wwPDB EM Validation Summary Report

Nov 2, 2022 – 06:02 AM EDT

PDB ID	:	5TAW
EMDB ID	:	EMD-8387
Title	:	Structure of rabbit RyR1 (ryanodine dataset, all particles)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.40 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:

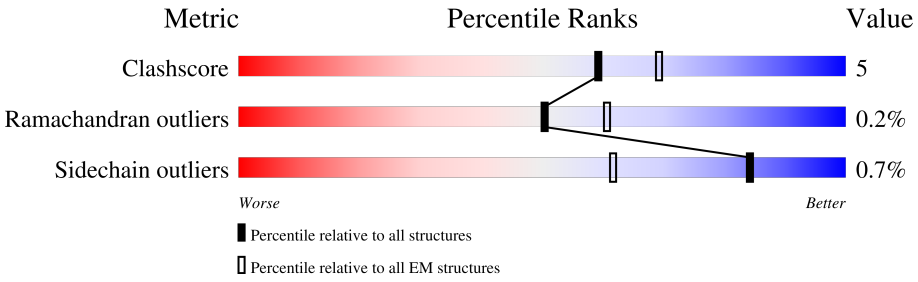
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.40 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	108	30% 83% 16% ·
1	F	108	31% 81% 18% ·
1	H	108	31% 81% 18% ·
1	J	108	29% 81% 18% ·
2	B	4416	43% 84% 11% 5%
2	E	4416	43% 84% 10% 5%
2	G	4416	43% 84% 11% 5%
2	I	4416	43% 84% 11% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 121276 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

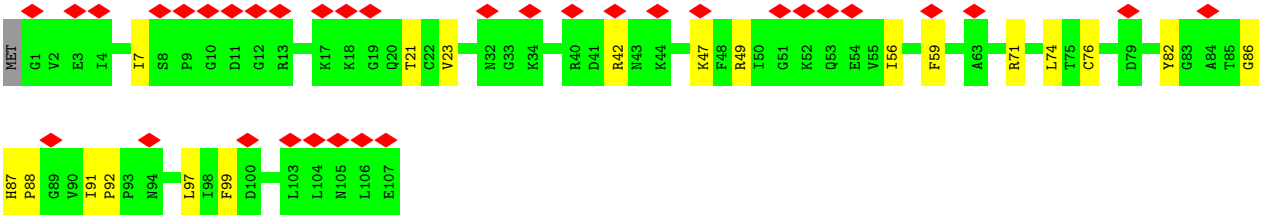
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0

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.

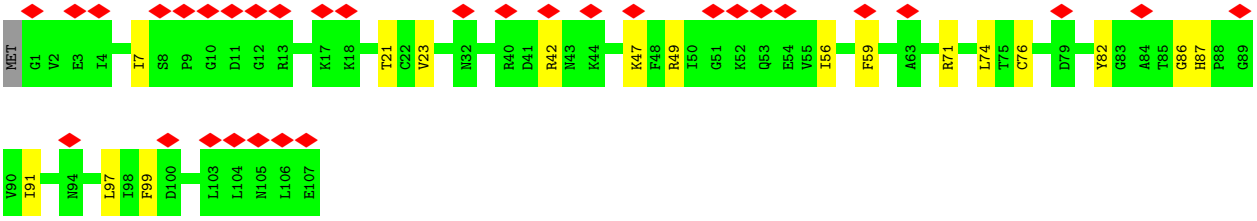
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



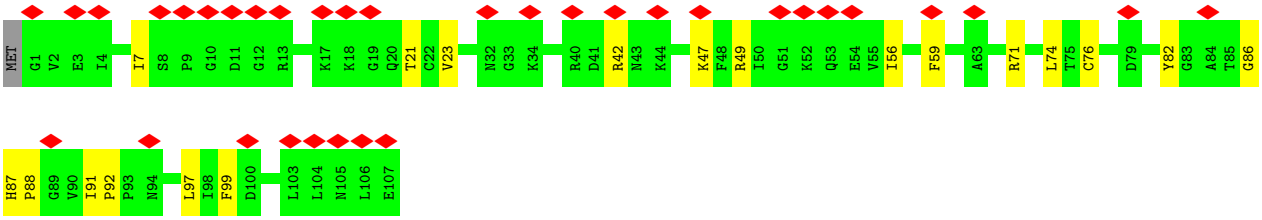
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



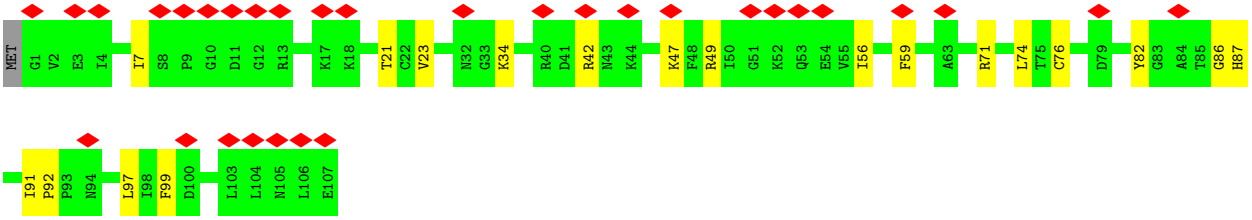
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



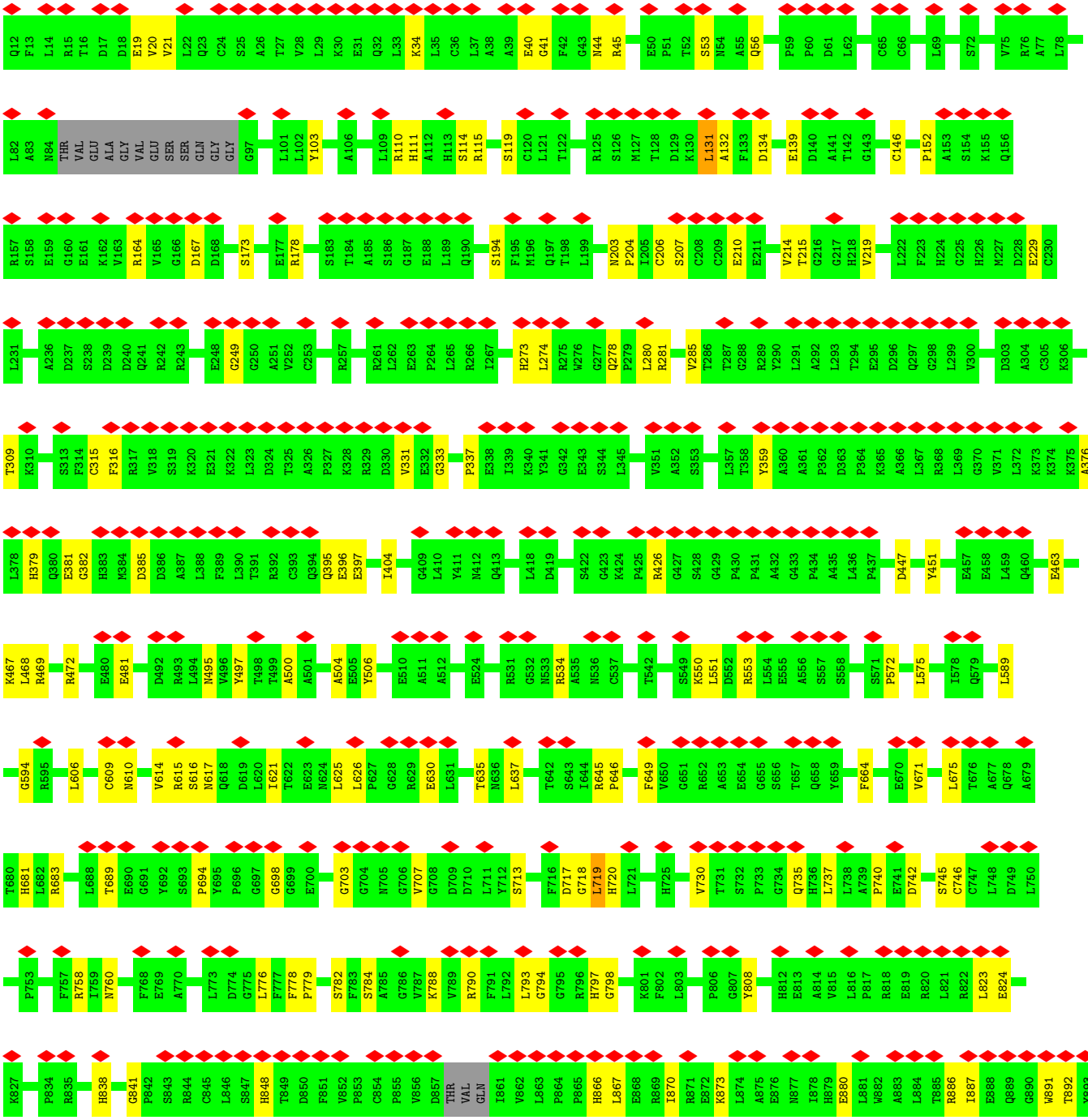
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

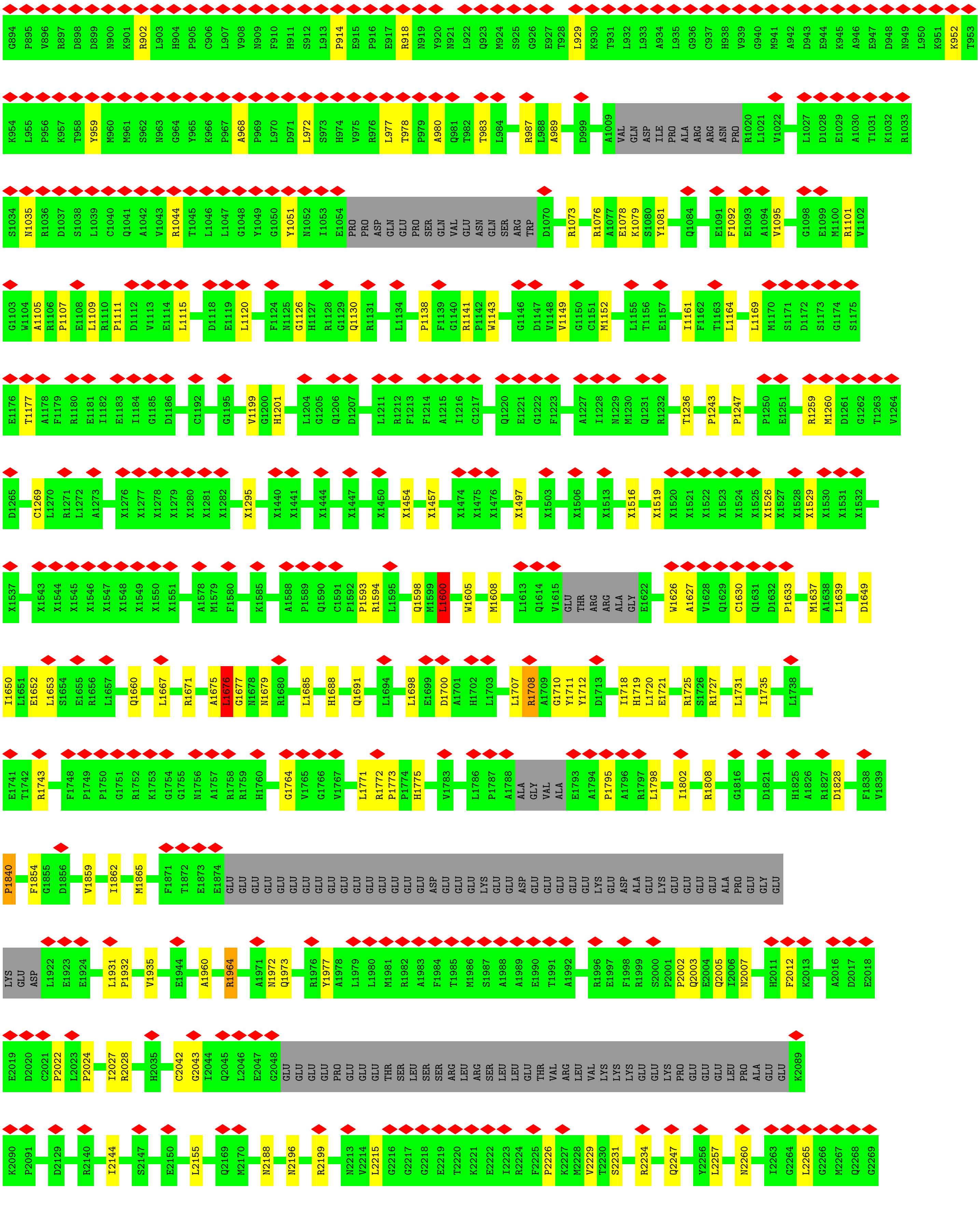
Chain J:



• Molecule 2: Ryanodine receptor 1

Chain B:

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K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 R987 L988 A989 D999 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 L1027 D1028 E1029 A1030 T1031 K1032 R1033
S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 R1076 A1077 E1078 K1079 S1080 Y1081 Q1084 E1091 F1092 E1093 A1094 V1095 G1098 E1099 M1100 R1101 V1102
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E1176 T1177 A1178 F1179 R1180 E1181 I1182 E1183 I1184 G1185 D1186 C1192 G1195 V1199 G1200 H1201 L1204 G1205 Q1206 D1207 L1211 R1212 F1213 F1214 A1215 I1216 C1217 Q1220 E1221 G1222 F1223 A1227 I1228 N1229 M1230 Q1231 R1232 T1236 P1243 P1247 P1250 E1251 R1259 M1260 D1261 G1262 T1263 V1264
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X1537 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 X1551 A1578 M1579 F1580 K1585 A1588 P1589 Q1590 C1591 P1592 P1593 R1594 L1595 Q1598 M1599 L1600 W1605 M1608 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 D1649
I1650 L1651 E1652 L1653 S1654 E1655 R1656 L1657 Q1660 L1667 R1671 A1675 L1676 G1677 N1678 N1679 R1680 L1685 H1688 Q1691 L1694 L1698 E1699 D1700 A1701 H1702 L1703 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 R1725 S1726 R1727 L1731 I1735 L1738
E1741 T1742 R1743 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1764 V1765 G1766 V1767 L1771 R1772 P1773 P1774 H1775 V1783 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798 I1802 R1808 G1816 D1821 H1825 A1826 R1827 D1828 F1838 V1839
P1840 F1854 G1855 D1856 V1859 I1862 M1865 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU
LYS GLU ASP L1922 E1923 E1924 L1931 P1932 V1935 E1944 A1960 R1964 A1971 N1972 Q1973 R1976 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1996 E1997 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006 N2007 H2011 F2012 K2013 A2016 D2017 E2018
E2019 D2020 C2021 P2022 L2023 P2024 I2027 R2028 H2035 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089
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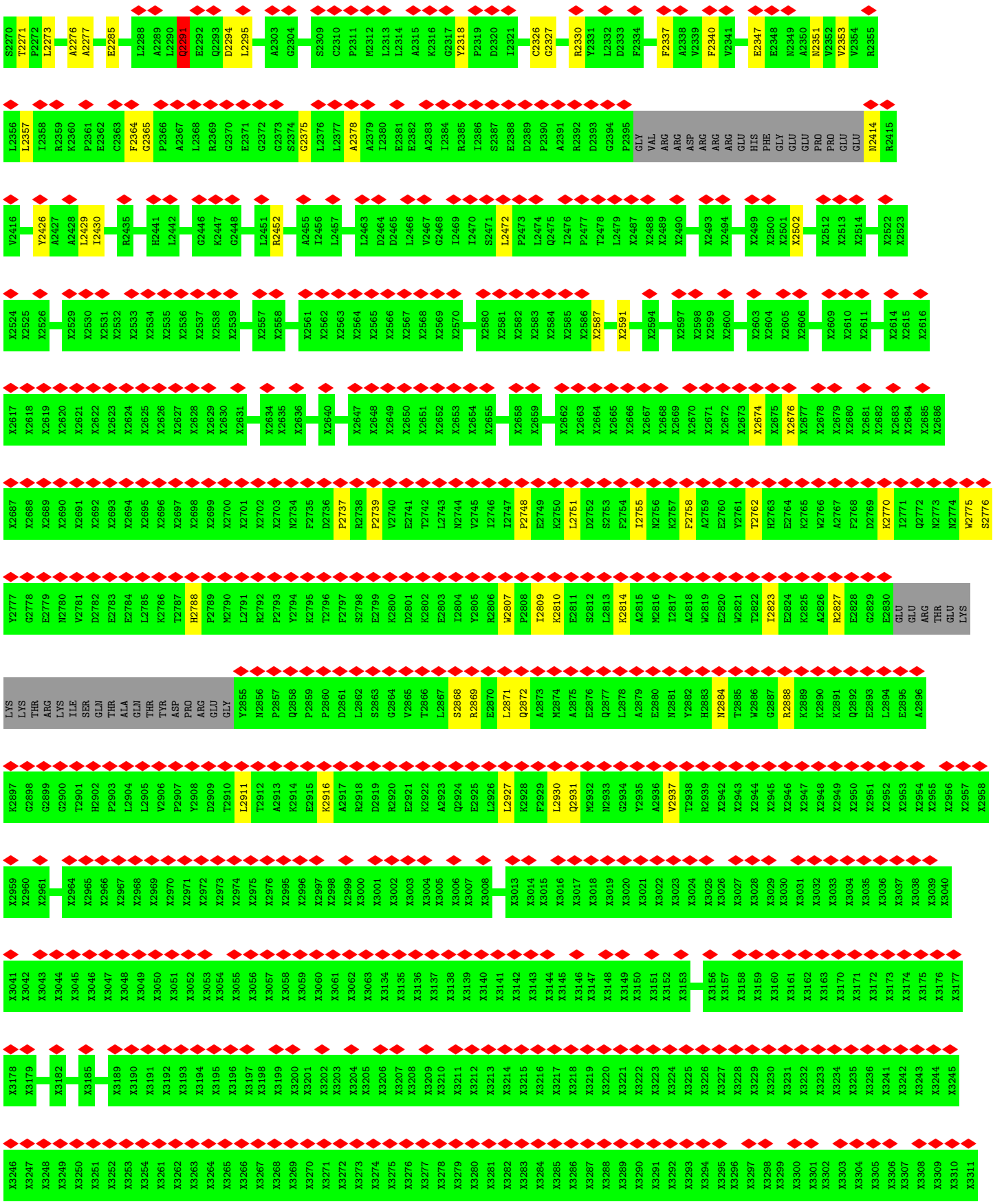
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L2356 L2357 I2358 R2359 K2360 P2361 E2362 C2363 F2364 G2365 P2366 A2367 L2368 R2369 G2370 E2371 G2372 G2373 S2374 G2375 L2376 L2377 A2378 A2379 I2380 E2381 E2382 A2383 I2384 R2385 I2386 S2387 E2388 D2389 P2390 A2391 R2392 D2393 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415
V2416 Y2426 K2427 A2428 L2429 I2430 R2435 H2441 L2442 G2446 K2447 G2448 L2451 R2452 A2455 I2456 L2457 L2463 D2464 D2465 L2466 V2467 G2468 I2469 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479 K2487 K2488 K2489 K2490 K2493 K2494 K2499 K2500 K2501 K2502 K2512 K2513 K2514 K2522 K2523
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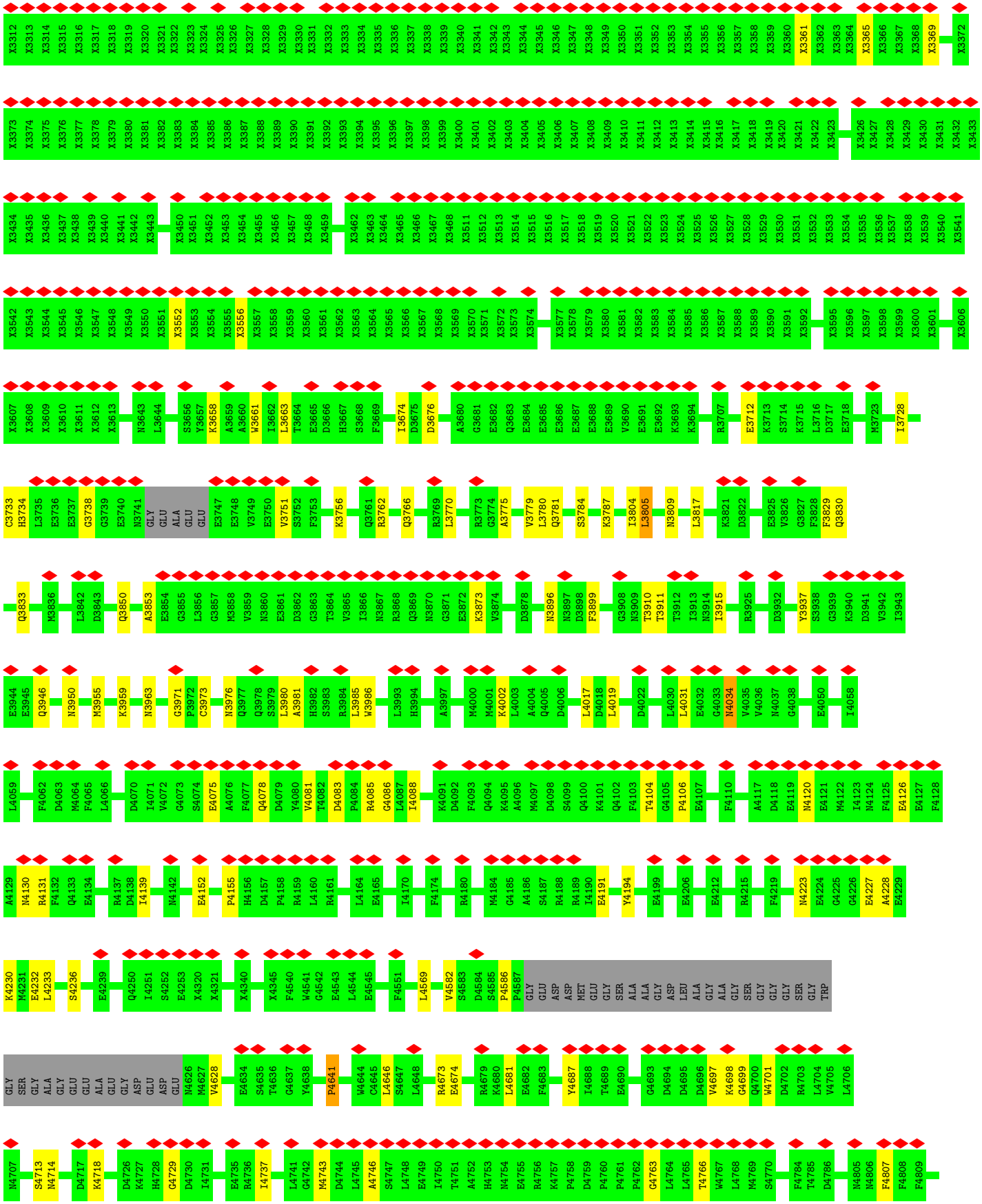
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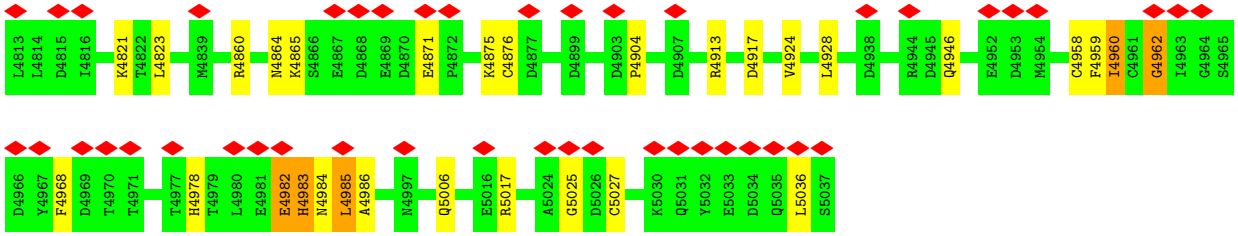
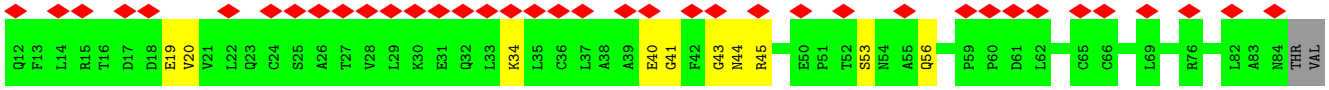
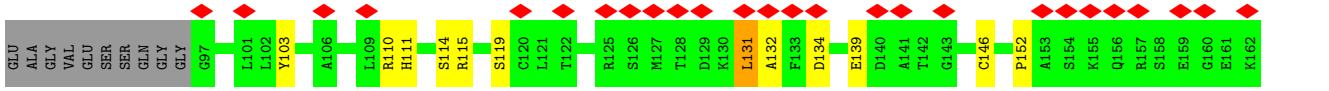
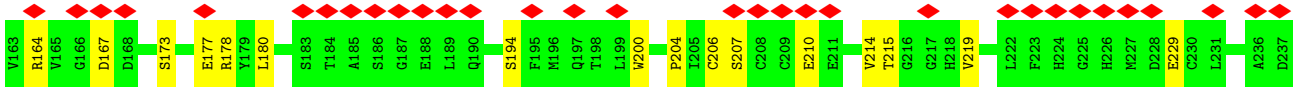


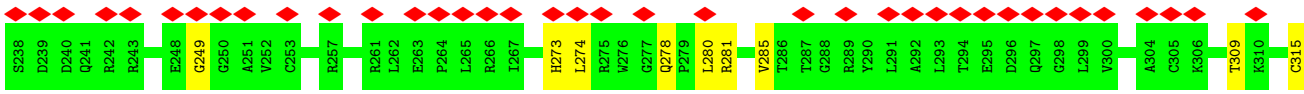
• Molecule 2: Ryanodine receptor 1

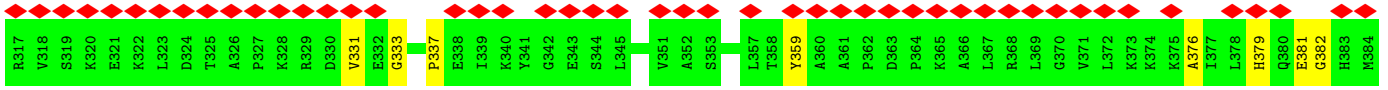
Chain G:

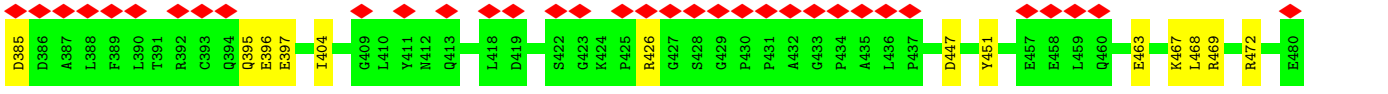


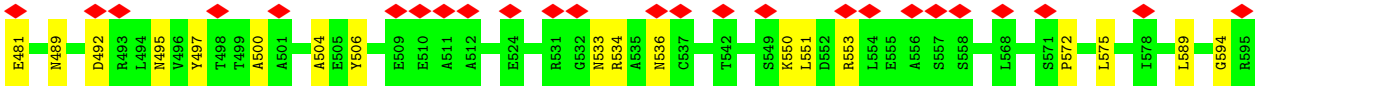


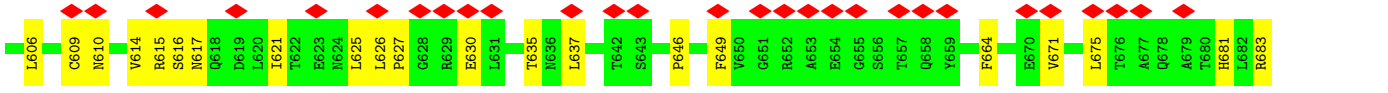


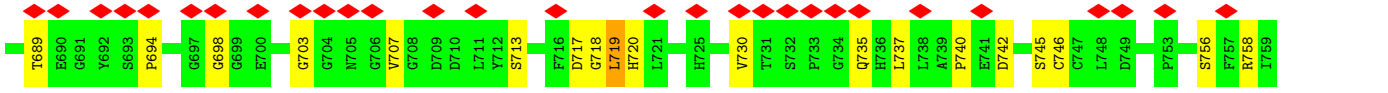


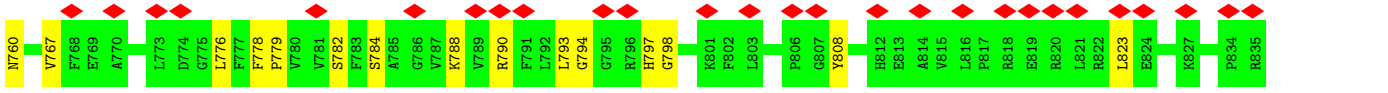


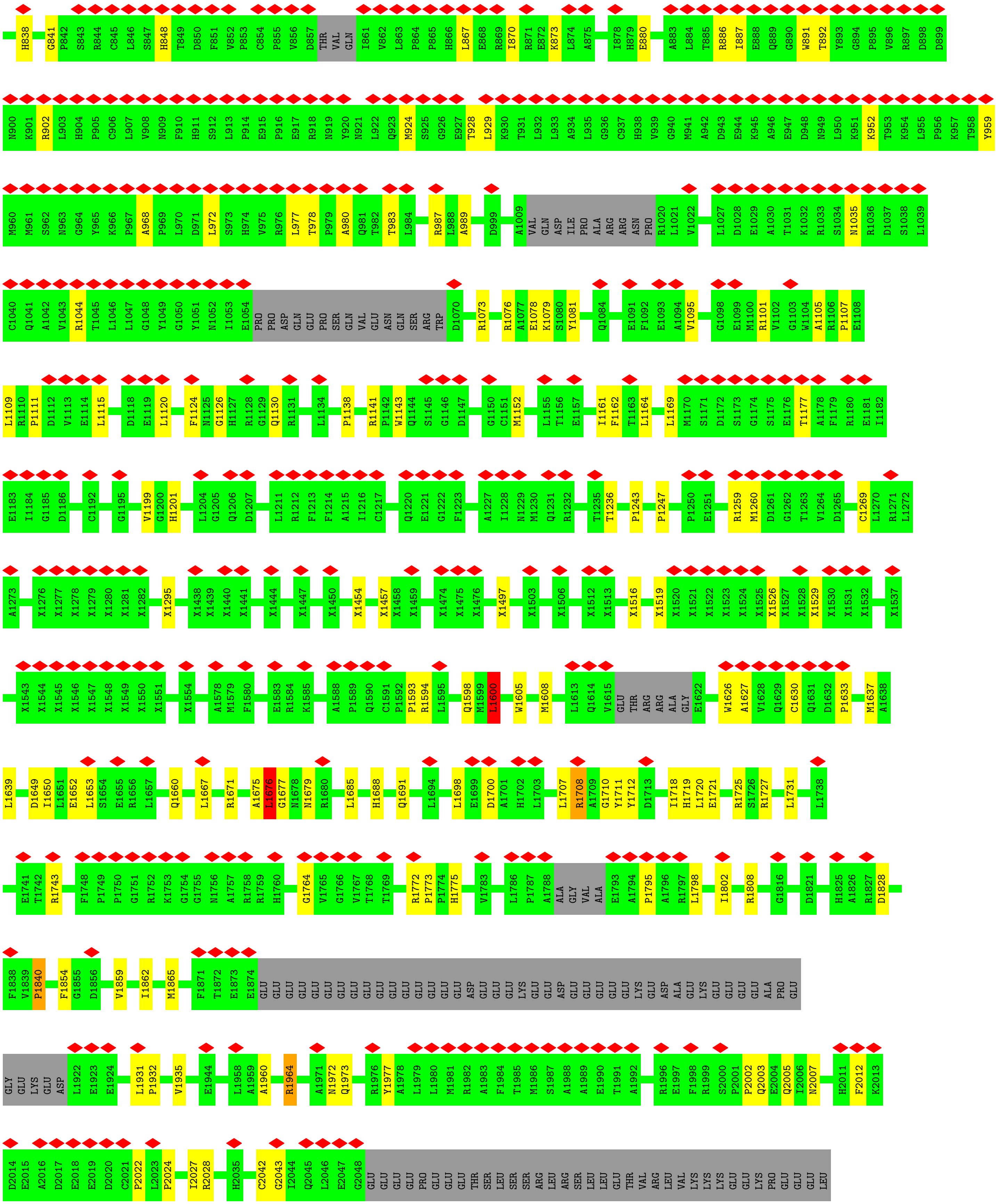








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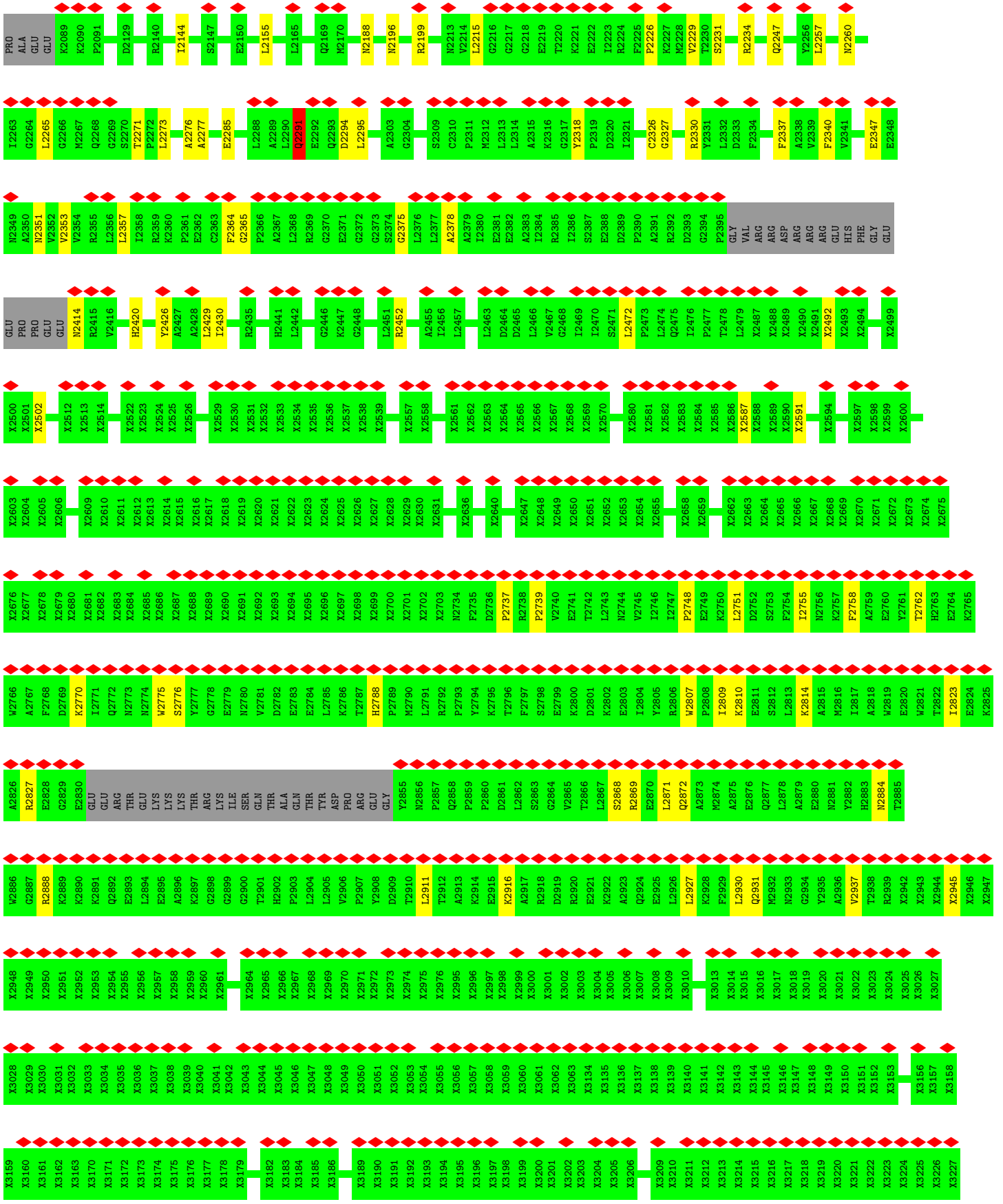
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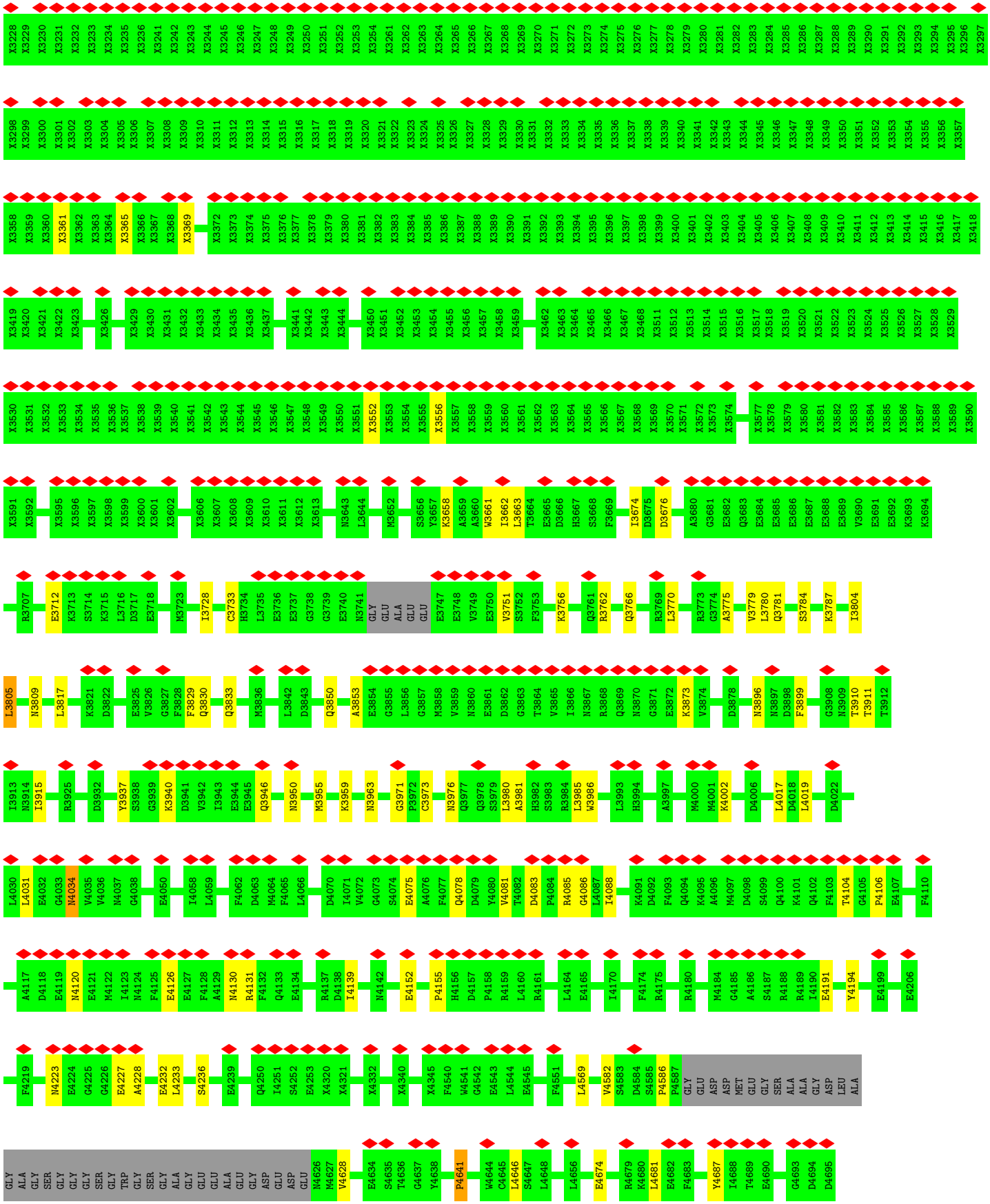
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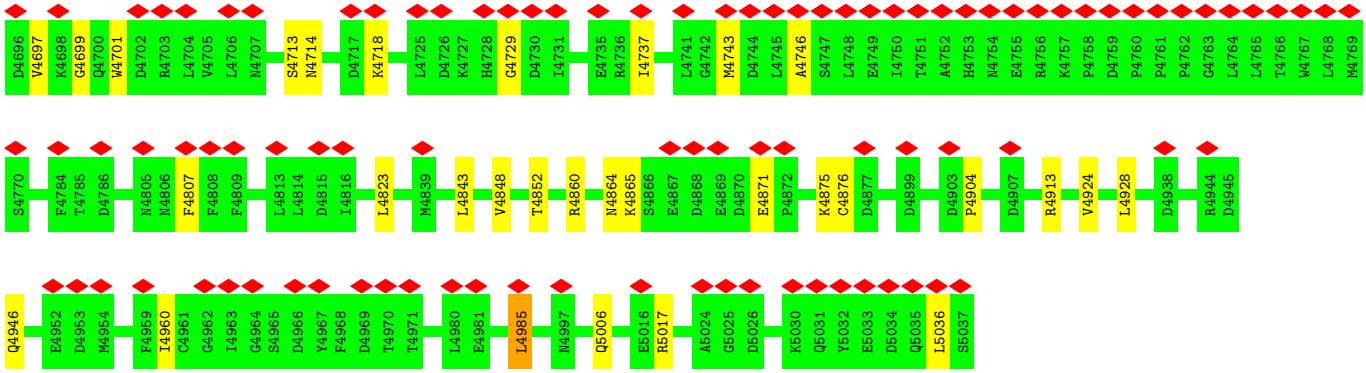

• Molecule 2: Ryanodine receptor 1

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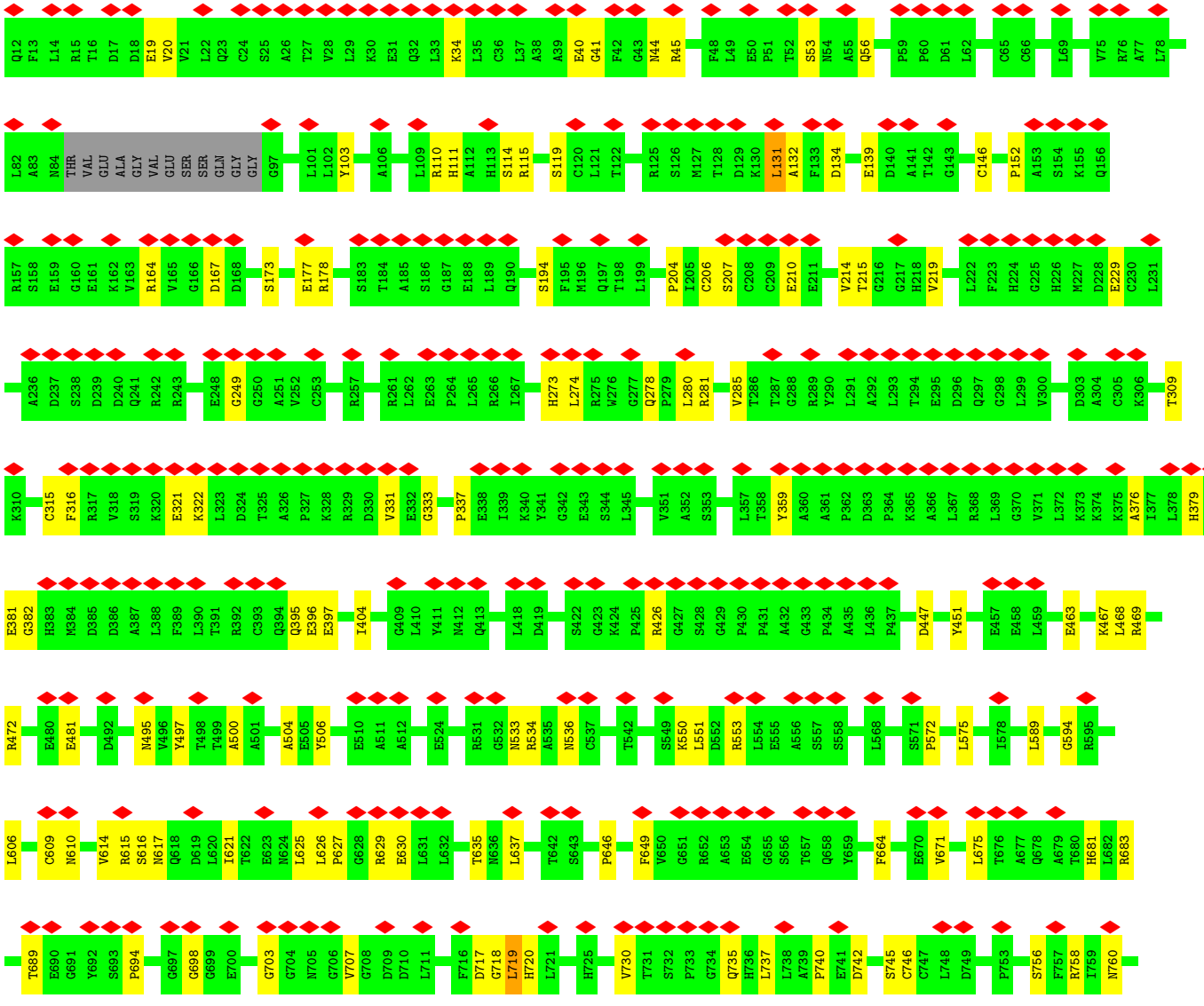

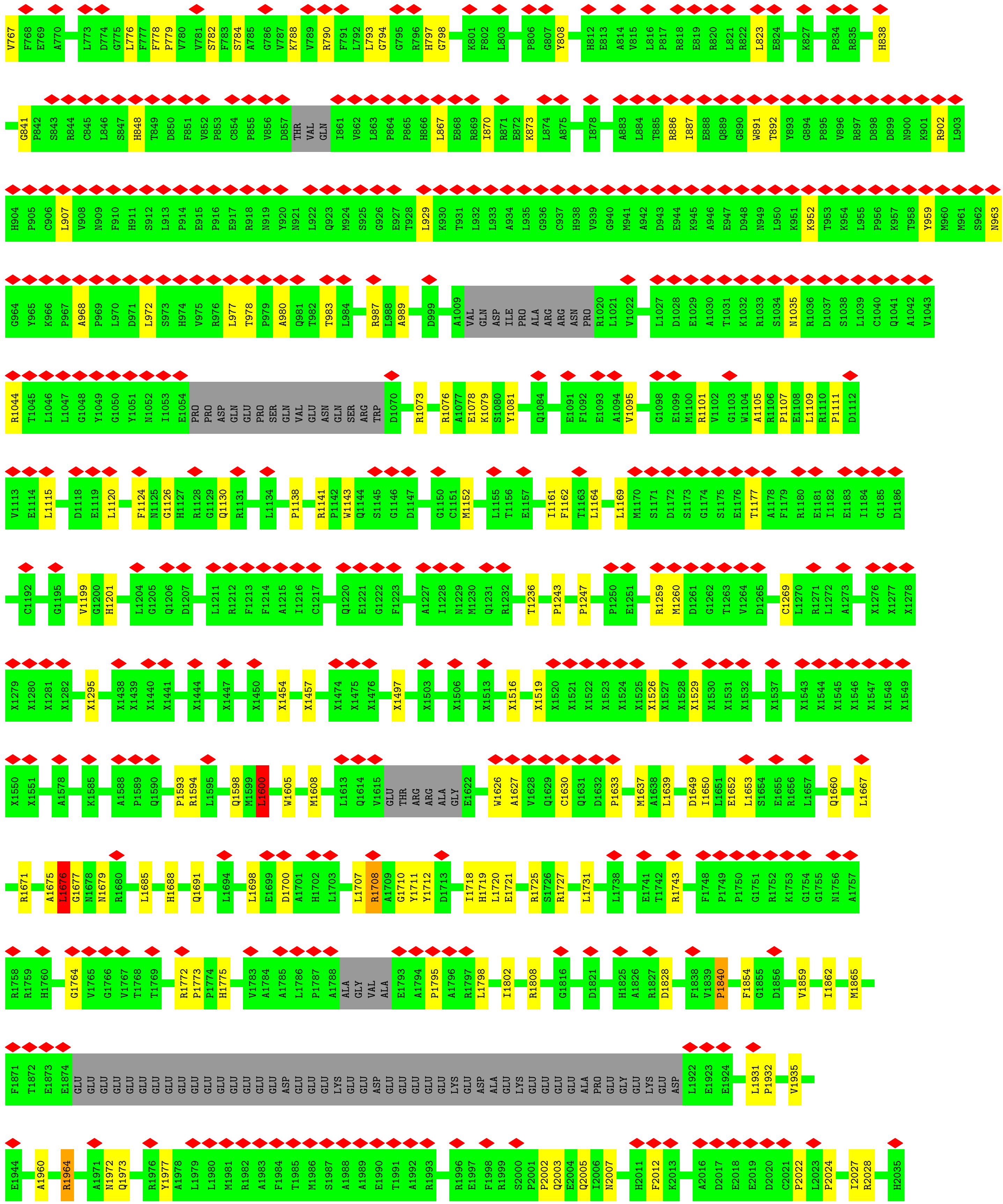
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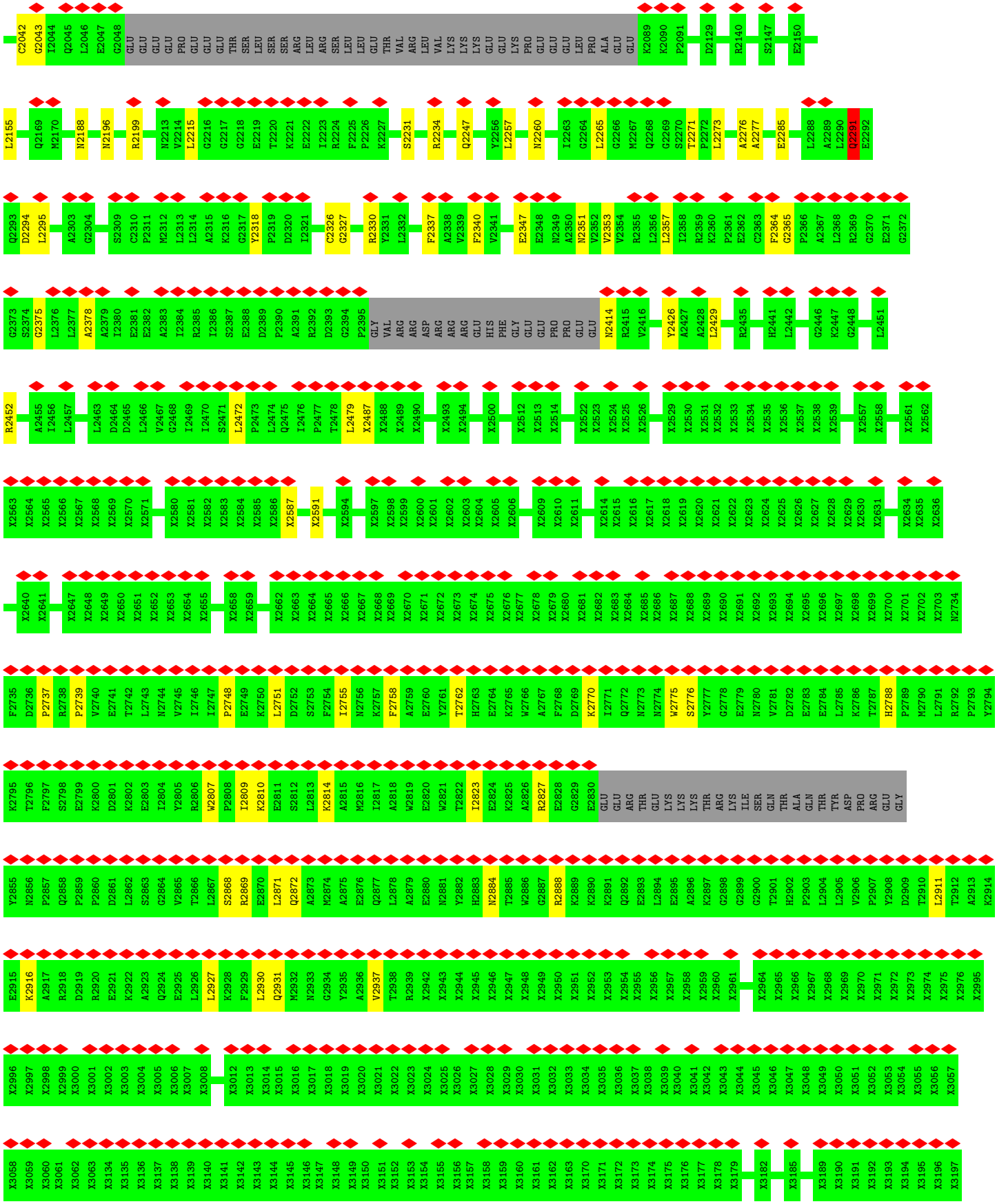
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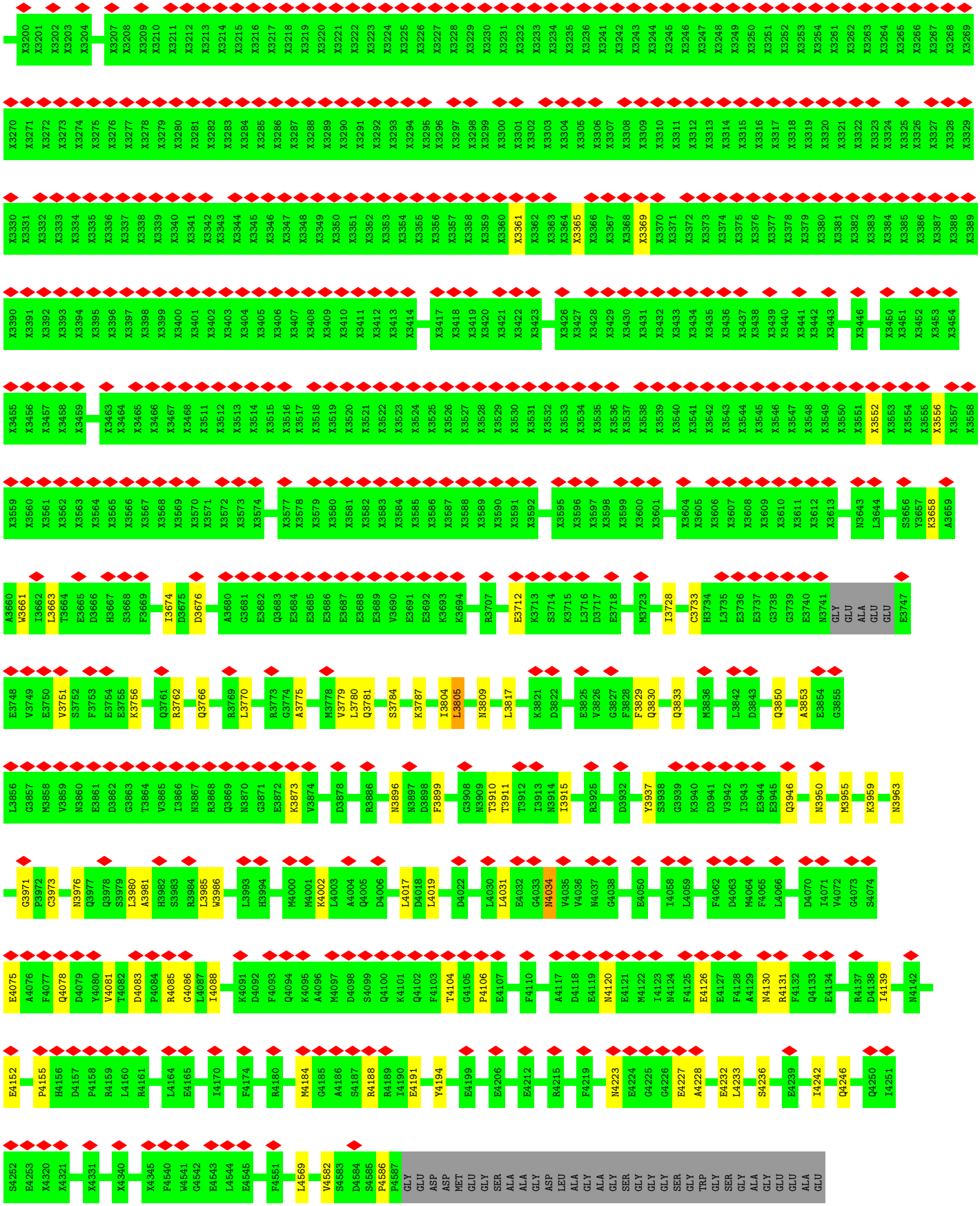
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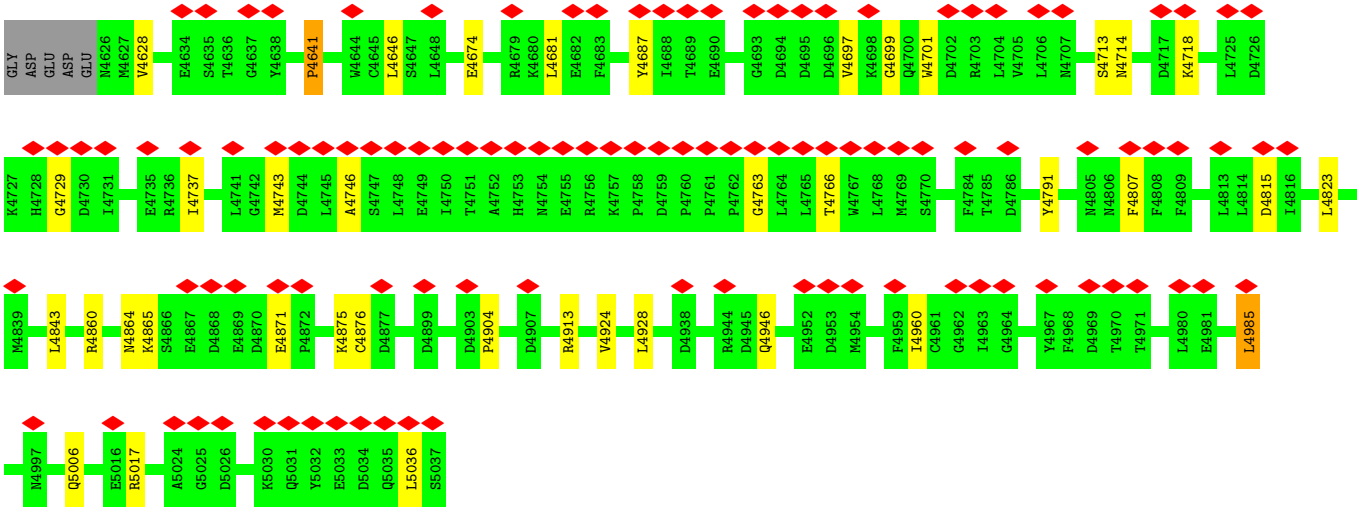
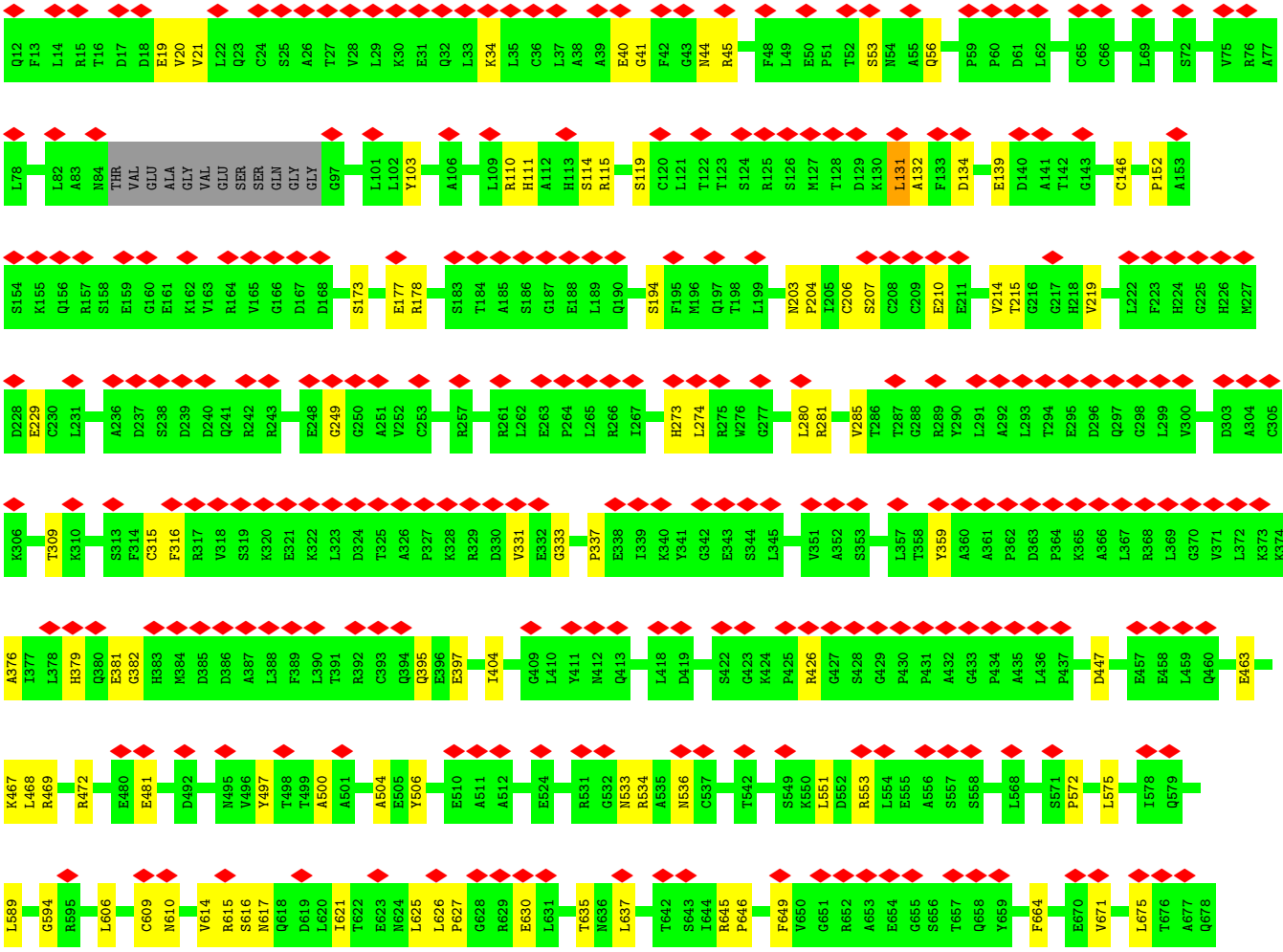
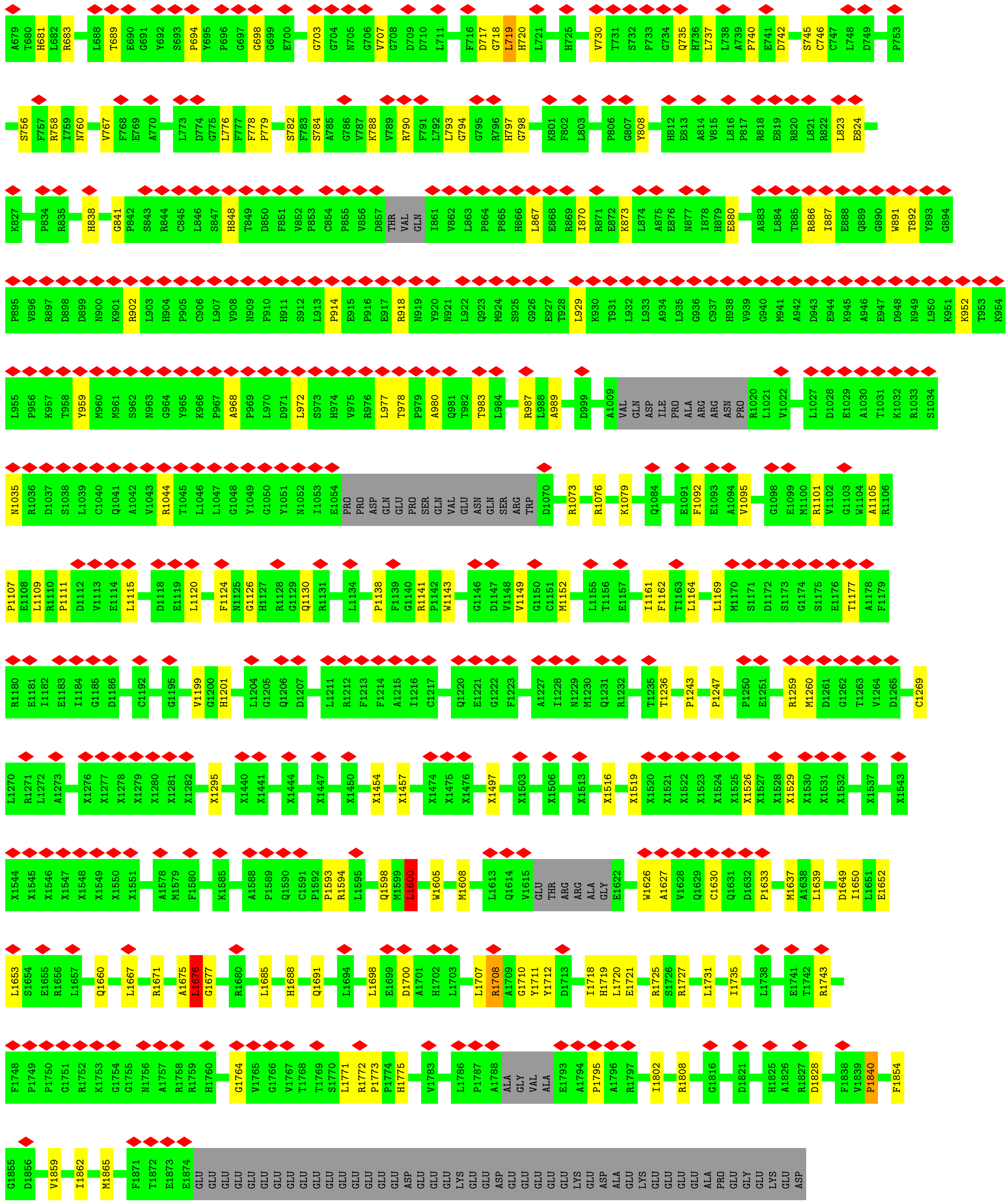


• Molecule 2: Ryanodine receptor 1

Chain E:

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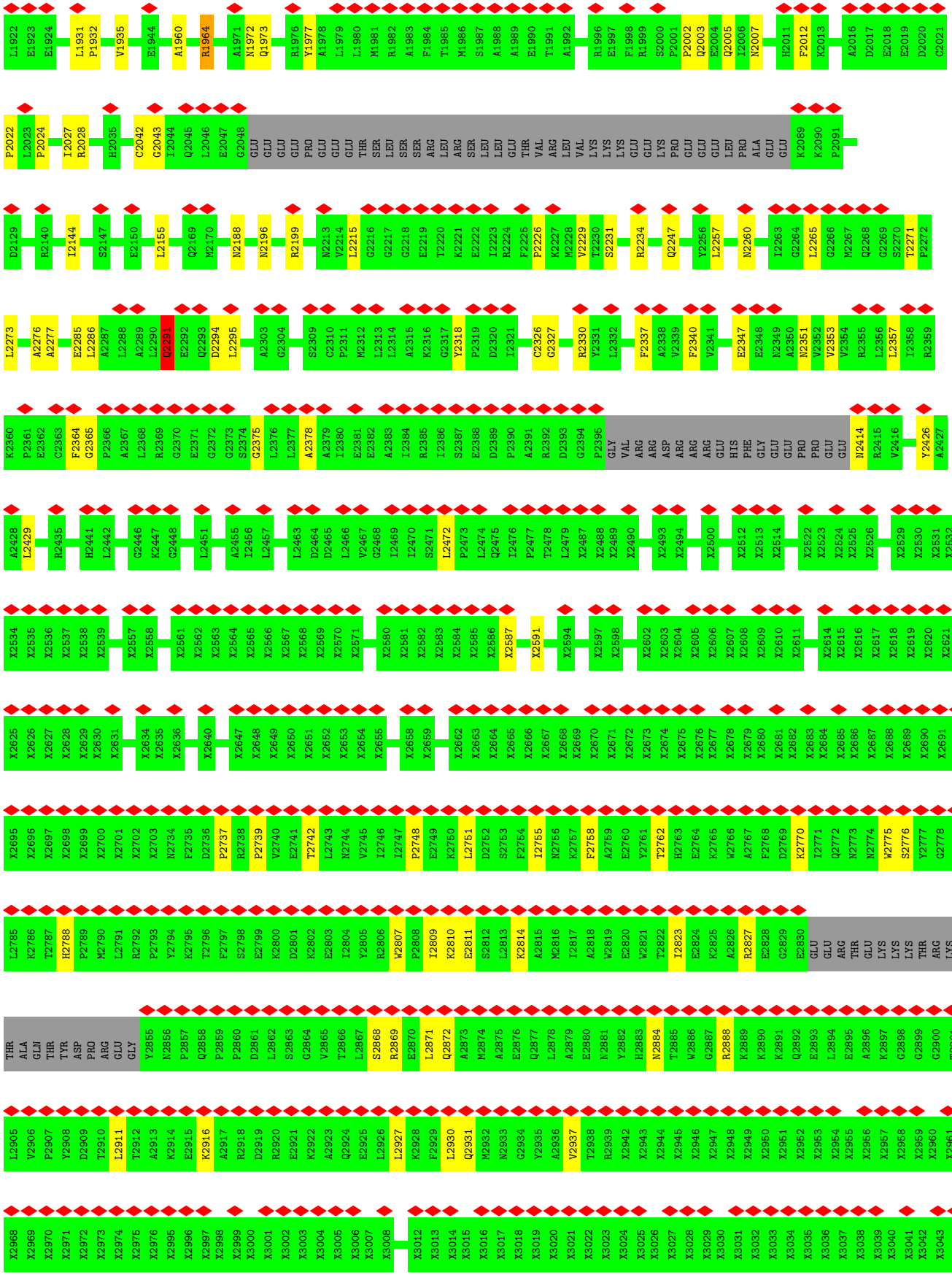
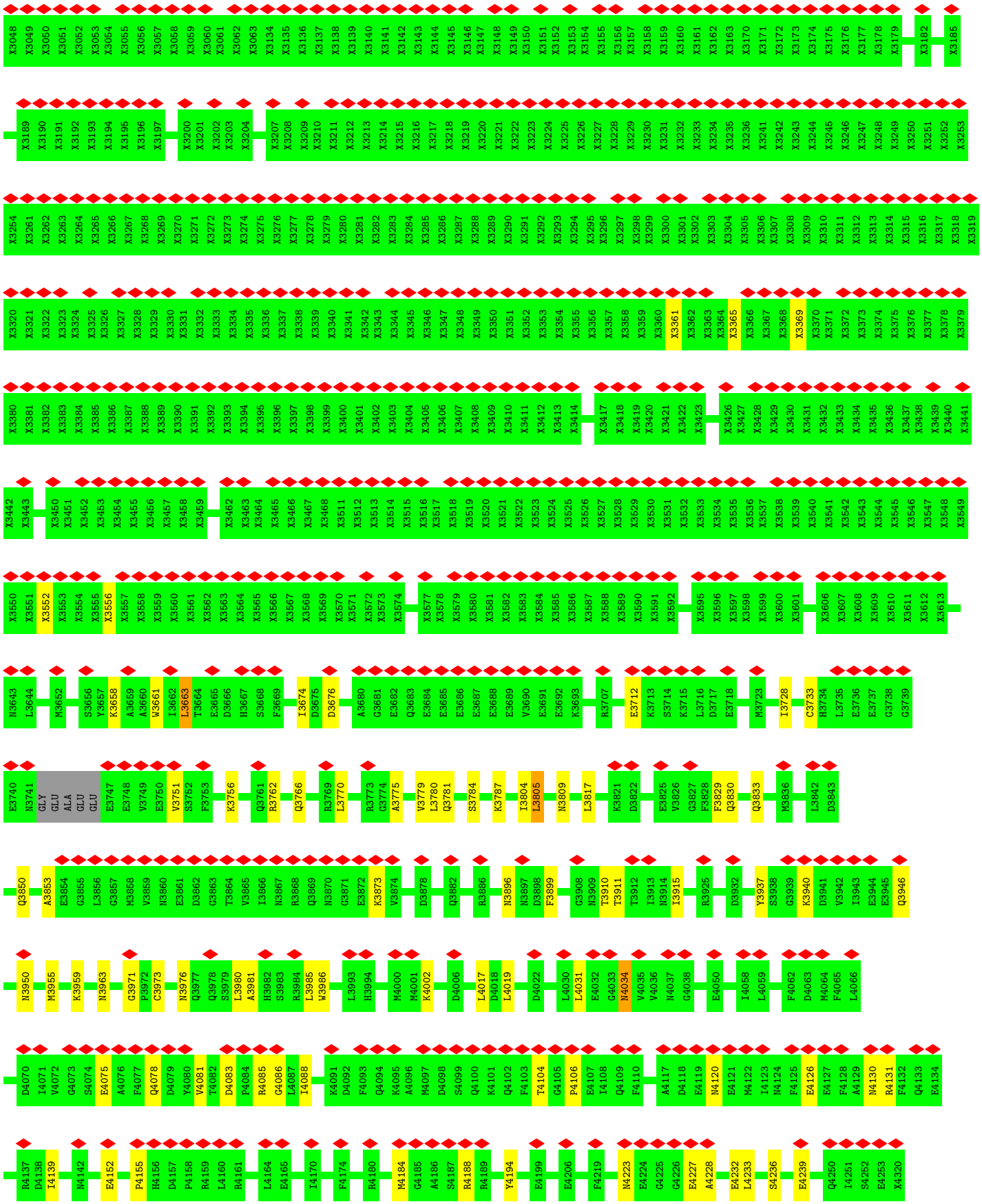
S756 F757 R758 I759 N760 V767 F768 E769 A770 L773 D774 G775 L776 F777 F778 P779 S782 F783 S784 A785 G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 H797 G798 K801 F802 L803 P806 G807 Y808 H812 E813 A814 V815 L816 P817 R818 E819 R820 L821 R822 L823 E824
K827 P834 R835 H838 G841 P842 S843 R844 C845 L846 S847 H848 T849 D850 F851 V852 P853 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894
P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954
L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 R987 L988 A989 D999 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 L1027 D1028 E1029 A1030 T1031 K1032 R1033 S1034
N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 R1076 K1079 Q1084 E1091 F1092 E1093 A1094 V1095 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106
P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 D1118 E1119 L1120 F1124 N1125 G1126 H1127 R1128 G1129 Q1130 R1131 L1134 P1138 F1139 G1140 R1141 P1142 W1143 G1146 D1147 V1148 V1149 G1150 C1151 M1152 L1155 T1156 E1157 I1161 F1162 T1163 L1164 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179
R1180 E1181 I1182 E1183 I1184 G1185 D1186 C1192 G1195 V1199 G1200 H1201 L1204 G1205 Q1206 D1207 L1211 R1212 F1213 F1214 A1215 I1216 C1217 Q1220 E1221 G1222 F1223 A1227 I1228 N1229 M1230 Q1231 R1232 T1235 T1236 P1243 P1247 P1250 E1251 R1259 M1260 D1261 G1262 T1263 V1264 D1265 C1269
L1270 R1271 L1272 A1273 X1276 X1277 X1278 X1279 X1280 X1281 X1282 X1295 X1440 X1441 X1444 X1447 X1450 X1454 X1457 X1474 X1475 X1476 X1497 X1503 X1506 X1513 X1516 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1532 X1537 X1543
X1544 X1545 X1546 X1547 X1548 X1549 X1550 X1551 A1578 M1579 F1580 K1585 A1588 P1589 Q1590 C1591 P1592 P1593 R1594 L1595 Q1598 M1599 L1600 W1605 M1608 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 D1649 I1650 L1651 E1652
L1653 S1654 E1655 R1656 L1657 Q1660 L1667 R1671 A1675 L1676 G1677 R1680 L1685 H1688 Q1691 L1694 L1698 E1699 D1700 A1701 H1702 L1703 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 R1725 S1726 R1727 L1731 I1735 L1738 E1741 T1742 R1743
F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 P1773 P1774 H1775 V1783 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 I1802 R1808 G1816 D1821 H1825 A1826 R1827 D1828 F1838 V1839 P1840 F1854
G1855 D1856 V1859 I1862 M1865 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP

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X3189 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3201 X3202 X3203 X3204 X3207 X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223 X3224 X3225 X3226 X3227 X3228 X3229 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253
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X3320 X3321 X3322 X3323 X3324 X3325 X3326 X3327 X3328 X3329 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344 X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3367 X3368 X3369 X3370 X3371 X3372 X3373 X3374 X3375 X3376 X3377 X3378 X3379
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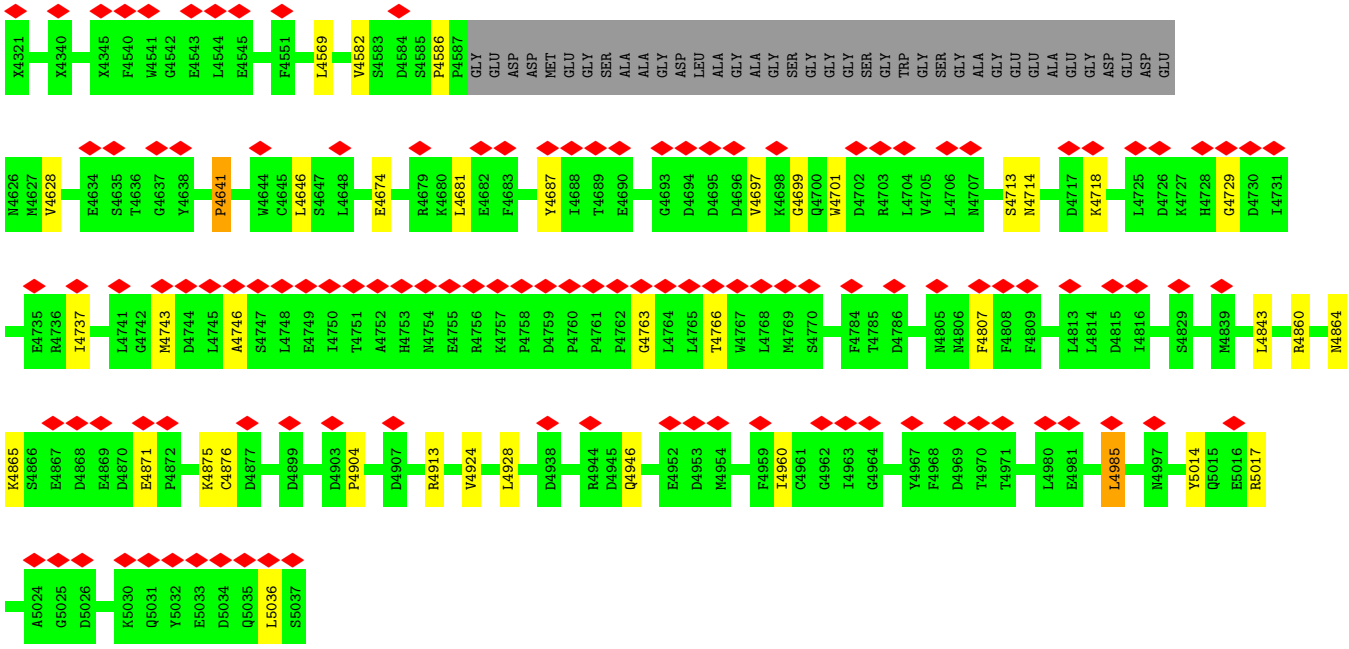
N3643 L3644 M3652 S3656 Y3657 K3658 A3659 A3660 W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 F3669 I3674 D3675 D3676 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 R3707 E3712 K3713 S3714 K3715 L3716 D3717 E3718 H3723 I3728 C3733 H3734 L3735 E3736 E3737 G3738 G3739
E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 Y3751 S3752 F3753 K3756 Q3761 R3762 Q3766 R3769 L3770 R3773 G3774 A3775 V3779 L3780 Q3781 S3784 K3787 I3804 L3805 N3809 L3817 K3821 D3822 E3825 V3826 G3827 F3828 F3829 Q3830 Q3833 M3836 L3842 D3843
Q3850 A3853 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 V3874 D3878 Q3882 R3886 N3896 N3897 D3898 F3899 G3908 N3909 T3910 T3911 T3912 I3913 N3914 I3915 R3925 D3932 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 E3944 E3945 Q3946
N3950 M3955 K3959 N3963 G3971 P3972 C3973 N3976 Q3977 Q3978 S3979 L3980 A3981 H3982 S3983 R3984 L3985 W3986 L3993 H3994 M4000 M4001 K4002 D4006 L4017 D4018 L4019 D4022 L4030 L4031 E4032 G4033 N4034 V4035 V4036 N4037 G4038 E4050 I4058 L4059 F4062 D4063 M4064 F4065 L4066
D4070 I4071 V4072 G4073 S4074 E4075 A4076 F4077 Q4078 D4079 V4080 V4081 T4082 D4083 P4084 R4085 G4086 L4087 I4088 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 E4107 I4108 Q4109 F4110 A4117 D4118 E4119 N4120 E4121 M4122 I4123 N4124 F4125 E4126 E4127 F4128 A4129 N4130 R4131 F4132 Q4133 E4134
R4137 D4138 I4139 N4142 E4152 P4155 H4156 D4157 P4158 R4159 L4160 R4161 L4164 E4165 I4170 F4174 R4180 M4184 G4185 A4186 S4187 R4188 R4189 Y4194 E4199 E4206 F4219 N4223 E4224 G4225 G4226 E4227 A4228 E4232 L4233 S4236 E4239 Q4250 I4251 S4252 E4253 X4320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A5024 G5025 D5026 K5030 Q5031 Y5032 E5033 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN

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	0.31	0/834	0.54	0/1123
1	F	0.31	0/834	0.54	0/1123
1	H	0.31	0/834	0.54	0/1123
1	J	0.31	0/834	0.54	0/1123
2	B	0.30	0/25428	0.54	5/34534 (0.0%)
2	E	0.30	0/25428	0.54	5/34534 (0.0%)
2	G	0.30	0/25428	0.54	5/34534 (0.0%)
2	I	0.30	0/25428	0.54	5/34534 (0.0%)
All	All	0.30	0/105048	0.54	20/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	7.62	132.81	115.30
2	I	131	LEU	CA-CB-CG	7.61	132.79	115.30
2	B	131	LEU	CA-CB-CG	7.59	132.75	115.30
2	G	131	LEU	CA-CB-CG	7.59	132.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1600	LEU	CA-CB-CG	6.68	130.67	115.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1720	LEU	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide

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	818	0	824	10	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24749	281	0
2	E	29499	0	24749	253	0
2	G	29499	0	24750	262	0
2	I	29499	0	24749	257	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102293	1081	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 5.

The worst 5 of 1081 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)
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.28	1.20
2:B:4230:LYS:HD2	2:B:4959:PHE:HE2	0.99	1.10
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.92	1.04
2:B:4983:HIS:CE1	2:B:5027:CYS:SG	2.57	0.98
2:B:4230:LYS:CD	2:B:4959:PHE:HE2	1.87	0.87

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	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2894 (90%)	333 (10%)	8 (0%)	47	81
2	E	3235/4416 (73%)	2898 (90%)	332 (10%)	5 (0%)	47	81
2	G	3235/4416 (73%)	2896 (90%)	334 (10%)	5 (0%)	47	81
2	I	3235/4416 (73%)	2898 (90%)	332 (10%)	5 (0%)	47	81
All	All	13360/18096 (74%)	11962 (90%)	1375 (10%)	23 (0%)	50	81

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4962	GLY
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG

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Mol	Chain	Res	Type
2	E	1708	ARG

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2473 (99%)	20 (1%)	81	89
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
All	All	10324/12444 (83%)	10253 (99%)	71 (1%)	84	90

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	719	LEU
2	E	1141	ARG
2	E	3805	LEU
2	G	1076	ARG
2	G	719	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	4983	HIS
2	E	3950	ASN
2	E	111	HIS
2	E	1679	ASN

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Mol	Chain	Res	Type
2	E	4806	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)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
2	I	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	4345:UNK	C	4540:PHE	N	73.65
1	B	4345:UNK	C	4540:PHE	N	73.61
1	I	4345:UNK	C	4540:PHE	N	73.61
1	E	4345:UNK	C	4540:PHE	N	73.59
1	G	3613:UNK	C	3639:THR	N	45.21

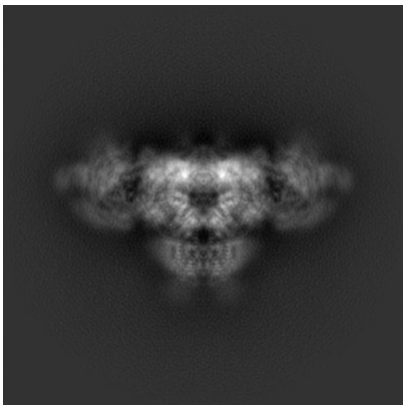
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8387. These allow visual inspection of the internal detail of the map and identification of artifacts.

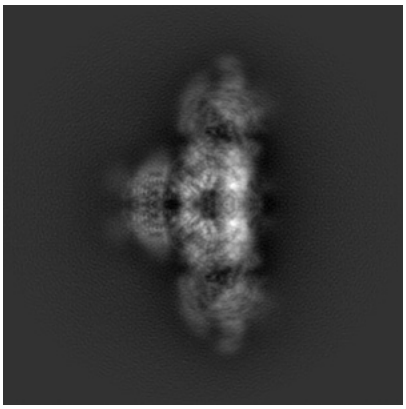
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

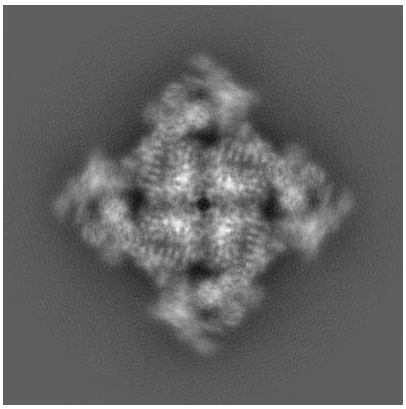
6.1.1 Primary map



X

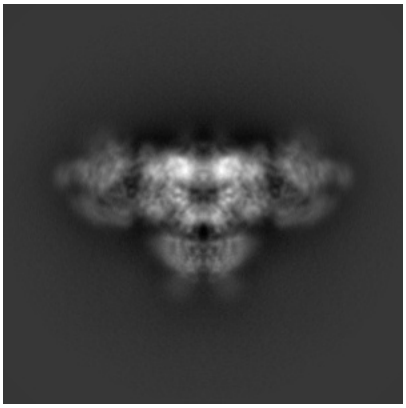


Y

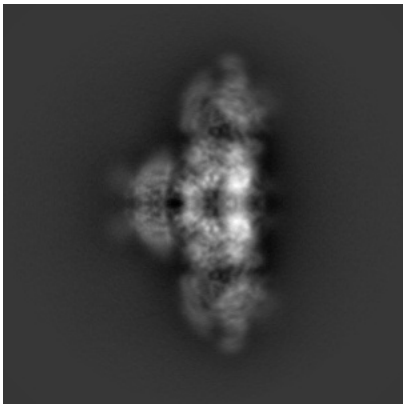


Z

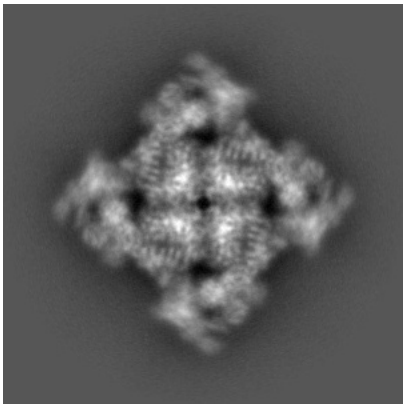
6.1.2 Raw map



X



Y

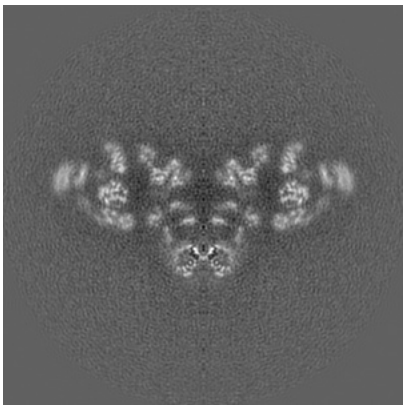


Z

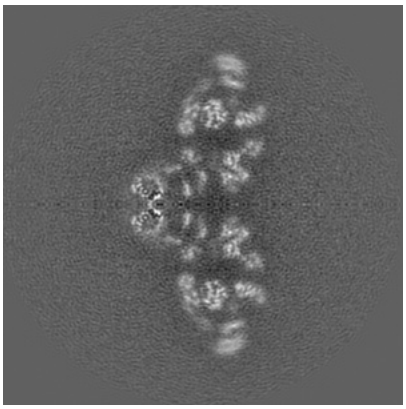
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

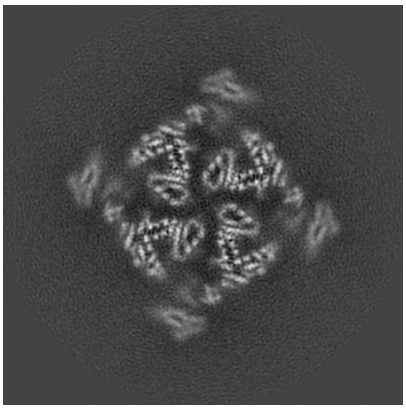
6.2.1 Primary map



X Index: 200

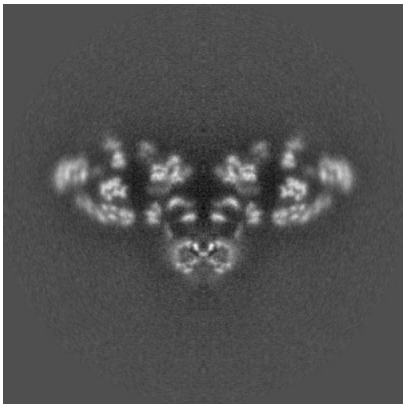


Y Index: 200

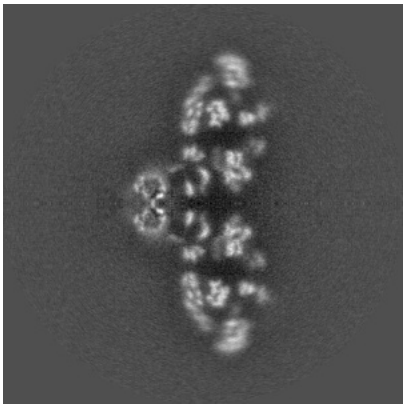


Z Index: 200

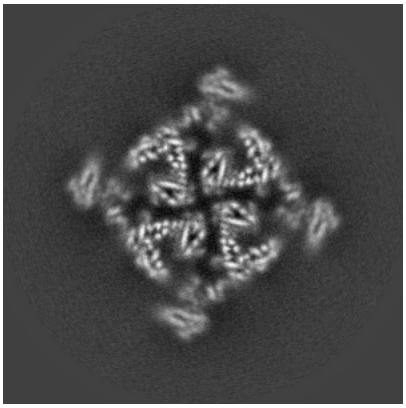
6.2.2 Raw map



X Index: 200



Y Index: 200

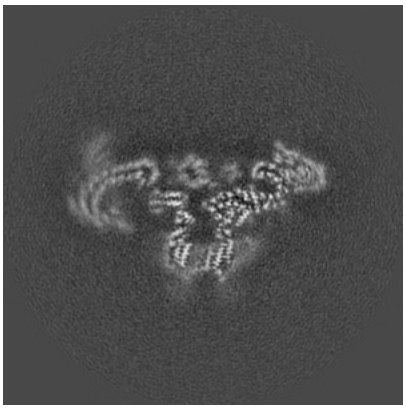


Z Index: 200

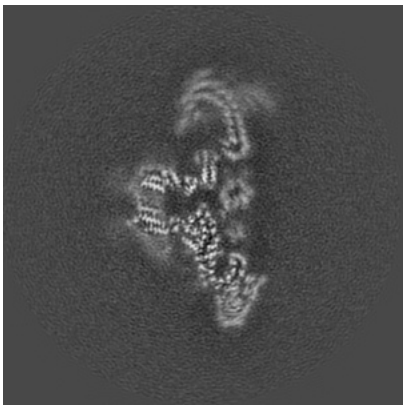
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

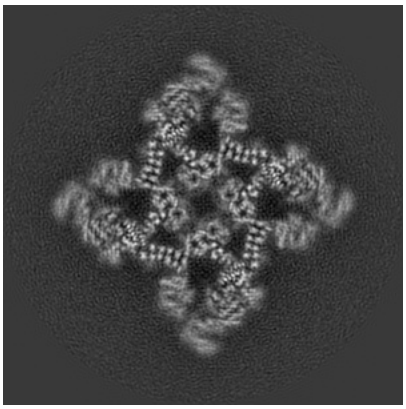
6.3.1 Primary map



X Index: 175

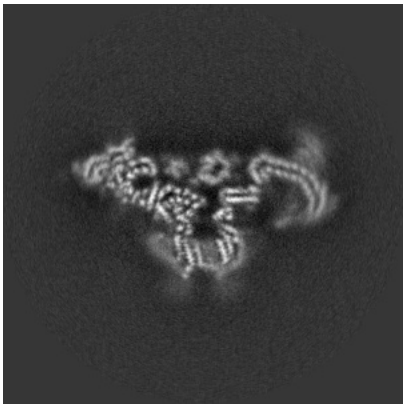


Y Index: 175

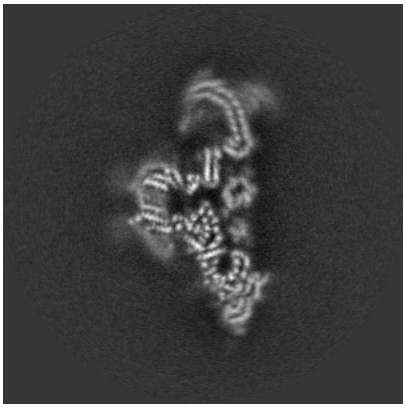


Z Index: 227

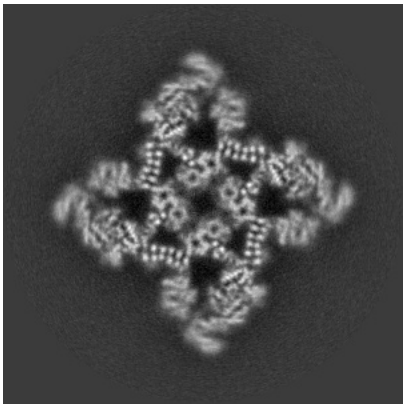
6.3.2 Raw map



X Index: 225



Y Index: 175

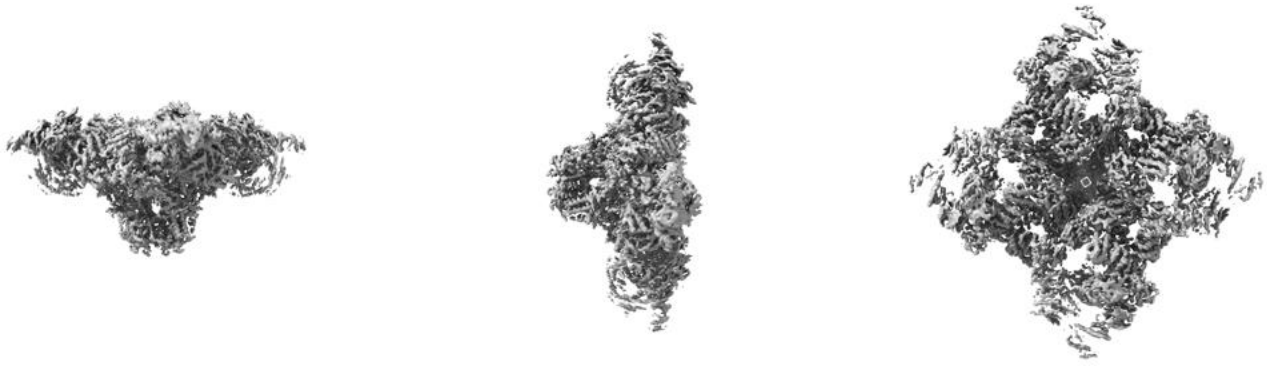


Z Index: 229

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 0.04. 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.

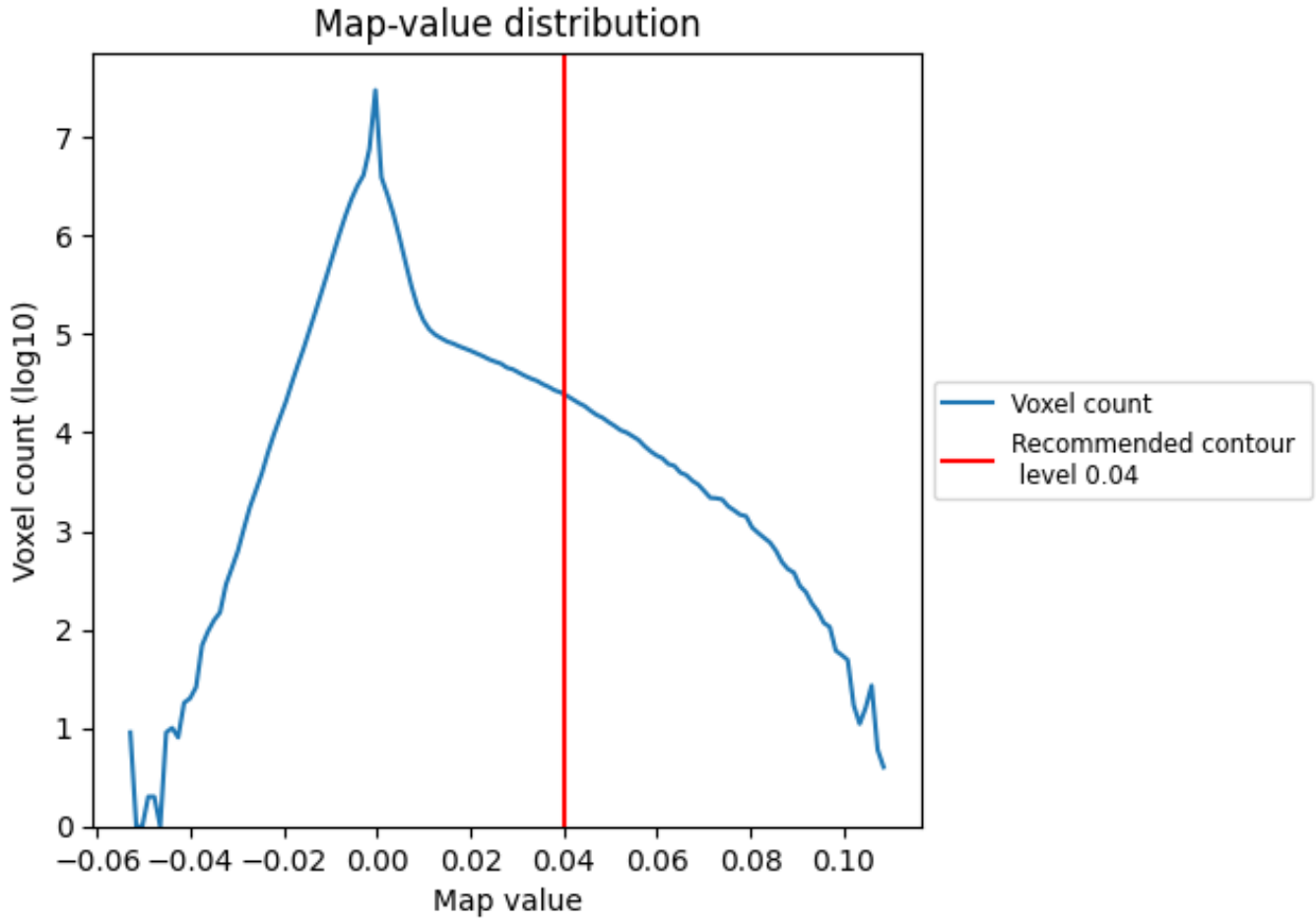
6.5 Mask visualisation (i)

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

7 Map analysis

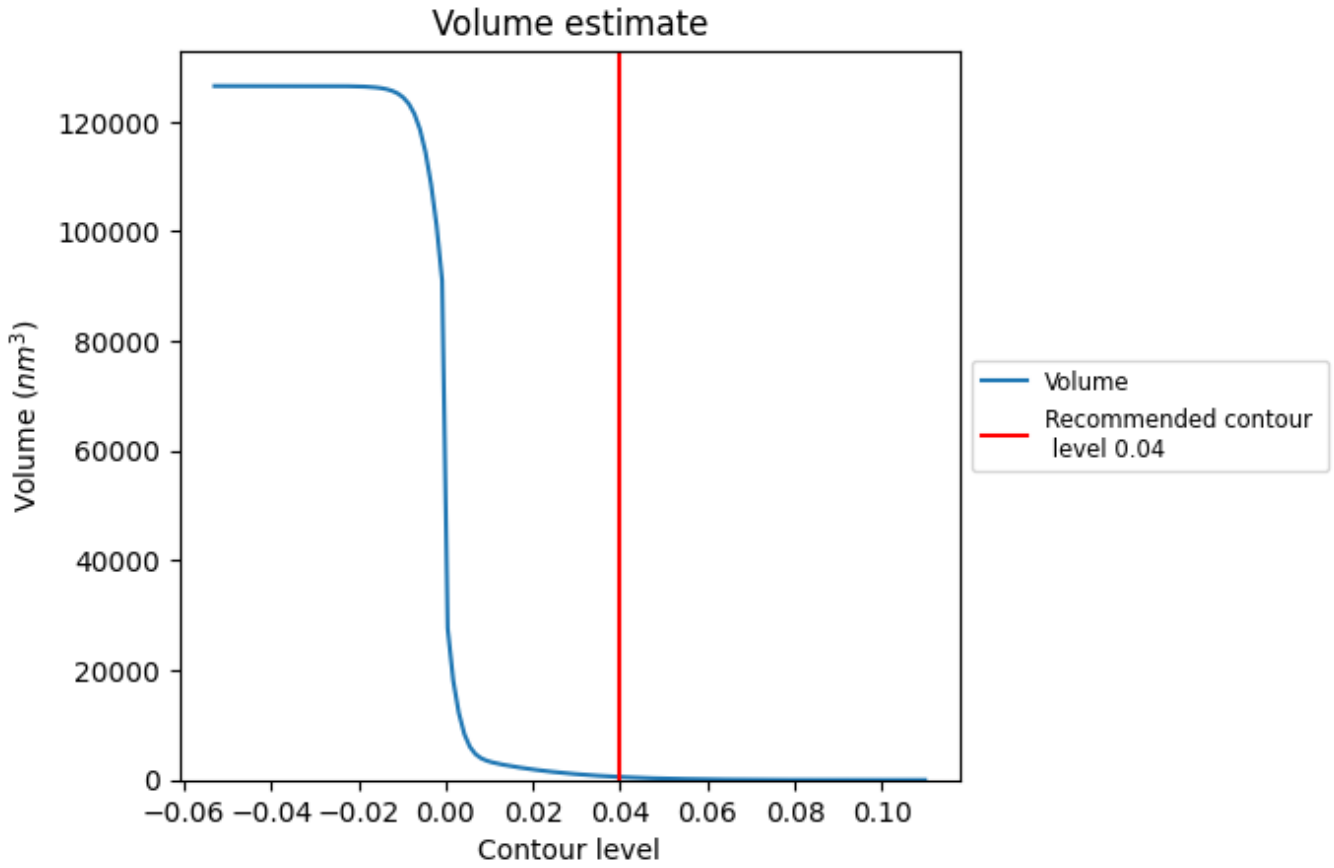
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

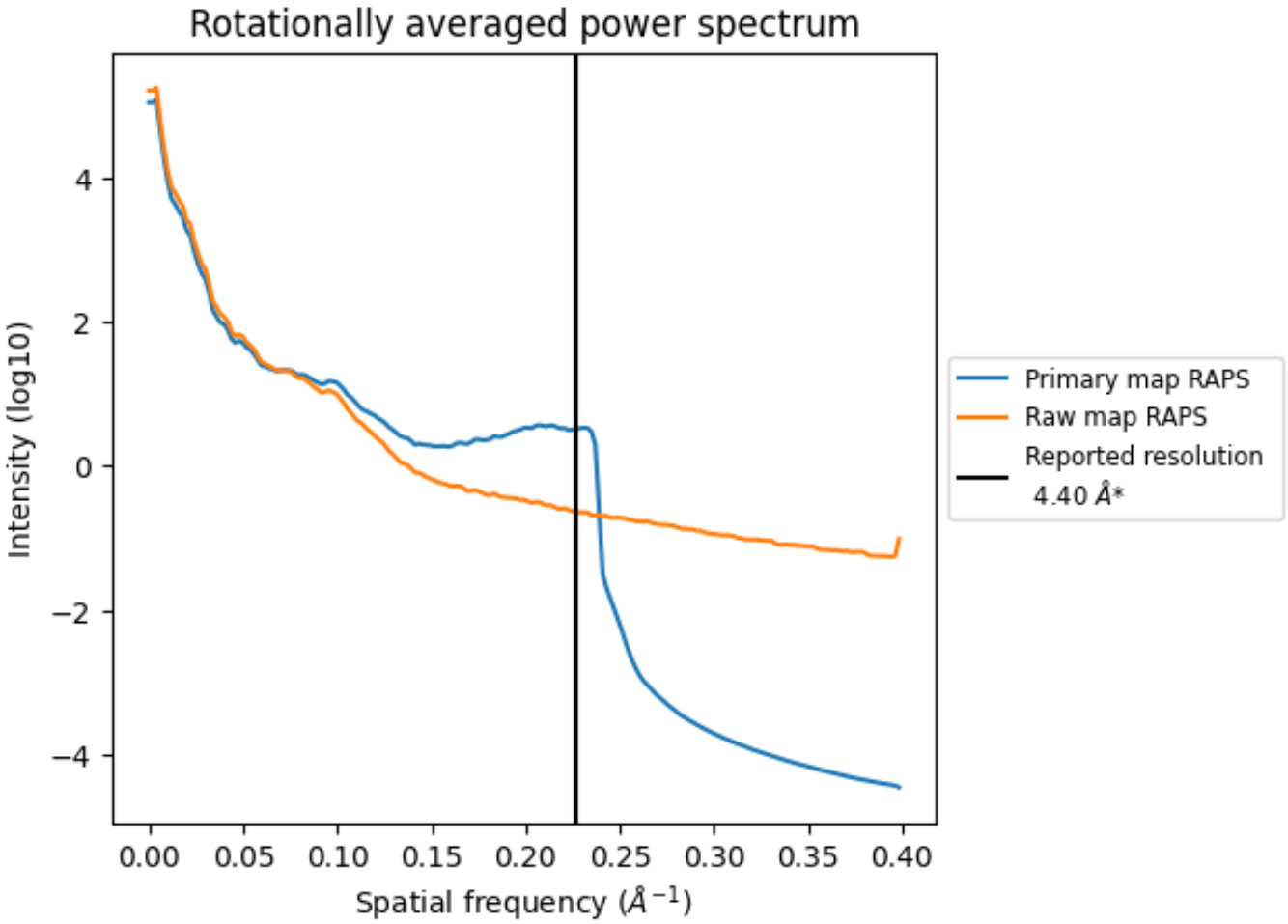
7.2 Volume estimate (i)



The volume at the recommended contour level is 547 nm^3; this corresponds to an approximate mass of 494 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)

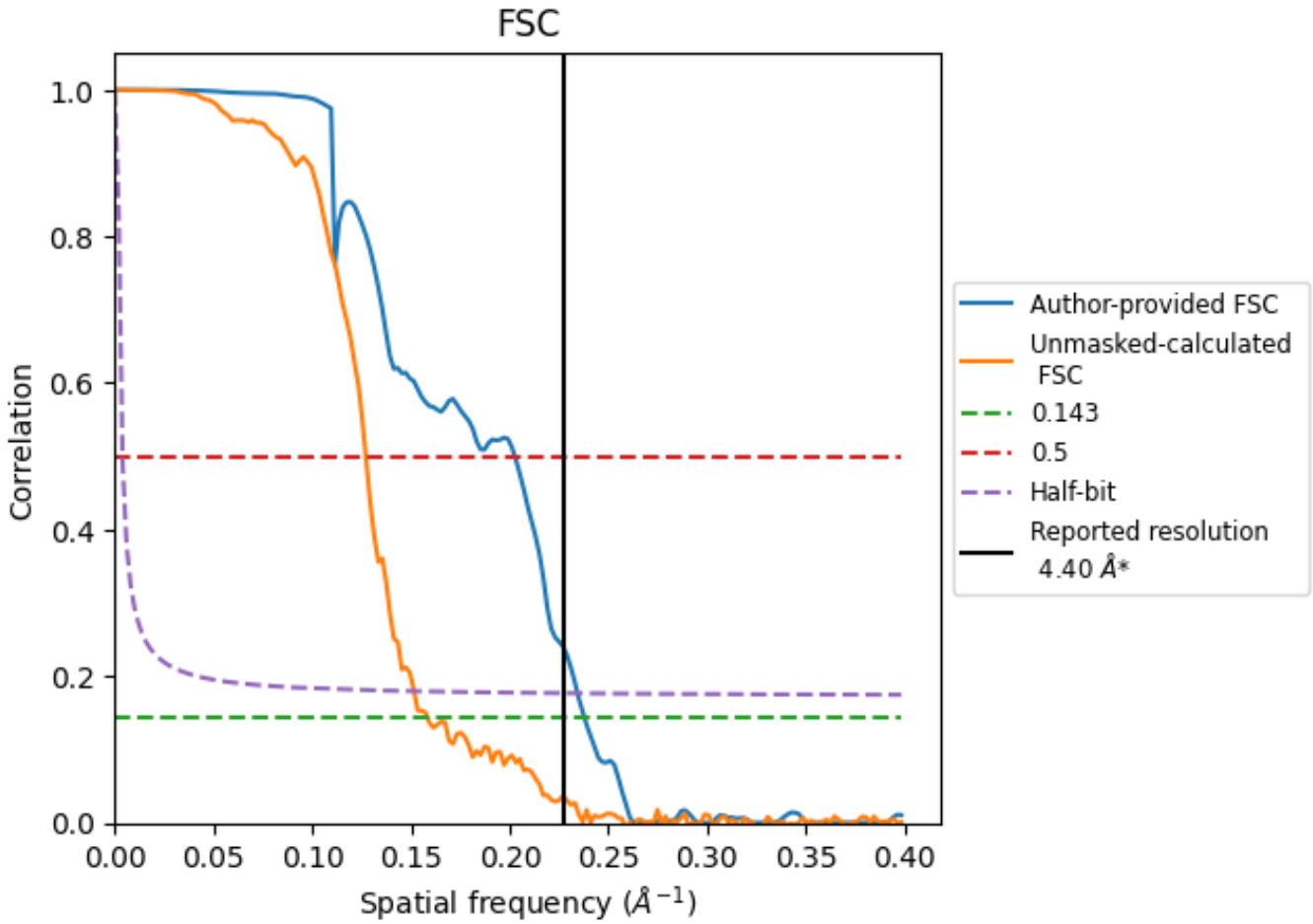


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

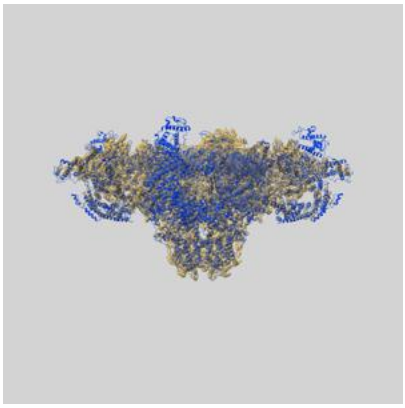
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.20	4.94	4.27
Unmasked-calculated*	6.31	7.87	6.60

*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 6.31 differs from the reported value 4.4 by more than 10 %

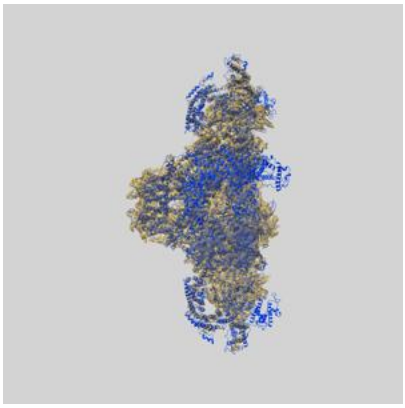
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8387 and PDB model 5TAW. Per-residue inclusion information can be found in section 3 on page 5.

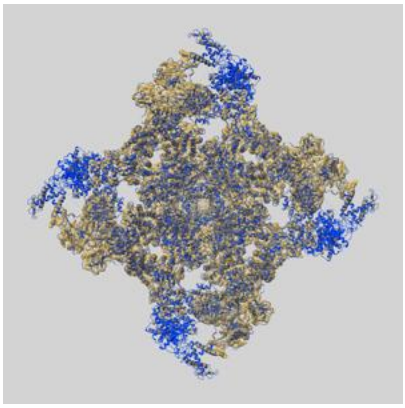
9.1 Map-model overlay



X



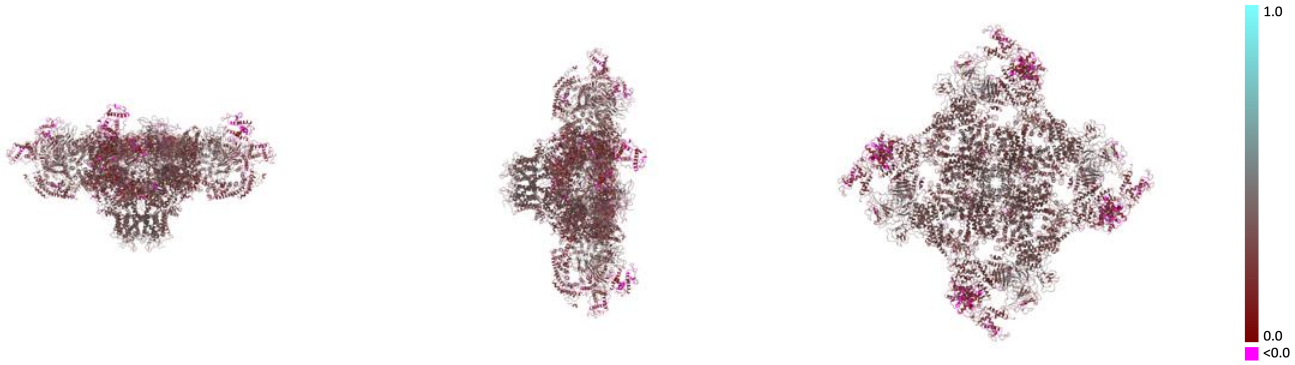
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

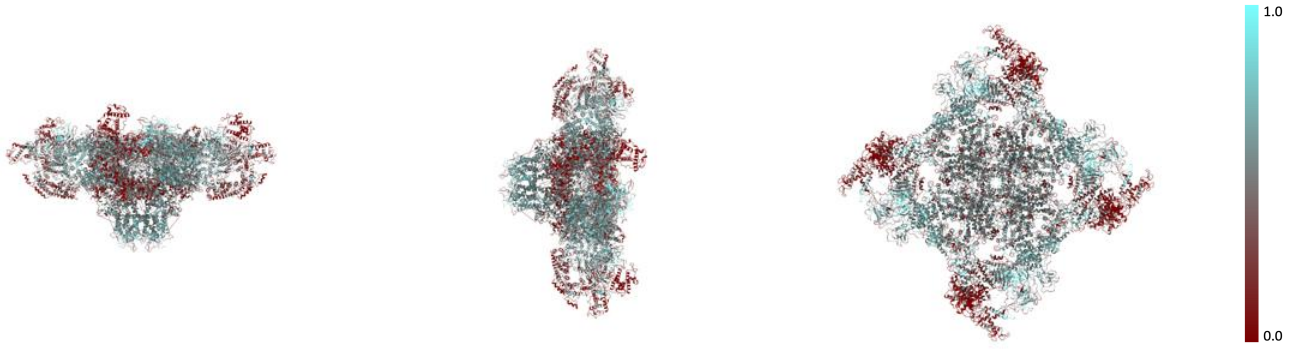
9.2 Q-score mapped to coordinate model



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.

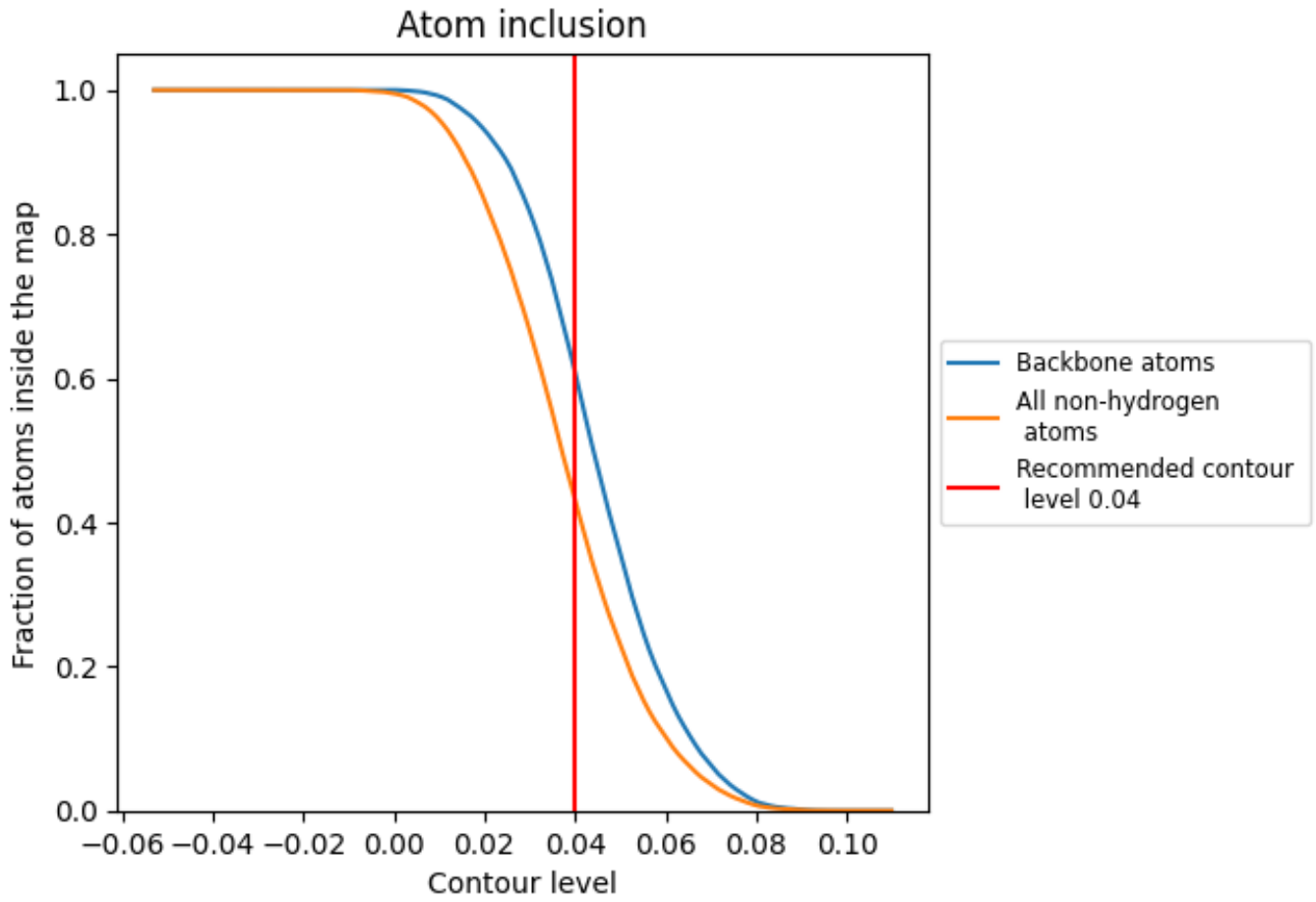
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 43% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4322	0.2790
A	0.4975	0.3250
B	0.4305	0.2780
E	0.4301	0.2780
F	0.4938	0.3290
G	0.4312	0.2780
H	0.4950	0.3280
I	0.4298	0.2780
J	0.4988	0.3270