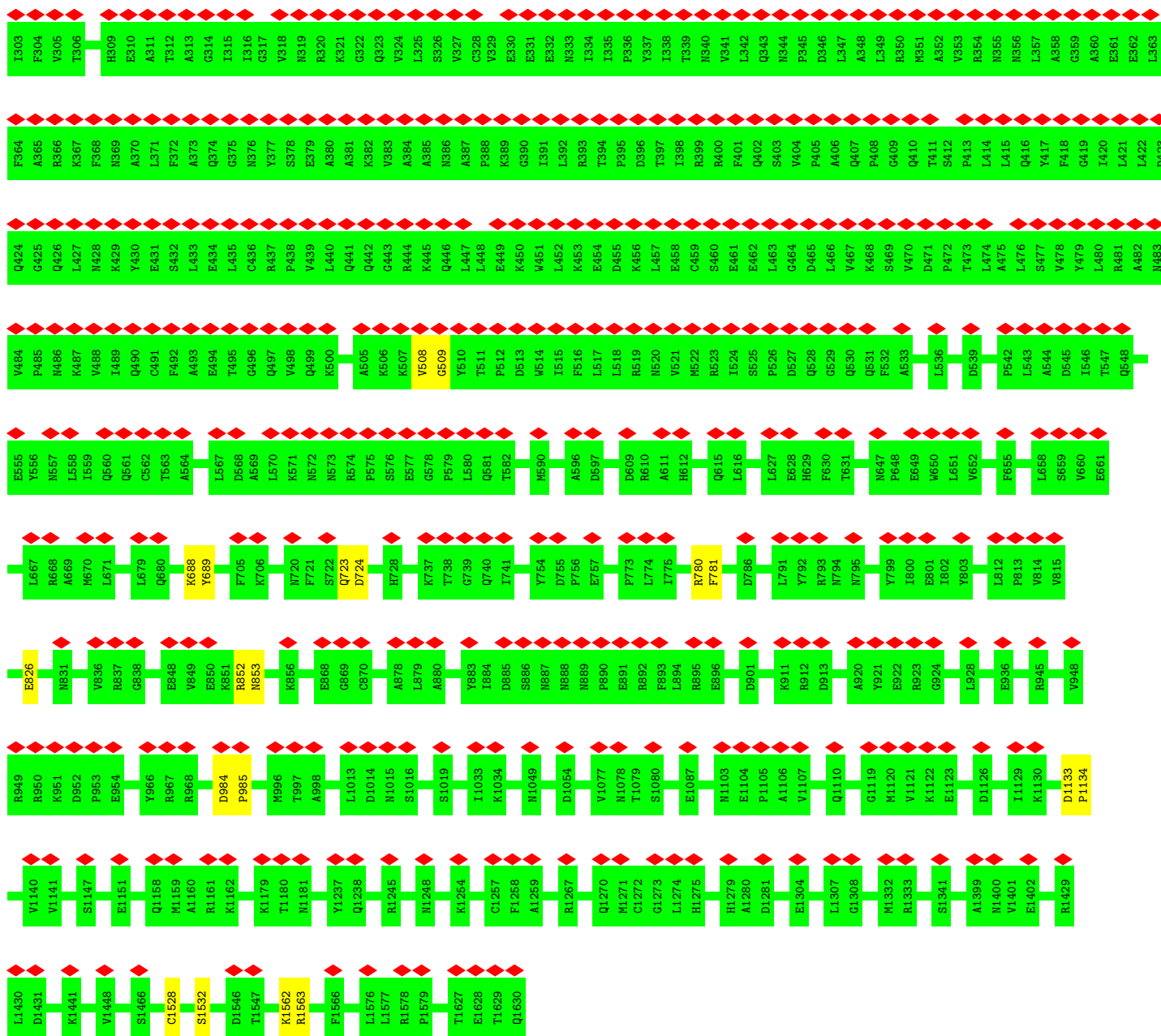




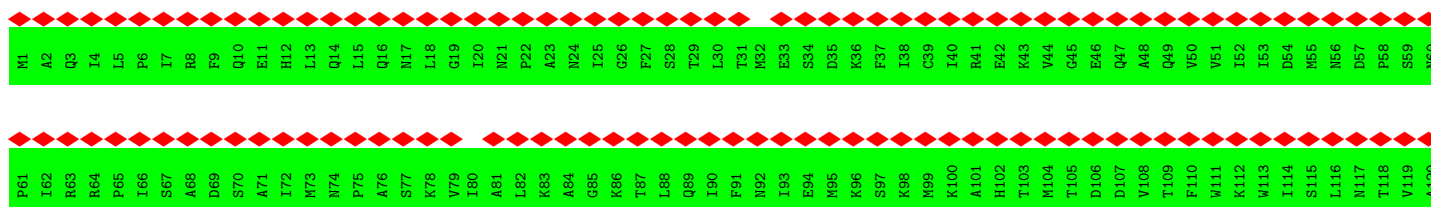
• Molecule 1: Clathrin heavy chain



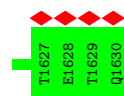




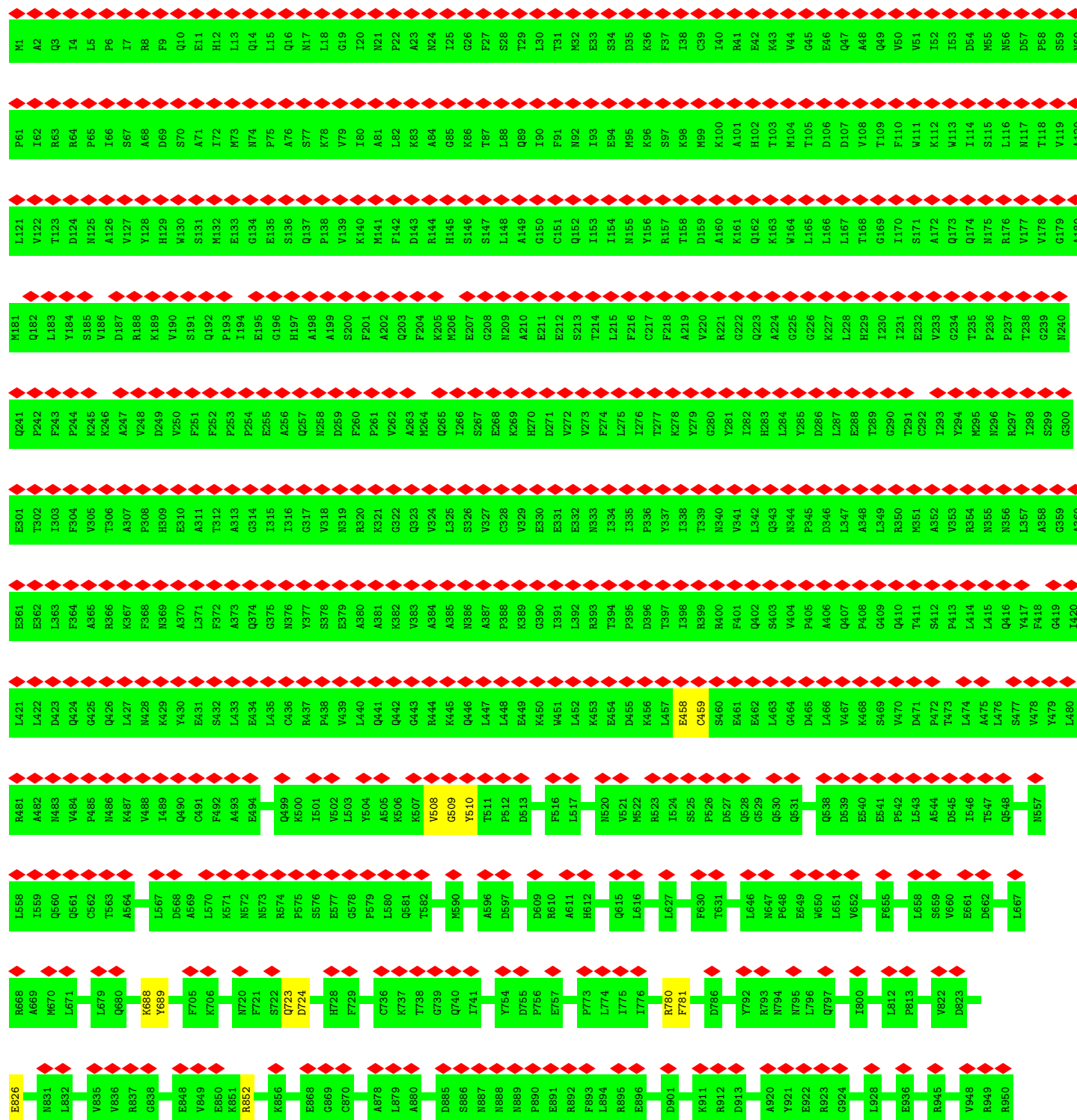
• Molecule 1: Clathrin heavy chain



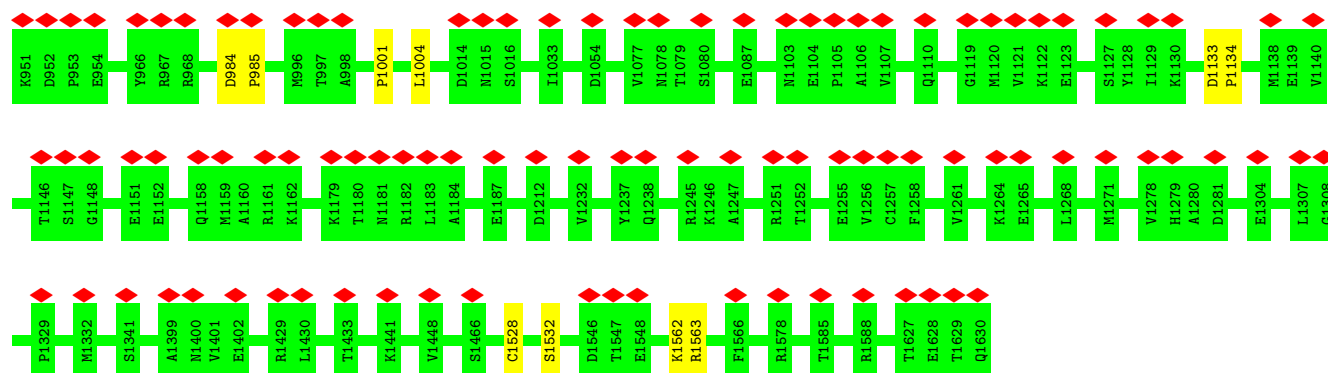
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F1266	K1130	R949	G838	R668	Q560	V488	L427	K367	P308	A247	V186	D124
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D1281	T966	T966	V846	Q680	L567	E494	L433	A373	G314	P253	P193	S131
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L1307	D984	D984	V849	Y689	L570	Q497	C436	N376	G317	A256	G196	G134
G1308	M1149	M1149	E850	F705	K571	V498	R437	Y377	V318	Q257	H197	S135
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K1162	S1016	S1016	E872	C736	Q581	Y510	L447	A387	C328	I266	R144	R144
K1179	V1017	V1017		K737	T582		L448	P388	V329	S267	E207	H145
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N1181	S1019	S1019	L879	Q739	I515	W514	K450	G390	E331	K269	N209	S147
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L1183	H1021	H1021		I741	D597	L517	K453	R393	R333	V272	E212	E211
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D1546	V1077	V1077	F893	R780	H629	D527	E462	Q402	L342	I281	R221	K161
T1547	N1078	N1078	L894	F781	F630	Q528	L463	S403	Q343	I282	G222	Q162
K1562	T1079	T1079	R895	D786	T631	G529	Q464	V404	N344	H283	Q223	K163
R1563	S1080	S1080	E896			Q530	D465	P405	P346	L284	A224	L164
F1566	E1087	E1087	D901	Y792	D635	F532	L466	A406	D346	Y285	G225	L165
L1576	M1103	M1103	K911	R794	L646	A533	V467	Q407	A348	D286	G226	L166
K1246	E1104	E1104	R912	N795	N647	Q534	K468	P408	L349	L287	K227	L167
A1247	P1105	P1105	D913	I800	P648	M535	S469	G409	R350	E288	G169	T168
N1248	A1106	A1106	A920	E826	E649	Q538	V470	Q410	N351	G290	I230	I170
S1249	V1107	V1107	E826	R827	W650	D539	D471	T411	T291	I291	I231	S171
T1250	Q1110	Q1110	Y921	V652	L651	E540	P472	S412	C292	G292	G232	A172
R1251	G1119	G1119	D827	F655	V652	E541	L474	P413	I293	I293	V233	Q173
D1262	M1120	M1120	V828	I829	F655	P542	A475	L414	Y294	K234	G234	Q174
	V1121	V1121	K830	R831	L658	L543	V478	Q416	M295	G235	G234	N175
			N831		S659	A544	Y479	Y417	L357	T235	P236	R176
			E936		V660	D545	Y479	F418	A358	R297	F237	V177
						I546	L480	G359	L357	I298	T237	G178
						T547	R481	A419	A360	S299	P238	V178
						Q548	A482	I420	E361	G300	G239	G179
							N483	L422	E362	E301	N240	A180
							V484	L422	L363	T302	Q241	M181
											P240	Q182



● Molecule 1: Clathrin heavy chain







• Molecule 2: Clathrin light chain A



• Molecule 2: Clathrin light chain A



• Molecule 2: Clathrin light chain A



• Molecule 2: Clathrin light chain A





- Molecule 2: Clathrin light chain A



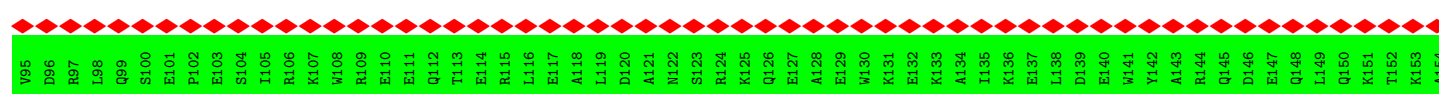
- Molecule 2: Clathrin light chain A



- Molecule 2: Clathrin light chain A



- Molecule 2: Clathrin light chain A



N155	N156	R157	V158	A159	D160	E161	A162	F163	Y164
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● Molecule 2: Clathrin light chain A



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	M122	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
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## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 ( $\text{\AA}$ )	873.6, 873.6, 873.6	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.8, 2.8, 2.8	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	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.

The worst 5 of 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

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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

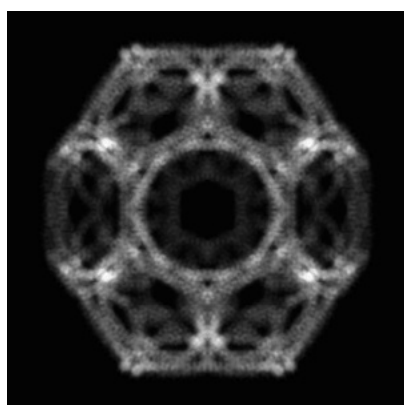
## 6 Map visualisation [i](#)

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.

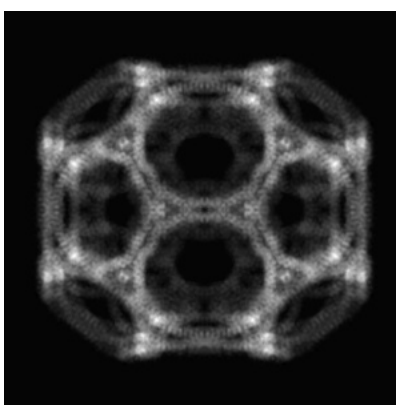
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

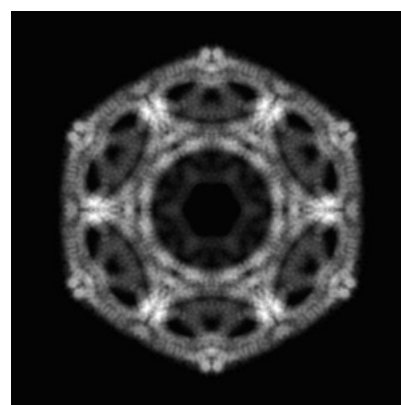
#### 6.1.1 Primary map



X



Y

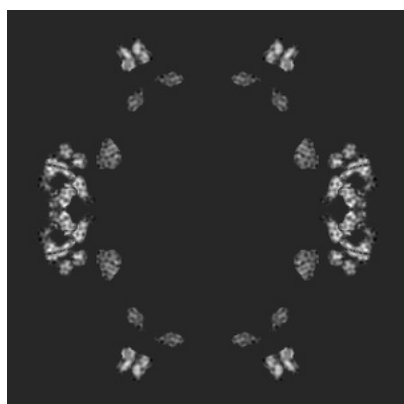


Z

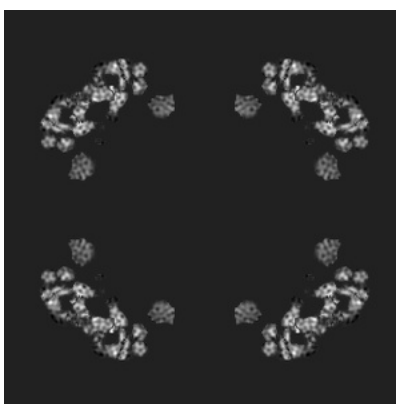
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

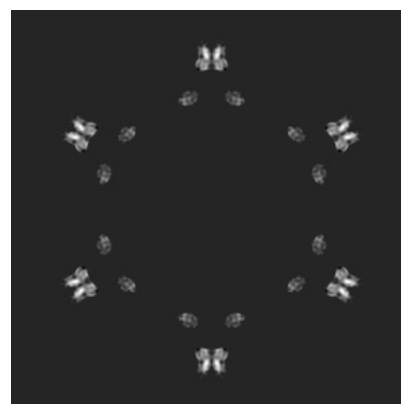
#### 6.2.1 Primary map



X Index: 156



Y Index: 156



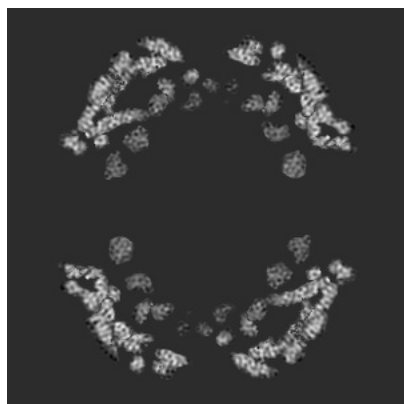
Z Index: 156



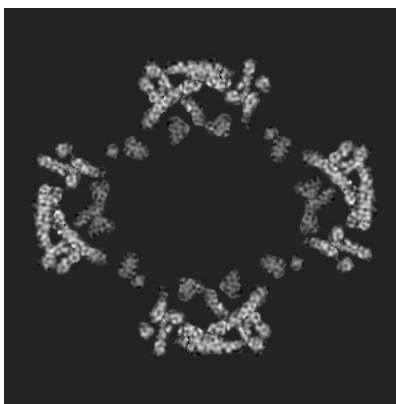
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

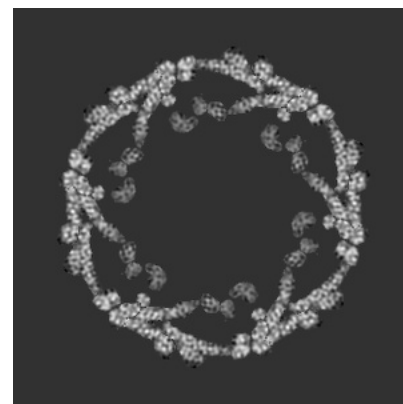
### 6.3.1 Primary map



X Index: 114



Y Index: 101

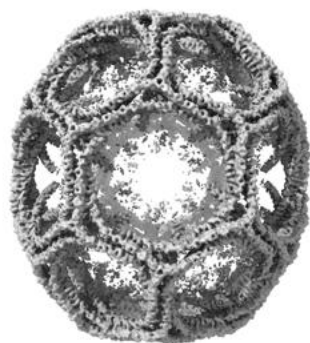


Z Index: 205

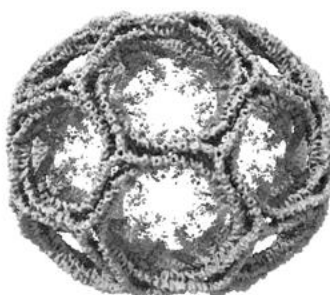
The images above show the largest variance slices of the map in three orthogonal directions.

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

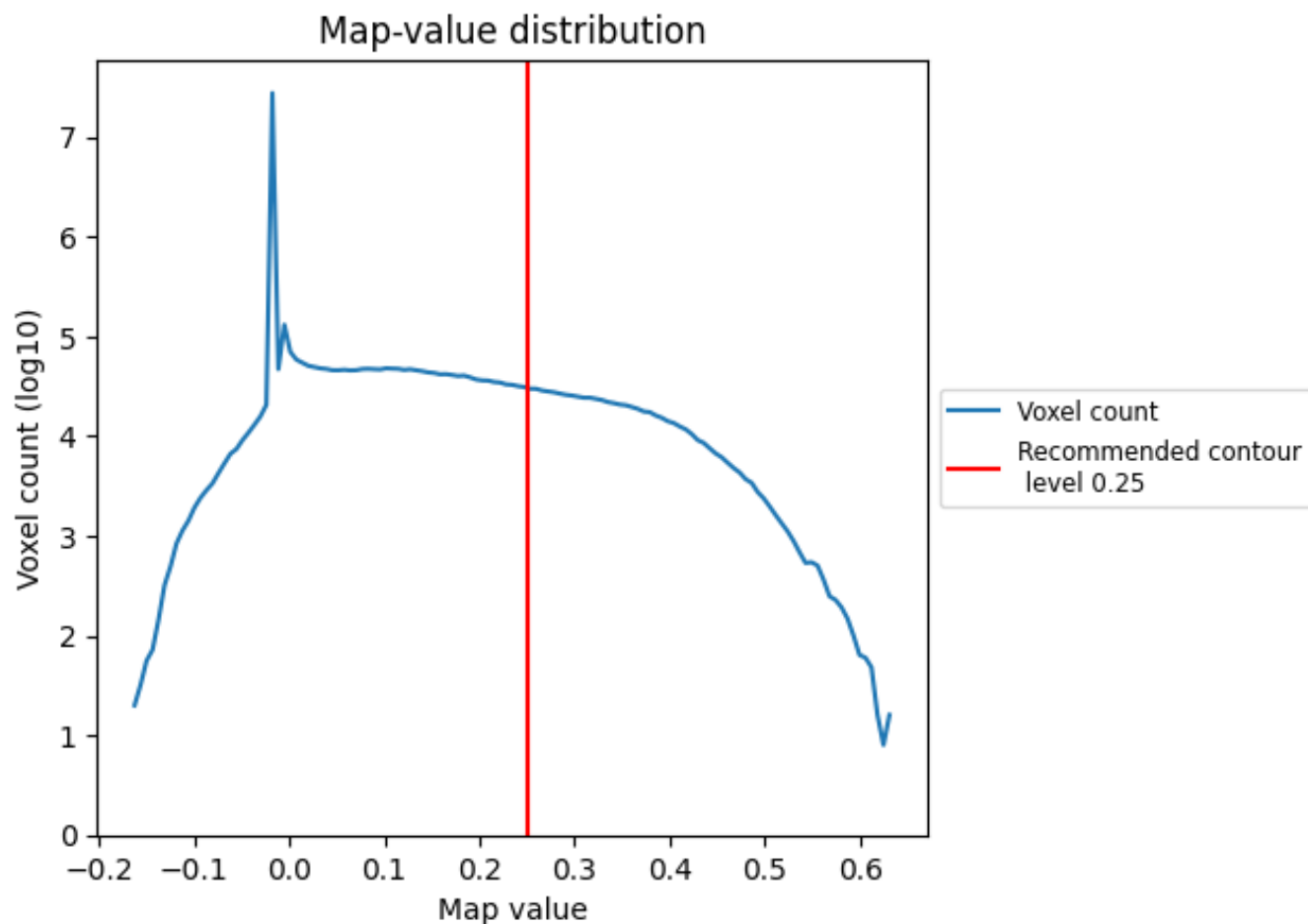
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

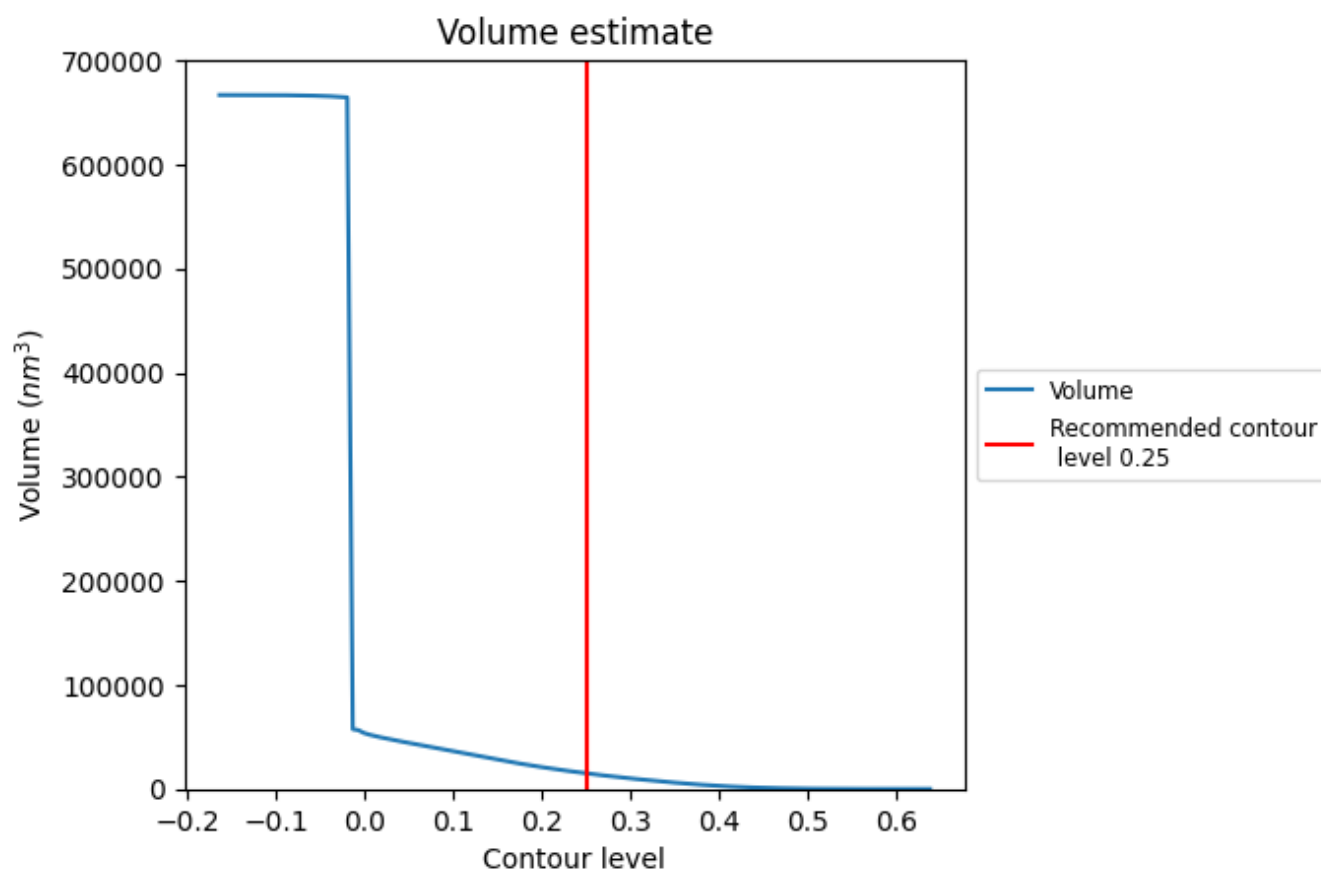
This section contains the results of statistical analysis of the map.

### 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.

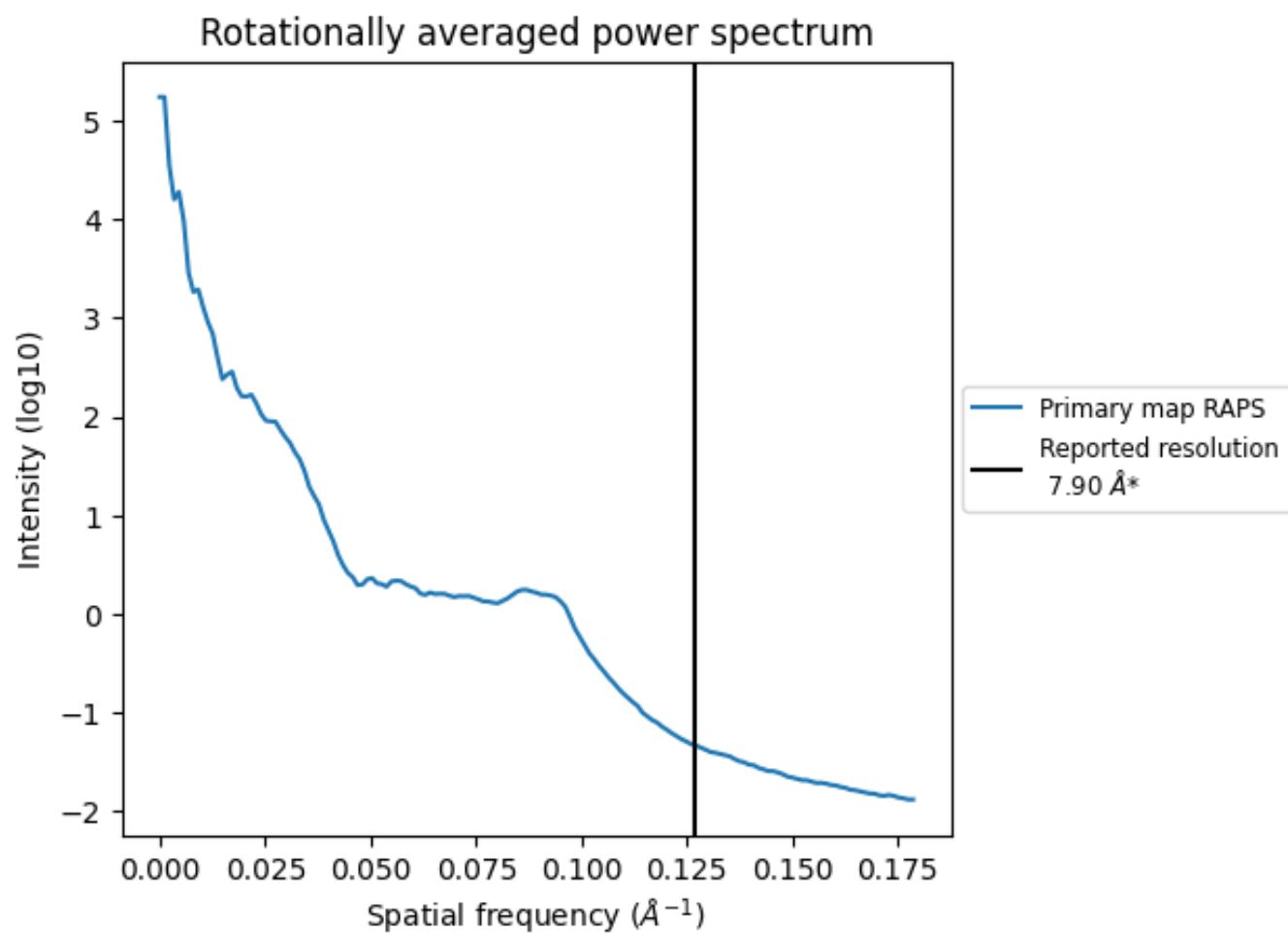
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 15047  $\text{nm}^3$ ; 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.127 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

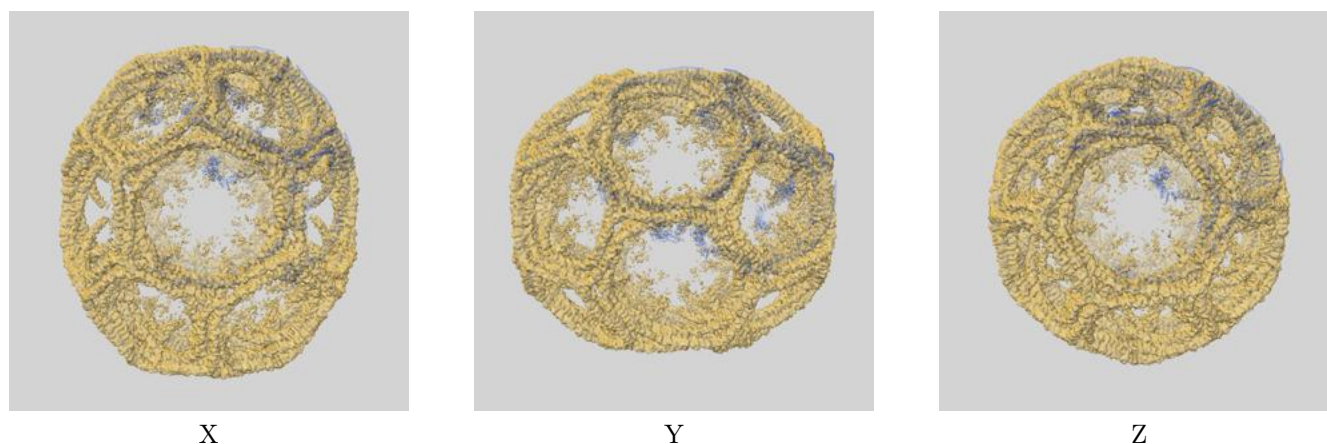
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

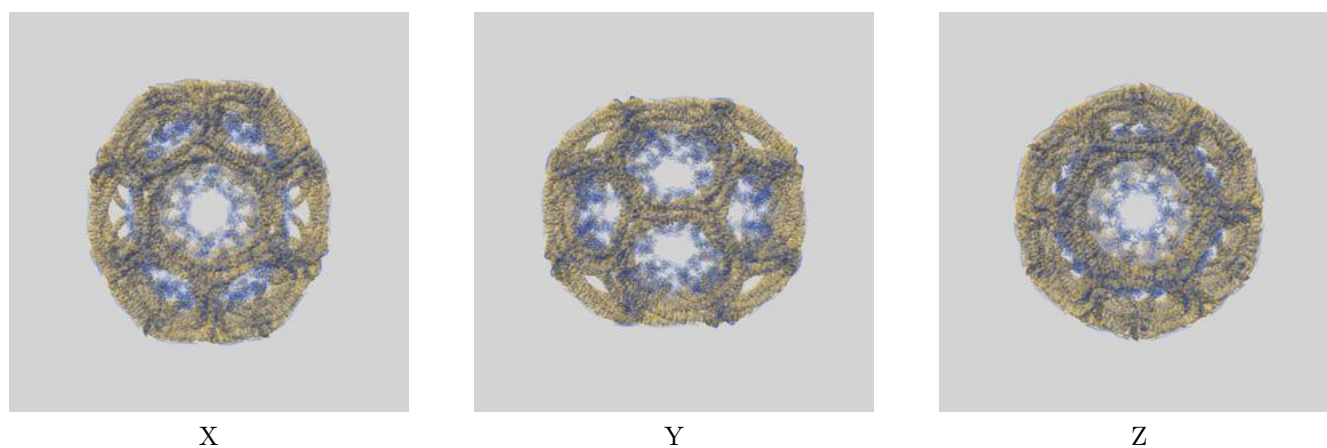
This section contains information regarding the fit between EMDB map EMD-5119 and PDB model 3IYV. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)



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



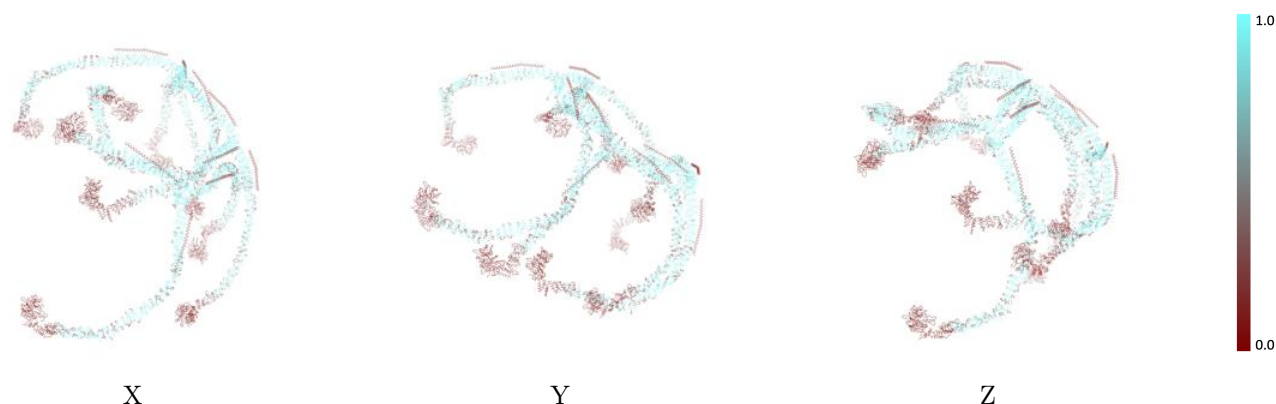
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

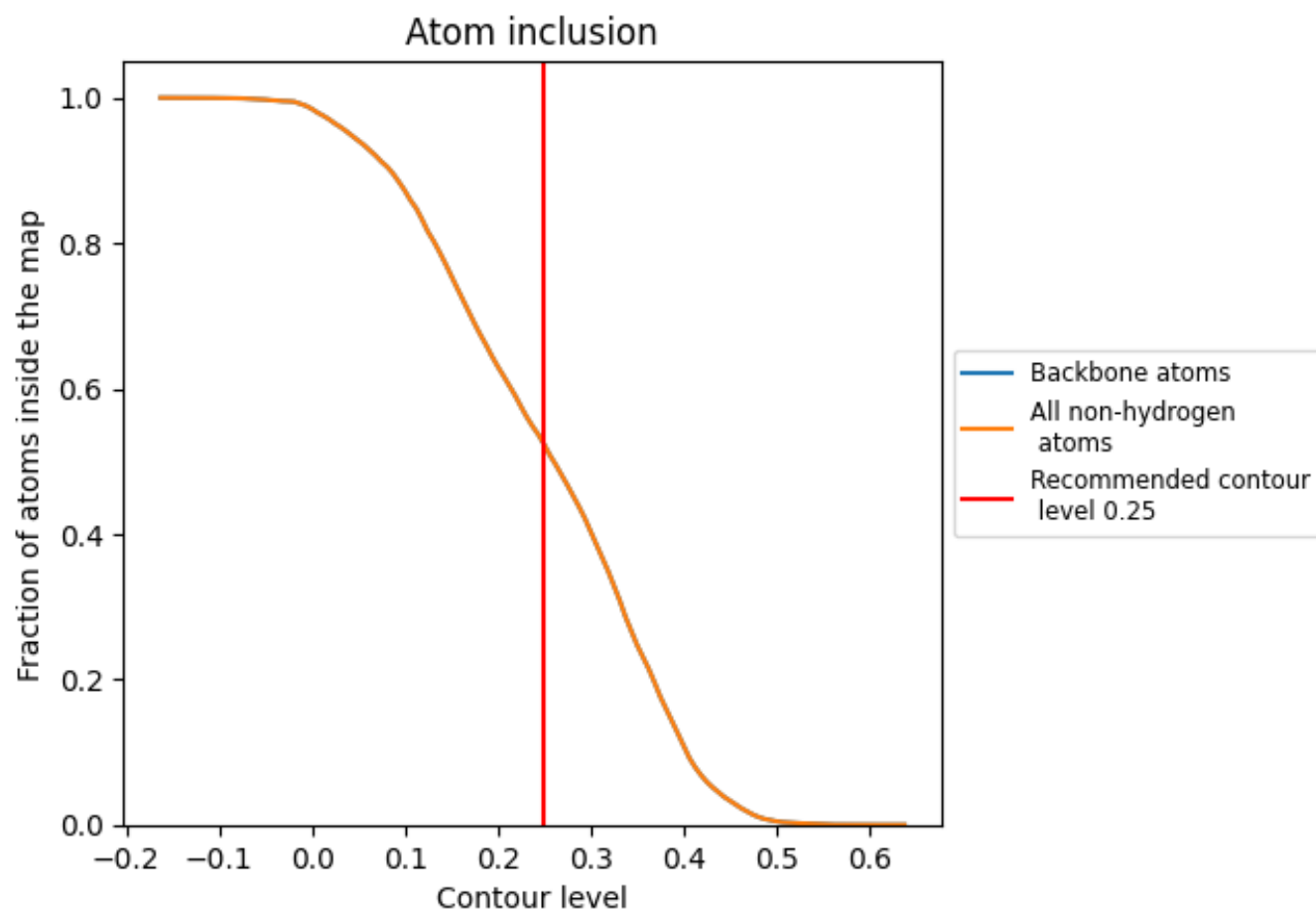
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 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	 0.5228	 0.0550
A	 0.5380	 0.0530
B	 0.5552	 0.0610
C	 0.5601	 0.0620
D	 0.5442	 0.0580
E	 0.5387	 0.0570
F	 0.5387	 0.0580
G	 0.5491	 0.0630
H	 0.5374	 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

