wwPDB EM Validation Summary Report

Dec 11, 2022 – 12:19 pm GMT

PDB ID	:	6SCT
EMDB ID	:	EMD-0126
Title	:	Cryo-EM structure of the consensus triskelion hub of the clathrin coat complex
Authors	:	Morris, K.L.; Cameron, A.D.; Sessions, R.; Smith, C.J.
Deposited on	:	2019-07-25
Resolution	:	4.69 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

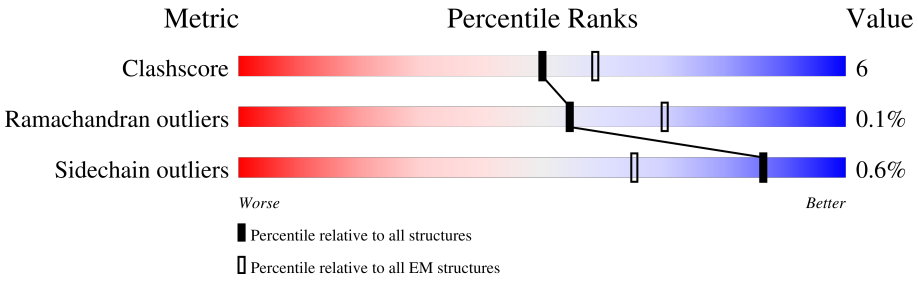
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.69 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	17% 20% · 77%
1	B	1675	35% 34% 6% 60%
1	C	1675	24% 22% 5% 74%
1	F	1675	17% 19% · 77%
1	G	1675	35% 34% 6% 60%
1	H	1675	24% 22% · 74%
1	K	1675	17% 19% · 77%
1	L	1675	35% 34% 6% 60%

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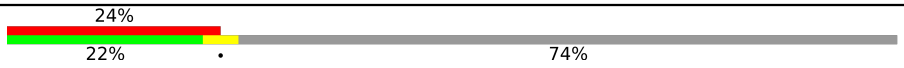
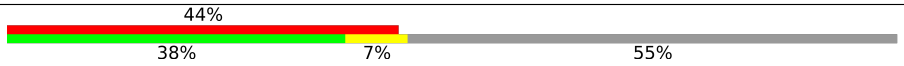
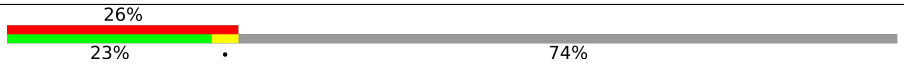
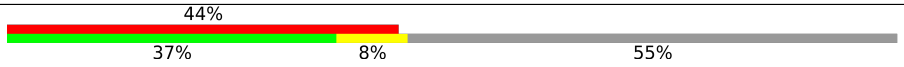
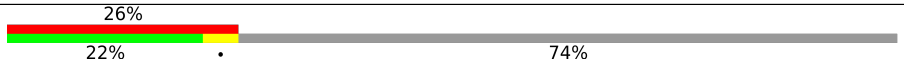
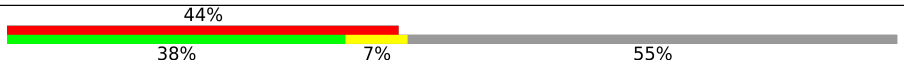
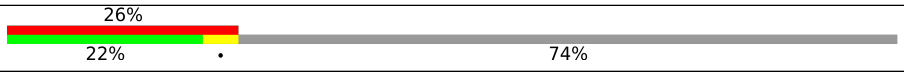
Mol	Chain	Length	Quality of chain
1	M	1675	
2	D	229	
2	E	229	
2	I	229	
2	J	229	
2	N	229	
2	O	229	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40680 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	379	Total 3168	C 2037	N 528	O 584	S 19	0	0
1	B	666	Total 5405	C 3438	N 927	O 1015	S 25	0	0
1	C	441	Total 3598	C 2293	N 615	O 675	S 15	0	0
1	F	379	Total 3168	C 2037	N 528	O 584	S 19	0	0
1	K	379	Total 3168	C 2037	N 528	O 584	S 19	0	0
1	G	666	Total 5405	C 3438	N 927	O 1015	S 25	0	0
1	L	666	Total 5405	C 3438	N 927	O 1015	S 25	0	0
1	H	441	Total 3598	C 2293	N 615	O 675	S 15	0	0
1	M	441	Total 3598	C 2293	N 615	O 675	S 15	0	0

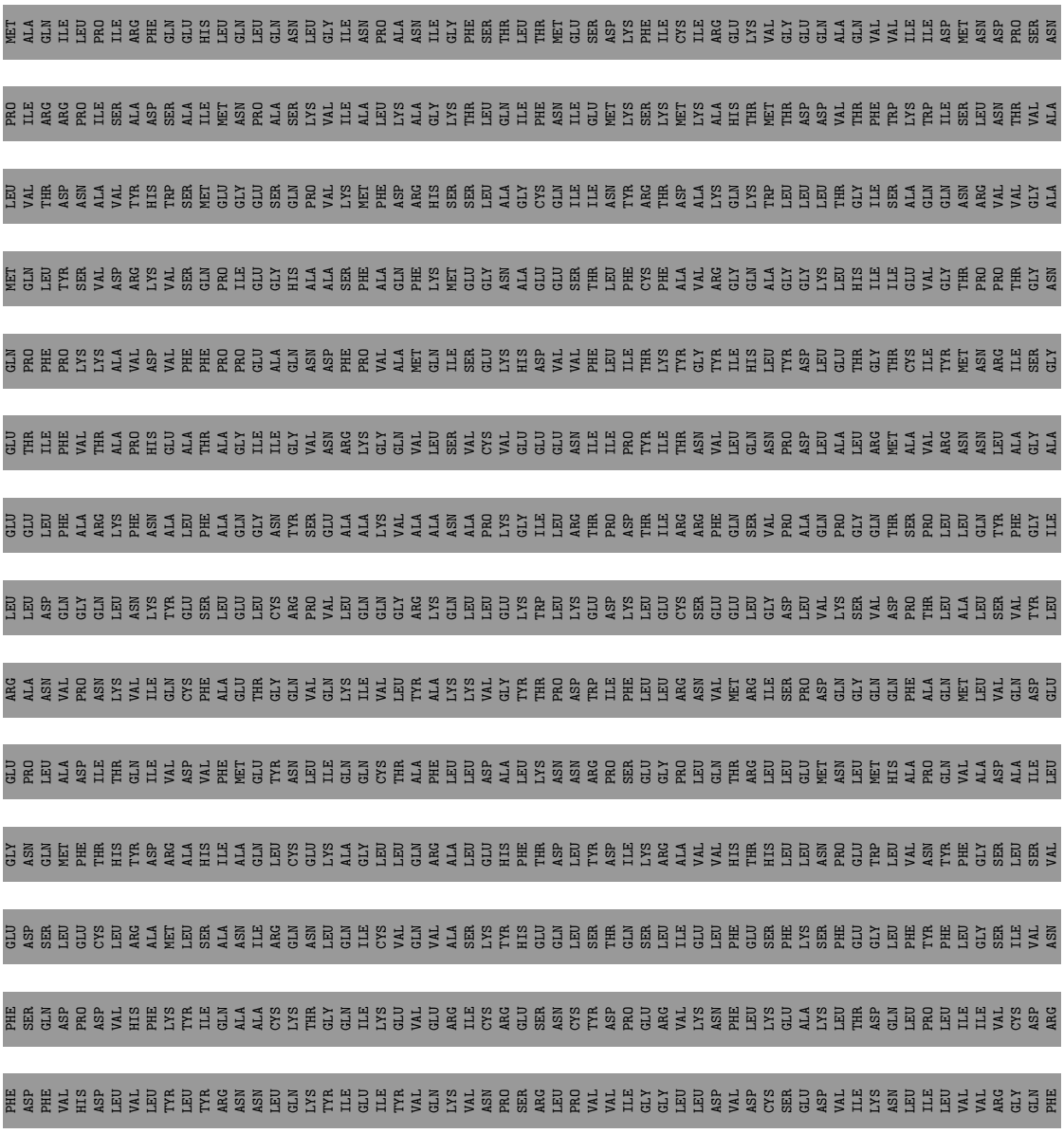
- Molecule 2 is a protein called Clathrin light chain.

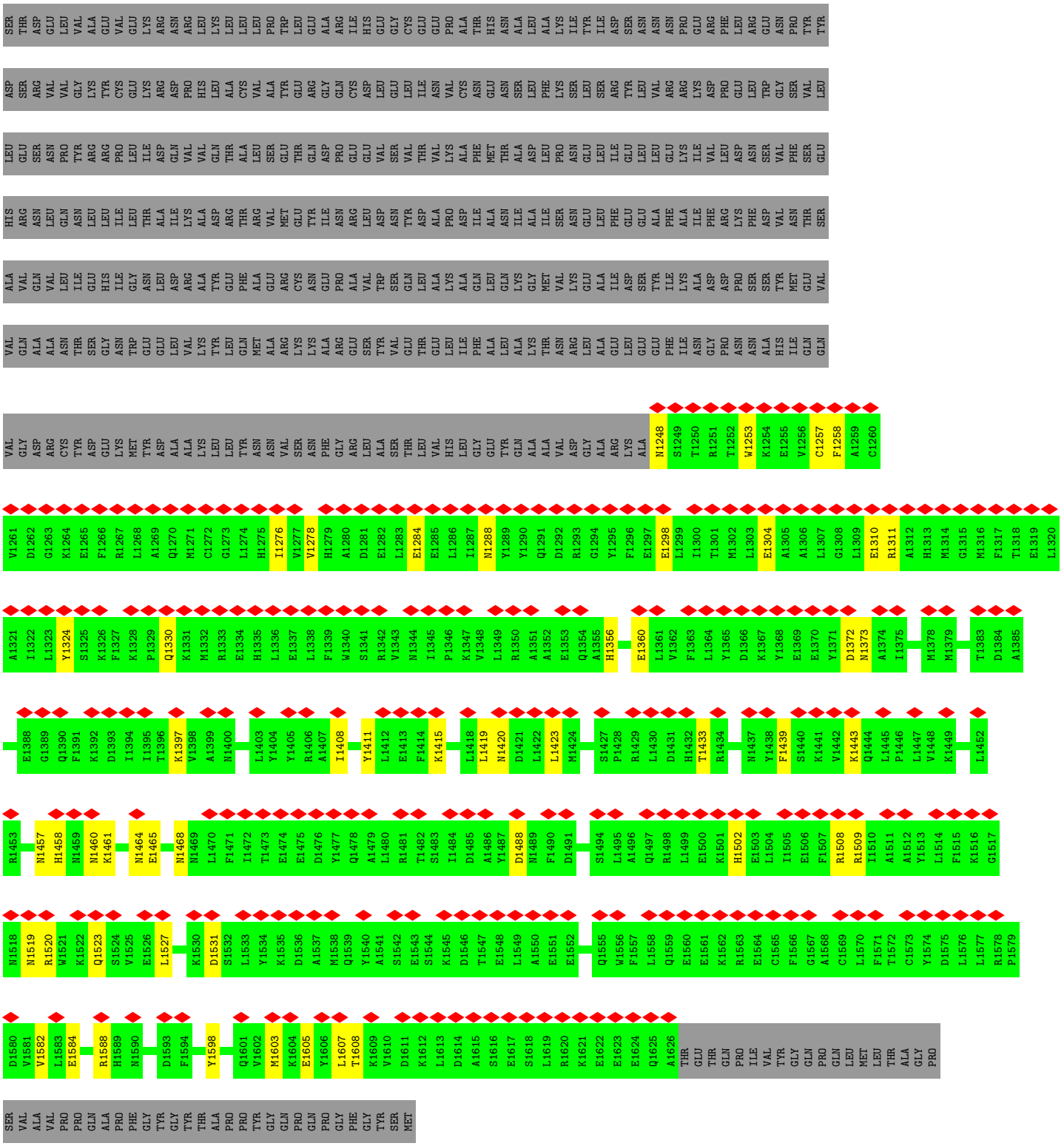
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	104	Total 875	C 539	N 165	O 168	S 3	0	0
2	E	59	Total 514	C 312	N 101	O 101		0	0
2	J	59	Total 514	C 312	N 101	O 101		0	0
2	O	59	Total 514	C 312	N 101	O 101		0	0
2	I	104	Total 875	C 539	N 165	O 168	S 3	0	0
2	N	104	Total 875	C 539	N 165	O 168	S 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Clathrin heavy chain





- Molecule 1: Clathrin heavy chain

Chain B:

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

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

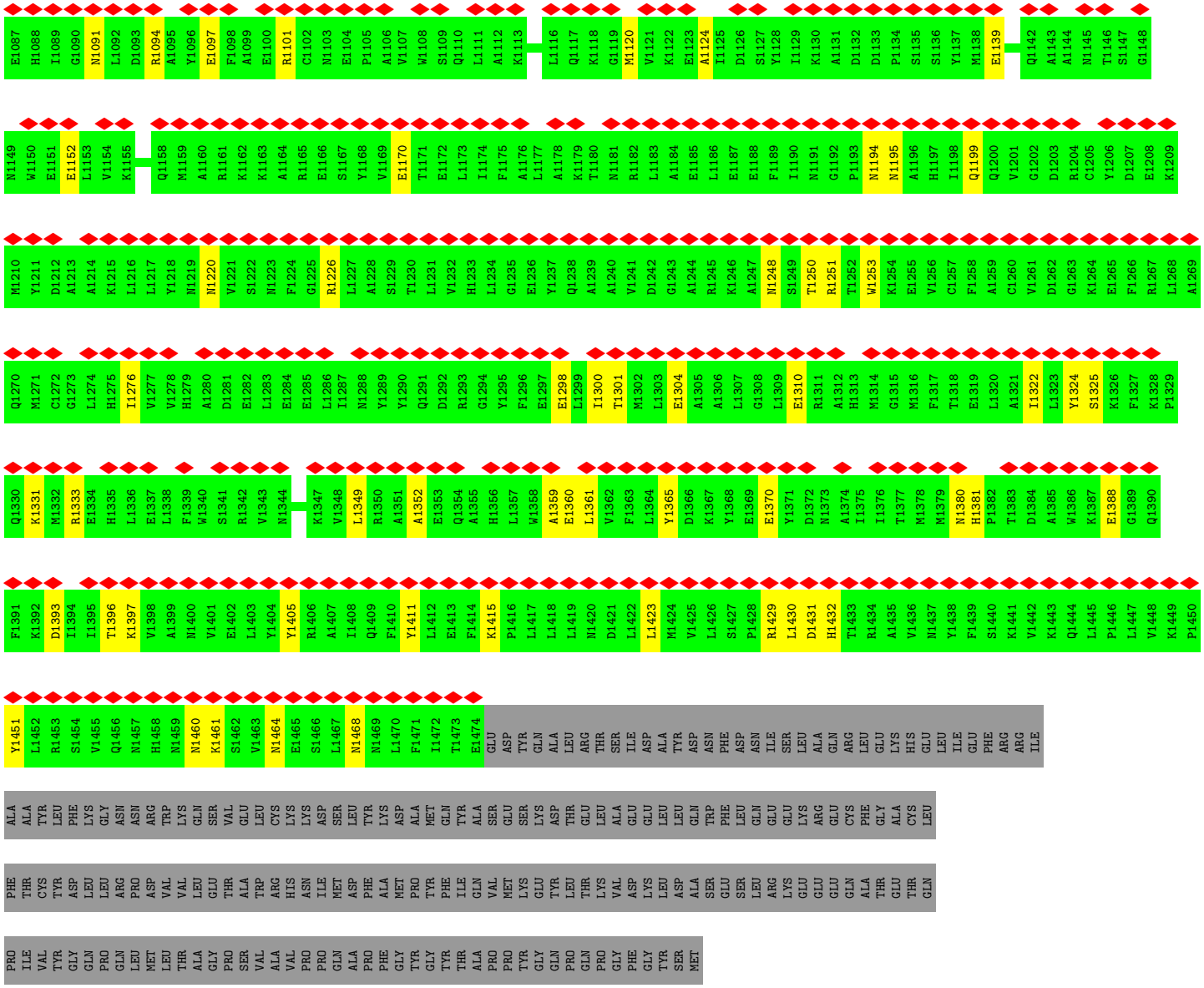
PHE ASP PHE VAL HIS ASP LEU VAL LEU TYR LEU TYR ARG ASN ASN LEU GLN LYS TYR ILE GLU ILE TYR VAL GLN LYS VAL ASN P809 S810 R811 L812 P813 V814 V815 I816 G817 G818 L819 L820 D821 V822 D823 C824 S825 E826 D827 V828 I829 K830 N831 L832 I833 L834 V835 V836 R837 G838 Q839 F840

S841 T842 D843 E844 L845 V846 A847 E848 V849 E850 K851 R852 N853 R854 L855 K856 L857 L858 L859 P860 W861 L862 E863 A864 R865 I866 H867 E868 G869 C870 E871 E872 P873 A874 T875 H876 N877 A878 L879 A880 K881 I882 Y883 I884 D885 S886 N887 N888 N889 P890 E891 R892 F893 L894 R895 E896 N897 P898 Y899 Y900

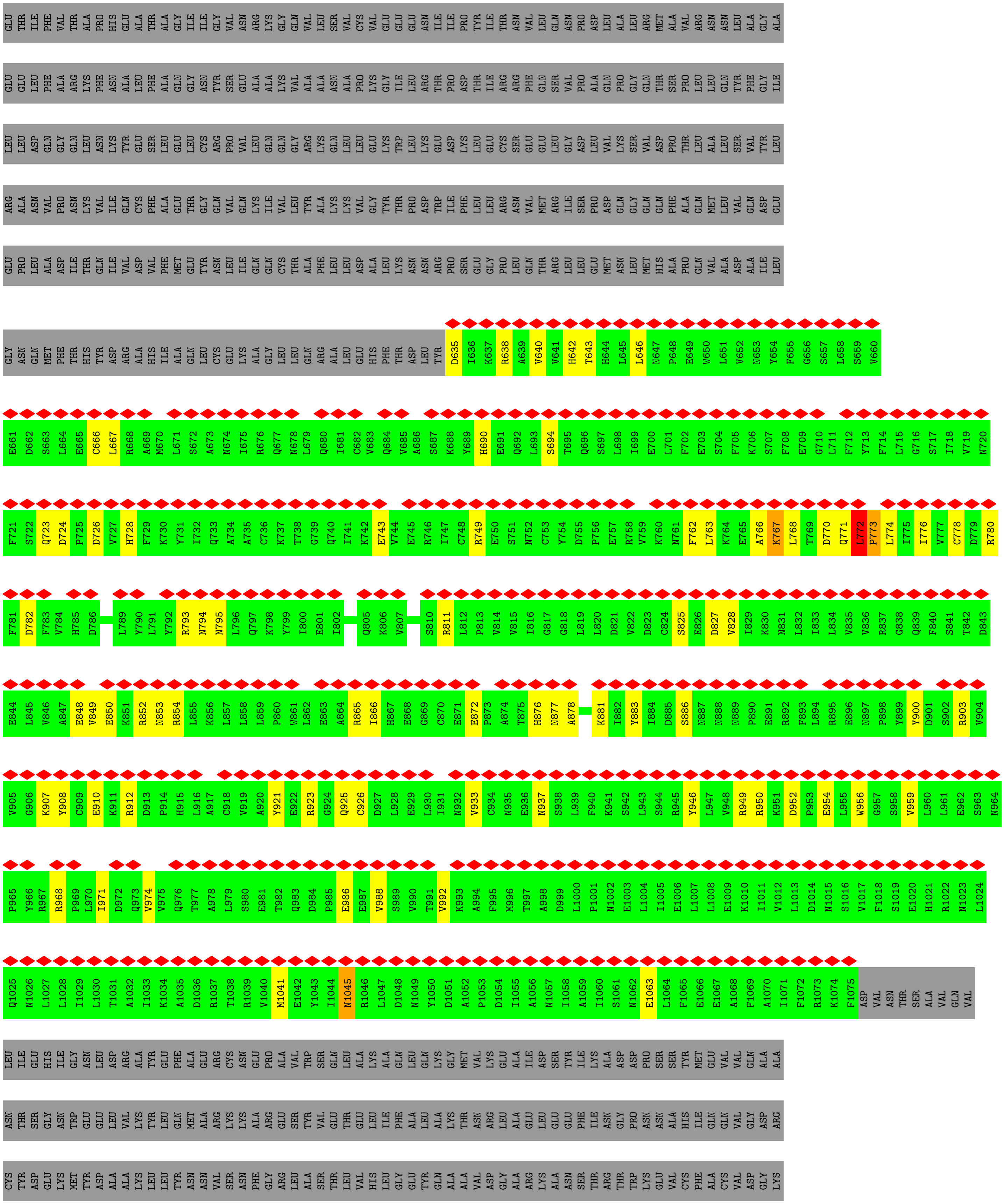
D901 S902 R903 V904 V905 G906 K907 Y908 C909 E910 K911 R912 D913 P914 H915 L916 A917 C918 V919 A920 Y921 E922 R923 G924 Q925 C926 D927 L928 E929 L930 I931 N932 V933 C934 N935 E936 N937 S938 L939 F940 K941 R945 Y946 L947 V948 R949 R950 K951 D952 P953 E954 L955 W956 G957 S958 V959 L960 L961 E962

S963 N964 P965 Y966 R967 R968 P969 L970 I971 D972 Q973 V974 V975 Q976 T977 A978 L979 S980 E981 T982 Q983 D984 P985 E986 E987 V988 S989 V990 T991 V992 K993 A994 F995 M996 T997 A998 D999 L1000 P1001 N1002 E1003 L1004 I1005 E1006 L1007 L1008 E1009 K1010 I1011 V1012 L1013 D1014 N1015 S1016 V1017 F1018 S1019 E1020 H1021 R1022

N1023 N1026 L1027 L1028 I1029 L1030 T1031 A1032 I1033 K1034 A1035 D1036 R1037 T1038 R1039 E1042 Y1043 I1044 N1045 R1046 L1047 D1048 N1049 Y1050 D1051 A1052 P1053 D1054 I1055 A1056 N1057 I1060 S1061 N1062 E1063 L1064 F1065 E1066 E1067 A1068 F1069 A1070 I1071 F1072 R1073 K1074 F1075 D1076 V1077 N1078 T1079 S1080 Q1083 V1084 L1085 I1086



- Molecule 1: Clathrin heavy chain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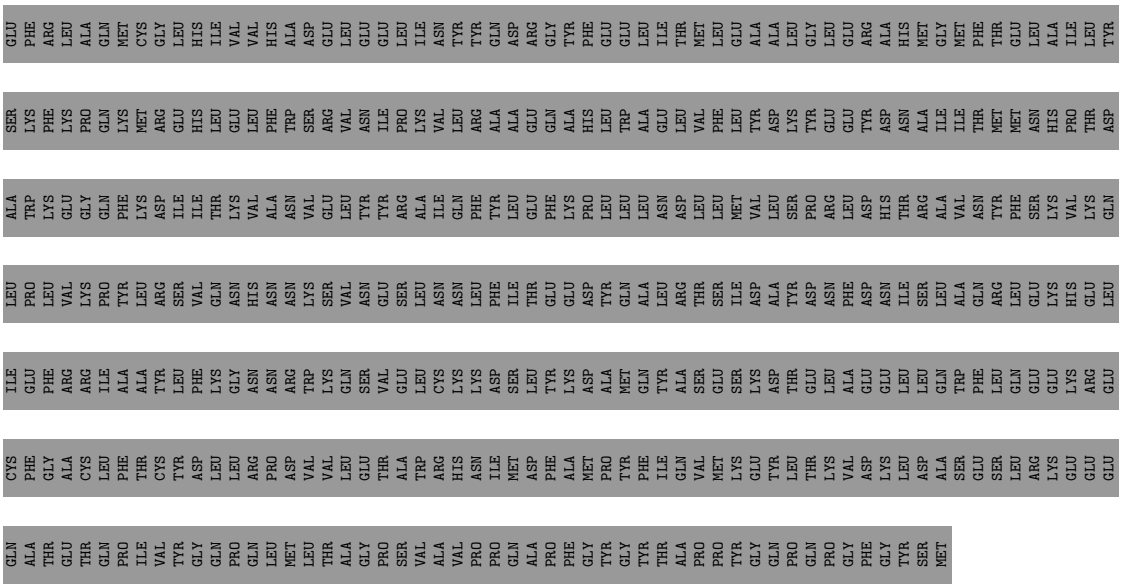
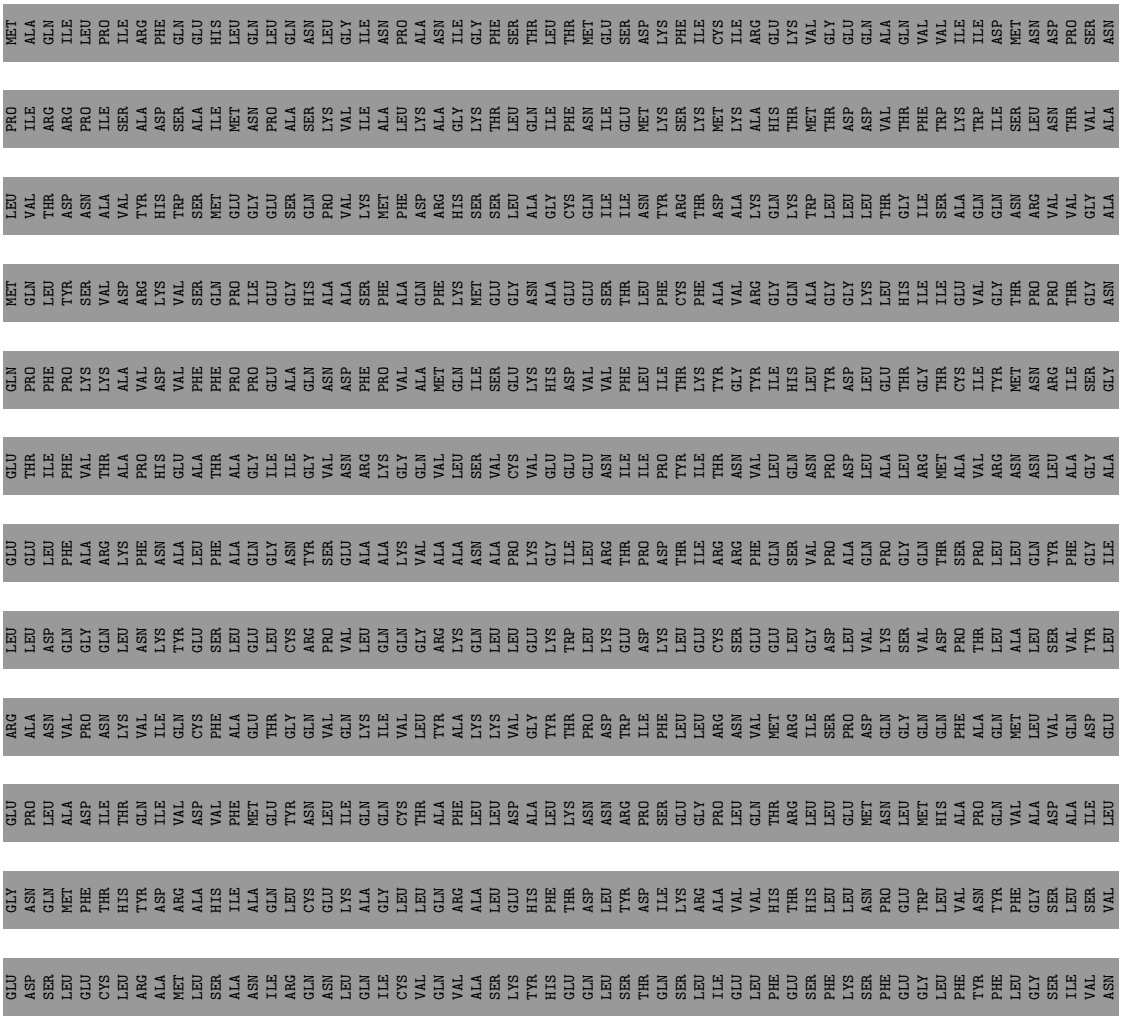
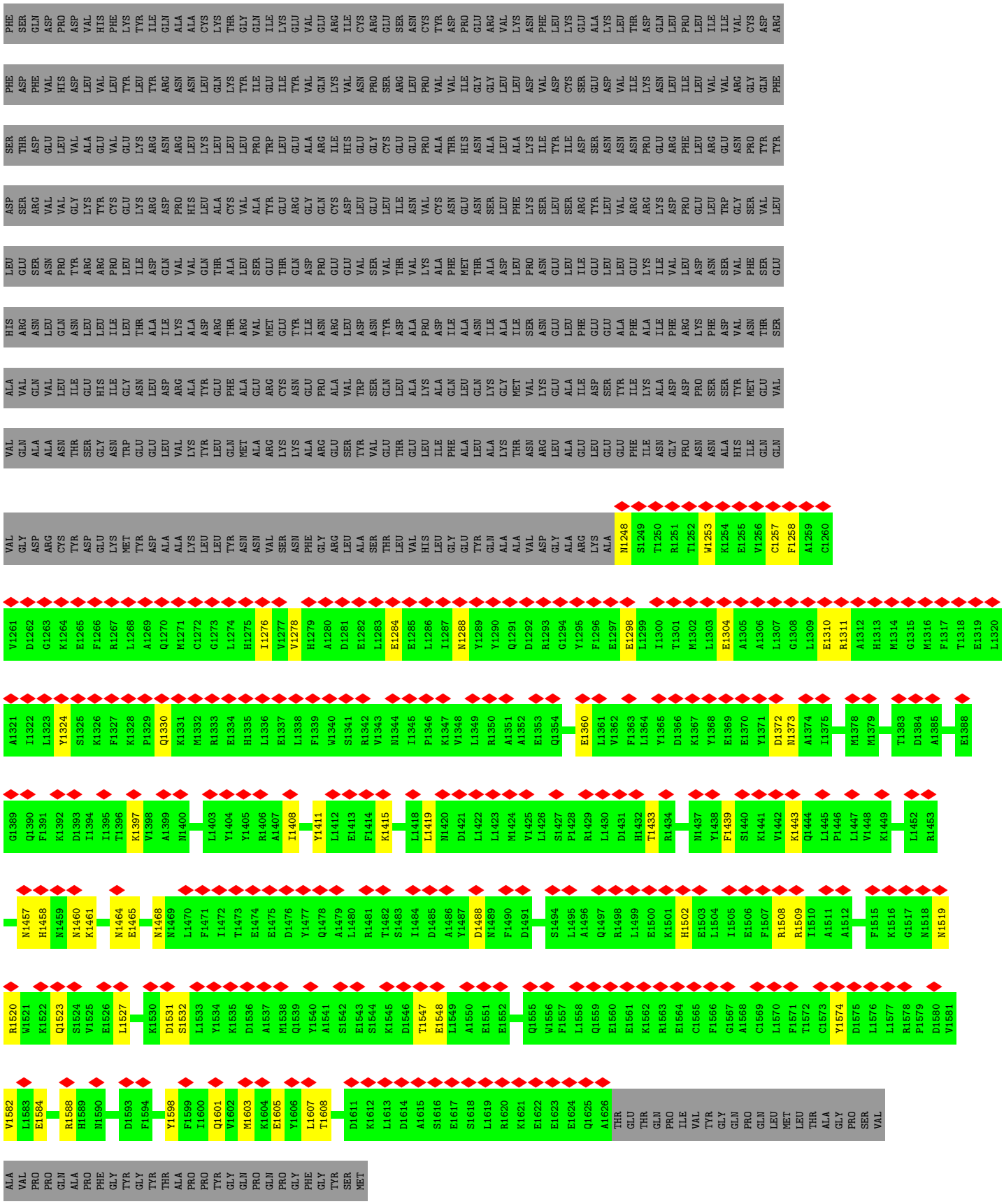
GLU GLU LEU PHE ALA ARG LYS PHE ASN ALA LEU PHE ALA GLN GLY ASN TYR SER GLU ALA ALA LYS VAL ALA ALA ASN ALA PRO LYS GLY ILE LEU ARG THR PRO ASP THR ILE ARG ARG PHE GLN SER VAL PRO ALA GLN PRO GLY GLN THR SER PRO LEU LEU GLN TYR PHE GLY ILE
LEU LEU ASP GLN GLY GLN LEU ASN LYS TYR GLU SER LEU GLU LEU CYS ARG PRO VAL LEU GLN 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 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 VAL ASP VAL 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 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 D635 I636 K637 R638 A639 V640 V641 H642 T643 H644 L645 L646 N647 P648 E649 W650 L651 V652 N653 Y654 F655 G656 S657 L658 S659 V660
E661 D662 S663 L664 E665 C666 L667 R668 A669 M670 L671 S672 A673 N674 I675 R676 Q677 N678 L679 Q680 I681 C682 V683 Q684 V685 A686 S687 K688 Y689 H690 E691 Q692 L693 S694 T695 Q696 S697 L698 I699 E700 L701 F702 E703 S704 F705 K706 S707 F708 E709 G710 L711 F712 Y713 F714 L715 G716 S717 I718 V719 N720
F721 S722 Q723 D724 P725 D726 V727 H728 F729 K730 Y731 I732 Q733 A734 A735 C736 K737 T738 G739 Q740 I741 K742 E743 V744 E745 R746 I747 C748 R749 E750 S751 N752 C753 Y754 D755 P756 E757 R758 V759 K760 N761 F762 L763 K764 E765 A766 K767 L768 T769 D770 Q771 L772 P773 L774 I775 I776 V777 C778 D779 R780
F781 D782 F783 V784 H785 D786 L789 Y790 L791 Y792 R793 N794 N795 L796 Q797 K798 Y799 I800 E801 I802 Q805 K806 V807 S810 R811 L812 P813 V814 V815 I816 G817 G818 L819 L820 D821 V822 D823 C824 S825 E826 D827 V828 I829 K830 N831 L832 I833 L834 V835 V836 R837 G838 Q839 F840 S841 T842 D843
E844 L845 V846 A847 E848 V849 E850 K851 R852 N853 R854 L855 K856 L857 L858 L859 P860 W861 L862 E863 A864 R865 I866 H867 E868 G869 C870 E871 E872 P873 A874 T875 H876 N877 A878 K881 I882 Y883 I884 D885 S886 N887 N888 N889 P890 E891 R892 F893 L894 R895 E896 N897 P898 Y899 Y900 D901 S902 R903 V904
V905 G906 K907 Y908 C909 E910 K911 R912 D913 P914 H915 L916 A917 C918 V919 A920 Y921 E922 R923 G924 Q925 C926 D927 L928 E929 L930 I931 N932 V933 C934 N935 E936 N937 S938 L939 F940 K941 S942 L943 S944 R945 Y946 L947 V948 R949 R950 K951 D952 P953 E954 L955 W956 G957 S958 V959 L960 L961 E962 S963 N964
P965 Y966 R967 R968 P969 L970 I971 D972 Q973 V974 V975 Q976 T977 A978 L979 S980 E981 T982 Q983 D984 P985 E986 E987 V988 S989 V990 T991 V992 K993 A994 F995 M996 T997 A998 D999 L1000 P1001 N1002 E1003 L1004 I1005 E1006 L1007 L1008 E1009 K1010 I1011 V1012 L1013 D1014 N1015 S1016 V1017 F1018 S1019 E1020 H1021 R1022 N1023 L1024
Q1025 N1026 L1027 L1028 I1029 L1030 T1031 A1032 I1033 K1034 A1035 D1036 R1037 T1038 R1039 V1040 M1041 E1042 Y1043 I1044 N1045 R1046 L1047 D1048 N1049 Y1050 D1051 A1052 P1053 D1054 I1055 A1056 N1057 I1058 A1059 I1060 S1061 N1062 E1063 L1064 F1065 E1066 E1067 A1068 F1069 A1070 I1071 F1072 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 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 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



- Molecule 1: Clathrin heavy chain

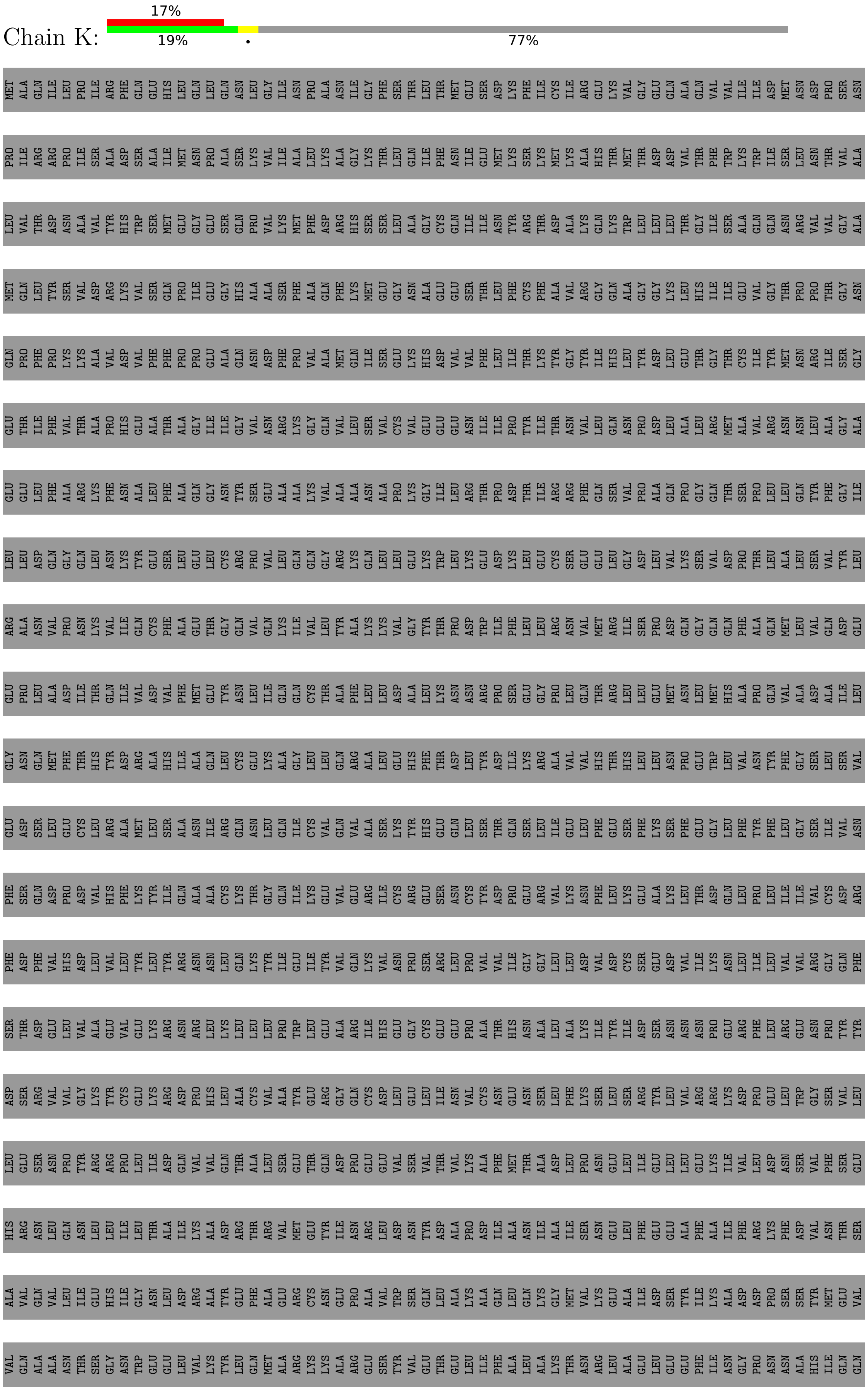
Chain F:

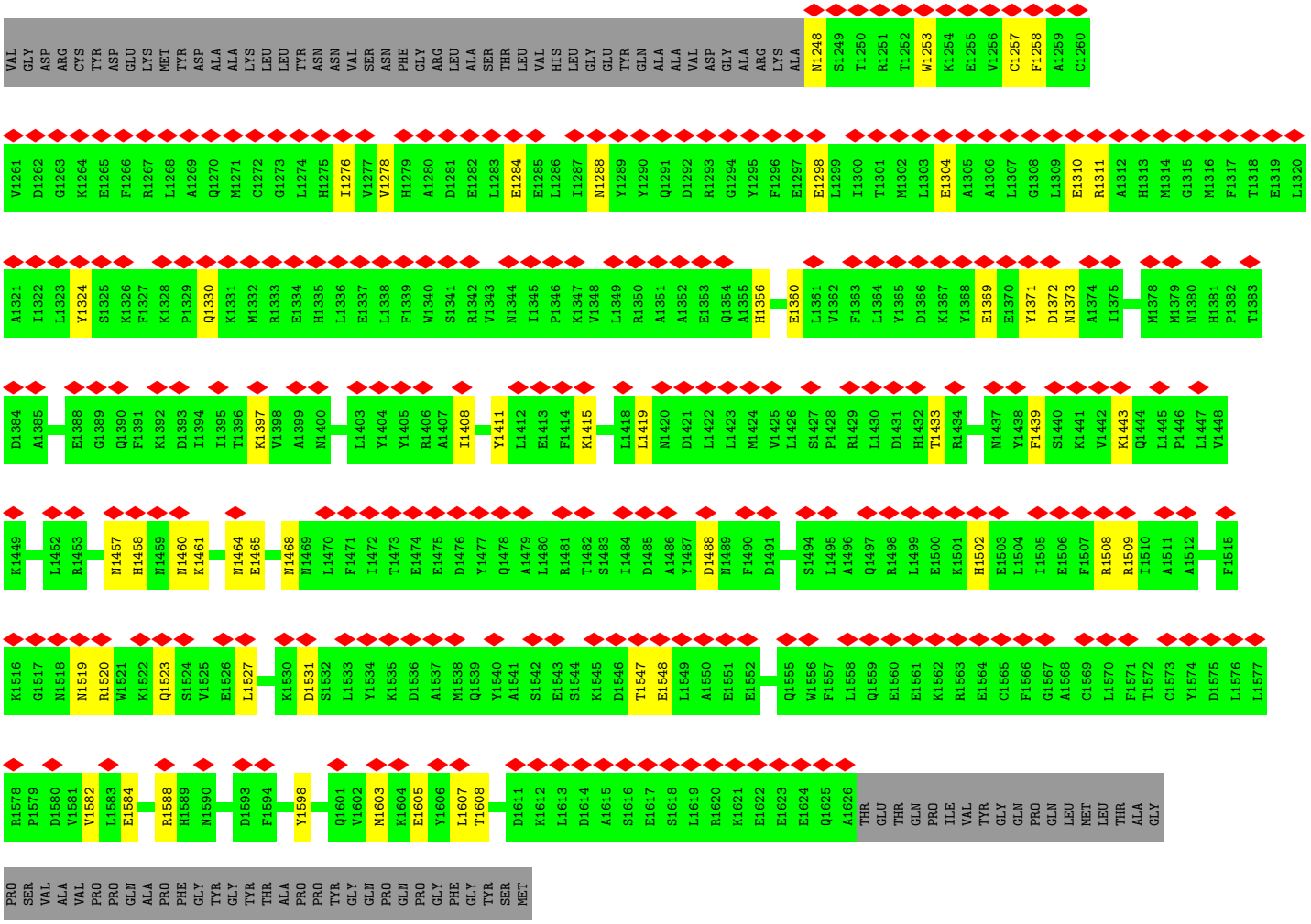




• Molecule 1: Clathrin heavy chain

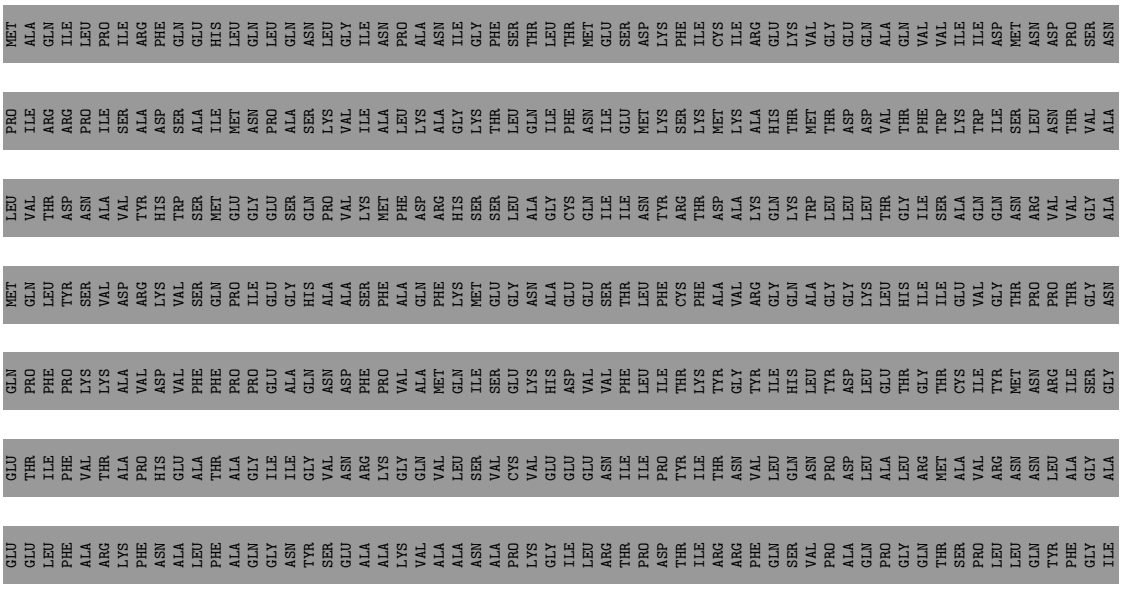
Chain K:

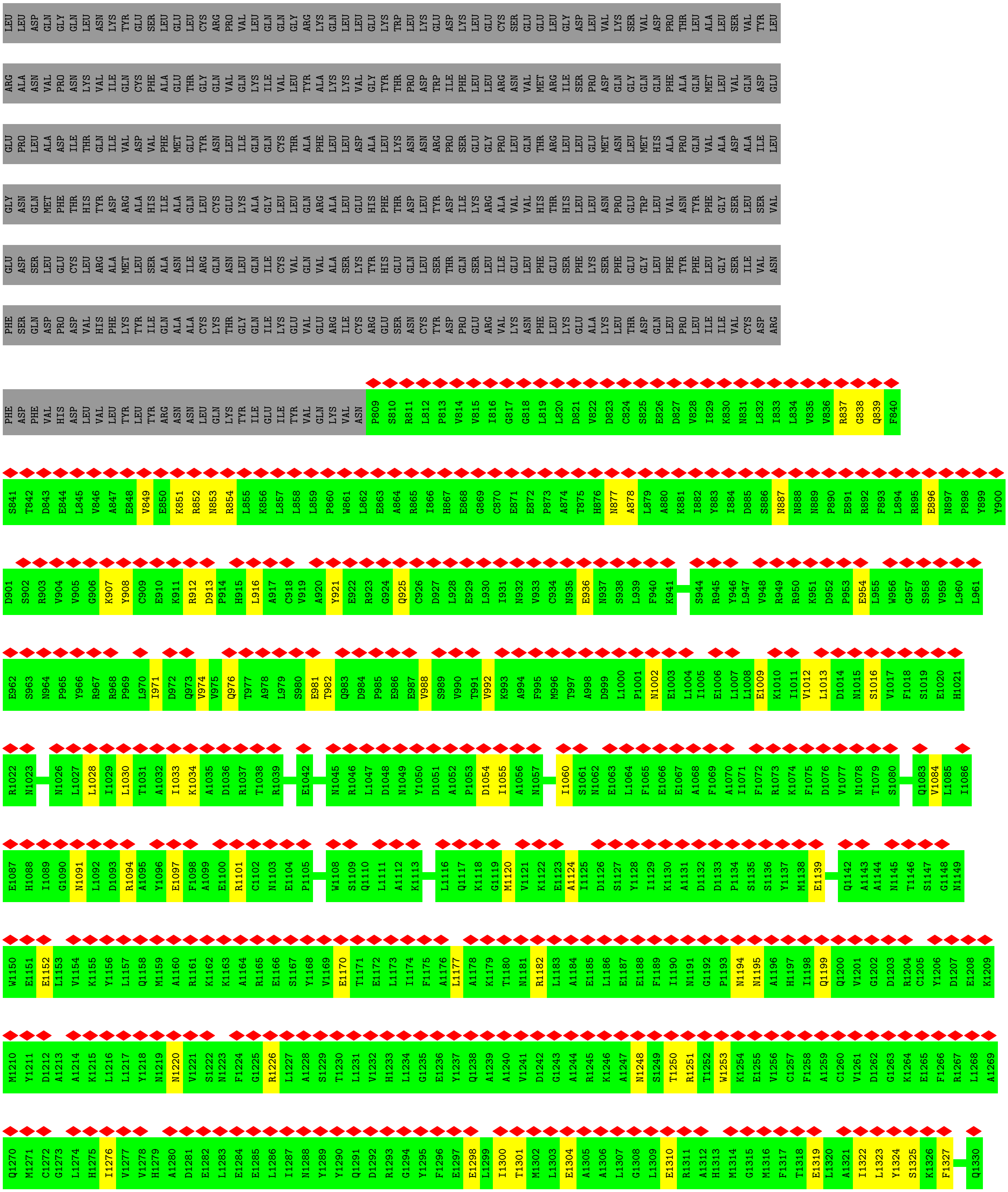




• Molecule 1: Clathrin heavy chain

Chain G:

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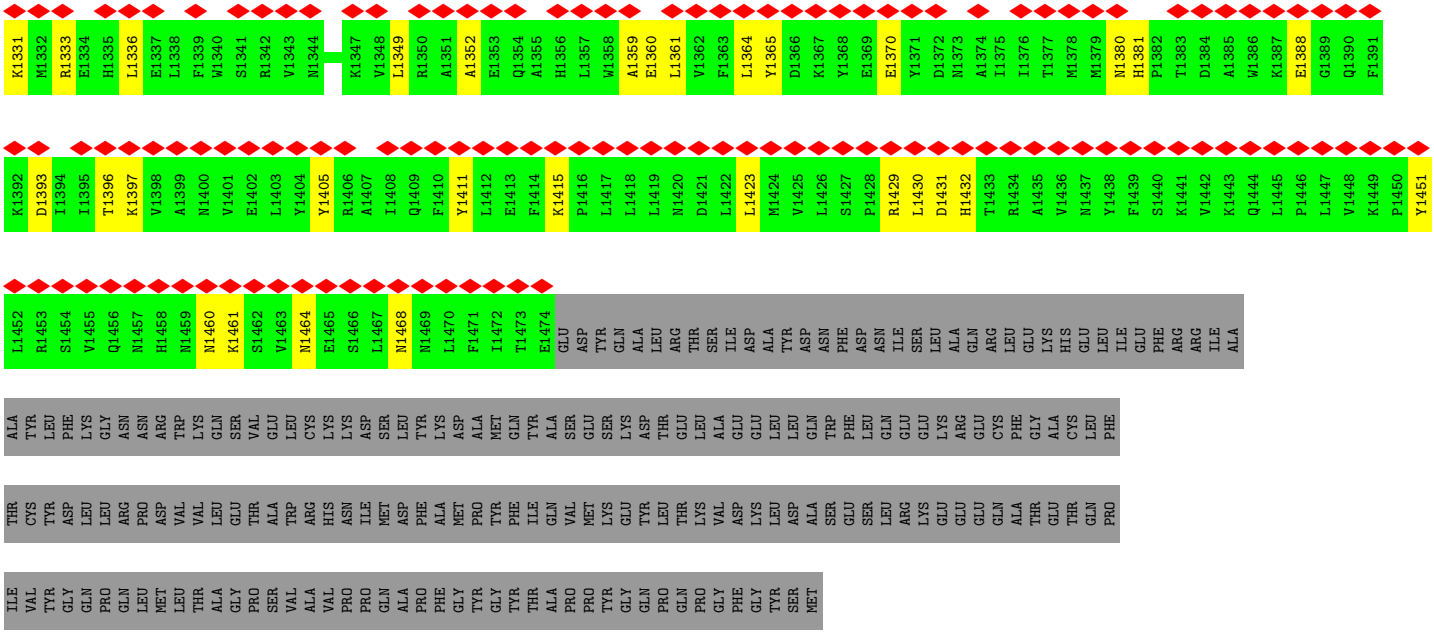
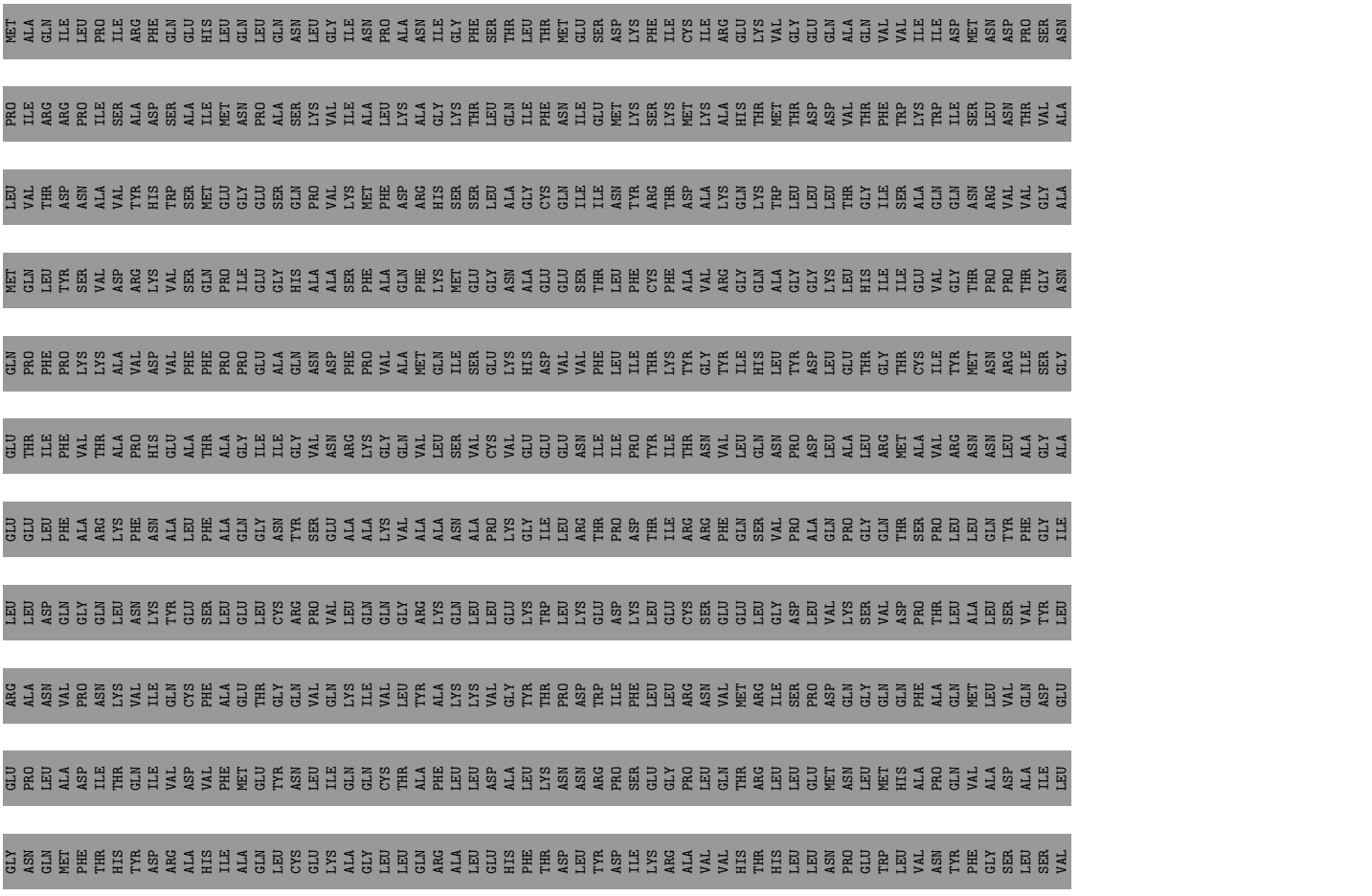
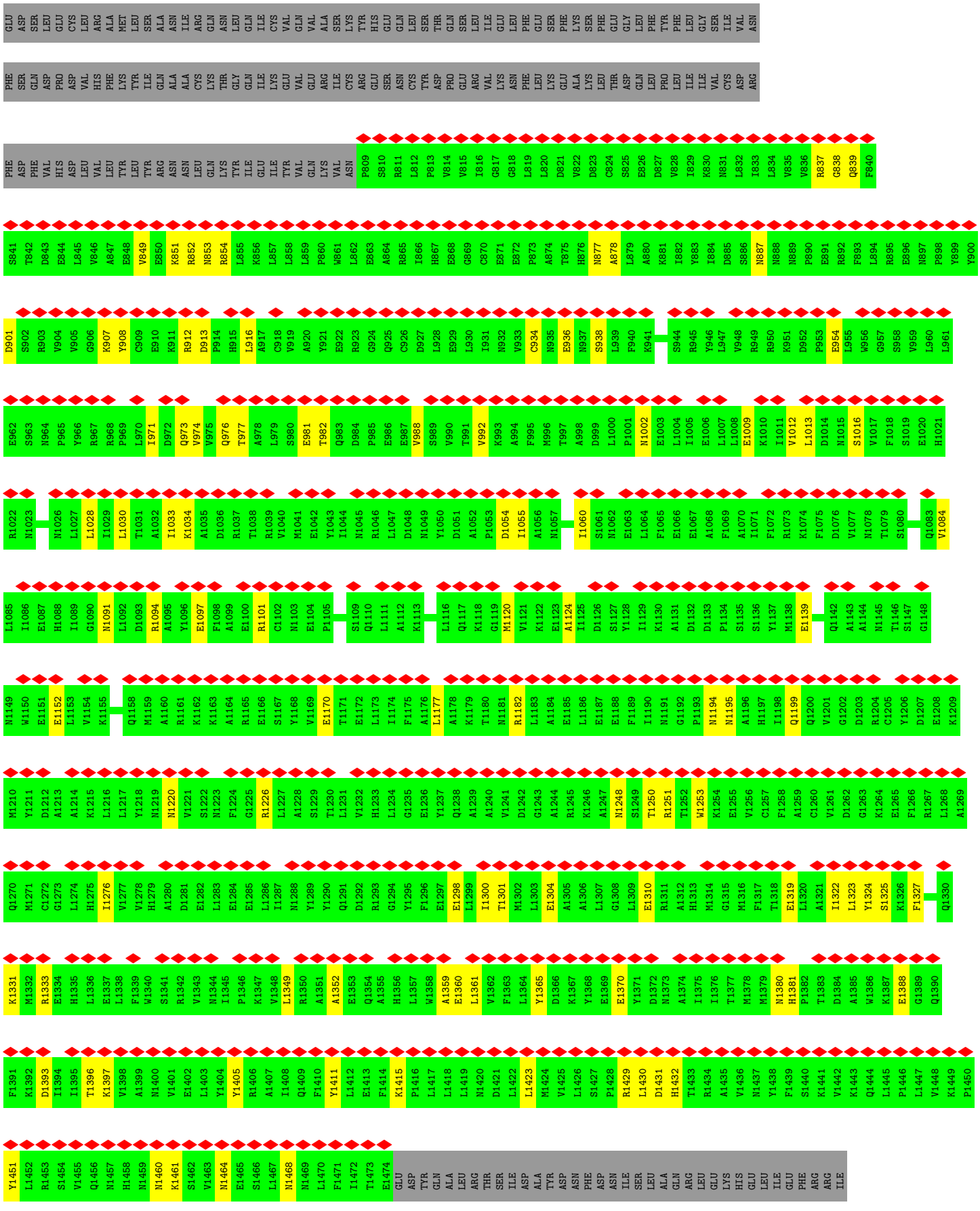
ARG ALA ASN VAL PRO ASN LYS VAL ILE GLN CYS PHE ALA GLU THR GLY GLN VAL GLN LYS ILE VAL LEU TYR ALA LYS LYS VAL GLY TYR THR PRO ASP TRP ILE PHE LEU LEU ARG ASN VAL MET ARG ILE SER PRO ASP GLN GLY GLN GLN PHE ALA GLN MET LEU VAL GLN ASP GLU
GLU PRO LEU ALA ASP ILE THR GLN ILE VAL ASP VAL PHE MET GLU TYR 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 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 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 CYS LEU ARG ALA MET LEU SER ALA ASN ILE ARG GLN ASN LEU GLN ILE CYS VAL GLN VAL ALA SER LYS TYR HIS GLU GLN LEU SER THR GLN SER LEU ILE GLU LEU PHE GLU SER PHE LYS SER PHE GLY 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 ILE VAL CYS 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 P809 S810 R811 L812 P813 V814 V815 I816 G817 G818 L819 L820 D821 V822 D823 C824 S825 E826 D827 V828 I829 K830 N831 L832 I833 L834 V835 V836 R837 G838 Q839 F840
S841 T842 D843 E844 L845 V846 A847 E848 V849 E850 K851 R852 N853 R854 L855 K856 L857 L858 L859 P860 W861 L862 E863 A864 R865 I866 H867 E868 G869 C870 E871 E872 P873 A874 T875 H876 N877 A878 L879 A880 K881 I882 Y883 I884 D885 S886 N887 N888 N889 P890 E891 R892 F893 L894 R895 E896 N897 P898 Y899 Y900
D901 S902 R903 V904 V905 G906 K907 Y908 C909 E910 K911 R912 D913 P914 H915 L916 A917 C918 V919 A920 Y921 E922 R923 G924 Q925 C926 D927 L928 E929 L930 I931 N932 V933 C934 N935 E936 N937 S938 L939 F940 K941 S944 R945 Y946 L947 V948 R949 R950 K951 D952 P953 E954 L955 W956 G957 S958 V959 L960 L961
E962 S963 N964 P965 Y966 R967 R968 P969 L970 I971 D972 Q973 V974 V975 Q976 T977 A978 L979 S980 E981 T982 Q983 D984 P985 E986 E987 V988 S989 V990 T991 V992 K993 A994 F995 M996 T997 A998 D999 L1000 P1001 N1002 E1003 L1004 I1005 E1006 L1007 L1008 E1009 K1010 I1011 V1012 L1013 D1014 N1015 S1016 V1017 F1018 S1019 E1020 H1021
R1022 N1023 N1026 L1027 L1028 I1029 L1030 T1031 A1032 I1033 K1034 A1035 D1036 R1037 T1038 R1039 E1042 N1045 R1046 L1047 D1048 N1049 Y1050 D1051 A1052 P1053 D1054 I1055 A1056 N1057 I1060 S1061 N1062 E1063 L1064 F1065 E1066 E1067 A1068 F1069 A1070 I1071 F1072 R1073 K1074 F1075 D1076 V1077 N1078 T1079 S1080 Q1083 V1084 L1085 I1086
E1087 H1088 I1089 G1090 N1091 L1092 D1093 R1094 A1095 Y1096 E1097 F1098 A1099 E1100 R1101 C1102 N1103 E1104 P1105 W1108 S1109 Q1110 L1111 A1112 K1113 L1116 Q1117 K1118 G1119 M1120 V1121 K1122 E1123 A1124 I1125 D1126 S1127 Y1128 I1129 K1130 A1131 D1132 D1133 P1134 S1135 S1136 Y1137 M1138 E1139 Q1142 A1143 A1144 N1145 T1146 S1147 G1148 N1149
W1150 E1151 E1152 L1153 V1154 K1155 Y1156 L1157 Q1158 M1159 A1160 R1161 K1162 K1163 A1164 R1165 E1166 S1167 Y1168 V1169 E1170 T1171 E1172 L1173 I1174 F1175 A1176 L1177 A1178 K1179 T1180 N1181 R1182 L1183 A1184 E1185 L1186 E1187 E1188 F1189 I1190 N1191 G1192 P1193 N1194 N1195 A1196 H1197 I1198 Q1199 Q1200 V1201 G1202 D1203 R1204 C1205 Y1206 D1207 E1208 K1209
M1210 Y1211 D1212 A1213 A1214 K1215 L1216 L1217 Y1218 N1219 N1220 V1221 S1222 N1223 F1224 G1225 R1226 L1227 A1228 S1229 T1230 L1231 V1232 H1233 L1234 G1235 E1236 Y1237 Q1238 A1239 A1240 V1241 D1242 G1243 A1244 R1245 K1246 A1247 N1248 S1249 T1250 R1251 T1252 W1253 K1254 E1255 V1256 C1257 F1258 A1259 C1260 V1261 D1262 G1263 K1264 E1265 F1266 R1267 L1268 A1269
Q1270 M1271 C1272 G1273 L1274 H1275 I1276 V1277 V1278 H1279 A1280 D1281 E1282 L1283 E1284 E1285 L1286 I1287 N1288 Y1289 Y1290 Q1291 D1292 R1293 G1294 Y1295 F1296 E1297 E1298 L1299 I1300 T1301 M1302 L1303 E1304 A1305 A1306 L1307 G1308 L1309 E1310 R1311 A1312 H1313 M1314 G1315 M1316 F1317 T1318 E1319 L1320 A1321 I1322 L1323 Y1324 S1325 K1326 F1327 Q1330



- Molecule 1: Clathrin heavy chain

Chain L:

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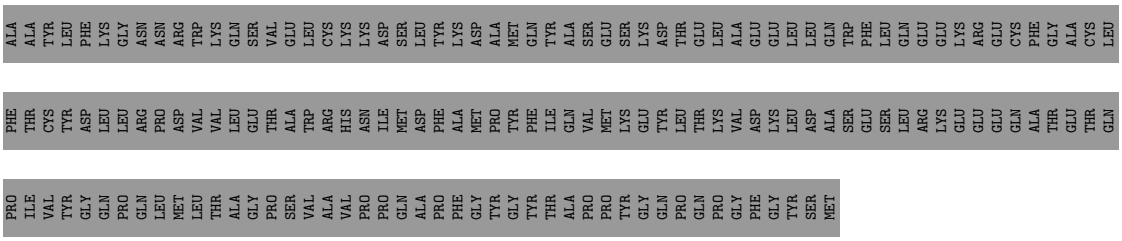
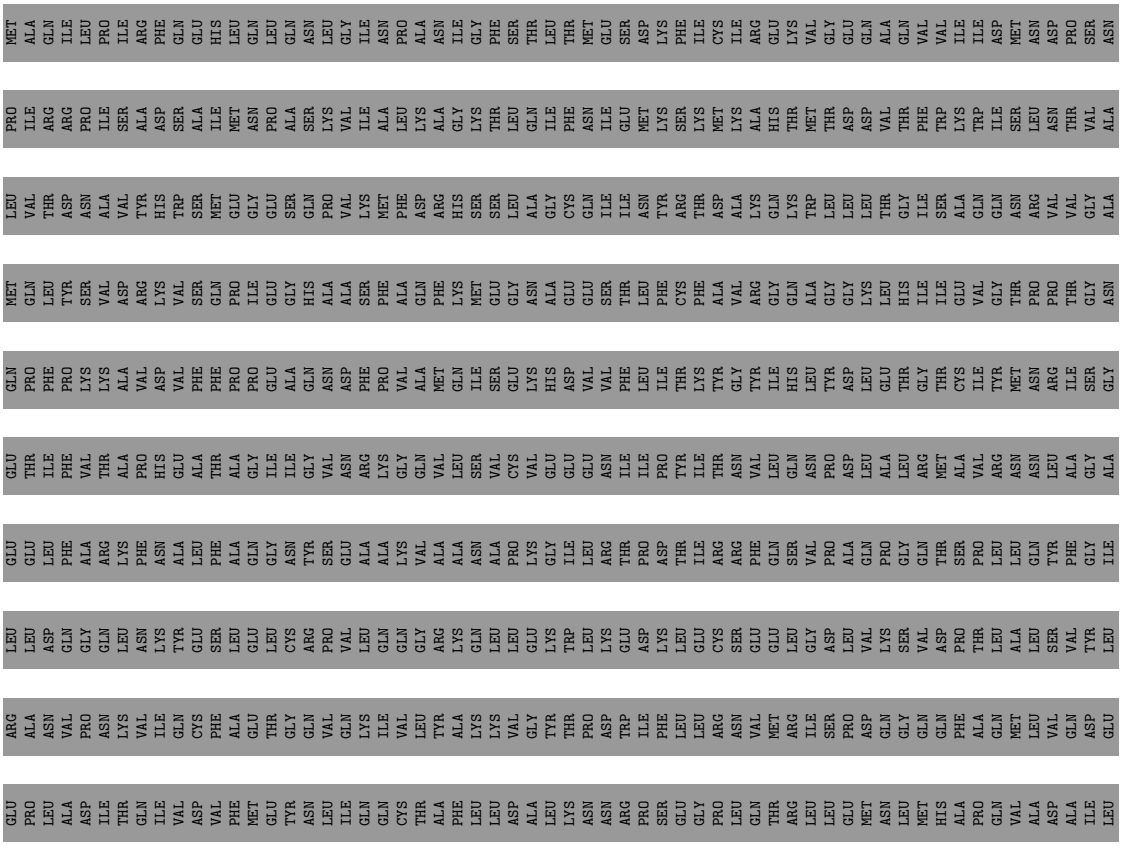
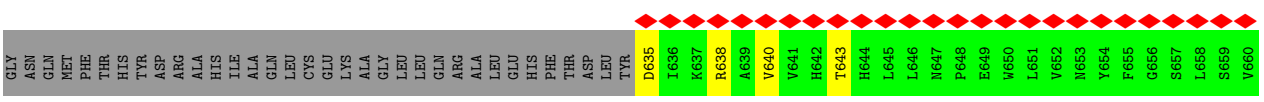
PHE SER GLN ASP PRO ASP VAL HIS PHE LYS TYR ILE GLN ALA ALA CYS LYS LYS THR GLY GLN ILE LYS GLU VAL GLU ARG ILE CYS ARG GLU SER ASN CYS TYR ASP PRO GLU ARG VAL LYS ASN PHE LEU LYS GLU ALA LYS LEU THR ASP GLN LEU PRO LEU ILE ILE VAL CYS ASP ARG
PHE ASP PHE VAL HIS ASP LEU VAL LEU TYR LEU TYR ARG ASN ASN LEU GLN LYS TYR ILE GLU ILE TYR VAL GLN LYS VAL ASN P809 S810 R811 L812 P813 V814 V815 I816 G817 G818 L819 L820 D821 V822 D823 C824 S825 E826 D827 V828 I829 K830 N831 L832 I833 L834 V835 V836 R837 G838 Q839 F840
S841 T842 D843 E844 L845 V846 A847 E848 V849 E850 K851 R852 N853 R854 L855 K856 L857 L858 L859 P860 W861 L862 E863 A864 R865 I866 H867 E868 G869 C870 E871 E872 P873 A874 T875 H876 N877 A878 L879 A880 K881 I882 Y883 I884 D885 S886 N887 M888 N889 P890 E891 R892 F893 L894 R895 E896 N897 P898 Y899 Y900
D901 S902 R903 V904 V905 G906 K907 Y908 C909 E910 K911 R912 D913 P914 H915 L916 A917 C918 V919 A920 Y921 E922 R923 G924 Q925 C926 D927 L928 E929 L930 I931 N932 V933 C934 N935 E936 N937 S938 L939 F940 K941 S944 R945 Y946 L947 V948 R949 R950 K951 D952 P953 E954 L955 W956 G957 S958 V959 L960 L961
E962 S963 N964 P965 Y966 R967 R968 P969 L970 I971 D972 Q973 V974 V975 Q976 T977 A978 L979 S980 E981 T982 Q983 D984 P985 E986 E987 V988 S989 V990 T991 V992 K993 A994 F995 M996 T997 A998 D999 L1000 P1001 N1002 E1003 L1004 I1005 E1006 L1007 L1008 E1009 K1010 I1011 V1012 L1013 D1014 N1015 S1016 V1017 F1018 S1019 E1020 H1021
R1022 N1023 N1026 L1027 L1028 I1029 L1030 T1031 A1032 I1033 K1034 A1035 D1036 R1037 T1038 R1039 V1040 M1041 E1042 Y1043 I1044 N1045 R1046 L1047 D1048 N1049 Y1050 D1051 A1052 P1053 D1054 I1055 A1056 N1057 I1060 S1061 N1062 E1063 L1064 F1065 E1066 E1067 A1068 F1069 A1070 I1071 F1072 R1073 K1074 F1075 D1076 V1077 N1078 T1079 S1080 Q1083 V1084
L1085 I1086 E1087 H1088 I1089 G1090 N1091 L1092 D1093 R1094 K1095 Y1096 E1097 F1098 A1099 E1100 R1101 C1102 N1103 E1104 P1105 S1109 Q1110 L1111 A1112 K1113 L1116 Q1117 K1118 G1119 M1120 V1121 K1122 E1123 A1124 I1125 D1126 S1127 Y1128 I1129 K1130 A1131 D1132 D1133 P1134 S1135 S1136 Y1137 M1138 E1139 Q1142 A1143 A1144 N1145 T1146 S1147 G1148
N1149 W1150 E1151 E1152 L1153 V1154 K1155 Q1158 M1159 A1160 R1161 K1162 K1163 A1164 R1165 E1166 S1167 Y1168 V1169 E1170 T1171 E1172 L1173 I1174 F1175 A1176 L1177 A1178 K1179 T1180 N1181 R1182 L1183 A1184 E1185 L1186 E1187 E1188 F1189 I1190 N1191 G1192 P1193 N1194 N1195 A1196 H1197 I1198 Q1199 Q1200 V1201 G1202 D1203 R1204 C1205 Y1206 D1207 E1208 K1209
M1210 Y1211 D1212 A1213 A1214 K1215 L1216 L1217 Y1218 N1219 N1220 V1221 S1222 N1223 F1224 G1225 R1226 L1227 A1228 S1229 T1230 L1231 V1232 H1233 L1234 G1235 E1236 Y1237 Q1238 A1239 A1240 V1241 D1242 G1243 A1244 R1245 K1246 A1247 N1248 S1249 T1250 R1251 T1252 W1253 K1254 E1255 V1256 C1257 F1258 A1259 C1260 V1261 D1262 G1263 K1264 E1265 F1266 R1267 L1268 A1269
Q1270 M1271 C1272 G1273 L1274 H1275 I1276 V1277 V1278 H1279 A1280 D1281 E1282 L1283 E1284 E1285 L1286 I1287 N1288 Y1289 Y1290 Q1291 D1292 R1293 G1294 Y1295 F1296 E1297 E1298 L1299 I1300 T1301 M1302 L1303 E1304 A1305 A1306 L1307 G1308 L1309 E1310 R1311 A1312 H1313 M1314 G1315 M1316 F1317 T1318 E1319 L1320 A1321 I1322 L1323 Y1324 S1325 K1326 F1327 Q1330
K1331 M1332 R1333 E1334 H1335 L1336 E1337 L1338 F1339 W1340 S1341 R1342 V1343 N1344 I1345 P1346 K1347 V1348 L1349 R1350 A1351 A1352 E1353 Q1354 A1355 H1356 L1357 W1358 A1359 E1360 L1361 V1362 F1363 L1364 Y1365 D1366 K1367 Y1368 E1369 E1370 Y1371 D1372 N1373 A1374 I1375 I1376 T1377 M1378 M1379 N1380 H1381 P1382 T1383 D1384 A1385 W1386 K1387 E1388 G1389 Q1390
F1391 K1392 D1393 I1394 I1395 T1396 K1397 V1398 A1399 N1400 V1401 E1402 L1403 Y1404 Y1405 R1406 A1407 I1408 Q1409 F1410 Y1411 L1412 E1413 F1414 K1415 P1416 L1417 L1418 L1419 N1420 D1421 D1422 L1423 M1424 V1425 L1426 S1427 P1428 R1429 L1430 D1431 H1432 T1433 R1434 A1435 V1436 N1437 Y1438 F1439 S1440 K1441 V1442 K1443 Q1444 L1445 P1446 L1447 V1448 K1449 P1450
Y1451 L1452 R1453 S1454 V1455 Q1456 N1457 H1458 N1459 N1460 K1461 S1462 V1463 N1464 E1465 S1466 L1467 L1468 N1469 L1470 F1471 I1472 T1473 E1474 GLU ASP TYR GLN ALA LEU ARG THR SER ILE ASP ALA TYR ASP ASN PHE ASP ASN ILE SER LEU ALA GLN ARG LEU GLU LYS HIS GLU LEU ILE GLU PHE ARG ARG ILE

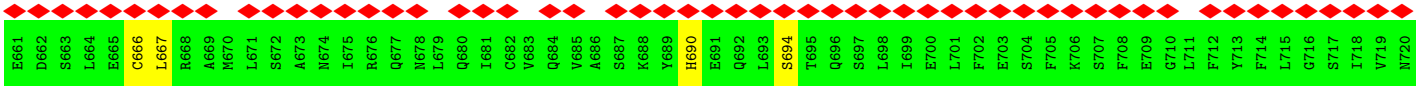


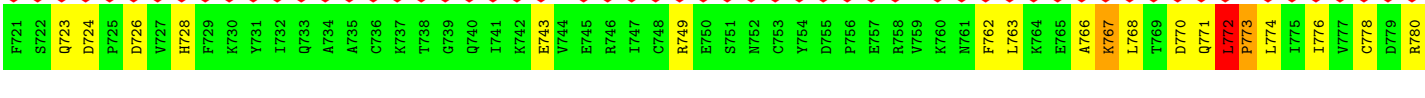
• Molecule 1: Clathrin heavy chain

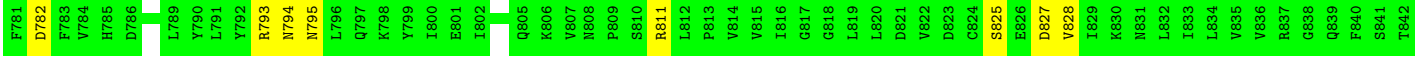
Chain H:

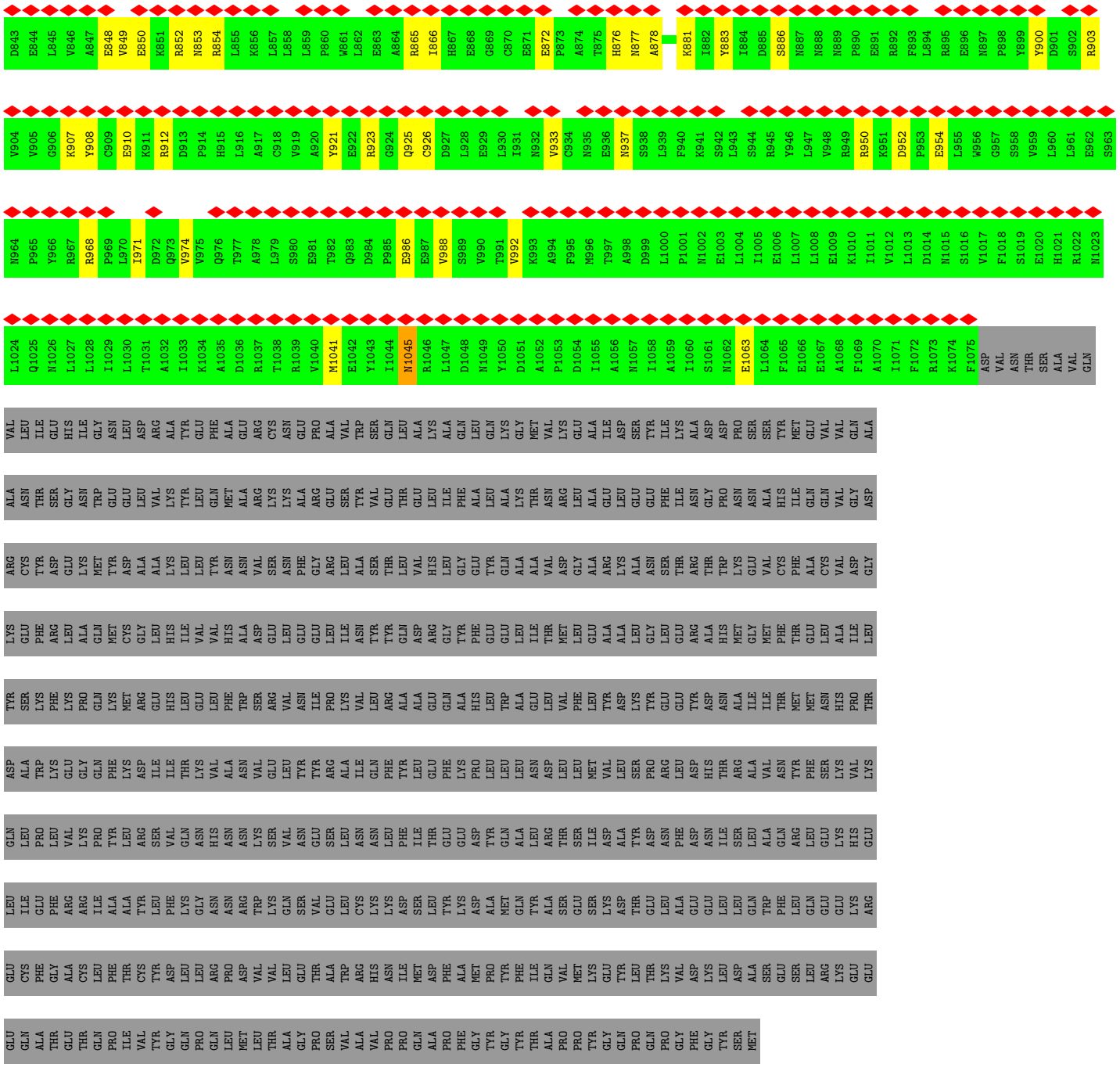






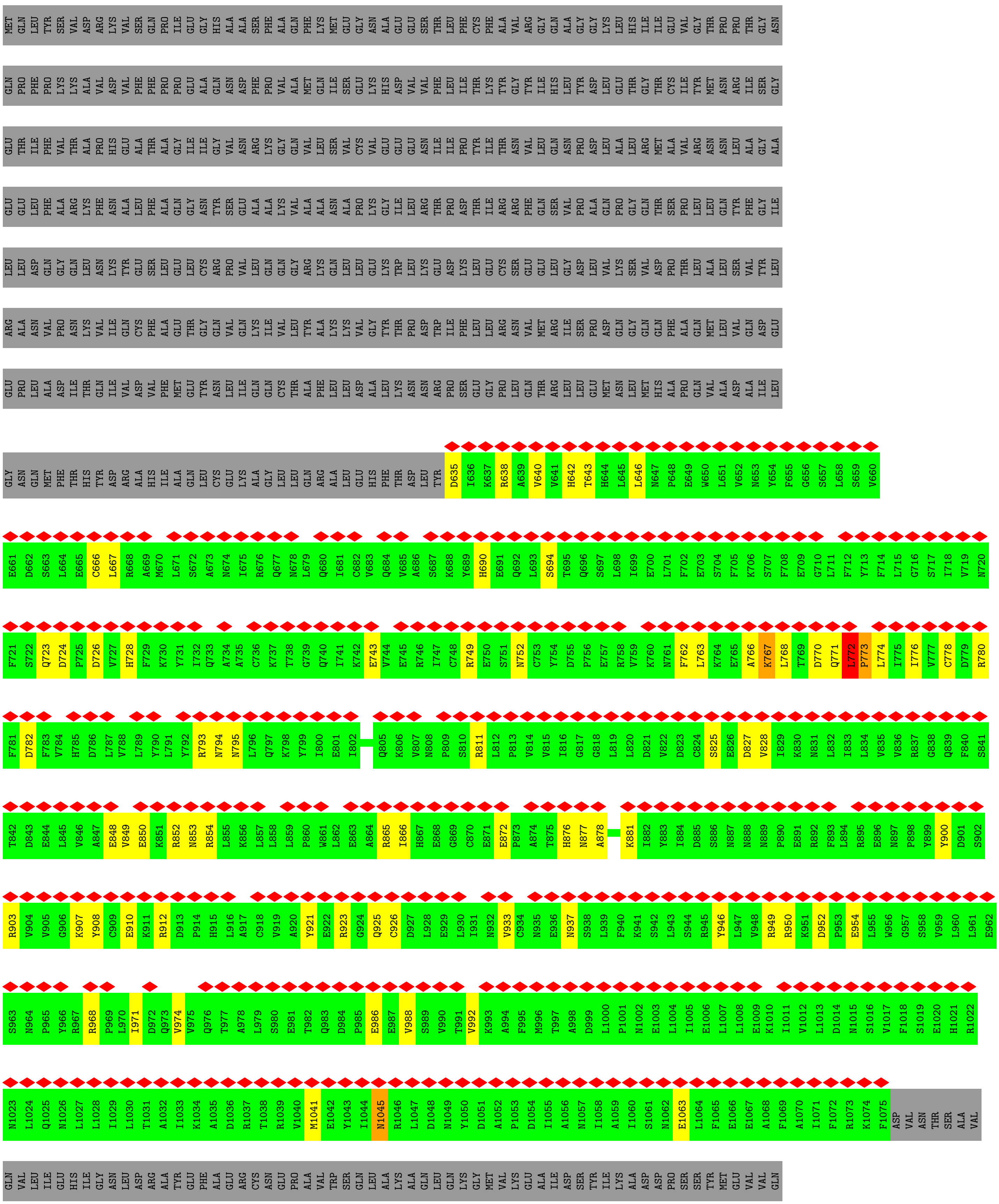


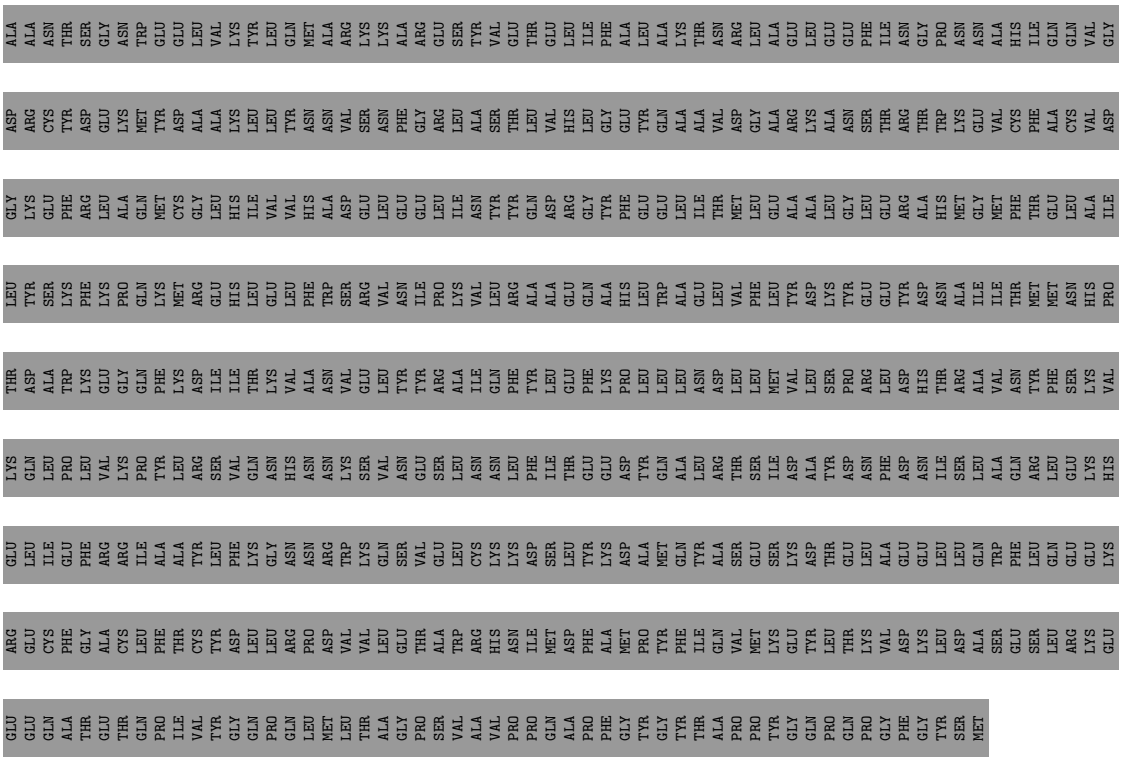




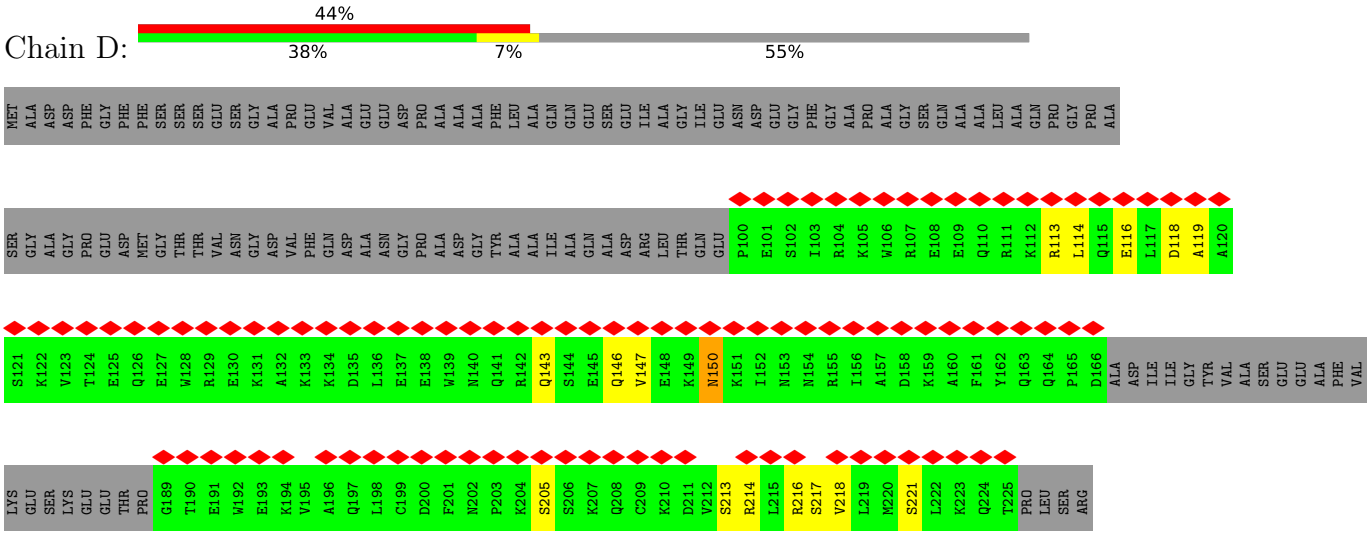
- Molecule 1: Clathrin heavy chain

Chain M:

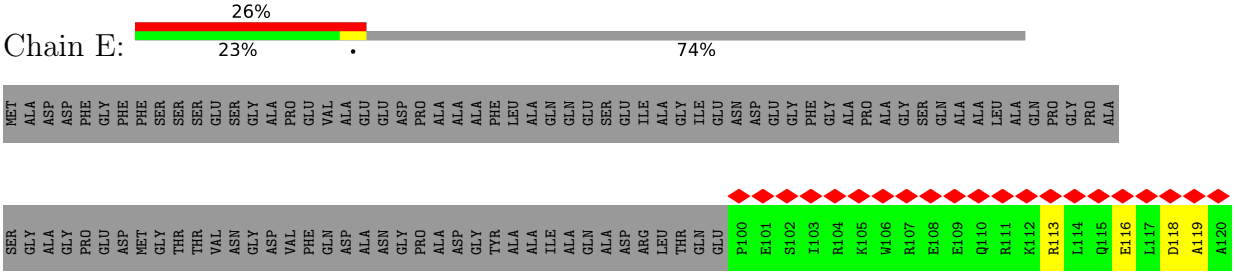

MET GLN LEU TYR SER VAL ASP ARG LYS VAL SER GLN PRO ILE GLU GLY HIS ALA ALA SER PHE ALA GLN PHE LYS MET GLU GLY ASN ALA GLU GLU SER THR LEU PHE CYS PHE ALA VAL ARG GLY GLN ALA GLY LYS LEU HIS ILE ILE GLU VAL GLY THR PRO PRO THR GLY ASN
GLN PRO PHE PRO LYS LYS ALA VAL ASP VAL PHE PHE PRO PRO GLU ALA GLN 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 SER VAL CYS VAL GLU GLU GLU ASN ILE ILE PRO TYR ILE THR ASN VAL LEU GLN ASN PRO ASP LEU ALA LEU ARG MET ALA VAL ARG ASN ASN LEU ALA GLY ALA
GLU GLU LEU PHE ALA ARG LYS PHE ASN ALA LEU PHE ALA GLN GLY ASN TYR SER GLU 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 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 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 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 VAL ASP VAL 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 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 D635 I636 K637 R638 A639 V640 V641 H642 T643 H644 L645 L646 N647 P648 E649 W650 L651 V652 N653 Y654 F655 G656 S657 L658 S659 V660
E661 D662 S663 L664 E665 C666 L667 R668 A669 M670 L671 S672 A673 N674 I675 R676 Q677 N678 L679 Q680 I681 C682 V683 Q684 V685 A686 S687 K688 Y689 H690 E691 Q692 L693 S694 T695 Q696 S697 L698 I699 E700 L701 F702 E703 S704 F705 K706 S707 F708 E709 G710 L711 F712 Y713 F714 L715 G716 S717 I718 V719 N720
F721 S722 Q723 D724 P725 D726 V727 H728 F729 K730 Y731 I732 Q733 A734 A735 C736 K737 T738 G739 Q740 I741 K742 E743 V744 E745 R746 I747 C748 R749 E750 S751 N752 C753 Y754 D755 P756 E757 R758 V759 K760 N761 F762 L763 K764 E765 A766 K767 L768 T769 D770 Q771 L772 P773 L774 I775 I776 V777 C778 D779 R780
F781 D782 F783 V784 H785 D786 L787 V788 L789 Y790 L791 Y792 R793 N794 N795 L796 Q797 K798 Y799 I800 E801 I802 Q805 K806 V807 N808 P809 S810 R811 L812 P813 V814 V815 I816 G817 G818 L819 L820 D821 V822 D823 C824 S825 E826 D827 V828 I829 K830 N831 L832 I833 L834 V835 V836 R837 G838 Q839 F840 S841
T842 D843 E844 L845 V846 A847 E848 V849 E850 K851 R852 N853 R854 L855 K856 L857 L858 L859 P860 W861 L862 E863 A864 R865 I866 H867 E868 G869 C870 E871 E872 P873 A874 T875 H876 N877 A878 K881 I882 Y883 I884 D885 S886 N887 N888 N889 P890 E891 R892 F893 L894 R895 E896 N897 P898 Y899 Y900 D901 S902
R903 V904 V905 G906 K907 Y908 C909 E910 K911 R912 D913 P914 H915 L916 A917 C918 V919 A920 Y921 E922 R923 G924 Q925 C926 D927 L928 E929 L930 I931 N932 V933 C934 N935 E936 N937 S938 L939 F940 K941 S942 L943 S944 R945 Y946 L947 V948 R949 R950 K951 D952 P953 E954 L955 W956 G957 S958 V959 L960 L961 E962
S963 N964 P965 Y966 R967 R968 P969 L970 I971 D972 Q973 V974 V975 Q976 T977 A978 L979 S980 E981 T982 Q983 D984 P985 E986 E987 V988 S989 V990 T991 V992 K993 A994 F995 M996 T997 A998 D999 L1000 P1001 N1002 E1003 L1004 I1005 E1006 L1007 L1008 E1009 K1010 I1011 V1012 L1013 D1014 N1015 S1016 V1017 F1018 S1019 E1020 H1021 R1022
N1023 L1024 Q1025 N1026 L1027 L1028 I1029 L1030 T1031 A1032 I1033 K1034 A1035 D1036 R1037 T1038 R1039 V1040 M1041 E1042 Y1043 I1044 N1045 R1046 L1047 D1048 N1049 Y1050 D1051 A1052 P1053 D1054 I1055 A1056 N1057 I1058 A1059 I1060 S1061 N1062 E1063 L1064 F1065 E1066 E1067 A1068 F1069 A1070 I1071 F1072 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

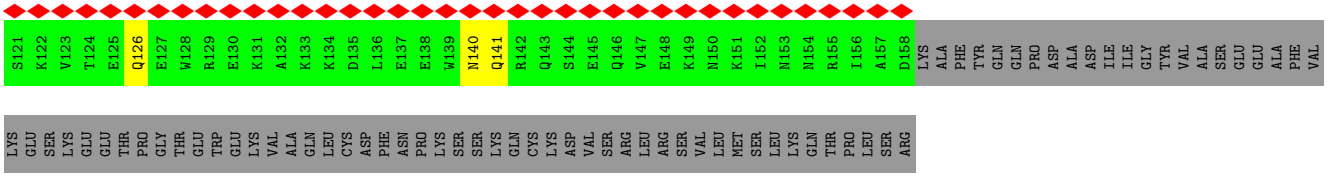


• Molecule 2: Clathrin light chain



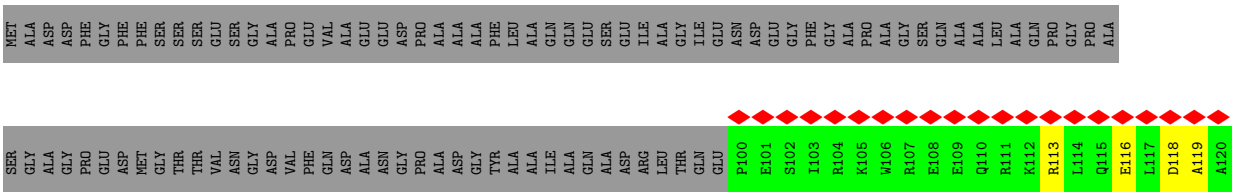
• Molecule 2: Clathrin light chain





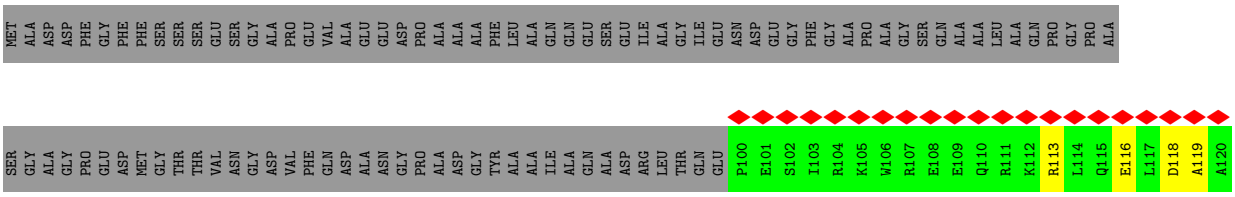
• Molecule 2: Clathrin light chain

Chain J:



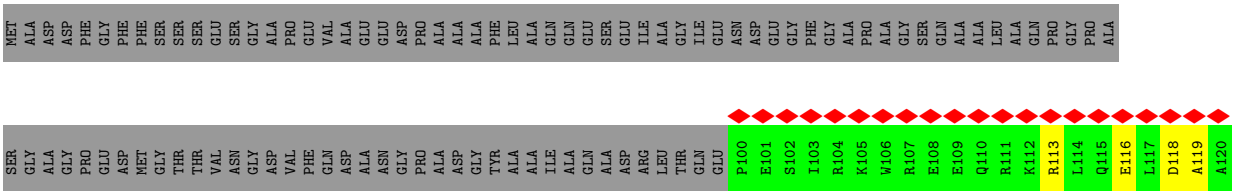
• Molecule 2: Clathrin light chain

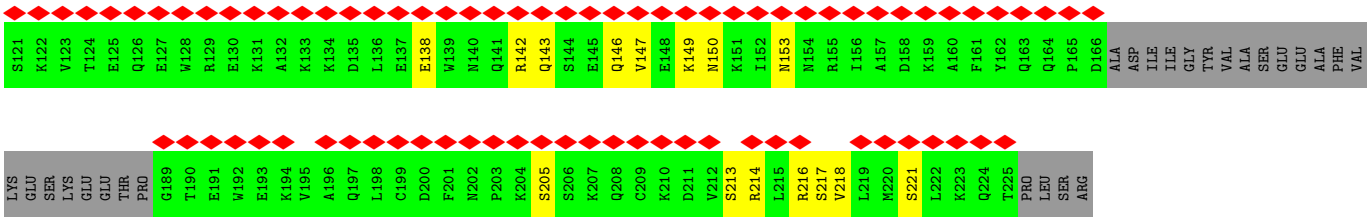
Chain O:



• Molecule 2: Clathrin light chain

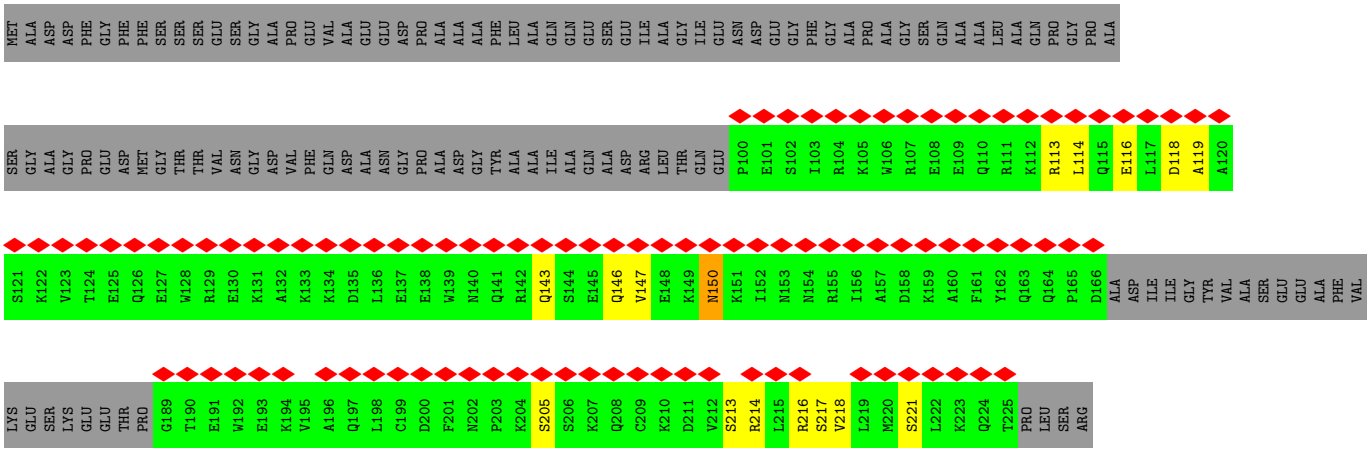
Chain I:





• Molecule 2: Clathrin light chain

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	313406	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 ($e^-/Å^2$)	69	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	82111	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.374	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.195	Depositor
Map size (Å)	436.48, 436.48, 436.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.705, 1.705, 1.705	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	0.30	0/3240	0.50	0/4375
1	B	0.28	0/5513	0.49	0/7468
1	C	0.29	0/3667	0.52	0/4970
1	F	0.30	0/3240	0.50	0/4375
1	G	0.29	0/5513	0.49	0/7468
1	H	0.29	0/3667	0.52	0/4970
1	K	0.30	0/3240	0.50	0/4375
1	L	0.29	0/5513	0.49	0/7468
1	M	0.29	0/3667	0.52	0/4970
2	D	0.28	0/887	0.51	0/1183
2	E	0.27	0/520	0.57	0/692
2	I	0.28	0/887	0.51	0/1183
2	J	0.28	0/520	0.56	0/692
2	N	0.28	0/887	0.51	0/1183
2	O	0.28	0/520	0.56	0/692
All	All	0.29	0/41481	0.51	0/56064

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	3168	0	3118	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5405	0	5359	61	0
1	C	3598	0	3592	58	0
1	F	3168	0	3118	35	0
1	G	5405	0	5359	65	0
1	H	3598	0	3592	53	0
1	K	3168	0	3118	36	0
1	L	5405	0	5359	65	0
1	M	3598	0	3592	56	0
2	D	875	0	872	8	0
2	E	514	0	508	4	0
2	I	875	0	872	9	0
2	J	514	0	508	5	0
2	N	875	0	872	8	0
2	O	514	0	508	5	0
All	All	40680	0	40347	488	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 488 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:772:LEU:H	1:C:773:PRO:HD2	1.22	1.03
1:H:772:LEU:H	1:H:773:PRO:HD2	1.22	1.00
1:M:772:LEU:H	1:M:773:PRO:HD2	1.22	1.00
1:H:763:LEU:HB3	1:H:768:LEU:HD11	1.46	0.97
1:C:763:LEU:HB3	1:C:768:LEU:HD11	1.46	0.97

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	377/1675 (22%)	351 (93%)	26 (7%)	0	100	100
1	B	664/1675 (40%)	620 (93%)	44 (7%)	0	100	100
1	C	439/1675 (26%)	389 (89%)	48 (11%)	2 (0%)	29	68
1	F	377/1675 (22%)	351 (93%)	26 (7%)	0	100	100
1	G	664/1675 (40%)	620 (93%)	44 (7%)	0	100	100
1	H	439/1675 (26%)	391 (89%)	46 (10%)	2 (0%)	29	68
1	K	377/1675 (22%)	351 (93%)	26 (7%)	0	100	100
1	L	664/1675 (40%)	620 (93%)	44 (7%)	0	100	100
1	M	439/1675 (26%)	389 (89%)	48 (11%)	2 (0%)	29	68
2	D	100/229 (44%)	95 (95%)	5 (5%)	0	100	100
2	E	57/229 (25%)	57 (100%)	0	0	100	100
2	I	100/229 (44%)	95 (95%)	5 (5%)	0	100	100
2	J	57/229 (25%)	57 (100%)	0	0	100	100
2	N	100/229 (44%)	95 (95%)	5 (5%)	0	100	100
2	O	57/229 (25%)	57 (100%)	0	0	100	100
All	All	4911/16449 (30%)	4538 (92%)	367 (8%)	6 (0%)	54	85

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	772	LEU
1	H	772	LEU
1	M	772	LEU
1	C	773	PRO
1	H	773	PRO

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	342/1471 (23%)	341 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	587/1471 (40%)	585 (100%)	2 (0%)	92 95
1	C	405/1471 (28%)	401 (99%)	4 (1%)	76 86
1	F	342/1471 (23%)	341 (100%)	1 (0%)	92 95
1	G	587/1471 (40%)	585 (100%)	2 (0%)	92 95
1	H	405/1471 (28%)	401 (99%)	4 (1%)	76 86
1	K	342/1471 (23%)	341 (100%)	1 (0%)	92 95
1	L	587/1471 (40%)	585 (100%)	2 (0%)	92 95
1	M	405/1471 (28%)	401 (99%)	4 (1%)	76 86
2	D	96/184 (52%)	94 (98%)	2 (2%)	53 72
2	E	55/184 (30%)	55 (100%)	0	100 100
2	I	96/184 (52%)	95 (99%)	1 (1%)	76 86
2	J	55/184 (30%)	55 (100%)	0	100 100
2	N	96/184 (52%)	94 (98%)	2 (2%)	53 72
2	O	55/184 (30%)	55 (100%)	0	100 100
All	All	4455/14343 (31%)	4429 (99%)	26 (1%)	86 92

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	907	LYS
1	H	907	LYS
2	N	150	ASN
1	H	772	LEU
1	H	1045	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	889	ASN
1	M	889	ASN
2	I	150	ASN
2	I	153	ASN

5.3.3 RNA

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.

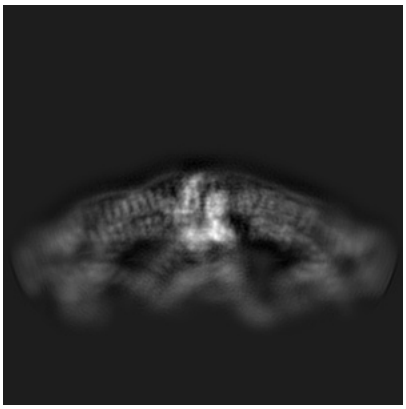
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0126. These allow visual inspection of the internal detail of the map and identification of artifacts.

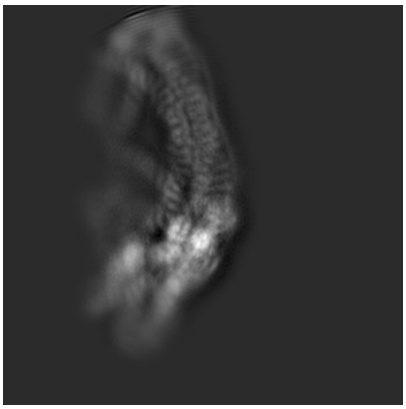
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

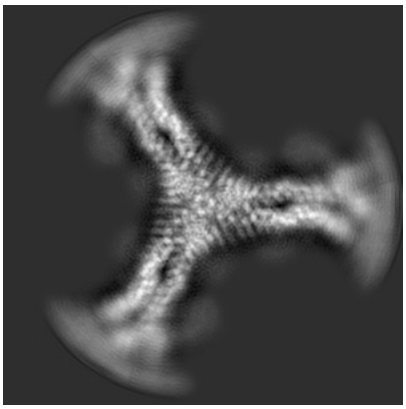
6.1.1 Primary map



X

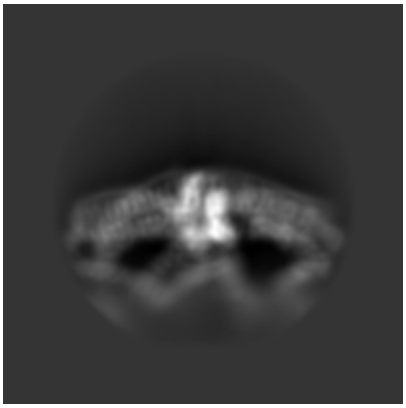


Y

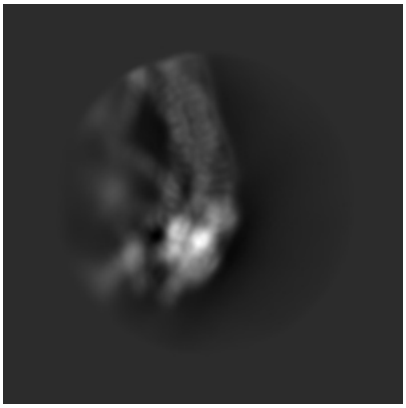


Z

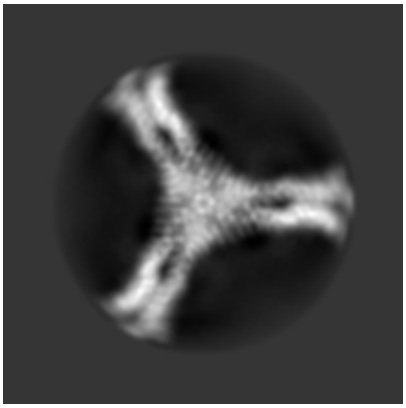
6.1.2 Raw map



X



Y

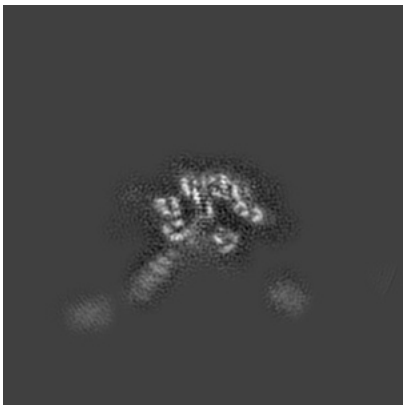


Z

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

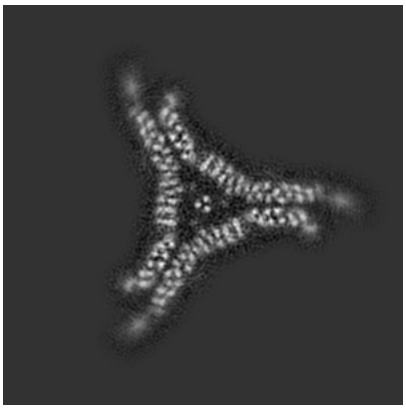
6.2 Central slices (i)

6.2.1 Primary map



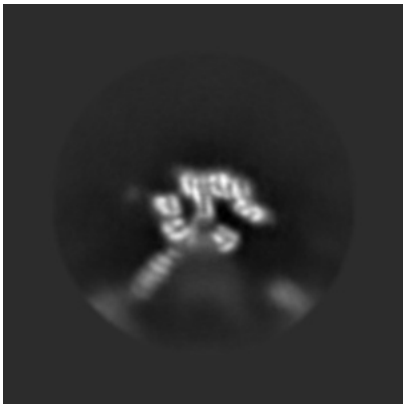
X Index: 128

Y Index: 128

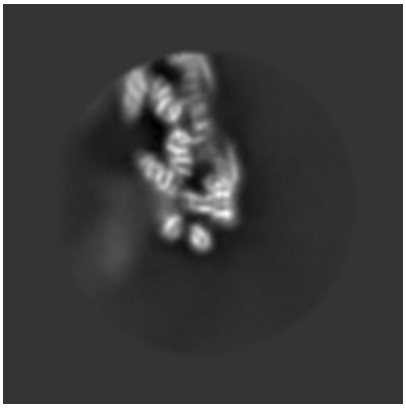


Z Index: 128

6.2.2 Raw map



X Index: 128



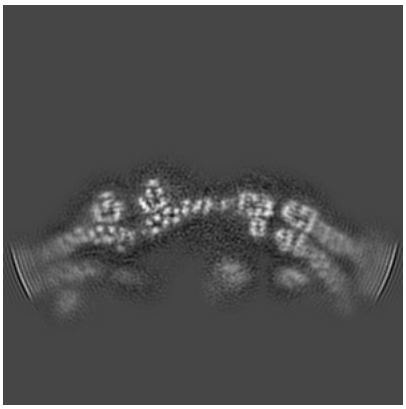
Y Index: 128

Z Index: 128

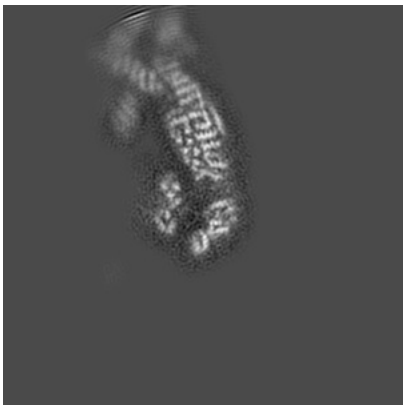
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

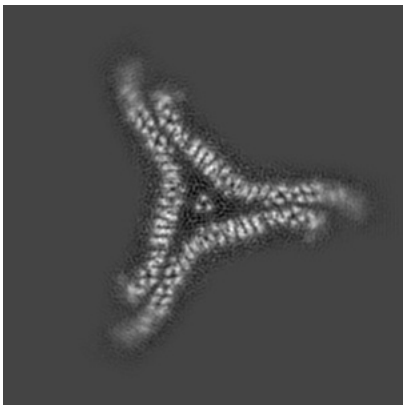
6.3.1 Primary map



X Index: 101



Y Index: 117



Z Index: 124

6.3.2 Raw map

X Index: 100

Y Index: 120

Z Index: 124

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 0.195. 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.

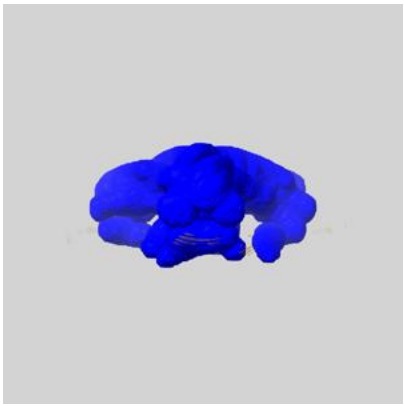
6.5 Mask visualisation (i)

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

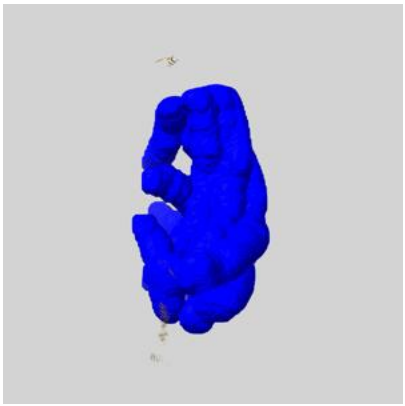
A mask typically either:

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

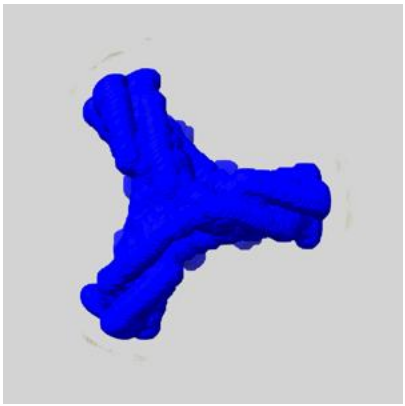
6.5.1 emd_0126_msk_1.map (i)



X



Y

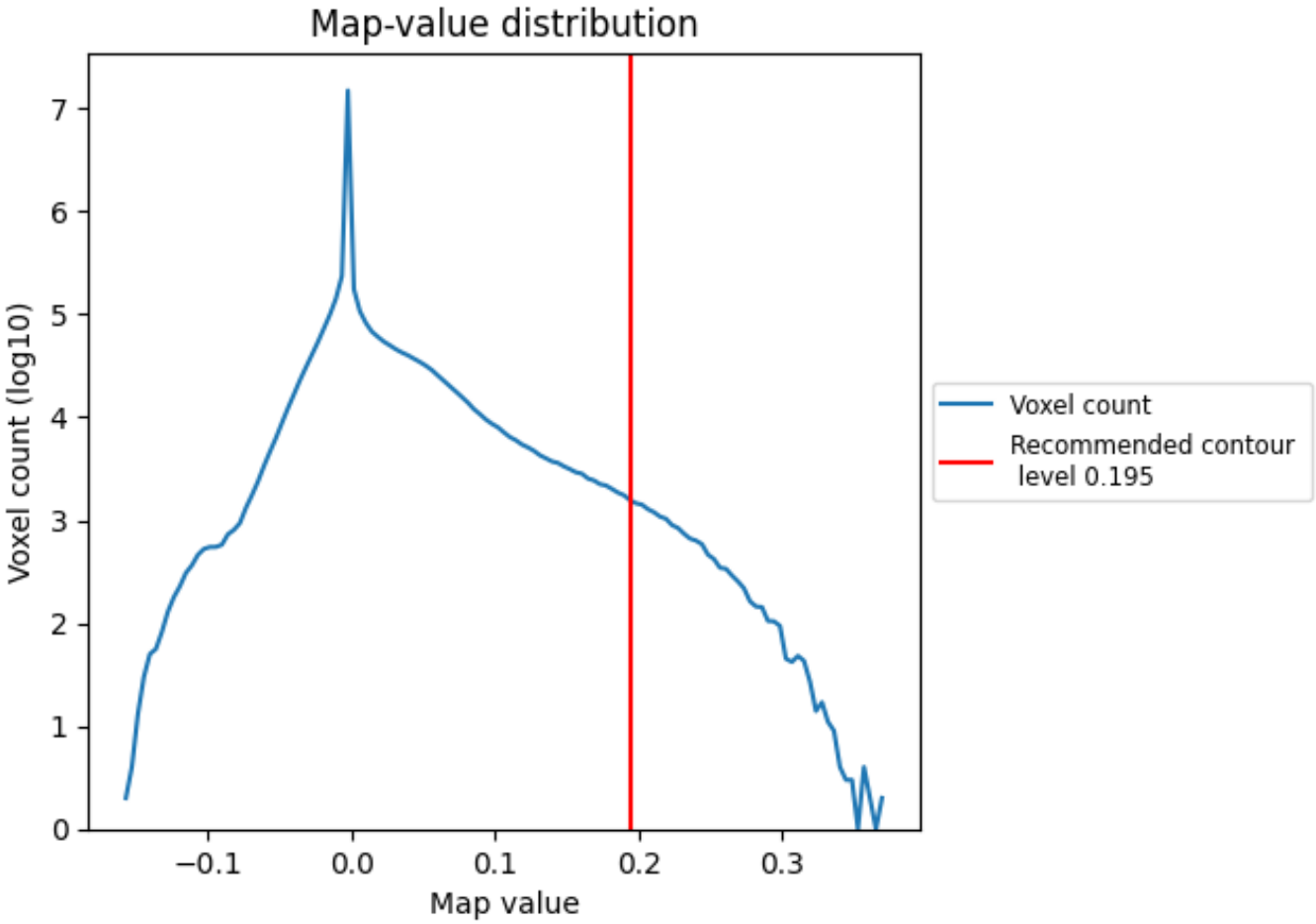


Z

7 Map analysis

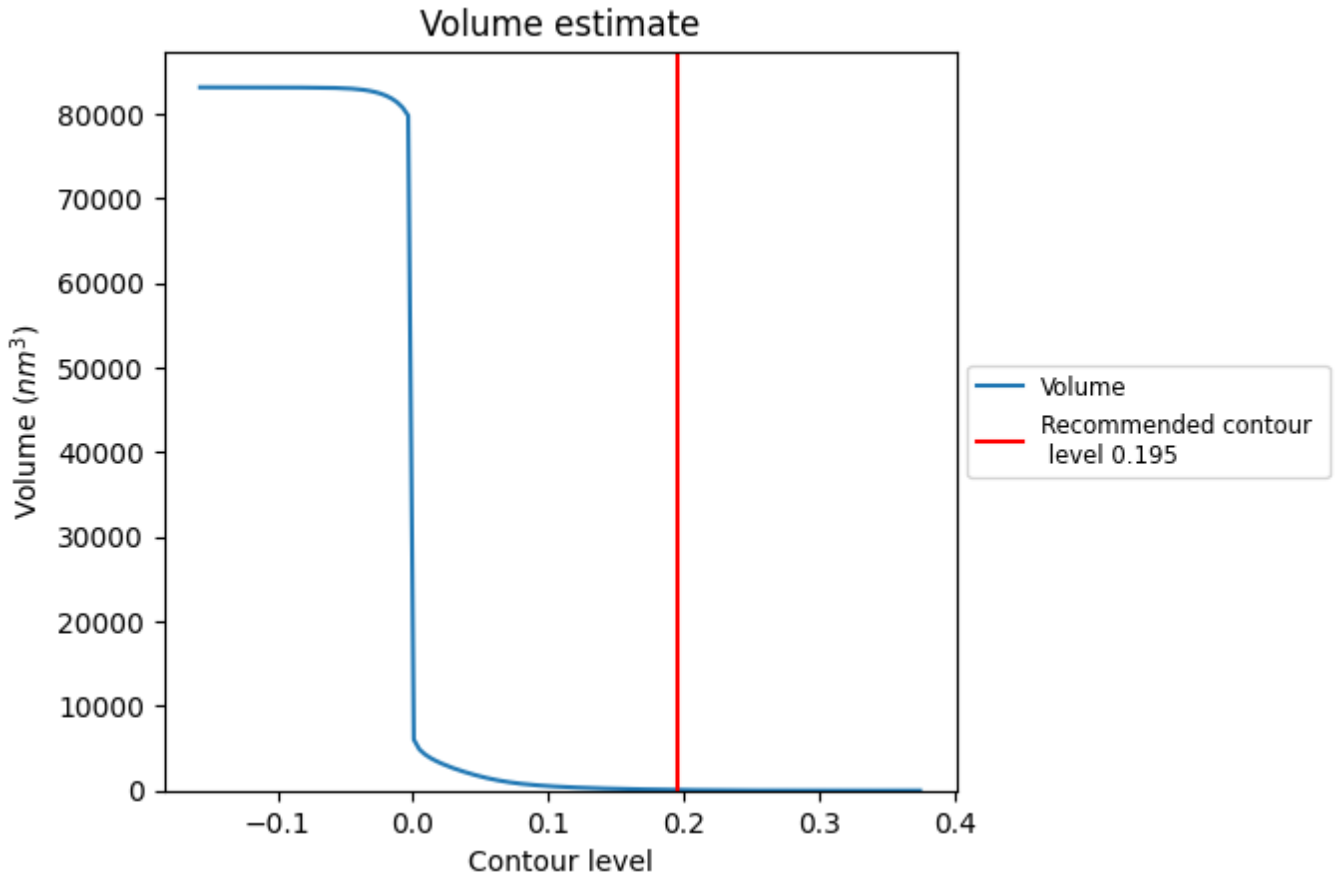
This section contains the results of statistical analysis of the map.

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.

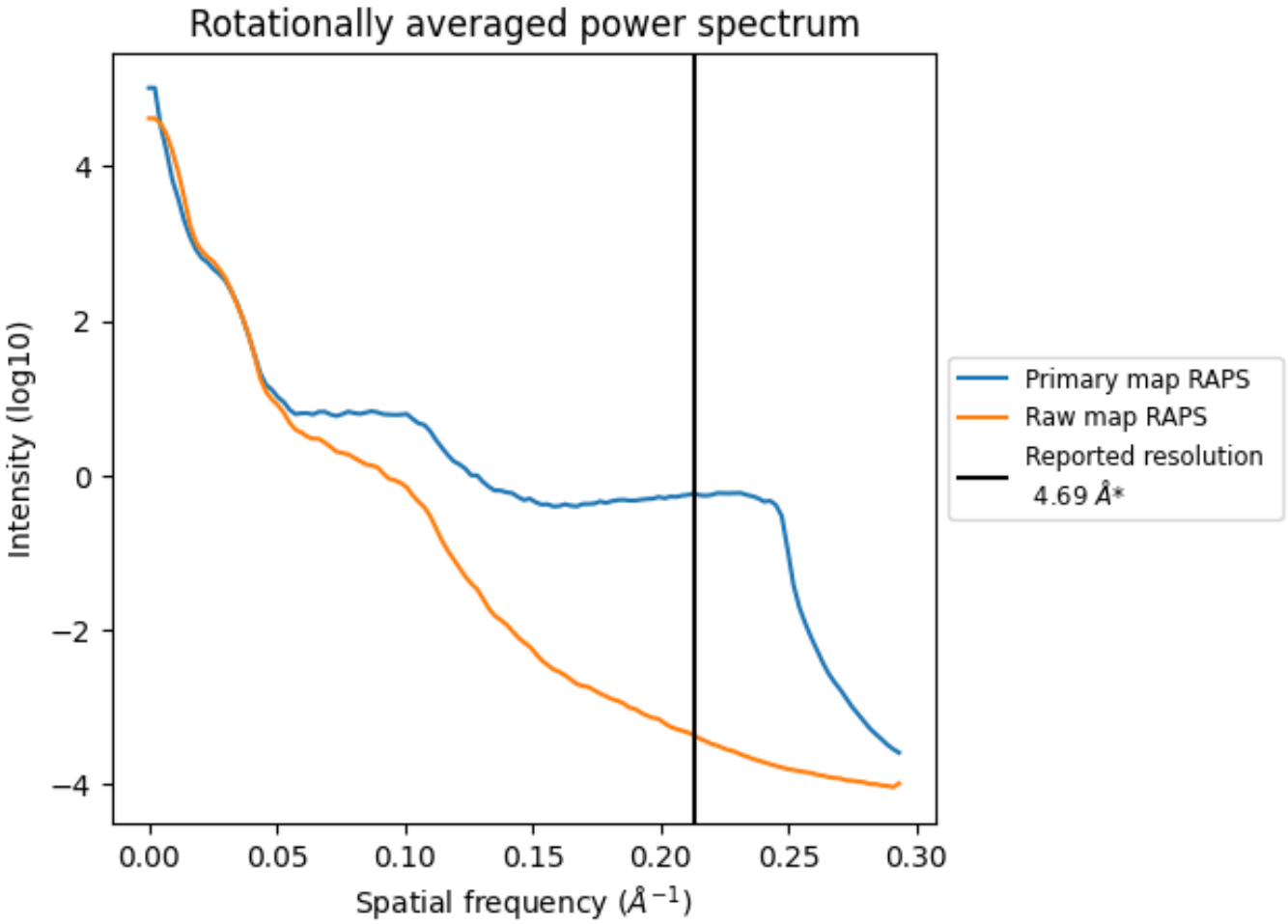
7.2 Volume estimate (i)



The volume at the recommended contour level is 82 nm^3; this corresponds to an approximate mass of 74 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)

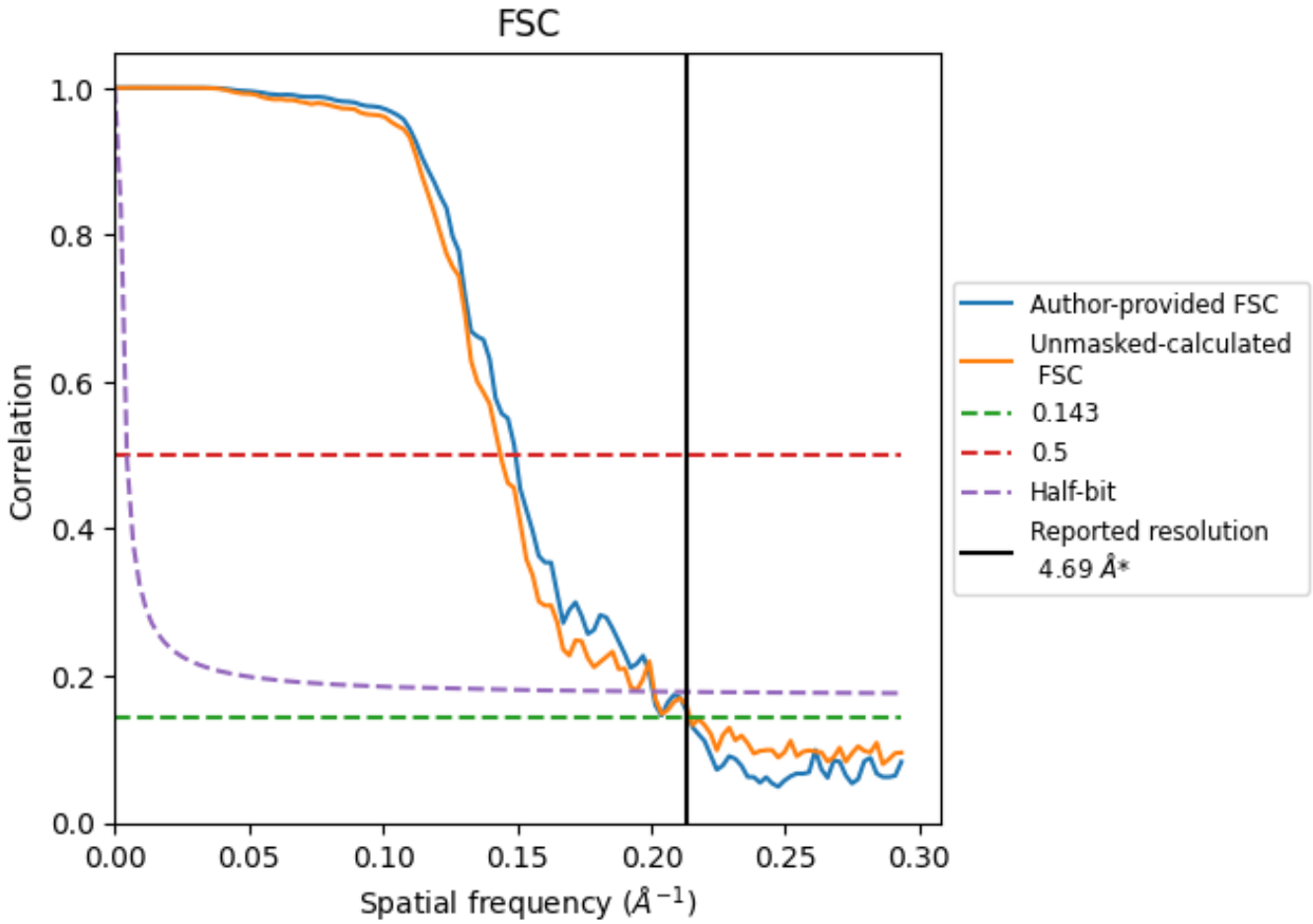


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

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 0.213 Å^{-1}

8.2 Resolution estimates (i)

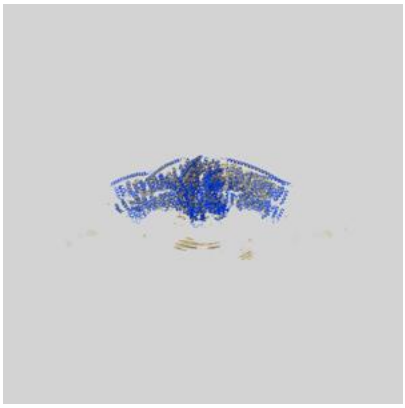
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.69	-	-
Author-provided FSC curve	4.67	6.69	4.98
Unmasked-calculated*	4.66	6.95	4.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

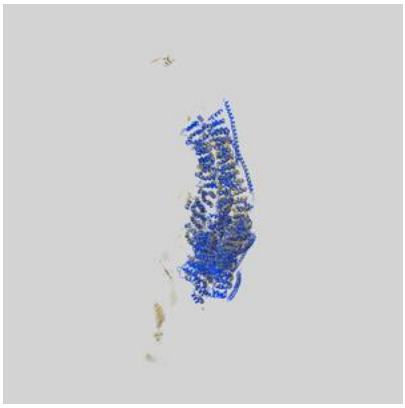
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0126 and PDB model 6SCT. Per-residue inclusion information can be found in section 3 on page 5.

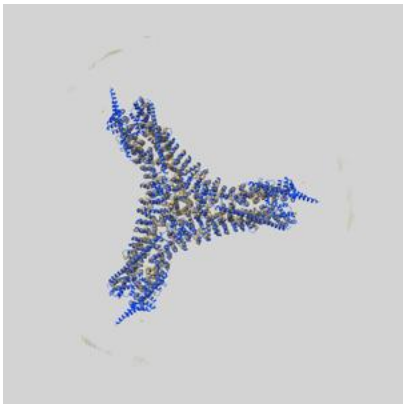
9.1 Map-model overlay



X



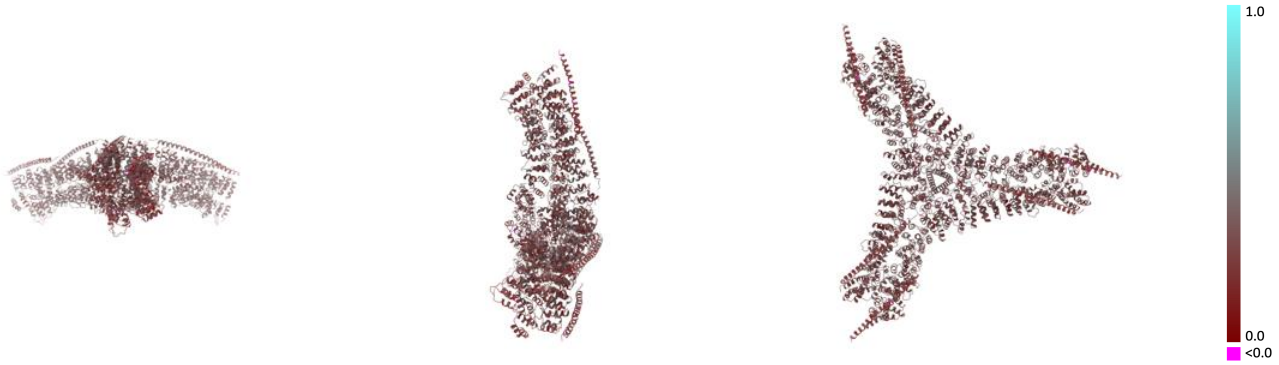
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.195 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.

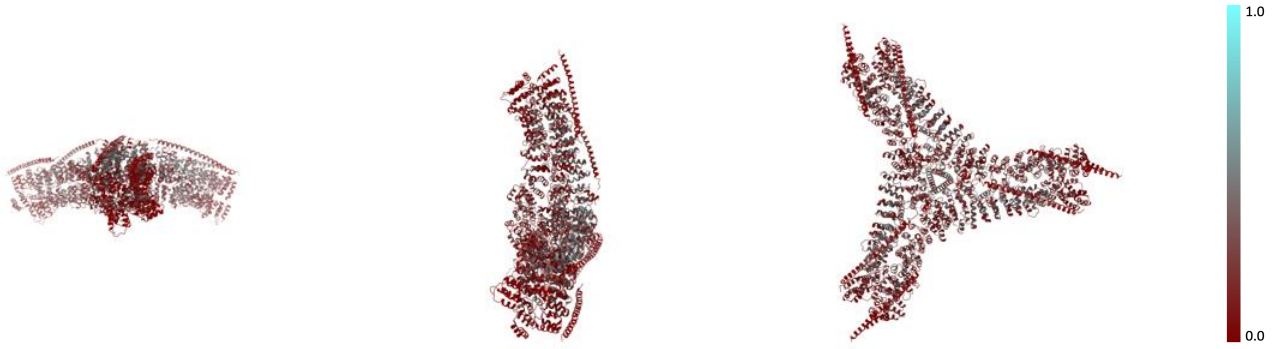
9.2 Q-score mapped to coordinate model (i)



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.

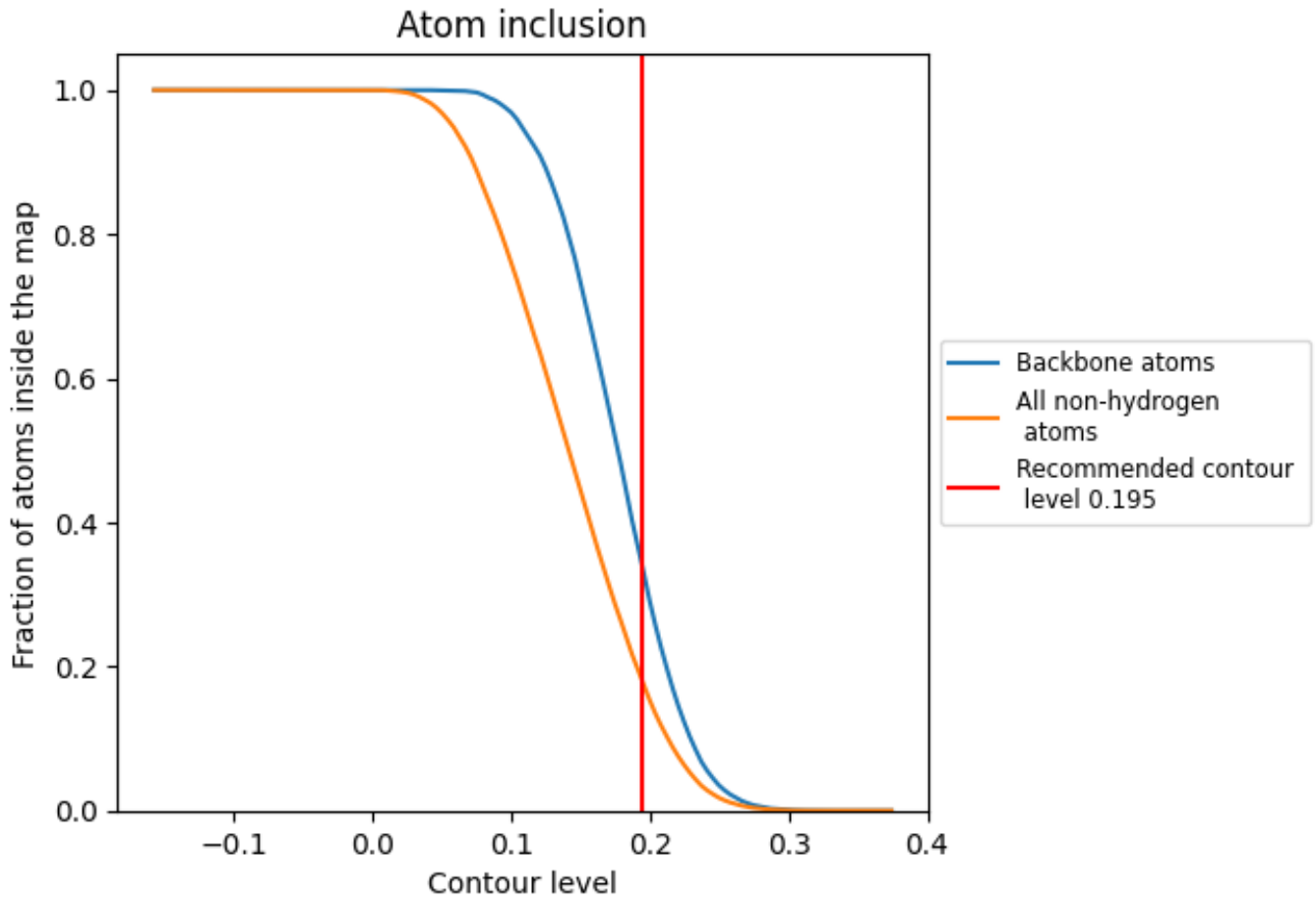
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.195).

9.4 Atom inclusion (i)



At the recommended contour level, 34% of all backbone atoms, 18% 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 (0.195) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1785	0.2970
A	0.2841	0.3140
B	0.1677	0.2980
C	0.1366	0.2890
D	0.1162	0.2920
E	0.0221	0.2180
F	0.2857	0.3160
G	0.1687	0.2990
H	0.1355	0.2910
I	0.1150	0.2890
J	0.0262	0.2210
K	0.2864	0.3170
L	0.1677	0.2980
M	0.1386	0.2890
N	0.1103	0.2910
O	0.0342	0.2180